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Publication Date

1990-12-01



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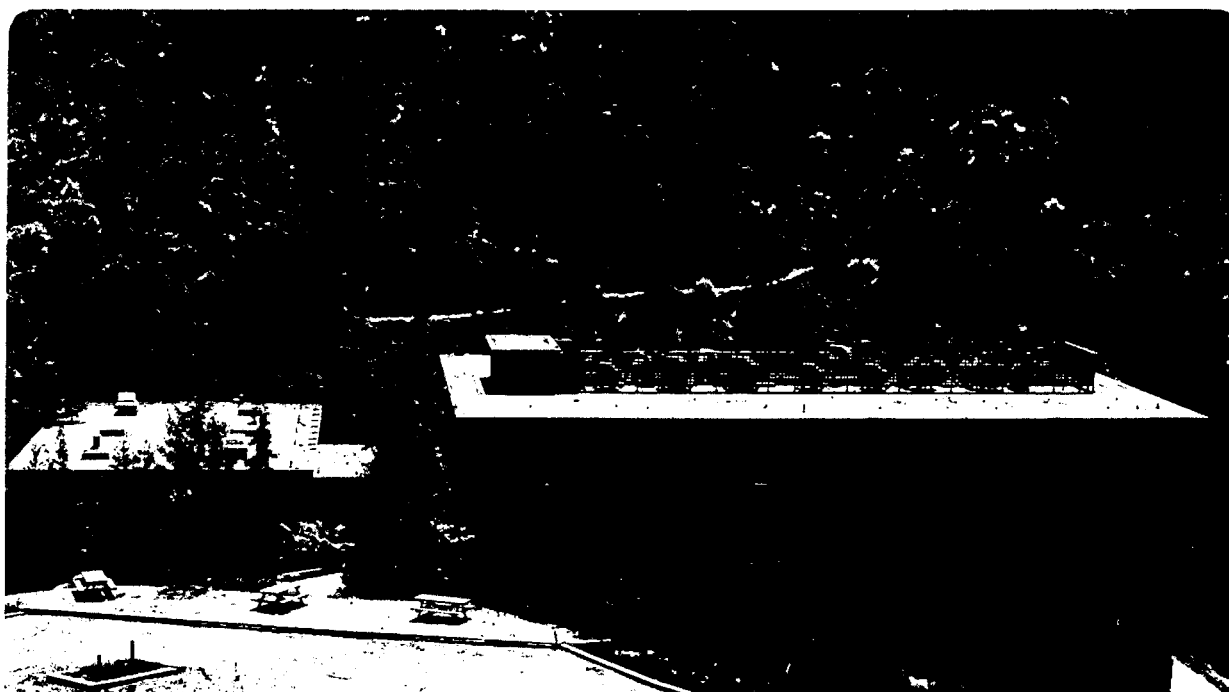
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Computer Programs for Simulation of Electrodeposition

K.G. Jordan and C.W. Tobias

December 1990



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COMPUTER PROGRAMS FOR SIMULATION OF ELECTRODEPOSITION

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December 1990

This work was supported by the Assistant Secretary for Conservation and Renewable Energy, Deputy Assistant Secretary for Utility Technologies, Office of Energy Management, Advanced Utility Concepts Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

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Introduction

In this report, FORTRAN programs and subroutines useful for modelling moving boundaries in electrochemical systems are listed. These programs were used by Kenneth Guy Jordan¹ to simulate moving boundaries during electrodeposition in presence of transport limited additives that acted either by (i) blocking the electrode to electrodeposition, or (ii) dissolving the electrode instantaneously upon their arrival, lowering the current efficiency. The programs were also used to analyze the behavior of evolving surface profiles during periodic current reversal.

The following elements of programming style were used:

- (1) Local subroutines (subroutines used only by that program) are listed in alphabetical order in the program listing, following the END of the main program module,
- (2) Global subroutines (subroutines used by more than one program) are listed in alphabetical order in the subroutine file listing following the program listings. The global subroutine files are ECFSUBS, ECBSUBS, SUBS, or MATHSUBS.
- (3) Variables in common blocks are defined in "Include" files. These files contain the declarations, common block, and description of the variables. The statements in the file are incorporated into the FORTRAN programs during compilation by using the INCLUDE statement. The "Include" files are listed in alphabetical order following the subroutines.

There are two distinct sets of programs: one set based on the finite element method, and another set based on the boundary element method. Both sets are written in FORTRAN for VAX/VMS. In the following, the intended sequence for using the programs, as well as the purpose of the program, the input required, and the output generated are briefly described.

¹ K.G. Jordan, "Levelling Of Microprofiles In Electrodeposition", Ph. D. Thesis, U.C. Berkeley, Dec (1990)

Overview of Finite Element Method Programs

There are six basic programs in the set using FEM. The intended order of use is to first run ECFMESH, then ECFDEFINE, followed by ECFPREPRO, and ECFCOMPUTE. The results from ECFCOMPUTE may be prepared for graphs by then running ECFPLOT, and ECFISO. A brief description of each program follows

ECFMESH

This program takes a concise geometric description of the FEM problem to be solved from a *.MAC file (see subroutine ReadECFMac) and generates mesh used to solve the problem: the boundary node numbers, locations, and condition, as well as node numbers and locations. The description of the FEM problem is written into *.HDR, *.MSH, *.BC, *.PAR, *.RES and *.NAM files. (See subroutines WriteMeshHdr, WriteMesh, WriteBC, WritePar, and WriteRes)

ECFDEFINE

This program allows a new FEM problem description to be entered, or an old FEM problem description to be modified. Information is read from and written to all the files that describe the problem (see subroutine WriteFEMUser.)

ECFPREPRO

This program computes the bandwidth for the FEM problem. It reads the entire FEM problem description (see subroutine ReadFEMUser) but only the mesh header file *.HDR is written (see subroutine WriteMeshHdr.)

ECFCOMPUTE

This program uses the Galerkin Finite Element Method to calculate the solution to the current distribution or convective-diffusion problem described in the files created by ECFMESH, ECFDEFINE, and ECFPREPRO. The entire FEM problem description is read (see subroutine ReadFEMUser), the results calculated, only the results are written (file *.RES, see subroutine WriteRes.)

ECFPLOT

This program takes the FEM results and prepares them for use a suitable graphics package such as *TELL-A-GRAPH*, or a user program that uses the package *DISSPLA*. The entire FEM problem description is read, and files created with X,Y data isopotential or iso-concentration contours (*.ISO), as well as concentration of potential values on the boundary (*.VAL) and the slopes of these on the boundary (*.SLP).

ECFISO

This program will take data from a *.ISO file and generate a graph using the *DISSPLA* graphics package.

Overview of Boundary Element Method Programs

There are five programs in the set that uses the boundary element method. These are usually run in the order, ECBPAR, ECBPREPRO, ECBM, ECBINT, and ECBPLOT. A brief description of each program follows.

ECBPAR

This program reads a concise description of the type of BEM problem to be solved from a *.DIM file (see subroutine ReadUserParams), creates an appropriate *.PAR file (see subroutine WritePar), and prints a report on the problem to be solved (see subroutine PrintUserParams.)

ECBPREPRO

This program reads a concise geometrical description of the BEM problem to be solved (including boundary conditions) from file *.MAC (see subroutine ReadMAC) and creates the boundary mesh, stored in file *.MSH (see subroutine WriteMesh), and the source points, stored in file *.SRC (see subroutine WriteSrc).

ECBM

This program uses the boundary element method to solve potential problems, or simultaneous diffusion and potential problems, for the current distributions in electrochemical systems with moving boundaries. The BEM problem description is read from files *.PAR, *.MSH, and *.MAC. Time vs. maximum profile depth is stored in file *.TD. The location of the moving boundary is stored in a series of files named *.BND. The final results are stored in *.MSH.

ECBINT

This program reads the solution from *.MSH and a list of internal points from *.INT (see subroutine ReadInt), and computes the value of the potential at all of the internal points.

The value of the potential at all of the internal points is written to file *.INT.

ECBPLOT

From the results generated by ECBM, this program generates files suitable for use in a number of graphics packages, such as *TELL-A-GRAF*, *DISSPLA*, or *LOTUS*. The x,y locations of the nodes are placed in file ECBPLOT.NOD; the x,y locations of the source points are written to file ECBPLOT.SRC. If desired, the user can cause solution values to be stored in file ECBPLOT.SOL, and BC values to be stored in ECBPLOT.SET. This program will also perform an integration of the flux along a given portion of the boundary. This is useful for computing cell resistances.

PROGRAM ECFMesh

```

C MakeMesh Program Takes FEM.MAC input file and generates
C   BdNodes()
C   NLoc(,)      x
C   Nodes(,) x
C   NoOfBDNodes
C   NoOfDim      x
C   NoOfElems   x
C   NoOfNodes   x

INCLUDE 'ECFHDR.INC'
INCLUDE 'ECFMAC.INC'

INTEGER MacElm,FilLen
LOGICAL Shared(4)
CHARACTER*80 FileName

CALL ChInp('File name? (no extension)',FileName)
CALL StringLength(FileName,FilLen)

CALL ReadECFMac(FileName(1:FilLen)//'.MAC')

DO MacElm=1,NoOfMacElem

  Shared(1)=.FALSE.
  Shared(2)=.FALSE.
  Shared(3)=.FALSE.
  Shared(4)=.FALSE.

  CALL SharedSides(MacElm,Shared)
  IF (MacElemType(MacElm).EQ.'S') THEN
    CALL ProcSqrMacElm(MacElm,Shared)
  ELSE IF (MacElemType(MacElm).EQ.'T') THEN
    CALL ProcTriMacElm(MacElm,Shared)
  ELSE
    WRITE(*,*) 'Error: Unknown macro element type=',
& MacElemType(MacElm)
    STOP 'ECFMesh: Main Program'
  END IF
END DO

CALL GenerateBDNodes
ECFMesh=.TRUE.

CALL PrintMacReport

CALL WriteMeshHdr(FileName(1:FilLen)//'.HDR')
CALL WriteMesh(FileName(1:FilLen)//'.MSH')
CALL WriteBC(FileName(1:FilLen)//'.BC')
CALL WritePar(FileName(1:FilLen)//'.PAR')
CALL WriteRes(FileName(1:FilLen)//'.RES')

OPEN(UNIT=1,FILE=FileName(1:FilLen)//'.NAM',STATUS='NEW',
& FORM='FORMATTED')
WRITE(1,*) '***,FileName(1:FilLen)//'.HDR',***
WRITE(1,*) '***,FileName(1:FilLen)//'.MSH',***
WRITE(1,*) '***,FileName(1:FilLen)//'.MAC',***

```

```

WRITE(1,*) ''',FileName(1:FilLen)//'.BC',''''
WRITE(1,*) ''',FileName(1:FilLen)//'.PAR',''''
WRITE(1,*) ''',FileName(1:FilLen)//'.RES',''''
WRITE(1,*) ''',FileName(1:FilLen)//'.ISO',''''
WRITE(1,*) ''',FileName(1:FilLen)//'.SLP',''''
WRITE(1,*) '''' ''''
WRITE(1,*) '''' ''''
CLOSE(1)

```

```

STOP 'MakeMesh: Normal End'
END

```

C ***** GenerateBDNodes

```

SUBROUTINE GenerateBDNodes

```

```

INCLUDE 'ECFHDR.INC'
INCLUDE 'ECFMSH.INC'
INCLUDE 'ECFMAC.INC'

```

```

LOGICAL SideNotFound
INTEGER BDSeg,BDSegp1,MacElem,MacSeg,MacSegp1,M,Vert1,Vert2
INTEGER Upper

```

```

DO BDSeg=1,NoOfMacBDNodes

```

```

    CALL IncrementI(BDSeg,BDSegp1,1,NoOfMacBDNodes)
    SideNotFound=.TRUE.

```

C The following DO Loop locates the side on the boundary.

```

    DO MacElem=1,NoOfMacElem
        CALL GetUpper(MacElemType(MacElem),Upper)
        DO MacSeg=1,Upper

```

```

            CALL IncrementI(MacSeg,MacSegp1,1,Upper)

```

```

            Vert1=MacElemVert(MacElem,MacSeg)
            Vert2=MacElemVert(MacElem,MacSegp1)

```

```

            IF ((Vert1.EQ.MacBDNodes(BDSeg)).AND.
& (Vert2.EQ.MacBDNodes(BDSegp1)) ) THEN

```

```

                MacBDNodeNo(Vert1)=NoOfBDNodes+1

```

```

D          WRITE(*,5) Vert1,NoOfBDNodes+1
5          FORMAT(X,'Mac BD Node No ',I5,' is Boundary Node ',I5)
          SideNotFound=.FALSE.

```

```

                DO M=1,NoOfMacElem(MacElem,MacSeg)

```

```

                    NoOfBDNodes=NoOfBDNodes+1

```

```

                    BDNodes(NoOfBDNodes)=SharedNodes(MacElem,MacSeg,M)

```

```

D          WRITE(*,10) NoOfBDNodes,BDNodes(NoOfBDNodes)
10         FORMAT(X,'    BDNodes(',I5,')=',I5)

```

```

                END DO

```

```

            END IF

```

```

        END DO

```

```

    END DO

```



```

IF (SideNotFound) THEN
  WRITE(*,*) 'Error: Boundary Side not found.'
  WRITE(*,*) '   BD Seg=',BDSeg
  STOP 'In Routine: GenerateBDNodes'
END IF

```

```

END DO

```

```

RETURN
END

```

```

C ***** MakeSpine

```

```

SUBROUTINE MakeSpine(StaPtX,StaPtY,EndPtX,EndPtY,
& NoOfMicElems,SpaType,SpaFac,
& SpineX,SpineY)

```

```

C StaPtX,Y   Starting Point Location
C EndPtX,Y   Ending Point Location
C NoOfMicElems   The number of microelements that must be on this side
C SpaType     Spacing Type for microelements
C SpaFac     Spacing Factor for microelements
C SpineX()    X Locations for spine
C SpineY()    Y Locations for spine.

```

```

INTEGER NoOfMicElems
REAL*8 StaPtX,StaPtY,EndPtX,EndPtY,SpineX(*),SpineY(*),SpaFac
CHARACTER*(*) SpaType

```

```

INTEGER I

```

```

IF (SpaType.EQ.'LIN') THEN

```

```

  SpineX(1)=StaPtX
  SpineY(1)=StaPtY

```

```

  DO I=1,NoOfMicElems
    SpineX(I)=StaPtX + (EndPtX-StaPtX) * FLOAT(I-1)
& / FLOAT(NoOfMicElems)
    SpineY(I)=StaPtY + (EndPtY-StaPtY) * FLOAT(I-1)
& / FLOAT(NoOfMicElems)
  END DO

```

```

  SpineX(NoOfMicElems+1)=EndPtX
  SpineY(NoOfMicElems+1)=EndPtY

```

```

ELSE

```

```

  WRITE(*,*) 'Error: Unknown Spacing Type=',SpaType
  STOP 'In Routine: MakeSpine'

```

```

END IF

```

```

RETURN
END

```

```

C ***** PrintMacReport

```

```
SUBROUTINE PrintMacReport
```

```
INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFGauss.INC'
INCLUDE 'ECFMsh.INC'
INCLUDE 'ECFMAC.INC'
```

```
INTEGER I,J,MacNodeNo,Upper
CHARACTER*80 Dummy,Output
```

```
CALL PrintProbHeader
WRITE(*,*) ' '
```

```
C 123456789a123456789b123456789c123456789d123456789e12
C ----- Macro Vertices & Elements
C                    iii   iii
C 123456789a123456789b123456789c123456789d123456789e123456789 1234567
```

```
WRITE(*,300) NoOfMacVert,NoOfMacElem
300 FORMAT(X,52('-'),' Macro Vertices & Elements' /
& X,59X,I4,7X,I4)
```

```
WRITE(*,*) ' '
WRITE(*,310)
310 FORMAT(X,23X,'Vertex No',3X,'X Coord',7X,'Y Coord')
WRITE(*,*) ' '
```

```
DO I=1,NoOfMacVert
WRITE(*,320) I,MacVertX(I),MacVertY(I)
END DO
320 FORMAT(X,25X,I4,4X,G11.4,3X,G11.4)
```

```
C 123456789a12345 123 1234567
C Vertex No X Coord Y Coord
C      iii  sd.dddde+dd sd.dddde+dd
C 123456789a12345 1234123456789a1123
```

```
C MACRO----- MICRO-----
C Elem Vertex Spacing Elems Vertex Bdry
C No Type Factor No Node
C      iii  iii  aaaa sd.dddde+dd  iii  iii  iii
C 1234 1234 1234 123456789a1 1234 1234 1234
```

```
WRITE(*,*) ' '
WRITE(*,340)
```

```
DO I=1,NoOfMacElem
MacNodeNo=MacBDNodeNo(MacElemVert(I,1))
IF (MacNodeNo.NE.0) THEN
WRITE(*,350) I,MacElemType(I),
& MacElemVert(I,1),SpaType(I,1),SpaFac(I,1),
& NoOfMicElm(I,1),BDNodes(MacNodeNo),MacNodeNo
ELSE
WRITE(*,350) I,MacElemType(I),
& MacElemVert(I,1),SpaType(I,1),SpaFac(I,1),
& NoOfMicElm(I,1),BDNodes(MacNodeNo)
END IF
```

```

CALL GetUpper(MacElemType(I),Upper)

DO J=2,Upper
  MacNodeNo=MacBDNodeNo(MacElemVert(I,J))
  IF (MacNodeNo.NE.0) THEN
    WRITE(*,360) MacElemVert(I,J),SpaType(I,J),SpaFac(I,J),
    & NoOfMicElm(I,J),BDNodes(MacNodeNo),MacNodeNo
  ELSE
    WRITE(*,360) MacElemVert(I,J),SpaType(I,J),SpaFac(I,J),
    & NoOfMicElm(I,J),BDNodes(MacNodeNo)
  END IF
END DO
WRITE(*,*) ''
END DO

340  FORMAT(X,7X,'MACRO',27('-'),5X,'MICRO',15('-'))/
    & X,7X,'Elem Vertex Spacing',12X,'Elems Vertex Bdry'/,
    & X,8X,'No',12X,'Type Factor',18X,'No Node'./)

c
12345
C1234567 123456789a123456789b1234567 123456789a12345
C 123 12345 123456789a12 12 123
C12345678 123456789a1 123 123456789a12345678 12345
C1234567 1234 123 12 12345 1234 1234

350  FORMAT(X,7X,I4,A1,3X,I4,3X,A4,2X,G11.4,5X,I4,4X,I4,.,4X,I4)
360  FORMAT(X,7X,4X,4X,I4,3X,A4,2X,G11.4,5X,I4,4X,I4,.,4X,I4)

RETURN
END

C ***** ProcSqrMacElm

SUBROUTINE ProcSqrMacElm(MacElm,Shared)

C Process MacroElement

INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFMsh.INC'
INCLUDE 'ECFMAC.INC'

INTEGER MacElm
LOGICAL Shared(*)

REAL*8 SpineX12(MaxNoOfMicVert),SpineY12(MaxNoOfMicVert)
REAL*8 SpineX23(MaxNoOfMicVert),SpineY23(MaxNoOfMicVert)
REAL*8 SpineX34(MaxNoOfMicVert),SpineY34(MaxNoOfMicVert)
REAL*8 SpineX41(MaxNoOfMicVert),SpineY41(MaxNoOfMicVert)
REAL*8 SpineX(MaxNoOfMicVert),SpineY(MaxNoOfMicVert)
REAL*8 StaPtX,StaPtY,EndPtX,EndPtY
INTEGER MicNode,Point,MicSta,MicEnd,Error,I,J

C Make Spine for First, Second, Third, and Fourth Sides
C (The following calls are really typing aids to the call of MakeSpine)

CALL SideSpine(MacElm,1,2,1,SpineX12,SpineY12)
CALL SideSpine(MacElm,2,3,2,SpineX23,SpineY23)

```

```
CALL SideSpine(MacElm,4,3,1,SpineX34,SpineY34)
CALL SideSpine(MacElm,1,4,2,SpineX41,SpineY41)
```

C Store Spine Into Mesh (for side 4)

```
C +3+ Spine Side definition. | 4-3 Loc. Vert. Def.
C 4 2           | ||
C +1+           | 1-2
```

```
IF (Shared(1)) THEN
  MicSta=2
ELSE
  MicSta=1
END IF
```

```
IF (Shared(3)) THEN
  MicEnd=NoOfMicElm(MacElm,2)
ELSE
  MicEnd=NoOfMicElm(MacElm,2)+1
END IF
```

```
D WRITE(*,20) MicSta,MicEnd
20 FORMAT(X,'Square Macro Elem: Start=',I5,' End=',I5)
```

```
IF (.NOT.Shared(4)) THEN
  CALL TransferSpine(MicSta,MicEnd,MacElm,4,1,
& SpineX41,SpineY41)
END IF
```

C Now do spines next to side 4

```
DO MicNode=2,NoOfMicElm(MacElm,1)
```

C Locate Intersections Between Crossing Spines

C Store first point on next spine.

```
SpineX(1)=SpineX12(MicNode)
SpineY(1)=SpineY12(MicNode)
```

C Store last point on next spine.

```
SpineX(NoOfMicElm(MacElm,2)+1)=SpineX34(MicNode)
SpineY(NoOfMicElm(MacElm,2)+1)=SpineY34(MicNode)
```

C Find intermediate points.

```
DO Point=2,NoOfMicElm(MacElm,2)
```

```
CALL ComputeIntersection(SpineX(1),SpineY(1),
& SpineX(NoOfMicElm(MacElm,2)+1),
& SpineY(NoOfMicElm(MacElm,2)+1),
& SpineX41(Point),SpineY41(Point),
& SpineX23(Point),SpineY23(Point),
& SpineX(Point),SpineY(Point),Error)
```

```
IF (Error.NE.0) THEN
  WRITE(*,*) 'Error: Spines do not intersect.'
```

```

      STOP 'In Routine: ProcMacElm'
    END IF
  END DO

```

```

C IF--- Store node numbers of possible shared nodes. (on side 1)
C CALL- Transfer spine locations into Nodes(). Save node numbers
C IF--- Store node numbers of possible shared nodes. (on side 3)

```

```

      IF (MicSta.EQ.1) THEN
        SharedNodes(MacElm,1,MicNode)=NoOfNodes+1
D      WRITE(*,10) MacElm,1,MicNode,NoOfNodes+1
10     FORMAT(X,'SQRSharedNodes(',I5,',',I5,',',I5,')=' ,I5)
      END IF
      CALL TransferSpine(MicSta,MicEnd,0,0,MicNode,SpineX,SpineY)
      IF (MicEnd.EQ.NoOfMicElm(MacElm,2)+1) THEN
        SharedNodes(MacElm,3,NoOfMicElm(MacElm,3)+2-MicNode)
& =NoOfNodes
D      WRITE(*,10) MacElm,3,NoOfMicElm(MacElm,3)+2-MicNode,
D      & NoOfNodes
      END IF

```

```

    END DO

```

```

C If Side 2 is not shared, (last side parallel to side 4), store it.

```

```

      IF (.NOT.Shared(2))
& CALL TransferSpine(MicSta,MicEnd,MacElm,2,
& NoOfMicElm(MacElm,1)+1,
& SpineX23,SpineY23)

```

```

C Store corner nodes as appropriate

```

```

C Side 4

```

```

      SharedNodes(MacElm,1,1)
& = SharedNodes(MacElm,4,NoOfMicElm(MacElm,4)+1)
      SharedNodes(MacElm,3,NoOfMicElm(MacElm,3)+1)
& = SharedNodes(MacElm,4,1)
D      WRITE(*,10) MacElm,1,1,SharedNodes(MacElm,1,1)
D      WRITE(*,10) MacElm,3,NoOfMicElm(MacElm,3)+1,
D      & SharedNodes(MacElm,4,1)

```

```

C Side 2

```

```

      SharedNodes(MacElm,3,1)
& = SharedNodes(MacElm,2,NoOfMicElm(MacElm,2)+1)
      SharedNodes(MacElm,1,NoOfMicElm(MacElm,1)+1)
& = SharedNodes(MacElm,2,1)
D      WRITE(*,10) MacElm,3,1,SharedNodes(MacElm,3,1)
D      WRITE(*,10) MacElm,1,NoOfMicElm(MacElm,3)+1,
D      & SharedNodes(MacElm,2,1)
D      WRITE(*,*) ' '

```

```

C Store node #s of mesh along shared sides of macro element.

```

```

      DO I=1,NoOfMicElm(MacElm,2)+1

```

```

      IF (Shared(2)) MacNodes(NoOfMicElm(MacElm,1)+1,I)
& =SharedNodes(MacElm,2,I)
      IF (Shared(4)) MacNodes(1,I)
& =SharedNodes(MacElm,4,NoOfMicElm(MacElm,4)+2-I)
      END DO

```

```

      DO I=1,NoOfMicElm(MacElm,1)+1
      IF (Shared(1)) MacNodes(I,1)
& =SharedNodes(MacElm,1,I)
      IF (Shared(3)) MacNodes(I,NoOfMicElm(MacElm,2)+1)
& =SharedNodes(MacElm,3,NoOfMicElm(MacElm,3)+2-I)
      END DO

```

C Use saved node numbers to generate NLoc matrix, and element type.

```

      DO J=1,NoOfMicElm(MacElm,1)
      DO I=1,NoOfMicElm(MacElm,2)
      NoOfElems=NoOfElems+1
      ElemType(NoOfElems)='S'
      NLoc(NoOfElems,1)=MacNodes(J,I)
      NLoc(NoOfElems,2)=MacNodes(J+1,I)
      NLoc(NoOfElems,3)=MacNodes(J+1,I+1)
      NLoc(NoOfElems,4)=MacNodes(J,I+1)
      END DO

```

```

      END DO

```

```

      RETURN
      END

```

C ***** ProcTriMacElm

```

      SUBROUTINE ProcTriMacElm(MacElm,Shared)

```

C Process MacroElement

```

      INCLUDE 'ECFHdr.INC'
      INCLUDE 'ECFMsh.INC'
      INCLUDE 'ECFMAC.INC'

```

```

      INTEGER MacElm
      LOGICAL Shared(*)

```

```

      REAL*8 SpineX12(MaxNoOfMicVert),SpineY12(MaxNoOfMicVert)
      REAL*8 SpineX21(MaxNoOfMicVert),SpineY21(MaxNoOfMicVert)
      REAL*8 SpineX32(MaxNoOfMicVert),SpineY32(MaxNoOfMicVert)
      REAL*8 SpineX31(MaxNoOfMicVert),SpineY31(MaxNoOfMicVert)

```

```

      REAL*8 SpineX(MaxNoOfMicVert),SpineY(MaxNoOfMicVert)
      REAL*8 StaPtX,StaPtY,EndPtX,EndPtY
      INTEGER MicNode,Point,MicSta,MicEnd,Error,I,J,Upper

```

C Make Spine for First, Second, Third, and Fourth Sides

C (The following calls are really typing aids to the call of MakeSpine)

```

      CALL SideSpine(MacElm,2,1,1,SpineX21,SpineY21)
      CALL SideSpine(MacElm,1,2,1,SpineX12,SpineY12)
      CALL SideSpine(MacElm,3,2,2,SpineX32,SpineY32)
      CALL SideSpine(MacElm,3,1,3,SpineX31,SpineY31)

```

```

C + Spine Side definition. | 2 Loc. Vert. Def.
C 21 | |
C +3+ | 3-1

```

C Store Spine Into Mesh for side 2.

```

IF (Shared(3)) THEN
  MicSta=2
ELSE
  MicSta=1
END IF

```

```

Upper=NoOfMicElm(MacElm,2)+1
IF (Shared(1)) THEN
  MicEnd=Upper-1
ELSE
  MicEnd=Upper
END IF

```

```

D WRITE(*,20) MicSta,MicEnd
20 FORMAT(X,'Triang Macro Elem: Start=',I5,' End=',I5)

```

```

IF (.NOT.Shared(2))
& CALL TransferSpine(MicSta,MicEnd,MacElm,2,1,
& SpineX32,SpineY32)

```

C Now do spines next to side 2

```

DO MicNode=2,NoOfMicElm(MacElm,3)

```

C MicEnd must be decreased by one for each subsequent spine.

```

MicEnd=MicEnd-1
Upper=Upper-1

```

C Locate Intersections Between Crossing Spines

C Store first point on next spine.

```

SpineX(1)=SpineX31(MicNode)
SpineY(1)=SpineY31(MicNode)

```

C Store last point on next spine.

```

SpineX(Upper)=SpineX21(MicNode)
SpineY(Upper)=SpineY21(MicNode)

```

C Find intermediate points.

```

DO Point=2,Upper-1

```

```

CALL ComputeIntersection(SpineX(1),SpineY(1),
& SpineX(Upper),SpineY(Upper),
& SpineX32(Point),SpineY32(Point),
& SpineX12(Point),SpineY12(Point),
& SpineX(Point),SpineY(Point),Error)

```

```

IF (Error.EQ.2) THEN

```

```

        WRITE(*,*) 'Error: Spines do not intersect.'
        STOP 'In Routine: ProcMacElm'
    END IF

```

```

    END DO

```

```

C IF--- Store node numbers of possible shared nodes. (on side 1)
C CALL- Transfer spine locations into Nodes(). Save node numbers
C IF--- Store node numbers of possible shared nodes. (on side 3)

```

```

        IF (MicSta.EQ.1) THEN
            SharedNodes(MacElm,3,MicNode)
            & =NoOfNodes+1
        D    WRITE(*,10) MacElm,3,MicNode,
        D    & NoOfNodes+1
        10    FORMAT(X,'TRISharedNodes(',I5,',',I5,',',I5,')=',I5)
            END IF
            CALL TransferSpine(MicSta,MicEnd,0,0,MicNode,SpineX,SpineY)
            IF (MicEnd.EQ.Upper) THEN
                SharedNodes(MacElm,1,NoOfMicElm(MacElm,1)+2-MicNode)
                & =NoOfNodes
        D    WRITE(*,10) MacElm,1,NoOfMicElm(MacElm,1)+2-MicNode,
        D    & NoOfNodes
            END IF
        END DO

```

```

        IF ((.NOT.Shared(1)).AND(.NOT.Shared(3))) THEN
            NoOfNodes=NoOfNodes+1
            SharedNodes(MacElm,1,1)=NoOfNodes
            SharedNodes(MacElm,3,NoOfMicElm(MacElm,3)+1)=NoOfNodes
            Nodes(NoOfNodes,1)=MacVertX(MacElemVert(MacElm,1))
            Nodes(NoOfNodes,2)=MacVertY(MacElemVert(MacElm,1))
            MacNodes(NoOfMicElm(MacElm,3)+1,1)=NoOfNodes
        END IF

```

```

C Store corner nodes as appropriate

```

```

C Side 2

```

```

        SharedNodes(MacElm,1,NoOfMicElm(MacElm,1)+1)
        & = SharedNodes(MacElm,2,1)
        SharedNodes(MacElm,3,1)
        & = SharedNodes(MacElm,2,NoOfMicElm(MacElm,2)+1)

        D    WRITE(*,10) MacElm,1,NoOfMicElm(MacElm,1)+1,
        D    & SharedNodes(MacElm,2,1)
        D    WRITE(*,10) MacElm,3,1,SharedNodes(MacElm,3,1)

```

```

C Side 1

```

```

        SharedNodes(MacElm,1,1)
        & = SharedNodes(MacElm,3,NoOfMicElm(MacElm,3)+1)
        D    WRITE(*,10) MacElm,1,1,SharedNodes(MacElm,1,1)

        D    WRITE(*,*) ' '

```

```

C Store node #s of mesh along shared sides of macro element.

```



```

DO I=1,NoOfMicElm(MacElm,1)+1

  IF (Shared(1)) MacNodes(I,NoOfMicElm(MacElm,2)+2-I)
& =SharedNodes(MacElm,1,NoOfMicElm(MacElm,1)+2-I)

  IF (Shared(2)) MacNodes(1,I)
& =SharedNodes(MacElm,2,NoOfMicElm(MacElm,2)+2-I)

  IF (Shared(3)) MacNodes(I,1)
& =SharedNodes(MacElm,3,I)

END DO

```

C Use saved node numbers to generate NLoc matrix, and element type.

```

DO J=1,NoOfMicElm(MacElm,3)

  DO I=1,NoOfMicElm(MacElm,2)-J
    NoOfElems=NoOfElems+1
    ElemType(NoOfElems)='S'
    NLoc(NoOfElems,1)=MacNodes(J,I)
    NLoc(NoOfElems,2)=MacNodes(J+1,I)
    NLoc(NoOfElems,3)=MacNodes(J+1,I+1)
    NLoc(NoOfElems,4)=MacNodes(J,I+1)
  END DO

  NoOfElems=NoOfElems+1
  ElemType(NoOfElems)='T'
  I=NoOfMicElm(MacElm,2)+1-J
  NLoc(NoOfElems,1)=MacNodes(J,I)
  NLoc(NoOfElems,2)=MacNodes(J+1,I)
  NLoc(NoOfElems,3)=MacNodes(J,I+1)

END DO

RETURN
END

```

C ***** ReadECFMAC

```

SUBROUTINE ReadECFMAC(FileName)

  INCLUDE 'ECFHDR.INC'
  INCLUDE 'ECFGauss.INC'
  INCLUDE 'ECFMAC.INC'

  CHARACTER(*) FileName
  INTEGER I,J,NoOfVert
  LOGICAL FileEXIST

  INQUIRE(FILE=FileName,EXIST=FileExist)
  IF (.NOT.FileExist) THEN
    WRITE(*,*) 'Error: Unknown File Name=',FileName
    CALL LIB$SPAWN('TYPE ECFMAC.STR')
    STOP 'In Routine: ReadECFMAC'
  END IF

  OPEN(UNIT=1,FILE=FileName,STATUS='OLD',FORM='FORMATTED')

```

```

READ(1,*) BasisDeg,Tolerance,NoOfGaussPts,MaxNoOfIter
READ(1,*) NoOfEqu,NoOfDim
READ(1,*) Debugging,Convection,PolyFlow,Guess,Nonnegative

```

C Read Macro Vertices

```

READ(1,*) NoOfMacVert
DO I=1,NoOfMacVert
  READ(1,*) MacVertX(I),MacVertY(I)
END DO

```

C Read Macro Elements

```

READ(1,*) NoOfMacElem
DO I=1,NoOfMacElem
  READ(1,*) MacElemType(I)

  CALL GetUpper(MacElemType(I),NoOfVert)

  READ(1,*) (MacElemVert(I,J),J=1,NoOfVert)
  READ(1,*) (NoOfMicElm(I,J),J=1,NoOfVert)

```

```

IF (MacElemType(I).EQ.'S') THEN

```

C Square Macro Element

```

  NoOfMicElm(I,3)=NoOfMicElm(I,1)
  NoOfMicElm(I,4)=NoOfMicElm(I,2)

```

```

ELSE

```

C Triangular Macro Element

```

  NoOfMicElm(I,2)=NoOfMicElm(I,1)
  NoOfMicElm(I,3)=NoOfMicElm(I,1)

```

```

END IF

```

C The following DO-Loop to check that number of micro elements on each
C side is less than the maximum number of micro elements that this program
C can handle.

```

DO J=1,NoOfVert
  IF (NoOfMicElm(I,J).GE.MaxNoOfMicVert) THEN
    WRITE(*,*) 'Error: Too many microelements! Either'
    WRITE(*,*) '  a) reduce number of microelements, or'
    WRITE(*,*) '  b) increase MaxNoOfMicVert in ECFMAC.INC'
    WRITE(*,*) '      and recompile programs.'
    WRITE(*,*) '      NoOfMicElm=',NoOfMicElm(I,J)
    WRITE(*,*) '      MaxNoOfMicVert=',MaxNoOfMicVert
    STOP 'In Routine: ReadECFMAC'
  END IF
END DO
READ(1,*) (SpaType(I,J),J=1,NoOfVert)
READ(1,*) (SpaFac(I,J),J=1,NoOfVert)
END DO

```

C Read the macrovertices on the boundary

```

READ(1,*) NoOfMacBDNodes

DO I=1,NoOfMacBDNodes
  READ(1,*) MacBDNodes(I)
END DO

```

CLOSE(1)

C FEM.MAC File Structure

```
c BasisDeg,Tolerance,NoOfGaussPts,MaxNoOfIter      )- goes to mesh hdr file
c NoOfEqu,NoOfDim                                   )
c Debugging,Convection,PolyFlow,Guess,Nonnegative  )
```

```
C NoOfMacVert                                     )- goes to mesh file
C X1,Y1
C X2,Y2
C ...
C XN,YN
```

C NoOfMacElm

```
C MacElemType
C MacVert1,MacVert2,MacVert3,MacVert4
C NoOfMicElm12,23,34,41
C SpaType12,23,34,41
C SpaFac12,23,34,41
```

C ...

```
C NoOfMacBDNodes
C MacBDNodes(1)
C ...
C MacBDNodes(N)
```

RETURN
END

C ***** SharedSides

SUBROUTINE SharedSides(MacElm,Shared)

INCLUDE 'ECFMAC.INC'

LOGICAL Shared(*)

INTEGER MacElm,PrevElm,K,L,M,Kp1,Lp1,Km1

INTEGER UpperPrev,UpperMac

CALL GetUpper(MacElemType(MacElm),UpperMac)

DO PrevElm=1,MacElm-1

CALL GetUpper(MacElemType(PrevElm),UpperPrev)

DO K=1,UpperMac

CALL IncrementI(K,Kp1,1,UpperMac)

DO L=1,UpperPrev

CALL IncrementI(L,Lp1,1,UpperPrev)

IF (
& (MacElemVert(MacElm,K).EQ.MacElemVert(PrevElm,Lp1)).AND.

```

& (MacElemVert(MacElem,Kp1).EQ.MacElemVert(PrevElm,L)) ) THEN

D          WRITE(*,10) MacElem,K,PrevElm,L
10         FORMAT(X,'Note: Mac Elem ',I5,' Side ',I5,
& ' is shared with Mac Elem ',I5,' Side ',I5)
          Shared(K)=.TRUE.
          NoOfMicElm(MacElem,K)=NoOfMicElm(PrevElm,L)

          DO M=1,NoOfMicElm(MacElem,K)+1
            SharedNodes(MacElem,K,M)
& =SharedNodes(PrevElm,L,NoOfMicElm(MacElem,K)+2-M)
          END DO

          CALL IncrementI(K,Km1,-1,UpperMac)
          SharedNodes(MacElem,Kp1,1)=SharedNodes(MacElem,K,
& NoOfMicElm(MacElem,K)+1)
          SharedNodes(MacElem,Km1,
& NoOfMicElm(MacElem,Km1)+1)=SharedNodes(MacElem,K,1)
          END IF

        END DO
      END DO
    END DO

    RETURN
  END

C ***** SideSpine

SUBROUTINE SideSpine(MacElem,StaVert,EndVert,Side,SpineX,SpineY)

C MacElem      The current macro element being processed
C StaVert      The local macro vertex for starting point.
C EndVert      The local macro vertex for ending point.
C Side         The side of the mesh.
C SpineX       The X locations on the spine
C SpineY       The Y locations on the spine

  INCLUDE 'ECFMAC.INC'

  REAL*8 SpineX(*),SpineY(*)
  INTEGER MacElem,StaVert,EndVert,Side

  REAL*8 StaPtX,StaPtY,EndPtX,EndPtY

  StaPtX=MacVertX(MacElemVert(MacElem,StaVert))
  StaPtY=MacVertY(MacElemVert(MacElem,StaVert))

  EndPtX=MacVertX(MacElemVert(MacElem,EndVert))
  EndPtY=MacVertY(MacElemVert(MacElem,EndVert))

  CALL MakeSpine(StaPtX,StaPtY,EndPtX,EndPtY,
& NoOfMicElm(MacElem,Side),
& SpaType(MacElem,Side),SpaFac(MacElem,Side),
& SpineX,SpineY)

  RETURN
END

```

C ***** TransferSpine

 SUBROUTINE TransferSpine(MicSta,MicEnd,MacElm,MacSide,SpeNode,
 & SpineX,SpineY)

C This subroutine stores the node locations from one spine into Nodes.

 INCLUDE 'ECFHDR.INC'
 INCLUDE 'ECFMAC.INC'
 INCLUDE 'ECFMSH.INC'

C SpineX() X Locations
C SpineY() Y Locations
C MacElm
C MacSide
C SpeNode
C MicSta 1st (local) mic node number
C MicEnd last (local) mic node number

 INTEGER MicSta,MicEnd,MacElm,MacSide,SpeNode
 REAL*8 SpineX(*),SpineY(*)
 INTEGER MicNod

 DO MicNod=MicSta,MicEnd
 NoOfNodes=NoOfNodes+1

 IF (NoOfNodes.GT.MaxNoOfNodes) THEN
 WRITE(*,*) 'Error: Too many micro nodes.'
 WRITE(*,*) ' Maximum allowed=',MaxNoOfNodes
 WRITE(*,*) ' Either scale back, or increase ',
& 'MaxNoOfNodes in ECFHDR.INC'
 WRITE(*,*) ' and recompile.'
 STOP 'In Routine: TransferSpine'
 END IF

 IF (MacSide.EQ.4) THEN

 SharedNodes(MacElm,MacSide,
& NoOfMicElm(MacElm,MacSide)+2-MicNod)=NoOfNodes
D WRITE(*,10) MacElm,MacSide,
D & NoOfMicElm(MacElm,MacSide)+2-MicNod,NoOfNodes
10 FORMAT(X,'TFRSharedNodes(',I5,',',I5,',',I5,')=',I5)

 ELSE IF (MacSide.EQ.2) THEN

 IF (MacElemType(MacElm).EQ.'S') THEN
 SharedNodes(MacElm,MacSide,MicNod)=NoOfNodes
D WRITE(*,10) MacElm,MacSide,MicNod,NoOfNodes
 ELSE
 SharedNodes(MacElm,MacSide,
& NoOfMicElm(MacElm,MacSide)+2-MicNod)=NoOfNodes
D WRITE(*,10) MacElm,MacSide,
D & NoOfMicElm(MacElm,MacSide)+2-MicNod,NoOfNodes
 END IF

 END IF

 Nodes(NoOfNodes,1)=SpineX(MicNod)

```
Nodes(NoOfNodes,2)=SpineY(MicNod)
  IF (SpeNode.GT.0) MacNodes(SpeNode,MicNod)=NoOfNodes
END DO

RETURN
END
```

PROGRAM ECFDefine

```

C This program get the problem definition from the user.
C Written by: Ken Jordan           8/1/87
C Modified by: Mike Armstrong     9/1/87
C   Added multiple equations.
C Modified by: Ken Jordan         9/24/87
C   Debugged multiple equations.
C Modified by: Ken Jordan         10/22/87
C   Added: EC Problem Report (prints parameters used to solve EC problem)
C   Added: Uses POLYFLOW Boundary Node numbers, converts to EC bdnodes
C   internally.

C *****
C Variables
C *****

C *****
C Subroutines
C *****

C ComputeCLoc      Computes the contents of the CLoc matrix.
C ComputeCorners  Computes the location of the corner points based
C                 on the boundary node numbers from polymesh and the
C                 degree of the basis functions.
C DefineBC        Allows the user to define the upper, lower electrode
C                 potential, and the type of current distribution.
C DefineECFParams
C PrintProb       Writes a report on the CRT about the FEM problem
C                 to be solved.
C SetCoef
C Titles
C WriteFEMUser    Writes the FEM.* files for later reading by
C                 FEM2dBAND
C WriteRes()      Writes the C and CLoc variables

C *****
C Main Program Follows
C *****

```

```

INCLUDE 'ECFNam.INC'
INCLUDE 'ECFHdr.INC'

```

```

CHARACTER*80 MenuTitle/'EC Problem Modification'/,
& MenuTxt(13)/
1 'Code To',
2 ', ',
3 'P  Print a problem report',
4 ', ',
5 'F  Modify FEM Parameters',
7 'B  Modify Boundary Conditions',
8 'C  Modify Convection or Kinetics Parameters',
9 'N  Modify File Names',
a ', ',
1 'X  Exit (saves modifications & recomputes first guess)',
2 'Q  Quit (forgets modifications)',
3 ', ',
4 '?  Repeats this list/'

```

```

CHARACTER*80 MenuPrompt/'Enter a Code'/
CHARACTER*1 MenuResps(8)/'P','F','B','C','N','X','Q','?'/
& DefResp/'X'/,Resp
INTEGER NTxt/13/,NResps/8/

INTEGER Length
LOGICAL FileExist,Editing,Another,Reset,OldProb
CHARACTER*80 FileName/'FEM.NAM'/

CALL Titles

1 CALL EditCh('Names file?',FileName)

IF (FileName.NE.' ') THEN

    INQUIRE(File=FileName,Exist=FileExist)
    IF (FileExist) THEN

        WRITE(*,*) 'Reading data from old files'
        CALL ReadNames(FileName)
        CALL ReadFEMUser
        IF (.NOT.ECFMesh) CALL UnComputeCorners
        CALL PrintProb(FileName)
        OldProb=.TRUE.

    ELSE

        OldProb=.FALSE.
        CALL Defaults

        CALL StringLength(FileName,Length)
        Length=MAX(Length,1)

        WRITE(*,*) 'Warning: File ',FileName(1:Length),
& ' doesn''t exist.'
        WRITE(*,*) '          I am assuming that you are entering',
& ' data for a new problem.'

    END IF

ELSE

    OldProb=.FALSE.
    FileExist=.FALSE.
    CALL Defaults
    WRITE(*,*) 'Getting data for a new problem!'

END IF

IF (FileExist) THEN

    Editing=.TRUE.
    DO WHILE(Editing)

        CALL Menu(MenuTitle,MenuTxt,NTxt,MenuPrompt,
& MenuResps,NResps,DefResp,Resp)

```

C P=print problem report

C F=Method, Problem Parameters
 C B=Boundary Conditions
 C C=Kinetics, Convection Parameters
 C N=File Names Definition

C X=Exit (saves modifications)
 C Q=Quit (no modifications saved)

```

    IF (Resp.EQ.'P') CALL PrintProb(FileName)

    IF (Resp.EQ.'F') CALL DefineECFParams(FileName)
    IF (Resp.EQ.'B') CALL DefineBC
    IF (Resp.EQ.'C') CALL DefinePar
    IF (Resp.EQ.'N') CALL DefineNames(FileName)

    IF (Resp.EQ.'X') Editing=.FALSE.
    IF (Resp.EQ.'Q') STOP 'Quit--No Modifications Saved!'
  
```

END DO

ELSE

```
CALL DefineECFParams(FileName)
```

```
CALL DefineBC
```

```
CALL DefinePar
```

```
CALL DefineNames(FileName)
```

END IF

IF (.NOT.ECFMesh) THEN

C The mesh was generated using POLYMESH.

```

WRITE(*,*) 'Transferring mesh from polymesh file'
CALL ComputeCorners
  
```

C The following call transfers the mesh from the polyflow file to
 C a EC file.

```
CALL MeshTransfer
```

END IF

C Compute the number of coefficients. Check to make sure we have enough memory
 C to solve this problem.

```

NoOfCoef=NoOfEqu*NoOfNodes
IF (NoOfCoef.GT.MaxNoOfCoef) THEN
  WRITE(*,*) 'Error: No of coefficients is too large.'
  WRITE(*,*) '      NoOfCoef=',NoOfCoef
  WRITE(*,*) '      MaxNoOfCoef=',MaxNoOfCoef
  STOP 'ECFDEFINE: Abnormal End'
END IF
  
```

C The following call computes the matrix CLoc used to locate the
 C coefficients for each equation.

```
CALL ComputeCLoc
```

C The following call computes a first guess for the coefficients

```
IF (OldProb) THEN
  CALL YorN('Reset Coefficients?',Reset)
ELSE
  Reset=.TRUE.
END IF
```

```
IF (Reset) CALL SetCoef
```

C The following two calls store the information for later use by FEM2D

```
CALL WriteNames(FileName)
CALL WriteFEMUser
```

```
CALL EditYorN('Another?',Another)
IF (Another) GOTO 1
```

```
STOP 'Normal End'
END
```

C ***** ComputeCLoc

```
SUBROUTINE ComputeCLoc
```

```
INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFMsh.INC'
INCLUDE 'ECFRes.INC'
INTEGER I,ElemCol,ElemRow,J,NodeNo,K,
& LocNodes((MaxNoOfBasisDeg+1)**(MaxNoOfDim))
INTEGER Upper
```

C The following DO-Loop Computes the CLoc (or NOP) Matrix
C (Currently set up for BasisDeg=1 or 2) from NLoc, the node numbers
C for each element.

```
IF ((BasisDeg.NE.1).AND.(BasisDeg.NE.2)) THEN
  WRITE(*,*) 'Error: Degree of Basis Functions incorrect.'
  WRITE(*,*) '   BasisDeg=',BasisDeg
  STOP 'In Routine: ComputeCLoc'
END IF
```

```
DO I=1,NoOfElems
  CALL GetUpper(ElemType(I),Upper)
  DO K=1,Upper
    DO J=1,NoOfEqu
```

C This is the most efficient way to store coefficients.

C Coefficients are numbers C1=node1,eq1, c2=node1,eq2,...

```
CALL ComputeCoefLoc(NLoc(I,K),J,CLoc(J,I,K))
```

D WRITE(*,*) 'NLoc',I,K,Nloc(I,K)

D WRITE(*,*) 'CLoc',J,I,K,CLoc(J,I,K)

C For Coefficients stored as C1=node1, eq1; c2=node2, eq1,...

C CLoc(J,I,K)=NLoc(I,K)-(J-1)*NoOfNodes

```

        END DO
    END DO
END DO

```

```

RETURN
END

```

C ***** ComputeCorners

```

SUBROUTINE ComputeCorners

```

C This subroutine computes the corner points for the problem based
C on the corner points from the POLYFLOW Mesh, and on the BasisDeg chosen
C by the user.

```

    INCLUDE 'ECFHdr.INC'
    INCLUDE 'ECFbc.INC'

```

```

    INTEGER Equ,Cnr

```

```

    IF ((BasisDeg.EQ.1).OR.(BasisDeg.EQ.3)) THEN
        DO Equ=1,NoOfEqu
            DO Cnr=1,NoOfCorners(Equ)
                Corners(Equ,Cnr)=(Corners(Equ,Cnr)+1)/2
            END DO
        END DO
    END IF

```

```

RETURN
END

```

C ***** Defaults

```

SUBROUTINE Defaults

```

```

    INCLUDE 'ECFNam.INC'
    INCLUDE 'ECFHdr.INC'
    INCLUDE 'ECFGauss.INC'

```

```

    MeshHdrFile='EC.HDR'
    MeshFile='EC.MSH'
    BCFile='EC.BC'
    ParFile='EC.PAR'

```

```

    ResFile='EC.RES'
    PlotFile='EC.ISO'
    SlopeFile='EC.SLP'

```

```

    NoOfEqu=1
    NoOfDim=2
    BasisDeg=1
    Tolerance=0.00001
    NoOfGaussPts=4
    MaxNoOfITer=10

```

```

    Debugging=.FALSE.
    Convection=.FALSE.
    PolyFlow=.TRUE.

```

Guess=.FALSE.

Nonnegative=.FALSE.

RETURN
END

C ***** DefineBC

SUBROUTINE DefineBC

C This subroutine allows the user to define the type of current distribution
C and the voltage at the upper and lower plates (Vu,VI)

INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFbc.INC'

INTEGER I,Ip1,Equ,J
INTEGER Corn(MaxNoOfCorners)

CHARACTER*80 Prompt,Dummy
LOGICAL Inputting,EntKin

CHARACTER*80 BCMenuTitle/'Boundary Condition Selection',
& BCMenuTxt(13)/
1 'Code Boundary Condition',
2 ', '
3 ' P Primary Current Distribution ',
4 ' (Surface is equipotential)',
5 ' S Secondary Current Distribution',
6 ' (Current depends on voltage near surface)',
7 ' I Insulator',
8 ' (No current through surface)',
9 ' E Essential',
a ' (Potential at surface set by external subroutine',
1 ' N Natural',
2 ' (Current at surface set by external subroutine',
3 ' ? Repeats this list'/
CHARACTER*80 MenuPrompt
CHARACTER*1 BCMenuResps(6)/'P','S','I','E','N','?'/,
& DefResp/'?'/,UsrResp
INTEGER BCNTxt/13/,BCNResps/6/

CHARACTER*80 KIMenuTitle/'Kinetics Selection',
& KIMenuTxt(6)/
1 'Code Electrode Kinetics Selected',
2 ', '
3 ' BV Butler Volmer',
4 ' LI Linear',
5 ' TA Tafel',
6 ' ? Repeats this list'/
CHARACTER*2 KIMenuResps(4)/'BV','LI','TA','?'/,KIDefResp/'?'/,
& KIUsrResp
INTEGER KINTxt/6/,KINResps/4/

DO Equ=1,NoOfEqu
EntKin=.FALSE.

```
WRITE(*,*) ' '
WRITE(*,*) 'BC Conditions-----'
```

C The following statements get the corner points from the user for
C equation #L

```
IF (NoOfEqu.GT.1) WRITE(*,*) 'For Equation ',Equ
WRITE(*,*) ' '
```

```
DO J=1,NoOfCorners(Equ)
  Corn(J)=Corners(Equ,J)
END DO
```

```
CALL CodeI(Corn,NoOfCorners(Equ),Dummy)
```

```
IF (ECFMesh) THEN
  WRITE(*,*) 'Mesh generated by ECFMESH'
ELSE
  WRITE(*,*) 'Mesh generated by POLYMESH'
END IF
```

```
CALL EditCh(
& 'Enter Corner Points (boundary node #s)?',Dummy)
```

```
CALL DecodeI(Dummy,Corn,NoOfCorners(Equ),MaxNoOfCorners)
DO J=1,NoOfCorners(Equ)
  Corners(Equ,J)=Corn(J)
END DO
```

C The following statements and DO-loop allow the user to select the
C current distribution. (Primary or Secondary)

```
DO I=1,NoOfCorners(Equ)
```

```
  CALL IncrementI(I,Ip1,1,NoOfCorners(Equ))
```

```
  WRITE(MenuPrompt,FMT=27) I,Equ,
& Corners(Equ,I),Corners(Equ,Ip1)
27  FORMAT('Boundary Condition for side ',I2,
& ' Equ ',I2,' (Nodes ',I3,' to ',I3,')')
```

```
  DefResp=BCs(Equ,I)
  IF (DefResp.EQ.' ') DefResp='?'
```

```
  Inputting=.TRUE.
  DO WHILE (Inputting)
    CALL Menu(bcMenuTitle,bcMenuTxt,bcNTxt,MenuPrompt,
& bcMenuResps,bcNResps,DefResp,UsrResp)
    Inputting=(UsrResp.EQ.'?')
  END DO
  BCs(Equ,I)=UsrResp
```

C The following statements get whatever parameters are required for the
C boundary condition.

```
  IF ((BCs(Equ,I).EQ.'S').OR.(BCs(Equ,I).EQ.'P')) THEN
30  WRITE(Prompt,FMT=30) I,Equ,BCs(Equ,I)
    FORMAT('Voltage applied to side ',I2,
```

```

& ' Equ ',I2,' (BC=',A1,')'
  CALL EditDP(Prompt,BCPar(Equ,I))

  IF (BCs(Equ,I).EQ.'S') EntKin=.TRUE.

  ELSE IF (BCs(Equ,I).EQ.'E') THEN

    WRITE(Prompt,FMT=31) I,Equ,BCs(Equ,I)
31    FORMAT('Essential Parameter? (side',I2,
& ' equ ',I2,') (BC=',A1,')'
    CALL EditDP(Prompt,BCPar(Equ,I))

    ELSE IF (BCs(Equ,I).EQ.'N') THEN

    WRITE(Prompt,FMT=32) I,Equ,BCs(Equ,I)
32    FORMAT('Natural Parameter? (side',I2,
& ' equ ',I2,') (BC=',A1,')'
    CALL EditDP(Prompt,BCPar(Equ,I))

    ELSE IF (BCs(Equ,I).EQ.'I') THEN
      BCPAr(Equ,I)=0
    END IF

  END DO

C Get the kinetics code to use for this problem.

  IF (EntKin) THEN
10    WRITE(MenuPrompt,Fmt=10) Equ
    FORMAT('Kinetics Code? (Eqn ',I2,')')

    KIDefResp=Kinetics(Equ)
    IF (KiDefResp.EQ.' ') KIDefResp='?'

    Inputting=.TRUE.
    DO WHILE (Inputting)
      CALL Menu(KIMenuTitle,KIMenuTxt,KINTxt,
& MenuPrompt,KIMenuResps,KINResps,KIDefResp,KIUsrResp)
      Inputting=(KIUsrResp.EQ.'?')
    END DO
    Kinetics(Equ) =KiUsrResp
  ELSE
    Kinetics(Equ)= ' '
  END IF

END DO

RETURN
END

```

C ***** DefineECFParams

```

SUBROUTINE DefineECFParams(FileName)

```

```

  INCLUDE 'ECFHdr.INC'
  INCLUDE 'ECFGauss.INC'

```

```

  CHARACTER*(*) FileName

```

CHARACTER*3 Code
 CHARACTER*80 Dummy
 INTEGER Length

C The following CALL obtains the tolerance for testing convergence of the
 C Newton-Raphson iterations.

```

OPEN(UNIT=1,STATUS='NEW',FORM='FORMATTED',FILE='ECFDEF.TMP')

IF (Convection) THEN
  IF (PolyFlow) THEN
    Code='PFC'
  ELSE
    Code='EXC'
  END IF
ELSE IF (Binary) THEN
  Code='BIN'
ELSE IF (Supporting) THEN
  Code='SUP'
ELSE
  Code='LAP'
END IF

WRITE(1,*) '','','Code,''' '' Problem Code:'
WRITE(1,*) ' ' '' PFC=polyflow convective-diffusion'
WRITE(1,*) ' ' '' EXC=external convective-diffusion'
WRITE(1,*) ' ' '' BIN, SUP=',
& 'binary, or supporting electrolyte'
WRITE(1,*) ' ' '' LAP=Laplace''s Equation',
& ' for potential or conc.'
WRITE(1,*) ' '

WRITE(1,*) BasisDeg,' '' Degree of Basis Functions (0-2)'
WRITE(1,*) NoOfGaussPts,
& ' '' No. of Gaussian Integration Points ',
& '(1-',MaxNoOfGaussPts,')'
WRITE(1,*) NoOfDim,' ''Number of dimensions (2)'
WRITE(1,*) NoOfEqu,' ''Number of Equations (1-)'
WRITE(1,*) MaxNoOfIter,' ''Maximum number of NR Iterations'
WRITE(1,*) Tolerance,' '' Convergence Tolerance'
WRITE(1,*) ' '

WRITE(1,*) Debugging,' ''T if debugging'
WRITE(1,*) Guess,' '' T for external first guess routine'
WRITE(1,*) Nonnegative,
& ' '' T for nonegative coeff. constraint'

WRITE(1,*) ' '
CALL StringLength(FileName,Length)
WRITE(1,*) 'FEM Method Parameters-----'
WRITE(1,*) 'File: ',FileName(1:Length)
CLOSE(1)

CALL LIB$SPAWN('EDIT ECFDEF.TMP')

OPEN(UNIT=1,STATUS='OLD',FORM='FORMATTED',FILE='ECFDEF.TMP')

READ(1,*) Code
```

```

10  READ(1,10) Dummy(1:1)
    FORMAT(A1)
    READ(1,10) Dummy(1:1)
    READ(1,10) Dummy(1:1)
    READ(1,10) Dummy(1:1)
    READ(1,10) Dummy(1:1)

    IF (Code.EQ.'PFC') THEN
        Convection=.TRUE.
        Polyflow=.TRUE.
        Binary=.FALSE.
        Supporting=.FALSE.
    ELSE IF (Code.EQ.'EXC') THEN
        Convection=.TRUE.
        Polyflow=.FALSE.
        Binary=.FALSE.
        Supporting=.FALSE.
    ELSE IF (Code.EQ.'BIN') THEN
        Convection=.FALSE.
        Binary=.TRUE.
        Supporting=.FALSE.
    ELSE IF (Code.EQ.'LAP') THEN
        Convection=.FALSE.
        Binary=.FALSE.
        Supporting=.FALSE.
    ELSE IF (Code.EQ.'SUP') THEN
        Convection=.FALSE.
        Binary=.FALSE.
        Supporting=.TRUE.
    ELSE
        WRITE(*,*) 'Error: Unknown problem code.'
    END IF

    READ(1,*) BasisDeg

    IF ((BasisDeg.LT.0).OR.(BasisDeg.GT.2)) THEN
        WRITE(*,*) 'Error: Degree of Basis Functions is out of range'
    END IF

    READ(1,*) NoOfGaussPts
    IF ((NoOfGaussPts.GT.MaxNoOfGaussPts)
    & .OR.(NoOfGaussPts.LT.1)) THEN
        WRITE(*,*) 'Error: No. of gauss pts is out of range.'
    END IF

    READ(1,*) NoOfDim
    READ(1,*) NoOfEqu

    READ(1,*) MaxNoOfIter
    READ(1,*) Tolerance
    READ(1,10) Dummy(1:1)

    READ(1,*) Debugging
    READ(1,*) Guess
    READ(1,*) Nonnegative

    CLOSE(1)

```



```
RETURN
END
```

```
C ***** DefineNames
```

```
  SUBROUTINE DefineNames(FileName)
```

```
    INCLUDE 'ECFHdr.INC'
    INCLUDE 'ECFNam.INC'
    CHARACTER*(*) FileName
```

```
C The following lines put in default names
```

```
  WRITE(*,*) 'File Names Selection-----'
```

```
  WRITE(*,*) ' '
  WRITE(*,*) '***** Mesh Source File *****'
  WRITE(*,*) ' '
```

```
  CALL GetFileName(
& 'PolyFlow Mesh File to transfer to EC Mesh?',
& MeshSrcFile)
```

```
  WRITE(*,*) ' '
  WRITE(*,*) '***** Input Files for ECCompute *****'
  WRITE(*,*) ' '
```

```
  CALL EditCh('Names file?',FileName)
  WRITE(*,*) ' '
```

```
  CALL EditCh('EC Mesh Header File?',MeshHdrFile)
  CALL EditCh('EC Mesh File?',MeshFile)
  CALL EditCh('BC File?',BCFile)
  CALL EditCh('Miscellaneous Parameters File?',ParFile)
```

```
  IF (Convection.AND.PolyFlow) THEN
```

```
    WRITE(*,*) ' '
    WRITE(*,*) '***** Velocity Profile Files From POLYFLOW '
& 'Program *****'
    WRITE(*,*) ' '
```

```
    CALL GetFileName('Polyflow Mesh Filename?',PFMeshFile)
    CALL GetFileName('Polyflow Results FileName?',PFCoeffFile)
```

```
  END IF
```

```
  WRITE(*,*) ' '
  WRITE(*,*) '***** Output Files from ECCompute *****'
  WRITE(*,*) ' '
```

```
  CALL EditCh('Results File?',ResFile)
  WRITE(*,*) ' '
  WRITE(*,*) '***** Graphics Files from FEM2dPlot *****'
  WRITE(*,*) ' '
  CALL EditCh('Plot File?',PlotFile)
  CALL EditCh('Slope File?',SlopeFile)
```

```
RETURN
END
```

C ***** DefinePar

```
SUBROUTINE DefinePar
```

C This subroutine will allow the user to define the various parameters used
C in the problem.

```
INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFPar.INC'
INCLUDE 'ECFbc.INC'
```

```
LOGICAL Kinet
INTEGER I,Equ
```

```
Kinet=.FALSE.
DO Equ=1,NoOfEqu
  DO I=1,NoOfCorners(Equ)
    Kinet=Kinet.OR.(BCs(Equ,I).EQ.'S')
  END DO
```

```
IF (Kinet) THEN
```

```
  IF (.NOT.Binary) THEN
    WRITE(*,*) ' '
    WRITE(*,*) ' WagnerLin = Kappa R T / L F i0'
  ELSE
```

C For Binary or Supporting cases.

```
  WRITE(*,*) ' '
  WRITE(*,*) ' WagnerLin = 2 F D1 Cref / L i0'
  END IF
  CALL EditDP('WagnerLin?',WagnerLin)
  CALL EditDP('Anodic Transfer Coefficient',aA)
  CALL EditDP('Cathodic Transfer Coefficient',aC)
```

```
  IF ((Binary).OR.(Supporting)) THEN
    CALL EditDP('Integration Constant (binary)?',BinaryK2)
  END IF
```

```
  IF (Supporting) THEN
    CALL EditDP('Integration Constant (supporting)?',
& SupportingK3)
  END IF
  END IF
```

```
  IF (Convection) THEN
    CALL EditDP('Peclet number?',Peclet)
  END IF
  END DO
```

```
RETURN
END
```

C ***** MeshTransfer

SUBROUTINE MeshTransfer

C This subroutine will generate NLoc(,) and Nodes(,) from data in a polyflow
C mesh file generated by POLYMESH

```
INCLUDE 'ECFNam.INC'
INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFMsh.INC'
INCLUDE 'POLYMesh.INC'
```

```
INTEGER I,NodeMax,Zero/0/,Nv,J,Stp
LOGICAL Triangular
```

```
CALL ReadPFMesh(MeshSrcFile)
```

C Transfer the boundary node information

```
NoOfBDNodes=0
```

```
IF ((BasisDeg.EQ.1).OR.(BasisDeg.EQ.3)) THEN
  Stp=2
ELSE IF (BasisDeg.EQ.2) THEN
  Stp=1
END IF
```

C Check Limits too see if max no of ... needs to be set higher.

```
IF (PolyNBd/Stp.GT.MaxNoOfNodes) THEN
  WRITE(*,*) 'Error: too many nodes. Problem can''t be'
  WRITE(*,*) '      solved by present program configuration'
  WRITE(*,*) '      Max No Of Nodes=',MaxNoOfNodes
  WRITE(*,*) '      Cur No Of Nodes=',PolyNBd/Stp
  STOP '(ECFDEFINE) In Routine: MeshTransfer'
END IF
```

```
IF (PolyNElem.GT.MaxNoOfNodes) THEN
  WRITE(*,*) 'Error: Too many mesh elements. Either decrease',
& ' the size of the mesh,'
  WRITE(*,*) '      or increase MaxNoOfNodes in ECFHDR.INC'
  WRITE(*,*) '      PolyNElem=',PolyNElem
  WRITE(*,*) '      MaxNoOfNodes=',MaxNoOfNodes
  STOP '(ECFDEFINE) In Routine: MeshTransfer'
END IF
```

```
DO I=1,PolyNbd,Stp
  NoOfBDNodes=NoOfBDNodes+1
  BdNodes(NoOfBDNodes)=PolyBDNod(I)
END DO
```

C Find the maximum node number and Transfer the node numbers to NLoc

```
NodeMax=0
DO I=1,PolyNElem
  IF (PolyNod(9,I).EQ.Zero) THEN
    Triangular=.TRUE.
  ELSE
    Triangular=.FALSE.
  END IF
```

```

IF (BasisDeg.EQ.1) THEN

  IF (Triangular) THEN
    Nv=3
  ELSE
    Nv=4
  END IF

ELSE IF (BasisDeg.EQ.2) THEN

  IF (Triangular) THEN
    Nv=6
  ELSE
    Nv=9
  END IF

ELSE

  Nv=0
  WRITE(*,*) 'Error: Routine not written for BasisDeg=',
& BasisDeg
  WRITE(*,*) '      BasisDeg must be 1 or 2'
  STOP 'In routine: MeshTransfer'

END IF

C Make NLoc

DO J=1,Nv
  IF (NodeMax.LT.PolyNod(J,I)) NodeMax=PolyNod(J,I)
  NLoc(I,J)=PolyNod(J,I)
END DO

END DO

C Transfer the node locations from POLYX, POLYY to Nodes(,)

IF (NodeMax.GT.MaxNoOfNodes) THEN
  WRITE(*,*) 'Error: Too many nodes. Number of Nodes = ',NodeMax
  WRITE(*,*) '      Max Number of Nodes = ',MaxNoOfNodes
  WRITE(*,*) '      Either decrease mesh, or increase MaxNoOfNodes',
& ' in ECFHDR.INC'
  WRITE(*,*) '      and recompile, relink ECF programs.'
  STOP 'ECFDEFINE=In Routine: MeshTransfer-Abnormal End'
END IF

DO I=1,NodeMax
  Nodes(I,1)=PolyX(I)
  Nodes(I,2)=PolyY(I)
END DO

NoOfElems=PolyNElem
NoOfNodes=NodeMax

RETURN
END

```

C ***** PrintProb

SUBROUTINE PrintProb(NamesFile)

C This subroutine outputs a report on the problem defined by the user.

INCLUDE 'ECFHdr.INC'
 INCLUDE 'ECFGauss.INC'
 INCLUDE 'ECFbc.INC'
 INCLUDE 'ECFPar.INC'
 INCLUDE 'ECFNam.INC'

INTEGER I,L,J,Equ,Length
 INTEGER Corn(MaxNoOfCorners)
 LOGICAL Kinet
 CHARACTER*80 Dummy,Output
 CHARACTER*(*) NamesFile

CALL PrintProbHeader

WRITE(*,230) NoOfElems,NoOfNodes,Nlc,NoOfBDNodes,Nuc

230 FORMAT(X,7X,'Number of Elements: ',I6/,
 & X,10X,'Number of Nodes: ',I6,4X,'Codiagonals: lower=',I4,
 & /,X,' Number of Boundary Nodes: ',I6,18X,'upper=',I4)

C 1234567 1234 12
 C Number of Elements: iiiiii
 C Number of Nodes: iiiiii Codiagonals: lower=iiii
 C Number of Boundary Nodes: iiiiii upper=iiii
 C 1 123456789a12345678

C +-----+

WRITE(*,10)
 10 FORMAT(X,58('-',) ' Boundary Conditions')

C 123456789a123456789b123456789c123456789d123456789e12345678
 C ----- Boundary Conditions

C 123456789a123456789b123456789c123456789d123456789e1
 C Equation ii iii Corners: aaa
 C 123456789a1234567
 C Side iii: BC (a) BC Parm (dd.ddddd e+dd) Kinetics (aa)

DO L=1,NoOfEqu

DO J=1,NoOfCorners(L)
 Corn(J)=Corners(L,J)
 END DO

Dummy=' '
 CALL CodeI(Corn,NoOfCorners(L),Dummy)

IF (NoOfEqu.EQ.1) THEN
 21 WRITE(*,21) NoOfCorners(1),Dummy
 FORMAT(X,' ',2X,3X,I3,' Corners: ',A51)
 ELSE
 WRITE(*,20) L,NoOfCorners(L),Dummy

```

20      FORMAT(X,'Equation ',I2,3X,I3,' Corners: ',A51)
      END IF

      DO I=1,NoOfCorners(L)
        IF (I.EQ.L) THEN
          IF (Kinetics(L).NE.' ') THEN
            WRITE(*,30) I,BCs(L,I),BCPar(L,I),Kinetics(L)
          ELSE
            WRITE(*,30) I,BCs(L,I),BCPar(L,I)
          END IF
        ELSE
          WRITE(*,30) I,BCs(L,I),BCPar(L,I)
        END IF
      END DO
30      FORMAT(X,17X,'Side ',I3,': BC (' ,A1,') Param. (' ,G14.7,
      & ')',:,' Kinetics (' ,A2,')')
      END DO
      END DO

```

C ++++++

```

      Kinet=.FALSE.
      DO Equ=1,NoOfEqu
        DO I=1,NoOfCorners(Equ)
          Kinet=Kinet.OR.(BCs(Equ,I).EQ.'S')
        END DO
      END DO

```

```

C 123456789a123456789b123456789c123456789d123456789e123
C ----- Miscellaneous Parameters
C      123456789a12      1234      1234
C Constants:      R=dddddddddddddd F=dddddddddddddd T=dddddddddddddd
C Transport Parameters: K=dddddddddddddd Pe=dddddddddddddd
C Kinetic Parameters: i0=dddddddddddddd aA=dddddddddddddd aC=dddddddddddddd

```

```

      IF (Kinet.OR.Convection) THEN
        WRITE(*,100)
100      FORMAT(X,53('-'),' Miscellaneous Parameters')
120      FORMAT(X,'Transport Parameters:Pe=',G14.7)
130      FORMAT(X,'Kinetic Parameters: Wa=',G14.7, aA=',G14.7,
      & ' aC=',G14.7)
135      FORMAT(X,'Kinetic Par.:      k2=',G14.7)

        IF (Convection) THEN
          WRITE(*,120) Peclet
        ELSE IF (Binary) THEN
          WRITE(*,130) WagnerLin,aA,aC
          WRITE(*,135) Binaryk2
        ELSE
          WRITE(*,130) WagnerLin,aA,aC
        END IF

```

END IF

C ++++++

```

C 123456789a123456789b123456789c123456789d123456789e123456789f1234567
C ----- File Names

```

```

WRITE(*,300)
300  FORMAT(X,67('-', ' File Names')

C      123456789a123456789b123456789c123456789      123456789a12345
C Input Files:                                     Names File: AAAAAAAAAAAAAAAAAA

      WRITE(*,310) NamesFile
310  FORMAT(X,'Input Files:',34X,'Names File: ',A20)
C 123      123456789a12345

C (PolyFlow Mesh Source: AAAAAAAAAAAAAAAAAA)

      IF (.NOT.ECFMesh) THEN
      CALL StringLength(MeshSrcFile,Length)
      WRITE(*,320) MeshSrcFile(1:Length)
320  FORMAT(X,' (PolyFlow Mesh Source: ',A<Length>,)')
      END IF

C 123456789a123      1234
C      Mesh Header: AAAAAAAAAAAAAAAAAA Mesh: AAAAAAAAAAAAAAAAAA

      WRITE(*,330) MeshHdrFile,MeshFile
330  FORMAT(X,13X,'Mesh Header: ',A20,4X,'Mesh: ',A20)

C 12345
C Boundary Conditions: AAAAAAAAAAAAAAAAAA
C Miscellaneous Parameters: AAAAAAAAAAAAAAAAAA
C

      WRITE(*,340) BCFile,ParFile
340  FORMAT(X,5X,'Boundary Conditions: ',A20,/,X,
& 'Miscellaneous Parameters: ',A20,/)

C Velocity Profile Files:
C      123456789a123456789b123      123456789a123456789b
C Polyflow Mesh: AAAAAAAAAAAAAAAAAAAAAAAAAA Polyflow Results: AAAAAAAAAAAAAAAAAAAAAAAAAA
C

      IF (Convection.AND.PolyFlow) THEN
      WRITE(*,350) PFMeshFile,PFCoefFile
350  FORMAT(X,'Velocity Profile Files: ',/,X,
& 'Polyflow Mesh File: ',A20,3X,'Polyflow Results: ',A20,/)
      END IF

C Output Files:
C 123456
C Results: AAAAAAAAAAAAAAAAAAAAAAAAAA
C 123456789      123
C Plot: AAAAAAAAAAAAAAAAAAAAAAAAAA Slope: AAAAAAAAAAAAAAAAAAAAAAAAAA

      WRITE(*,360) ResFile,PlotFile,SlopeFile
360  FORMAT(X,'Output Files: ',/,X,
& 6X,'Results: ',A20,/,X,
& 9X,'Plot: ',A20,3X,'Slope: ',A20)

      RETURN
      END

```

C ***** SetCoef

SUBROUTINE SetCoef

C This subroutine sets up the values of the potential for the first guess.

C (Note, currently the subroutine will only handle 1st

C order basis functions)

```
INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFMsh.INC'
INCLUDE 'ECFRes.INC'
INCLUDE 'ECFbc.INC'
```

```
REAL*8 dV,Avg,X(MaxNoOfDim)
INTEGER J,NodeNo,K,Equ,Side,Sidep1,Elem,Upper
```

```
IF ((BasisDeg.GT.2).OR.(BasisDeg.LT.0)) THEN
  WRITE(*,*) 'Warning: illegal degree of basis functions'
  WRITE(*,*) '      BasisDeg=',BasisDeg
  STOP 'In routine: SetCoef'
END IF
```

```
DO Equ=1,NoOfEqu
```

```
  IF (.NOT.Guess) THEN
```

```
    Avg=0.0
    DO Side=1,NoOfCorners(Equ)
      Avg=Avg+BCPar(Equ,Side)
    END DO
    Avg=Avg/(NoOfCorners(Equ)-2)
```

```
  END IF
```

C The following do-loop makes the first guess for coefficients

```
IF ((Binary).OR.(Supporting)) THEN
  Avg=ABS(Avg)
END IF
```

```
DO Elem=1,NoOfElems
  CALL GetUpper(ElemType(Elem),Upper)
  DO J=1,Upper
```

```
    IF (.NOT.Guess) THEN
      C(CLoc(Equ,Elem,J))=Avg
    ELSE
      DO K=1,NoOfDim
        X(K)=Nodes(NLoc(Elem,J),K)
      END DO
      CALL FirstGuess(1,Elem,X,C(CLoc(Equ,Elem,J)))
    END IF
```

```
  END DO
```

```
END DO
```

```
END DO
```

C The following DO-Loop sets the voltage of the plate for primary

C current distribution.

```

DO Equ=1,NoOfEqu
  DO Side=1,NoOfCorners(Equ)

    CALL IncrementI(Side,Side1,1,NoOfCorners(Equ))

    IF (BCs(Equ,Side).EQ.'P') THEN

      DO J=Corners(Equ,Side),Corners(Equ,Side1)
        C((BDNodes(J)-1)*NoOfEqu+Equ)=BCPar(Equ,Side)
      END DO

    ELSE IF (BCs(Equ,Side).EQ.'E') THEN

      IF (Corners(Equ,Side).LE.Corners(Equ,Side1)) THEN

        DO J=Corners(Equ,Side),Corners(Equ,Side1)
          DO K=1,NoOfDim
            X(K)=Nodes(BDNodes(J),K)
          END DO
          CALL Essential(Side,1,X,BCPar(Equ,Side),
& C((BDNodes(J)-1)*NoOfEqu+Equ))
        END DO

      ELSE

        DO J=Corners(Equ,Side),NoOfBDNodes
          DO K=1,NoOfDim
            X(K)=Nodes(BDNodes(J),K)
          END DO
          CALL Essential(Side,1,X,BCPar(Equ,Side),
& C((BDNodes(J)-1)*NoOfEqu+Equ))
        END DO

        DO J=1,Corners(Equ,Side1)
          DO K=1,NoOfDim
            X(K)=Nodes(BDNodes(J),K)
          END DO
          CALL Essential(Side,1,X,BCPar(Equ,Side),
& C((BDNodes(J)-1)*NoOfEqu+Equ))
        END DO

      END IF

    END IF
  END DO
END DO

RETURN
END

```

C ***** Titles

SUBROUTINE Titles

C This subroutine prints the run-time-message that lets the user know
C the name of the program being run, etc.

```
WRITE(*,*) 'Program ECFDefine'  
WRITE(*,*) 'Version 2'  
WRITE(*,*) ''  
WRITE(*,*) 'This program allows the user to define the type'  
WRITE(*,*) 'of problem the FEM program will solve'  
WRITE(*,*) ''
```

```
RETURN  
END
```

```
C ***** UnComputeCorners
```

```
SUBROUTINE UnComputeCorners
```

```
C This subroutine computes the corner points of the polyflow mesh based  
C on the corner points for the problem and on the BasisDeg chosen  
C by the user.
```

```
INCLUDE 'ECFHdr.INC'  
INCLUDE 'ECFbc.INC'
```

```
INTEGER Equ,Cmr
```

```
IF ((BasisDeg.EQ.1).OR.(BasisDeg.EQ.3)) THEN  
  DO Equ=1,NoOfEqu  
    DO Cmr=1,NoOfCorners(Equ)  
      Corners(Equ,Cmr)=2*Corners(Equ,Cmr)-1  
    END DO  
  END DO  
END IF
```

```
RETURN  
END
```

```
C *
```

PROGRAM ECFPrePro

C This program computes the bandwidth for the EC problem.

C Written by: Ken Jordan

C Modified by: Mike Armstrong

C Debugged by: Ken Jordan

C *****

C VARIABLES

C *****

INCLUDE 'ECFNam.INC'

INCLUDE 'ECFHdr.INC'

INCLUDE 'ECFMsh.INC'

CHARACTER*72 FileName

INTEGER Elm,I,J,BandWidth,MaxN,MinN,MaxDiff,Upper

C *****

C Main Program

C *****

C The following call reads the values of variables that define the problem and
C solution technique (BasisDeg, NoOfElems, NoOfNodes, NoOfXElems, NoOfYElems,
C Tolerance)

CALL GetFileName('Names file?',FileName)

CALL ReadNames(FileName)

CALL ReadFEMUser

C New routine to calculate bandwidth based on max difference between node
C number on each element.

MaxDiff=1

DO Elm=1,NoOfElems

MaxN=NLoc(Elm,1)

MinN=MaxN

CALL GetUpper(ElemType(Elm),Upper)

DO I=2,Upper

MaxN=MAX(MaxN,NLoc(Elm,I))

MinN=MIN(MinN,NLoc(Elm,I))

END DO

MaxDiff=MAX(MaxDiff,MaxN-MinN)

END DO

Nuc=MaxDiff

Nlc=MaxDiff

Bandwidth=Nlc+Nuc+1

WRITE(*,*) 'Number of Lower Codiagonals=',Nlc

```
WRITE(*,*) 'Number of Upper Codiagonals=',Nuc  
WRITE(*,*) ' Bandwidth=',Bandwidth  
WRITE(*,*) 'Matrix Order=',NoOfCoef,',',NoOfCoef
```

```
CALL WriteMeshHdr(MeshHdrFile)
```

```
STOP 'Normal End'  
END
```

PROGRAM ECFCompute

C This program uses the galerkin method in two dimensions to
C solve migration-diffusion problems.

C The differential equation is:

$$C \frac{d^2\Phi}{dy^2} + \frac{d^2\Phi}{dx^2} - Pe (V_x \frac{d\Phi}{dX} + V_y \frac{d\Phi}{dY}) = 0$$

C with the following possible boundary conditions,

- C Constant Potential
- C Arbitrary Potential Profile
- C Insulator (Slope=0)
- C Constant Slope
- C Tafel, Linear, or BV Kinetics (Slope dependent on overpotential)

C Written by: Ken Jordan 4/2/86

C Modified 8/3/87

C *****
C Variables
C *****

C Converged .TRUE. when solution has converged.
C FileName The name of the names file. (Contains file names
C for reading remaining data. E.g. HULL.NAM)

C *****
C Subroutines
C *****

C Internal

- C AdjustForKinetics Computes the BC for secondary current distribution.
- C AdjustForKnown Resets R and RJacobian for known coefficients.
- C AssembleBC Adjusts the R, RJacobian matrices for the
C boundary conditions.
- C AssembleMatrices Assembles the R, RJacobian matrices.
- C VecNormDP Compares 2-norm of dC to Tolerance to check for
C convergence
- C ComputeDelPotDotNorm Computes the normal wall current (used in secondary
C current distribution boundary conditions.)
- C ComputeIsoPara Given the Element number, and PhiZeta, computes
C XZeta, and the determinant of the jacobian.
- C ComputePot Computes the value of the potential and the potential
C derivative.
- C NewtonRaphson Performs the newton-raphson technique to solve the
C differential equation.
- C PrintCLoc Prints the contents of the CLoc matrix.
- C PrintMat Prints the Jacobian Matrix, and the Residual Vector
- C PrintNodes Prints the node locations
- C PrintResults Prints the coefficients and parameter settings used
C to run problem.

C UpdateC Adds dC to C and stores result in C
 C ZeroRJ Zeros the R,RJacobian,dRdP vectors.

C External

C Compute1DPhi Computes the value of the local weighting functions
 C Phi and dPhi/dZeta() (Zeta() is the local variable) in
 C 1 dimension.
 C Compute2DPhi Computes the value of the local weighting functions
 C and derivatives for 2D.
 C GaussPtsWts Generates the Gauss Pts and Wts in two vectors for
 C 1-6 Gaussian Quadrature integration points.

C *****
 C Files
 C *****

C *.BC Contains the boundary conditions
 C *.CMP Comparison between two slope files.
 C *.HDR Contains problem header information. (i.e. No of coefficients,
 C Number of dimensions, Number of equations...)
 C *.ISO Contains the data needed for isopotential plots.
 C *.MSH Contains the mesh and node locations and boundary node locations
 C *.NAM Contains the names of the files to use in solving the problem
 C E.g. *.NAM defines the filenames for *.bc, *.hdr, *.par, *.msh,
 C *.msh
 C *.PAR Contains parameter information. E.g. Kinetic parameters such
 C as the exchange current density, the transfer coefficients...
 C *.RES Contains the Coefficients and CLoc(,,)
 C *.SLP Contains slope at the boundary

C *****
 C Main Program Follows
 C *****

INCLUDE 'ECFHdr.INC'
 INCLUDE 'ECFNam.INC'
 INCLUDE 'ECFGauss.INC'

LOGICAL Converged
 CHARACTER*80 FileName
 INTEGER NoOfIterations,TotalIterations

*** IMSL workspace for DLSARB. The workspace is based on N, NLCA, and
 *** NUCA, where N = 377, NLCA = 27, and NUCA = 27 are given.

COMMON /WORKSP/ RWKSP
 REAL RWKSP(3343481)
 CALL IWKIN(3343481)

C The following call reads the values of variables that
 C define the problem and solution technique (BasisDeg, NoOfElems,
 C NoOfNodes,NoOfXElems,NoOfYElems,Tolerance)

CALL GetFileName('Names file?',FileName)

IF (FileName.EQ.' ') THEN
 WRITE(*,*) 'Error: No file name entered.'

```

      STOP 'In Program: ECFCompute'
    END IF

```

```

      CALL ReadNames(FileName)

```

```

      CALL ReadFEMUser

```

```

      IF (Convection.AND.PolyFlow) THEN
        CALL ReadPFMesh(PFMeshFile)
        CALL ReadPFCoef(PFCoefFile)
      END IF

```

C The following call obtains the Gauss Points and Weights for
C integrals over the interval 0 to 1.

```

      CALL GaussPtsWts(NoOfGaussPts,Pts,Wts)
      CALL TriPtsWts

```

```

      IF (Debugging) THEN
        CALL PrintNodes
        CALL PrintCLOC
      END IF

```

```

      TotalIterations=0

```

```

      CALL NewtonRaphson(NoOfIterations,Converged)

```

```

      CALL WriteRes(ResFile)

```

```

      IF (Converged) THEN

```

```

        TotalIterations=TotalIterations+NoOfIterations
        IF (Debugging) THEN
          CALL PrintNodes
          CALL PrintResults(TotalIterations,TotalIterations)
        END IF

```

```

      ELSE

```

```

        STOP 'Abnormal End: Not Converged, try continuation?'

```

```

      END IF

```

```

      STOP 'Normal End'
    END

```

C ***** AdjustForKinetics

```

      SUBROUTINE AdjustForKinetics(Nodals,Phi1D,DelPotDotNorm,
& DelPotDotNormPot,WtsJx,dR)

```

```

      INCLUDE 'ECFHdr.INC'
      INCLUDE 'ECFRes.INC'
      INCLUDE 'ECFCal.INC'

```

```

      INTEGER Nodals(*),BandCol
      REAL*8 Phi1D(*),WtsJx,dR,DelPotDotNorm,DelPotDotNormPot

```

```
INTEGER LocRow,LocCol
```

```
C The following statements and DO-Loops adjust the residual and jacobian
C for the boundary conditions on a plate when there are kinetics.
```

```
DO LocRow=1,BasisDeg+1
```

```
  R(Nodals(LocRow))=R(Nodals(LocRow))-WtsJx*
  & DelPotDotNorm*Phi1D(LocRow)*dR
```

```
  DO LocCol=1,BasisDeg+1
```

```
    CALL ComputeBandCol(Nodals(LocRow),Nodals(LocCol),BandCol)
    RJacobian(BandCol,Nodals(LocRow))=
    & RJacobian(BandCol,Nodals(LocRow))
    & +WtsJx*Phi1D(LocRow)*Phi1D(LocCol)*DelPotDotNormPot
    & *dR
```

```
  END DO
```

```
END DO
```

```
RETURN
```

```
END
```

```
C ***** AdjustForKnown
```

```
SUBROUTINE AdjustForKnown(CNodals,Val)
```

```
C This subroutine sets the appropriate residual and jacobian
C elements to zero or one for known coefficients (i.e. b.c.'s like
C T=1 at X=3...)
C This subroutine is usually called by AJUSTFORBC
```

```
INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFRes.INC'
INCLUDE 'ECFCal.INC'
```

```
INTEGER CNodals(*)
```

```
INTEGER I,BandCol,LocRow
REAL*8 Val
```

```
DO LocRow=1,BasisDeg+1
```

```
  C(CNodals(LocRow))=Val
```

```
  R(CNodals(LocRow))=0.0
```

```
  DO I=1,NoOfCoef
```

```
    CALL ComputeBandCol(CNodals(LocRow),I,BandCol)
```

```
    IF ((BandCol.GT.0).AND.(BandCol.LE.Nuc+Nlc+1)) THEN
```

```
      RJacobian(BandCol,CNodals(LocRow))=0.0
```

```
    END IF
```

```
  END DO
```

```
  CALL ComputeBandCol(CNodals(LocRow),CNodals(LocRow),
& BandCol)
```

```
  RJacobian(BandCol,CNodals(LocRow))=1.0
```

```
END DO
```

```
RETURN
```

```
END
```

```
C ***** AdjustForNatural
```



```
SUBROUTINE AdjustForNatural(Nodals,Phi1D,BCPar,WtsJx,dR)
```

```
INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFCal.INC'
```

C Variables

```
C Phi1D      1D Phis (At Surface)
C WtsJx      Wts(Jx)
```

```
INTEGER Nodals(*)
REAL*8 Phi1D(*),WtsJx,dR,BCPar
```

```
INTEGER LocRow
```

C The following statements and DO-Loops adjust the residual
C for the natural boundary conditions.

```
DO LocRow=1,BasisDeg+1
  R(Nodals(LocRow))=R(Nodals(LocRow))-WtsJx*
  & BCPAr*Phi1D(LocRow)*dR
END DO
```

```
RETURN
END
```

C ***** AssembleBC

```
SUBROUTINE AssembleBC
```

C This subroutine adjusts the Jacobian and Residual vector for the essential
C boundary conditions. The variables passed are described in the main
C program.

```
INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFGauss.INC'
INCLUDE 'ECFMsh.INC'
INCLUDE 'ECFbc.INC'
```

```
INTEGER I,J,Jp1,Equ
```

C The following IF-THEN blocks check to see that the basis degree is in
C the range that is used by the program.

```
IF ((BasisDeg.NE.1).AND.(BasisDeg.NE.2)) THEN
  WRITE(*,*) 'Warning: BasisDeg is not 1 or 2.'
  WRITE(*,*) '      BasisDeg=',BasisDeg
  STOP 'In routine: AssembleBC'
END IF
```

```
DO Equ=1,NoOfEqu
  DO J=1,NoOfCorners(Equ)
```

```
    CALL IncrementI(J,Jp1,1,NoOfCorners(Equ))
```

```
    IF ((BCs(Equ,J).EQ.'P').OR.(BCs(Equ,J).EQ.'E')) THEN
```

C For the primary current distribution, the value of the potential at the

C upper and lower plates is known. These are essential b.c.'s
 C BC type P or E

```

    IF (Corners(Equ,J).LE.Corners(Equ,Jp1)) THEN
      CALL SubKnown(Corners(Equ,J),Corners(Equ,Jp1)-1,
& Equ,J)
    ELSE
      CALL SubKnown(Corners(Equ,J),NoOfBDNodes,Equ,J)
      CALL SubKnown(1,Corners(Equ,Jp1)-1,Equ,J)
    END IF

    ELSE IF (BCs(Equ,J).EQ.'S') THEN

```

C For secondary current distribution

```

    IF (Corners(Equ,J).LE.Corners(Equ,Jp1)) THEN
      CALL SubSecondary(Corners(Equ,J),Corners(Equ,Jp1)-1,
& Equ,J)
    ELSE
      CALL SubSecondary(Corners(Equ,J),NoOfBDNodes,Equ,J)
      CALL SubSecondary(1,Corners(Equ,Jp1)-1,Equ,J)
    END IF

    ELSE IF (BCs(Equ,J).EQ.'N') THEN

```

C For natural boundary condition (slope set)

C (No need to call if condition is insulator, because, slope =0, adds

C nothing to residual or jacobian)

```

    IF (Corners(Equ,J).LE.Corners(Equ,Jp1)) THEN
      CALL SubNatural(Corners(Equ,J),Corners(Equ,Jp1)-1,
& Equ,J)
    ELSE
      CALL SubNatural(Corners(Equ,J),NoOfBDNodes,Equ,J)
      CALL SubNatural(1,Corners(Equ,Jp1)-1,Equ,J)
    END IF

```

END IF

END DO
 END DO

RETURN
 END

C ***** AssembleMatrices

SUBROUTINE AssembleMatrices

C Internal Variables

```

C NoOfGaussPts    The number of points to use in the Gaussian
C                quadrature approximation of the integration.
C Phi()           The value of the Local Weighting function at the current
C                gauss point. (Phi(1) is local weighting function 1,
C                while Phi(2) is local weighting function 2.)
C PhiZeta()       The slope of the weighting functions at the
C                current gauss point.

```

```

INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFMsh.INC'
INTEGER Elem,Equ

IF (NoOfDim.NE.2) THEN
  WRITE(*,*) 'Warning: NoOfDim is not 2'
  WRITE(*,*) '      The code must be altered!'
  STOP 'In Routine: AssembleMatrices'
END IF

```

C The following CALL zeros the residual vector and the jacobian

```
CALL ZeroRJ
```

```
DO Equ=1,NoOfEqu
```

C The following DO-LOOP loops over the number of elements

```
DO Elem=1,NoOfElems
```

```

IF (ElemType(Elem).EQ.'S') THEN
  CALL AssembleSquare(Equ,Elem)
ELSE IF (ElemType(Elem).EQ.'T') THEN
  CALL AssembleTriangle(Equ,Elem)
END IF

```

```
END DO
```

```
END DO
```

```
RETURN
```

```
END
```

C ***** AssembleSquare

```
SUBROUTINE AssembleSquare(Equ,Elem)
```

C Internal Variables

```

C NoOfGaussPts      The number of points to use in the Gaussian
C                   quadrature approximation of the integration.
C Phi()             The value of the Local Weighting function at the current
C                   gauss point. (Phi(1) is local weighting function 1,
C                   while Phi(2) is local weighting function 2.)
C PhiZeta()         The slope of the weighting functions at the
C                   current gauss point.

```

```

INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFGauss.INC'
INCLUDE 'ECFMsh.INC'
INCLUDE 'ECFRes.INC'
INCLUDE 'ECFCal.INC'
INCLUDE 'ECFPar.INC'

```

```

REAL*8 Zeta(MaxNoOfDim),XZeta(MaxNoOfDim,MaxNoOfDim),DetXZeta,
& Vlcty(MaxNoOfDim)
REAL*8 PHI((MaxNoOfBasisDeg+1)**MaxNoOfDim),
& PhiZeta(MaxNoOfDim,(MaxNoOfBasisDeg+1)**MaxNoOfDim),
& PhiX(MaxNoOfDim,(MaxNoOfBasisDeg+1)**MaxNoOfDim),

```

```

& Pot(MaxNoOfEqu),PotX(MaxNoOfDim,MaxNoOfEqu),
& dX(MaxNoOfDim),X(MaxNoOfDim)
  INTEGER LocRow,LocCol,Elem,J,Jx,Jy,BandCol,Equ,Upper

```

C The following DO-LOOP loops over the Gauss Points (performing the gaussian quadrature numerical integration). It forms the R Jacobian matrix and the R vector in an element by element fashion.

```

  CALL GetUpper(ElemType(Elem),Upper)

  DO Jx=1,NoOfGaussPts
  DO Jy=1,NoOfGaussPts

    Zeta(1)=Pts(Jx)
    Zeta(2)=Pts(Jy)

    CALL Compute2DPhis(Zeta,Phi,PhiZeta)
    CALL ComputeIsoPara(Elem,PhiZeta,XZeta,DetXZeta
& ,Upper)
    CALL ComputePhiX(Upper,PhiZeta,XZeta,DetXZeta,PhiX)
    CALL ComputePot(Elem,Upper,Phi,PhiX,Pot,PotX)

```

C The following call computes the velocity in the zeta(1) and C the zeta(2) directions. To do this, it needs to know the C current values of Zeta(1) and Zeta(2), as well as the current C element number.

```

  IF (Convection) THEN
    CALL ComputeLoc(Phi,Elem,X)
    CALL Velocity(X,Vlcty)
  END IF

```

```

  DO LocRow=1,Upper

```

C The following statements compute the Residual vector

```

    R(CLoc(Equ,Elem,LocRow))=R(CLoc(Equ,Elem,LocRow))
& +Wts(Jx)*Wts(Jy)*(PotX(1,Equ)*PhiX(1,LocRow)+
& PotX(2,Equ)*PhiX(2,LocRow))*DetXZeta

    IF (Convection) THEN
      R(CLoc(Equ,Elem,LocRow))=R(CLoc(Equ,Elem,LocRow))
& +Wts(Jx)*Wts(Jy)*(Peclet*Phi(LocRow)*
& (Vlcty(1)*PotX(1,Equ)+Vlcty(2)*PotX(2,Equ)))*DetXZeta
    END IF

    DO LocCol=1,Upper

```

C The following statements compute the Jacobian

```

    CALL ComputeBandCol(CLoc(Equ,Elem,LocRow),
& CLoc(Equ,Elem,LocCol),BandCol)

    RJacobian(BandCol,CLoc(Equ,Elem,LocRow))=
& RJacobian(BandCol,CLoc(Equ,Elem,LocRow))-Wts(Jx)*Wts(Jy)*
& (PhiX(1,LocRow)*PhiX(1,LocCol)+
& PhiX(2,LocRow)*PhiX(2,LocCol))*DetXZeta

```

```

      IF (Convection) THEN
        RJacobian(BandCol,CLoc(Equ,Elem,LocRow))=
& RJacobian(BandCol,CLoc(Equ,Elem,LocRow))-Wts(Jx)*Wts(Jy)*
& (Peclet*Phi(LocRow)*(Vlcty(1)*PhiX(1,LocCol)+
& Vlcty(2)*PhiX(2,LocCol)))*DetXZeta
      END IF

```

```

    END DO
  END DO
END DO
END DO

```

```

RETURN
END

```

C ***** AssembleTriangle

```

SUBROUTINE AssembleTriangle(Equ,Elem)

```

C Internal Variables

```

C NoOfGaussPts      The number of points to use in the Gaussian
C                   quadrature approximation of the integration.
C Phi()             The value of the Local Weighting function at the current
C                   gauss point. (Phi(1) is local weighting function 1,
C                   while Phi(2) is local weighting function 2.)
C PhiZeta()         The slope of the weighting functions at the
C                   current gauss point.

```

```

INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFTriPts.INC'
INCLUDE 'ECFMsh.INC'
INCLUDE 'ECFRes.INC'
INCLUDE 'ECFCal.INC'
INCLUDE 'ECFPar.INC'

```

```

REAL*8 Zeta(MaxNoOfDim),XZeta(MaxNoOfDim,MaxNoOfDim),DetXZeta,
& Vlcty(MaxNoOfDim)
REAL*8 PHI((MaxNoOfBasisDeg+1)**MaxNoOfDim),
& PhiZeta(MaxNoOfDim,(MaxNoOfBasisDeg+1)**MaxNoOfDim),
& PhiX(MaxNoOfDim,(MaxNoOfBasisDeg+1)**MaxNoOfDim),
& Pot(MaxNoOfEqu),PotX(MaxNoOfDim,MaxNoOfEqu),
& dX(MaxNoOfDim),X(MaxNoOfDim)
INTEGER LocRow,LocCol,Elem,J,Jx,Jy,BandCol,Equ,Upper

```

C The following DO-LOOP loops over the Gauss Points (performing the gaussian quadrature numerical integration). It forms the RJacobian matrix and the R vector in an element by element fashion.

```

CALL GetUpper(ElemType(Elem),Upper)
DO Jx=1,NoOfTriPts

  Zeta(1)=TriPts(Jx,1)
  Zeta(2)=TriPts(Jx,2)

  CALL ComputeTriPhis(Zeta,Phi,PhiZeta)
  CALL ComputeIsoPara(Elem,PhiZeta,XZeta,DetXZeta,Upper)
  CALL ComputePhiX(Upper,PhiZeta,XZeta,DetXZeta,PhiX)

```

```
CALL ComputePot(Elem,Upper,Phi,PhiX,Pot,PotX)
```

C The following call computes the velocity in the zeta(1) and
C the zeta(2) directions. To do this, it needs to know the
C current values of Zeta(1) and Zeta(2), as well as the current
C element number.

```
IF (Convection) THEN
  CALL ComputeLoc(Phi,Elem,X)
  CALL Velocity(X,Vlcty)
END IF
```

```
DO LocRow=1,Upper
```

C The following statements compute the Residual vector

```
R(CLoc(Equ,Elem,LocRow))=R(CLoc(Equ,Elem,LocRow))
& +TriWts(Jx)*(PotX(1,Equ)*PhiX(1,LocRow)+
& PotX(2,Equ)*PhiX(2,LocRow))*DetXZeta
```

```
IF (Convection) THEN
  R(CLoc(Equ,Elem,LocRow))=R(CLoc(Equ,Elem,LocRow))
& +TriWts(Jx)*(Peclet*Phi(LocRow)*
& (Vlcty(1)*PotX(1,Equ)+Vlcty(2)*PotX(2,Equ)))*DetXZeta
END IF
```

```
DO LocCol=1,Upper
```

C The following statements compute the Jacobian

```
CALL ComputeBandCol(CLoc(Equ,Elem,LocRow),
& CLoc(Equ,Elem,LocCol),BandCol)
```

```
RJacobian(BandCol,CLoc(Equ,Elem,LocRow))=
& RJacobian(BandCol,CLoc(Equ,Elem,LocRow))-TriWts(Jx)*
& (PhiX(1,LocRow)*PhiX(1,LocCol)+
& PhiX(2,LocRow)*PhiX(2,LocCol))*DetXZeta
```

```
IF (Convection) THEN
  RJacobian(BandCol,CLoc(Equ,Elem,LocRow))=
& RJacobian(BandCol,CLoc(Equ,Elem,LocRow))-TriWts(Jx)*
& (Peclet*Phi(LocRow)*(Vlcty(1)*PhiX(1,LocCol)+
& Vlcty(2)*PhiX(2,LocCol)))*DetXZeta
END IF
```

```
END DO
END DO
END DO
```

```
RETURN
END
```

C ***** ComputeBandCol

```
SUBROUTINE ComputeBandCol(Row,Col,BandCol)
```

C This function computes the column in a banded matrix given the
C row and column of a square matrix, and (from ECFHdr) the number of

C lower columns (Nlc)

```
INCLUDE 'ECFHdr.INC'
INTEGER Row,Col,BandCol
```

```
BandCol=Col+Nlc+1-Row
```

```
RETURN
END
```

C ***** ComputeDelPotDotNorm

```
SUBROUTINE ComputeDelPotDotNorm(V,Kinetics,Pot,DelPotDotNorm,
& DelPotDotNormPot)
```

C This subroutine computes the normal current/conductivity (DelPotDotNorm) and
C the derivative of the normal current/conductivity (DelPotDotNormPot) with
C respect to potential for a given wall voltage (V) and electrolyte potential
C (Pot)

```
INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFPar.INC'
```

```
REAL*8 Pot,DelPotDotNorm,DelPotDotNormPot,V,Curr,CurrPot
CHARACTER*(*) Kinetics
```

```
REAL*8 Eta,dEtaPot
REAL*8 C2,dPotdC2,CurrC2,C1,C3,dC1dC2
```

```
IF ((BINARY).OR.(Supporting)) THEN
```

C This block handles butler-volmer kinetic conditions for a 1:1 binary
C electrolyte where metal is depositing. The exchange current density is
C assumed to vary with the surface concentration to the first power.

```
C2=Pot
Pot= LOG(C2/BinaryK2)
dPotdC2= 1.0/ C2
```

```
Eta=(v-Pot)
dEtaPot= -1.0
```

```
IF (Binary) THEN
```

```
  C1=C2
  dC1dC2=1.0
```

```
ELSE IF (Supporting) THEN
```

```
  C3=BinaryK2*SupportingK3/C2
  C1=C2-C3
```

```
  dC1dC2=1.0+BinaryK2*SupportingK3/(C2*C2)
```

```
END IF
```

```
Curr = 1.0/WagnerLin * c1 * (EXP(aA*Eta)-EXP(-aC*Eta))
```

```
CurrC2 = 1.0/WagnerLin *
```

```
& ((+dC1dC2+aA*dEtaPot*dPotdC2*c1)*EXP(aA*Eta) +
& (-dC1dC2+aC*dEtaPot*dPotdC2*c1)*EXP(-aC*Eta))
```

C The following two variables would be better named (for this block of code
C only) DelC2DotNorm and DelC2DotNormC2

```

DelPotDotNorm = Curr
DelPotDotNormPot= CurrC2

```

```

ELSE

```

C The following definition for the overpotential ($V > 0$, $Pot > 0$) gives $\eta < 0$ for C cathodic current.

```

Eta=(V-Pot)
dEtaPot=-1.0

```

```

IF (Kinetics.EQ.'BV') THEN

```

```

    Curr = 1.0/WagnerLin * (EXP(aA*Eta)-EXP(-aC*Eta))
    CurrPot = 1.0/WagnerLin
    & *(aA*EXP(aA*Eta)+aC*EXP(-aC*Eta))*dEtaPot

```

```

    DelPotDotNorm = Curr
    DelPotDotNormPot = CurrPot

```

```

ELSE IF (Kinetics.EQ.'LIN') THEN

```

```

    Curr = (aA+aC)*Eta/WagnerLin
    CurrPot =(aA+aC)*dEtaPot/WagnerLin

```

```

    DelPotDotNorm=Curr
    DelPotDotNormPot=CurrPot

```

```

ELSE IF (Kinetics.EQ.'USER') THEN

```

```

    CALL UserKinetics(V,Pot,DelPotDotNorm,DelPotDotNormPot)

```

```

ELSE

```

```

    WRITE(*,*) 'Error: Unknown Kinetics=',Kinetics
    STOP 'ECFCompute: In Routine: ComputeDelPotDotNorm'

```

```

END IF

```

```

END IF

```

```

RETURN
END

```

C ***** ComputeTangent

```

SUBROUTINE ComputeTangent(Phi1DZeta,Nodals,dX,dY)

```

C The following DO Loop computes the change in pathlength for a change in C zeta (integration variable)

```

INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFMsh.INC'

```

```

REAL*8 dX,dY,Phi1DZeta(*)
INTEGER Nodals(*),K

```

```

dX=0.0

```



```

dY=0.0
DO K=1,BasisDeg+1
  dX=dX+Nodes(Nodals(K),1)*Phi1DZeta(K)
  dY=dY+Nodes(Nodals(K),2)*Phi1DZeta(K)
END DO

```

```

RETURN
END

```

C ***** GETNODALS

```

SUBROUTINE GetNodals(I,Equ,Nodals,CNodals)

```

```

INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFMsh.INC'

```

```

INTEGER I,Equ
INTEGER Nodals(*),CNodals(*)

```

```

INTEGER K,IpK

```

C The following DO-loop loads the nodal locations for the current element
C into Nodals(*), and coefficient locations into CNodals()

```

DO K=0,BasisDeg
  CALL IncrementI(I,IpK,K,NoOfBDNodes)
  Nodals(K+1)=BDNodes(IpK)
  CALL ComputeCoefLoc(BDNodes(IpK),Equ,CNodals(K+1))
END DO

```

```

RETURN
END

```

C ***** NewtonRaphson

```

SUBROUTINE NewtonRaphson(NoOfIterations,Converged)

```

C This subroutine uses the iterative Newton Raphson technique to obtain a
C solution to the differential equation.

```

INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFCal.INC'
INCLUDE 'ECFRes.Inc'

```

```

INTEGER NoOfIterations
LOGICAL Converged,FirstLoop

```

```

REAL*8 NormR,NormdC,LastNormdC,dC(MaxNoOfCoef)
INTEGER I,J
REAL*8 VecNormDP
EXTERNAL VecNormDP

```

C The following DO-LOOP Performs the Newton-Raphson iterations.

```

Converged=.FALSE.
LastNormdC=0.0
NormdC=SQRT(Tolerance)
NoOfIterations=0

```

```
FirstLoop=.TRUE.
```

```
DO WHILE(.NOT.Converged)
```

```
C The following CALLS assemble the matrices used in the Newton-Raphson
C technique, and solve the set of simultaneous equations, and Updatec the
C coefficient vector.
```

```
CALL AssembleMatrices
```

```
C Note: the following call adjusts the residual and Jacobian for the
C essential and natural b.c.'s
```

```
CALL AssembleBC
```

```
IF (Debugging) CALL PrintMat
```

```
C The following statements prepare for and solve the system of linear
C equations. The subroutine DLSARB is an IMSL subroutine for solving
C a banded system of equations.
```

```
CALL DLSARB(NoOfCoef,RJacobian,MaxBandWidth,Nlc,Nuc,
& R,2,dC)
```

```
C The following DO-Loop transfers the coefficient values from the DLSARB
C routine to the dC() vector.
```

```
IF (NonNegative) THEN
  DO I=1,NoOfCoef
    IF (dC(I)+C(I).LT.0) dC(I)=-C(I)
  END DO
END IF
```

```
C The following statements check the norm of the change in coefficients
C for quadratic convergence.
```

```
LastNormdC=NormdC
NormdC=VecNormDP(NoOfCoef,dC)
```

```
IF ((.NOT.FirstLoop).AND.(NormdC.GT.1000)) THEN
  WRITE(*,*) 'Warning: Guesses might be diverging.'
  WRITE(*,*) '  Current Guess Norm=',NormdC
  WRITE(*,*) '  Last Guess Norm=',LastNormdC
END IF
FirstLoop=.FALSE.
```

```
CALL UpdateC(dC)
```

```
NormR=VecNormDP(NoOfCoef,R)
Converged=((NormR.LT.tolerance).OR.(NormdC.LT.Tolerance))
```

```
C The following WRITE statement prints the 2-norm of dC for
C each iteration. This allows the user to check for quadratic
C convergence.
```

```
90 WRITE(*,90) NormdC,NormR
  FORMAT(X,10X,
& 'dC=',G14.5,;, 'Residual=',G14.5)
```

```

C      hC=ggggggggggggggg Residual=ggggggggggggggg
      NoOfIterations=NoOfIterations+1

```

C The following IF-THEN block prevents the subroutine from performing
C more than MaxNoOfIter iterations.

```

      IF (NoOfIterations.GT.MaxNoOfIter) THEN
        WRITE(*,*) 'Warning: number of newton-raphson iterations'
        WRITE(*,*) 'exceeds ',MaxNoOfIter
        STOP 'In routine: NewtonRaphson'
      END IF

```

```

      END DO

```

C The following write statement concludes the report for this newton iteration
C (# of Iterations, and whether or not the last two steps
C converged quadratically)

```

      IF (LastNormdC**2.LT.NormdC) THEN
        WRITE(*,100) NoOfIterations
100    FORMAT(X,' **** ',14X,' # of Iterations:',I3,
      & ' UNQUADRATIC CONVERGENCE')
      ELSE
        WRITE(*,101) NoOfIterations
101    FORMAT(X,' ',14X,' # of Iterations:',I3,
      & ' >= Quadratic Convergence')
      END IF

      IF ((NormdC.GT.0).AND.(LastNormdC.GT.0).AND.(LastNormdC.LT.1))
      & WRITE (*,110) LOG(NormdC)/LOG(LastNormdC)
110    FORMAT(/,X,' Order of Convergence=',G14.7,/)

      IF (NormR.GT.Tolerance)
      & WRITE(*,*) 'Warning: Residual is greater than ',Tolerance

      RETURN
      END

```

C ***** PrintCLoc

```

      SUBROUTINE PrintCLoc

```

C This subroutine prints the CLoc matrix for user verification.

```

      INCLUDE 'ECFHdr.INC'
      INCLUDE 'ECFRes.INC'

      INTEGER I,J,K

      WRITE(*,99)
99    FORMAT(X,'Matrix CLoc',/,
      & X,'Eqn Elem Local Coefficients',/,
      & X,'      1      2      3      4',/)

      DO I=1,NoOfElems
        DO J=1,NoOfEqu
          WRITE(*,100) J,I,(CLoc(J,I,K),K=1,(BasisDeg+1)**NoOfDim)
100    FORMAT(X,I2,3X,I2,3X,<(BasisDeg+1)**NoOfDim>(I4,XX))

```

```

      END DO
    END DO

```

```

C Eqn Elem Local Nodes
C iixxxiixxx...

```

```

      RETURN
    END

```

```

C ***** PrintMat

```

```

      SUBROUTINE PrintMat

```

```

C The following subroutine prints the jacobian and residual vectors. This
C subroutine is useful for debugging the program.

```

```

      INCLUDE 'ECFHdr.INC'
      INCLUDE 'ECFCal.INC'

```

```

      INTEGER I,J

```

```

      WRITE(*,*) ' '
      WRITE(*,*) ' Jacobian '
      WRITE(*,*) ' '

```

```

      DO I=1,NoOfCoef
        WRITE(*,*) '--- ROW ('I,')'
        WRITE(*,10) (RJacobian(J,I),J=1,Nlc+1+Nuc)
      END DO

```

```

10      WRITE(*,*) '--- END '
      FORMAT(X,8(G10.3))

```

```

      WRITE(*,*) ' '
      WRITE(*,*) ' Residual Vector'
      WRITE(*,*) ' '

```

```

      WRITE(*,10) (R(I),I=1,NoOfCoef)

```

```

      RETURN
    END

```

```

C ***** PrintNodes

```

```

      SUBROUTINE PrintNodes

```

```

C The following subroutine prints the node locations.

```

```

      INCLUDE 'ECFHdr.INC'
      INCLUDE 'ECFMsh.INC'

```

```

      INTEGER I,K

```

```

      WRITE(*,*) ' '
      WRITE(*,*) ' Node Locations'
      WRITE(*,*) ' '

```

```

      DO I=1,NoOfNodes
        WRITE(*,100) I,(Nodes(I,K),K=1,NoOfDim)
      END DO

```

```

      END DO
100  FORMAT(X,'Node(',I3,')=(',F10.5,<NoOfDim-1>(',',F10.5,')')
      RETURN
      END

```

C ***** PrintResults

```

      SUBROUTINE PrintResults(TotalIterations,NoOfTimeSteps)

      INCLUDE 'ECFHdr.INC'
      INCLUDE 'ECFRes.INC'
      INTEGER I,TotalIterations,NoOfTimeSteps

      WRITE(*,*) '-----'
10    WRITE(*,10) TotalIterations,NoOfTimeSteps
      FORMAT(X,'Final Coefficients (',I6,' iterations)'/,
      & X,' (',I6,' Total Iterations)')
      WRITE(*,*) ' '

11    WRITE(*,11) BasisDeg,NoOfElems
      FORMAT(X,' ',10X,
      & ' Degree of Basis Functions=',I1,' No Of Elems=',I3)

13    WRITE(*,13) NoOfNodes
      FORMAT(X,' ',10X,
      & ' No Of Nodes=',I3,/)

      DO I=1,NoOfCoef
        WRITE(*,100) I,C(I)
      END DO
100  FORMAT(X,'C(',I3,')=',F10.5)

      RETURN
      END

```

C ***** SubKnown

```

      SUBROUTINE SubKnown(Start,End,Equ,J)

```

C This subroutine loops over known coefficients, and calls a subroutine
C that sets them to zero.

```

      INTEGER Start,End,Equ,J

      INCLUDE 'ECFHdr.INC'
      INCLUDE 'ECFbc.INC'

      INTEGER Nodals(MaxNoOfBasisDeg+1),J
      INTEGER CNodals(MaxNoOfBasisDeg+1)

      DO I=Start,End,BasisDeg
        CALL GetNodals(I,Equ,Nodals,CNodals)
        CALL AdjustForKnown(CNodals,BCPar(Equ,J))
      END DO

      RETURN
      END

```

C ***** SubNatural

SUBROUTINE SubNatural(Start,End,Equ,Side)

C This subroutine loops over boundary nodes that have Natural boundary
C conditions.

INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFGauss.INC'
INCLUDE 'ECFMsh.INC'
INCLUDE 'ECFCal.INC'
INCLUDE 'ECFbc.INC'

INTEGER Start,End,Equ,Side

REAL*8 dX,dY,dR,
& Phi1D(MaxNoOfBasisDeg+1),Phi1DZeta(MaxNoOfBasisDeg+1)
INTEGER Jx,Nodals(MaxNoOfBasisDeg+1),IpK,I,K
INTEGER CNodals(MaxNoOfBasisDeg+1)

C I Boundary Node index

C K Local Node Index

DO I=Start,End,BasisDeg

CALL GetNodals(I,Equ,Nodals,CNodals)

C The following DO-loop loops over the integration points.

DO Jx=1,NoOfGaussPts

C The following statements compute the slope of the path with respect to
C the integration parameter at the Gauss Point.

CALL Compute1DPhis(BasisDeg,Pts(Jx),Phi1D,Phi1DZeta)
CALL ComputeTangent(Phi1DZeta,Nodals,dX,dY)
dR=SQRT(dX*dX+dY*dY)

CALL AdjustForNatural(CNodals,Phi1D,
& BCPar(Equ,Side),Wts(Jx),dR)

END DO

END DO

RETURN

END

C ***** SubSecondary

SUBROUTINE SubSecondary(Start,End,Equ,Side)

C This subroutine loops over boundary nodes that have secondary boundary
C conditions.

INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFGauss.INC'
INCLUDE 'ECFMsh.INC'
INCLUDE 'ECFRes.INC'

```
INCLUDE 'ECFCal.INC'
INCLUDE 'ECFbc.INC'
```

```
INTEGER Start,End,Equ,Side
```

```
REAL*8 dX,dY,dR,Phi1D(MaxNoOfBasisDeg+1),
& Phi1DZeta(MaxNoOfBasisDeg+1)
REAL*8 Pot,DelPotDotNorm,DelPotDotNormPot
INTEGER Jx,Nodals(MaxNoOfBasisDeg+1),IpK,I,K
INTEGER CNodals(MaxNoOfBasisDeg+1)
```

C The following DO-loop goes along the boundary.

```
DO I=Start,End,BasisDeg

CALL GetNodals(I,Equ,Nodals,CNodals)
```

C The following DO-loop loops over the integration points.

```
DO Jx=1,NoOfGaussPts
```

C The following statements compute the slope of the path length vs. the
C integration variable at the integration point.

```
CALL Compute1DPhis(BasisDeg,Pts(Jx),Phi1D,Phi1DZeta)
CALL ComputeTangent(Phi1DZeta,Nodals,dX,dY)
dR=SQRT(dX*dX+dY*dY)
```

C The following DO-loop compute the potential at the boundary location.

```
Pot=0.0
DO K=1,(BasisDeg+1)
  Pot=Pot+C(CNodals(K))*Phi1D(K)
END DO
```

C The following CALL computes (Del Potential).(Unit Normal) and
C $d[(\text{Del Potential}).(\text{Unit Normal})]/d[\text{Potential}]$

```
CALL ComputeDelPotDotNorm(BCPar(Equ,Side),Kinetics(Equ),
& Pot,DelPotDotNorm,DelPotDotNormPot)
```

```
CALL AdjustForKinetics(CNodals,
& Phi1D,DelPotDotNorm,DelPotDotNormPot,Wts(Jx),dR)
```

```
END DO
END DO
```

```
RETURN
END
```

C ***** TriPtsWts

```
SUBROUTINE TriPtsWts
INCLUDE 'ECFTriPts.INC'
```

C See Burnett p 596 for other than NoOfTriPts=4

C (Note: weights are divided by 2 as indicated in formula given on p 596

C Gaussian integration points for a triangular element.

```

NoOfTriPts=4

TriPts(1,1)=1.0/3.0
TriPts(1,2)=1.0/3.0
TriWts(1)=-27.0/48.0/2.0

TriPts(2,1)=1.0/5.0
TriPts(2,2)=1.0/5.0
TriWts(2)=25.0/48.0/2.0

TriPts(3,1)=3.0/5.0
TriPts(3,2)=1.0/5.0
TriWts(3)=25.0/48.0/2.0

TriPts(4,1)=1.0/5.0
TriPts(4,2)=3.0/5.0
TriWts(4)=25.0/48.0/2.0

RETURN
END

```

C ***** UpdateC

```

SUBROUTINE UpdateC(dC)

```

C This subroutine Updates the coefficients C() by adding the correction
C dC() to them.

```

INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFRes.INC'

REAL*8 dC(*),Norm
INTEGER I,K

DO I=1,NoOfCoef
  C(I)=C(I)+dC(I)
  IF (Debugging) WRITE(*,*) 'C(',I,')=',C(I)
END DO

RETURN
END

```

C ***** ZeroRJ

```

SUBROUTINE ZeroRJ

```

C This subroutine zeros the residual vector, the jacobian, and the continuance
C vector

```

INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFCal.INC'

INTEGER I,J

DO I=1,NoOfCoef
  R(I)=0.0
  DO J=1,Nuc+Nlc+1
    RJacobian(J,I)=0.0
  
```



```
END DO  
END DO  
  
RETURN  
END
```

c *

PROGRAM ECFPlot

C This program reads a results file and makes a plot file

C Written by: Ken Jordan 8/29/87

C *****

C Variables

C *****

C FileName The name of the names file. (Contains file names
C for reading remaining data.)

C *****

C Files

C *****

C *.BC Contains the boundary conditions
C *.HDR Contains problem header information. (i.e. No of coefficients,
C Number of dimensions, Number of equations...)
C *.PAR Contains parameter information. E.g. Kinetic parameters such
C as the exchange current density, the transfer coefficients...
C *.MSH Contains the mesh and node locations and boundary node locations
C *.RES Contains the Coefficients and CLoc(,.)
C *.NAM Contains the names of the files to use in solving the problem
C E.g. *.NAM defines the filenames for *.bc, *.hdr, *.par, *.msh,
C *.msh
C *.iso Contains the data needed for isopotential plots.
C *.SLP contains slope along boundary.

C *****

C Main Program Follows

C *****

```

INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFNam.INC'
CHARACTER*80 FileName,ValFile
```

C The following call reads the values of variables that
C define the problem and solution technique (BasisDeg, NoOfElems,
C NoOfNodes,NoOfXElems,NoOfYElems,Tolerance)

```

CALL GetFileName('Names file?',FileName)
CALL ReadNames(FileName)
```

```

CALL ReadFEMUser
```

```

CALL FindIso(PlotFile)
CALL PlotBdrySlope(SlopeFile)
ValFile='Bdry.Val'
CALL PlotBdryVal(ValFile)
```

```

STOP 'Normal End'
END
```

C ***** ComputeLocStep

```

SUBROUTINE ComputeLocStep(BDNodeLoc,dX,XBase)
```

C The following statements compute the step to take and in which
C direction on the local element.

```
INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFGauss.INC'
```

```
INTEGER BDNodeLoc
REAL*8 dX(*),XBase(*)
```

C For Square Elements, there are four cases:

```
C 4-3 B,BP1= 1,2 dX(1)=1.0/NoOfGaussPts dX(2)=0
C ||      2,3 dX(1)=0 dX(2)=1.0/NoOfGaussPts
C 1-2      3,4 dX(1)=-1.0/NoOfGaussPts dX(2)=0
C          4,1 dX(1)=0 dX(2)=-1.0/NoOfGaussPts
```

```
dX(1)=0.0
dX(2)=0.0
```

```
IF (BDNodeLoc.EQ.1) THEN
```

```
  XBase(1)=0.0
  XBase(2)=0.0
  dX(1)=1.0/NoOfGaussPts
```

```
ELSE IF (BDNodeLoc.EQ.2) THEN
```

```
  XBase(1)=1.0
  XBase(2)=0.0
  dX(2)=1.0/NoOfGaussPts
```

```
ELSE IF (BDNodeLoc.EQ.3) THEN
```

```
  XBase(1)=1.0
  XBase(2)=1.0
  dX(1)=-1.0/NoOfGaussPts
```

```
ELSE IF (BDNodeLoc.EQ.4) THEN
```

```
  XBase(1)=0.0
  XBase(2)=1.0
  dX(2)=-1.0/NoOfGaussPts
```

```
ELSE
```

```
  WRITE(*,*) 'Error: Location of Boundary node in Local Element'
  WRITE(*,*) '      is unknown.'
  WRITE(*,*) '      Local Element Location=',BDNodeLoc
  WRITE(*,*) '      Perhaps basis degree is larger than one?'
  STOP 'In Routine: ComputeLocStep'
```

```
END IF
```

```
RETURN
END
```

C ***** ComputeNormal

```
SUBROUTINE ComputeNormal(BdNode,BDNodeP1,UnitNormal)
```

C This subroutine computes the outward pointing unit normal given the boundary
 C node number. The normal is perpendicular to the line segment from BdNode
 C to BdNode+1.

```

    INCLUDE 'ECFHdr.INC'
    INCLUDE 'ECFMsh.INC'

    REAL*8 UnitNormal(*),Distance,dX(MaxNoOfDim),Sum
    INTEGER BdNode,BdNodeP1,I

    Sum=0.0
    DO I=1,NoOfDim
      dX(I) = Nodes(BDNodes(BdNodeP1),I)-Nodes(BDNodes(BdNode),I)
      Sum=Sum+dX(I)*dX(I)
    END DO
    Distance=SQRT(Sum)
  
```

C UnitDistance(1)= dX(1)/Distance
 C UnitDistance(2)= dX(2)/Distance

```

    UnitNormal(1) = dX(2)/Distance
    UnitNormal(2) = -dX(1)/Distance
  
```

```

    RETURN
  END
  
```

C ***** FindIso

```

    SUBROUTINE FindIso(FileName)
  
```

C This subroutine compute the location of isopotential points and stores
 C them in file FileName.

```

    INCLUDE 'ECFHdr.INC'
    INCLUDE 'ECFMsh.INC'
    INCLUDE 'ECFRes.INC'
    INCLUDE 'ECFPar.INC'

    PARAMETER MaxNoOfPot=25
    CHARACTER*(*) FileName
    REAL*8 PotMax,PotMin,dPot,Pots(MaxNoOfPot+1),Zero/0.0,One/1.0/,
    & XPts(MaxNoOfPot+1,2*MaxNoOfNodes),
    & YPts(MaxNoOfPot+1,2*MaxNoOfNodes),
    & XTemp(2*MaxNoOfNodes),YTemp(2*MaxNoOfNodes)
    REAL*8 C3Min,C3Max
    INTEGER NoOfPPts(MaxNoOfPot+1),I,J,K,L,RNode,LNode,
    & Pointer(2*MaxNoOfNodes),Kp1,NoOfPot,Upper,FilLen
  
```

C The following statements find the max and min potentials.

```

    PotMax=C(1)
    PotMin=C(1)

    DO I=1,NoOfCoef
      PotMax=MAX(PotMax,C(I))
      PotMin=MIN(PotMin,C(I))
    END DO
  
```

```

WRITE(*,*) ' '
WRITE(*,*) ' Iso Potential Plot Information: File ',FileName
WRITE(*,*) ' '
IF (.NOT.(Binary).OR.(Supporting)) THEN
  WRITE(*,*) 'Maximum Potential Found:',PotMax
  WRITE(*,*) 'Minimum Potential Found:',PotMin
ELSE
  WRITE(*,*) 'Maximum Potential Found:',LOG(PotMax/BinaryK2)
  WRITE(*,*) 'Minimum Potential Found:',LOG(PotMin/BinaryK2)
  WRITE(*,*) ' '
  IF (.NOT.Supporting) THEN
    WRITE(*,*) 'Maximum Concentration Found:',PotMax
    WRITE(*,*) 'Minimum Concentration Found:', PotMin
  ELSE
    C3Min=BinaryK2*SupportingK3/PotMax
    C3Max=BinaryK2*SupportingK3/PotMin

    WRITE(*,*) 'Maximum Concentration 3 Found:',C3Max
    WRITE(*,*) 'Minimum Concentration 3 Found:',C3Min
    WRITE(*,*) ' '
    WRITE(*,*) 'Maximum Concentration 2 Found:',PotMax
    WRITE(*,*) 'Minimum Concentration 2 Found:', PotMin
  END IF
END IF

WRITE(*,*) ' '

CALL IInp('No Of Iso- curves?',NoOfPot)
CALL EditDP('Maximum ',PotMax)
CALL EditDP('Minimum ',PotMin)

```

C The following statements find the (NoOfPot+1) isopotentials that will be C plotted.

```

dPot=(PotMax-PotMin)/Float(NoOfPot)

DO L=1,NoOfPot+1
  Pots(L)=PotMin+(L-1)*dPot
END DO

CALL PlotPots(NoOfPot,Pots,FileName)

IF ((Binary).OR.(Supporting)) THEN

```

C The following statements find the (NoOfPot+1) isopotentials that will be C plotted.

```

dPot=(LOG(PotMax/BinaryK2)-LOG(PotMin/BinaryK2))
& /Float(NoOfPot)

DO L=1,NoOfPot+1
  Pots(L)=LOG(PotMin/BinaryK2)+(L-1)*dPot
  Pots(L)=BinaryK2*EXP(Pots(L))
END DO

CALL StringLength(FileName,FillLen)
CALL PlotPots(NoOfPot,Pots;FileName(1:FillLen)//'Pot')

```

```

END IF

IF (Supporting) THEN
  dPot=(C3Max-C3Min)/Float(NoOfPot)

  DO L=1,NoOfPot+1
    Pots(L)=C3Min+(L-1)*dPot
    Pots(L)=BinaryK2*SupportingK3/(Pots(L))
  END DO

  CALL StringLength(FileName,FilLen)
  CALL PlotPots(NoOfPot,Pots,FileName(1:FilLen))/'C3'

END IF

RETURN
END

```

C ***** LocateGlobalElem

```

SUBROUTINE LocateGlobalElem(BDNode,BDNodeP1,Elem,BDNodeLoc)

INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFMsh.INC'

INTEGER BDNode,BDNodeP1,Elem,BDNodeLoc,LocNode
LOGICAL BDNodeFound,BDNodeP1Found

```

C This subroutine locates the global element containing the current boundary
C node and the next boundary node.

C Loop over elements
C Check to see if BDNode Found
C Check to see if BDNodeP1 Found.

```

BDNodeFound=.FALSE.
BDNodeP1Found=.FALSE.

```

```

Elem=0

```

```

DO WHILE(.NOT.(BDNodeFound.AND.BDNodeP1Found))

```

```

  Elem=Elem+1
  IF (Elem.GT.NoOfElems) THEN
    WRITE(*,*) 'Error: Boundary nodes not found in any element',
    & ' (Searched ',NoOfElems,' elements)'
    WRITE(*,*) '   Boundary Node Numbers:',BDNode
    WRITE(*,*) '   ',BDNodes(BDNode),BDNodes(BDNodeP1)
    STOP 'In Routine: LocateGlobalElem'
  END IF

```

```

  BDNodeFound=.FALSE.
  BDNodeP1Found=.FALSE.

```

C Search all the outside nodes (Squares: 1,2,3,4,5,6,7,8)
C (Triangles: 1,2,3,4,5,6)

```

DO LocNode=1,8

```

```

      IF (NLoc(Elem,LocNode).EQ.BDNodes(BdNode)) THEN
        BDNNodeFound=.TRUE.
        BDNNodeLoc=LocNode
      END IF
      IF (NLoc(Elem,LocNode).EQ.BDNodes(BdNodeP1)) BDNNodeP1Found=.TRUE.
    END DO

```

```

  END DO

```

C We return when Elem has BDNode and BDNodeP1 on it!

```

  RETURN
END

```

C ***** Plot1Slope

```

  SUBROUTINE Plot1Slope(J,Upper,Elem)

```

```

    INCLUDE 'ECFHdr.INC'
    INCLUDE 'ECFMsh.INC'
    INCLUDE 'ECFPlot.INC'

```

```

    INTEGER J,Upper,Elem

```

```

    INTEGER K

```

```

    REAL*8 Cx,Xs(MaxNoOfDim)

```

```

    REAL*8 Zeta(MaxNoOfDim),XZeta(MaxNoOfDim,MaxNoOfDim),DetXZeta

```

```

    REAL*8 PHI((MaxNoOfBasisDeg+1)**MaxNoOfDim),

```

```

    & PhiZeta(MaxNoOfDim,(MaxNoOfBasisDeg+1)**MaxNoOfDim),

```

```

    & PhiX(MaxNoOfDim,(MaxNoOfBasisDeg+1)**MaxNoOfDim),

```

```

    & Pot(MaxNoOfEqu),PotX(MaxNoOfDim,MaxNoOfEqu)

```

```

    DO K=1,NoOfDim

```

```

      Zeta(K)=XBase(K)+J*dX(K)

```

```

    END DO

```

```

    IF (ElemType(Elem).EQ.'S') THEN

```

```

      CALL Compute2DPhis(Zeta,Phi,PhiZeta)

```

```

    ELSE

```

```

      CALL ComputeTriPhis(Zeta,Phi,PhiZeta)

```

```

    END IF

```

```

    CALL ComputeIsoPara(Elem,PhiZeta,XZeta,DetXZeta,Upper)

```

```

    CALL ComputePhiX(Upper,PhiZeta,XZeta,DetXZeta,PhiX)

```

```

    CALL ComputePot(Elem,Upper,Phi,PhiX,Pot,PotX)

```

C The following DO-Loop computes the dot product between PotX and C Normal.

```

    Cx=0

```

```

    DO K=1,NoOfDim

```

```

      Cx=Cx+Normal(K)*PotX(K,1)

```

```

    END DO

```

C The next few lines compute the change in distance between the last C computation and this one.

```

    XLast=X

```

```
YLast=Y
```

```
CALL ComputeLoc(Phi,Elem,Xs)
```

```
X=Xs(1)
```

```
Y=Xs(2)
```

```
Distance=Distance+SQRT((X-XLast)**2+(Y-YLast)**2)
```

C The next line writes the distance and the slope computed into a file.

```
WRITE(1,*) Distance,Cx
```

```
RETURN
```

```
END
```

C ***** PlotBdrySlope

```
SUBROUTINE PlotBdrySlope(FileName)
```

C This subroutine computes the slope of the potential at the boundary.

```
INCLUDE 'ECFHdr.INC'
```

```
INCLUDE 'ECFGauss.INC'
```

```
INCLUDE 'ECFMsh.INC'
```

```
INCLUDE 'ECFPlot.INC'
```

```
CHARACTER*(*) FileName
```

```
INTEGER I,J,K,BDNode,BDNodeP1,Elem,LocNode,BDNodeLoc
```

```
INTEGER Upper
```

```
OPEN(UNIT=1,FILE=FileName,STATUS='NEW',FORM='FORMATTED')
```

```
WRITE(1,*) NoOfBDNodes*(NoOfGaussPts+1)
```

```
Distance=0
```

```
X=Nodes(BDNodes(1),1)
```

```
Y=Nodes(BDNodes(1),2)
```

C The following DO-Loop loops over the boundary nodes.

```
DO BdNode=1,NoOfBDNodes
```

```
    CALL IncrementI(BDNode,BDNodeP1,1,NoOfBDNodes)
```

```
    CALL ComputeNormal(BdNode,BdNodeP1,Normal)
```

```
    CALL LocateGlobalElem(BDNode,BDNodeP1,Elem,BDNodeLoc)
```

```
    CALL ComputeLocStep(BDNodeLoc,dX,XBase)
```

```
    CALL GetUpper(ElemType(Elem),Upper)
```

C The following DO-Loop Loops over the gauss points and computes the value
C of the potential and the potential slope at at each point on the boundary.

```
    IF (ElemType(Elem).EQ.'T') THEN
```

```
        CALL Plot1Slope(NoOfGaussPts/2,Upper,Elem)
```

```
    ELSE
```

```
        DO J=0,NoOfGaussPts
```

```
            CALL Plot1Slope(J,Upper,Elem)
```

```
        END DO
```



```

      END IF
    END DO

```

```

    CLOSE(1)
    CLOSE(2)
    CLOSE(3)

```

```

    RETURN
  END

```

C ***** PlotBdryVal

```

  SUBROUTINE PlotBdryVal(FileName)

```

C This subroutine computes the value of the potential at the boundary.

```

    INCLUDE 'ECFHdr.INC'
    INCLUDE 'ECFGauss.INC'
    INCLUDE 'ECFMsh.INC'

```

```

    CHARACTER*(*) FileName
    INTEGER I,J,K,BDNode,BDNodeP1,Elem,LocNode,BDNodeLoc
    INTEGER Upper
    REAL*8 Distance,X,Y,XLast,YLast,Xs(MaxNoOfDim)
    REAL*8 Normal(MaxNoOfDim),dX(MaxNoOfDim),XBase(MaxNoOfDim),
    & Zeta(MaxNoOfDim),XZeta(MaxNoOfDim,MaxNoOfDim),DetXZeta
    REAL*8 PHI((MaxNoOfBasisDeg+1)**MaxNoOfDim),
    & PhiZeta(MaxNoOfDim,(MaxNoOfBasisDeg+1)**MaxNoOfDim),
    & PhiX(MaxNoOfDim,(MAXNoOfBasisDeg+1)**MaxNoOfDim),
    & Pot(MaxNoOfEqu),PotX(MaxNoOfDim,MaxNoOfEqu)

```

```

    OPEN(UNIT=1,FILE=FileName,STATUS='NEW',FORM='FORMATTED')
    WRITE(1,*) NoOfBDNodes*(NoOfGaussPts+1)

```

```

    Distance=0
    X=Nodes(BDNodes(1),1)
    Y=Nodes(BDNodes(1),2)

```

C The following DO-Loop loops over the boundary nodes.

```

    DO BdNode=1,NoOfBDNodes

      BDNodeP1=BdNode+1
      IF (BDNodeP1.GT.NoOfBDNodes) BDNodeP1=1

      CALL LocateGlobalElem(BDNode,BDNodeP1,Elem,BDNodeLoc)
      CALL ComputeLocStep(BDNodeLoc,dX,XBase)
      CALL GetUpper(ElemType(Elem),Upper)

```

C The following DO-Loop Loops over the gauss points and computes the value C of the potential and the potential slope at at each point on the boundary.

```

    DO J=0,NoOfGaussPts

      DO K=1,NoOfDim
        Zeta(K)=XBase(K)+J*dX(K)
      END DO

```

```

IF (ElemType(Elem).EQ.'S') THEN
  CALL Compute2DPhis(Zeta,Phi,PhiZeta)
ELSE
  CALL ComputeTriPhis(Zeta,Phi,PhiZeta)
END IF

CALL ComputeIsoPara(Elem,PhiZeta,XZeta,DetXZeta,Upper)
CALL ComputePhiX(Upper,PhiZeta,XZeta,DetXZeta,PhiX)
CALL ComputePot(Elem,Upper,Phi,PhiX,Pot,PotX)

```

C The next few lines compute the change in distance between the last
C computation and this one.

```

XLast=X
YLast=Y

CALL ComputeLoc(Phi,Elem,Xs)

X=Xs(1)
Y=Xs(2)

Distance=Distance+SQRT((X-XLast)**2+(Y-YLast)**2)

```

C The next line writes the distance and the slope computed into a file.

```

WRITE(1,*) Distance,Pot(1)

END DO
END DO

CLOSE(1)
CLOSE(2)
CLOSE(3)

RETURN
END

```

C ***** PlotPots

```

SUBROUTINE PlotPots(NoOfPot,Pots,FileName)

INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFMsh.INC'
INCLUDE 'ECFRes.INC'

PARAMETER MaxNoOfPot=25

INTEGER NoOfPts
REAL*8 Pots(*),PotMax,PotMin
CHARACTER*(*) FileName

REAL*8 Zero/0.0/,One/1.0/,
& XPts(MaxNoOfPot+1,2*MaxNoOfNodes),
& YPts(MaxNoOfPot+1,2*MaxNoOfNodes),
& XTemp(2*MaxNoOfNodes),YTemp(2*MaxNoOfNodes)
  INTEGER NoOfPPts(MaxNoOfPot+1),I,J,K,L,RNode,LNode,
& Pointer(2*MaxNoOfNodes),Kp1,NoOfPot,Upper

```

C Open the file that will contain endpoints of segments to be plotted.

```
OPEN(UNIT=1,FORM='FORMATTED',FILE=FileName,STATUS='NEW')
```

C The following statements Loop through elements.

```
DO J=1,NoOfElems
```

```
CALL GetUpper(ElemType(J),Upper)
```

C The following DO-Loop clears the number of pts found at a given potential
C for the element.

```
DO L=1,NoOfPot+1
  NoOfPPts(L)=0
END DO
```

C The following DO-Loop loops through the local segments.

```
DO K=1,Upper
```

```
CALL IncrementI(K,Kp1,1,Upper)
```

```
PotMax=MAX(C(CLoc(1,J,K)),C(CLoc(1,J,Kp1)))
PotMin=MIN(C(CLoc(1,J,K)),C(CLoc(1,J,Kp1)))
```

C Next, we loop over all the isopotential values.

```
DO L=1,NoOfPot+1
```

C The following IF-THEN block locates all the points on the boundary
C of the element that have potential values we are interested in.

```
IF ((Pots(L).GE.PotMin).AND.(Pots(L).LE.PotMax)) THEN
  NoOfPPts(L)=NoOfPPts(L)+1
  CALL Interp1D(C(CLoc(1,J,K)),Nodes(NLoc(J,K),1),
& C(CLoc(1,J,Kp1)),Nodes(NLoc(J,Kp1),1),Pots(L),
& XPts(L,NoOfPPts(L)))
  CALL Interp1D(C(CLoc(1,J,K)),Nodes(NLoc(J,K),2),
& C(CLoc(1,J,Kp1)),Nodes(NLoc(J,Kp1),2),Pots(L),
& YPts(L,NoOfPPts(L)))
END IF
```

```
END DO
END DO
```

C The following statements store the points found for this element into
C the plot file.

```
DO L=1,NoOfPot+1
  IF (NoOfPPts(L).GT.1) THEN
    DO I=1,NoOfPPts(L)-1
      WRITE(1,*) XPts(L,I),YPts(L,I),Pots(L)
      WRITE(1,*) XPts(L,I+1),YPts(L,I+1),Pots(L)
    END DO
  END IF
END DO
```

```

END DO

CLOSE(1)

RETURN

END

```

C ***** Subroutine Calls

C Internal Subroutines (ECFPLOT.FOR)

```

c   SUBROUTINE ComputeLocStep(BDNodeLoc,dX,XBase)
c   SUBROUTINE ComputeNormal(BdNode,BDNodeP1,UnitNormal)
c   SUBROUTINE FindIso(FileName)
c   SUBROUTINE LocateGlobalElem(BDNode,BDNodeP1,Elem,BDNodeLoc)
c   SUBROUTINE PlotBdrySlope(FileName)
c   SUBROUTINE PlotBdryVal(FileName)

```

C Calls to Internal Subroutines

```

c   CALL ComputeLocStep(BDNodeLoc,dX,XBase)
c   CALL ComputeLocStep(BDNodeLoc,dX,XBase)
c   CALL ComputeNormal(BdNode,BdNodeP1,Normal)
c   CALL FindIso(PlotFile)
c   CALL LocateGlobalElem(BDNode,BDNodeP1,Elem,BDNodeLoc)
c   CALL LocateGlobalElem(BDNode,BDNodeP1,Elem,BDNodeLoc)
c   CALL PlotBdrySlope(SlopeFile)
c   CALL PlotBdryVal(ValFile)

```

C Calls to External Subroutines (ECFSUBS.FOR)-----F.E.M. routines

```

c   CALL Compute2DPhis(Zeta,Phi,PhiZeta)
c   CALL Compute2DPhis(Zeta,Phi,PhiZeta)
c   CALL ComputeIsoPara(Elem,PhiZeta,XZeta,DetXZeta)
c   CALL ComputeIsoPara(Elem,PhiZeta,XZeta,DetXZeta)
c   CALL ComputeLoc(Phi,Elem,Xs)
c   CALL ComputeLoc(Phi,Elem,Xs)
c   CALL ComputePhiX(PhiZeta,XZeta,DetXZeta,PhiX)
c   CALL ComputePhiX(PhiZeta,XZeta,DetXZeta,PhiX)
c   CALL ComputePot(Elem,Phi,PhiX,Pot,PotX)
c   CALL ComputePot(Elem,Phi,PhiX,Pot,PotX)
c   CALL ReadMesh(MeshFile)
c   CALL ReadMeshHdr(MeshHdrFile)
c   CALL ReadNames(FileName)
c   CALL ReadRes(ResFile)

```

C Calls To External Subroutines (SUBS.FOR)-----General Routines

```

c   CALL EditDP('Maximum Potential',PotMax)
c   CALL EditDP('Minimum Potential',PotMin)
c   CALL GetFileName('Names file?',FileName)
c   CALL Iinp('No Of Isopotential curves?',NoOfPot)

```

C Calls To External Subroutines (MATHSUBS.FOR)-----Math Routines

```

c   CALL Interp1D(C(CLoc(1,J,K)),Nodes(NLoc(J,K),1),
c   CALL Interp1D(C(CLoc(1,J,K)),Nodes(NLoc(J,K),2),

```

```
PROGRAM ECFiso
```

```
C This program will read an *.ISO file and plot the contours.
```

```
INCLUDE '[KJ.DATA]PLOTABL.INC'
```

```
INTEGER Length,NoOfPlots,NoOfSegs
```

```
REAL Pot1,Pot2,X1,X2,Y1,Y2
```

```
CHARACTER TermType*3,File*80
```

```
C Get Plotter and Set It Up
```

```
CALL GetPlotter(TermType)
```

```
C The following statements will read the data from the data file.
```

```
NoOfPlots=0
```

```
File='*'
```

```
DO WHILE(File.NE.' ')
```

```
File=' '
```

```
CALL LIB$SPAWN('DIR [...]*.ISO')
```

```
CALL GetFileName('Iso-potential plot file?',File)
```

```
CALL StringLength(File,Length)
```

```
IF ((Length.EQ.0).AND.(NoOfPlots.EQ.0)) THEN
```

```
WRITE(*,*) 'Error: no filename entered.'
```

```
ELSE IF (Length.GT.0) THEN
```

```
NoOfPlots=NoOfPlots+1
```

```
CALL GetMaxMin(File,NoOfSegs)
```

```
Title=File
```

```
XLabel='X'
```

```
YLabel='Y'
```

```
CALL GetLabels
```

```
CALL PlotCurve(TermType,File,NoOfSegs)
```

```
END IF
```

```
END DO
```

```
CALL DonePl
```

```
WRITE(*,*) 'Normal End: ',NoOfPlots,' plots.'
```

```
STOP
```

```
END
```

```
C ***** GetLabels
```

```
SUBROUTINE GetLabels
```

```
INCLUDE '[KJ.DATA]PLOTABL.INC'
```

```
INTEGER Length
```

```

REAL T

OPEN(UNIT=2,FILE='PLOT.LAB',STATUS='UNKNOWN',
& FORM='FORMATTED')
CALL StringLength(Title,Length)
WRITE(2,*) '','',Title(1:Length),'', ''Title''
CALL SStringLength(XLabel,Length)
WRITE(2,*) '','',XLabel(1:Length),'', '',XMin,XMax,
& ', ''XLabel'', XMin, XMax'
WRITE(2,*) LogX, ''LogX''
CALL StringLength(YLabel,Length)
WRITE(2,*) '','',YLabel(1:Length),'', '',YMin,YMax,
& ', ''YLabel'', YMin, YMax'
WRITE(2,*) LogY, ''LogY''
CLOSE(2)
CALL LIB$SPAWN('EDIT PLOT.LAB')

OPEN(UNIT=2,FILE='PLOT.LAB',STATUS='UNKNOWN',
& FORM='FORMATTED')
READ(2,*) Title
READ(2,*) XLabel,XMin,XMax
READ(2,*) LogX
READ(2,*) YLabel,YMin,YMax
READ(2,*) LogY
CLOSE(2)

c WRITE(*,*) 'You must enter a title.'
c CALL EditCh('Title?',Title)

C Get X & Y Axis type and label

c CALL GetAxis('X',XLabel,XMin,XMax,LogX)
c CALL GetAxis('Y',YLabel,YMin,YMax,LogY)

RETURN
END

C ***** GetMaxMin

SUBROUTINE GetMaxMin(File,NoOfSegs)

INTEGER NoOfSegs
CHARACTER*(*) File
REAL X1,Y1,Pot1
REAL X2,Y2,Pot2
INCLUDE '[KJ.DATA]PLOT.LABL.INC'

NoOfSegs=0

OPEN(UNIT=1,FILE=File,STATUS='OLD',FORM='FORMATTED')

90 READ(1,*,END=100) X1,Y1,Pot1
READ(1,*,END=100) X2,Y2,Pot2

NoOfSegs=NoOfSegs+1

IF (NoOfSegs.EQ.1) THEN
  XMin=MIN(X1,X2)

```

```

        YMin=MIN(Y1,Y2)
        XMax=MAX(X1,X2)
        YMax=MAX(Y1,Y2)
    ELSE
        XMin=MIN(XMin,X2)
        YMin=MIN(YMin,Y2)
        XMax=MAX(XMax,X2)
        YMax=MAX(YMax,Y2)

        XMin=MIN(XMin,X1)
        YMin=MIN(YMin,Y1)
        XMax=MAX(XMax,X1)
        YMax=MAX(YMax,Y1)
    END IF

    GOTO 90

100  CLOSE(1)

    RETURN
    END

C ***** PlotCurve

```

```

SUBROUTINE PlotCurve(TermType,File,NoOfSegs)

```

```

CHARACTER*(*) TermType,File
INTEGER NoOfSegs

```

```

INCLUDE '[KJ.DATA]PLOTLABEL.INC'

```

```

INTEGER I,J,K,Length
PARAMETER MaxNoOfPoints=2

```

```

REAL PtsX(MaxNoOfPoints),PtsY(MaxNoOfPoints)
CHARACTER X1*30,Y1*30,Ti*30
REAL Pot1,Pot2

```

```

C Set up the Graphics output using DISSPLA

```

```

CALL SetPlotter(TermType)

```

```

CALL Height(0.25)
CALL StringLength(Title,Length)
IF (Length.GT.0) CALL Headin(Title,Length,1.1,1)

```

```

CALL StringLength(XLabel,Length)
CALL XName(XLabel,Length)
CALL StringLength(YLabel,Length)
CALL YName(YLabel,Length)

```

```

CALL YAXANG(0.0)
CALL Graf(XMin,'SCALE',XMax,YMin,'SCALE',YMax)

```

```

CALL NoChek

```

```

OPEN(UNIT=1,FILE=File,STATUS='OLD',FORM='FORMATTED')

```

```
DO I=1,NoOfSegs
    READ(1,*,END=200) PtsX(1),PtsY(1),Pot1
    READ(1,*,END=200) PtsX(2),PtsY(2),Pot2

    CALL Marker(0)
    CALL Curve(PtsX,PtsY,2,0)

END DO
200 : CLOSE(1)
    CALL EndPI(0)

RETURN
END
```


C File ECSUBS.FOR

C ***** Compute2DPhis

SUBROUTINE Compute2DPhis(Zeta,Phi,PhiZeta)

C This subroutine computes the values of the local weighting functions, and
C the values of their slopes.

C Input Variables

C Zeta(NoOfDim) The value of the local variable at which to evaluate the
C functions.

C(In COMMON BasisDeg=degree of basis functions, 3 are hermite cubics)
C(NoOfDim)

C Output Variables

C Phi() Phi(1) is the first local weighting function evaluated at
C local node. Phi(2) is the second.

C PhiZeta(NoOfDim,) These are the derivates (with respect to zeta)
C evaluated at zeta(i).

INCLUDE 'ECFHdr.INC'

REAL*8 Phi((MaxNoOfBasisDeg+1)**MaxNoOfDim),
& PhiZeta(NoOfDim,(MaxNoOfBasisDeg+1)*MaxNoOfDim),
& Zeta(NoOfDim)

IF (NoOfDim.NE.2) THEN
WRITE(*,*) 'Warning: NoOfDim is not 2'
STOP 'In Routine: Compute2DPhis'
END IF

IF (BasisDeg.EQ.1) THEN

C The following local bilinear basis functions are based on the
C numbering scheme shown below:

C 4-3
C ||
C 1-2

Phi(1)=(1.0-Zeta(1)) *(1.0-Zeta(2))
Phi(4)=(1.0-Zeta(1)) *(Zeta(2))
Phi(2)=(Zeta(1)) *(1.0-Zeta(2))
Phi(3)=(Zeta(1)) *(Zeta(2))

PhiZeta(1,1)=-1.0 *(1.0-Zeta(2))
PhiZeta(1,4)=-1.0 *(Zeta(2))
PhiZeta(1,2)=1.0 *(1.0-Zeta(2))
PhiZeta(1,3)=1.0 *(Zeta(2))

PhiZeta(2,1)=(1.0-Zeta(1)) *(-1.0)
PhiZeta(2,4)=(1.0-Zeta(1)) *(1.0)
PhiZeta(2,2)=(Zeta(1)) *(-1.0)
PhiZeta(2,3)=(Zeta(1)) *(1.0)

```
ELSE IF (BasisDeg.EQ.2) THEN
```

```
C The following local biquadratic basis functions are based on the
C numbering scheme shown below:
```

```
C 4-7-3
C | |
C 8 9 6
C | |
C 1-5-2
```

```
ELSE
```

```
WRITE(*,*) 'Warning: Higher order basis functions not
WRITE(*,*) 'yet programmed for 2D'
STOP 'In Routine: Compute2DPhis'
```

```
END IF
```

```
RETURN
END
```

```
C ***** ComputeCoefLoc
```

```
SUBROUTINE ComputeCoefLoc(NLoca,J,CLoca)
```

```
C This subroutine is used to compute coefficient locations.
```

```
INTEGER NLoca,J,CLoca
```

```
INCLUDE 'ECFHdr.INC'
```

```
CLoca=(NLoca-1)*NoOfEqu + J
```

```
RETURN
END
```

```
C ***** ComputeIsoPara
```

```
SUBROUTINE ComputeIsoPara(Elem,PhiZeta,XZeta,DetXZeta,Upper)
```

```
C This subroutine computes XZeta (dx(j)/dzeta(i)) (j=col, i=row) and DetXZeta
C (Det XZeta) where XZeta is the jacobian for the isoparametric transformation
C between the global element (represented by the x's) and the local element
C (represented by the zeta's)
```

```
INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFMsh.INC'
```

```
C Note: written for BasisDeg=1
```

```
REAL*8 XZeta(MaxNoOfDim,MaxNoOfDim),DetXZeta,
& PhiZeta(MaxNoOfDim,(MaxNoOfBasisDeg+1)**MaxNoOfDim),
& IsoJacobian(MaxNoOfDim,MaxNoOfDim)
```

```
INTEGER Elem,I,J,K,Upper
```

```
C The following DO-loop loops over the global dimensions.
```

```
DO J=1,NoOfDim
```

C The following DO-Loop loops over the local dimensions.

```
DO I=1,NoOfDim
  XZeta(I,J)=0.0
```

C The following DO-Loop computes the value of XZeta(I,J)=
C sum (x(I,K).PhiZeta(K,J)

```
DO K=1,Upper
  XZeta(I,J)=XZeta(I,J)
  & +PhiZeta(I,K)*Nodes(NLoc(Elem,K),J)
END DO
```

```
END DO
END DO
```

C The following statement computes the determinant of the transformation
C Jacobian for 2 dimensions.

```
DetXZeta=XZeta(1,1)*XZeta(2,2)-XZeta(1,2)*XZeta(2,1)
```

```
IF (DetXZeta.EQ.0.0) THEN
  WRITE(*,*) 'Error: Determinant of Jacobian is ZERO!'
  STOP 'In Routine: ComputeIsoPara'
END IF
```

```
RETURN
END
```

C ***** ComputeLoc

```
SUBROUTINE ComputeLoc(Phi,Elem,X)
```

C Given the element number and the Basis Functions at the Desired point,
C This subroutine computes the location within the element of the local
C point (i.e. the point in the transformed domain)

C Phi() The basis functions evaluated at the point in the local element
C Elem The global element number
C X() The global location of the local point.

```
INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFMsh.INC'
```

```
REAL*8 X(MaxNoOfDim),Phi((MaxNoOfBasisDeg+1)**MaxNoOfDim)
INTEGER Elem,I,J,Upper
```

```
CALL GetUpper(ElemType(Elem),Upper)
DO I=1,NoOfDim
  X(I)=0.0
  DO J=1,Upper
    X(I)=X(I)+Nodes(NLoc(Elem,J),I)*Phi(J)
  END DO
END DO
```

```
RETURN
```

END

C ***** ComputePhiX

SUBROUTINE ComputePhiX(Upper,PhiZeta,XZeta,DetXZeta,PhiX)

C This subroutine computes PhiX from PhiZeta and the Jacobian of the
C isoparametric mapping.

INCLUDE 'ECFHdr.INC'

REAL*8 PhiZeta(MaxNoOfDim,(MaxNoOfBasisDeg+1)**MaxNoOfDim),
& PhiX(MaxNoOfDim,(MaxNoOfBasisDeg+1)**MaxNoOfDim)
REAL*8 XZeta(MaxNoOfDim,MaxNoOfDim),DetXZeta
INTEGER I,Upper

IF (NoOfDim.EQ.1) THEN

C Inverse is easy

DO I=1,BasisDeg+1
PhiX(1,I)=PhiZeta(1,I)
END DO

ELSE IF (NoOfDim.EQ.2) THEN

C Inverse of 2x2 is known

IF (DetXZeta.EQ.0.0) THEN
WRITE(*,*) 'Error: Attempting to divide by zero!'
WRITE(*,*) ' DetXZeta=0.0!'
STOP 'In Routine: ComputePhiX'
END IF

DO I=1,Upper
PhiX(1,I)=(XZeta(2,2)*PhiZeta(1,I)-
& XZeta(1,2)*PhiZeta(2,I))/DetXZeta
PhiX(2,I)=(XZeta(1,1)*PhiZeta(2,I)-
& XZeta(2,1)*PhiZeta(1,I))/DetXZeta
END DO

ELSE

WRITE(*,*) 'Error: NoOfDim too great! I can''t invert'
WRITE(*,*) ' the isoparametric mapping!'
WRITE(*,*) ' NoOfDim=',NoOfDim
STOP 'In Routine: ComputePhiX'

END IF

RETURN
END

C ***** ComputePot

SUBROUTINE ComputePot(Elem,Upper,Phi,PhiX,Pot,PotX)

C This subroutine computes the local value of the potential and the derivative

C of the potential with respect to the local coordinates.

```
INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFRes.INC'
```

```
INTEGER Elem,J,K,I,Upper
REAL*8 Pot(MaxNoOfEqu),PotX(MaxNoOfDim,MaxNoOfEqu),
& Phi((MaxNoOfBasisDeg+1)**MaxNoOfDim),
& PhiX(MaxNoOfDim,(MaxNoOfBasisDeg+1)**MaxNoOfDim),
& dX(MaxNoOfDim)
```

C The following DO-Loops zero the Pot and PotZeta matrices

```
DO K=1,NoOfEqu
  Pot(K)=0.0
  DO I=1,NoOfDim
    PotX(I,K)=0.0
  END DO
END DO
```

C The following DO-Loop computes the CONC(i) and slope PotZeta(I,K)

```
DO I=1,NoOfEqu
  DO J=1,Upper
    Pot(I)=Pot(I)+C(CLoc(I,Elem,J))*Phi(J)
    DO K=1,NoOfDim
      PotX(K,I)=PotX(K,I)
& + C(CLoc(I,Elem,J))*PhiX(K,J)
    END DO
  END DO
END DO

RETURN
END
```

C ***** ComputeTriPhis

```
SUBROUTINE ComputeTriPhis(Zeta,Phi,PhiZeta)
```

```
INCLUDE 'ECFHdr.INC'
```

```
REAL*8 Zeta(MaxNoOfDim)
REAL*8 Phi((MaxNoOfBasisDeg+1)**MaxNoOfDim)
REAL*8 PhiZeta(MaxNoOfDim,(MaxNoOfBasisDeg+1)**MaxNoOfDim)
```

```
IF (BasisDeg.NE.1) THEN
  WRITE(*,*) 'Error: basis functions for triangular elements'
  WRITE(*,*) ' are only known for basis degree=1'
  WRITE(*,*) ' BasisDeg=',BasisDeg
  STOP 'In Routine: ComputeTriPhis'
END IF
```

```
Phi(1)=1-Zeta(1)-Zeta(2)
Phi(2)=Zeta(1)
Phi(3)=Zeta(2)
```

```
PhiZeta(1,1)=-1.0
PhiZeta(2,1)=1.0
```

```
PhiZeta(1,2)=1.0
PhiZeta(2,2)=0.0
```

```
PhiZeta(1,3)=0.0
PhiZeta(2,3)=1.0
```

```
RETURN
END
```

C ***** Essential

```
SUBROUTINE Essential(Side,Eqn,X,BCPar,C)
```

C This subroutine is used to set essential boundary conditions.
C Input Variables

C Side The side number currently set to its essential boundary condition
C X0 The location of the node
C BCPar The bc input parameter assigned to the ith side.
C Eqn The equation number.

C Output Variables

C C The values of the coefficients at the node for equations

```
REAL*8 X(*),BCPar,C
INTEGER Side,Eqn
```

```
WRITE(*,*) 'Warning: external subroutine ESSENTIAL has not been',
& 'linked into'
WRITE(*,*) ' ECDEFINE. Please refer to users manual.'
```

```
RETURN
END
```

C ***** FirstGuess

```
SUBROUTINE FirstGuess(Eqn,Elem,X,C)
```

C This subroutine is used to make a first guess for the coefficients.

C Input Variables

C Elem The current element.
C X0 The location of the node
C Eqn The equation number.

C Output Variables

C C The values of the coefficients at the node for equations

```
REAL*8 X(*),C
INTEGER Elem,Eqn
```

```
WRITE(*,*) 'Warning: external subroutine FIRSTGUESS has not been',
& 'linked into'
WRITE(*,*) ' ECDEFINE. Please refer to users manual.'
```

```
RETURN
END
```

```
C ***** GetFEMProb
```

```
SUBROUTINE GetFEMProb(Prompt,FileName)
```

```
CHARACTER*(*) FileName,Prompt
INTEGER Length,PrLen
LOGICAL FileExist
```

```
CALL StringLength(Prompt,PrLen)
CALL EditCh('Names file for '//Prompt(1:PrLen)//'? ',FileName)
```

```
IF (FileName.NE.' ') THEN
```

```
  INQUIRE(File=FileName,Exist=FileExist)
  IF (FileExist) THEN
```

```
    WRITE(*,*) 'Reading data from old files'
    CALL ReadNames(FileName)
    CALL ReadFEMUser
```

```
  ELSE
```

```
    CALL StringLength(FileName,Length)
    Length=MAX(Length,1)
```

```
    WRITE(*,*) 'Error: File ',FileName(1:Length),
& ' doesn't exist.'
    STOP 'In Routine: GetFEMProb'
```

```
  END IF
```

```
ELSE
```

```
  STOP 'In Routine: GetFEMProblem Normal End'
END IF
```

```
RETURN
END
```

```
C ***** GetUpper
```

```
SUBROUTINE GetUpper(ElemType,Upper)
```

```
CHARACTER*1 ElemType
INTEGER Upper
```

```
INCLUDE 'ECFHdr.INC'
```

```
C This routine only works for BasisDeg=1
```

```
IF (ElemType.EQ.'S') THEN
```

```
C Square type of element
```

```
  Upper=(BasisDeg+1)**NoOfDim
```

```
ELSE IF (ElemType.EQ.'T') THEN
```

```
C Triangular type of element
```

```
Upper=3
IF (BasisDeg.NE.1) THEN
  WRITE(*,*) 'Error: Can't handle orders higher than 1 with'
  WRITE(*,*) '      triangular elements'
  STOP 'In Routine: GetUpper'
END IF
```

```
ELSE
```

```
C Unknown
```

```
WRITE(*,*) 'Error: Unknown type of element=',ElemType
STOP 'In Routine: GetUpper'
```

```
END IF
```

```
RETURN
END
```

```
C ***** PrintProbHeader
```

```
SUBROUTINE PrintProbHeader
```

```
INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFGauss.INC'
INCLUDE 'ECFbc.INC'
INCLUDE 'ECFNam.INC'
```

```
CHARACTER*80 Output
```

```
C ++++++
```

```
C 123456789a123456789b123456789c123456789d12345
```

```
C ----- Finite Element Method Parameters
```

```
200 WRITE(*,200)
    FORMAT(X,45('-'),' Finite Element Method Parameters')
```

```
Output=' '
```

```
C          123456789a123456
IF (Guess) Output='Ext. 1st Guess '
```

```
IF (Convection) THEN
```

```
IF (PolyFlow) THEN
```

```
C          123456789a1234
```

```
Output='PF Convection '//Output
```

```
ELSE
```

```
Output='External Conv '//Output
```

```
END IF
```

```
ELSE IF (Binary) THEN
```

```
Output='Binary Elec. '//Output
```

```
ELSE
```

```
Output=' '//Output
```



```

      END IF

      IF (ECFMesh) THEN
C      123456789
        Output='ECF Mesh '//Output
      ELSE
        Output='PF Mesh '//Output
      END IF

      IF (Debugging) THEN
C      123456
        Output='DEBUG '//Output
      ELSE
        Output=' '//Output
      END IF

      WRITE(*,210) Output,NoOfDim,NoOfEqu
210    FORMAT(X,A50,I2,' dimensions, ',I3,' equations')

C 123456789a123456789b123456789c123456789d123456789e
C DEBUGGING CONVECTION EXTERNAL 1ST GUESS      ii dimensions, iii equations

      WRITE(*,220) BasisDeg,Tolerance,NoOfGaussPts,MaxNoOfIter
220    FORMAT(X,'Degree of Basis Functions: ',I3,
& ' Convergence Tolerance: ',G14.7/,
& X,' Number of Gauss Points: ',I3,6X,
& 'Maximum No. NR Iter: ',I3)

C 123      1234
C Degree of Basis Functions: iii Convergence Tolerance: dddddddddddddd
C Number of Gauss Points: iii Maximum No. NR Iter: iii
C      123456

      RETURN
      END

C ***** ReadBC

      SUBROUTINE ReadBC(FileName)

      INCLUDE 'ECFHdr.INC'
      INCLUDE 'ECFbc.INC'
      INTEGER I,J
      CHARACTER*(*) FileName

C The following statements read the boundary conditions

      OPEN(UNIT=1,FILE=FileName,STATUS='OLD',FORM='FORMATTED')

      DO J=1,NoOfEqu
        READ(1,*) NoOfCorners(J)
        DO I=1,NoOfCorners(J)
          READ(1,*) Corners(J,I),BCs(J,I),Kinetics(I),BCPar(J,I)
        END DO
      END DO

      CLOSE(1)

```

```

RETURN
END

```

C ***** ReadFEMUser

```

SUBROUTINE READFEMUser

```

C This subroutine read the file FEM.IN created by WriteFEMUser

```

INCLUDE 'ECFNam.INC'

```

```

CALL ReadMeshHdr(MeshHdrFile)
CALL ReadMesh(MeshFile)
CALL ReadBC(BCFile)
CALL ReadRes(ResFile)
CALL ReadPar(ParFile)

```

```

RETURN
END

```

C ***** ReadMesh

```

SUBROUTINE ReadMesh(FileName)

```

```

INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFMsh.INC'
CHARACTER*(*) FileName
INTEGER I,J,K

```

C The following statements read the node locations

```

OPEN(UNIT=1,FILE=FileName,STATUS='OLD',FORM='FORMATTED')

```

```

DO I=1,NoOfNodes
  DO J=1,NoOfDim
    READ(1,*) Nodes(I,J)
  END DO
END DO

```

C The following statements read the NLOC matrix for finding the
C node numbers for various element locations.

```

DO J=1,NoOfElems
  READ(1,*) ElemType(J)
  DO K=1,(BasisDeg+1)**NoOfDim
    READ(1,*) NLoc(J,K)
  END DO
END DO

```

C The following statements read the number of the nodes on the boundary.

```

DO I=1,NoOfBDNodes
  READ(1,*) BDNodes(I)
END DO

```

```

CLOSE(1)

```

```

RETURN

```

END

C ***** ReadMeshHdr

SUBROUTINE ReadMeshHdr(FileName)

INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFGauss.INC'

CHARACTER*(*) FileName
LOGICAL FileExist

C The following statements read the degree of the basis functions, tolerance
C No of elements, nodes, boundary nodes, coefficients
C and debugging or convection flags, as well as file names.

INQUIRE(FILE=FileName,EXIST=FileExist)
IF (.NOT.FileExist) THEN
 WRITE(*,*) 'Error: File ',FileName,', does not exist.'
 STOP 'In Routine: ReadMeshHdr (ECFSUBS)'
END IF

OPEN(UNIT=1,FILE=FileName,STATUS='OLD',FORM='FORMATTED')

READ(1,*) BasisDeg,Tolerance,NoOfGaussPts,MaxNoOfIter
READ(1,*) NoOfEqu,NoOfDim
READ(1,*) NoOfElems,NoOfNodes,NoOfBDNodes
READ(1,*) NoOfCoef,Nlc,Nuc
READ(1,*) Debugging,Convection,PolyFlow,Guess,Nonnegative
READ(1,*) ECFMesh,Binary,Supporting

CLOSE(1)

RETURN
END

C ***** ReadNames

SUBROUTINE ReadNames(FileName)

INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFNam.INC'

CHARACTER*(*) FileName

OPEN(UNIT=1,FILE=FileName,STATUS='OLD',FORM='FORMATTED')

READ(1,*) MeshHdrFile
READ(1,*) MeshFile
READ(1,*) MeshSrcFile
READ(1,*) BCFile
READ(1,*) ParFile
READ(1,*) ResFile
READ(1,*) PlotFile
READ(1,*) SlopeFile

READ(1,*) PFMeshFile
READ(1,*) PFCoefFile

CLOSE(1)

RETURN
END

C ***** ReadPFCoef

SUBROUTINE ReadPFCoef(FileName)

INCLUDE 'POLYCOEF.INC'

INTEGER io1/1/J
CHARACTER*(*) FileName

OPEN(UNIT=IO1,FILE=FILENAME,STATUS='OLD',FORM='UNFORMATTED')

READ(io1) PolyNVers
READ(io1) PolyNTot,PolyNComp,PolyNNodeR,PolyVerTr
READ(io1) PolyTitle
READ(io1) (PolyFil1(J),J=1,PolyNComp)
READ(io1) (PolyFil2(J),J=1,PolyNComp)

IF (PolyNVers.NE.20) THEN
WRITE(*,*) 'Error: Expecting to read data from the version'
WRITE(*,*) ' 20 Polyflow.'
WRITE(*,*) ' NVers=',PolyNVers
STOP 'In Routine: ReadPFCoef'
END IF

READ(io1) PolyCase,PolyAx,PolyFluid,PolyStres
READ(io1) PolyTestRH,PolyTestZ

IF (PolyCase.NE.1) THEN
WRITE(*,*) 'Error: Expecting to read data for PolyFlow'
WRITE(*,*) ' for ICASE=1'
WRITE(*,*) ' ICASE=',PolyCase
STOP 'In Routine: ReadPFCoef'
END IF

READ (io1) PolyFac,PolyTNat,PolyExpO,PolyRO

IF (PolyNTot.GT.PolyMaxNoOfZ) THEN
WRITE(*,*) 'Error: Too many coefficients!'
WRITE(*,*) ' PolyNTot=',PolyNTot
WRITE(*,*) ' PolyMaxNoOfZ=',PolyMaxNoOfZ
STOP 'In Routine: ReadPFCoef'
END IF

READ (io1) (PolyZ(J),J=1,PolyNTot)

CLOSE(IO1)

RETURN
END

C ***** ReadPFMesh

SUBROUTINE ReadPFMesh(FileName)

```

INCLUDE 'PolyMesh.INC'
CHARACTER*(*) FileName
INTEGER I,J,Io1/1/,K
LOGICAL Error,FileExists

Error=.FALSE.
INQUIRE(File=FileName,Exist=FileExists)
IF (.NOT.FileExists) THEN
  WRITE(*,*) 'Error: The filename doesn't exist.'
  WRITE(*,*) '   FileName=',FileName
  STOP 'In Routine: ReadPFMesh'
END IF

OPEN(UNIT=io1,FILE=Filename,STATUS='OLD',FORM='FORMATTED')

READ (io1,100) PolyNVert,PolyNNode,PolyNBd,PolyNElem

IF (PolyNElem.GT.PolyMaxNElem) THEN
  WRITE(*,*) 'Error: PolyNElem is larger than PolyMaxNElem'
  WRITE(*,*) '   PolyNElem=',PolyNElem
  WRITE(*,*) '   PolyMaxNElem=',PolyMaxNElem
  Error=.TRUE.
END IF

IF (PolyNBd.GT.PolyMaxNBd) THEN
  WRITE(*,*) 'Error: PolyNBd is larger than PolyMaxNBd'
  WRITE(*,*) '   PolyNBd=',PolyNBd
  WRITE(*,*) '   PolyMaxNBd=',PolyMaxNBd
  ERROR=.TRUE.
END IF

IF (PolyNNode.GT.PolyMaxNNode) THEN
  WRITE(*,*) 'Error: PolyNNode is larger than PolyMaxNNode'
  WRITE(*,*) '   PolyNNode=',PolyNNode
  WRITE(*,*) '   PolyMaxNNode=',PolyMaxNNode
  ERROR=.TRUE.
END IF

IF (Error) STOP 'In Routine: ReadPFMesh'

DO I=1,PolyNElem
  READ(io1,100) (PolyNod(J,I),J=1,9)
  FORMAT(20I4)
END DO

READ(io1,100) (PolyBDNod(K),K=1,PolyNBd)
DO I=1,PolyNNode
  READ(io1,200) PolyX(I),PolyY(I)
  FORMAT(2E14.7)
END DO

CLOSE(io1)

RETURN
END

C ***** ReadPar

```

```

SUBROUTINE ReadPar(FileName)

INCLUDE 'ECFPar.INC'
CHARACTER*(*) FileName

OPEN(UNIT=1,STATUS='OLD',FORM='FORMATTED',FILE=FileName)

READ(1,*) WagnerLin,aA,aC
READ(1,*) Peclet
READ(1,*) BinaryK2,SupportingK3

CLOSE(1)

RETURN
END

```

C ***** ReadRes

```

SUBROUTINE ReadRes(FileName)

INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFRes.INC'
INTEGER I,J,K
CHARACTER*(*) FileName

OPEN(UNIT=1,FILE=FileName,STATUS='OLD',FORM='FORMATTED')

DO I=1,NoOfCoef
  READ(1,*) C(I)
END DO

DO I=1,NoOfEqu
  DO J=1,NoOfElems
    DO K=1,(BasisDeg+1)**NoOfDim
      READ(1,*) CLoc(I,J,K)
    END DO
  END DO
END DO

CLOSE(1)

RETURN
END

```

C ***** SearchForPFElem

```

SUBROUTINE SearchForPFElem(X,PFElem,Triangular)

```

C The following subroutine searches the Polyflow mesh element by element.

C The polyflow element containing the point X is returned.

C X() We wish to find the polyflow element containing this point.

C PFElem The polyflow element number containing X, or 0 if no

C element found.

C Triangular Set to .TRUE. if the polyflow element is triangular

```

INCLUDE 'ECFHdr.INC'
INCLUDE 'POLYMesh.INC'

```

```
REAL*8 X(MaxNoOfDim),ThetaSum,p1x,p1y,p2x,p2y,
& Pi/3.141592/
```

```
INTEGER PFElem,Nv,I,J,Jp1
LOGICAL Triangular
```

```
DO I=1,PolyNElem
```

```
Triangular=(PolyNod(8,I).EQ.0).AND.(PolyNod(9,I).EQ.0)
ThetaSum=0.0
```

```
IF (Triangular) THEN
```

```
  Nv=3
```

```
ELSE
```

```
  Nv=4
```

```
END IF
```

C The following statements compute the angles

```
DO J=1,Nv
```

```
  Jp1=J+1
```

```
  IF (Jp1.GT.Nv) Jp1=1
```

```
  p1X=PolyX(PolyNod(J,I))-X(1)
```

```
  p1Y=PolyY(PolyNod(J,I))-X(2)
```

```
  p2X=PolyX(PolyNod(Jp1,I))-X(1)
```

```
  p2Y=PolyY(PolyNod(Jp1,I))-X(2)
```

```
  IF (((P1X.EQ.0.0).AND.(P1Y.EQ.0.0)).OR.
& ((P2X.EQ.0.0).AND.(P2Y.EQ.0.0))) THEN
```

```
    PFElem=I
```

```
    RETURN
```

```
  END IF
```

```
  ThetaSum=ThetaSum+ACOS((p1X*p2X+p1Y*p2Y)/
& SQRT((P1X**2+P1Y**2)*(P2X**2+P2Y**2)))
```

```
END DO
```

```
IF (ThetaSum.GE.2.0*Pi) THEN
```

```
  PFElem=I
```

```
  RETURN
```

```
END IF
```

```
END DO
```

```
PFElem=0
```

```
RETURN
```

```
END
```

C ***** Velocity

```
SUBROUTINE Velocity(X,Vlcty)
```

C The subroutine computes the velocity Vlcty() calculated by PolyFlow at the C location X().

```
REAL*8 X(*),Vlcty(*)
LOGICAL Found
```

```
INCLUDE 'ECFHdr.INC'
INCLUDE 'PolyMesh.INC'
INCLUDE 'PolyCoef.INC'
```

```
PARAMETER Np=9
```

```
INTEGER Elem,PFElem,Indx(Np),NoOfPhis,I,J
REAL PtMat(Np,Np),PhiCoef(Np,Np),Col(Np),Phis(Np)
LOGICAL Triangular
```

```
IF (.NOT.PolyFlow) THEN
  WRITE(*,*) 'Error: No external subroutine linked into ECCOMPUTE.FOR'
  WRITE(*,*) '      for computing velocity'
  STOP 'In Routine: Velocity (internal)'
END IF
```

```
DO I=1,NoOfDim
  Vlcty(I)=0.0
END DO
```

```
CALL SearchForPFElem(X,PFElem,Triangular)
```

C PFElem is zero when no polyflow element could be found. The following
C IF-THEN block tests for this and if true, tells the user and stops the
C program.

```
IF (PFElem.EQ.0) THEN
  IF (PolyFlow) THEN
    WRITE(*,*) 'Error: point X() not found',
    & ' within polyflow mesh'
  ELSE
    WRITE(*,*) 'Error: point X() not found',
    & ' within external subroutine Velocity'
  END IF

  DO I=1,NoOfDim
    WRITE(*,*) '      X(',I,')=',X(I)
  END DO
  STOP 'In Routine: Velocity (internal)'
END IF
```

C The following do-loop makes the inverse of the matrix that will be used to
C compute phis for PolyFlow elements

```
IF (Triangular) THEN
  NoOfPhis=6
ELSE
  NoOfPhis=9
END IF
```

```
DO I=1,NoOfPhis
```

```
  PtMat(I,1)=1.0
  PtMat(I,2)=PolyX(PolyNod(I,PFElem))
```



```

PtMat(I,3)=PolyY(PolyNod(I,PFElem))
PtMat(I,4)=PolyX(PolyNod(I,PFElem))*PolyY(PolyNod(I,PFElem))
PtMat(I,5)=PolyX(PolyNod(I,PFElem))*PolyX(PolyNod(I,PFElem))
PtMat(I,6)=PolyY(PolyNod(I,PFElem))*PolyY(PolyNod(I,PFElem))

```

```

IF (.NOT.Triangular) THEN
  PtMat(I,7)=PolyX(PolyNod(I,PFElem))
  & *PolyY(PolyNod(I,PFElem))*PolyY(PolyNod(I,PFElem))
  PtMat(I,8)=PolyX(PolyNod(I,PFElem))
  & *PolyX(PolyNod(I,PFElem))*PolyY(PolyNod(I,PFElem))
  PtMat(I,9)=PolyX(PolyNod(I,PFElem))
  & *PolyX(PolyNod(I,PFElem))*PolyY(PolyNod(I,PFElem))
  & *PolyY(PolyNod(I,PFElem))
END IF

```

```

END DO

```

C The following CALL finds the inverse of the matrix

```

CALL MatInv(PtMat,PhiCoef,Indx,Col,NoOfPhis,Np)

```

C The following Statements compute the position vector Col
C for use in computing the Phis at the point X()

```

Col(1)=1
Col(2)=X(1)
Col(3)=X(2)
Col(4)=X(1)*X(2)
Col(5)=X(1)*X(1)
Col(6)=X(2)*X(2)

```

```

IF (.NOT.Triangular) THEN
  Col(7)=X(1)*X(2)*X(2)
  Col(8)=X(1)*X(1)*X(2)
  Col(9)=X(1)*X(1)*X(2)*X(2)
END IF

```

C The following DO-Loop computes the PHis for the PolyFlow Element

```

DO I=1,NoOfPhis
  Phis(I)=0.0

  DO J=1,NoOfPhis
    Phis(I)=Phis(I)+PhiCoef(J,I)*Col(J)
  END DO
END DO

```

C The following DO-loop computes the velocity in x and y directions.

```

DO I=1,NoOfDim
  Vlcty(I)=0.0

  DO J=1,NoOfPhis
    Vlcty(I)=Vlcty(I)+Phis(J)*
    & PolyZ(PolyNod(J,PFElem)+(I-1)*PolyNNode)
  END DO
END DO

```

```
RETURN
END
```

C ***** WriteBC

```
SUBROUTINE WriteBC(FileName)
```

```
INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFbc.INC'
INTEGER I,J
CHARACTER*(*) FileName
```

C The following statements Write the boundary conditions

```
OPEN(UNIT=1,FILE=FileName,STATUS='NEW',FORM='FORMATTED')
```

```
DO J=1,NoOfEqu
  WRITE(1,*) NoOfCorners(J)
  DO I=1,NoOfCorners(J)
    WRITE(1,*) Corners(J,I),',',BCs(J,I),',',
& Kinetics(I),',',BCPar(J,I)
  END DO
END DO
```

```
CLOSE(1)
```

```
RETURN
END
```

C ***** WriteFEMUser

```
SUBROUTINE WriteFEMUser
```

```
INCLUDE 'ECFNam.INC'
INCLUDE 'ECFHdr.INC'
```

```
CALL WriteMeshHdr(MeshHdrFile)
CALL WriteMesh(MeshFile)
CALL WriteBC(BCFile)
CALL WriteRes(ResFile)
CALL WritePar(ParFile)
```

```
RETURN
END
```

C ***** WriteMesh

```
SUBROUTINE WriteMesh(FileName)
```

```
INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFMsh.INC'
CHARACTER*(*) FileName
INTEGER I,J,K
```

C The following statements Write the node locations

```
OPEN(UNIT=1,FILE=FileName,STATUS='NEW',FORM='FORMATTED')
```

```

DO I=1,NoOfNodes
  DO J=1,NoOfDim
    Write(1,*) Nodes(I,J)
  END DO
END DO

```

C The following statements Write the NLOC matrix for finding the
C node numbers for various element locations.

```

DO J=1,NoOfElems
  WRITE(1,*) '','','ElemType(J),'''
  DO K=1,(BasisDeg+1)**NoOfDim
    Write(1,*) NLoc(J,K)
  END DO
END DO

```

C The following statements Write the number of the nodes on the boundary.

```

DO I=1,NoOfBDNodes
  Write(1,*) BDNodes(I)
END DO

CLOSE(1)

RETURN
END

```

C ***** WriteMeshHdr

```

SUBROUTINE WriteMeshHdr(FileName)

INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFGauss.INC'

CHARACTER*(*) FileName

```

C The following statements Write the degree of the basis functions, tolerance
C No of elements, nodes, boundary nodes, coefficients
C and debugging or convection flags, as well as file names.

```

OPEN(UNIT=1,FILE=FileName,STATUS='NEW',FORM='FORMATTED')

Write(1,*) BasisDeg,',','Tolerance,',','NoOfGaussPts,',','MaxNoOfIter
Write(1,*) NoOfEqu,',','NoOfDim
Write(1,*) NoOfElems,',','NoOfNodes,',','NoOfBDNodes
Write(1,*) NoOfCoef,Nlc,Nuc
Write(1,*) Debugging,',','Convection,',','PolyFlow,',','Guess,
& ',','Nonnegative
WRITE(1,*) ECFMesh,',','Binary,',','Supporting

CLOSE(1)

RETURN
END

```

C ***** WriteNames

```

SUBROUTINE WriteNames(FileName)

```

```
INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFNam.INC'
```

```
CHARACTER*(*) FileName
INTEGER Length
```

```
OPEN(UNIT=1,FILE=FileName,STATUS='NEW',FORM='FORMATTED')
```

```
CALL StringLength(MeshHdrFile,Length)
Write(1,*) ' ',MeshHdrFile(1:Length),' '
CALL StringLength(MeshFile,Length)
Write(1,*) ' ',MeshFile(1:Length),' '
CALL StringLength(MeshSrcFile,Length)
Write(1,*) ' ',MeshSrcFile(1:Length),' '
CALL StringLength(BCFile,Length)
Write(1,*) ' ',BCFile(1:Length),' '
CALL StringLength(ParFile,Length)
Write(1,*) ' ',ParFile(1:Length),' '
CALL StringLength(ResFile,Length)
Write(1,*) ' ',ResFile(1:Length),' '
```

```
CALL StringLength(PlotFile,Length)
WRITE(1,*) ' ',PlotFile(1:Length),' '
CALL StringLength(SlopeFile,Length)
WRITE(1,*) ' ',SlopeFile(1:Length),' '
```

```
CALL StringLength(PFMeshFile,Length)
IF (Length.LE.0) Length=1
Write(1,*) ' ',PFMeshFile(1:Length),' '
CALL StringLength(PFCoeffFile,Length)
IF (Length.LE.0) Length=1
Write(1,*) ' ',PFCoeffFile(1:Length),' '
```

```
CLOSE(1)
```

```
RETURN
END
```

```
C ***** WritePar
```

```
SUBROUTINE WritePar(FileName)
```

```
INCLUDE 'ECFPar.INC'
CHARACTER*(*) FileName
```

```
OPEN(UNIT=1,STATUS='NEW',FORM='FORMATTED',FILE=FileName)
```

```
Write(1,*) WagnerLin,' ',aA,' ',aC
Write(1,*) Peclet
WRITE(1,*) BinaryK2,SupportingK3
```

```
CLOSE(1)
```

```
RETURN
END
```

```
C ***** WriteRes
```

```
SUBROUTINE WriteRes(FileName)

INCLUDE 'ECFHdr.INC'
INCLUDE 'ECFRes.INC'

INTEGER I,J,K
CHARACTER*(*) FileName

OPEN(UNIT=1,FILE=FileName,STATUS='NEW',FORM='FORMATTED')

DO I=1,NoOfCoef
  WRITE(1,*) C(I)
END DO

DO I=1,NoOfEqu
  DO J=1,NoOfElems
    DO K=1,(BasisDeg+1)**NoOfDim
      WRITE(1,*) CLoc(I,J,K)
    END DO
  END DO
END DO

CLOSE(1)

RETURN
END
```

C Include File: ECFbc.INC

C Written by: Ken Jordan

Date: 8/3/87

C This INCLUDE file defines and dimensions the variables in COMMON block
C FEMbc. The variables are described in program FEM2d.FOR

C ----- Parameters

C MaxNoOfCorners The maximum number of boundary condition changes
C allowed. (i.e. the maximum number of insulators, electrodes,
C ...)

C ----- Variables

C BCPar(j,i) The voltage to apply to side i for equation j.
C This may also be a parameter used for computing
C boundary values for side i and equation j.
C BCs(,) The type of boundary condition to apply to each
C side (BCs(i) applies to Nodes(Corners(i))-Nodes(Corners(i+1))
C The first index is the equation number.
C Corners(,) The node numbers for the corners. The first index is the
C equation number, the second index is the corner number,
C the contents are the boundary node number for the corner.
C Kinetics() The type of kinetics to use for each side.
C NoOfCorners The number of corner points

C ----- Declarations

PARAMETER MaxNoOfCorners=4
COMMON /ECFbc/ Corners,NoOfCorners,BCs,Kinetics,BCPar

INTEGER Corners(MaxNoOfEqu,MaxNoOfCorners),
& NoOfCorners(MaxNoOfEqu)
REAL*8 BCPar(MaxNoOfEqu,MaxNoOfCorners)
CHARACTER*1 BCs(MaxNoOfEqu,MaxNoOfCorners)
CHARACTER*2 Kinetics(MaxNoOfCorners)

C Include File: ECFCal.INC

C Written By: Ken Jordan

Date: 8/3/87

C This INCLUDE file defines and dimensions the variables in COMMON block

C FEMCalcs. The variables are described in program FEM2d.FOR

C Note: Assumes FEMMesh.INC precedes it.

C ----- Variables

C R() The Residual vector for the last guess.

C RJacobian(,) The jacobian (dR(i)/dcoefficient(j))

C ----- Declarations

COMMON /ECFCal/R,RJacobian

REAL*8 R(MaxNoOfCoef),RJacobian(MaxBandWidth,MaxNoOfCoef)

C Include File: ECFEqu.INC
C Written By: Ken Jordan

C This file is only used when integrating concentrations (e.g. in binary,
C supporting or complex problems to get k's)

C Equ The equation number being solved. Should be 1 for binary and
C supporting

C Species The species number being integrated
C 1=depositing species
C 2=depositing species anion
C 3=supporting cation

INTEGER Equ,Species
COMMON /ECFEQU/Equ,Species

C Include File: ECFGauss
C Written By: Ken Jordan

7/10/90

C This file contains declarations for gaussian integration points.

C NoOfGaussPts The number of points used in the numerical integration.
C Pts(NoOfGaussPts) The points to be used in the evaluation of the
C integral.
C Wts(NoOfGaussPts) The weights to be used at each Gauss point.

PARAMETER MaxNoOfGaussPts=5

COMMON /ECFGauss/ Pts,Wts,NoOfGaussPts

INTEGER NoOfGaussPts

DOUBLE PRECISION Pts(MaxNoOfGaussPts),Wts(MaxNoOfGaussPts)

C Include File: ECFHdr.INC

C Written by: Ken Jordan

Date: 8/3/87

C This include file defines and dimensions variables in COMMON block ECFHdr

C ----- Parameters

C MaxNoOfNodes The maximum number of nodes allowed (A Parameter)
 C MaxBandWidth The maximum bandwidth for the problem
 C MaxNoOfEqu The maximum number of equations the ECF program can handle
 C MaxNoOfDim The maximum number of dimensions
 C MaxNoOfBasisDeg The maximum degree of basis functions.
 C MaxNoOfCoef The maximum number of coefficients

C ----- Variables

C BasisDeg The number 1 for linear Lagrange Basis Functions
 C 2 for quadratic Lagrange Basis Functions
 C 3 for cubic Hermite Basis Functions
 C Convection .TRUE. if the user wishes to include convective terms
 C (program computes velocity in subroutine)
 C Binary .TRUE. if the user is solving a binary electrolyte problem.
 C (program uses kappa for diffusivity, kinetics have conc. dep.)
 C Supporting .TRUE. if the user is solving a tertiary electrolyte problem.
 C Debugging .TRUE. if want CLoc, RJacobian, ... printed out between
 C iterations
 C Guess .TRUE. if the user wants the first guess computed in
 C program ECDEFINE.
 C MaxNoOfIter The maximum number of iterations allowed before NewtonRaphson
 C routine stops
 C Nlc The number of lower codiagonals for the RJacobian Matrix
 C NoOfBDNodes The number of nodes on the boundary
 C NoOfDim The number of dimensions.
 C NoOfElems The number of elements
 C NoOfEqu The number of equations being solved
 C NoOfNodes The number of distinct nodes
 C Nonnegative .TRUE. if the coefficients are not allowed to be negative.
 C Nuc The number of upper codiagonals for the RJacobian Matrix
 C PolyFlow .TRUE. if the program is to use POLYFLOW results for Convection.
 C Tolerance The norm of the C(N+1)-C(N) must be less than this for
 C solution to be considered converged.
 C ECFMesh .TRUE. if mesh was generated by ECFMESH (.FALSE. if mesh
 c was generated by POLYMESH)

C ----- Declarations

PARAMETER MaxNoOfNodes=2000
 PARAMETER MaxBandWidth=100
 PARAMETER MaxNoOfEqu=1
 PARAMETER MaxNoOfDim=2
 PARAMETER MaxNoOfBasisDeg=3
 PARAMETER MaxNoOfCoef=MaxNoOfEqu*MaxNoOfNodes

COMMON /ECFHdr/ BasisDeg,Tolerance,MaxNoOfIter,
 & NoOfDim,NoOfEqu,
 & NoOfElems,NoOfNodes,NoOfBDNodes,
 & NoOfCoef,Nlc,Nuc,
 & Debugging,Convection,Guess,PolyFlow,Nonnegative,

& ECFMesh,Binary,Supporting

INTEGER BasisDeg,NoOfElems,NoOfNodes,NoOfBDNodes,
& NoOfCoef,NoOfDim,NoOfEqu,Nlc,Nuc,MaxNoOfIter
LOGICAL Debugging,Convection,PolyFlow,Guess,Nonnegative
LOGICAL ECFMesh,Binary,Supporting
REAL*8 Tolerance

C Include File: ECFHdr2.INC

C Written by: Ken Jordan

Date: 8/3/87

C This include file defines and dimensions variables in COMMON block ECFHdr2

C ----- Variables

- C BasisDeg2 The number 1 for linear Lagrange Basis Functions
- C 2 for quadratic Lagrange Basis Functions
- C 3 for cubic Hermite Basis Functions
- C NoOfDim2 The number of dimensions.
- C NoOfElems2 The number of elements
- C NoOfEqu2 The number of equations being solved
- C NoOfNodes2 The number of distinct nodes

C ----- Declarations

COMMON /ECFHdr2/ BasisDeg2,NoOfDim2,NoOfEqu2,NoOfElems2,NoOfNodes2,
& NoOfCoef2

INTEGER BasisDeg2,NoOfElems2,NoOfNodes2,
& NoOfCoef2,NoOfDim2,NoOfEqu2

C Include File: ECFMAC.INC
 C Written By: Ken Jordan

C Parameters

C MaxNoOfMacVert
 C MaxNoOfMacElem
 C MaxNoOfMicVert

C Variables

C NoOfMacVert The number of macrovertices.
 C MacVertX() X location of macrovertices
 C MacVertY() Y location of macrovertices

C NoOfMacElem The number of macro elements
 C MacElemType() 'S' for square elements, 'T' for triangular.
 C MacElemVert(,4) Macrovertex numbers that make up the element
 C (Macro element number, vertex number)
 C The following conventions apply:

C Square macro elements
 C 4-3 +3+
 C || <- Vert. No. 4 2 <- Side No.
 C 1-2 +1+

C Triangular Macro Elements
 C 2 *
 C | C
 C || |C
 C *_* <- Vert. No. 2-1
 C 3_ *_ 1 *-3-*

C NoOfMicElm(,4) (Mac Elem No, Side), number of microelements to split
 C the side up into.
 C SpaType(,4) (Mac Elem No, Side), spacing to use on the side.
 C 'LIN' for linear spacing (currently the only type
 C known
 C SpaFac(,4) (Mac Elem No, Side), factor for spacing on the side.

c NoOfMacBDNodes The number of macrovertices on the boundary
 c MacBDNodeNo(MaxNoOfMacVert)
 C The micro node number of the macro vertex. Used
 C in printing reports on mesh, and in setting up B.C.
 c MacBDNodes(MaxNoOfMacVert)
 C The macrovertex numbers in the order that make up the
 C boundary.

c MacNodes(MaxNoOfMicVert+1,MaxNoOfMicVert+1)
 C (MicNode X, Mic Node Y)
 C The node numbers of the microvertices in the whole
 C macroelement. Two cases.

C Square macro element.
 C
 c 1,2--2,2--3,2 etc.
 c | | |
 c 1,1--2,1--3,1

C Triangular Macro Element

C	1,3		
C	c	C	1,2--2,2
c	b	c	1,1--2,1--3,1

c SharedNodes(MaxNoOfMacElem,4,MaxNoOfMicVert+1)

C (Mac Elem No, Side, Micro Vert. No)

C The node numbers of micro vertices on the sides of each

C macro element.

PARAMETER MaxNoOfMacVert=10

PARAMETER MaxNoOfMacElem=10

PARAMETER MaxNoOfMicVert=50

INTEGER NoOfMacVert,NoOfMacElem,

& MacElemVert(MaxNoOfMacElem,4),NoOfMicElm(MaxNoOfMacElem,4)

INTEGER SharedNodes(MaxNoOfMacElem,4,MaxNoOfMicVert+1)

INTEGER MacNodes(MaxNoOfMicVert+1,MaxNoOfMicVert+1)

INTEGER MacBDNodes(MaxNoOfMacVert),NoOfMacBDNodes

INTEGER MacBDNodeNo(MaxNoOfMacVert)

REAL*8 MacVertX(MaxNoOfMacVert),MacVertY(MaxNoOfMacVert),

& SpaFac(MaxNoOfMacElem,4)

CHARACTER*4 SpaType(MaxNoOfMacElem,4)

CHARACTER*1 MacElemType(MaxNoOfMacElem)

COMMON /ECFMAC/NoOfMacVert,NoOfMacElem,MacElemVert,NoOfMicElm,

& MacVertX,MacVertY,SpaFac,SpaType,SharedNodes,MacNodes,

& NoOfMacBDNodes,MacBDNodes,MacBDNodeNo,MacElemType

C Include File: ECFMsh.INC
 C Written by: Ken Jordan

Date: 8/3/87

C This include file defines and dimensions variables in COMMON block
 C ECFMsh. Read to and written from ReadMesh, WriteMesh()

C ----- Variables

C BdNodes() The vertex number of nodes on the boundary. (In order
 C around the boundary.)

C NLoc(.) The first index is the global element number (numbered
 C from the lower left corner and up)
 C The second index is the local node number
 C (1-> (BasisDeg+1)^(NoOfDim))
 C The contents are the Node location in matrix NODES.

C Nodes(.) The location of the nodes.
 C The first index is the node number (1-> NoOfNodes)
 C The second index is coordinate number (1=x, 2=y)

C ElemType() The type of element 'S' for square and 'T' for triangular.

C ----- Declarations

COMMON /ECFMsh/ Nodes,NLoc,BDNodes,ElemType

INTEGER NLoc(MaxNoOfNodes,(MaxNoOfBasisDeg+1)**MaxNoOfDim),
 & BDNodes(MaxNoOfNodes)
 REAL*8 Nodes(MaxNoOfNodes,MaxNoOfDim)
 CHARACTER*1 ElemType(MaxNoOfNodes)

C Include File: ECFMsh2.INC

C Written by: Ken Jordan

Date: 8/3/87

C This include file defines and dimensions variables in COMMON block
C ECFMsh. Read to and written from ReadMesh, WriteMesh()

C ----- Variables

C NLoc2(,) The first index is the global element number (numbered
C from the lower left corner and up)
C The second index is the local node number
C (1-> (BasisDeg+1)^(NoOfDim)
C The contents are the Node location in matrix NODES.

C Nodes2(,) The location of the nodes.
C The first index is the node number (1-> NoOfNodes)
C The second index is coordinate number (1=x, 2=y)

C ElemType2() The type of element 'S' for square and 'T' for triangular.

C ----- Declarations

COMMON /ECFMsh2/ Nodes2,NLoc2,ElemType2

INTEGER NLoc2(MaxNoOfNodes,(MaxNoOfBasisDeg+1)**MaxNoOfDim)
REAL*8 Nodes2(MaxNoOfNodes,MaxNoOfDim)
CHARACTER*1 ElemType2(MaxNoOfNodes)

C Include File: ECFNam.INC

C Written by: Ken Jordan

Date: 8/11/87

C ----- Variables

C BCFile The name of the *.BC file.
 C MeshFile The filename for the *.MSH file
 C MeshHdrFile The filename for the *.HDR file
 C MeshSrcFile The filename of the polyflow mesh file that serves as the
 C source for the *.MSH file
 C ParFile The name of the *.PAR file.
 C PFMeshFile The filename for the hydrodynamic flow mesh. (from POLYFLOW)
 C PFCoeffFile The filename for the hydrodynamic coefficients(from POLYFLOW)
 C PlotFile The name of the *.ISO file containing line segments
 C of constant value.
 C ResName The filename for the results file (also used for
 C first guess.)
 C SlopeFile The name of the *.SLP file containing the slope of coefficients
 C along the boundary.

C ----- Declarations

CHARACTER*72 MeshHdrFile,MeshFile,MeshSrcFile,BCFile,ParFile,
 & PlotFile

CHARACTER*72 PFMeshFile,PFCoeffFile,ResFile,SlopeFile

COMMON /ECFNam/MeshHdrFile,MeshFile,BCFile,ParFile,
 & ResFile,PFMeshFile,PFCoeffFile,PlotFile,SlopeFile,
 & MeshSrcFile

C Include File: ECFPar.INC

C Written by: Ken Jordan

Date: 8/3/87

C This INCLUDE file defines and dimensions the variables in COMMON block

C ECFPar. The variables are described here. They

C represent parameters used to define kinetic and convection conditions.

C ----- Variables

C Kinetic Variables

C WagnerKLin Linear wagner number for kinetics to ohmic

C kappa R T / L F i0

C aA The anodic transfer Coefficient

C aC The cathodic transfer Coefficient

C BinaryK2 Integration constant when considering binary electrolyte

C SupportingK3 Integration constant when considering supporting electrolyte.

C Convection Variables

C Peclet The peclet number for convection problems

C ----- Declarations

COMMON /ECFPar/ WagnerLin,aA,aC,Peclet,
& BinaryK2,SupportingK3

REAL*8 aA,aC,WagnerLin

REAL*8 Peclet,BinaryK2,SupportingK3

```
C Include File: ECFPlot.INC
C Written By: Ken Jordan
```

```
C This file contains variables used internally to program ecfplot and
C subroutines. This file just saves retyping all of this stuff in each routine
C and in each call pass list.
```

```
C XBase()      The starting point for the current segment
C dX()         The total step across the segment (if straight)
C Distance     The total distance moved along the boundary so far.
C X,Y         The current X,Y location plotted.
C XLast,YLast The last x,y locatio plotted.
C Normal()    The outward pointing unit normal to the surface.
```

```
REAL*8 Distance,X,Y,XLast,YLast
REAL*8 XBase(MaxNoOfDim),dX(MaxNoOfDim),
& Normal(MaxNoOfDim)
```

```
COMMON /ECFPlot/Distance,X,Y,XLast,YLast,XBase,dX,Normal
```

C Include File: ECFRes.INC

C Written by: Ken Jordan

Date: 8/11/87

C This file contains the dimensions and common block necessary for accessing
C the ECF results.

C ----- Variables

C C() The coefficients for the basis functions.
C CLoc(,,) The first index is the equation number (1=potential)
C The second index is the global element number (numbered
C from the lower left corner and up)
C The third index is the local node number (1-> (BasisDeg+1)^2)
C The contents are the Global Coef location.
C (Some people call this the NOP array)

C ----- Declarations

COMMON /ECFRes/C,CLoc

INTEGER CLoc(MaxNoOfEqu,MaxNoOfNodes,
& (MaxNoOfBasisDeg+1)**(MaxNoOfDim))
REAL*8 C(MaxNoOfCoef)

C Include File: ECFRes2.INC

C Written by: Ken Jordan

Date: 8/11/87

C This file contains the dimensions and common block necessary for accessing
C the ECF results.

C ----- Variables

C C2() The coefficients for the basis functions.
C CLoc2(,,) The first index is the equation number (1=potential)
C The second index is the global element number (numbered
C from the lower left corner and up)
C The third index is the local node number (1-> (BasisDeg+1)^2)
C The contents are the Global Coef location.
C (Some people call this the NOP array)

C ----- Declarations

COMMON /ECFRes2/C2,CLoc2

INTEGER CLoc2(MaxNoOfEqu,MaxNoOfNodes,
& (MaxNoOfBasisDeg+1)**(MaxNoOfDim))
REAL*8 C2(MaxNoOfCoef)

C Include File: ECFTriPts.INC
C Written By: Ken Jordan

C This file contains integration points to use for triangular elements.
C Currently, only NoOfTriPts=4 is allowed. See Burnett, p 596 for others

COMMON /ECFTriPts/NoOfTriPts, TriPts, TriWts

INTEGER NoOfTriPts
REAL*8 TriPts(10,2), TriWts(10)

C Include File: PolyCoef.INC

C Written By: Ken Jordan

Date: 8/5/87

C This include file contains the declarations and common block necessary
C to access the polyflow coefficient data.

C ----- Variables

C PolyNVers The polyflow version number that made the coefficient file.
C PolyNtot The total number of coefficients.
C PolyNComp The number of ??
C PolyNNodeR ?
C PolyVerTr ?
C PolyTitle The title
C PolyFil1(*)
C PolyFil2(*)
C PolyCase The type of problem that POLYFLOW solved
C PolyAx ?
C PolyFluid ?
C PolyStres ?
C PolyTestRH ?
C PolyTestZ ?
C PolyFac ?
C PolyTNat ?
C PolyExpO ?
C PolyRO
C PolyZ(*) The Coefficient Values at each node location
C Stored in the form U1, U2, U3, ... UNNode,
C V1, ...
C P1, ...
C Psi1, ...

C ----- Declarations

PARAMETER PolyMaxNoOfZ=8000

INTEGER PolyNVers,PolyNTot,PolyNComp,PolyNNodeR,PolyVerTr

INTEGER PolyTitle(19)

INTEGER PolyFil1(20),PolyFil2(20),PolyCase,PolyAx,PolyFluid

INTEGER PolyStres

REAL*8 PolyTestRH,PolyTestZ,PolyFac,PolyTNat,PolyExpO,PolyRO

REAL*8 PolyZ(PolyMaxNoOfZ)

COMMON /PolyCoef/PolyNVers,PolyNTot,PolyNComp,PolyNNodeR,
& PolyVerTr,PolyTitle,PolyFil1,PolyFil2,PolyCase,PolyAx,
& PolyFluid,PolyStres,PolyTestRH,PolyTestZ,PolyFac,PolyTNat,
& PolyExpO,PolyRo,PolyZ

C Include File: PolyMesh.INC

C Written by: Ken Jordan

Date: 8/5/87

C This file contains the declarations and common block required to
C read the polyflow mesh.

C ----- Variables

C PolyNVert The number of vertices
C PolyNNode The number of nodes
C PolyNBd The number of points on the boundary
C PolyNElem The number of elements
C PolyNod(9,*) The nodes locations for each element
C PolyBDNod(*) The ?? Boundary nodes
C PolyX(*) The X points of the mesh
C PolyY(*) The Y Points of the mesh

C ----- Declarations

PARAMETER PolyMaxNElem=1300

PARAMETER PolyMaxNBd=360

PARAMETER PolyMaxNNode=5400

INTEGER PolyNVert,PolyNNode,PolyNBd,PolyNElem

INTEGER PolyNod(9,PolyMaxNElem)

INTEGER PolyBDNod(PolyMaxNBd)

REAL PolyX(PolyMaxNNode),PolyY(PolyMaxNNode)

COMMON /PolyMesh/PolyNVert,PolyNNode,PolyNBd,PolyNElem,
& PolyNod,PolyBDNod,PolyX,PolyY

PROGRAM ECBPAR

C This program generates the *.PAR file

```

CHARACTER*80 FileName
INTEGER FilLen

CALL ChInp('Dimensional File? (No .DIM)',FileName)

CALL StringLength(FileName,FilLen)
CALL ReadUserParams(FileName(1:FilLen)//'.DIM')
CALL PrintUserParams(FileName(1:FilLen)//'.DIM')
CALL WritePar(FileName(1:FilLen)//'.PAR')

STOP 'Normal End'
END

```

C ***** PrintUserParams

```

SUBROUTINE PrintUserParams(FileName)

```

```

CHARACTER*(*) FileName

```

```

INCLUDE 'ECBPPar.INC'
INCLUDE 'ECBPPar2.INC'

```

```

INTEGER FilLen

```

```

10  FORMAT(X,55('*'), ' Constants & Parameters')

```

```

C 123456789a123456789b123456789c123456789d123456789e12345

```

C ***** Constants & Parameters

```

20  FORMAT(X, ' Fundamental: ',7X, 'F = ',F12.0, ' C/mol')

```

```

C          1234567 123456789a12
C Fundamental:   F = dddd.de+dd C/mol

```

```

30  FORMAT(X, ' Additive: C Bulk = ',G10.3, ' mol/l' /
& X,19X, ' D = ',G10.3, ' cm^2/s')

```

```

35  FORMAT(X, 'Current Revrsl: CRRatio=',G10.3,
& ' i cathodic/i anodic',
& /,X, ' WaLinPCR=',G10.3)

```

```

C 123      12      123456789
C Additive: C Bulk = d.ddde+dd mol/l
C 123456789a123456789
C          D = d.ddde+dd cm^2/s

```

```

40  FORMAT(X,4X, ' Kinetic: alpha A = ',F6.3,
& 11X, ' i0 = ',F7.2, ' mA/cm^2',
& /,X,13X, ' alpha C = ',F6.3)

```

```

C 1234      12345123456789a1 123456
C Kinetic: alpha A = d.ddd      i0 = ddd.dd mA/cm^2
C 123456789a123      123456789
C          alpha C = d.ddd

```

```

50   FORMAT(X,' Electrolyte: kappa =',F6.3,' mho/cm')
C   Electrolyte: kappa = d.ddd mho/cm

60   FORMAT(X,'Characteristic: xstar =',G12.4,' microns',
& /X,      '          phistar =',G12.4,' V',
& /X,      '          istar =',G12.4,' mA/cm^2',
& 5X,'idep =',G12.4,' mA/cm^2',
& /X,      '          ',12X, '          ',
& 5X,'BC 4 =',G12.4,
& /X,      '          tstar =',G12.4,' s')

C           123456
C Characteristic: xstar = ddd.d microns
C           istar = ddd.ddd mA/cm^2
C           12345678
C           phistar = ddd.ddd V

70   FORMAT(X,78('*'))

C       1       2       3       4       5       6       7
C 123456789a123456789b123456789c123456789d123456789e123456789f123456789g12345678
C *****

WRITE(*,10)
CALL StringLength(FileName,FilLen)
WRITE(*,*) 'File=',FileName(1:FilLen)
WRITE(*,*) ''
WRITE(*,20) F
WRITE(*,*) ''
IF (CorLev) THEN
  WRITE(*,30) CaBulk,Da
  WRITE(*,*) ''
END IF
IF (PerRev) THEN
  WRITE(*,35) CRRatio,WaLinPCR
END IF
WRITE(*,40) aA,i0,aC
WRITE(*,*) ''
WRITE(*,50) kappa
WRITE(*,*) ''
WRITE(*,60) xstar,phistar,istar,idep,(idep/istar),tstar
WRITE(*,*) ''
WRITE(*,70)
WRITE(*,*) ''
WRITE(*,80)
WRITE(*,*) ''
IF (CorLev) THEN
  WRITE(*,90) WagLin,Corros,WagLin/(idep/i0),idep/i0
ELSE
  IF (PerRev) THEN
    WRITE(*,*) '  A N O D I C'
    WRITE(*,*) ''
    WRITE(*,91) WagLin,WagLin/(idep/i0),idep/i0
    WRITE(*,*) ''
    WRITE(*,*) '  C A T H O D I C'
    WRITE(*,*) ''
    WRITE(*,91) WagLin*WaLinPCR,

```

```

& WagLin*WaLinPCR/(idep*CRRatio/i0),idep*CRRatio/i0
  ELSE
    WRITE(*,91) WagLin,WagLin/(idep/i0),idep/i0
  END IF
END IF
WRITE(*,*) ' '
WRITE(*,70)
WRITE(*,*) ' '

80  FORMAT(X,57('*'),' Dimensionless Groups')

C 123456789a123456789b123456789c123456789d123456789e1234567
C ***** Dimensionless Groups

90  FORMAT(X,6X,'WagLin =',G11.4,31X,'Corrosion =',G11.4,
& /, X,6X,'WagTaf =',G11.4,
& /X, 'Nonlinearity =',G11.4)
91  FORMAT(X,6X,'WagLin =',G11.4,
& /, X,6X,'WagTaf =',G11.4,
& /X, 'Nonlinearity =',G11.4)

C 123456      123456789a1123456789a123456789b123456789c1
C   WagLin = d.dddde+dd                      Corrosion = d.dddde+dd
C Nonlinearity = d.dddde+dd

      RETURN
      END

C ***** ReadUserParams

      SUBROUTINE ReadUserParams(FileName)

      INCLUDE 'ECBHdr.INC'
      INCLUDE 'ECBPar.INC'
      INCLUDE 'ECBPar2.INC'
      INCLUDE 'ECGaus.INC'
      INCLUDE 'ECBMAC.INC'

      CHARACTER*(*) FileName

C Read the data in the kinetics file (usually called corros.dat, filename
C.is set in *.PAR file for the problem)

      OPEN(UNIT=1,FILE=FileName,STATUS='OLD',FORM='FORMATTED')

      READ(1,*) F
c          96487
      READ(1,*) CaBulk,Da, kappa
c          mol/l, cm^2/s/ohm-cm
      READ(1,*) nelec,aA,aC,i0
c          mA/cm^2
      READ(1,*) xstar, PhiStar
c          um, V
      READ(1,*) rho, MW
C          g/cc, g/mol
      READ(1,*) idep
c          mA/cm^2

```

```

READ(1,*) Axisymmetric,CorLev,Spline3D,PerRev
READ(1,*) MaxIter,SrcFactor,Tolerance
READ(1,*) KineticsFile
READ(1,*) NoOfDim,BasisDeg,NoOfGaussPts
READ(1,*) CRRatio,WaLinPCR
IF (PerRev) THEN
  READ(1,*) NoOfPCR
  READ(1,*) PCRMax
END IF
CLOSE(1)

```

C Compute characteristic quantities

```

C      istar = (kappa * PhiStar / xstar ) * 10**7
C          mA/cm2

C      tstar = rho * nelec * F * xstar / ( MW * istar ) / 10
C          s

```

C Compute Dimensionless Groups

```

WagLin = istar / i0
Corros = ( Da * nelec * F * CaBulk / Idep / Xstar ) * 10**4

```

c Note: Corros must be multiplied by (Xstar/delta)(istar/idep)
C to get the correct physical meaning. (>1=corrosion, <1=net dep)

```

RETURN
END

```

C ***** WritePar

```

SUBROUTINE WritePar(FileName)

```

```

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBPar.INC'
INCLUDE 'ECBPAR2.INC'
INCLUDE 'ECCGaus.INC'

```

```

CHARACTER*(*) FileName
LOGICAL FileExist
INTEGER Length,I,Version,KinLen

```

```

Version=6

```

```

OPEN(UNIT=1,FILE=FileName,STATUS='NEW',FORM='FORMATTED')
WRITE(1,*) Version

```

```

WRITE(1,*) NoOfDim,',',BasisDeg,',',NoOfGaussPts
WRITE(1,*) Spline3D,',',Axisymmetric
WRITE(1,*) CorLev,',',PerRev
WRITE(1,*) Corros
WRITE(1,*) NoOfPCR,',',CRRatio,',',WaLinPCR,',',PCRMax
WRITE(1,*) SrcFactor,',',Tolerance,',',MaxIter
WRITE(1,*) WagLin
WRITE(1,*) aA,',',aC
CALL StringLength(KineticsFile,KinLen)
IF (KinLen.GT.0) THEN

```

```
WRITE(1,*) ''',KineticsFile(1:KinLen),'''
ELSE
WRITE(1,*) ''',''
END IF
WRITE(1,*) tstar,istar

WRITE(1,*) ' '
WRITE(1,*) 'Dim, BasisDeg, GaussPts'
WRITE(1,*) 'Spline 3 d?, Axisymmetric ?'
WRITE(1,*) 'Corrosive Levelling?, Periodic Current Reversal?'
WRITE(1,*) 'Corrosion #'
WRITE(1,*) 'NoOfPCR, CRRatio, WaLinPCR, PCRMax'
WRITE(1,*) 'Src Factor, Tolerance, Max Iter'
WRITE(1,*) 'Wagner Number for Linear Kinetics'
WRITE(1,*) 'alpha A, alpha C'
WRITE(1,*) 'Kinetics Filename'
WRITE(1,*) ' t star, i star'
CLOSE(1)

RETURN
END
```

```

PROGRAM ECBPrePro

CHARACTER*80 FileName
INTEGER Length,I,Lgth
LOGICAL User

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMsh.INC'
INCLUDE 'ECBPar.INC'
INCLUDE 'ECBMac.INC'

COMMON /WORKSP/ RWKSP
REAL RWKSP(250000)
CALL IWKIN(250000)

```

C This program read macro vertices and bc's and makes the *.MSH & *.SRC
C file

```

CALL Titles
CALL ChInp('Filename? (No extension)',FileName)
CALL UpperCaseCh(FileName)
CALL StringLength(FileName,Length)

User=(FileName(1:Length).EQ.'USER')
IF (.NOT.User) THEN
  IF ((FileName(Length:Length).EQ.'A').OR.
& (FileName(Length:Length).EQ.'B')) THEN
    CALL ReadPar(FileName(1:Length-1)//'.PAR')
  ELSE
    CALL ReadPar(FileName(1:Length)//'.PAR')
  END IF
ELSE
  BasisDeg=1
END IF
CALL ReadMac(FileName(1:Length)//'.MAC')

IF (NoOfMacElems.GT.1) CALL LocateTrans
CALL MakeNodeMap
CALL WriteMac(FileName(1:Length)//'.MAC')

CALL MakeMeshPts(.FALSE.,.FALSE.)
CALL PrintMacroElems(FileName)

IF (.NOT.User) THEN
  CALL WriteMesh(FileName(1:Length)//'.MSH')
  WRITE(*,*) FileName(1:Length),'.MSH has been created'

  CALL MakeSrcPts
  CALL WriteSrc(FileName(1:Length)//'.SRC')
  WRITE(*,*) FileName(1:Length),'.SRC has been created.'

ELSE

  OPEN(UNIT=1,FILE='USER.ORIG',STATUS='NEW',FORM='FORMATTED')
  WRITE(1,*) NoOfCoords
  DO I=1,NoOfCoords-1
    WRITE(1,*) Coords(I,1),Coords(I,2)
  END DO

```

```

        WRITE(1,*) MacVertX(MacIndx(NoOfMacElems,2)),
& MacVertY(MacIndx(NoOfMacElems,2))
        CLOSE(1)
        WRITE(*,*) 'USER.ORIG has been created.'

    END IF

    STOP 'ECBPrePro: Normal Completion'
    END

```

C ***** CopyMactoTMac

```

SUBROUTINE CopyMactoTMac(I,Offset)

    INCLUDE 'ECBMac.INC'
    INCLUDE 'ECBTMac.INC'
    INTEGER I,J,Offset

    TMacBCType(I+Offset)=MacBCType(I)
    TMacBCVal(I+Offset)=MacBCVal(I)
    TNoOfMicElems(I+Offset)=NoOfMicElems(I)
    DO J=1,2
        TMacIndx(I+Offset,J)=MacIndx(I,J)
    END DO
    DO J=1,3
        TMacPar(I+Offset,J)=MacPar(I,J)
    END DO
    TMacRatio(I+Offset)=MacRatio(I)
    TMacShape(I+Offset)=MacShape(I)
    TMacSpac(I+Offset)=MacSpac(I)

    RETURN
    END

```

C ***** CopyTMactoMac

```

SUBROUTINE CopyTMactoMac

    INCLUDE 'ECBMac.INC'
    INCLUDE 'ECBTMac.INC'
    INTEGER I,J

    DO I=1,NoOfMacElems
        MacBCType(I)=TMacBCType(I)
        MacBCVal(I)=TMacBCVal(I)
        NoOfMicElems(I)=TNoOfMicElems(I)
        DO J=1,2
            MacIndx(I,J)=TMacIndx(I,J)
        END DO
        DO J=1,3
            MacPar(I,J)=TMacPar(I,J)
        END DO
        MacRatio(I)=TMacRatio(I)
        MacShape(I)=TMacShape(I)
        MacSpac(I)=TMacSpac(I)
    END DO

```

```
RETURN
END
```

C ***** CreateMacTrans

```
SUBROUTINE CreateMacTrans(I,IPlus1,Offset)
```

```
INCLUDE 'ECBMac.INC'
INCLUDE 'ECBTMac.INC'
INTEGER I,J,Offset,IPlus1
```

```
TMacBCType(I+Offset)=MacBCType(I)
TNoOfMicElems(I+Offset)=1
```

```
TMacRatio(I+Offset)=1.0
TMacShape(I+Offset)='TRNS'
TMacSpac(I+Offset)='EQU'
DO J=1,3
  TMacPar(I+Offset,J)=0
END DO
```

```
MacVertX(NoOfMacVert+1)=
& 0.95*(MacVertX(MacIndx(IPlus1,1)) - MacVertX(MacIndx(IPlus1,2)))
& + MacVertX(MacIndx(IPlus1,2))
MacVertY(NoOfMacVert+1)=
& 0.95*(MacVertY(MacIndx(IPlus1,1)) - MacVertY(MacIndx(IPlus1,2)))
& + MacVertY(MacIndx(IPlus1,2))
```

```
MacVertX(TMacIndx(I+Offset-1,2))=
& 0.95*(MacVertX(TMacIndx(I+Offset-1,2)) -
& MacVertX(TMacIndx(I+Offset-1,1)))
& + MacVertX(TMacIndx(I+Offset-1,1))
MacVertY(TMacIndx(I+Offset-1,2))=
& 0.95*(MacVertY(TMacIndx(I+Offset-1,2)) -
& MacVertY(TMacIndx(I+Offset-1,1)))
& + MacVertY(TMacIndx(I+Offset-1,1))
```

```
MacIndx(IPlus1,1)=NoOfMacVert+1
TMacIndx(I+Offset,1)=TMacIndx(I+Offset-1,2)
TMacIndx(I+Offset,2)=MacIndx(IPlus1,1)
```

```
NoOfMacVert=NoOfMacVert+1
```

```
RETURN
END
```

C ***** LocateTrans

```
SUBROUTINE LocateTrans
```

C This subroutine locates 'trans'-elements. Those elements that must span
C between two regions with different boundary conditions, but the same BC
C type (e.g. NAT, 0, to NAT, 1)

```
INCLUDE 'ECBMac.INC'
INCLUDE 'ECBTMac.INC'
```

```
INTEGER I,Offset,IPlus1
```



```

LOGICAL MacNat
EXTERNAL MacNat

Offset=0
DO I=1,NoOfMacElems
  CALL CopyMactoTMac(I,Offset)
  CALL IncrementI(I,IPlus1,1,NoOfMacElems)
  IF ( ( MacNat(MacBCType(I))
& .EQ. MacNat(MacBCType(IPlus1)) ) .AND.
& ( MacBCVal(I) .NE. MacBCVal(IPlus1) ) .AND.
& ( (MacShape(IPlus1) .NE. 'TRNS') .AND.
& (MacShape(I) .NE. 'TRNS') ) ) THEN
    Offset=Offset+1
    CALL CreateMacTrans(I,IPlus1,Offset)
  END IF
END DO
NoOfMacElems=NoOfMacElems+Offset

CALL CopyTMactoMac

RETURN
END

```

C ***** PrintMacroElems

```

SUBROUTINE PrintMacroElems(FileName)

INCLUDE 'ECBMac.INC'

INTEGER LOutput/6/,I,Length,MSFLen
CHARACTER*(*) FileName
CHARACTER*20 FileN

FileN=Filename
CALL StringLength(FileN,Length)

WRITE(LOutput,100)
100  FORMAT(X,80('*'))

C          123456789a123456789b
WRITE(LOutput,250) 'Macro Element Report',FileN
250  FORMAT(X,30X,A20,<30-Length>X,A<Length>)

WRITE(LOutput,100)

WRITE(LOutput,500)
500  FORMAT(X/,X,18X,'---- MACROVERTICES ----',/
& X,18X,'Point',10X,'X',18X,'Y',/)

C 123456789a123456
c  ---- MACROVERTICES ----
C 123  123456789a 123456789a12345678
c  Point      X          Y

510  FORMAT(X,19X,I3,2(5X,G14.5))
C 1234  12345          12345
c  iii   gggggggggggggg  gggggggggggggg

```

```

DO I=1,NoOfMacVert
  WRITE(LOutput,510) I,MacVertX(I),MacVertY(I)
END DO

WRITE(LOutput,600)
600  FORMAT(X,/,X,15X,'Micro',6X,'Boundary',27X,'MicroNodes' /
    & X,'Element Type Elements Type Value',10X,
    & 'MacroVertices Start End' /)
C 123456789a12345 123456 123456789a123456789b1234567
C      Micro      Boundary      MicroNodes
C      12 1      12 123 123456789a1      12 12
C Element Type Elements Type Value      MacroVertices Start End

610  FORMAT(X,2X,I3,4X,A4,3X,I3,5X,A4,3X,G14.5,X,2(X,I4),
    & 5X,I4,2X,I4)
611  FORMAT(X,9X,A)
615  FORMAT(X,9X,A4,.,3X,'Spacing Factor:',G14.5)
616  FORMAT(X,9X,A4,.,3X,' Spacing File:',A)
C      123456789a12345
C 12 1234 123 12345 123 12 12345 12
C iii aaaa iii xaaaaax gggggggggggggg iiiiii iiiiii
c      (transition)
620  FORMAT(X,2X,I3,4X,A4,3X,I3,5X,A4,3X,' (transition) ',
    & X,2(X,I4),5X,I4,2X,I4)

DO I=1,NoOfMacElems
  IF (MacShape(I).NE.'TRNS') THEN

    WRITE(LOutput,610) I,MacShape(I),NoOfMicElems(I),
    & MacBCType(I),MacBCVal(I),MacIndx(I,1),MacIndx(I,2),
    & MacStart(I),MacEnd(I)

    IF (MacShape(I).EQ.'USER') THEN
      CALL StringLength(MacBdryFile,MSFLen)
      WRITE(LOutput,611) MacBdryFile(1:MSFLen)
    END IF

    IF (MacSpac(I).EQ.'USER') THEN
      CALL StringLength(MacSpaFile(I),MSFLen)
      WRITE(LOutput,616) MacSpac(I),MacSpaFile(I)(1:MSFLen)
    ELSE IF (MacSpac(I).EQ.'LOG') THEN
      WRITE(LOutput,615) MacSpac(I),MacRatio(I)
    ELSE
      WRITE(LOutput,615) MacSpac(I)
    END IF

  ELSE

    WRITE(LOutput,620) I,MacShape(I),NoOfMicElems(I),
    & MacBCType(I),MacIndx(I,1),MacIndx(I,2),
    & MacStart(I),MacEnd(I)

  END IF

  IF ((MacIndx(I,1).GT.NoOfMacVert).OR.
    & (MacIndx(I,2).GT.NoOfMacVert)) THEN
    WRITE(*,*) 'Error: MacIndx is out of range. Mac Elem=',I
    WRITE(*,*) ' MacIndx=',MacIndx(I,1),MacIndx(I,2)
  END IF

```

```
      STOP 'In Routine: PrintMacroElems'  
    END IF  
  END DO
```

```
  RETURN  
  END
```

C ***** Titles

```
  SUBROUTINE Titles
```

```
  WRITE(*,*) ' PROGRAM: ECBPrePro           2/23/88'  
  WRITE(*,*) 'Written by: Ken Jordan       Version 2'  
  WRITE(*,*) ''  
  WRITE(*,*) 'This program reads input from the data file'  
  WRITE(*,*) '*.MAC and generates output files *.MSH & *.SRC'  
  WRITE(*,*) ''  
  WRITE(*,*) 'These files are used as input for program ECB'  
  WRITE(*,*) ''  
  WRITE(*,*) 'This program generates the BEM Mesh from the Macro'  
  WRITE(*,*) 'mesh stored in *.MAC'  
  WRITE(*,*) ''
```

```
  RETURN  
  END
```

program ECBM

C This program will solve for the current distribution and move boundaries
C for various levelling problems.

```

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMsh.INC'
INCLUDE 'ECBCal.INC'
INCLUDE 'ECBBC.INC'
INCLUDE 'ECBSrc.INC'
INCLUDE 'ECBPar.INC'
INCLUDE 'ECGaus.INC'
INCLUDE 'ECGLOG.INC'
INCLUDE 'ECBMac.INC'
INCLUDE 'ECBMOVE.INC'
INCLUDE 'ECBTime.INC'

```

```

CHARACTER*80 FileName
INTEGER FilLen,I

```

C Declarations required by IMSL

```

COMMON /WORKSP/ RWKSP
REAL RWKSP(136973)
CALL IWKIN(136973)

```

C ----- Initialize Problem

C -----
C The following CALLS obtain from the user the name of the problem he is
C solving and time stepping criteria.

```

CALL ChInp('Filename?',FileName)
WRITE(*,*) ' '

CALL DPInp(' Start Time (in seconds)',Time)
CALL DPInp(' End Time',EndTime)
CALL DPInp('Desired dTime',DesdTime)
WRITE(*,*) ' '

CALL DPInp('Desired Maximum dX per time step (unitless)',DesdX)
WRITE(*,*) ' '

```

C -----
C The following CALLS read data from files describing the BEM problem to solve.

```

CALL StringLength(FileName,FilLen)
CALL ReadPar(Filename(1:FilLen)//'.PAR')
IF (CorLev) THEN
  CALL ReadMesh(Filename(1:FilLen)//'.Msh')
  CALL ReadMac(FileName(1:FilLen)//'.MAC')
ELSE
  CALL ReadMesh(Filename(1:FilLen)//'.Msh')
  CALL ReadMac(FileName(1:FilLen)//'.MAC')
END IF

IF (PerRev) THEN

```

C Save time step for use in periodically reversing the current

```
DeltaTime=Endtime
END IF
```

C Note, the following two calls can be replaced by IMSL routines.

```
CALL GauLeg(NoOfGaussPts,GaussPts,GaussWts)
NoOfGauLogPts=NoOfGaussPts
CALL GauLog(NoOfGauLogPts,GauLogPts,GauLogWts)
```

C -----
C Make dimensional quantities dimensionless

```
Time=Time/tstar
EndTime=EndTime/tstar
DesdTime=DesdTime/tstar
MaxTimeCounter=1.5*(EndTime-Time)/DesdTime
LastTime=.FALSE.
TimeCounter=1
```

```
OPEN(UNIT=3,FILE=Filename(1:FilLen)//'.TD',STATUS='NEW',
& FORM='FORMATTED')
WRITE(3,*) 1000
```

```
IF (PerRev) THEN
```

```
IF (PCRMax) THEN
CALL PerCurRevMax(FileName)
ELSE
CALL PerCurRev(FileName)
END IF
```

```
ELSE
```

```
CALL TimeLoop(FileName)
```

```
END IF
```

```
CLOSE(3)
```

```
STOP 'Normal End'
END
```

C ***** AdjustForPr

```
SUBROUTINE AdjustForPr(St,En)
```

```
INTEGER St,En
```

```
INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMac.INC'
INCLUDE 'ECBPar.INC'
INCLUDE 'ECBBC.inc'
INTEGER I
```

```
DO I=MacStart(St),MacEnd(En)
```

```
D WRITE(*,*) 'Old BC Value:',I,BCValues(I)
```

```

      BCValues(I)= - BCValues(I)*CRRatio
D      WRITE(*,*) '      New:',I,BCValues(I)
      END DO

      DO I=St,En
      MacBCVal(I)= - MacBCVal(I)*CRRatio
      END DO

      RETURN
      END

```

C ***** Bem

SUBROUTINE Bem

C This subroutine solves the BEM problem posed in the include files.

```

      INCLUDE 'ECBHdr.INC'
      INCLUDE 'ECBPar.INC'

```

```

      REAL*8 dBCValues(MaxNoOfCoords),MagDiff,MagBC,MagdBC
      INTEGER NoOfdBCValues,Iteration
      LOGICAL Convergence,SolvedOnce

```

```

      REAL*8 VecNormDP
      EXTERNAL VecNormDP

```

C Make set of source points

```

      CALL MakeSrcPts

```

C Assemble G & H Matrices, and re-arrange into A & C

```

      CALL AssembleGH
      CALL AssembleAC

```

```

      Iteration=0
      SolvedOnce=.FALSE.
      Convergence=.FALSE.

```

```

      DO WHILE(.NOT.Convergence)

```

C Solve the system BemG.SolValues= (BemH.BCValues) for SolValues

```

      CALL BemMatSol(SolvedOnce)

```

C Iterate to solve kinetic BCValues

```

      CALL NewtonRaphson(Iteration,
      & NoOfdBCValues,dBCValues,MagDiff,MagBC)
      IF (NoOfdBCValues.GT.0) THEN

```

C Test for convergence on kinetic boundary condition

```

      MagdBC=VecNormDP(NoOfdBCValues,dBCValues)
      Convergence=(MagdBC.LT.Tolerance)
      Convergence=Convergence.AND.(MagDiff.LT.Tolerance)
      IF (MagBC.NE.0) Convergence=Convergence.AND.

```

& (MagdBC/MagBC.LT.Tolerance)

C Increment Number of Iterations, and print iteration status report

```

      Iteration=Iteration+1
      IF (MagBC.EQ.0) THEN
        WRITE(*,10) Iteration,MagDiff,MagdBC
      ELSE
        WRITE(*,10) Iteration,MagDiff,MagdBC,MagdBC/MagBC
      END IF
10    FORMAT(X,'Iter ',I3,2X,'Ik-Ip=',G13.6,2X,
      & 'dBC=',G13.6,2X,'dBC/BC=',G13.6)
cIter iii Ik-Ip=ggggggggggggg dBC=ggggggggggggg dBC/BC=ggggggggggggg

```

C Check to see that we haven't iterated too many times.

```

      IF (Iteration.GE.MaxIter)
        & CALL ErrMaxIter(NoOfdBCValues,dBCValues)

      CALL UpdateBCValues(NoOfdBCValues,dBCValues)

      ELSE
        Convergence=.TRUE.
      END IF

      END DO

```

C If we have been iterating on a kinetic bc, re-solve the BEM equations
C before returning.

```

      IF (NoOfdBCValues.GT.0) CALL BemMatSol(SolvedOnce)

      RETURN
      END

```

C ***** BemMatSol

```

      SUBROUTINE BemMatSol(SolvedOnce)

      LOGICAL SolvedOnce

      INCLUDE 'ECBHdr.INC'
      INCLUDE 'ECBMsh.INC'
      INCLUDE 'ECBCal.INC'
      INCLUDE 'ECBBC.INC'

      REAL*8 VecB(MaxNoOfCoords)

      CALL MatVecMultDP(MaxNoOfCoords,NoOfCoords,BemH,
      & BCValues,VecB)
      IF (SolvedOnce) THEN
        CALL SolveRelEq(VecB,SolValues)
      ELSE
        CALL SolveSimEq(BemG,VecB,NoOfCoords,SolValues,
      & MaxNoOfCoords)
        SolvedOnce=.TRUE.
      END IF

```

```
RETURN
END
```

C ***** CopyInsPoints

```
SUBROUTINE CopyInsPoints(Ntc,NodeMap,Elem,Coords)
```

C Passed Variables

```
INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMOVE.INC'
```

```
INTEGER Ntc,Elem,
& NodeMap(MaxNoOfCoords,MaxBasisDeg+1)
REAL*8 Coords(MaxNoOfCoords,MaxNoOfDim)
```

C Local Variables

```
INTEGER Loc
```

```
DO Loc=BasisDeg+1,2,-1
  CALL CopyPoint(NodeMap(Elem,Loc),Coords,NoOfIns,Ins)
```

```
  Ntc=Ntc+1
  IF (Ntc.EQ.1) First=NoOfIns
  IF (Ntc.EQ.2) Second=NoOfIns
```

```
  NextToLast=NoOfIns
```

```
END DO
```

```
RETURN
END
```

C ***** CurReversal

```
SUBROUTINE CurReversal
```

```
INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBPar.INC'
INCLUDE 'ECBTime.INC'
```

C The following CALLs adjust the current bc's for Current Reversal

```
CALL AdjustForPr(3,5)
CALL AdjustForPr(1,1)
```

```
WagLin=WagLin*WaLinPCR
DeltaTime=DeltaTime/CRRatio
DesdTime=DesdTime/CRRatio
```

```
EndTime=Time+DeltaTime/tstar
MaxTimeCounter=1.5*(EndTime-Time)/DesdTime+TimeCounter
LastTime=.FALSE.
```

C The following lines place the current reversal message into the output file.

```
WRITE(*,*) ' '
```



```

WRITE(*,*) 'Reversing Current! ',
& 'Current Ratio Final/Initial=',CRRatio
WRITE(*,*) '
& '      Wa(lin) PCR =',WaLinPCR
WRITE(*,*) '      Delta Time=',DeltaTime
WRITE(*,*) '
RETURN
END

```

C ***** ErrMaxIter

```

SUBROUTINE ErrMaxIter(NoOfdBCValues,dBCValues)

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMsh.INC'
INCLUDE 'ECBBC.INC'

INTEGER J,I,NoOfdBCValues
REAL*8 dBCValues(*),Factor,VecNormDP,MagdBC
LOGICAL KineticBC
EXTERNAL KineticBC,VecNormDP

MagdBC=VecNormDP(NoOfdBCValues,dBCValues)
IF (MagdBC.GT.1.0) THEN
  Factor=MAX(MIN(0.9D0,2.0D0/MagdBC),0.2D0)
ELSE
  Factor=1.0
END IF

WRITE(*,*) 'Error: Maximum number of iterations reached'
WRITE(*,*) 'ECBM: (In Routine: Bem) Abnormal End'

WRITE(*,5)
5  FORMAT(/,X,'      dBC Value  BC Value  Sol Value',/)
10 FORMAT(X,I3,3X,G11.4,3X,G11.4,3X,G11.4)

C  dBC Value  BC Value  Sol Value
C iii gggggggggggg gggggggggggg gggggggggggg
C  md.ddddemdd
c  12345678901

J=1
DO I=1,NoOfCoords
  IF (KineticBC(BCType(I))) THEN
    WRITE(*,10) I,dBCValues(J)*Factor,
& BCValues(I)-dBCValues(J)*Factor,SolValues(I)
    J=J+1
  END IF
END DO

STOP 'In Routine: Bem'
END

```

C ***** IntegrateBnddX

```

REAL*8 FUNCTION IntegrateBnddX(Dummy)

```

```

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMsh.INC'
INCLUDE 'ECBMac.INC'
INCLUDE 'ECBMove.INC'

INTEGER NoOfX,I
LOGICAL Dummy
REAL*8 X(MaxNoOfCoords),Y(MaxNoOfCoords),
& Break(MaxNoOfCoords),CSCoef(4,MaxNoOfCoords)
REAL*8 LowerLim,UpperLim,DCSITG
EXTERNAL DCSITG

IF (.NOT.Dummy) THEN

    NoOfX=NoOfMicElems(1)*BasisDeg+1

    DO I=1,NoOfX
        X(I)=Coords(I,1)
        Y(I)=Coords(I,2)
D    WRITE(*,*) I,' X=',X(I),' Y=',Y(I)
    END DO

    LowerLim=Coords(1,1)
    UpperLim=Coords(NoOfX,1)

ELSE

    NoOfX=NoOfMoved
    DO I=1,NoOfX
        X(I)=Moved(I,1)
        Y(I)=Moved(I,2)
D    WRITE(*,*) I,' X=',X(I),' Y=',Y(I)
    END DO

    LowerLim=Moved(1,1)
    UpperLim=Moved(NoOfX,1)

END IF

C Compute Integral

CALL DCSAKM(NoOfX,X,Y,Break,CSCoef)

D    WRITE(*,*) 'Lower Limit=',LowerLim
D    WRITE(*,*) 'Upper Limit=',UpperLim

IntegrateBnddX=DCSITG(LowerLim,UpperLim,NoOfX-1,Break,CSCoef)

RETURN
END

C ***** MakeIns

SUBROUTINE MakeIns(ElemStart,ElemEnd,NodeMap,Coords,NoOfElems,
& FileName)

C Passed Variables

```

```

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMOVE.INC'

```

```

INTEGER Coord,ElemStart,ElemEnd,
& NodeMap(MaxNoOfCoords,MaxBasisDeg+1),NoOfElems
REAL*8 Coords(MaxNoOfCoords,MaxNoOfDim)
CHARACTER*(*) FileName

```

C Local Variables

```

INTEGER Elem,Loc,Ntc
LOGICAL FirstExec/.TRUE./,InsExt/.FALSE./
REAL*8 BegPtX,BegPtY,EndPtX,EndPtY

```

```

COMMON /MakeInsYar/InsExt,FirstExec

```

```

IF (FirstExec) CALL ReadInsExt(BegPtX,BegPtY,EndPtX,EndPtY,
& InsExt,FileName)

```

```

IF (InsExt) THEN
  NoOfIns=1
  Ins(1,1)=BegPtX
  Ins(1,2)=BegPtY
ELSE
  NoOfIns=0
END IF

```

C Forces the 1st point on the boundary to be an endpoint for an element

```

IF ((ElemEnd+1).LE.(ElemStart-1)) THEN
  Ntc=0
  DO Elem=ElemStart-1,ElemEnd+1,-1
    CALL CopyInsPoints(Ntc,NodeMap,Elem,Coords)
  END DO

```

```

ELSE
  Ntc=0
  DO Elem=ElemStart-1,1,-1
    CALL CopyInsPoints(Ntc,NodeMap,Elem,Coords)
  END DO

```

```

  DO Elem=NoOfElems,ElemEnd+1,-1
    CALL CopyInsPoints(Ntc,NodeMap,Elem,Coords)
  END DO

```

```

END IF

```

```

CALL CopyPoint(NodeMap(ElemEnd+1,1),Coords,NoOfIns,Ins)
Last=NoOfIns

```

```

IF (InsExt) THEN

```

```

  NoOfIns=NoOfIns+1

```

```

  Ins(NoOfIns,1)=EndPtX
  Ins(NoOfIns,2)=EndPtY

```

```

END IF

IF (dXdN(1).GT.0) THEN
  IF (InsExt) THEN
    StaRev=.TRUE.
    Second=1
  ELSE
    WRITE(*,*) 'Error: Moving boundary off of insulator!'
    WRITE(*,*) '   This error could be corrected by creating'
    WRITE(*,*) '   a *.EXT file.'
    STOP 'In Routine: MakeIns'
  END IF
ELSE
  StaRev=.FALSE.
END IF

IF (dXdN(NoOfMoved).GT.0) THEN
  IF (InsExt) THEN
    EndRev=.TRUE.
    NextToLast=NoOfIns
  ELSE
    WRITE(*,*) 'Error: Moving boundary off of insulator!'
    STOP 'In Routine: MakeIns'
  END IF
ELSE
  EndRev=.FALSE.
END IF

CALL AcuteAngles

FirstExec=.FALSE.

RETURN
END

```

C ***** MakedXdN

```

SUBROUTINE MakedXdN(ElemStart,ElemEnd)

```

C Passed Variables

```

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMsh.INC'
INCLUDE 'ECBBC.INC'
INCLUDE 'ECBBC2.INC'
INCLUDE 'ECBPAR.INC'
INCLUDE 'ECBMOVE.INC'
INCLUDE 'ECBTIME.INC'

```

```

INTEGER ElemStart,ElemEnd

```

C Internal Variables

```

INTEGER NoOfSmooth,Offset,Elem,Loc,I,Coord,LastC

```

```

LOGICAL FirstTime/.TRUE./

```

```

REAL*8 Im(MaxNoOfCoords),Ia(MaxNoOfCoords)

```

```

REAL*8 SmoothX(MaxNoOfCoords),SmoothF(MaxNoOfCoords)
REAL*8 OrigX(MaxNoOfCoords),LastOrig
REAL*8 Breaka(MaxNoOfCoords),CSCoefa(4,MaxNoOfCoords)
REAL*8 Breakm(MaxNoOfCoords),CSCoefm(4,MaxNoOfCoords)
REAL*8 Ratio,Factor

```

C External Functions

```

REAL*8 DCSVAL,SlopeVal,DCSITG
EXTERNAL DCSVAL,SlopeVal,DCSITG

```

C The following DO-loop computes the local metal and corrosive agent flux.

```

NoOfdXdN=0

LastOrig=0.0
LastC=NodeMap(ElemStart,1)

DO Elem=ElemStart,ElemEnd
  DO Loc=1,BasisDeg+1
    Coord=NodeMap(Elem,Loc)
    NoOfdXdN=NoOfdXdN+1

    Im(NoOfdXdN)=
    & SlopeVal(Natural(Coord),BCValues(Coord),SolValues(Coord))

    IF (CorLev) THEN

```

C Compute Flux of Additive at point and equivalent corrosion current density
C from additive.

```

      Ia(NoOfdXdN)=
      & SlopeVal(Natural2(Coord),BCValues2(Coord),SolValues2(Coord))

      ELSE
        Ia(NoOfdXdN)=0
      END IF

```

C Calculate distances used to smooth c.d.

```

      OrigX(NoOfdXdN)=SQRT(
      & (Coords(Coord,1)-Coords(LastC,1))
      & *(Coords(Coord,1)-Coords(LastC,1))
      & +(Coords(Coord,2)-Coords(LastC,1))
      & *(Coords(Coord,2)-Coords(LastC,1)) )+LastOrig
      SmoothX(NoOfdXdN)=OrigX(NoOfdXdN)

      LastC=Coord
      LastOrig=OrigX(NoOfdXdN)

      END DO
    END DO

```

C Smooth dXdN *) Remove Duplicate X Values.

```

NoOfSmooth=NoOfdXdN
Offset=0
DO I=1,NoOfSmooth-1

```

```

      IF (SmoothX(I-Offset).EQ.SmoothX(I+1)) THEN
        Offset=Offset+1
      END IF
      SmoothX(I-Offset+1)=SmoothX(I+1)
      IF (CorLev) Ia(I-Offset+1)=Ia(I+1)
      Im(I-Offset+1)=Im(I+1)
    END DO
    NoOfSmooth=NoOfSmooth-Offset

```

C Smooth dXdN *) Call IMSL Smoothing routine.

```

      IF (CorLev) CALL DCSSCV(NoOfSmooth,SmoothX,Ia,2,Breaka,CSCCoefa)
      CALL DCSSCV(NoOfSmooth,SmoothX,Im,2,Breakm,CSCCoefm)

```

```

      IF (CorLev) THEN

```

C Ratio= additive / current

```

          Ratio=DCSITG(SmoothX(1),SmoothX(NoOfSmooth),
            & NoOfSmooth-1,Breaka,CSCCoefa)
            & / DCSITG(SmoothX(1),SmoothX(NoOfSmooth),
            & NoOfSmooth-1,Breakm,CSCCoefm)

```

C First time through the loop, we must compute Factor = Corros <i> / <Na>

```

          IF (FirstTime) Factor=Corros/Ratio
          WRITE(*,*) ' Corros=',Ratio*Factor

```

```

          ELSE IF (PerRev) THEN

```

```

            WRITE(*,*) ' Im=',DCSITG(SmoothX(1),SmoothX(NoOfSmooth),
            & NoOfSmooth-1,Breakm,CSCCoefm),' Time=',Time*tstar

```

```

          END IF

```

```

          NoOfdXdN=0
          DO Elem=ElemStart,ElemEnd
            DO Loc=1,BasisDeg+1
              NoOfdXdN=NoOfdXdN+1

```

```

              Im(NoOfdXdN)=DCSVAL(OrigX(NoOfdXdN),NoOfSmooth-1,
            & Breakm,CSCCoefm)
              IF (CorLev) THEN
                Ia(NoOfdXdN)=DCSVAL(OrigX(NoOfdXdN),NoOfSmooth-1,
            & Breaka,CSCCoefa)
              ELSE
                Ia(NoOfdXdN)=0.0
              END IF

```

```

              dXdN(NoOfdXdN)=Im(NoOfdXdN)-Factor*Ia(NoOfdXdN)

```

```

D          WRITE(*,*) 'NoOfdXdN ',NoOfdXdN,' X',SmoothX(NoOfdXdN)
          END DO
        END DO

```

```

        FirstTime=.FALSE.

```

```

        RETURN

```

END

C ***** PerCurRev

SUBROUTINE PerCurRev(FileName)

CHARACTER*80 FileName

INTEGER PCRCounter

INCLUDE 'ECBHdr.INC'

INCLUDE 'ECBPar.INC'

INCLUDE 'ECBMac.INC'

IF (NoOfMacElems.LT.6) THEN

WRITE(*,*) 'Error: Improper configuration for ',
& 'solution of periodic'
WRITE(*,*) ' current reversal problem.'
WRITE(*,*) ' Use 4 sides w/ 2 transition elements'
STOP 'ECBM: In Subroutine: PerCurRev'
END IF

IF (MacBCVal(4).GE.0) THEN

WRITE(*,*) 'Current Initially Cathodic=','
& MacBCVal(4)*istar,'mA/cm2'
ELSE
WRITE(*,*) 'Current Initially Anodic =','
& MacBCVal(4)*istar,'mA/cm2'
END IF

DO PCRCounter=1,NoOfPCR

CALL TimeLoop(FileName)

C The following call updates the boundary conditions

CALL CurReversal

CALL TimeLoop(FileName)

IF (PCRCounter.LT.NoOfPCR) THEN

CRRatio=1/CRRatio
WaLinPCR=1/WaLinPCR

CALL CurReversal

CRRatio=1/CRRatio
WaLinPCR=1/WaLinPCR

END IF

END DO

RETURN

END

C ***** PerCurRevMax

```
SUBROUTINE PerCurRevMax(FileName)
```

```
CHARACTER*80 FileName
INTEGER PCRCounter,FilLen
```

```
INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMsh.INC'
INCLUDE 'ECBPar.INC'
INCLUDE 'ECBMac.INC'
INCLUDE 'ECBMOVE.INC'
INCLUDE 'ECBTime.INC'
```

```
INTEGER ElemStart,ElemEnd,Elem,Loc,I
LOGICAL BdryFileExist,Iterating
REAL*8 IntOrig,IntCurr,IntegrateBnddX,dAdis,dAdep,dh,h
REAL*8 FirstX,FirstY,LastX,LastY,BigdTime
REAL*8 BigdMaxTC
EXTERNAL IntegrateBnddX
```

```
CALL StringLength(FileName,FilLen)
```

```
IF (NoOfMacElems.LT.4) THEN
  WRITE(*,*) 'Error: Improper configuration for ',
& 'solution of periodic'
  WRITE(*,*) '    current reversal problem with',
& ' maximum levelling.'
  WRITE(*,*) '    Use 4 sides (ESS,NAT,ESS,NAT)'
  STOP 'ECBM: In Subroutine: PerCurRevMax'
END IF
```

```
IF (Time.GT.0) THEN
  WRITE(*,*) 'Warning: Start time reset to zero.'
END IF
Time=0.0
BigdTime=EndTime-Time
BigdMaxTC=MaxTimeCounter
```

```
WRITE(*,*) 'Current Initially Anodic: Maximum Levelling Case.'
```

C Moving boundary is always the first macro element.

C (Note: NoOfMicElems(1) is the number of microelements on the moving part C of the boundary. The program assumes that parts A & B have the same moving C part of the boundary, with identical discretization.)

```
ElemStart=1
ElemEnd=NoOfMicElems(1)
```

```
IntOrig=IntegrateBnddX(.FALSE.)
```

```
DO PCRCounter=1,NoOfPCR
```

```
  CALL TimeLoop(FileName)
```

```
  IntCurr=IntegrateBnddX(.FALSE.)
  dAdis=ABS(IntOrig-IntCurr)
  IntOrig=IntCurr
```



```

      h=dAdis/(ABS(
& MacVertX(MacIndx(1,1))
& - MacVertX(MacIndx(1,2)) ))

```

```

      WRITE(*,*) 'Reversing Current! '

```

```

C ----- Boundary Movement

```

```

C Store coordinates in mesh into temporary storage (Moved), then compute
C the normal to every point on the surface (Nx), and current density at those
C points (dXdN)

```

```

C -----
C The following DO-LOOP stores the 'current density' at each point of the moving
C boundary; the result is stored in matrix dXdN.

```

```

      NoOfdXdN=0
      DO Elem=ElemStart,ElemEnd
        DO Loc=1,BasisDeg+1
          NoOfdXdN=NoOfdXdN+1
          dXdN(NoOfdXdN)=-1.0
        END DO
      END DO

```

```

C -----

```

```

C The following CALL computes the 'normal' at each point of the moving
C boundary; the result is stored in matrix Nx.

```

```

      CALL MakeMoved(ElemStart,ElemEnd,NodeMap,Coords)
      CALL ComputeNx(ElemEnd-ElemStart+1)

```

```

C The following DO-loop iterates on h until dAdep=dAdis -----

```

```

      dh=100*Tolerance
      Iterating=.TRUE.
      DO WHILE (Iterating)

```

```

C Moved;1
D      CALL WriteMoved

```

```

C Move the points.

```

```

      CALL Move(h)

```

```

C Moved;2
D      CALL WriteMoved

```

```

C Store coordinates not being moved in Ins

```

```

      CALL MakeIns(ElemStart,ElemEnd,NodeMap,Coords,NoOfElems,
& Filename)

```

```

C Search for intersections, and recompute moved boundary w/o intersections

```

```

      CALL RemoveLocIntersects

```

```

C Moved;3
D      CALL WriteMoved

```

```

c      CALL RemoveBdryIntersects
cC Moved;4
cD      CALL WriteMoved

```

```

      CALL RemoveInsIntersects
C Moved;5
D      CALL WriteMoved

```

C Compute next change in h.

```

      IntCurr = IntegrateBnddX(.TRUE.)
      dAdep = ABS(IntOrig-IntCurr)
      dh = (h/dAdep)*(dAdis-dAdep)
      WRITE(*,100) h,dh,dAdep,dAdis
100    FORMAT(X,'h=',G14.7,' dh=',G14.7,' dAdep=',G14.7,
& ' dAdis=',G14.7)
      h = h+dh
      Iterating=(dh/h.GT.Tolerance)

```

```

      END DO
      IntOrig=IntCurr

```

```

      CALL WriteMBF(MacBdryFile)

```

```

      FirstX=Moved(1,1)
      FirstY=Moved(1,2)
      LastX=Moved(NoOfMoved,1)
      LastY=Moved(NoOfMoved,2)

```

```

      CALL ReMakeMesh(FileName(1:FilLen),FirstX,FirstY,
& LastX,LastY,.FALSE.)

```

```

      CALL WriteBND(1,FILENAME(1:FilLen)//'.BND',
& ElemStart,ElemEnd,NodeMap,Coords,Time*tstar)

```

```

C -----
C The following IF-THEN block resets time constants for the
C next anodic dissolution step.

```

```

      IF (PCRCounter.LT.NoOfPCR) THEN
        WRITE(*,*) 'Reversing Current! '
        EndTime=Time+BigdTime
        LastTime=.FALSE.
        MaxTimeCounter=TimeCounter+BigdMaxTC
        CALL MakeMoved(ElemStart,ElemEnd,NodeMap,Coords)
      END IF

```

```

      END DO
      CALL WriteMesh(FileName(1:FilLen)//'.MSH')

```

```

      RETURN
      END

```

```

C ***** ReMakeMesh

```

```

      SUBROUTINE ReMakeMesh(FileName,X1,Y1,X2,Y2,Smooth)

```

C X1,Y1, and X2,Y2 are the starting and ending points for the moved element

C of the macro mesh.

```

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMac.INC'
INCLUDE 'ECBPar.INC'

CHARACTER*(*) FileName
REAL*8 X1,Y1,X2,Y2
LOGICAL SaveKinetic/.TRUE./,Smooth

```

C Alter macro info

```

IF (CorLev) CALL ReadMac(FileName//'.MAC')

MacVertX(1)=X1
MacVertY(1)=Y1

MacVertX(2)=X2
MacVertY(2)=Y2

MacShape(1)='USR'
CALL MakeNodeMap
CALL MakeMeshPts(SaveKinetic,Smooth)

RETURN
END

```

C ***** ReadInsExt

```

SUBROUTINE ReadInsExt(BegPtX,BegPtY,EndPtX,EndPtY,InsExt,FileName)

LOGICAL InsExt
REAL*8 BegPtX,BegPtY,EndPtX,EndPtY
CHARACTER*(*) FileName
INTEGER FilLen

CALL StringLength(FileName,FilLen)
INQUIRE(FILE=FileName(1:FilLen)//'.EXT',EXIST=InsExt)
IF (InsExt) THEN

  OPEN(UNIT=1,FILE=FileName(1:FilLen)//'.EXT',
& STATUS='OLD',FORM='FORMATTED')
  READ(1,*) BegPtX,BegPtY
  READ(1,*) EndPtX,EndPtY
  CLOSE(1)

  WRITE(*,10)
  WRITE(*,20) FileName(1:FilLen)//'.EXT'
  WRITE(*,30) BegPtX,BegPtY
  WRITE(*,40) EndPtX,EndPtY
  WRITE(*,50)

END IF
RETURN

```

C The following comments document the extended insulator report.

C 123456789a123456789b123456789c13456789d123456789e123456789

```

C -----Insulator Extension
C 123456789a123
C      >> Insulator extended beyond solution domain <<
C 123456789a123456789b1234      123456789a
C      Start: ( d.ddde+dd, d.ddde+dd)
C      Finish: ( d.ddde+dd, d.ddde+dd)
C 123456789a123456789b123456789c123456789d123456789e123456789f123456789g12345678
C -----

```

```

10  FORMAT(X,59('*'),' Insulator Extension')
20  FORMAT(X,13X,'>> Insulator Extended Beyond Solution Domain: ',
    & A,' <<')
30  FORMAT(X,24X,'Start: (',G10.3,',',G10.3,')')
40  FORMAT(X,23X,'Finish: (',G10.3,',',G10.3,')')
50  FORMAT(X,78('*'))

```

END

```

C ***** SaveECBbc

```

SUBROUTINE SaveECBbc

```

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMsh.INC'
INCLUDE 'ECBbc.INC'
INCLUDE 'ECBbc2.INC'

```

INTEGER I

```

DO I=1,NoOfCoords
  BCValues2(I)=BCValues(I)
  SolValues2(I)=SolValues(I)
  Natural2(I)=Natural(I)
END DO

```

RETURN
END

```

C ***** SlopeVal

```

```

REAL*8 FUNCTION SlopeVal(Nat,BCV,SolV)
LOGICAL Nat
REAL*8 BCV,SolV

```

```

IF (Nat) THEN
  SlopeVal=BCV
ELSE
  SlopeVal=SolV
END IF

```

RETURN
END

```

C ***** TimeLoop

```

SUBROUTINE TimeLoop(FileName)

C The subroutine performs the Time Iteration Loop

```

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMsh.INC'
INCLUDE 'ECBCal.INC'
INCLUDE 'ECBBC.INC'
INCLUDE 'ECBsrc.INC'
INCLUDE 'ECBPar.INC'
INCLUDE 'ECGaus.INC'
INCLUDE 'ECGLOG.INC'
INCLUDE 'ECBMac.INC'
INCLUDE 'ECBMOVE.INC'
INCLUDE 'ECBTIME.INC'

```

```
CHARACTER*(*) FileName
```

```

INTEGER ElemStart,ElemEnd,Elem,Loc,I,FilLen
LOGICAL BdryFileExist
REAL*8 FirstX,FirstY,LastX,LastY
REAL*8 MaxXdN,MinXdN

```

```
CALL StringLength(FileName,FilLen)
```

```
DO WHILE(.NOT.LastTime)
```

```
  IF (CorLev) THEN
```

```
  C ----- Compute the concentration distribution
```

```
  C Set up for DifEq A
```

```
  D      WRITE(*,*) 'Solving Differential Equation A--Concentration'
        CALL Bem
```

```
  C Save what we need from Dif Eq A for Dif Eq B
```

```
        CALL SaveECBbc
      END IF
```

```
  C ----- Compute the current distribution
```

```
  C Set up for Dif Eq B
```

```
  C Read the macro file for part B of the problem (the part that computes the
  C current distribution)
```

```
    IF (CorLev) THEN
```

```
      CALL ReadMac(FileName(1:FilLen)//'B.MAC')
```

```
  C Read the mesh file for part B.
```

```
    CALL ReadMesh(FileName(1:FilLen)//'B.MSH')
  D      WRITE(*,*) 'Solving Differential Equation B--Potential'
```

```
    ELSE
```

```
  D      WRITE(*,*) 'Solving Differential Equation----Potential'
```

```
    END IF
```

```
  C Solve current distribution problem
```

CALL Bem

C ----- Boundary Movement

C Moving boundary is always the first macro element.

C (Note: NoOfMicElems(1) is the number of microelements on the moving part
C of the boundary. The program assumes that parts A & B have the same moving
C part of the boundary, with identical discretization.)

```
ElemStart=1
ElemEnd=NoOfMicElems(1)
```

C Store coordinates in mesh into temporary storage (Moved), then compute
C the normal to every point on the surface (Nx), and current density at those
C points (dXdN)

C -----
C The following CALL stores the moving boundary into a temporary location,
C array Moved.

```
CALL MakeMoved(ElemStart,ElemEnd,NodeMap,Coords)
C Moved;1
D CALL WriteMoved
```

C -----
C The following CALL computes the 'current density' at each point of the moving
C boundary; the result is stored in matrix dXdN.

```
CALL MakedXdN(ElemStart,ElemEnd)
```

C The maximum motion of the boundary determines the maximum allowable time
C step. For the time step, we choose the minimum of desired time step, and
C the largest time step allowed by the maximum current density on the boundary.

```
CALL VecExtremaDP(dXdN,NoOfMoved,MaxdXdN,MindXdN)
MaxdXdN=MAX(ABS(MaxdXdN),ABS(MindXdN))
```

```
MotdTime=DesdX/MaxdXdN
dTime=MIN(DesdTime,MotdTime)
```

```
IF (dTime.LE.0) THEN
  WRITE(*,*) 'Error: dTime < 0.0!'
  STOP 'In Program :ECBM'
END IF
```

C -----
C The following IF-THEN-ELSE block determines if this is the last time we
C run the Time-Iteration Loop

```
IF (Time+dTime.GT.EndTime) THEN
  dTime=EndTime-Time
  LastTime=.TRUE.
ELSE
  LastTime=.FALSE.
END IF
```

```
IF (TimeCounter.GT.MaxTimeCounter) LastTime=.TRUE.
```

C -----
 C The following CALL computes the 'normal' at each point of the moving
 C boundary; the result is stored in matrix Nx.

CALL ComputeNx(ElemEnd-ElemStart+1)

C -----
 C Move the points.

CALL Move(dTime)

C Moved;2

D CALL WriteMoved

C -----
 C Store coordinates not being moved in Ins

CALL MakeIns(ElemStart,ElemEnd,NodeMap,Coords,NoOfElems,
 & Filename)

C -----
 C Search for intersections, and recompute moved boundary w/o intersections

CALL RemoveLocIntersects

C Moved;3

D CALL WriteMoved

c CALL RemoveBdryIntersects

cC Moved;4

cD CALL WriteMoved

CALL RemoveInsIntersects

C Moved;5

D CALL WriteMoved

C -----
 C Save moved nodes for generating new mesh

```
INQUIRE(FILE=MacBdryFile,EXIST=BdryFileExist)
IF (BdryFileExist) THEN
  OPEN(UNIT=1,FILE=MacBdryFile,STATUS='OLD',FORM='FORMATTED')
ELSE
  OPEN(UNIT=1,FILE=MacBdryFile,STATUS='NEW',FORM='FORMATTED')
  WRITE(*,*) 'Warning: Moving boundary must have shape type USER'
  STOP 'ECBM: Abnormal End'
END IF
```

```
WRITE(1,*) NoOfMoved
DO I=1,NoOfMoved
  WRITE(1,*) Moved(I,1),Moved(I,2)
END DO
CLOSE(1)
```

```
FirstX=Moved(1,1)
FirstY=Moved(1,2)
LastX=Moved(NoOfMoved,1)
LastY=Moved(NoOfMoved,2)
```

C -----
 C Next, use the current distribution to compute the boundary movement

```

    Time=Time+dTime
    TimeCounter=Timecounter+1

    IF (.NOT.PerRev) THEN
      WRITE(*,20) TimeCounter,Time*tstar
20    FORMAT(X,'Boundary ;',I4,' corresponds to time=',G14.7,' secs')
    END IF

    WRITE(3,*) Time*tstar,Moved(NoOfMoved,2)-Moved(1,2)

```

C -----
 C The following calls recompute the mesh based on the new boundary

```

    IF (CorLev) THEN
      CALL ReMakeMesh(FileName(1:FilLen)//'B',FirstX,FirstY,
& LastX,LastY,TRUE.)
      CALL WriteMesh(FileName(1:FilLen)//'B.MSH')

      CALL ReMakeMesh(FileName(1:FilLen)//'A',FirstX,FirstY,
& LastX,LastY,TRUE.)
      CALL WriteMesh(FileName(1:FilLen)//'A.MSH')
    ELSE
      CALL ReMakeMesh(FileName(1:FilLen),FirstX,FirstY,
& LastX,LastY,TRUE.)
      CALL WriteMesh(FileName(1:FilLen)//'.MSH')
    END IF

    IF (.NOT.PerRev) THEN
      CALL WriteBND(1,FILENAME(1:FilLen)//'.BND',
& ElemStart,ElemEnd,NodeMap,Coords,Time*tstar)
    END IF

    END DO

    IF (PerRev) THEN
      CALL WriteBND(1,FILENAME(1:FilLen)//'.BND',
& ElemStart,ElemEnd,NodeMap,Coords,Time*tstar)
      WRITE(*,*) FILENAME(1:FilLen)//'.BND', ' written for ',Time*tstar
    END IF

    RETURN
  END

```

C ***** WriteArray

```

SUBROUTINE WriteArray(NoOfElem,Array)

REAL*8 Array(*)
INTEGER NoOfElem,I

OPEN(UNIT=1,FILE='ARRAY.DAT',STATUS='NEW',FORM='FORMATTED')
WRITE(1,*) NoOfElem

DO I=1,NoOfElem
  WRITE(1,*) I,Array(I)

```



```

END DO
CLOSE(1)
RETURN
END

```

C ***** WriteBND

```

SUBROUTINE WriteBND(LunO,Name,ElemStart,ElemEnd,NodeMap,Coords,
& Time)

```

```

INCLUDE 'ECBHdr.INC'
REAL*8 Coords(MaxNoOfCoords,MaxNoOfDim),Time
INTEGER NoOfOrig,LunO,I,K,NodeMap(MaxNoOfCoords,MaxBasisDeg+1)
INTEGER Elem,Loc,ElemStart,ElemEnd
CHARACTER*(*) Name

IF (.NOT.((LunO.EQ.6).OR.(LunO.EQ.5))) THEN
  OPEN(UNIT=LunO,FILE=Name,FORM='FORMATTED',STATUS='NEW')
END IF

WRITE(LunO,*) (ElemEnd-ElemStart+1)*BasisDeg+1
DO Elem=ElemStart,ElemEnd
  DO Loc=1,BasisDeg
    WRITE(LunO,*) (Coords(NodeMap(Elem,Loc),K),K=1,NoOfDim)
  END DO
END DO
WRITE(LunO,*) (Coords(NodeMap(ElemEnd,BasisDeg+1),K),K=1,NoOfDim)
WRITE(LunO,*) Time
IF (.NOT.((LunO.EQ.6).OR.(LunO.EQ.5))) THEN
  CLOSE(LunO)
END IF

RETURN
END

```

C ***** WriteMBF

```

SUBROUTINE WriteMBF(MacBdryFile)

```

```

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMove.INC'

CHARACTER*(*) MacBdryFile
INTEGER I
LOGICAL BdryFileExist

```

C Save moved nodes for generating new mesh

```

INQUIRE(FILE=MacBdryFile,EXIST=BdryFileExist)
IF (BdryFileExist) THEN
  OPEN(UNIT=1,FILE=MacBdryFile,STATUS='OLD',FORM='FORMATTED')
ELSE
  OPEN(UNIT=1,FILE=MacBdryFile,STATUS='NEW',FORM='FORMATTED')
  WRITE(*,*) 'Warning: Moving boundary must have shape type USER'
  STOP 'ECBM: (Subroutine WriteMBF) Abnormal End'
END IF

```

```
WRITE(1,*) NoOfMoved
DO I=1,NoOfMoved
  WRITE(1,*) Moved(I,1),Moved(I,2)
END DO
CLOSE(1)
```

```
RETURN
END
```

C ***** WriteMoved

```
SUBROUTINE WriteMoved
```

```
INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMOVE.INC'
```

```
INTEGER I
```

```
OPEN(UNIT=1,FILE='MOVED.DAT',STATUS='NEW',FORM='FORMATTED')
```

```
WRITE(1,*) NoOfMoved
DO I=1,NoOfMoved
  WRITE(1,*) Moved(I,1),Moved(I,2)
END DO
```

```
CLOSE(1)
RETURN
END
```

c *

PROGRAM ECBINT

C This program will be used to compute potential at internal points,
 C after a current distribution problem has been solved.

```

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMsh.INC'
INCLUDE 'ECBCal.INC'
INCLUDE 'ECBBC.INC'
INCLUDE 'ECBSrc.INC'
INCLUDE 'ECBPar.INC'
INCLUDE 'ECGaus.INC'
INCLUDE 'ECGLOG.INC'

```

```

INTEGER Length
CHARACTER*80 File/'ECB'/

```

```

CALL Titles
CALL EditCh('Filename? (No extension)',File)
CALL StringLength(File,Length)

```

```

CALL ReadPar(FILE(1:Length)//'.PAR')
CALL ReadMesh(FILE(1:Length)//'.Msh')

```

```

CALL GauLeg(NoOfGaussPts,GaussPts,GaussWts)
NoOfGauLogPts=NoOfGaussPts
CALL GauLog(NoOfGauLogPts,GauLogPts,GauLogWts)

```

```

CALL ReadInt(File(1:Length)//'.INT')
CALL ComputeInt
CALL WriteInt(File(1:Length)//'.INT')

```

```

STOP 'ECB: Normal Completion'
END

```

C ***** Titles

SUBROUTINE Titles

```

WRITE(*,*) ' PROGRAM: ECBINT           10/20/89'
WRITE(*,*) 'Written by: Ken Jordan       Version 1'
WRITE(*,*) ' '
WRITE(*,*) 'This program reads input from the data files'
WRITE(*,*) '* .PAR, * .MSH, and * .INT; generates output files'
WRITE(*,*) '* .INT'
WRITE(*,*) ' '
WRITE(*,*) 'This program solves for the potential at the internal'
WRITE(*,*) 'points specified in the * .INT input files.'
WRITE(*,*) ' '

```

```

RETURN
END

```

```
PROGRAM ECBPlot
```

```
INCLUDE 'ECBHDR.INC'
INCLUDE 'ECBMsh.INC'
INCLUDE 'ECBSrc.INC'
INCLUDE 'ECBMac.INC'
INCLUDE 'ECBBC.INC'
INCLUDE 'ECBEIm.INC'
INCLUDE 'ECBINT.INC'
INCLUDE '[KJ.DATA]PLOTABL.INC'
INCLUDE 'ECBPARG.INC'
```

```
CHARACTER*80 FileName
CHARACTER*1 SubProb
INTEGER Start,End,FLen
LOGICAL IntFile
```

```
CALL GetFileName(FileName,FLen)
```

C Read and process the data for later use.

```
CALL ReadPar(FileName(1:FLen)//'.PAR')
IF (CorLev) THEN
  DO WHILE ((SubProb.NE.'A').AND.(SubProb.NE.'B'))
    CALL ChInp('Sub Problem A or B? (A or B)?',SubProb)
  END DO
  FileName(FLen+1:)=SubProb
  FLen=FLen+1
END IF
```

```
CALL ReadMac(FileName(1:FLen)//'.MAC')
CALL ReadMesh(FileName(1:FLen)//'.MSH')
CALL ReadSrc(FileName(1:FLen)//'.SRC')
```

```
INQUIRE(FILE=FileName(1:FLen)//'.INT',EXIST=Intfile)
IF (Intfile) THEN
  CALL ReadInt(FileName(1:FLen)//'.INT')
END IF
```

C Put Source Points into a plottable file

```
CALL PlotSrc
```

C Put Node Points into a plottable file

```
CALL PlotNod
```

C Read, Process & Plot internal points

```
IF (IntFile) CALL ProcessInt
```

C Process set and solved for values.

```
CALL MeshReport
```

```
CALL StartEnd(Start,End)
```

```
IF (Start.GT.0) CALL ProcessSolSet(Start,End)
```

C Tell user where plotted data is.

```
WRITE(*,*) ' '
WRITE(*,*) ' ECBPLOT.NOD   Node Points (x,y)'
WRITE(*,*) ' ECBPLOT.SRC   Source Points (x,y)'
WRITE(*,*) ' '

```

```
STOP 'ECBPlot: Normal End'
END

```

C ***** GetFileName

```
SUBROUTINE GetFileName(FileName,FLen)

```

C Get filename.

```
CHARACTER(*) FileName
LOGICAL FileExist
INTEGER FLen

FileExist=.FALSE.
DO WHILE(.NOT.FileExist)
  CALL EditCh('Enter Problem Name?',FileName)
  CALL StringLength(FileName,FLen)
  IF (FLen.LE.0) STOP 'ECBPlot (GetFileName): No name Entered'
  INQUIRE(FILE=FileName(1:FLen)//'.PAR',EXIST=FileExist)
  IF (.NOT.FileExist) THEN
    WRITE(*,*) 'Error: File '//FileName(1:FLen)//'.PAR '
    WRITE(*,*) '      doesn''t exist.'
  END IF
END DO

RETURN
END

```

C ***** MeshReport

```
SUBROUTINE MeshReport

INCLUDE 'ECBHDR.INC'
INCLUDE 'ECBMsh.INC'
INCLUDE 'ECBMac.INC'

WRITE(*,*) ' '
WRITE(*,*) ' Preparing to Plot BC and Solution Values'
WRITE(*,*) ' '

WRITE(*,*) 'Minimum Element Number=',1
WRITE(*,*) 'Maximum Element Number=',NoOfElems

RETURN
END

```

C ***** PlotInt

```
SUBROUTINE PlotInt(Pot,Con)

INCLUDE 'ECBHDR.INC'

```

```

INCLUDE 'ECBINT.INC'

INTEGER J,K,Loc,NoOfPts,I,Con
LOGICAL Between
REAL PtsX(MaxNoOfCoords),PtsY(MaxNoOfCoords)
REAL*8 XPt,YPt,Pot
CHARACTER*3 Ext(10)/'CN1','CN2','CN3','CN4','CN5','CN6','CN7',
&'CN8','CN9','CNA'/

WRITE(*,*) 'Plotting Internal Points ',Pot

NoOfPts=0
DO J=1,NoOfSpines
  DO K=1,IntPerSpine-1
    Loc=(J-1)*IntPerSpine+K

    Between= (( (InternalPot(Loc).LE.Pot) .AND.
& (Pot.LE.InternalPot(Loc+1)) ) .OR.
& ( (InternalPot(Loc).GE.Pot) .AND.
& (Pot.GE.InternalPot(Loc+1)) ))
    IF (Between) THEN
      NoOfPts=NoOfPts+1
      CALL Interp1d(InternalPot(Loc),InternalPts(Loc,1),
& InternalPot(Loc+1),InternalPts(Loc+1,1),
& Pot,XPt)
      PtsX(NoOfPts)=XPt

      CALL Interp1d(InternalPot(Loc),InternalPts(Loc,2),
& InternalPot(Loc+1),InternalPts(Loc+1,2),
& Pot,YPt)
      PtsY(NoOfPts)=YPt
      WRITE(*,10) XPt,YPt
10      FORMAT(X,10X,G12.4,2X,G12.4)
    END IF
  END DO
END DO

IF (NoOfPts.GT.0) THEN
  OPEN(UNIT=1,FILE='ECBPLOT.'//EXT(Con),
& STATUS='NEW',FORM='FORMATTED')
  WRITE(1,*) NoOfPts, Pot,',','Potential'
  DO I=1,NoOfPts
    WRITE(1,*) PtsX(I),PtsY(I)
  END DO
  CLOSE(1)
END IF

RETURN
END

C ***** PlotNod

SUBROUTINE PlotNod

INTEGER I
INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMsh.INC'

```

```

OPEN(UNIT=1,FILE='ECBPLOT.NOD',STATUS='NEW',FORM='FORMATTED')
WRITE(1,*) NoOfCoords
DO I=1,NoOfCoords
  WRITE(1,*) Coords(I,1),Coords(I,2)
END DO
CLOSE(1)

RETURN
END

```

C ***** PlotSolSet

```

SUBROUTINE PlotSolSet(NoOfSC,TotDist,Dist,BCPtsY,SolPtsY)

INTEGER NoOfSC,J
INCLUDE 'ECBHdr.INC'
REAL Dist(MaxNoOfCoords),BCPtsY(MaxNoOfCoords),
& SolPtsY(MaxNoOfCoords)
REAL*8 TotDist

OPEN (UNIT=1,FILE='ECBPLOT.SOL',STATUS='NEW',FORM='FORMATTED')
OPEN (UNIT=2,FILE='ECBPLOT.SET',STATUS='NEW',FORM='FORMATTED')

WRITE(1,*) NoOfSC
WRITE(2,*) NoOfSC

DO J=1,NoOfSC
  WRITE(1,*) Dist(J)/TotDist,SolPtsY(J)
  WRITE(2,*) Dist(J)/TotDist,BCPtsY(J)
END DO

CLOSE(1)
CLOSE(2)

RETURN
END

```

C ***** PlotSrc

```

SUBROUTINE PlotSrc

INTEGER I
INCLUDE 'ECBHDR.INC'
INCLUDE 'ECBSRC.INC'

```

C Put Source Points into a plottable file

```

OPEN(UNIT=1,FILE='ECBPLOT.SRC',STATUS='NEW',FORM='FORMATTED')
WRITE(1,*) NoOfSrc
DO I=1,NoOfSrc
  WRITE(1,*) Src(I,1),Src(I,2)
END DO
CLOSE(1)

RETURN
END

```

C ***** ProcessData

```

SUBROUTINE ProcessData(I,Elem,Loc,IntegrandX,Integrand,TotDist,Dist,
& BCPtsY,SolPtsY)

```

```

INCLUDE 'ECBHDR.INC'
INCLUDE 'ECBMsh.INC'
INCLUDE 'ECBEIm.INC'
INCLUDE 'ECBPar.INC'
INCLUDE 'ECBBC.INC'

```

```

INTEGER I,Elem,Loc
REAL Dist(MaxNoOfCoords),BCPtsY(MaxNoOfCoords),
& SolPtsY(MaxNoOfCoords)
REAL*8 TotDist
REAL*8 Integrand(MaxNoOfCoords),IntegrandX(MaxNoOfCoords)

```

```

IntegrandX(I)=TotDist
IF (ElemNat(Elem)) THEN
  Integrand(I)=BCValues(NodeMap(Elem,Loc))
ELSE
  Integrand(I)=SolValues(NodeMap(Elem,Loc))
END IF
IF (Axisymmetric) Integrand(I)=Integrand(I)*ElemR(1,Loc)

```

```

SolPtsY(I)=SolValues(NodeMap(Elem,Loc))

```

```

Dist(I)=TotDist
BCPtsY(I)=BCValues(NodeMap(Elem,Loc))

```

```

RETURN
END

```

```

C ***** ProcessInt

```

```

SUBROUTINE ProcessInt

```

```

INTEGER NoOfPot,I
INCLUDE 'ECBHDR.INC'
INCLUDE 'ECBINT.INC'

```

```

REAL*8 Pot,PotMax,PotMin

```

```

C Read, Process & Plot internal points

```

```

CALL MatExtremaDP(InternalPot,NoOfInternal,PotMax,PotMin)

```

```

OPEN(UNIT=3,FILE='POT.INT',STATUS='OLD',FORM='FORMATTED')
READ(3,*) NoOfPot
DO I=1,NoOfPot
  READ(3,*) Pot
  CALL PlotInt(Pot,I)
END DO
CLOSE(3)

```

```

RETURN
END

```

```

C ***** ProcessSolSet

```



```

SUBROUTINE ProcessSolSet(Start,End)

  INCLUDE 'ECBHdr.INC'
  INCLUDE 'ECBEIm.INC'

  INTEGER I,Start,End,Elem,Loc
  REAL Dist(MaxNoOfCoords),BCPtsY(MaxNoOfCoords),
& SolPtsY(MaxNoOfCoords)
  REAL*8 TotDist,Seg
  REAL*8 Integrand(MaxNoOfCoords),IntegrandX(MaxNoOfCoords)
  REAL*8 Break(MaxNoOfCoords),CSCoef(4,MaxNoOfCoords)

  REAL*8 DCSITG
  EXTERNAL DCSITG

  TotDist=0.0

  I=1
  DO Elem=Start,End

    CALL GetElemR(Elem)

    DO Loc=1,BasisDeg

      Seg=SQRT((ElemR(1,Loc+1)-ElemR(1,Loc))**2+
& (ElemR(2,Loc+1)-ElemR(2,Loc))**2)

      CALL ProcessData(I,Elem,Loc,IntegrandX,Integrand,TotDist,Dist,
& BCPtsY,SolPtsY)

      TotDist=TotDist+Seg
      I=I+1

    END DO

  END DO

  CALL ProcessData(I,End,BasisDeg+1,IntegrandX,Integrand,
& TotDist,Dist,BCPtsY,SolPtsY)

C Store Data in Plot Files

  CALL PlotSolSet(I,TotDist,Dist,BCPtsY,SolPtsY)

C Carry out integration

  CALL DCSAKM(I,integrandx,Integrand,Break,CSCoef)
  WRITE(*,*) '1/Integral=',1/DCSITG(0.0,TotDist,I-1,Break,CSCoef)

  WRITE(*,*) ''
  WRITE(*,*) ' ECBPLOT.SOL ',
& 'Solution Values, Relative TotDistance'
  WRITE(*,*) ' ECBPLOT.SET ',
& 'Proscribed Values, Relative TotDistance'
  WRITE(*,*) ''

  RETURN
  END

```

C ***** StartEnd

SUBROUTINE StartEnd(Start,End)

INCLUDE 'ECBHDR.INC'

INCLUDE 'ECBMsh.INC'

INTEGER Start,End,T

C Get the Start and End Element

CALL EditI('Starting Elem Number? (<=0 to quit)',Start)

IF (Start.GT.0) THEN

CALL EditI('Ending Elem Number?',End)

IF (Start.GT.End) THEN

T=Start

Start=End

End=T

END IF

Start=MAX(1,Start)

Start=MIN(NoOfElems,Start)

End=MIN(End,NoOfElems)

End=MAX(End,1)

ELSE

End=0

END IF

RETURN

END

c *

C File: ECBSUBS.FOR

C Boundary Movement subroutines.

```

C      REAL*8 FUNCTION CrossProduct2D(Ax,Ay,Bx,By)
C      REAL*8 FUNCTION DotProduct(Ax,Ay,Az,Bx,By,Bz)
C      REAL*8 FUNCTION GeomSeries(Ratio,NoOfTerms)
C      LOGICAL FUNCTION MacNat(BCType)

c      SUBROUTINE AddOne(NoOfM,M,X,Y)
c      SUBROUTINE ChkIsoPara(Mac)
c      SUBROUTINE ChkIsoParaErr(Dim,Mic,MajorError)
c      SUBROUTINE ComputeBdry(Moved,NoOfMoved,
cglobal SUBROUTINE ComputeNx(Moved,NoOfElems,Nx)
c      SUBROUTINE ComputePrevElem(Elem,PrevElems)
c      SUBROUTINE ComputeRelativeSpacing(...)
cglobal SUBROUTINE CopyPoint(Coord,Orig,NoOfMoved,Moved)
c      SUBROUTINE CopyPoint2(Coord,Orig,NoOfMoved,Moved)
c      SUBROUTINE LocateIntersects(Sign,NoOfMoved,Moved,
c      SUBROUTINE MakeCoord(X,Y,MicNod,MacElm,SaveKinetic)
c      SUBROUTINE MakeElemBC
c      SUBROUTINE MakeMacElem(Mac,SaveKinetic,Smooth)
c      SUBROUTINE MakeMeshPts(SaveKinetic,Smooth)
cglobal SUBROUTINE MakeMoved(ElemStart,ElemEnd,NodeMap,Orig,
cglobal SUBROUTINE MakeNodeMap
cglobal SUBROUTINE Move(NoOfMoved,Moved,dXdN,Nx,dt)
c      SUBROUTINE ObtAngAtBdryBeg(Ins,NoOfIns,...
c      SUBROUTINE ObtAngAtBdryEnd(Ins,NoOfIns,...
c      SUBROUTINE ObtAngErr
cglobal SUBROUTINE ReadMac(FileName)
cglobal SUBROUTINE RemoveBdryIntersects(NoOfMoved,Moved)
c      SUBROUTINE RemoveBdryAfter(NoOfMoved,Moved,I,XInt,YInt)
c      SUBROUTINE RemoveBdryBefore(NoOfMoved,Moved,I,XInt,YInt)
cglobal SUBROUTINE RemoveInsIntersects(Orig,Ins,NoOfIns,
cglobal SUBROUTINE RemoveLocIntersects(NoOfMoved,Moved)

c      SUBROUTINE ShpCir(MacElm,SaveKinetic)
c      SUBROUTINE ShpFlat(MacElm,SaveKinetic)
c      SUBROUTINE ShpFlatHiPt(MacElm,MaxY)
c      SUBROUTINE ShpLine(MacElm,SaveKinetic)
c      SUBROUTINE ShpPrev(MacElm,SaveKinetic)
c      SUBROUTINE ShpSine(MacElm,SaveKinetic)
c      SUBROUTINE ShpTRNS(MacElm,SaveKinetic)
c      SUBROUTINE ShpUser(MacElm,SaveKinetic,Smooth)

c      SUBROUTINE WriteMac(FileName)
c      SUBROUTINE XY2T(X,Y,T)

```

C Read/Write subroutines

```

c      SUBROUTINE ErrorFilename(Filename,RoutineName)
c      SUBROUTINE ErrorVersion(Version,FileName,RoutineName)
c      SUBROUTINE ReadCal(FileName)
c      SUBROUTINE ReadMesh(FileName)
c      SUBROUTINE ReadPar(FileName)
c      SUBROUTINE ReadSrc(FileName)
c      SUBROUTINE WriteCal(FileName)
c      SUBROUTINE WriteMesh(FileName)

```

c SUBROUTINE WriteSrc(FileName)

C Boundary Element Routines.

c SUBROUTINE AssembleAC
 c SUBROUTINE AssembleGH
 c SUBROUTINE Integrate(Nodes)

C Kinetic Boundary Condition routines for BEM method.

c SUBROUTINE NewtonRaphson(NoOfdBCValues,dBCValues,MagDiff)
 c SUBROUTINE UpdateBCValues(dBCValues)
 c SUBROUTINE ECBKinetics(KinTyp,Slope,Pot,Coord)
 c SUBROUTINE Kinetics(Slope,Pot,Elem,X,Y)

C Miscellaneous I/O routines for BEM.

c SUBROUTINE GetElemR(Elem)
 c SUBROUTINE GetSrcPoint(Source)
 c SUBROUTINE TestForSingularity(Singularity)
 c SUBROUTINE PrintMesh(Lun)
 c SUBROUTINE PrintPar
 c SUBROUTINE PrintSrc(Lun)

C ***** AcuteAngles

SUBROUTINE AcuteAngles

C The following subroutine determine if the angles between the moving
 C boundary and the insulator on either side are acute.

INCLUDE 'ECBHdr.INC'
 INCLUDE 'ECBMOVE.INC'

REAL*8 NCross

C External Functions

REAL*8 CrossProduct2D
 EXTERNAL CrossProduct2D

D WRITE(*,10) 'Moved',Moved(1,1),Moved(1,2),1
 D WRITE(*,10) 'Ins First',Ins(First,1),Ins(First,2),First
 D WRITE(*,10) 'Ins Second',Ins(Second,1),Ins(Second,2),Second
 D WRITE(*,*) ' '
 D WRITE(*,10) 'Ins NxtLst',Ins(NextToLast,1),Ins(NextToLast,2),
 D & NextToLast
 D WRITE(*,10) 'Ins Last',Ins(Last,1),Ins(Last,2),Last
 D WRITE(*,10) 'Moved',Moved(NoOfMoved,1),Moved(NoOfMoved,2),
 D & NoOfMoved
 10 FORMAT(X,A15,G10.3,2X,G10.3,.:2X,I4)

C The following lines check the beginning of the moving boundary

NCross=CrossProduct2D(Moved(1,1)-Ins(First,1),
 & Moved(1,2)-Ins(First,2),
 & Ins(Second,1)-Ins(First,1),
 & Ins(Second,2)-Ins(First,2))

```

D      IF (StaRev) THEN
D          WRITE(*,*) 'Bdry Start Moving Backwards'
D      ELSE
D          WRITE(*,*) 'Bdry Start Moving Forwards'
D      END IF

D      WRITE(*,*) 'Cross Product=',NCross
        AcuteAngleBefore=((NCross.GT.0.0).AND.(StaRev)).OR.
        & ((NCross.LT.0.0).AND.(NOT.StaRev)))

```

```

        NoAngleBefore=(NCross.EQ.0.0)

```

```

D      IF (AcuteAngleBefore) THEN
D          WRITE(*,*) 'At Moving Bdry Start: Acute Angle'
D      ELSE
D          WRITE(*,*) 'At Moving Bdry Start: Obtuse Angle'
D      END IF

```

C The following lines determine if the angle between the end of the boundary
C and the insulator is acute.

```

D      WRITE(*,*) ' '
        NCross=CrossProduct2D(Moved(NoOfMoved,1)-Ins(Last,1),
        & Moved(NoOfMoved,2)-Ins(Last,2),
        & Ins(NextToLast,1)-Ins(Last,1),
        & Ins(NextToLast,2)-Ins(Last,2))

```

```

D      IF (EndRev) THEN
D          WRITE(*,*) 'Bdry End Moving Backwards'
D      ELSE
D          WRITE(*,*) 'Bdry End Moving Forwards'
D      END IF

```

```

D      WRITE(*,*) 'Cross Product=',NCross
        AcuteAngleAfter=((NCross.GT.0.0).AND.(NOT.EndRev)).OR.
        & ((NCross.LT.0.0).AND.(EndRev)))
        NoAngleAfter=(NCross.EQ.0.0)

```

```

D      IF (AcuteAngleAfter) THEN
D          WRITE(*,*) ' At Moving Bdry End: Acute Angle'
D      ELSE
D          WRITE(*,*) ' At Moving Bdry End: Obtuse Angle'
D      END IF

```

```

        RETURN
        END

```

C ***** AddOne

```

        SUBROUTINE AddOne(NoOfM,M,X,Y)

```

C This subroutine adds the coordinates x,y to the list of coordinates
C stored in M.

```

        INTEGER NoOfM
        REAL*8 X,Y
        INCLUDE 'ECBHdr.INC'

```

```
REAL*8 M(MaxNoOfCoords,MaxNoOfDim)
```

```
NoOfM=NoOfM+1
M(NoOfM,1)=X
M(NoOfM,2)=Y
```

```
RETURN
END
```

```
C ***** AssembleAC
```

```
SUBROUTINE AssembleAC
```

```
INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMsh.INC'
INCLUDE 'ECBCal.INC'
INCLUDE 'ECBBC.INC'
```

```
INTEGER Row,Col,Elem,LastCol
REAL*8 Temp
```

C Re-arrange matrices G and H so that G will multiply the vector of unknowns.
 C Before this subroutine is executed, G multiplies
 C the natural conditions, so we must exchange the Column with its counterpart
 C in H. After this routine is executed, G multiplies the unknowns; H, the
 C knows.

```
DO Col=1,NoOfCoords
  IF (Natural(Col)) THEN
    DO Row=1,NoOfCoords
      Temp = BemH(Row,Col)
      BemH(Row,Col)= -BemG(Row,Col)
      BemG(Row,Col)= -Temp
    END DO
  END IF
END DO

RETURN
END
```

```
C ***** AssembleGH
```

```
SUBROUTINE AssembleGH
```

C This subroutine
 C 1) formulates G (stored in BemG)
 C 2) formulates H (stored in BEMH)
 C Note: the following is set up for 2nd order basis functions

C Common Variables

```
INCLUDE 'ECBPar.INC'
INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMsh.INC'
INCLUDE 'ECGaus.INC'
INCLUDE 'ECBG.INC'
INCLUDE 'ECBCal.INC'
```

C Internal Variables

```

      INTEGER Elem,Row,Col,Loc
      INCLUDE 'EcbElm.INC'
      REAL*8 Sum

```

C Clear the BemG and BemH Matrices

```

      CALL MatZeroDP(MaxNoOfCoords,NoOfCoords,NoOfCoords,BemG)
      CALL MatZeroDP(MaxNoOfCoords,NoOfCoords,NoOfCoords,BemH)

```

C The following DO-Loop performs the integration by Element, computing
 C the components of the G and H matrices

```

      DO Elem=1,NoOfElems
        CALL PrepInt(Elem)
        CALL Integrate(Elem)
      END DO

```

C Obtain diagonal elements of H.

```

      DO Row=1,NoOfCoords
        BEMH(Row,Row)=0.0
        Sum=0.0
        DO Col=1,NoOfCoords
          Sum=Sum+BEMH(Row,Col)
        END DO
        BemH(Row,Row)=-Sum
      END DO

```

```

      RETURN
      END

```

C ***** Axi2B3

```

      REAL*8 FUNCTION Axi2B3(GaussPt)

```

C For an Axisymmetric Problem, with 2nd Order basis functions,
 C this function returns the bounded portion of the integrand for
 C loc=3

```

      INCLUDE 'ECBHDR.INC'
      REAL*8 GaussPt

```

```

      REAL*8 Den,A,B,UstarB,KB,RBig,Eta
      REAL*8 R(MaxNoOfDim), IsoJacob
      REAL*8 Phi(MaxBasisDeg+1)

```

C From Common ElcmR

```

      Eta=1-GaussPt
      CALL AxiSub(Eta,3,A,B,Den,R,IsoJacob,Phi,RBig)

```

```

      KB=A+B*LOG(Den)-B*LOG(RBig)
      UStarB=2*KB/SQRT(Den)
      Axi2B3 = UStarB*IsoJacob*r(1)*Phi(3)

```

```

      RETURN

```

END

C ***** Axi2B2

REAL*8 FUNCTION Axi2B2(GaussPt)

C For an Axisymmetric Problem, with 2nd Order basis functions,
C this function returns the bounded portion of the integrand
C for loc=2

REAL*8 GaussPt,Eta

INCLUDE 'ECBHDR.INC'
REAL*8 Den,A,B,UstarB,KB,RBig
REAL*8 R(MaxNoOfDim), IsoJacob
REAL*8 Phi(MaxBasisDeg+1)

C From Common ElemR

Eta=(1.0-GaussPt)/2.0
CALL AxiSub(Eta,2,A,B,Den,R,IsoJacob,Phi,RBig)

KB=A+B*LOG(Den)-B*LOG(RBig)
UStarB=KB/SQRT(Den)
Axi2B2 = UStarB*IsoJacob*r(1)*Phi(2)

Eta=(1.0+GaussPt)/2.0
CALL AxiSub(Eta,2,A,B,Den,R,IsoJacob,Phi,RBig)

KB=A+B*LOG(Den)-B*LOG(RBig)
UStarB=KB/SQRT(Den)
Axi2B2 = Axi2B2 + UStarB*IsoJacob*r(1)*Phi(2)

RETURN
END

C ***** Axi2B1

REAL*8 FUNCTION Axi2B1(GaussPt)

C For an Axisymmetric Problem, with 2nd Order basis functions,
C this function returns the bounded portion of the integrand for
C loc=1

REAL*8 GaussPt

INCLUDE 'ECBHDR.INC'
REAL*8 Den,A,B,UstarB,KB,RBig
REAL*8 R(MaxNoOfDim), IsoJacob
REAL*8 Phi(MaxBasisDeg+1)

C From Common ElemR

CALL AxiSub(GaussPt,1,A,B,Den,R,IsoJacob,Phi,RBig)

KB=A+B*LOG(Den)-B*LOG(RBig)
UStarB=2*KB/SQRT(Den)
Axi2B1 = UStarB*IsoJacob*r(1)*Phi(1)

RETURN
END

C ***** Axi2U3

REAL*8 FUNCTION Axi2U3(GaussPt)

C For an Axisymmetric Problem, with 2nd Order basis functions,
C this function returns the unbounded portion of the integrand for
C loc=3 (Note: the unbounded LN(1/GaussPt) term is NOT included. This
C is accounted for in the integration routine points and weights)

REAL*8 GaussPt

INCLUDE 'ECBHDR.INC'
REAL*8 Den,A,B,UstarU,KU,RBig,Eta
REAL*8 R(MaxNoOfDim), IsoJacob
REAL*8 Phi(MaxBasisDeg+1)

C From Common ElemR

Eta=1-GaussPt
CALL AxiSub(Eta,3,A,B,Den,R,IsoJacob,Phi,RBig)

KU=2*B
UStarU=2*KU/SQRT(Den)

Axi2U3 = UStarU*IsoJacob*r(1)*Phi(3)

RETURN
END

C ***** Axi2U2

REAL*8 FUNCTION Axi2U2(GaussPt)

C For an Axisymmetric Problem, with 2nd Order basis functions,
C this function returns the unbounded portion of the integrand for
C loc=2 (Note: the unbounded LN(1/GaussPt) term is NOT included. This
C is accounted for in the integration routine points and weights)

REAL*8 GaussPt

INCLUDE 'ECBHDR.INC'
REAL*8 Den,A,B,UstarU,KU,Eta,RBig
REAL*8 R(MaxNoOfDim), IsoJacob
REAL*8 Phi(MaxBasisDeg+1)

C From Common ElemR

Eta=(1.0-GaussPt)/2.0
CALL AxiSub(Eta,2,A,B,Den,R,IsoJacob,Phi,RBig)

KU=B
UStarU=2*KU/SQRT(Den)

Axi2U2 = UStarU*IsoJacob*r(1)*Phi(2)

```

Eta=(1.0+GaussPt)/2.0
CALL AxiSub(Eta,2,A,B,Den,R,IsoJacob,Phi,RBig)

```

```

KU=B
UStarU=2*KU/SQRT(Den)

```

```

Axi2U2 = Axi2U2 + UStarU*IsoJacob*r(1)*Phi(2)

```

```

RETURN
END

```

```

C ***** Axi2U1

```

```

REAL*8 FUNCTION Axi2U1(GaussPt)

```

```

C For an Axisymmetric Problem, with 2nd Order basis functions,
C this function returns the unbounded portion of the integrand for
C loc=1 (Note: the unbounded LN(1/GaussPt) term is NOT included. This
C is accounted for in the integration routine points and weights)

```

```

REAL*8 GaussPt

```

```

INCLUDE 'ECBHDR.INC'
REAL*8 Den,A,B,UstarU,KU,RBig
REAL*8 R(MaxNoOfDim), IsoJacob
REAL*8 Phi(MaxBasisDeg+1)

```

```

C From Common ElemR

```

```

CALL AxiSub(GaussPt,1,A,B,Den,R,IsoJacob,Phi,RBig)

```

```

KU=2*B
UStarU=2*KU/SQRT(Den)

```

```

Axi2U1 = UStarU*IsoJacob*r(1)*Phi(1)

```

```

RETURN
END

```

```

C ***** AxiSub

```

```

SUBROUTINE AxiSub(GaussPt,Loc,A,B,Den,R,IsoJacob,Phi,RBig)

```

```

INCLUDE 'ECBHDR.INC'
INCLUDE 'ECBPAN.INC'
INCLUDE 'ECBELM.INC'

```

```

INTEGER Loc
REAL*8 GaussPt,A,B,Den,R(*),IsoJacob,Phi(*),RBig

```

```

REAL*8 M,M1,dRdZeta(MaxNoOfDim),PhiZeta(MaxBasisDeg+1)

```

```

C From Common ElemR, SourceR

```

```

C Functions

```

```

REAL*8 IsoJacobian
EXTERNAL IsoJacobian

```

C From Common BasisDeg, ElemR, SourceR

```
CALL Compute1DPhis(BasisDeg,GaussPt,Phi,PhiZeta)
CALL ComputeRZ(Phi,R)
```

```
Den = (R(1)+SourceR(1))*(R(1)+SourceR(1)) +
& (r(2)-SourceR(2))*(r(2)-SourceR(2))
M=4*r(1)*SourceR(1)/Den
```

```
IF (M.GE.1) THEN
  WRITE(*,*) ' M=',M,' Den=',Den
  WRITE(*,*) ' R=',R(1),R(2)
  WRITE(*,*) ' Source=',SourceR(1),SourceR(2)
  WRITE(*,*) 'GaussPt=',GaussPt,' Loc=',Loc
  WRITE(*,*) ' '
END IF
```

```
CALL KelpCocf(M,M1,A,B)
```

```
IsoJacob=IsoJacobian(PhiZeta,dRdZeta)
```

```
CALL ComputeRBig(GaussPt,Loc,RBig)
```

```
RETURN
END
```

C ***** ChkIsoPara

```
SUBROUTINE ChkIsoPara(Mac)
```

```
INTEGER MAC
INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBEIm.INC'
INCLUDE 'ECBMac.INC'
```

```
INTEGER PrevElems,Mic,Dim
REAL*8 Test
```

```
LOGICAL MajorError
```

```
CALL ComputePrevElem(Mac,PrevElems)
DO Mic=PrevElems+1,PrevElems+NoOfMicElems(Mac)
```

```
MajorError=.FALSE.
CALL GetElemR(Mic)
```

```
DO Dim=1,NoOfDim
```

```
Test=ElemR(Dim,1) + ElemR(Dim,3) - 2.0 * ElemR(Dim,2)
```

```
IF (Test.NE.0.0) THEN
```

```
Test= (ElemR(Dim,1) - ElemR(Dim,3))/Test
IF (ABS(Test).LE.2.0) CALL ChkIsoParaErr(Dim,Mic,MajorError)
```

```
END IF
END DO
END DO
```

```
RETURN
END
```

```
C ***** ChkIsoParaErr
```

```
SUBROUTINE ChkIsoParaErr(Dim,Mic,MajorError)
```

```
INTEGER Dim,Mic
LOGICAL MajorError
```

```
INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBEIm.INC'
INCLUDE 'ECBMsh.INC'
```

```
IF (.NOT.MajorError) THEN
  MajorError=.TRUE.
```

```
ELSE
```

```
  WRITE(*,*) ' '
  WRITE(*,*) ' Error: isoparametric mapping from global ',
& 'element to local element is definitely not 1-1'
  WRITE(*,*) ' '
  WRITE(*,*) '      Element # ',Mic
  WRITE(*,*) ' '
  WRITE(*,*) '      ElemR(,1)',ElemR(1,1),ElemR(2,1)
  WRITE(*,*) '      ElemR(,2)',ElemR(1,2),ElemR(2,2)
  WRITE(*,*) '      ElemR(,3)',ElemR(1,3),ElemR(2,3)
  WRITE(*,*) ' '
  WRITE(*,*) '      NodeMap(,1..3)',NodeMap(Mic,1),
& NodeMap(Mic,2),NodeMap(Mic,3)
```

```
  CALL WriteMesh('ISOPARA.ERR')
```

```
  STOP 'In Routine: ChkIsoPara (ChkIsoParaErr)'
END IF
```

```
RETURN
END
```

```
c ***** CirLinNtrsxn
```

```
SUBROUTINE CirLinNtrsxn(X1,Y1,X2,Y2,Xc,Yc,R,
& XInt1,YInt1,XInt2,YInt2,Error)
```

```
C Input Variables -----
```

```
REAL*8 X1,Y1,X2,Y2,Xc,Yc,R
```

```
C X1,Y1      Starting point of line segment
C X2,Y2      Ending point of line segment
```

```
C Xc,YcCenter of Circle
C R      Radius of Circle
```

```
C Output Variables -----
```

```
REAL*8 XInt1,YInt1,XInt2,YInt2
INTEGER Error
```

C XInt1,YInt1 First intersection between circle and line segment
 C XInt2,YInt2 Second intersection between circle and line segment

C Error 0 if only 1 intersection 1 is on the line segment
 C 1 if two intersections are on the line segment
 C 2 if no intersections are on the line segment, but are on the line
 C 3 if no intersections are on the line.

C Internal Variables -----

REAL*8 Xhat,Yhat,dX,dY,b_2a_y,c_a_y,b_2a_x,c_a_x,DiscX,DiscY
 REAL*8 Temp
 LOGICAL Tangent,One,Two

C Xhat,Yhat x1-xc, y1-yc
 C dx,dy x1-x2,y1-y2
 C b_2a_y dx(yhat dx - xhat dy)/(dx dx + dy dy)
 C c_a_y (r r dy dy - (xhat dy - yhat dx)^2)/(dx dx + dy dy)
 C b_2a_x dy(xhat dy ...
 C c_a_y (r r dx dx ...

xhat=x1-xc
 yhat=y1-yc

dx=x1-x2
 dy=y1-y2

b_2a_y = dx*(yhat*dx - xhat*dy) / (dx*dx + dy*dy)
 b_2a_x = dy*(xhat*dy - yhat*dx) / (dx*dx + dy*dy)

c_a_y = (r*r*dy*dy -
 & (xhat*dy - yhat*dx)*(xhat*dy - yhat*dx))
 & / (dx*dx + dy*dy)
 c_a_x = (r*r*dx*dx -
 & (xhat*dy - yhat*dx)*(xhat*dy - yhat*dx))
 & / (dx*dx + dy*dy)

DiscX = b_2a_x*b_2a_x + c_a_x
 DiscY = b_2a_y*b_2a_y + c_a_y

Tangent=.FALSE.
 IF (DiscY.LT.0) THEN

Error=3
 RETURN

ELSE IF ((DiscY.EQ.0).AND.(DiscX.EQ.0)) THEN

XInt1=b_2a_x
 YInt1=b_2a_y

XInt2=b_2a_x
 YInt2=b_2a_y

Tangent=.TRUE.

ELSE IF ((DiscY.EQ.0).AND.(DiscX.GT.0)) THEN

```
XInt1 = b_2a_x + SQRT(DiscX)
YInt1 = b_2a_y
```

```
XInt2 = b_2a_x - SQRT(DiscX)
YInt2 = b_2a_y
```

```
ELSE IF ((DiscY.GT.0).AND.(DiscX.EQ.0)) THEN
```

```
XInt1 = b_2a_x
YInt1 = b_2a_y + SQRT(DiscY)
```

```
XInt2 = b_2a_x
YInt2 = b_2a_y - SQRT(DiscY)
```

```
ELSE IF ((DiscY.GT.0).AND.(DiscX.GT.0)) THEN
```

```
XInt1 = b_2a_x + SQRT(DiscX)
YInt1 = dy/dx * ( xInt1 - xhat) + yhat
```

```
XInt2 = b_2a_x - SQRT(DiscX)
YInt2 = dy/dx * ( xInt2 - xhat) + yhat
```

```
END IF
```

```
XInt1=XInt1 + xc
YInt1=YInt1 + yc
```

```
XInt2=XInt2 + xc
YInt2=YInt2 + yc
```

```
One = ( ((MIN(X1,X2).LE.XInt1).AND.(XInt1.LE.MAX(X1,X2)))
& .AND.
& ((MIN(Y1,Y2).LE.YInt1).AND.(YInt1.LE.MAX(Y2,Y1))) )
```

```
Two = ( ((MIN(X1,X2).LE.XInt2).AND.(XInt2.LE.MAX(X1,X2)))
& .AND.
& ((MIN(Y1,Y2).LE.YInt2).AND.(YInt2.LE.MAX(Y2,Y1))) )
```

```
IF (Tangent) THEN
```

```
IF (One) THEN
  Error=0
ELSE
  Error=2
END IF
```

```
ELSE
```

```
IF (One.AND.Two) THEN
  Error=1
ELSE IF (One) THEN
  Error=0
ELSE IF (Two) THEN
  Error=0
```

```
Temp=XInt1
XInt1=XInt2
XInt2=Temp
```

```

Temp=YInt1
YInt1=YInt2
YInt2=Temp

```

```

ELSE
  Error=2
END IF
END IF

```

```

RETURN
END

```

```

C ***** CirPts

```

```

SUBROUTINE CirPts(Xc,Yc,X1,Y1,X2,Y2,NPts,PtsX,PtsY,Clockwise)

```

```

C This subroutine generates points on a circular arc
C (centered at xc,yc) starting with (x1,y1) and ending with (x2,y2)

```

```

C Input Variables -----

```

```

REAL*8 Xc,Yc,X1,Y1,X2,Y2
LOGICAL Clockwise

```

```

C Xc,Yc Center of the Circle
C X1,Y1 First Point on Circular Arc
C X2,Y2 Last Point on Circular Arc
C Clockwise .TRUE. for a clockwise circle

```

```

C Output Variables -----

```

```

INTEGER NPts
REAL*8 PtsX(*),PtsY(*)

```

```

C NPts The number of points on the arc
C PtsX(*) X coordinate locations
C PtsY(*) Y coordinate locations

```

```

C Internal Variables -----

```

```

REAL*8 T1,T2,TStp,T,R
INTEGER I
INCLUDE '[kj.for.util]pi.inc'

```

```

C External Functions -----

```

```

REAL*8 Mag
EXTERNAL Mag

```

```

R=(MAG(X1-Xc,Y1-Yc)+MAG(X2-Xc,Y2-Yc))/2

```

```

CALL XY2T(X1-Xc,Y1-Yc,T1)
CALL XY2T(X2-Xc,Y2-Yc,T2)

```

```

IF ((ABS(T1-T2).LT.0.01)
& .OR.(ABS(T1-T2).GT.(2.0*Pi-0.01))) THEN
  NPts=2

```

```

ELSE
  IF (Clockwise) THEN
    DO WHILE(T1.LE.T2)
      T1=T1+2.0*Pi
    END DO
  ELSE
    DO WHILE(T1.GE.T2)
      T1=T1-2.0*Pi
    END DO
  END IF

  NPts=ABS((T2-T1)*18.0/Pi)+2
  TStp=(T2-T1)/(NPts-1)

  T=T1+TStp
  DO I=2,NPts-1
    PtsX(I)=Xc+R*COS(T)
    PtsY(I)=Yc+R*SIN(T)
    T=T+TStp
  END DO

  END IF

  PtsX(1)=X1
  PtsY(1)=Y1
  PtsX(Npts)=X2
  PtsY(Npts)=Y2

  RETURN
END

```

C ***** ComputeBdry

SUBROUTINE ComputeBdry(Spa,NoOfSpa,Smooth,Spl3D)

C This subroutine computes the new y coordinates based on Spa. An IMSL Cubic
C Spline routine is used to generate the new boundary points from moved points.

C Input Variables -----

C UserPts() Locations of X and Y Coordinates to use in Spline
C NoOfUserPts Number of X,Y Coordinates to use spline with.
C Spa() Location of X coordinates to find Y coordinates (using Spline)
C NoOfSpa Number of X locs at which we wish to find Y locs.
C Smooth .TRUE. if smoothing spline is to be used.

C Output Variables -----

C UserPts() Desired Locations of X and Y Coordinates

```

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBPar.INC'
INCLUDE 'ECBMove.INC'

```

```

REAL*8 PtsX(MaxNoOfCoords),PtsY(MaxNoOfCoords)
REAL*8 Spa(*),OrigSpa(MaxNoOfCoords)
REAL*8 YBreak(MaxNoOfCoords),YCSCoef(4,MaxNoOfCoords)

```



```

REAL*8 XBreak(MaxNoOfCoords),XCSCoef(4,MaxNoOfCoords)
INTEGER I,J,NoOfSpa,Offset

LOGICAL Smooth,Spl3D

REAL*8 DCSVAL
EXTERNAL DCSVAL

DO I=1,NoOfMoved
  PtsX(I)=Moved(I,1)
  PtsY(I)=Moved(I,2)
END DO

IF (Spl3D) THEN

c   IF (Smooth) THEN
c     WRITE(*,*) 'Error: Smoothing Not implemented in this version'
c   END IF

D   WRITE(*,*) 'ComputeBdry: Calling ComputeRelativeSpacing'
    CALL ComputeRelativeSpacing(Moved,NoOfMoved,OrigSpa)

    Offset=0
    DO I=1,NoOfMoved-1
      IF (ABS(OrigSpa(I-Offset)-OrigSpa(I+1))
& .LE.Tolerance/100.0) THEN
        Offset=Offset+1
      END IF
      OrigSpa(I-Offset+1)=OrigSpa(I+1)
      PtsX(I-Offset+1)=PtsX(I+1)
      PtsY(I-Offset+1)=PtsY(I+1)
    END DO
    NoOfMoved=NoOfMoved-Offset

    IF (Smooth) THEN

C Use Shape smoothing spline

D     WRITE(*,*) 'Calling DCSSCV from ComputeBdry:',
D   & ' x(1..',NoOfMoved,')'
      CALL DCSSCV(NoOfMoved,OrigSpa,PtsX,2,XBreak,XCSCoef)
D     WRITE(*,*) 'Calling DCSSCV from ComputeBdry:',
D   & ' y(1..',NoOfMoved,')'
      CALL DCSSCV(NoOfMoved,OrigSpa,PtsY,2,YBreak,YCSCoef)

    ELSE

C Use Akima Spline

D     WRITE(*,*) 'Calling DCSAKM from ComputeBdry:',
D   & ' x(1..',NoOfMoved,')'
      CALL DCSAKM(NoOfMoved,OrigSpa,PtsX,XBreak,XCSCoef)
D     WRITE(*,*) 'Calling DCSSCV from ComputeBdry:',
D   & ' y(1..',NoOfMoved,')'
      CALL DCSSCV(NoOfMoved,OrigSpa,PtsY,YBreak,YCSCoef)

    END IF

```

C Generate the new points from the old X locations.

```

      DO J=1,NoOfSpa
        Moved(J,1)=DCSVAL(Spa(J),NoOfMoved-1,XPBreak,XCSCoef)
        Moved(J,2)=DCSVAL(Spa(J),NoOfMoved-1,YPBreak,YCSCoef)
      END DO

      ELSE

      Offset=0
      DO I=1,NoOfMoved-1
        IF (ABS(PtsX(I-Offset)-PtsX(I+1))
& .LE.Tolerance/100) THEN
          Offset=Offset+1
        END IF
        PtsX(I-Offset+1)=PtsX(I+1)
        PtsY(I-Offset+1)=PtsY(I+1)
      END DO
      NoOfMoved=NoOfMoved-Offset

      IF (NoOfMoved.LE.3) THEN
        DO J=1,NoOfSpa
          Moved(J,1)=Spa(J)
          IF (PtsX(NoOfMoved).EQ.PtsX(1)) THEN
            WRITE(*,*) 'Error: X points are not varying.'
            STOP 'In Routine: ComputeBdry'
          END IF
          Moved(J,2)=PtsY(NoOfMoved)-(PtsY(NoOfMoved)-PtsY(1))
& / (PtsX(NoOfMoved)-PtsX(1)) * (PtsX(NoOfMoved)-Spa(J))
        END DO
      ELSE

      IF (Smooth) THEN

      D      WRITE(*,*) 'Calling DCSSCV from ComputeBdry: ',
      D & 'y(x(1..',NoOfMoved,')'
          CALL DCSSCV(NoOfMoved,PtsX,PtsY,2,YPBreak,YCSCoef)

      ELSE

      D      WRITE(*,*) 'Calling DCSAKM from ComputeBdry: ',
      D & 'y(x(1..',NoOfMoved,')'
          CALL DCSAKM(NoOfMoved,PtsX,PtsY,YPBreak,YCSCoef)

      END IF

      DO J=1,NoOfSpa
        Moved(J,1)=Spa(J)
        Moved(J,2)=DCSVAL(Spa(J),NoOfMoved-1,YPBreak,YCSCoef)
      END DO
      END IF

      END IF

      NoOfMoved=NoOfSpa

      RETURN
      END

```

C ***** ComputeInt

SUBROUTINE ComputeInt

C This subroutine (for internal points)

C 0) stores the internal points into the source points
 C 1) formulates G (stored in BemG)
 C 2) formulates H (stored in BemH)
 C 3) computes Pot for internal points

C Note: the following is set up for 2nd order basis functions

C Note: the source points ARE destroyed by this subroutine, so, it

C should always be called last, after the BEM problem has been solved
 C and saved.

C Common Variables

INCLUDE 'ECBHdr.INC'
 INCLUDE 'ECGaus.INC'
 INCLUDE 'ECBBC.INC'
 INCLUDE 'ECBCal.INC'
 INCLUDE 'ECBINT.INC'
 INCLUDE 'ECBG.INC'
 INCLUDE 'ECBMsh.INC'
 INCLUDE 'ECBPar.INC'
 INCLUDE 'ECBSRC.INC'
 INCLUDE '[kj.for.util]pi.inc'

C Internal Variables

INTEGER Elem,Row,Col,Loc,I,J
 REAL*8 U,Q
 INCLUDE 'EcbElm.INC'

C Clear the BemG and BemH Matrices

CALL MatZeroDP(MaxNoOfCoords,NoOfCoords,NoOfCoords,BemG)
 CALL MatZeroDP(MaxNoOfCoords,NoOfCoords,NoOfCoords,BemH)

C Store the internal points into the source points

NoOfSrc=NoOfInternal
 DO I=1,NoOfInternal
 DO J=1,NoOfDim
 Src(I,J)=InternalPts(I,J)
 END DO
 END DO

C The following DO-Loop performs the integration by Element, computing
 C the components of the G and H matrices

DO Elem=1,NoOfElcms
 CALL PrepInt(Elem)
 CALL Integrate(Elem)
 END DO

C Compute the value of the potential at the internal points.

```

DO I=1,NoOfInternal
  InternalPot(I)=0.0
  DO J=1,NoOfCoords

    IF (Natural(J)) THEN
      U=SolValues(J)
      Q=BCValues(J)
    ELSE
      U=BCValues(J)
      Q=SolValues(J)
    END IF

    InternalPot(I)=InternalPot(I)+
    & BemG(I,J)*Q-BemH(I,J)*U

  END DO
  InternalPot(I)=InternalPot(I)/(2.0*Pi)
END DO

RETURN
END

```

C ***** ComputeNx

SUBROUTINE ComputeNx(NoOfElems)

C This subroutine computes the unit normals for all the boundary points.
C K is a counter variable. Assumes moving boundary has been placed into MOVE

```

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBEIm.INC'
INCLUDE 'ECBMOVE.INC'

INTEGER Elem,Loc,K,Dim,NoOfElems
REAL*8 dRdZeta(MaxNoOfDim),
& Zeta, Norm, Phi(MaxBasisDeg+1), PhiZeta(MaxBasisDeg+1)
REAL*8 DeltaX, DeltaY

REAL*8 VecNormDP
EXTERNAL VecNormDP

K=0
DO Elem=1,NoOfElems

```

C Transfer points from global Moved matrix to local ELEMNR matrix

```

DO Loc=1,BasisDeg+1
  K=K+1
  DO Dim=1,NoOfDim
    ElemR(Dim,Loc)=Moved(K,Dim)
  END DO
END DO

```

C Compute the normal to each element at each node

```

D WRITE(*,*) 'ComputeNx: ElemR'
D WRITE(*,*) ' (1)',ElemR(1,1),ElemR(2,1)
D WRITE(*,*) ' (2)',ElemR(1,2),ElemR(2,2)

```

D IF (BasisDeg+1.GT.2) WRITE(*,*) ' (,3)',ElemR(1,3),ElemR(2,3)

DeltaX=ElemR(1,2)-ElemR(1,1)

DeltaY=ElemR(2,2)-ElemR(2,1)

Norm=SQRT(DeltaX*DeltaX+DeltaY*DeltaY)

Nx(K+1-BasisDeg-1,1) =-DeltaY/Norm

Nx(K+1-BasisDeg-1,2) = DeltaX/Norm

D WRITE(*,*) ' Nx(,1)=',-DeltaY/Norm,K+1-BasisDeg-1

D WRITE(*,*) ' Nx(,2)=' , DeltaX/Norm

DO Loc=2,BasisDeg

DeltaX=ElemR(1,Loc)-ElemR(1,Loc-1)

DeltaY=ElemR(2,Loc)-ElemR(2,Loc-1)

DeltaX=DeltaX+ElemR(1,Loc+1)-ElemR(1,Loc)

DeltaY=DeltaY+ElemR(2,Loc+1)-ElemR(2,Loc)

Norm=SQRT(DeltaX*DeltaX+DeltaY*DeltaY)

Nx(K+Loc-BasisDeg-1,1) =-DeltaY/Norm

Nx(K+Loc-BasisDeg-1,2) = DeltaX/Norm

D WRITE(*,*) ' Nx(,1)=',-DeltaY/Norm,K+Loc-BasisDeg-1

D WRITE(*,*) ' Nx(,2)=' , DeltaX/Norm

END DO

Loc=BasisDeg+1

DeltaX=ElemR(1,Loc)-ElemR(1,Loc-1)

DeltaY=ElemR(2,Loc)-ElemR(2,Loc-1)

Norm=SQRT(DeltaX*DeltaX+DeltaY*DeltaY)

Nx(K+Loc-BasisDeg-1,1) =-DeltaY/Norm

Nx(K+Loc-BasisDeg-1,2) = DeltaX/Norm

D WRITE(*,*) ' Nx(,1)=',-DeltaY/Norm,K+Loc-BasisDeg-1

D WRITE(*,*) ' Nx(,2)=' , DeltaX/Norm

END DO

RETURN

END

C ***** ComputePrevElem

SUBROUTINE ComputePrevElem(Elem,PrevElems)

C Computes the previous number of micro-elements (PrevElem) from
C macro-element(1) to macro-element(Elem).

INTEGER Elem,PrevElems

INCLUDE 'ECBMAC.INC'

INTEGER J

PrevElems=0

DO J=1,Elem-1

PrevElems=PrevElems+NoOfMicElems(J)

END DO

RETURN
END

C ***** ComputerRBig

SUBROUTINE ComputerRBig(GaussPt,Loc,RBig)

INCLUDE 'ECBHDR.INC'

INCLUDE 'ECBEIm.INC'

INTEGER Loc

REAL*8 GaussPt,RBig

REAL*8 RBigr,RBigz

IF (Loc.EQ.1) THEN

 RBig = ElemR(1,1)*(-3+2*GaussPt)
 & + ElemR(1,2)*4*(1-GaussPt)
 & + ElemR(1,3)*(2*GaussPt-1)
 RBigz = ElemR(2,1)*(-3+2*GaussPt)
 & + ElemR(2,2)*4*(1-GaussPt)
 & + ElemR(2,3)*(2*GaussPt-1)

ELSE IF (Loc.EQ.2) THEN

 RBigr = ElemR(1,1)*(1-GaussPt)
 & - ElemR(1,2)*(1-2*GaussPt)
 & - ElemR(1,3)*GaussPt
 RBigz = ElemR(2,1)*(1-GaussPt)
 & - ElemR(2,2)*(1-2*GaussPt)
 & - ElemR(2,3)*GaussPt

ELSE IF (Loc.EQ.3) THEN

 RBigr = ElemR(1,1)*(1-2*GaussPt)
 & + ElemR(1,2)*4*GaussPt
 & - ElemR(1,3)*(1+2*GaussPt)
 RBigz = ElemR(2,1)*(1-2*GaussPt)
 & + ElemR(2,2)*4*GaussPt
 & - ElemR(2,3)*(1+2*GaussPt)

ELSE

 WRITE(*,*) 'Error: Information for computing RBig has'
 WRITE(*,*) ' not been entered for Loc=',Loc
 STOP 'In Routine: ComputerRBig'

END IF

RBig = RBigr*RBigR + RBigZ*RBigZ

RETURN

END

C ***** ComputerRZ

SUBROUTINE ComputerRZ(Phi,R)

C This subroutine computes the isoparametric transformation

C Input Variables

C Phi(1),Phi(2),Phi(3) The basis functions evaluated at the gauss point.
C ElemR(MaxNoOfDim,*) The three coordinates on the element.

C Output Variables

C R,Z The coordinates of the current point on the integration path.

```
INCLUDE 'ECBHdr.INC'
```

```
INCLUDE 'ECBEIm.INC'
REAL*8 Phi(*),R(*)
INTEGER Loc,J
```

```
CALL VecZeroDP(NoOfDim,R)
```

```
DO Loc=1,BasisDeg+1
  DO J=1,NoOfDim
    R(J)=R(J)+Phi(Loc)*ElemR(J,Loc)
  END DO
END DO
```

```
RETURN
END
```

C ***** CrossProduct2D

```
REAL*8 FUNCTION CrossProduct2D(Ax,Ay,Bx,By)
```

```
REAL*8 Ax,Ay,Bx,By
```

C Compute | A x B |

C	I	J	K
C	ax	ay	0
C	bx	by	0

```
CrossProduct2D=Ax*By-Bx*Ay
```

```
RETURN
END
```

C ***** ComputeRelativeSpacing

```
SUBROUTINE ComputeRelativeSpacing(Moved,NoOfMoved,Spacing)
```

```
INCLUDE 'ECBHdr.INC'
```

```
REAL*8 Moved(MaxNoOfCoords,MaxNoOfDim),Spacing(*),IncLength
INTEGER I,NoOfMoved
REAL*8 Mag
EXTERNAL Mag
```

```
Spacing(1)=0.0
```

```

DO I=2,NoOfMoved
  IncLength=MAG(Moved(I,1)-Moved(I-1,1),Moved(I,2)-Moved(I-1,2))
  Spacing(I)=Spacing(I-1)+IncLength
END DO

```

```

IF (Spacing(NoOfMoved).EQ.0) THEN
  WRITE(*,*) 'Error: Boundary has no length!'
  STOP 'In Routine: ComputeRelativeSpacing'
END IF

```

```

DO I=2,NoOfMoved-1
  Spacing(I)=Spacing(I)/Spacing(NoOfMoved)
END DO
Spacing(NoOfMoved)=1.0

```

```

RETURN
END

```

C ***** CopyPoint

```

SUBROUTINE CopyPoint(Coord,Orig,NoOfMoved,Moved)

```

```

  INCLUDE 'ECBHdr.INC'

```

```

  INTEGER NoOfMoved,Coord,J
  REAL*8 Moved(MaxNoOfCoords,MaxNoOfDim),
& Orig(MaxNoOfCoords,MaxNoOfDim)

```

```

  NoOfMoved=NoOfMoved+1
  CALL CopyPoint2(Coord,Orig,NoOfMoved,Moved)

```

```

  RETURN
END

```

C ***** CopyPoint2

```

SUBROUTINE CopyPoint2(Coord,Orig,NoOfMoved,Moved)

```

```

  INCLUDE 'ECBHdr.INC'

```

```

  INTEGER NoOfMoved,Coord,J
  REAL*8 Moved(MaxNoOfCoords,MaxNoOfDim),
& Orig(MaxNoOfCoords,MaxNoOfDim)

```

```

  DO J=1,NoOfDim
    Moved(NoOfMoved,J)=Orig(Coord,J)
  END DO

```

```

  RETURN
END

```

C ***** DotProduct

```

REAL*8 FUNCTION DotProduct(Ax,Ay,Az,Bx,By,Bz)

```

```

  REAL*8 Ax,Ay,Az,Bx,By,Bz

```

```

  DotProduct=Ax*Bx+Ay*By+Az*Bz

```



```
RETURN
END
```

```
C ***** ECBKinetics
```

```
  SUBROUTINE ECBKinetics(Pot,KinTyp,Slope,SlopePot,Coord)
```

```
C Given the kinetics type, and the potential slope, this subroutine computes
C the potential.
```

```
  INCLUDE 'ECBHdr.INC'
  INCLUDE 'ECBPar.INC'
  INCLUDE 'ECBMsh.INC'
```

```
  INTEGER Coord,Elem
  CHARACTER*(*) KinTyp
  REAL*8 Pot,SlopePot,Slope
  LOGICAL Ok
```

```
  Ok=.TRUE.
```

```
  IF (KinTyp.EQ.'BV') THEN
    Slope = - (EXP(aA*Pot)-EXP(-aC*Pot)) / WagLin
    SlopePot = - (aA*EXP(aA*Pot)+aC*EXP(-aC*Pot)) / WagLin
  ELSE IF (KinTyp.EQ.'LIN') THEN
    Slope = - Pot*(aA+aC) / WagLin
    SlopePot = - (aA+aC) / WagLin
  ELSE IF (KinTyp.EQ.'TAFA') THEN
    Slope = - EXP(aA*Pot) / WagLin
    SlopePot = - aA*EXP(aA*Pot) / WagLin
  ELSE IF (KinTyp.EQ.'TAFC') THEN
    Slope = - EXP(-aC*Pot) / WagLin
    SlopePot = aC*EXP(-aC*Pot) / WagLin
  ELSE IF (KinTyp.EQ.'USR') THEN
    CALL Kinetics(Pot,Coords(Coord,1),Coords(Coord,2),Coord,
& Slope,SlopePot,Ok)
  END IF
```

```
  IF (.NOT.Ok) THEN
    WRITE(*,10) Coord,Coords(Coord,1),Coords(Coord,2)
10  FORMAT(X,'      Out of range at ',I3,
& '(,G9.2,',',G9.2,')')
  END IF
```

```
  RETURN
  END
```

```
C ***** ErrSing
```

```
  SUBROUTINE ErrSing
```

```
C This subroutine prints the error message for singularities that the program
C cannot handle.
```

```
  WRITE(*,*) 'Error: Current Program cannot compute for'
  WRITE(*,*) '      singularities. Use source points outside'
  WRITE(*,*) '      of domain of interest.'
  STOP 'In Routine: Integrate'
```

END

C ***** ErrorFileName

SUBROUTINE ErrorFilename(Filename,RoutineName)

CHARACTER*(*) FileName,RoutineName
INTEGER Length

CALL StringLength(FileName,Length)
WRITE(*,*) 'Error: Filename "',FileName(1:Length),
& "' doesn't exist.'
WRITE(*,*) 'In Routine: '//RoutineName

STOP
END

C ***** ErrorVersion

SUBROUTINE ErrorVersion(Version,FileName,RoutineName)

CHARACTER*(*) fileName,RoutineName
INTEGER Version

WRITE(*,*) 'Error: unable to read this version.'
WRITE(*,*) ' Version=',Version
WRITE(*,*) ' Filename=',FileName
WRITE(*,*) 'In Routine: '//RoutineName

STOP
END

C ***** GaussInt

SUBROUTINE GaussInt(BemG,BemH,Loc)

INCLUDE 'ECGaus.INC'
INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBPar.INC'
INCLUDE 'ECBG.INC'
INCLUDE 'EcbElm.INC'

C Passed Variables

INTEGER Loc
REAL*8 BemG,BemH

C Internal Variables

REAL*8 Dist2,Gc,Hc,UBJacob,Cor,Den,M
INTEGER Gs

C Functions

REAL*8 UStar,QStar
EXTERNAL UStar,QStar

C Subroutine Code

```

DO Gs=1,NoOfGaussPts
  IF (GPhi(Gs,Loc).NE.0.0) THEN
    IF (Axisymmetric) THEN
      Den=(GR(Gs,1)+SourceR(1))*(GR(Gs,1)+SourceR(1))
      & + (GR(Gs,2)-SourceR(2))*(GR(Gs,2)-SourceR(2))
      M=4.0D0*GR(Gs,1)*SourceR(1)/Den
      IF (M.GE.1.0) THEN
        WRITE(*,*) ' M=',M,' Gs=',Gs
        WRITE(*,*) ' R=',Gr(Gs,1),Gr(Gs,2)
        WRITE(*,*) ' SourceR=',SourceR(1),SourceR(2)
        WRITE(*,*) ' ElemR=',ElemR(1,1),ElemR(2,1)
        WRITE(*,*) ' ,ElemR(1,2),ElemR(2,2)
        WRITE(*,*) ' ,ElemR(1,3),ElemR(2,3)
        WRITE(*,*) ' '
      END IF
    END IF

    Dist2=(GR(Gs,1)-SourceR(1))**2 + (GR(Gs,2)-SourceR(2))**2

    Gc=UStar(Dist2,Gs,Den,M)*GaussWts(Gs)*GIsoJacob(Gs)
    BEMG = BEMG + Gc*GPhi(Gs,Loc)

```

C Note: the Hc term does not need to be multiplied by the isojacobian here
 C because this has already been done when computing the normal.

```

Hc=QStar(Dist2,Gs,Den,M)*GaussWts(Gs)
BEMH = BEMH + Hc*GPhi(Gs,Loc)

```

```

END IF
END DO

```

```

RETURN
END

```

C ***** GeomSeries

```

REAL*8 FUNCTION GeomSeries(Ratio,NoOfTerms)

```

C This function returns the value of the sum of the geometric series
 C sum(J=0,NoOfTerms) of (Ratio**J)

```

REAL*8 Ratio
INTEGER NoOfTerms,J

GeomSeries=0.0D0
DO J=0,NoOfTerms
  GeomSeries=GeomSeries+Ratio**J
END DO

```

```

RETURN
END

```

C ***** GetElemR

```

SUBROUTINE GetElemR(Elem)

```

```

INCLUDE 'ECBHdr.INC'

```

```

INCLUDE 'ECBEIm.INC'
INCLUDE 'ECBMsh.INC'
INTEGER Elem,Loc,Dim

DO Loc=1,BasisDeg+1
  DO Dim=1,NoOfDim
    ElemR(Dim,Loc)=Coords(NodeMap(Elem,Loc),Dim)
  END DO
END DO

RETURN
END

```

C ***** GetSpa

```

SUBROUTINE GetSpa(MacElm,Spa,NoOfSpa)

```

```

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBPar.INC'
INCLUDE 'ECBMac.INC'
INCLUDE 'ECBMove.INC'
INTEGER NoOfSpa,MacElm
REAL*8 Spa(*)

```

```

INTEGER I,J
REAL*8 D,X

```

```

IF (MacSpac(MacElm).EQ.'=CRV') THEN

```

```

D   WRITE(*,*) 'GetSpa: Calling ComputeRelativeSpacing'
    CALL ComputeRelativeSpacing(Moved,NoOfMoved,Spa)
    CALL ReMesh(NoOfMicElems(MacElm)+1,Spa,NoOfMoved,Moved)
    NoOfSpa=NoOfMicElems(MacElm)*BasisDeg
    Spa(NoOfSpa+1)=1.0
    DO I=NoOfMicElems(MacElm),1,-1
      Spa( (I-1)*BasisDeg+1 )=Spa(I)
      D=Spa( I*BasisDeg+1)-Spa( (I-1)*BasisDeg+1 )
      DO J=1,BasisDeg-1
        Spa(I*BasisDeg+1-J)=Spa((I-1)*BasisDeg+1)+
& D*FLOAT(J)/FLOAT(BasisDeg)
      END DO
    END DO

```

```

ELSE

```

C Calculate Spacing

```

    CALL ShpSpacing(MacElm,NoOfSpa,Spa)

```

```

END IF

```

```

RETURN
END

```

C ***** GetSrcPoint

```

SUBROUTINE GetSrcPoint(Source)

```

```

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBSrc.INC'
INCLUDE 'ECBPar.INC'
INCLUDE 'ECBEIm.INC'

```

```

INTEGER Source,I

```

```

IF ((Source.LT.1).OR.(Source.GT.NoOfSrc)) THEN
  WRITE(*,*) 'Error: Source point is out of range!'
  WRITE(*,*) '   Source Point # =',Source
  WRITE(*,*) '   Range=(1, 'NoOfSrc,')'
  STOP 'In routine: GetSourcePoint'
END IF

```

```

DO I=1,NoOfDim
  SourceR(I)=Src(Source,I)
END DO

```

```

RETURN
END

```

C ***** IntAxis

```

SUBROUTINE IntAxis(GiiB,GiiU,SingLoc)

```

```

INCLUDE 'ECGaus.INC'
INCLUDE 'ECGLOG.INC'

```

```

INTEGER SingLoc
REAL*8 GiiB,GiiU

```

C Functions

```

REAL*8 Axi2b3,Axi2b2,Axi2b1,Axi2u3,Axi2u2,Axi2u1
EXTERNAL Axi2b3,Axi2b2,Axi2b1,Axi2u3,Axi2u2,Axi2u1

```

```

IF (SingLoc.EQ.3) THEN
  CALL GaussQuad(NoOfGaussPts,GaussPts,GaussWts,
& Axi2B3,GiiB)
  CALL GaussQuad(NoOfGauLogPts,GauLogPts,GauLogWts,
& Axi2U3,GiiU)
  ELSE IF (SingLoc.EQ.2) THEN
  CALL GaussQuad(NoOfGaussPts,GaussPts,GaussWts,
& Axi2B2,GiiB)
  CALL GaussQuad(NoOfGauLogPts,GauLogPts,GauLogWts,
& Axi2U2,GiiU)
  ELSE IF (SingLoc.EQ.1) THEN
  CALL GaussQuad(NoOfGaussPts,GaussPts,GaussWts,
& Axi2B1,GiiB)
  CALL GaussQuad(NoOfGauLogPts,GauLogPts,GauLogWts,
& Axi2U1,GiiU)
END IF

```

```

RETURN
END

```

C ***** IntPlan

```
SUBROUTINE IntPlan(GiiB,GiiU,SingLoc)
```

```
REAL*8 GiiB,GiiU
INTEGER SingLoc
```

```
REAL*8 Pla2b3,Pla2b2,Pla2b1,Pla2u3,Pla2u2,Pla2u1
EXTERNAL Pla2b3,Pla2b2,Pla2b1,Pla2u3,Pla2u2,Pla2u1
```

```
INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBEIm.INC'
INCLUDE 'ECGaus.INC'
INCLUDE 'ECGLOG.INC'
```

```
REAL*8 RSeg
```

```
IF (BasisDeg.EQ.1) THEN
```

```
C Gii for Planar 1st degree basis functions
```

```
    RSeg=SQRT(
    & (ElemR(1,2)-ElemR(1,1))*(ElemR(1,2)-ElemR(1,1)) +
    & (ElemR(2,2)-ElemR(2,1))*(ElemR(2,2)-ElemR(2,1)) )
```

```
    GiiB=RSeg/2*(1-LOG(RSeg))
    GiiU=0.0
```

```
ELSE IF (BasisDeg.EQ.2) THEN
```

```
C Gii for Planar 2nd degree basis functions
```

```
    IF (SingLoc.EQ.3) THEN
        CALL GaussQuad(NoOfGaussPts,GaussPts,GaussWts,
        & Pla2B3,GiiB)
        CALL GaussQuad(NoOfGauLogPts,GauLogPts,GauLogWts,
        & Pla2U3,GiiU)
    ELSE IF (SingLoc.EQ.2) THEN
        CALL GaussQuad(NoOfGaussPts,GaussPts,GaussWts,
        & Pla2B2,GiiB)
        CALL GaussQuad(NoOfGauLogPts,GauLogPts,GauLogWts,
        & Pla2U2,GiiU)
    ELSE IF (SingLoc.EQ.1) THEN
        CALL GaussQuad(NoOfGaussPts,GaussPts,GaussWts,
        & Pla2B1,GiiB)
        CALL GaussQuad(NoOfGauLogPts,GauLogPts,GauLogWts,
        & Pla2U1,GiiU)
    END IF
```

```
ELSE
    CALL ErrSing
END IF
```

```
RETURN
END
```

```
C ***** Integrate
```

```
SUBROUTINE Integrate(Elem)
```

C This subroutine performs the integrations for all source points over an
C element.

```
INCLUDE 'ECGaus.INC'
INCLUDE 'ECGLOG.INC'
INCLUDE 'ECBPar.INC'
```

```
INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMsh.INC'
INCLUDE 'ECBCal.INC'
INCLUDE 'ECBG.INC'
INCLUDE 'ECBSRC.INC'
```

C Input Variables

```
INTEGER Elem
INCLUDE 'ECBELM.INC'
```

C Internal Variables

```
LOGICAL Singularity
INTEGER Source,Loc,I,SingLoc

REAL*8 Dist2,DTemp,Small/1.0D-05/,Gc,Hc
REAL*8 GiiU,GiiB
```

C Code Follows

C The following Do-Loop performs the integration along the element for each
C source point.

```
DO Source=1,NoOfSrc

  CALL GetSrcPoint(Source)
  CALL TestForSingularity(Singularity,SingLoc)

  DO Loc=1,BasisDeg+1
    IF (SingLoc.NE.Loc) THEN
```

C Integrate over elements w/o singularities

```
      CALL GaussInt(BEMG(Source,NodeMap(Elem,Loc)),
& BEMH(Source,NodeMap(Elem,Loc)),Loc)
```

```
    ELSE
```

C Integrate over elements w/ singularities:

```
      IF (Axisymmetric) THEN
```

C Axisymmetric Elements w/ singularities

```
        IF (BasisDeg.NE.2) CALL ErrSing
        CALL IntAxis(GiiB,GiiU,SingLoc)
```

```
      ELSE
```

C Planar elements w/ singularities

```

        CALL IntPlan(GiiB,GiiU,SingLoc)

        END IF

        BemG(Source,NodeMap(Elem,Loc)) =
& BemG(Source,NodeMap(Elem,Loc)) + GiiB + GiiU

        END IF
    END DO
END DO

RETURN
END

C ***** IsoJacobian

    REAL*8 FUNCTION IsoJacobian(PhiZeta,dRdZeta)

C This subroutine computes the jacobian for the iso-parametric transformation.

    INCLUDE 'ECBHdr.INC'

    INCLUDE 'EcbElm.INC'
    REAL*8 PhiZeta(*),dRdZeta(MaxNoOfDim)
    REAL*8 VecNormDP
    EXTERNAL VecNormDP

    CALL ComputeRZ(PhiZeta,dRdZeta)
    IsoJacobian=VecNormDP(NoOfDim,dRdZeta)

    RETURN
    END

C ***** Kinetics

    SUBROUTINE Kinetics(Pot,X,Y,Coord,Slope,SlopePot,Ok)

C Return the potential as a function of the slope in potential

    INTEGER Coord
    REAL*8 Pot,Slope,SlopePot,X,Y
    LOGICAL Ok

    WRITE(*,*) 'Error: Kinetics routine has not been written'
    Ok=.FALSE.

    RETURN
    END

C ***** KineticBC

    LOGICAL FUNCTION KineticBC(BCType)

    CHARACTER*(*) BCType

    KineticBC=(BCType.EQ.'LIN').OR.(BCType.EQ.'TAFA')
& .OR.(BCType.EQ.'TAFC').OR.(BCType.EQ.'BV').OR.

```



```
& (BCType.EQ.'USR')
```

```
RETURN
END
```

```
C ***** LocateIntersects
```

```
SUBROUTINE LocateIntersects(Sign,I,J,XInt,YInt,Error)
```

```
INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMOVE.INC'
```

```
REAL*8 XInt,YInt
INTEGER Sign,I,J,ErrorInt
```

```
INTEGER Ilimits(2),Jlimits(2)
LOGICAL Error
```

```
D WRITE(*,*) '-----: LocateIntersects'
```

```
Error=.FALSE.
IF (Sign.GT.0) THEN
  Ilimits(1)=1
  Ilimits(2)=NoOfMoved-1
  Jlimits(1)=1
  Jlimits(2)=NoOfIns-1
ELSE
  Ilimits(1)=NoOfMoved
  Ilimits(2)=2
  Jlimits(1)=NoOfIns
  Jlimits(2)=2
END IF
```

```
C Outer loop, goes down moved boundary points
```

```
DO I=Ilimits(1),Ilimits(2),Sign
```

```
D WRITE(*,*) ' I=',I
D WRITE(*,*) ' M1 ',Moved(I,1),Moved(I,2)
D WRITE(*,*) ' M2 ',Moved(I+Sign,1),Moved(I+Sign,2)
```

```
C Inner loop, goes down insulator points.
```

```
DO J=Jlimits(1),Jlimits(2),Sign
  CALL ComputeIntersection(Moved(I,1),Moved(I,2),
    & Moved(I+Sign,1),Moved(I+Sign,2),
    & Ins(J,1),Ins(J,2),
    & Ins(J+Sign,1),Ins(J+Sign,2),XInt,YInt,ErrorInt)
```

```
D WRITE(*,*) 'J=',J, ErrorInt=',ErrorInt
D WRITE(*,*) ' I1 ',Ins(J,1),Ins(J,2)
D WRITE(*,*) ' I2 ',Ins(J+Sign,1),Ins(J+Sign,2)
```

```
IF (ErrorInt.EQ.0) THEN
D WRITE(*,*) 'Int=',XInt,YInt
RETURN
END IF
END DO
```

```

      END DO

      WRITE(*,*) 'Warning: no intersection found between ',
& 'moved boundary and insulator.'
      WRITE(*,*) '      Time step is probably too big.'
      WRITE(*,*) ' Sign=',Sign
      WRITE(*,*) ' MOVED=',Moved(ILimits(1),1),Moved(ILimits(1),2)
      WRITE(*,*) '      ',Moved(ILimits(2),1),Moved(ILimits(2),2)
      WRITE(*,*) ' INS=',Ins(JLimits(1),1),Ins(JLimits(1),2)
      WRITE(*,*) '      ',Ins(JLimits(2),1),Ins(JLimits(2),2)

      WRITE(*,*) 'In Routine: LocateIntersects'
      Error=.TRUE.

      END

C ***** MacNat

      LOGICAL FUNCTION MacNat(BCType)

C This function returns .TRUE. if BCType represents a natural boundary
C condition.

      CHARACTER*(*) BCType
      LOGICAL KineticBC
      EXTERNAL KineticBC

      IF (BCType.EQ.'CRNT') THEN
          MacNat=.TRUE.
      ELSE IF (KineticBC(BCType)) THEN

C For Kinetic BCs, the potential is guessed at and the current is solved
C for using BEM. Then potential is re-guessed using Newton-Raphson or
C Picard scheme.

          MacNat=.FALSE.
      ELSE IF (BCType.EQ.'NAT') THEN
          MacNat=.TRUE.
      ELSE IF (BCType.EQ.'ESS') THEN
          MacNat=.FALSE.
      ELSE
          WRITE(*,*) 'Error: Unknown Boundary Condition Type=',BCType
          STOP 'In Function: MacNat'
      END IF

      RETURN
      END

C ***** Mag

      REAL*8 FUNCTION Mag(X,Y)

      REAL*8 X,Y

      Mag=SQRT(X*X+Y*Y)

      RETURN
      END

```

C ***** MakeCoord

SUBROUTINE MakeCoord(X,Y,MicNod,MacElm,SaveKinetic)

INCLUDE 'ECBHdr.INC'
 INCLUDE 'ECBMsh.INC'
 INCLUDE 'ECBBC.INC'
 INCLUDE 'ECBMac.INC'
 INCLUDE 'ECBPar.INC'

INTEGER MicNod,MacElm
 REAL*8 X,Y
 LOGICAL KineticBC,SaveKinetic,MacNat
 EXTERNAL KineticBC,MacNat

Coords(MicNod,1)=X
 Coords(MicNod,2)=Y

BCType(MicNod)=MacBCType(MacElm)
 Natural(MicNod)=MacNat(MacBCType(MacElm))

IF (MacBCType(MacElm).EQ.'CRNT') THEN

C BC Type CRNT no longer allowed.

WRITE(*,*) 'Error: Mac BC Type "CRNT" is no longer allowed.'
 WRITE(*,*) ' Use BC Type "NAT" instead.'
 STOP 'In Routine: MakeCoord'

ELSE IF (KineticBC(MacBCType(MacElm))) THEN

IF (.NOT.SaveKinetic) THEN
 BCValues(MicNod)=MacBCVal(MacElm)
 SolValues(MicNod)=0.0D0
 END IF

ELSE IF (MacBCType(MacElm).EQ.'NAT') THEN

BCValues(MicNod)=MacBCVal(MacElm)
 SolValues(MicNod)=0.0D0

ELSE IF (MacBCType(MacElm).EQ.'ESS') THEN

BCValues(MicNod)=MacBCVal(MacElm)
 SolValues(MicNod)=0.0D0

END IF

RETURN
 END

C ***** MakeElemBC

SUBROUTINE MakeElemBC

C Get BC conditions for element from mid node (or first node if BasisDeg=1)

INCLUDE 'ECBHdr.INC'

```

INCLUDE 'ECBMsh.INC'
INCLUDE 'ECBBC.INC'
INCLUDE 'ECBPar.INC'

```

```

INTEGER I

```

```

DO I=1,NoOfElems
  ElemNat(I)=Natural(NodeMap(I,BasisDeg))
  ElemBCType(I)=BCType(NodeMap(I,BasisDeg))
END DO

```

```

RETURN
END

```

```

C ***** MakeMacElem

```

```

SUBROUTINE MakeMacElem(Mac,SaveKinetic,Smooth)

```

```

INTEGER Mac,MacPlus1,Indx,Mic,Dim,PrevElems,MacPrev,MacNext
LOGICAL SaveKinetic,Smooth,MacNat,TransNext
EXTERNAL MacNat
CHARACTER*4 Shp,NextShp
REAL*8 MaxY,Test,MinY

```

```

INCLUDE 'ECBMac.INC'
INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMsh.INC'
INCLUDE 'ECBPar.INC'
INCLUDE 'ECBBC.INC'
INCLUDE 'ECBEIm.INC'

```

```

C Compute Coord Locations

```

```

Shp=MacShape(Mac)
CALL IncrementI(Mac,MacPlus1,1,NoOfMacElems)
MacNext=MacPlus1
NextShp=MacShape(MacNext)

```

```

IF (NextShp.EQ.'TRNS') THEN
  TransNext=.TRUE.
  CALL IncrementI(MacPlus1,MacNext,1,NoOfMacElems)
  NextShp=MacShape(MacNext)
ELSE
  TransNext=.FALSE.
END IF

```

```

IF (NextShp.EQ.'FLAT') THEN
  CALL ShpFlatHiPt(MacNext,MaxY)
  IF (TransNext) THEN
    MacVertY(MacIndx(MacPlus1,2))=
& MaxY+MacPar(MacNext,1)
    MacVertY(MacIndx(MacPlus1,1))=
& MacVertY(MacIndx(MacPlus1,2))-0.05
    MacVertY(MacIndx(Mac,2))=
& MacVertY(MacIndx(MacPlus1,1))
  ELSE
    MacVertY(MacIndx(Mac,2))=MaxY+MacPar(MacNext,1)
  END IF

```

ELSE IF (NextShp.EQ.'FLTL') THEN

C Flat spaced from low point.

```

CALL ShpFlatLoPt(MacNext,MinY)
IF (TransNext) THEN
  MacVertY(MacIndx(MacPlus1,2))=
& MinY+MacPar(MacNext,1)
  MacVertY(MacIndx(MacPlus1,1))=
& MacVertY(MacIndx(MacPlus1,2))-0.05
  MacVertY(MacIndx(Mac,2))=
& MacVertY(MacIndx(MacPlus1,1))
ELSE
  MacVertY(MacIndx(Mac,2))=MinY+MacPar(MacNext,1)
END IF

```

ELSE IF (NextShp.EQ.'PREV') THEN

C Must compute Prev boundary & Store Loc of MacroVertex

D WRITE(*,*) ' MakeMacElem:First Call to ShpPrev'
CALL ShpPrev(MacPlus1,SaveKinetic)

IF (TransNext) THEN

```

MacVertX(MacIndx(MacPlus1,2))=
& MacVertX(MacIndx(MacNext,1))
MacVertY(MacIndx(MacPlus1,2))=
& MacVertY(MacIndx(MacNext,1))

```

```

MacVertX(MacIndx(MacPlus1,1))=
& MacVertX(MacIndx(MacNext,1))
MacVertY(MacIndx(MacPlus1,1))=
& MacVertY(MacIndx(MacNext,1))-0.05

```

```

MacVertX(MacIndx(Mac,2))=
& MacVertX(MacIndx(MacPlus1,1))
MacVertY(MacIndx(Mac,2))=
& MacVertY(MacIndx(MacPlus1,1))

```

ELSE

```

MacVertX(MacIndx(Mac,2))=
& MacVertX(MacIndx(MacNext,1))
MacVertY(MacIndx(Mac,2))=
& MacVertY(MacIndx(MacNext,1))

```

END IF

END IF

IF (Shp.EQ.'LINE') THEN

CALL ShpLine(Mac,SaveKinetic)

ELSE IF (Shp.EQ.'TRNS') THEN

IF (MacBCVal(MacPlus1).EQ.0.0) THEN

CALL IncrementI(Mac,MacPrev,-1,NoOfMacElems)

```

      MacVertX(MacIndx(Mac,1))=MacVertX(MacIndx(MacPrev,2))
      MacVertY(MacIndx(Mac,1))=MacVertY(MacIndx(MacPrev,2))

      MacVertX(MacIndx(Mac,2))=MacVertX(MacIndx(MacPrev,2))
      MacVertY(MacIndx(Mac,2))=MacVertY(MacIndx(MacPrev,2))-0.05

      END IF

      MacVertX(MacIndx(MacPlus1,1))=
& MacVertX(MacIndx(Mac,2))
      MacVertY(MacIndx(MacPlus1,1))=
& MacVertY(MacIndx(Mac,2))

      CALL ShpTrns(Mac,SaveKinetic)

      ELSE IF (Shp.EQ.'SINE') THEN
        CALL ShpSine(Mac,SaveKinetic)
      ELSE IF (Shp.EQ.'CIR') THEN
        CALL ShpCir(Mac,SaveKinetic)
      ELSE IF ((Shp.EQ.'USER').OR.
& (Shp.EQ.'USR')) THEN
        CALL ShpUser(Mac,SaveKinetic,Smooth)
      ELSE IF (Shp.EQ.'PREV') THEN
D      WRITE(*,*) ' MakeMacElem:Second Call to ShpPrev'
        CALL ShpPrev(Mac,SaveKinetic)
      ELSE IF (Shp.EQ.'FLAT') THEN
        CALL ShpFlat(Mac,SaveKinetic)
      ELSE IF (Shp.EQ.'FLTL') THEN
        CALL ShpFltL(Mac,SaveKinetic)
      ELSE
        WRITE(*,*) 'Error: Unknown Mac Shp!=',Shp
        STOP 'In Routine: MakeMacElem'
      END IF

C Make the node at the end of the macroelement. If this is not a double
C node, it will be re-made in the next loop. However, we must have the last
C point on the element stored, so that we can next check the micro elements of
C the macro element to see that the iso-parametric transformation is 1-1.

      Indx=MacIndx(Mac,2)
      CALL MakeCoord(MacVertX(MacIndx(Mac,2)),MacVertY(MacIndx(Mac,2)),
& MacEnd(Mac),Mac,SaveKinetic)

C Check the x,y locations on micro elements to make sure the isoparametric
C mapping is (1-1).

      IF (BasisDeg.EQ.1) RETURN

      IF (BasisDeg.NE.2) THEN

        WRITE(*,*) 'Warning: Unable to test nodes for 1-1',
& ' isoparametric mapping'

      ELSE

D      WRITE(*,*) 'Shp ',Shp,' Mac',Mac
        CALL ChkIsoPara(Mac)

```

```

END IF

RETURN
END

```

C ***** MakeMeshPts

```

SUBROUTINE MakeMeshPts(SaveKinetic,Smooth)

```

```

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBPar.INC'
INCLUDE 'ECBMac.INC'
INCLUDE 'ECBMsh.INC'
INCLUDE 'ECBBC.INC'

```

```

INTEGER Mac,Sum
LOGICAL SaveKinetic,Smooth

```

```

CALL MatSumI(NoOfMicElems,1,NoOfMacElems,NoOfElems)

```

```

Sum=NoOfElems*BasisDeg

```

```

IF (Sum.GT.MaxNoOfCoords) THEN

```

```

    WRITE(*,*) 'Error: ',Sum,' coordinates have been specified.',

```

```

    & ' I only have room for ',MaxNoOfCoords,'

```

```

    WRITE(*,*) '    Increase the parameter MaxNoOfCoords in ',

```

```

    & 'ECBMsh.INC and recompile, or, alter the'

```

```

    WRITE(*,*) '    number of microelements specified in your',

```

```

    & ' *.MAC file.'

```

```

    STOP 'In routine: MakeMeshPts'

```

```

END IF

```

c IF (Smooth) WRITE(*,*) 'Smoothing Spline will be used!'

```

DO Mac=1,NoOfMacElems

```

```

    CALL MakeMacElem(Mac,SaveKinetic,Smooth)

```

```

END DO

```

```

CALL MakeElemBC

```

```

RETURN

```

```

END

```

C ***** MakeMoved

```

SUBROUTINE MakeMoved(ElemStart,ElemEnd,NodeMap,Coords)

```

C Passed Variables

C ElemStart Moving boundary starts with first point of

C microelement ElemStart

C ElemEnd Moving Boundary ends with last point of microelement ElemEnd

C Coords(.) (original) Coordinates of mesh

```

INCLUDE 'ECBHdr.INC'

```

```

INCLUDE 'ECBMOVE.INC'

```

```

INTEGER ElemStart,ElemEnd,

```

```

& NodeMap(MaxNoOfCoords,MaxBasisDeg+1)

```

```

REAL*8 Coords(MaxNoOfCoords,MaxNoOfDim)

```

```
INTEGER Elem,Loc
```

```
NoOfMoved=0
```

```
C Forces the 1st point on the boundary to be an endpoint for an element
```

```
D WRITE(*,*) ' MakeMoved: ElemStart=',ElemStart,
D & ' ElemEnd=',ElemEnd
```

```
DO Elem=ElemStart,ElemEnd
  DO Loc=1,BasisDeg+1
    CALL CopyPoint(NodeMap(Elem,Loc),Coords,NoOfMoved,Moved)
  END DO
END DO
```

```
Orig(1,1)=Moved(2,1)
Orig(1,2)=Moved(2,2)
Orig(2,1)=Moved(NoOfMoved-1,1)
Orig(2,2)=Moved(NoOfMoved-1,2)
```

```
RETURN
END
```

```
C ***** MakeNodeMap
```

```
SUBROUTINE MakeNodeMap
```

```
INTEGER Mac,Loc,I,PrevElem,MacPlus1
LOGICAL MacNat
EXTERNAL MacNat
```

```
INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMsh.INC'
INCLUDE 'ECBMac.INC'
```

```
NoOfCoords=1
DO Mac=1,NoOfMacElems
```

```
  MacStart(Mac)=NoOfCoords
```

```
C Compute NodeMap
```

```
CALL ComputePrevElem(Mac,PrevElem)
DO I=PrevElem+1,PrevElem+NoOfMicElems(Mac)
```

```
  DO Loc=1,BasisDeg+1
    NodeMap(I,Loc)=NoOfCoords
    NoOfCoords=NoOfCoords+1
  END DO
  NoOfCoords=NoOfCoords-1
```

```
END DO
```

```
C Make Corner Points if necessary (Double node where BC changes)
```

```
CALL IncrementI(Mac,MacPlus1,1,NoOfMacElems)
```

```
MacEnd(Mac)=NoOfCoords
```



```

      IF (MacNat(MacBCType(MacPlus1)).NE.MacNat(MacBCType(Mac)))
& NoOfCoords=NoOfCoords+1

```

```

      END DO

```

```

      NoOfCoords=NoOfCoords-1

```

```

      IF (MacNat(MacBCType(1)).EQ.MacNat(MacBCType(NoOfMacElems)))
& THEN

```

```

        CALL ComputePrevElem(NoOfMacElems,PrevElem)

```

```

        NodeMap(PrevElem+NoOfMacElems(NoOfMacElems),BasisDeg+1)=1

```

```

      END IF

```

```

      RETURN

```

```

      END

```

```

C ***** MakeSrcPts

```

```

      SUBROUTINE MakeSrcPts

```

```

        INCLUDE 'ECBHDR.INC'

```

```

        INCLUDE 'ECBSRC.INC'

```

```

        INCLUDE 'ECBPARG.INC'

```

```

        INCLUDE 'ECBMsh.INC'

```

```

        INCLUDE 'ECBBC.INC'

```

```

        INCLUDE '[kj.for.util]pi.inc'

```

```

        INCLUDE 'EcbElm.INC'

```

```

        REAL*8 R,Zeta,Phi(MaxBasisDeg+1),

```

```

& PhiZeta(MaxBasisDeg+1),dRdZeta(MaxNoOfDim),VecNormDP

```

```

        REAL*8 Norm,Nx(MaxNoOfDim)

```

```

        INTEGER I,Ip1,NSrc,Loc

```

```

        EXTERNAL VecNormDP

```

```

        NoOfSrc=NoOfCoords

```

```

        NSrc=0

```

```

        DO I=1,NoOfElems

```

```

            CALL GetElemR(I)

```

```

            R = SQRT( (ElemR(1,1)-ElemR(1,2))*(ElemR(1,1)-ElemR(1,2)) +

```

```

& (ElemR(2,1)-ElemR(2,2))*(ElemR(2,1)-ElemR(2,2)) ) +

```

```

& SQRT( (ElemR(1,2)-ElemR(1,3))*(ElemR(1,2)-ElemR(1,3)) +

```

```

& (ElemR(2,2)-ElemR(2,3))*(ElemR(2,2)-ElemR(2,3)) )

```

```

            DO Loc=1,BasisDeg+1

```

```

                Zeta=FLOAT(Loc-1)/FLOAT(BasisDeg)

```

```

                CALL Compute1DPhis(BasisDeg,Zeta,Phi,PhiZeta)

```

```

            CALL ComputeRZ(PhiZeta,dRdZeta)

```

```

            Norm=VecNormDP(NoOfDim,dRdZeta)

```

```

C Outward Pointing Normal.

```

```

      IF (Norm.NE.0) THEN

```

```

        Nx(1)= dRdZeta(2)/Norm

```

```

        Nx(2)=-dRdZeta(1)/Norm

```

```

      ELSE

```

```

        WRITE(*,*) 'Error: no normal to surface!'

```

```

WRITE(*,*) '      ElemR=',ElemR(1,1),ElemR(2,1)
WRITE(*,*) '           ',ElemR(1,2),ElemR(2,2)
WRITE(*,*) '           ',ElemR(1,3),ElemR(2,3)
WRITE(*,*) '      Loc=',Loc,' Elem=',I
Stop 'In routine: MakeSrcPts'
END IF

```

```

NSrc=NSrc+1
Src(NSrc,1)=Coords(NodeMap(I,Loc),1)+SrcFactor*Nx(1)*R
Src(NSrc,2)=Coords(NodeMap(I,Loc),2)+SrcFactor*Nx(2)*R
END DO

```

```

CALL IncrementI(I,IP1,1,NoOfCoords)
IF (ElemBCType(I).EQ.ElemBCType(IP1)) NSrc=NSrc-1

```

```

END DO

```

```

RETURN
END

```

C ***** Move

```

SUBROUTINE Move(dt)

```

C This subroutine moves the coords.

C Variables-----

C dt The size of the current time step.

```

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMOVE.INC'

```

```

INTEGER I,J
REAL*8 dt

```

```

DO I=1,NoOfMoved
  DO J=1,NoOfDim
    Moved(I,J)=Moved(I,J)-dXdN(I)*Nx(I,J)*dt
  END DO
END DO

```

```

RETURN
END

```

C ***** NewtonRaphson

```

SUBROUTINE NewtonRaphson(Iteration,NoOfdBCValues,
& dBCValues,MagDiff,MagBC)

```

C Newton Raphson Iteration Scheme. This is guaranteed to converge if our
C first guess is close enough to the solution. For Kinetics BCs, the
C current is solved for using BEM. The potential guess is adjusted
C until the current solved for does not differ from the current using
C kinetic relation.

```

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMsh.INC'

```

```

INCLUDE 'ECBCal.INC'
INCLUDE 'ECBPARG.INC'
INCLUDE 'ECBBC.INC'

```

```

REAL*8 dBCValues(*),MagDiff,MagBC
REAL*8 Jacobian(MaxNoOfCoords,MaxNoOfCoords),
& VecB1(MaxNoOfCoords),SlopePot,Slope,VecB(MaxNoOfCoords)
REAL*8 SlopePots(MaxNoOfCoords)
INTEGER NoOfdBCValues,JCol,JRow,I,J,Iteration
LOGICAL KineticBC
EXTERNAL KineticBC

```

```

MagDiff=0.0
MagBC=0.0

```

```

JCol=1

```

```

DO I=1,NoOfCoords
  IF (KineticBC(BCType(I))) THEN

```

```

    IF (Iteration.LT.1) THEN

```

```

C Compute the Bem Part of the Jacobian

```

```

    DO J=1,NoOfCoords
      VecB1(J)=BemH(J,I)
    END DO
    CALL SolveRelEq(VecB1,dBCValues)

```

```

    JRow=1
    DO J=1,NoOfCoords
      IF (KineticBC(BCType(J))) THEN
        Jacobian(JRow,JCol)=dBCValues(J)
        JRow=JRow+1
      END IF
    END DO

```

```

    ELSE
      Jacobian(JCol,JCol)=Jacobian(JCol,JCol)+SlopePots(JCol)
    END IF

```

```

C Compute the Kinetic Part of the Jacobian

```

```

    CALL ECBKinetics(BCValues(I),BCType(I),
& Slope,SlopePots(JCol),I)
    Jacobian(JCol,JCol)=Jacobian(JCol,JCol)-SlopePots(JCol)

```

```

C The following lines compute the B vector for the matrix equation
C Jacobian.dBCValues=VecB

```

```

    VecB(JCol)=- (SolValues(I)-Slope)
    MagDiff=MagDiff+VecB(JCol)*VecB(JCol)
    MagBC=MagBC+BCValues(I)*BCValues(I)

```

```

C Increment number of columns

```

```

    JCol=JCol+1

```

```

      END IF
    END DO

```

C The following line computes the number of Kinetic bc values

```

      NoOfdBCValues=JCol-1

      IF (NoOfdBCValues.LE.0) RETURN

      MagDiff=SQRT(MagDiff)
      MagBC=SQRT(MagBC)

```

C Call IMSL Routine DLSARG to get new BCValues by solving equation
C dBCValues=INV(Jacobian)VecB

```

      CALL DLSARG(NoOfdBCValues,Jacobian,MaxNoOfCoords,VecB,1,
& dBCValues)

      RETURN
    END

```

C ***** ObAngAtBdryBeg

```

SUBROUTINE ObAngAtBdryBeg

```

```

  INCLUDE 'ECBHdr.INC'
  INCLUDE 'ECBMOVE.INC'

```

```

  REAL*8 Xc,Yc,R,XInt1,YInt1,XInt2,YInt2
  REAL*8 PtsX(MaxNoOfCoords),PtsY(MaxNoOfCoords)
  INTEGER I,J,K,Error,NPts

```

```

  REAL*8 Mag
  EXTERNAL Mag

```

D WRITE(*,*) '-----: ObAngAtBdryBeg'

```

  Xc=Ins(First,1)
  Yc=Ins(First,2)
  R=Mag(Moved(1,1)-Xc,Moved(1,2)-Yc)

```

```

  IF (.NOT.StaRev) THEN

```

```

    DO J=First,NoOfIns-1
      CALL CirLinNtrxn(Ins(J,1),Ins(J,2),Ins(J+1,1),Ins(J+1,2),
& Xc,Yc,R,XInt1,YInt1,XInt2,YInt2,Error)
      IF (Error.EQ.0) GOTO 1
      IF (Error.EQ.1) THEN
        WRITE(*,*) 'Error: Moved boundary intersects insulator in'
        WRITE(*,*) '      two possible locations.'
        STOP 'In Routine: ObAngAtBdryBeg'
      END IF
    END DO
    CALL ObAngErr

```

```

  ELSE IF (First.NE.1) THEN

```

```

    J=1

```

```

      CALL CirLinNtrsxn(Ins(J,1),Ins(J,2),Ins(J+1,1),Ins(J+1,2),
& Xc,Yc,R,XInt1,YInt1,XInt2,YInt2,Error)
      IF (Error.EQ.1) THEN
        WRITE(*,*) 'Error: Moved boundary intersects insulator in'
        WRITE(*,*) '      two possible locations.'
        STOP 'In Routine: ObtAngAtBdryBeg'
      ELSE IF (Error.NE.0) THEN
        CALL ObtAngErr
      END IF

```

```

ELSE

```

```

      WRITE(*,*) 'Error: Start of boundary is moving backwards, and'
      WRITE(*,*) '      insulator is not extended.'
      WRITE(*,*) '      To extend the insulator, make a file: INS.EXT'
      WRITE(*,*) '      containing: x at Beg, y at Beg'
      WRITE(*,*) '      x at End, y at End'
      STOP 'In Routine: ObtAngAtBdryBeg'

```

```

END IF

```

```

1  CALL RemoveBdryBefore(NoOfIns,Ins,J,XInt1,YInt1)
   Last=Last-J+1
   NextToLast=NextToLast-J+1

```

```

C Use Counterclockwise circle for backward boundary movement,
C Clockwise circle for forward boundary movement.

```

```

      CALL CirPts(Xc,Yc,XInt1,YInt1,Moved(1,1),Moved(1,2),
& NPts,PtsX,PtsY,.NOT.StaRev)

```

```

10  FORMAT(X,A40,2X,G12.4,2X,G12.4)

```

```

D   WRITE(*,*) '      Bdry Start'
D   IF (.NOT.StaRev) THEN
D     WRITE(*,10) 'Counter-Clockwise Circle, Center:',Xc,Yc
D   ELSE
D     WRITE(*,10) 'Clockwise Circle, Center:',Xc,Yc
D   END IF
D   WRITE(*,10) 'From:',XInt1,YInt1
D   WRITE(*,10) 'To:',Moved(1,1),Moved(1,2)

```

```

      IF (NPts.EQ.2) THEN
        IF ((XInt1.EQ.Moved(1,1)).AND.(YInt1.EQ.Moved(1,2))) THEN
          RETURN
        END IF
      END IF

```

```

C Bump Points up to make room for new points

```

```

      DO I=NoOfMoved,1,-1
        DO K=1,NoOfDim
          Moved(I+NPts-1,K)=Moved(I,K)
        END DO
      END DO

```

```

C Add New Points

```

```

D   WRITE(*,*) 'Adding Points at Beginning:'
    DO I=1,NPts-1
      Moved(I,1)=PtsX(I)
      Moved(I,2)=PtsY(I)
D   WRITE(*,*) PtsX(I),PtsY(I)
    END DO
    NoOfMoved=NoOfMoved+NPts-1

    RETURN
    END

```

C ***** ObAngAtBdryEnd

```

SUBROUTINE ObAngAtBdryEnd

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMOVE.INC'

REAL*8 XInt1,YInt1,XInt2,YInt2,R,Xc,Yc
REAL*8 PtsX(MaxNoOfCoords),PtsY(MaxNoOfCoords)
INTEGER I,J,K>Error,NPts

REAL*8 Mag
EXTERNAL Mag

R=Mag(Moved(NoOfMoved,1)-Ins(Last,1),
& Moved(NoOfMoved,2)-Ins(Last,2))
Xc=Ins(Last,1)
Yc=Ins(Last,2)

IF (.NOT.EndRev) THEN

  DO J=Last,2,-1
    CALL CirLinNtrsxn(Ins(J,1),Ins(J,2),Ins(J-1,1),Ins(J-1,2),
& Xc,Yc,R,XInt1,YInt1,XInt2,YInt2>Error)
    IF (Error.EQ.0) GOTO 1
    IF (Error.EQ.1) THEN
      WRITE(*,*) 'Error: Moved boundary intersects insulator in'
      WRITE(*,*) '      two possible locations.'
      STOP 'In Routine: ObAngAtBdryEnd'
    END IF
  END DO
  CALL ObAngErr

ELSE IF (Last.NE.NoOfIns) THEN

  J=NoOfIns
  CALL CirLinNtrsxn(Ins(J,1),Ins(J,2),Ins(J-1,1),Ins(J-1,2),
& Xc,Yc,R,XInt1,YInt1,XInt2,YInt2>Error)
  IF (Error.EQ.1) THEN
    WRITE(*,*) 'Error: Moved boundary intersects insulator in'
    WRITE(*,*) '      two possible locations.'
    STOP 'In Routine: ObAngAtBdryEnd'
  ELSE IF (Error.NE.0) THEN
    CALL ObAngErr
  END IF

ELSE

```

```

WRITE(*,*) 'Error: End of boundary is moving backwards, and'
WRITE(*,*) '      insulator is not extended.'
WRITE(*,*) '      To extend the insulator, make a file: INS.EXT'
WRITE(*,*) '      containing: x at Beg, y at Beg'
WRITE(*,*) '      x at End, y at End'
WRITE(*,*) 'Last=',Last,'NoOfIns=',NoOfIns
STOP 'In Routine: ObtAngAtBdryEnd'

```

```
END IF
```

```
1 CALL RemoveBdryAfter(NoOfIns,Ins,J,XInt1,YInt1)
```

```
C Use clockwise circle for forward boundary movement, counterclockwise
C for backward movement.
```

```

D WRITE(*,*) ' Bdry End'
D IF (.NOT.EndRev) THEN
D WRITE(*,10) 'Clockwise Circle, Center:',Xc,Yc
D ELSE
D WRITE(*,10) 'Counter-Clockwise Circle, Center:',Xc,Yc
D END IF
D WRITE(*,10) 'From:',Moved(NoOfMoved,1),
D & Moved(NoOfMoved,2)
D WRITE(*,10) 'To:',XInt1,YInt1

```

```
CALL CirPts(Xc,Yc,Moved(NoOfMoved,1),Moved(NoOfMoved,2),
& XInt1,YInt1,NPts,PtsX,PtsY,.NOT.EndRev)
```

```
10 FORMAT(X,A40,2X,G12.4,2X,G12.4)
```

```
C Store new points.
```

```

IF (NPts.EQ.2) THEN
IF ((XInt1.EQ.Moved(NoOfMoved,1))
& .AND.(YInt1.EQ.Moved(NoOfMoved,2))) THEN
RETURN
END IF
END IF

```

```

D WRITE(*,*) 'Adding Points at Ending:'
DO I=2,NPts
Moved(NoOfMoved+I-1,1)=PtsX(I)
Moved(NoOfMoved+I-1,2)=PtsY(I)
D WRITE(*,*) PtsX(I),PtsY(I)
END DO

```

```
NoOfMoved=NoOfMoved+NPts-1
```

```
RETURN
END
```

```
C ***** ObtAngErr
```

```
SUBROUTINE ObtAngErr
```

```

WRITE(*,*) 'Error: No intersection found between insulator and',
& ' moved boundary.'
STOP 'In routine: ObtAngErr'

```

END

C ***** Picard

SUBROUTINE Picard(NoOfdBCValues,dBCValues,MagDiff)

C This subroutine uses a Picard iteration scheme instead of Newton-Raphson
 C type of iteration. The Picard scheme, if it converges, can be much faster
 C than the Newton-Raphson scheme. For Kinetic BCs, the current is solved for
 C using BEM. The potential guess is adjusted until the current solved for
 C does not differ from the current using kinetic relation.

INCLUDE 'ECBHdr.INC'
 INCLUDE 'ECBMsh.INC'
 INCLUDE 'ECBCal.INC'
 INCLUDE 'ECBBC.INC'

REAL*8 dBCValues(*),MagDiff,VecNormDP
 REAL*8 dBCValue,Jacobian(MaxNoOfCoords,MaxNoOfCoords),
 & VecB(MaxNoOfCoords),SlopePot
 REAL*8 Slope(MaxNoOfCoords),PotPert,PotUnpert
 INTEGER NoOfdBCValues,JCol,JRow,I,J
 LOGICAL KineticBC,FindSlope
 EXTERNAL KineticBC,VecNormDP

WRITE (*,*) 'Error: Picard routine called. This routine doesn''t'
 WRITE(*,*) 'currently work! Sorry...'

c MagDiff=0.0
 c FindSlope=.FALSE.
 c
 c dBCValue=0.0001
 c JCol=1
 c DO I=1,NoOfCoords
 c IF (KineticBC(BCType(I))) THEN
 c
 c CALL ECBKinetics(BCType(I),SolValues(I),PotUnpert,I,
 c & FindSlope)
 c dBCValues(JCol)=PotUnPert-BCValues(I)
 c MagDiff=MagDiff+dBCValues(JCol)*dBCValues(JCol)
 cc JCol=JCol+1
 c
 c END IF
 c END DO
 c
 c NoOfdBCValues=JCol-1
 c MagDiff=SQRT(MagDiff)

STOP 'In Routine: Picard'
 END

C ***** Pla2B3

REAL*8 FUNCTION Pla2B3(GaussPt)

C For an Planar Problem, with 2nd Order basis functions,
 C this function returns the bounded portion of the integrand for

C loc=3

```

INCLUDE 'ECBHDR.INC'
REAL*8 GaussPt

REAL*8 UstarB,RBig,Eta,IsoJacob,Phi(MaxBasisDeg+1)

```

C From Common ElemR

```

Eta=1-GaussPt
CALL PlaSub(Eta,3,IsoJacob,Phi,RBig)

```

```

UStarB=-0.5*LOG(RBig)
Pla2B3 = UStarB*IsoJacob*Phi(3)

```

```

RETURN
END

```

C ***** Pla2B2

```

REAL*8 FUNCTION Pla2B2(GaussPt)

```

C For an Planar Problem, with 2nd Order basis functions,
C this function returns the bounded portion of the integrand
C for loc=2

```

REAL*8 GaussPt

```

```

INCLUDE 'ECBHDR.INC'
REAL*8 UstarB,RBig,Eta,IsoJacob,Phi(MaxBasisDeg+1)

```

C From Common ElemR

```

Eta=(1.0-GaussPt)/2.0
CALL PlaSub(Eta,2,IsoJacob,Phi,RBig)

```

```

UStarB=-0.5*LOG(RBig)
Pla2B2 = UStarB*IsoJacob*Phi(2)/2.0

```

```

Eta=(1.0+GaussPt)/2.0
CALL PlaSub(Eta,2,IsoJacob,Phi,RBig)

```

```

UStarB=-0.5*LOG(RBig)
Pla2B2 = Pla2B2 + UStarB*IsoJacob*Phi(2)/2.0

```

```

RETURN
END

```

C ***** Pla2B1

```

REAL*8 FUNCTION Pla2B1(GaussPt)

```

C For an Planar Problem, with 2nd Order basis functions,
C this function returns the bounded portion of the integrand for
C loc=1

```

REAL*8 GaussPt

```

```

INCLUDE 'ECBHDR.INC'
REAL*8 UStarB,RBig,IsoJacob,Phi(MaxBasisDeg+1)

```

C From Common ElemR

```
CALL PlaSub(GaussPt,1,IsoJacob,Phi,RBig)
```

```
UStarB=-0.5*LOG(RBig)
Pla2B1 = UStarB*IsoJacob*Phi(1)
```

```
RETURN
END
```

C ***** Pla2U3

```
REAL*8 FUNCTION Pla2U3(GaussPt)
```

C For an Planar Problem, with 2nd Order basis functions,
C this function returns the unbounded portion of the integrand for
C loc=3 (Note: the unbounded LN(1/GaussPt) term is NOT included. This
C is accounted for in the integration routine points and weights)

```
REAL*8 GaussPt
```

```
INCLUDE 'ECBHDR.INC'
REAL*8 RBig,Eta,IsoJacob,Phi(MaxBasisDeg+1)
```

C From Common ElemR

```
Eta=1-GaussPt
CALL PlaSub(Eta,1,IsoJacob,Phi,RBig)
```

```
Pla2U3 = IsoJacob*Phi(3)
```

```
RETURN
END
```

C ***** Pla2U2

```
REAL*8 FUNCTION Pla2U2(GaussPt)
```

C For an Planar Problem, with 2nd Order basis functions,
C this function returns the unbounded portion of the integrand for
C loc=2 (Note: the unbounded LN(1/GaussPt) term is NOT included. This
C is accounted for in the integration routine points and weights)

```
REAL*8 GaussPt
```

```
INCLUDE 'ECBHDR.INC'
REAL*8 RBig,Eta,IsoJacob,Phi(MaxBasisDeg+1)
```

C From Common ElemR

```
Eta=(1.0-GaussPt)/2.0
CALL PlaSub(Eta,2,IsoJacob,Phi,RBig)
```

```
Pla2U2 = IsoJacob*Phi(2)/2.0
```

```

Eta=(1.0+GaussPt)/2.0
CALL PlaSub(Eta,2,IsoJacob,Phi,RBig)

```

```

Pla2U2 = Pla2U2 + IsoJacob*Phi(2)/2.0

```

```

RETURN
END

```

```

C ***** Pla2U1

```

```

REAL*8 FUNCTION Pla2U1(GaussPt)

```

```

C For an Planar Problem, with 2nd Order basis functions,
C this function returns the unbounded portion of the integrand for
C loc=1 (Note: the unbounded LN(1/GaussPt) term is NOT included. This
C is accounted for in the integration routine points and weights)

```

```

REAL*8 GaussPt

```

```

INCLUDE 'ECBHDR.INC'
REAL*8 RBig,IsoJacob,Phi(MaxBasisDeg+1)

```

```

C From Common ElemR

```

```

CALL PlaSub(GaussPt,1,IsoJacob,Phi,RBig)

```

```

Pla2U1 = IsoJacob*Phi(1)

```

```

RETURN
END

```

```

C ***** PlaSub

```

```

SUBROUTINE PlaSub(GaussPt,Loc,IsoJacob,Phi,RBig)

```

```

INCLUDE 'ECBHDR.INC'
INCLUDE 'ECBPARG.INC'

```

```

C From Common ElemR, SourceR
INCLUDE 'ECBELM.INC'

```

```

INTEGER Loc
REAL*8 GaussPt,IsoJacob,Phi(*),RBig

```

```

REAL*8 R(MaxNoOfDim)
REAL*8 dRdZeta(MaxNoOfDim),PhiZeta(MaxBasisDeg+1)

```

```

C Functions

```

```

REAL*8 IsoJacobian
EXTERNAL IsoJacobian

```

```

C From Common BasisDeg, ElemR, SourceR

```

```

CALL Compute1DPhis(BasisDeg,GaussPt,Phi,PhiZeta)
CALL ComputeRZ(Phi,R)

```

```

IsoJacob=IsoJacobian(PhiZeta,dRdZeta)

```

```
CALL ComputeRBig(GaussPt,Loc,RBig)
```

```
RETURN
END
```

```
C ***** PrepInt
```

```
  SUBROUTINE PrepInt(Elem)
```

```
C This subroutine prepares variables for use in the integration subroutine.
C Two things are accomplished here: 1) The node coordinates on the element
C are put into ElemR and 2) values that need only be calculated once for
C each element are computed, such as Isojacobian, Normal, ... at each
C gaussian integration point.
```

```
C Common Variables
```

```
  INCLUDE 'ECBPar.INC'
  INCLUDE 'ECBHdr.INC'
  INCLUDE 'ECBMsh.INC'
  INCLUDE 'ECGaus.INC'
  INCLUDE 'ECBG.INC'
  INCLUDE 'EcbElm.INC'
```

```
C Passed Variables
```

```
  INTEGER Elem
```

```
C Internal Variables
```

```
  INTEGER Gs,Loc,I
  REAL*8 R(MaxNoOfDim),dRdZeta(MaxNoOfDim),
  & IsoJacob,Normal(MaxNoOfDim)
  REAL*8 Phi(MaxBasisDeg+1),PhiZeta(MaxBasisDeg+1)
```

```
C Functions
```

```
  REAL*8 IsoJacobian
  EXTERNAL IsoJacobian
```

```
C Code Follows
```

```
  CALL GctElemR(Elem)
```

```
C The following DO-Loop computes variables of interest that only need
C to be calculated one time and stored, so that we save computing time
C when in the loop over source points.
```

```
  DO Gs=1,NoOfGaussPts
    CALL Compute1DPhis(BasisDeg,GaussPts(Gs),Phi,PhiZeta)
    CALL ComputeRZ(Phi,R)
    IsoJacob=IsoJacobian(PhiZeta,dRdZeta)
```

```
C The following two statements compute the outward pointing normal multiplied
C by IsoJacob.
```

```
  Normal(1) =+dRdZeta(2)
  Normal(2) =-dRdZeta(1)
```

```

      GIsoJacob(Gs)=IsoJacob
      DO I=1,NoOfDim
        GNormal(Gs,I)=Normal(I)
        GR(Gs,I)=R(I)
      END DO
      DO I=1,BasisDeg+1
        GPhi(Gs,I)=Phi(I)
      END DO
    END DO

    RETURN
  END

```

C ***** PrintMesh

```

SUBROUTINE PrintMesh(Lun,Msg)

```

```

  INTEGER Lun,I,K
  INCLUDE 'ECBHdr.INC'
  INCLUDE 'ECBMsh.INC'
  INCLUDE 'ECBBC.INC'
  LOGICAL LastNat
  CHARACTER*(*) Msg

```

```

1  FORMAT(X,80('*'))
2  FORMAT(X,A40,29X,'Mesh Report')
10 FORMAT(X,' Boundary Conditions',12X,'Coordinates',
  & /,X,' Nat BC Value Sol Value',5X,'i',7X,'X',9X,'Y',
  & /)
11 FORMAT(X,2X,A1,2X,G10.4,X,G10.4,3X,I3,2X,G10.4,X,G10.4)

```

```

C123          123456789a12
C Boundary Conditions      Coordinates
C1 12      12      12345 1234567 123456789
C Nat BC Value Sol Value  i    X    Y
C12 12      123  12
C a ddddddddd ddddddddd iii ddddddddd ddddddddd
C 123456789a 123456789a 123 123456789a 123456789a

```

```

  WRITE(Lun,1)
  WRITE(Lun,2) Msg
  WRITE(Lun,1)
  WRITE(Lun,*) ' '
  WRITE(Lun,10)
  LastNat=Natural(1)
  DO I=1,NoOfCoords
    IF (LastNat.NE.Natural(I)) WRITE(Lun,*) ' '
    LastNat=Natural(I)

    IF (Natural(I)) THEN
      WRITE(Lun,11) 'T',BCValues(I),
        & SolValues(I),I,
        & Coords(I,1),Coords(I,2)
    ELSE
      WRITE(Lun,11) 'F',BCValues(I),
        & SolValues(I),I,
        & Coords(I,1),Coords(I,2)
    END IF
  END DO

```

END DO

RETURN

END

C ***** PrintNodeMap

SUBROUTINE PrintNodeMap(Lun)

INTEGER Lun,I,K
 INCLUDE 'ECBHdr.INC'
 INCLUDE 'ECBMsh.INC'
 INCLUDE 'ECBBC.INC'

C 123

C Element Nodes

C iii iii,iii,iii,iii,...

C 123456

20 FORMAT(/,X,'Element Nodes',/)

30 FORMAT(X,X,I3,6X,I3,10(:,',',I3))

WRITE(Lun,20)

DO I=1,NoOfElems

WRITE(Lun,30) I,(NodeMap(I,K),K=1,BasisDeg+1)

END DO

RETURN

END

C ***** PrintSrc

SUBROUTINE PrintSrc(Lun)

INCLUDE 'ECBHdr.INC'
 INCLUDE 'ECBSrc.INC'

INTEGER Lun,I

C SOURCE POINTS

C 1 1234567 123456789a

C i X Y

C iii dddddddddd dddddddddd

C 123 123456789a 123456789a

10 FORMAT(X,'SOURCE POINTS',
 & /,X,' i',7X,'X',10X,'Y',
 & /)

20 FORMAT(X,I3,X,G10.4,X,G10.4)

WRITE(Lun,10)

DO I=1,NoOfSrc

WRITE(Lun,20) I,Src(I,1),Src(I,2)

END DO

RETURN

END

C ***** QStar

```
REAL*8 FUNCTION QStar(Dist2,Gs,Den,M)
```

```
INCLUDE 'ECBPar.INC'
```

C The following two include files are necessary for dimensioning items in
C the following third include file.
C QStar is multiplied by 2Pi

```
INCLUDE 'ECBHdr.INC'  
INCLUDE 'ECGaus.INC'  
INCLUDE 'ECBG.INC'  
INCLUDE 'ECBEIm.INC'
```

```
INTEGER Gs  
REAL*8 Dist2,Den,M  
REAL*8 T1,T2,T3,First,Second
```

```
REAL*8 KElliptic,EElliptic  
EXTERNAL KElliptic,EElliptic
```

```
IF (Axisymmetric) THEN
```

C The problem is an Axisymmetric.
C QStar is multiplied by 2Pi

```
T1 = KElliptic(M)
```

```
T2 = EElliptic(M)*  
& (SourceR(1)*SourceR(1)-GR(Gs,1)*GR(Gs,1)  
& + (Gr(Gs,2)-SourceR(2))*(Gr(Gs,2)-SourceR(2)))  
T2 = T2/((GR(Gs,1)-SourceR(1))*(GR(Gs,1)-SourceR(1))  
& + (Gr(Gs,2)-SourceR(2))*(Gr(Gs,2)-SourceR(2)))
```

```
T3 = 2.0*EElliptic(M) * (SourceR(2)-Gr(Gs,2))  
& / ((GR(Gs,1)-SourceR(1))*(GR(Gs,1)-SourceR(1))  
& + (Gr(Gs,2)-SourceR(2))*(Gr(Gs,2)-SourceR(2)))
```

```
QStar = ( (-T1+T2) * GNormal(Gs,1)  
& + T3 * GNormal(Gs,2) * Gr(Gs,1) )/SQRT(Den)
```

```
ELSE
```

C The problem is planar
C QStar is multiplied by 2Pi

```
QStar=( (SourceR(1)-GR(Gs,1)) * GNormal(Gs,1) +  
& (SourceR(2)-GR(Gs,2)) * GNormal(Gs,2) ) / (Dist2)
```

```
END IF
```

```
RETURN  
END
```

C ***** ReadCal

```
SUBROUTINE ReadCal(FileName)
```

```
INCLUDE 'ECBHdr.INC'
```

```

INCLUDE 'ECBMsh.INC'
INCLUDE 'ECBCal.INC'
CHARACTER*(*) FileName
INTEGER I,J,Version
LOGICAL FileExist

INQUIRE(FILE=FileName,EXIST=FileExist)
IF (.NOT.FileExist) CALL ErrorFileName(FileName,'ReadCalcs')

OPEN(UNIT=1,FILE=FileName,STATUS='OLD',FORM='FORMATTED')

READ(1,*) Version

IF (Version.EQ.1) THEN
  DO I=1,NoOfCoords
    DO J=1,NoOfCoords
      READ(1,*) BemG(I,J),BemH(I,J)
    END DO
  END DO
ELSE
  CALL ErrorVersion(Version,FileName,'ReadCal')
END IF

CLOSE(1)

RETURN
END

```

C ***** ReadInt

```

SUBROUTINE ReadInt(FileName)

INCLUDE 'ECBHDR.INC'
INCLUDE 'ECBINT.INC'

CHARACTER*(*) FileName
LOGICAL FileExist
INTEGER Version,I,K

INQUIRE(FILE=FileName,EXIST=FileExist)
IF (.NOT.FileExist) CALL ErrorFileName(FileName,'ReadInt')

OPEN(UNIT=1,FILE=FileName,STATUS='OLD',FORM='FORMATTED')
READ(1,*) Version

IF (Version.EQ.1) THEN
  READ(1,*) NoOfInternal,NoOfSpines,IntPerSpine
  DO I=1,NoOfInternal
    READ(1,*) (InternalPts(I,K),K=1,NoOfDim),InternalPot(I)
  END DO
ELSE IF (Version.EQ.0) THEN
  READ(1,*) NoOfInternal,NoOfSpines,IntPerSpine
  DO I=1,NoOfInternal
    READ(1,*) (InternalPts(I,K),K=1,NoOfDim)
  END DO
ELSE
  CALL ErrorVersion(Version,FileName,'ReadInt')
END IF

```


CLOSE(1)

RETURN
END

C ***** ReadMac

SUBROUTINE ReadMac(FileName)

C This subroutine reads the contents of the BEM.MAC file. This file contains
C the information required to make the BEM.INP file, the more detailed file
C used by the BEMLIN.FOR program for input.

INCLUDE 'ECBMAC.INC'
CHARACTER*(*) FileName
INTEGER I,Version,FLen
LOGICAL FileExist

INQUIRE (FILE=FileName,EXIST=FileExist)
IF (.NOT.FileExist) CALL ErrorFileName(FileName,'ReadMac')

OPEN(UNIT=1,FILE=FileName,STATUS='OLD',FORM='FORMATTED')

READ(1,*) Version
IF ((Version.NE.1).AND.(Version.NE.2).AND.(Version.NE.3))
& CALL ErrorVersion(Version,FileName,'ReadMac')

READ(1,*) NoOfMacVert
IF (NoOfMacVert.GT.MaxNoOfMacVert) THEN
WRITE(*,*) 'Error: Number of macro-vertices,'NoOfMacVert
WRITE(*,*) ' is larger than the maximum number of '
WRITE(*,*) ' macro-vertices allowed:',MaxNoOfMacVert
STOP 'In Routine: ReadMac'
END IF

CALL StringLength(FileName,FLen)

D WRITE(*,*) 'Reading File ',FileName(1:FLen),' Version:',Version
D WRITE(*,*) ' ',NoOfMacVert,' macro vertices'
DO I=1,NoOfMacVert
READ(1,*) MacVertX(I),MacVertY(I)
END DO

READ(1,*) NoOfMacElems
D WRITE(*,*) ' ',NoOfMacElems,' macro elems'
DO I=1,NoOfMacElems
READ(1,*) MacShape(I),NoOfMicElems(I),MacBCType(I),MacBCVal(I),
& MacSpac(I),MacRatio(I)
IF (MacShape(I).EQ.'LINE') THEN
READ(1,*) MacIndx(I,1),MacIndx(I,2)
ELSE IF (MacShape(I).EQ.'SINE') THEN
READ(1,*) MacIndx(I,1),MacIndx(I,2)
READ(1,*) MacPar(I,1),MacPar(I,2)

C $(Y-Y_0)=A*\sin((Par1*X+Par2)*\pi)$ A and Y0 are solved for

ELSE IF (MacShape(I).EQ.'CIR') THEN
READ(1,*) MacIndx(I,1),MacIndx(I,2)
READ(1,*) MacPar(I,1),MacPar(I,2)

C CIR, Radius is determined from center and starting mac vertex #

```

      ELSE IF ((MacShape(I).EQ.'USER').OR.
& (MacShape(I).EQ.'USR')) THEN
        IF (Version.LE.2) THEN
          READ(1,*) MacIndx(I,1),MacIndx(I,2)
          MacBdryFile='USER'
        ELSE
          READ(1,*) MacIndx(I,1),MacIndx(I,2),MacBdryFile
        END IF
      ELSE IF (MacShape(I).EQ.'TRNS') THEN
        READ(1,*) MacIndx(I,1),MacIndx(I,2)
      ELSE IF (MacShape(I).EQ.'PREV') THEN
        READ(1,*) MacIndx(I,1),MacIndx(I,2)
        READ(1,*) MacPar(I,1),MacPar(I,2),MacPar(I,3),MacPar(I,4)
      ELSE IF (MacShape(I).EQ.'FLAT') THEN
        READ(1,*) MacIndx(I,1),MacIndx(I,2)
        READ(1,*) MacPar(I,1),MacPar(I,2)
C      BL thickness, Element to space away from
      ELSE IF (MacShape(I).EQ.'FTL') THEN
        READ(1,*) MacIndx(I,1),MacIndx(I,2)
        READ(1,*) MacPar(I,1),MacPar(I,2)
C      BL thickness, Element to space away from
      ELSE
        WRITE(*,*) 'Error: Unknown Macro-Element Type:',MacShape(I)
        STOP 'In Routine: ReadMac'
      END IF
      IF (Version.GE.2) READ(1,*) MacStart(I),MacEnd(I)
      IF (MacSpac(I).EQ.'USER') READ(1,*) MacSpaFile(I)
    END DO
  CLOSE(1)
D  WRITE(*,*) ' '

  RETURN
  END

```

C ***** ReadMesh

```

SUBROUTINE ReadMesh(FileName)

  CHARACTER*(*) FileName
  INTEGER Length,Version,I,J
  LOGICAL FileExist

  INCLUDE 'ECBHdr.INC'
  INCLUDE 'ECBMsh.INC'
  INCLUDE 'ECBBC.Inc'

  INQUIRE(FILE=FileName,EXIST=FileExist)

  IF (.NOT.FileExist) CALL ErrorFileName(FileName,'ReadMesh')

  OPEN(UNIT=1,FILE=FileName,STATUS='OLD',FORM='FORMATTED')

  READ(1,*) Version

  IF ((Version.EQ.1).OR.(Version.EQ.2)) THEN

```

```

      READ(1,*) NoOfCoords
      DO I=1,NoOfCoords
        READ(1,*) (Coords(I,J),J=1,NoOfDim)
        READ(1,*) BCValues(I),SolValues(I),Natural(I),BCType(I)
      END DO

      READ(1,*) NoOfElems
      DO I=1,NoOfElems
        READ(1,*) (NodeMap(I,J),J=1,BasisDeg+1),ElemNat(I),
& ElemBCType(I)
      END DO

      IF (Version.EQ.1) THEN
        DO I=1,NoOfElems
          DO J=1,BasisDeg+1
            Natural(NodeMap(I,J))=ElemNat(I)
            BCType(NodeMap(I,J))=ElemBCType(I)
          END DO
        END DO
      END IF

      ELSE

        CALL ErrorVersion(Version,FileName,'ReadMesh')

      END IF
      CLOSE(1)

      RETURN
      END

```

C ***** ReadPar

```

SUBROUTINE ReadPar(FileName)

  INCLUDE 'ECBHdr.INC'
  INCLUDE 'ECBPar.INC'
  INCLUDE 'ECGaus.INC'

  CHARACTER*(*) FileName
  LOGICAL FileExist
  INTEGER Length,I,Version
  REAL*8 JohnNewman,IRatio

  INQUIRE(FILE=FileName,EXIST=FileExist)
  IF (.NOT.FileExist) CALL ErrorFileName(FileName,'ReadPar')

  OPEN(UNIT=1,FILE=FileName,STATUS='OLD',FORM='FORMATTED')
  READ(1,*) Version

  CorLev=.FALSE.
  Spline3D=.FALSE.
  MaxIter=25

  IF (Version.EQ.1) THEN
    READ(1,*) NoOfDim,BasisDeg,NoOfGaussPts
    READ(1,*) SrcFactor,Tolerance
    READ(1,*) Axisymmetric

```

```
      READ(1,*) JohnNewman,IRatio
      READ(1,*) aA,aC
      MaxIter=25
      WagLin= 1/ (JohnNewman*IRatio)
ELSE IF (Version.EQ.2) THEN
      READ(1,*) NoOfDim,BasisDeg,NoOfGaussPts
      READ(1,*) SrcFactor,Tolerance,MaxIter
      READ(1,*) Axisymmetric
      READ(1,*) JohnNewman,IRatio
      READ(1,*) aA,aC
      WagLin= 1/ (JohnNewman*IRatio)
ELSE IF (Version.EQ.3) THEN
      READ(1,*) NoOfDim,BasisDeg,NoOfGaussPts
      READ(1,*) Spline3D
      READ(1,*) SrcFactor,Tolerance,MaxIter
      READ(1,*) Axisymmetric
      READ(1,*) JohnNewman,IRatio
      READ(1,*) aA,aC
      WagLin= 1/ (JohnNewman*IRatio)
ELSE IF (Version.EQ.4) THEN
      READ(1,*) NoOfDim,BasisDeg,NoOfGaussPts
      READ(1,*) Spline3D
      READ(1,*) SrcFactor,Tolerance,MaxIter
      READ(1,*) Axisymmetric
      READ(1,*) JohnNewman,IRatio
      READ(1,*) aA,aC
      READ(1,*) KineticsFile
      WagLin= 1/ (JohnNewman*IRatio)
ELSE IF (Version.EQ.5) THEN
      READ(1,*) NoOfDim,BasisDeg,NoOfGaussPts
      READ(1,*) Spline3D, Axisymmetric
      READ(1,*) CorLev, PerRev
      READ(1,*) Corros, CRRatio,WaLinPCR
      READ(1,*) SrcFactor,Tolerance,MaxIter
      READ(1,*) WagLin
      READ(1,*) aA,aC
      READ(1,*) KineticsFile
      READ(1,*) tstar,istar
ELSE IF (Version.EQ.6) THEN
      READ(1,*) NoOfDim,BasisDeg,NoOfGaussPts
      READ(1,*) Spline3D, Axisymmetric
      READ(1,*) CorLev, PerRev
      READ(1,*) Corros
      READ(1,*) NoOfPCR,CRRatio,WaLinPCR,PCRMax
      READ(1,*) SrcFactor,Tolerance,MaxIter
      READ(1,*) WagLin
      READ(1,*) aA,aC
      READ(1,*) KineticsFile
      READ(1,*) tstar,istar
ELSE
      CALL ErrorVersion(Version,FileName,'ReadPar')
END IF

CLOSE(1)

RETURN
END
```

C ***** ReadSrc

```

SUBROUTINE ReadSrc(FileName)

  INCLUDE 'ECBHdr.INC'
  INCLUDE 'ECBSrc.INC'
  INCLUDE 'ECBMsh.INC'

  INTEGER Version,I,J
  CHARACTER*(*) FileName
  LOGICAL FileExist

  INQUIRE(FILE=FileName,EXIST=FileExist)
  IF (.NOT.FileExist) CALL ErrorFileName(FileName,'ReadSrc')

  OPEN(UNIT=1,FILE=FileName,STATUS='OLD',FORM='FORMATTED')

  READ(1,*) Version

  IF (Version.EQ.1) THEN
    READ(1,*) NoOfSrc

    IF (NoOfSrc.NE.NoOfCoords) THEN
      WRITE(*,*) 'Error: Number of source points is not equal to'
      WRITE(*,*) '  the number of coordinates.'
      WRITE(*,*) '  Filename=' FileName
      WRITE(*,*) '  NoOfSrc=' NoOfSrc
      WRITE(*,*) '  NoOfCoords=' NoOfCoords
      STOP 'In Routine: ReadSrc'
    END IF

    DO I=1,NoOfSrc
      READ(1,*) (Src(I,J),J=1,NoOfDim)
    END DO
  ELSE
    CALL ErrorVersion(Version,FileName,'ReadSrc')
  END IF
  CLOSE(1)

  RETURN
END

```

C ***** ReMesh

```

SUBROUTINE ReMesh(NoOfSpa,Spa,NoOfPos,Pos)

```

C This subroutine remeshes the nodal locations.

C Input Variables

```

C NoOfSpa    The desired number of Spacings
C Spa0      The original Spacing
C NoOfPos   The number of original spacings and positions Pos(i,1..2)
C Pos(,2)   The original values of the function whose curvature is
C           equidistributed.

```

C Output Variables

C Spa() The relocated Spacings

C Passed Variables

```
INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBRemesh.INC'
REAL*8 Spa(*),Pos(MaxNoOfCoords,MaxNoOfDim)
INTEGER NoOfSpa,NoOfPos
```

C Local Variables

```
INTEGER I,J,K
REAL*8 Curvature(MaxNoOfCoords),TSpa,LowerBound,UpperBound,
& PosX(MaxNoOfCoords),PosY(MaxNoOfCoords)
REAL*8 Error(MaxNoOfCoords),AvgError,Sum,YMax,YMin
REAL*8 XCSCoef(4,MaxNoOfCoords),XBreak(MaxNoOfCoords)
REAL*8 YCSCoef(4,MaxNoOfCoords),YBreak(MaxNoOfCoords)
REAL*8 Orig(MaxNoOfCoords),Slope
LOGICAL Changes,FileRead/.FALSE./
```

C Functions

```
REAL*8 DCSDER,DCSITG,DCSVAL
EXTERNAL DCSDER,DCSITG,DCSVAL
```

```
IF (.NOT.FileRead) THEN
  OPEN(UNIT=2,FILE='REMESH.ECB',STATUS='OLD',FORM='FORMATTED')
  READ(2,*) SpaFac
  READ(2,*) UpFac,LowFac
  CLOSE(2)
  FileRead=.TRUE.
END IF
```

```
DO I=1,NoOfPos
  Orig(I)=Spa(I)
  PosX(I)=Pos(I,1)
  PosY(I)=Pos(I,2)
END DO
```

```
D  WRITE(*,*) 'Calling DCSSCV from Remesh: x'
  CALL DCSSCV(NoOfPos,Spa,PosX,2,XBreak,XCSCoef)
D  WRITE(*,*) 'Calling DCSSCV from Remesh: y'
  CALL DCSSCV(NoOfPos,Spa,PosY,2,YBreak,YCSCoef)
```

C Compute the Curvature

```
DO I=1,NoOfPos
  Curvature(I)=SQRT(
& DCSDER(2,Spa(I),NoOfPos-1,XBreak,XCSCoef)**2 +
& DCSDER(2,Spa(I),NoOfPos-1,YBreak,YCSCoef)**2)
END DO
```

C Bound the Curvature

```
Sum=0.0
DO I=1,NoOfPos-1
  Sum=Sum+(Spa(I+1)-Spa(I))*
& (Curvature(I+1)+Curvature(I))/2.0D0
```

```

      END DO

      AvgError=Sum/(NoOfPos-1)

      UpperBound=AvgError*UpFac
      LowerBound=AvgError*LowFac

      DO I=1,NoOfPos
        Curvature(I)=MIN(UpperBound,Curvature(I))
        Curvature(I)=MAX(LowerBound,Curvature(I))
      END DO

C Compute New Integral Error

D   WRITE(*,*) 'Error'
D   WRITE(*,*) NoOfPos
D   WRITE(*,*) 1,0.0D0,Spa(1)

      Error(1)=0.0
      DO I=2,NoOfPos
        Error(I)=Error(I-1)+(Spa(I)-Spa(I-1))*
& (Curvature(I)+Curvature(I-1))/2.0D0
D   WRITE(*,*) I,Error(I),Spa(I)
      END DO
D   WRITE(*,*) ' '

      AvgError=Error(NoOfPos)/FLOAT(NoOfSpa-1)

C Now equi-distribute the residual error for each element.

C   Spa(1) keeps its original value.
C   Spa(NoOfSpa) keeps the endpoint value

      Spa(NoOfSpa)=Spa(NoOfPos)

      TSpa=0.0
      K=1
      DO I=2,NoOfSpa-1
        TSpa=TSpa+AvgError
        DO WHILE (TSpa.GT.Error(K+1))
          K=K+1
D   WRITE(*,*) ' Error:',K,Error(K),Orig(K)
        END DO
        Spa(I) = Orig(K) + (TSpa-Error(K)) *
& (Orig(K+1)-Orig(K))/
& (Error(K+1)-Error(K))
D   WRITE(*,*) 'Location',I,TSpa,Spa(I)
      END DO

      RETURN
      END

```

C ***** RemoveBdryAfter

```

      SUBROUTINE RemoveBdryAfter(NoOfMoved,Moved,I,XInt,YInt)

```

C Remove points between intersection (I,) and end from moved surface.
C The segment from Moved(I,) to Moved(I+1,) intersects with insulator.

C Moved(I)=intersection

```
INCLUDE 'ECBHdr.INC'
REAL*8 Moved(MaxNoOfCoords,MaxNoOfDim),XInt,YInt
INTEGER I,NoOfMoved
```

D WRITE(*,*) '-----: RemoveBdryAfter',I

```
Moved(I,1)=XInt
Moved(I,2)=YInt
```

```
NoOfMoved=I
```

```
RETURN
END
```

C ***** RemoveBdryBefore

```
SUBROUTINE RemoveBdryBefore(NoOfMoved,Moved,I,XInt,YInt)
```

C Remove points between start and intersection (I,I) from moved surface.

C The segment from Moved(I,) to Moved(I+1,) intersects with insulator.

C Moved(1)=intersection

C Moved(2)=Moved(I+1),...

```
INCLUDE 'ECBHdr.INC'
REAL*8 Moved(MaxNoOfCoords,MaxNoOfDim),XInt,YInt
INTEGER I,NoOfMoved
INTEGER K
```

D WRITE(*,*) '-----: RemoveBdryBefore',I

```
Moved(1,1)=XInt
Moved(1,2)=YInt
```

```
IF (I.EQ.1) RETURN
```

```
DO K=I+1,NoOfMoved
  Moved(K-I+1,1)=Moved(K,1)
  Moved(K-I+1,2)=Moved(K,2)
END DO
```

```
NoOfMoved=NoOfMoved-I+1
```

```
RETURN
END
```

C ***** RemoveBdryIntersects

```
SUBROUTINE RemoveBdryIntersects
```

```
INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBPar.INC'
INCLUDE 'ECBMOVE.INC'
```

```
INTEGER I,J,K,Error
LOGICAL Thinking
REAL*8 XInt,YInt,Dist
```



```

D  WRITE(*,*) '-----: RemoveBdryIntersects'
   I=2
   Thinking=(I.LT.NoOfMoved)
   DO WHILE(Thinking)

```

C Check following line segments for intersections with current line segment

```

   J=I+2
   IF (J.GT.NoOfMoved) THEN
     Error=0
   ELSE
     Error=1
     Dist=SQRT((Moved(I,1)-Moved(J-1,1))**2+
& (Moved(I,2)-Moved(J-1,2))**2)
     IF (Dist.LT.Tolerance*10.0D0) THEN
       Error=0
       XInt=(Moved(I,1)+Moved(J-1,1))/2.0D0
       YInt=(Moved(I,2)+Moved(J-1,2))/2.0D0
     END IF
   END IF

   DO WHILE(Error.NE.0)
     CALL ComputeIntersection(Moved(I-1,1),Moved(I-1,2),
& Moved(I,1),Moved(I,2),
& Moved(J-1,1),Moved(J-1,2),
& Moved(J,1),Moved(J,2),XInt,YInt,Error)
     IF (Error.NE.0) THEN
       J=J+1
       IF (J.GT.NoOfMoved) Error=0
     END IF
   END DO

   IF (J.LE.NoOfMoved) THEN

```

C Insert intersection point between node I-1 and node J.

```

     Moved(I,1)=XInt
     Moved(I,2)=YInt

```

C Remove nodes between I and J-1.

```

     DO K=J,NoOfMoved
       Moved(I+K+1-J,1)=Moved(K,1)
       Moved(I+K+1-J,2)=Moved(K,2)
     END DO
     NoOfMoved=NoOfMoved-(J-I)+1

```

C Recheck for intersections beginning with node I

```

     ELSE

```

C No intersection found with segment I, increment I to check for next segment.

```

     I=I+1

```

```

   END IF

```

```

   Thinking=(I.LT.NoOfMoved)

```

END DO

RETURN
END

C ***** RemoveInsIntersects

SUBROUTINE RemoveInsIntersects

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMOVE.INC'

REAL*8 XInt,YInt,R,R2
INTEGER I,J,K
LOGICAL Thinking,Error

D WRITE(*,*) '-----: RemoveInsIntersects'

C First check one end of boundary -----

IF (AcuteAngleBefore) THEN

C If Acute angle with insulator, then loop from start until intersection with
C conductor segment and insulator is found.

C Check for intersection between boundary and insulator.

CALL LocateIntersects(1,I,J,XInt,YInt,Error)

IF (.NOT.Error) THEN

IF (XInt.EQ.Moved(I+1,1).AND.(XInt.EQ.Moved(I+1,2))) I=I+1

CALL RemoveBdryBefore(NoOfMoved,Moved,I,XInt,YInt)

CALL RemoveBdryBefore(NoOfIns,Ins,J,XInt,YInt)

Last=Last-J+1

NextToLast=NextToLast-J+1

ELSE

WRITE(*,*) 'Warning: Treating nonintersection like',
& ' obtuse angle.'

C Use clockwise circle for forward boundary movement,

C Counterclockwise circle for backward boundary movement.

CALL ObtAngAtBdryBeg

END IF

ELSE IF (.NOT.NoAngleBefore) THEN

C Compute new point on boundary, add to beginning.

CALL ObtAngAtBdryBeg

END IF

C Second, check other end of boundary (Similar to Above Code) -----

IF (AcuteAngleAfter) THEN

C Check for intersection between boundary and insulator.

CALL LocateIntersects(-1,I,J,XInt,YInt,Error)

IF (.NOT.Error) THEN

D WRITE(*,*) 'Calling RemoveBdryAfter from RemoveInsIntersects'

D WRITE(*,*) ' I='I,' J='J

D WRITE(*,*) ' X='XInt,' Y='YInt

CALL RemoveBdryAfter(NoOfMoved,Moved,I,XInt,YInt)

CALL RemoveBdryAfter(NoOfIns,Ins,J,XInt,YInt)

ELSE

WRITE(*,*) 'Warning: Treating nonintersection like',
& ' obtuse angle.'

CALL ObtAngAtBdryEnd

END IF

ELSE IF (.NOT.NoAngleAfter) THEN

CALL ObtAngAtBdryEnd

END IF

D WRITE(*,*) ' :-----'

RETURN

END

C ***** RemoveLocIntersects

SUBROUTINE RemoveLocIntersects

C This subroutine averages the beginning endpoint with previous segments
C ending endpoint after a boundary has been moved.

INCLUDE 'ECBHdr.INC'

INCLUDE 'ECBPar.INC'

INCLUDE 'ECBMsh.INC'

INCLUDE 'ECBMOVE.INC'

INTEGER I,J,OffSet

REAL*8 Avg

D WRITE(*,*) '-----: RemoveLocIntersects'

DO I=BasisDeg+1,NoOfMoved-1,BasisDeg+1

DO J=1,NoOfDim

Avg=(Moved(I,J)+Moved(I+1,J))/2.0D0

Moved(I,J)=Avg

Moved(I+1,J)=Avg

END DO

END DO

C Remove Duplicate Points

Offset=0

DO I=2,NoOfMoved

IF ((Moved(I,1).EQ.Moved(I-Offset-1,1)).AND.

```

& (Moved(I,2).EQ.Moved(I-Offset-1,2))) THEN
  Offset=Offset+1
ELSE
  Moved(I-Offset,1)=Moved(I,1)
  Moved(I-Offset,2)=Moved(I,2)
END IF
END DO
NoOfMoved=NoOfMoved-Offset
D WRITE(*,*) '      ',Offset,'points removed :-----'

RETURN
END

```

C ***** ShpCir

```

SUBROUTINE ShpCir(MacElm,SaveKinetic)

```

```

  INCLUDE 'ECBHdr.INC'
  INCLUDE 'ECBMac.INC'
  INCLUDE 'ECBMsh.INC'
  INCLUDE '[KJ.FOR.UTIL]Pi.INC'

```

```

  INTEGER MacElm,Error,I,NoOfSpa
  REAL*8 X,Y,Xc,Yc,Radius,AngleStart,AngleEnd,Spa(MaxNoOfCoords)
  LOGICAL SaveKinetic

```

C Get center of circle.

```

  Xc=MacVertX(MacPar(MacElm,1))
  Yc=MacVertY(MacPar(MacElm,1))

```

C Compute the radius

```

  Radius=SQRT(
& (Xc-MacVertX(MacIndx(MacElm,1)))
& * (Xc-MacVertX(MacIndx(MacElm,1))) +
& (Yc-MacVertY(MacIndx(MacElm,1)))
& * (Yc-MacVertY(MacIndx(MacElm,1))) )

```

C Locate Start and End Angles

```

  CALL XY2T(MacVertX(MacIndx(MacElm,1))-Xc,
& MacVertY(MacIndx(MacElm,1))-Yc,AngleStart)
  CALL XY2T(MacVertX(MacIndx(MacElm,2))-Xc,
& MacVertY(MacIndx(MacElm,2))-Yc,AngleEnd)

```

```

  IF (MacPar(MacElm,2).GE.0) THEN

```

C Clockwise Circle

```

  DO WHILE(AngleStart.LE.AngleEnd)
    AngleStart=AngleStart+2.0*Pi
  END DO
  ELSE

```

C Counter-Clockwise Circle

```

  DO WHILE(AngleStart.GE.AngleEnd)

```

```

        AngleStart=AngleStart-2.0*Pi
      END DO
    END IF

    CALL ShpSpacing(MacElm,NoOfSpa,Spa)
    DO I=1,NoOfSpa
      X=Xc+Radius*COS(AngleStart+(AngleEnd-AngleStart)*Spa(I))
      Y=Yc+Radius*SIN(AngleStart+(AngleEnd-AngleStart)*Spa(I))
      CALL MakeCoord(X,Y,MacStart(MacElm)+(I-1),MacElm,SaveKinetic)
    END DO

    RETURN
  END

```

C ***** ShpFlat

```

SUBROUTINE ShpFlat(MacElm,SaveKinetic)

```

```

  INCLUDE 'ECBHdr.INC'
  INCLUDE 'ECBMac.INC'
  INCLUDE 'ECBMsh.INC'

```

```

  INTEGER MacElm,NoOfSpa,I
  LOGICAL SaveKinetic
  REAL*8 X,Y,Spa(MaxNoOfCoords),MaxY

```

C Note: Must Alter Endpoints for Start and End (Note: No TRNS elements!)

```

  CALL ShpFlatHiPt(MacElm,MaxY)
  Y=MaxY+MacPar(MacElm,1)
  MacVertY(MacIndx(MacElm,2))=Y

```

```

  CALL ShpSpacing(MacElm,NoOfSpa,Spa)
  DO I=1,NoOfSpa
    X=MacVertX(MacIndx(MacElm,1)) +
    & (MacVertX(MacIndx(MacElm,2)) - MacVertX(MacIndx(MacElm,1)))
    & * Spa(I)
    CALL MakeCoord(X,Y,MacStart(MacElm)+(I-1),MacElm,SaveKinetic)
  END DO

  RETURN
  END

```

C ***** ShpFlatHiPt

```

SUBROUTINE ShpFlatHiPt(MacElm,MaxY)

```

C This subroutine locates the high (maximum Y) point on macro element
 C MacPar(MacElm,2)

C This subroutine is used for FLAT mass transfer boundary layers located
 C above a profile below.

```

  INTEGER MacElm
  REAL*8 MaxY

  INCLUDE 'ECBHdr.INC'
  INCLUDE 'ECBMac.INC'

```

```

INCLUDE 'ECBPar.INC'
INCLUDE 'ECBMsh.INC'

INTEGER PrevMac,PrevElems,MicNod,K

PrevMac=MacPar(MacElm,2)
CALL ComputePrevElem(PrevMac,PrevElems)

MaxY=Coords(NodeMap(PrevElems+1,1),2)
DO MicNod=PrevElems+1,PrevElems+NoOfMicElems(PrevMac)
  DO K=1,BasisDeg+1
    IF (MaxY.LT.Coords(NodeMap(MicNod,K),2))
& MaxY=Coords(NodeMap(MicNod,K),2)
  END DO
END DO

RETURN
END

```

C ***** ShpFlatLoPt

```

SUBROUTINE ShpFlatLoPt(MacElm,MinY)

```

C This subroutine locates the low (minimum Y) point on macro element

C MacPar(MacElm,2)

C This subroutine is used for FLTL mass transfer boundary layers located

C above a profile below.

```

INTEGER MacElm
REAL*8 MinY

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMac.INC'
INCLUDE 'ECBPar.INC'
INCLUDE 'ECBMsh.INC'

INTEGER PrevMac,PrevElems,MicNod,K

PrevMac=MacPar(MacElm,2)
CALL ComputePrevElem(PrevMac,PrevElems)

MinY=Coords(NodeMap(PrevElems+1,1),2)
DO MicNod=PrevElems+1,PrevElems+NoOfMicElems(PrevMac)
  DO K=1,BasisDeg+1
    IF (MinY.GT.Coords(NodeMap(MicNod,K),2))
& MinY=Coords(NodeMap(MicNod,K),2)
  END DO
END DO

RETURN
END

```

C ***** ShpFltL

```

SUBROUTINE ShpFltL(MacElm,SaveKinetic)

```

```

INCLUDE 'ECBHdr.INC'

```

```

INCLUDE 'ECBMac.INC'
INCLUDE 'ECBMsh.INC'

INTEGER MacElm,NoOfSpa,I
LOGICAL SaveKinetic
REAL*8 X,Y,Spa(MaxNoOfCoords),MinY

```

C Note: Must Alter Endpoints for Start and End (Note: No TRNS elements!)

```

CALL ShpFlatLoPt(MacElm,MinY)
Y=MinY+MacPar(MacElm,1)
MacVertY(MacIndx(MacElm,2))=Y

CALL ShpSpacing(MacElm,NoOfSpa,Spa)
DO I=1,NoOfSpa
  X=MacVertX(MacIndx(MacElm,1)) +
& (MacVertX(MacIndx(MacElm,2)) - MacVertX(MacIndx(MacElm,1)))
& * Spa(I)
  CALL MakeCoord(X,Y,MacStart(MacElm)+(I-1),MacElm,SaveKinetic)
END DO

RETURN
END

```

C ***** ShpLine

```

SUBROUTINE ShpLine(MacElm,SaveKinetic)

```

C This subroutine generates the mesh points for line Shps. (Straight
C line segments between macro mesh pts)

```

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMac.INC'
INCLUDE 'ECBMsh.INC'

INTEGER MacElm,NoOfSpa,I
REAL*8 X,Y,Spa(MaxNoOfCoords)
LOGICAL SaveKinetic

CALL ShpSpacing(MacElm,NoOfSpa,Spa)
DO I=1,NoOfSpa
  X=MacVertX(MacIndx(MacElm,1)) +
& ( MacVertX(MacIndx(MacElm,2))
& - MacVertX(MacIndx(MacElm,1)) )
& * Spa(I)
  Y=MacVertY(MacIndx(MacElm,1)) +
& (MacVertY(MacIndx(MacElm,2))-MacVertY(MacIndx(MacElm,1)))
& * Spa(I)
  CALL MakeCoord(X,Y,MacStart(MacElm)+(I-1),MacElm,SaveKinetic)
END DO

RETURN
END

```

C ***** ShpPrev

```

SUBROUTINE ShpPrev(MacElm,SaveKinetic)

```

```

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBPar.INc'
INCLUDE 'ECBMac.INC'
INCLUDE 'ECBMsh.INC'
INCLUDE 'ECBMOVE.INC'

```

```

INTEGER MacElm,MicNod,NoOfSpa,PrevElems,
& ElemStart,ElemEnd,MacFollow,J,I
LOGICAL SaveKinetic,Smooth
REAL*8 X,Y,Spa(MaxNoOfCoords),D,Temp
REAL*8 dtime/1.0/

```

C Get nodes of previous element

```

MacFollow=MacPar(MacElm,2)
CALL ComputePrevElem(MacFollow,PrevElems)

ElemStart=PrevElems+1
ElemEnd=PrevElems+NoOfMicElems(MacFollow)
D WRITE(*,*) ' ShpPrev: ElemStart=',ElemStart,
D & ' ElemEnd=',ElemEnd

D WRITE(*,*) ' ShpPrev: Calling MakeMoved'
CALL MakeMoved(ElemStart,ElemEnd,NodeMap,Coords)
D WRITE(*,*) ' ShpPrev: NoOfMoved=',NoOfMoved

D WRITE(*,*) ' ShpPrev: First Moved Point=',
D & Moved(1,1),Moved(1,2)
D WRITE(*,*) ' ShpPrev: Last Moved Point=',
D & Moved(NoOfMoved,1),Moved(NoOfMoved,2)

DO MicNod=1,NoOfMoved
dXdN(MicNod)=-MacPar(MacElm,1)
END DO
D WRITE(*,*) ' ShpPrev: Calling ComputeNx'
CALL ComputeNx(ElemEnd-ElemStart+1)

```

C Move Previous Elements Nodes by boundary layer thickness

```

NoOfIns=4

Ins(1,1)=Moved(1,1)
Ins(1,2)=Moved(1,2)

Ins(2,1)=MacVertX(MacPar(MacElm,3))
Ins(2,2)=MacVertY(MacPar(MacElm,3))

Ins(3,1)=MacVertX(MacPar(MacElm,4))
Ins(3,2)=MacVertY(MacPar(MacElm,4))

Ins(4,1)=Moved(NoOfMoved,1)
Ins(4,2)=Moved(NoOfMoved,2)

D WRITE(*,*) ' ShpPrev: Calling Moved'
CALL Move(dTime)
D WRITE(*,*) ' ShpPrev: Last Moved Point=',
D & Moved(NoOfMoved,1),Moved(NoOfMoved,2)
D WRITE(*,*) ' ShpPrev: Calling RemoveLocIntersects'

```



```

CALL RemoveLocIntersects
D WRITE(*,*) ' ShpPrev: Last Moved Point=',
D & Moved(NoOfMoved,1),Moved(NoOfMoved,2)
D WRITE(*,*) ' ShpPrev: Calling RemoveBdryIntersects'
CALL RemoveBdryIntersects
D WRITE(*,*) ' ShpPrev: Last Moved Point=',
D & Moved(NoOfMoved,1),Moved(NoOfMoved,2)

```

```

StaRev=.FALSE.
EndRev=.FALSE.

```

```

First=1
Second=2

```

```

NextToLast=3
Last=4

```

```

D WRITE(*,*) ' ShpPrev: Calling AcuteAngles'
CALL AcuteAngles
D WRITE(*,*) ' ShpPrev: Calling RemoveInsIntersects'
CALL RemoveInsIntersects

```

C Save the intersection of the profile following boundary with the insulator
C on the far side. (The whole point of doing the previous steps.)

```

MacVertX(MacIndx(MacElm,1))=Moved(NoOfMoved,1)
MacVertY(MacIndx(MacElm,1))=Moved(NoOfMoved,2)

```

```

MacVertX(MacIndx(MacElm,2))=Moved(1,1)
MacVertY(MacIndx(MacElm,2))=Moved(1,2)

```

C Compute the location of the boundary at specified x locations
C Note: The orientation of Moved is the inverse of what it should be
C for SHPPREV.
C (e.g. it starts at the end of the element, and ends at the
C beginning of the element) The following lines reverse the Moved Pts
C to account for this.

```

DO I=1,(NoOfMoved+1)/2
CALL DpXCHNG(Moved(I,1),Moved(NoOfMoved-I+1,1))
CALL DpXCHNG(Moved(I,2),Moved(NoOfMoved-I+1,2))
END DO

```

```

CALL GetSpa(MacElm,Spa,NoOfSpa)

```

```

IF (MacSpac(MacElm).NE.'=CRV') THEN
DO I=1,NoOfSpa
X=MacVertX(MacIndx(MacElm,1)) +
& (MacVertX(MacIndx(MacElm,2)) - MacVertX(MacIndx(MacElm,1)))
& * Spa(I)
Spa(I)=X
END DO
END IF

```

```

D WRITE(*,*) ' ShpPrev: NoOfSpa=',NoOfSpa
D WRITE(*,*) ' : Calling ComputeBdry'

```

```

CALL ComputeBdry(Spa,NoOfSpa,Smooth,Spline3D)

```

C Transfer the node locations from moved to coords

```

      DO MicNod=1,NoOfSpa
D      WRITE(*,*) ' ShpPrev: Spa ',MicNod,Spa(MicNod)
D      WRITE(*,*) '      :',Moved(MicNod,1),Moved(MicNod,2)
      CALL MakeCoord(Moved(MicNod,1),Moved(MicNod,2),
& MacStart(MacElm)+MicNod-1,MacElm,SaveKinetic)
      END DO

      RETURN
      END

```

C ***** ShpSine

SUBROUTINE ShpSine(MacElm,SaveKinetic)

```

      INCLUDE 'ECBHdr.INC'
      INCLUDE 'ECBMac.INC'
      INCLUDE 'ECBMsh.INC'
      INCLUDE '[KJ.FOR.UTIL]Pi.INC'

```

```

      INTEGER MacElm,I,NoOfSpa
      REAL*8 X,Y,A,Y0,Spa(MaxNoOfCoords)
      LOGICAL SaveKinetic

```

C Compute Sine parameters

C $Y=Y0+A*\text{SIN}(Pi*(Par1*X+Par2))$

```

      A=(MacVertY(MacIdx(MacElm,1))-MacVertY(MacIdx(MacElm,2)))
& / (SIN( Pi*(MacPar(MacElm,1)*MacVertX(MacIdx(MacElm,1))
& + MacPar(MacElm,2) ))
& - SIN( Pi*(MacPar(MacElm,1)*MacVertX(MacIdx(MacElm,2))
& + MacPar(MacElm,2) )) )

```

```

      Y0=MacVertY(MacIdx(MacElm,1))-A*
& SIN(Pi*( MacPar(MacElm,1)*MacVertX(MacIdx(MacElm,1))
& + MacPar(MacElm,2) ))

```

```

      CALL ShpSpacing(MacElm,NoOfSpa,Spa)
      DO I=1,NoOfSpa
      X=MacVertX(MacIdx(MacElm,1)) +
& (MacVertX(MacIdx(MacElm,2))-MacVertX(MacIdx(MacElm,1)))
& *Spa(I)
      Y=Y0+A*SIN(Pi*( MacPar(MacElm,1)*X+MacPar(MacElm,2) ))
      CALL MakeCoord(X,Y,MacStart(MacElm)+(I-1),MacElm,SaveKinetic)
      END DO

```

```

      RETURN
      END

```

C ***** ShpSpacing

SUBROUTINE ShpSpacing(MacElm,NoOfSpa,Spa)

```

      INCLUDE 'ECBHdr.INC'
      INCLUDE 'ECBMac.INC'
      INCLUDE '[KJ.FOR.UTIL]Pi.INC'

```

```

INTEGER MacElm,NoOfSpa,I,Length,NoOfPts,TNoOfSpa
REAL*8 Spa(*),StepX

```

```

REAL*8 GeomSeries
EXTERNAL GeomSeries

```

```

NoOfSpa=NoOfMicElems(MacElm)*BasisDeg

```

```

Spa(1)=0.0
Spa(NoOfSpa+1)=1.0

```

```

TNoOfSpa=(NoOfSpa+1)/2
IF (MacSpac(MacElm).EQ.'EQU') THEN

```

```

IF (BasisDeg.EQ.2) THEN
  DO I=2,TNoOfSpa
    Spa(2*I-1)=FLOAT(I-1)/FLOAT(TNoOfSpa)
  END DO
  DO I=2,NoOfSpa,2
    Spa(I)=(Spa(I+1)+Spa(I-1))/2.0
  END DO
ELSE
  DO I=2,NoOfSpa
    Spa(I)=FLOAT(I-1)/FLOAT(NoOfSpa)
  END DO
END IF

```

```

ELSE IF (MacSpac(MacElm).EQ.'LOG') THEN

```

```

IF (BasisDeg.EQ.2) THEN
  StepX=1.0/GeomSeries(MacRatio(MacElm),TNoOfSpa-1)

  DO I=2,TNoOfSpa
    Spa(2*I-1) = Spa(2*(I-1)-1) + StepX
    StepX=StepX*MacRatio(MacElm)
  END DO
  DO I=2,NoOfSpa,2
    Spa(I)=(Spa(I+1)+Spa(I-1))/2.0
  END DO

```

```

ELSE

```

```

  StepX=1.0/GeomSeries(MacRatio(MacElm),NoOfSpa-1)

```

```

  DO I=2,NoOfSpa
    Spa(I) = Spa(I-1) + StepX
    StepX=StepX*MacRatio(MacElm)
  END DO

```

```

END IF

```

```

ELSE IF (MacSpac(MacElm).EQ.'CHEB') THEN

```

```

IF (BasisDeg.EQ.2) THEN

```

```

  DO I=2,TNoOfSpa
    Spa(2*I-1)=(1.0-COS((I-1)*Pi/TNoOfSpa))/2.0

```

```

      END DO

      DO I=2,NoOfSpa,2
        Spa(I)=(Spa(I+1)+Spa(I-1))/2.0
      END DO

      ELSE

        DO I=2,NoOfSpa
          Spa(I)=(1.0-COS((I-1)*Pi/NoOfSpa))/2.0
        END DO
      END IF

      ELSE IF (MacSpac(MacElm).EQ.'USER') THEN

        OPEN(UNIT=1,FILE=MacSpaFile(MacElm),STATUS='OLD',
& FORM='FORMATTED')
        READ(1,*) NoOfPts

        IF (NoOfPts.NE.NoOfSpa) THEN
          CLOSE(1)
          CALL StringLength(MacSpaFile(MacElm),Length)
          WRITE(*,*) 'Error: number of points in ',
& MacSpaFile(MacElm)(1:Length), ' is not ',NoOfSpa
          WRITE(*,*) '      ',MacSpaFile(MacElm)(1:Length), ' has ',
& NoOfPts, ' points'
          WRITE(*,*) '      Program cannot continue until this is ',
& 'corrected.'
          STOP 'In Routine: ShpUser'
        END IF

        DO I=1,NoOfSpa
          READ(1,*) Spa(I)
        END DO
        CLOSE(1)

      ELSE

        WRITE(*,*) 'Error: Unknown Spacing=',MacSpac(MacElm)
        STOP 'In Routine: ShpUser'

      END IF

      RETURN
      END

```

C ***** ShpTRNS

```

      SUBROUTINE ShpTRNS(MacElm,SaveKinetic)

```

C This subroutine generates the mesh points for line Shps. (Straight
C line segments between macro mesh pts)

```

      INCLUDE 'ECBHdr.INC'
      INCLUDE 'ECBPar.INC'
      INCLUDE 'ECBMac.INC'
      INCLUDE 'ECBMsh.INC'
      INCLUDE 'ECBBC.INC'

```

```

INTEGER MacElm,MicNod
REAL*8 StepX,StepY,X,Y,StepBC
LOGICAL SaveKinetic

```

C Compute the steps in the x and y directions for micro elements
 C between macro-end points MacElm and MacElm plus 1.

```

StepX=(MacVertX(MacIndx(MacElm,2))-MacVertX(MacIndx(MacElm,1)))/
& (NoOfMicElems(MacElm)*BasisDeg)
StepY=(MacVertY(MacIndx(MacElm,2))-MacVertY(MacIndx(MacElm,1)))/
& (NoOfMicElems(MacElm)*BasisDeg)
StepBC=(MacBCVal(MacElm+1)-MacBCVal(MacElm-1))/
& (NoOfMicElems(MacElm)*BasisDeg)

```

C Make the mesh points and boundary conditions

```

DO MicNod=0,BasisDeg*NoOfMicElems(MacElm)-1
  X=MacVertX(MacIndx(MacElm,1))+StepX*MicNod
  Y=MacVertY(MacIndx(MacElm,1))+StepY*MicNod
  MacBCVal(MacElm)=MacBCVal(MacElm-1)+StepBC*MicNod
  CALL MakeCoord(X,Y,MacStart(MacElm)+MicNod,MacElm,SaveKinetic)
END DO

RETURN
END

```

C ***** ShpUser

```

SUBROUTINE ShpUser(MacElm,SaveKinetic,Smooth)

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBPar.INC'
INCLUDE 'ECBMac.INC'
INCLUDE 'ECBMove.INC'

INTEGER MacElm,I,NoOfSpa,J
LOGICAL SaveKinetic,Smooth
REAL*8 Spa(MaxNoOfCoords),D,X

OPEN(UNIT=1,FILE=MacBdryFile,STATUS='OLD',FORM='FORMATTED')

READ(1,*) NoOfMoved
DO I=1,NoOfMoved
  READ(1,*) Moved(I,1),Moved(I,2)
END DO
CLOSE(1)

CALL GetSpa(MacElm,Spa,NoOfSpa)

```

C Compute the location of the boundary at specified x locations

```

D WRITE(*,*) ' ShpUser: NoOfMoved=',NoOfMoved
D WRITE(*,*) ' : NoOfSpa=',NoOfSpa
D WRITE(*,*) ' : Calling ComputeBdry'

IF (.NOT.Spline3D) THEN
  DO I=1,NoOfSpa
    X=MacVertX(MacIndx(MacElm,1)) +

```

```

& (MacVertX(MacIndx(MacElm,2)) - MacVertX(MacIndx(MacElm,1)))
& * Spa(I)
    Spa(I)=X
  END DO
END IF

CALL ComputeBdry(Spa,NoOfSpa,Smooth,Spline3D)

DO I=1,NoOfSpa
  CALL MakeCoord(Moved(I,1),Moved(I,2),
& MacStart(MacElm)+(I-1),MacElm,SaveKinetic)
END DO

RETURN
END

```

C ***** TestForSingularity

```

SUBROUTINE TestForSingularity(Singularity,SingLoc)

```

```

  INCLUDE 'ECBHdr.INC'

```

```

  INTEGER SingLoc
  INCLUDE 'EcbElm.INC'
  LOGICAL Singularity

```

```

  INTEGER J
  REAL*8 D,Small/1.0E-10/

```

C See if we need to correct for singularities. Singularity occurs when
C source point is the same as the current node. This can be avoided by
C choosing source points interior to the region.

```

  Singularity=.FALSE.

```

```

  SingLoc=0
  DO J=1,BasisDeg+1
    D=((SourceR(1)-ElemR(1,J))*(SourceR(1)-ElemR(1,J)) +
& (SourceR(2)-ElemR(2,J))*(SourceR(2)-ElemR(2,J)))
    IF (D.LT.Small*Small) THEN
      Singularity=.TRUE.
      SingLoc=J
      RETURN
    END IF
  END DO

RETURN
END

```

C ***** UpdateBCValues

```

SUBROUTINE UpdateBCValues(NoOfdBCValues,dBCValues)

```

```

  INCLUDE 'ECBHdr.INC'
  INCLUDE 'ECBMsh.INC'
  INCLUDE 'ECBBC.INC'

```

```

  INTEGER J,I,NoOfdBCValues

```

```

REAL*8 dBCValues(*),Factor,VecNormDP,MagdBC
LOGICAL KineticBC
EXTERNAL KineticBC,VecNormDP

```

C Based on the magnitude of the desired change in boundary values,
C use relaxation technique (scale down the desired step).

```

MagdBC=VecNormDP(NoOfdBCValues,dBCValues)
IF (MagdBC.GT.1.0) THEN
  Factor=MAX(MIN(0.9D0,2.0D0/MagdBC),0.2D0)
  WRITE(*,*) 'Factor=',Factor
ELSE
  Factor=1.0
END IF

```

```

J=1
DO I=1,NoOfCoords
  IF (KineticBC(BCType(I))) THEN
    BCValues(I)=BCValues(I)+dBCValues(J)*Factor
    J=J+1
  END IF
END DO

```

```

RETURN
END

```

C ***** UStar

```

REAL*8 FUNCTION UStar(Dist2,Gs,Den,M)

```

```

INCLUDE 'ECBPar.INC'
INCLUDE 'ECBHdr.INC'
INCLUDE 'ECGaus.INC'
INCLUDE 'ECBG.INC'
INCLUDE 'ECBEIm.INC'

```

```

INTEGER Gs
REAL*8 Dist2,Den,M

```

```

REAL*8 First,Second

```

```

REAL*8 KEIP
EXTERNAL KEIP

```

C Variables

C SourceR(*) Coordinates of the Source Point

```

IF (Axisymmetric) THEN

```

C The problem is Axisymmetric.

C UStar Multiplied by 2Pi

C Note: the Gr(Gs,1) term is here because it is not included in the computation
C of the isojacobian for axisymmetric problems.

```

UStar = 2.0D0*KEIP(M)*Gr(Gs,1)/SQRT(Den)

```

ELSE

C The problem is planar
C Ustar multiplied by 2Pi

UStar = -LOG(Dist2)/2.0D0

END IF

RETURN
END

C ***** WriteCal

SUBROUTINE WriteCal(FileName)

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMsh.INC'
INCLUDE 'ECBCal.INC'
CHARACTER*(*) FileName
LOGICAL FileExist
INTEGER I,J,Version/1/

INQUIRE(FILE=FileName,EXIST=FileExist)
IF (.NOT.FileExist) THEN
 OPEN(UNIT=1,FILE=FileName,STATUS='NEW',FORM='FORMATTED')
ELSE
 OPEN(UNIT=1,FILE=FileName,STATUS='OLD',FORM='FORMATTED')
END IF

WRITE(1,*) Version

DO I=1,NoOfCoords
 DO J=1,NoOfCoords
 WRITE(1,*) BemG(I,J),BemH(I,J),I,J
 END DO
END DO

CLOSE(1)

RETURN
END

C ***** WriteInt

SUBROUTINE WriteInt(FileName)

INCLUDE 'ECBHDR.INC'
INCLUDE 'ECBINT.INC'

CHARACTER*(*) FileName
LOGICAL FileExist
INTEGER Version,I,K

OPEN(UNIT=1,FILE=FileName,STATUS='NEW',FORM='FORMATTED')
WRITE(1,*) 1

WRITE(1,*) NoOfInternal,NoOfSpines,IntPerSpine


```

DO I=1,NoOfInternal
  WRITE(1,*) (InternalPts(I,K),K=1,NoOfDim),InternalPot(I)
END DO

```

```

CLOSE(1)

```

```

RETURN
END

```

```

C ***** WriteMac

```

```

SUBROUTINE WriteMac(FileName)

```

```

C This subroutine writes the contents of the BEM.MAC file. This file contains
C the information required to make the BEM.INP file, the more detailed file
C used by the BEMLIN.FOR program for input.

```

```

INCLUDE 'ECBMAC.INC'
CHARACTER*(*) FileName
INTEGER I,Version
LOGICAL FileExist

```

```

INQUIRE (FILE=FileName,EXIST=FileExist)
IF (.NOT.FileExist) CALL ErrorFileName(FileName,'ReadMac')

```

```

OPEN(UNIT=1,FILE=FileName,STATUS='NEW',FORM='FORMATTED',RECL=132)

```

```

WRITE(1,*) 3

```

```

IF (NoOfMacVert.GT.MaxNoOfMacVert) THEN
  WRITE(*,*) 'Error: Number of macro-vertices,',NoOfMacVert
  WRITE(*,*) ' is larger than the maximum number of '
  WRITE(*,*) ' macro-vertices allowed:',MaxNoOfMacVert
  STOP 'In Routine: WriteMac'
END IF

```

```

WRITE(1,*) NoOfMacVert

```

```

DO I=1,NoOfMacVert
  WRITE(1,*) MacVertX(I),', ',MacVertY(I)
END DO

```

```

WRITE(1,*) NoOfMacElems
DO I=1,NoOfMacElems
  WRITE(1,*) '','',MacShape(I),'','',NoOfMicElems(I),
& '','',MacBCTYPE(I),'','',MacBCVal(I),'','',
& MacSpac(I),'','',MacRatio(I)
  IF (MacShape(I).EQ.'LINE') THEN
    WRITE(1,*) MacIndx(I,1),MacIndx(I,2)
  ELSE IF (MacShape(I).EQ.'SINE') THEN
    WRITE(1,*) MacIndx(I,1),MacIndx(I,2)
    WRITE(1,*) MacPar(I,1),MacPar(I,2)

```

```

C (Y-Y0)=A*Sin(Par1*X+Par2)) A and Y0 are solved for

```

```

ELSE IF (MacShape(I).EQ.'CIR') THEN
  WRITE(1,*) MacIndx(I,1),MacIndx(I,2)
  WRITE(1,*) MacPar(I,1),MacPar(I,2)
ELSE IF ((MacShape(I).EQ.'USER').OR.

```

```

& (MacShape(I).EQ.'USR') THEN
  WRITE(1,*) MacIndx(I,1),MacIndx(I,2),',',MacBdryFile,''''
ELSE IF (MacShape(I).EQ.'TRNS') THEN
  WRITE(1,*) MacIndx(I,1),MacIndx(I,2)
ELSE IF (MacShape(I).EQ.'PREV') THEN
  WRITE(1,*) MacIndx(I,1),MacIndx(I,2)
  WRITE(1,*) MacPar(I,1),MacPar(I,2),MacPar(I,3),MacPar(I,4)
ELSE IF (MacShape(I).EQ.'FLAT') THEN
  WRITE(1,*) MacIndx(I,1),MacIndx(I,2)
  WRITE(1,*) MacPar(I,1),MacPar(I,2)
ELSE IF (MacShape(I).EQ.'FLTL') THEN
  WRITE(1,*) MacIndx(I,1),MacIndx(I,2)
  WRITE(1,*) MacPar(I,1),MacPar(I,2)
ELSE
  WRITE(*,*) 'Error: Unknown Macro-Element Type:',MacShape(I)
  STOP 'In Routine: WriteMac'
END IF
WRITE(1,*) MacStart(I),MacEnd(I)
IF (MacSpac(I).EQ.'USER') WRITE(1,*) '','',MacSpaFile(I),''''
END DO
CLOSE(1)

RETURN
END

```

C ***** WriteMesh

```

SUBROUTINE WriteMesh(fileName)

CHARACTER*(*) fileName
INTEGER Length,Version/1/,I,J
LOGICAL FileExist

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBMsh.INC'
INCLUDE 'ECBBC.Inc'

OPEN(UNIT=1,FILE=fileName,STATUS='UNKNOWN',FORM='FORMATTED')

WRITE(1,*) Version

WRITE(1,*) NoOfCoords
DO I=1,NoOfCoords
  WRITE(1,*) (Coords(I,J),J=1,NoOfDim)
  WRITE(1,*) BCValues(I),SolValues(I),Natural(I),
& ',','',BCType(I),''''
END DO

WRITE(1,*) NoOfElems
DO I=1,NoOfElems
  WRITE(1,*) (NodeMap(I,J),J=1,BasisDeg+1),ElemNat(I),
& ',','',ElemBCType(I),''''
END DO

CLOSE(1)

RETURN
END

```

C ***** WriteSrc

```

SUBROUTINE WriteSrc(FileName)

INCLUDE 'ECBHdr.INC'
INCLUDE 'ECBSrc.INC'
INCLUDE 'ECBMsh.INC'

INTEGER Version/1/,IJ
CHARACTER*(*) FileName
LOGICAL FileExist

OPEN(UNIT=1,FILE=FileName,STATUS='UNKNOWN',FORM='FORMATTED')

WRITE(1,*) Version

IF (Version.EQ.1) THEN
  WRITE(1,*) NoOfSrc

  IF (NoOfSrc.NE.NoOfCoords) THEN
    WRITE(*,*) 'Error: Number of source points is not equal to'
    WRITE(*,*) '  the number of coordinates.'
    WRITE(*,*) '  Filename=',FileName
    WRITE(*,*) '  NoOfSrc=',NoOfSrc
    WRITE(*,*) '  NoOfCoords=',NoOfCoords
    STOP 'In Routine: WriteSrc'
  END IF

  DO I=1,NoOfSrc
    WRITE(1,*) (Src(I,J),J=1,NoOfDim)
  END DO
ELSE
  CALL ErrorVersion(Version,FileName,'WriteSrc')
END IF

CLOSE(1)

RETURN
END

```

C ***** XY2T

```

SUBROUTINE XY2T(X,Y,T)

```

C This subroutine taken from Ken Jordan's Masters Thesis CalTech 1985

C This subroutine returns the angle, T, from the positive x-axis, of
C the point X,Y

```

REAL*8 X,Y,T,PI/3.1415926536/

IF (X.GT.0.0) THEN
  IF (Y.GE.0.0) THEN
    T=ATAN(Y/X)
  ELSE
    T=ATAN(Y/X)+2.0*PI
  END IF
END IF

```

```
IF (X.LT.0.0) T=ATAN(Y/X)+PI
```

```
IF (X.EQ.0.0) THEN
```

```
  IF (Y.GT.0.0) T=PI/2.0
```

```
  IF (Y.EQ.0.0) T=0.0
```

```
  IF (Y.LT.0.0) T=3.0*PI/2.0
```

```
END IF
```

```
RETURN
```

```
END
```

C Include File: ECBBC.INC

C Written by: Ken Jordan

Date: 3/18/88

C This file contains the declarations for the bc values and solution results.

C Used for reading/writing .BC files.

C ----- Variables

C BCType() The boundary condition for each node.
C 'ESS ' Essential Boundary Condition
C 'NAT ' Natural Boundary Condition
C 'CRNT' Natural condition where $dPot/dn=-Wagner$
C 'LIN ' Linear
C 'TAFA' Tafel Anodic
C 'TAFC' Tafel Cathodic
C 'BV ' Butler-Volmer
C 'USR ' User supplied (Function...)

C BCValues(*) The boundary condition value for each node
C ElemBCType(*) BC Kinetics Type for each element.
C ElemNat(*) Logical TRUE if element I has natural BC's.
C Natural(*) Logical True if BCValues(I) is a natural BC
C SolValues(*) if Natural(i) is true, then this is the essential value.
C if Natural(i) is false, then this is the natural value.

C ----- Declarations

REAL*8 BCValues(MaxNoOfCoords),SolValues(MaxNoOfCoords)
LOGICAL Natural(MaxNoOfCoords),ElemNat(MaxNoOfCoords)
CHARACTER*4 BCType(MaxNoOfCoords),ElemBCType(MaxNoOfCoords)

COMMON/ECBBC/BCValues,SolValues,Natural,ElemNat,
& BCType,ElemBCType

C Include File: ECBbc2
C Written By: Ken Jordan

8/24/88

C This file declares variables for saving old BEM problem boundary conditions
C and solution values

C ----- Variables

C Natural2(*) Logical True if BCValues(I) is a natural BC
C BCValues2(*) The boundary condition value for each node
C SolValues2(*) if Natural2(i) is true, then this is the essential value.
C if Natural2(i) is false, then this is the natural value.

C ----- Declarations

REAL*8 BCValues2(MaxNoOfCoords),SolValues2(MaxNoOfCoords)
LOGICAL Natural2(MaxNoOfCoords)

COMMON/ECBBC2/BCValues2,SolValues2,Natural2

C Include File: ECBCal
C Written by: Ken Jordan

Date: 3/18/88

C This file contains the declarations necessary to access the BEM Matrices
C BEMH(.) and BEMG(.).

C ----- Declarations

REAL*8 BEMH(MaxNoOfCoords,MaxNoOfCoords),
& BEMG(MaxNoOfCoords,MaxNoOfCoords)

COMMON /ECBCal/BemH,BemG

C Include File: ECBELM.INC
C Written by: Ken Jordan

8/10/88

C This include file declares the common block used to store the
C current local element coordinates, and the current source point for
C integration over the local element.

```
COMMON /ECBELM/ElemR,SourceR  
REAL*8 ElemR(MaxNoOfDim,MaxBasisDeg+1),SourceR(MaxNoOfDim)
```


C INCLUDE FILE: ECBG.INC
C Written by: Ken Jordan

7/29/88

C This file contains declarations for variables passed to UStar and QStar,
C such as GPhi, GR,GIsoJacob,GNormal, that only need to be calculated once
C for each gauss point on the element, and not for each source point.

REAL*8 GPhi(MaxNoOfGauss,MaxBasisDeg+1),
& GR(MaxNoOfGauss,MaxNoOfDim),GIsoJacob(MaxNoOfGauss),
& GNormal(MaxNoOfGauss,MaxNoOfDim)

COMMON /ECBG/GPhi,Gr,GIsoJacob,GNormal

C Include File: ECBHdr.INc

C Written by: Ken Jordan

Date: 3/18/88

C This include file contains the declarations for variables and parameters
C used to solve the BEM problem

C ----- Parameters

C MaxBasisDeg The maximum basis function allowed

C MaxNoOfCoords The maximum number of mesh points and source points

C allowed

C MaxNoOfDim The maximum dimension allowed.

C ----- Variables

C BasisDeg The degree of the basis functions.

C NoOfDim The actual number of dimensions specified by the user.

C ----- Declarations

PARAMETER MaxNoOfCoords=500

PARAMETER MaxNoOfDim=2

PARAMETER MaxBasisDeg=2

INTEGER NoOfDim,BasisDeg

COMMON /ECBHdr/NoOfDim,BasisDeg

C Include File: ECBINT.INC
C Written By: Ken Jordan

Date: 10/20/89

C This include file declares the internal points

C NoOfInternal The number of internal points
C NoOfSpines The number of spines
C IntPerSpine The number of internal points per spine
C InternalPts(,2) The locations of the internal Points.
C InternalPot() The potential at the internal points.

INTEGER NoOfInternal,NoOfSpines,IntPerSpine
REAL*8 InternalPts(MaxNoOfCoords,MaxNoOfDim),
& InternalPot(MaxNoOfCoords)

COMMON /ECBINT/ NoOfInternal,NoOfSpines,IntPerSpine,
& InternalPts,InternalPot

C Include File: ECBMac.INC
 C Written By: Ken Jordan

Date: 6/5/87

C This include file defines and dimensions the variables used in the ECBMAC
 C common block for setting up a mesh. The file is used by program ECBPrePro.

C ----- Parameters

C MaxNoOfMacVert is used to dimension the matrices used to read the BEM.MAC
 C file.

C ----- Variables

C NoOfMacElems The number of macro elements.
 C NoOfMacVert Number of macro vertices in the BEM.MAC file
 C NoOfMicElems() The number of elements for each macro element.
 C MacBCType() The b.c. to be applied to the element
 C 'ESS','NAT','CRNT','BV','LIN','TAFA','T AFC'
 C MacBCVal() The b.c. value for the element
 C Value of the potential in the node I if BCType(i)=0
 C Value of the potential derivative if BCType(i)=1
 C MacIndx(.) The first index is the macro element number,
 C If the macro element is a line then the contents for
 C second index=1 is the index number of the macro vertex
 C at the start of the line segment.
 C second index=2 is the index number of the macro vertex
 C at the end of the line segment.
 C MacPar(.) Parameters used for various macro element types.
 C 'LINE'
 C 'SINE' $Y=Y_0+A*\sin(\text{MacPar}(I,1)*X+\text{MacPar}(I,2))$
 C 'FLAT' Horizontal surface MacPar(I,1) above highest point
 C of MacroElement MacPar(I,2)
 C 'PREV' Surface of with shape of MacroElement MacPar(I,2)
 C spaced MacPar(I,1) away.
 C MacShape() The type of macro-element. Currently, the only type allowed
 C is 'LINE','SINE','FLAT','PREV','USER','CIR'
 C MacSpac() The spacing for the macro-element. (LOG, CHEB, EQU, =CRV,USR)
 C MacRatio() The spacing parameter for LOG spacing.
 C MacVertX() X coordinate of macro vertex
 C MacVertY() Y coordinate of macro vertex
 C MacSPAFile() The filename to use for user-defined spacings
 C MacBdryFile The filename to use for temporary storage of the moving
 C boundary

C ----- Declarations

COMMON /ECBMac/NoOfMacVert,MacVertX,MacVertY,NoOfMacElems,
 & MacShape,NoOfMicElems,MacBCType,MacBCVal,MacIndx,MacPar,
 & MacSpac,MacRatio,MacStart,MacEnd,MacSpaFile,MacBdryFile

PARAMETER MaxNoOfMacVert=10

INTEGER NoOfMacVert,NoOfMacElems,NoOfMicElems(MaxNoOfMacVert),
 & MacIndx(MaxNoOfMacVert,2),MacStart(MaxNoOfMacVert),
 & MacEnd(MaxNoOfMacVert)
 REAL*8 MacVertX(MaxNoOfMacVert),MacVertY(MaxNoOfMacVert),
 & MacBCVal(MaxNoOfMacVert),MacPar(MaxNoOfMacVert,4),

& MacRatio(MaxNoOfMacVert)

CHARACTER*4 MacShape(MaxNoOfMacVert),MacBCType(MaxNoOfMacVert),
& MacSpac(MaxNoOfMacVert)
CHARACTER*50 MacSpaFile(MaxNoOfMacVert),MacBdryFile

C *.MAC file structure

C NoOfMacVert

C MaxVertX(i),MacVertY(i)

C NoOfMacElems

C MacShape(i),NoOfMicElems(i),MacBCType(i),MacBCVal(i)

C MacIndx(i,1),MacIndx(i,2) for mac type 'LINE'

C MacIndx(i,1),MacIndx(i,2) for mac type 'SINE'

C MacPar(I,1),MacPar(I,2)

C Corners can be identified by changes in the BC Type

C Transition elements are identified by changes in the BC Value.

C Include File: ECBMove.INC

C Written By: Ken Jordan

10/18/89 (After the Big One)

C This file declares variables for the common block ECBMOVE. These variables
C are used in boundary movement

C NoOfIns Number of points in unmoving boundary
C Ins(,2) Points in unmoving boundary. (,1)=x, (,2)=y
C Orig(2,2) First Index: =1, second point on original surface
C =2, next to last point on original surface
C Second index: dimension, (=1,x), (=2,y)
C NoOfMoved Number of points in moving boundary
C Moved(,2) Points in moving boundary. (,1)=x, (,2)=y
C AcuteAngleBefore .TRUE. if an acute angle exists between moving and
C unmoving boundaries at start of moving boundary
C NoAngleBefore .TRUE. if moving and unmoving boundaries start
C at the same point.
C AcuteAngleAfter .TRUE. if an acute angle exists between moving and
C unmoving boundaries at end of moving boundary
C NoAngleAfter .TRUE. if the moving and unmoving boundaries end at
C the same point.
C Nx(,2) normal to point. (,1) x direction, (,2) y direction
C dXdN() current density to point.
C StaRev .TRUE. if the start of the moving boundary is moving backwards
C EndRev .TRUE. if the end of the moving boundary is moving backwards

INTEGER NoOfIns,NoOfMoved,NoOfdXdN

INTEGER First,Second,NextToLast,Last

LOGICAL AcuteAngleBefore,AcuteAngleAfter,StaRev,EndRev

LOGICAL NoAngleBefore,NoAngleAfter

REAL*8 Ins(MaxNoOfCoords,MaxNoOfDim)

REAL*8 Moved(MaxNoOfCoords,MaxNoOfDim)

REAL*8 Orig(2,MaxNoOfDim)

REAL*8 Nx(MaxNoOfCoords,MaxNoOfDim),dXdN(MaxNoOfCoords)

COMMON/ECBMOVE/NoOfIns,Ins,NoOfMoved,Moved,Orig,
& AcuteAngleBefore,AcuteAngleAfter,Nx,dXdN,StaRev,EndRev,
& First,Second,NextToLast,Last,NoAngleBefore,NoAngleAfter

C Include File: ECBMsh.INC

C Written by: Ken Jordan

Date: 3/18/88

C This include file declares the variables that contain the mesh.

C ----- Variables

C Coords(*,*) The coordinates of the node. The first index is the node
C number; the second index is the dimension number. The
C first dimension is always the R dimension

C NodeMap(,) The first index is the element number, the second index
C is the local node number. The contents are the index
C of the global node.

C NoOfCoords The number of coordinates in the mesh.

C NoOfElems The number of elements in the mesh.

C ----- Declarations

INTEGER NoOfCoords,NoOfElems,NodeMap(MaxNoOfCoords,MaxBasisDeg+1)
REAL*8 Coords(MaxNoOfCoords,MaxNoOfDim)

COMMON /ECBMsh/NoOfCoords,Coords,NoOfElems,NodeMap

C Include File: ECBPar.INc.

C Written by: Ken Jordan

Date: 3/18/88

C This include file declares the variables used for secondary current

C distributions (aA, aC, IRatio, JohnNewman) and for geometry

C (Axisymmetric, RInner)

C ----- Variables

C Kinetic Parameters

C aA Anodic transfer coefficient

C aC Cathodic transfer coefficient

C WagLin Wagner number for Linear Kinetics

C = $i_{star} / i_0 = \kappa R T / F x_{star} i_0$

C Nondimensionalization Constants

C tstar The quantity used to make time dimensionless

C = $\rho * n_{elec} * F * x_{star} / (MW * i_{star})$

C = $\rho n_{elec} F^2 x_{star}^2 / MW \kappa R T$

C istar The quantity used to make current density dimensionless

C = $\kappa \Phi_{Star} / x_{star}$

C = $\kappa R T / F x_{star}$

C CorLev .TRUE. if solving problem with corrosion and deposition

C at same time

C Corros Quantity used to scale corrosion current to deposition

C current.

C = $D_a F C_a Bulk / i_{star} x_{star}$

C Corros only has meaning if CorLev is .TRUE.

C (not ideal: better is = $N_a(local) F / i(local)$)

C = $D_a C_a Bulk F / i(local) \delta$

C where $\delta = MT BL$ thickness

C (it's the best we can do at present.)

C Periodic Current Reversal Parameters

C PerRev .TRUE. if solving periodic current reversal problem

C CRRatio Periodic Current Reversal Ratio (>0 always)

C (I init/I final). Only has meaning if PerRev=.TRUE.

C WaLinPCR Ratio of Linear Wagner Numbers for Periodic Current

C Reversal.

C NoOfPCR Number of times to reverse the current

C PCRMax .TRUE. if primary c.d. during dissolution, and uniform c.d.

C during deposition

C Method Parameters

C Axisymmetric .TRUE. if the problem is axisymmetric

C Spline3D .TRUE. if spline should be based on x(d),y(d),d

C .FALSE. if spline should be based on Y(x),x

C MaxIter Maximum number of iterations allowed before program

C quits when doing Newton Raphson technique

C SrcFactor Factor (>1) used to determine radius of circle that

C has source points on it.

C Tolerance Used to determine convergence tolerance for NR technique
C and to tell when two points are the same.

C BC Parameters

C KineticsFile filename containing data for user defined kinetics routine.

C ----- Declarations

INTEGER MaxIter,NoOfPCR
LOGICAL Axisymmetric,Spline3D,CorLev,PerRev,PCRMax
REAL*8 WagLin,aA,aC,Tolerance,SrcFactor,Corros,CRRatio
REAL*8 tstar, istar,WaLinPCR
CHARACTER*80 Kineticsfile

COMMON/ECBPar/ aA,aC,WagLin,tstar,istar,Corros,CRRatio,WALinPCR,
& Axisymmetric,CorLev,Spline3D,PerRev,
& Tolerance,SrcFactor,MaxIter,KineticsFile,
& PCRMax,NoOfPCR

C Include File: ECBPar2.INC

C This include file contains declarations and COMMON statements for the
C dimensional parameters describing the ECB problem.

C -----Input Parameters

C F

C CaBulk [mol/l], Da (Bulk Concentration, Diffusivity) Parameters For

C Corrosive Chemical

C Kappa Electrolyte Conductivity [1/ohm-cm]

C aA, aC, i0 [mA/cm2] Metal Electrodeposition Kinetics

C xstar [um],PhiStar [V] Geometry Scale (amplitude), Potential Scale

C -----Calculated Nondimensionalization Constants

C (phistar = RT/F)

C istar = kappa PhiStar / xstar

C -----Important Dimensionless Groups

C Waglin = istar / i0

C Corros = Da F CaBulk / i0 delta

REAL*8 F

REAL*8 CaBulk, Da, kappa

INTEGER nelec

REAL*8 i0

REAL*8 xstar, PhiStar

REAL*8 rho, MW

REAL*8 idep

COMMON /EcbPar2/F, CaBulk, Da, kappa, nelec, i0, xstar,
& PhiStar, rho, MW, idep

c Include File: ECBRemesh.INC

C Contains declarations for common block variables used in remeshing.

C Variables

C SpaFac Used to weight importance of spacing (0 = unimportant
c 1=equal in importance to curvature)
C UpFac Bound the curvature by avg error * Up Fac as maximum
C LowFac Bound the curvature by avg error * Low Fac as minimum
C SlopFac Bound the changes in curvature by (Max-Min)/TotDis/SlopFac

COMMON /ECBRemesh/SpaFac,UpFac,LowFac,SlopFac
REAL*8 SpaFac,UpFac,LowFac,SlopFac

C Include File: ECBSrc.INC

C Written by: Ken Jordan

Date: 3/18/88

C This include file declares the variables used to describe the source
C points.

C ----- Variables

C NoOfSrc The number of source points. (This should equal the number
C of nodes)

C Src(,) The coordinates of the source points. The first index is
C the source point number, the second index is the dimension

C ----- Declarations

INTEGER NoOfSrc

REAL*8 Src(MaxNoOfCoords,MaxNoOfDim)

COMMON /ECBSrc/NoOfSrc,Src

C Include File ECBTime.INC
C This file contains variables used by program ECBM to do time stepping.

C TimeCounter
C MaxTimeCounter
C Time
C dTime
C EndTime
C DesdX
C DesdTime
C MotdTime
C LastTime

INTEGER TimeCounter,MaxTimeCounter
REAL*8 Time,dTime,Endtime,DeltaTime
REAL*8 DesdX,DesdTime,MotdTime
LOGICAL LastTime

COMMON /ECBTime/Timecounter,MaxtimeCounter,Time,Dtime,endtime,
& DesdX,DesdTime,MotdTime,LastTime,DeltaTime

C Include File: ECBTMac.INC

C Written By: Ken Jordan

Date: 6/5/87

C This include file defines and dimensions the variables used in the ECBMAC
C common block for setting up a mesh. The file is used by program ECBPrePro.

C ----- Variables

C TNoOfMicElems() The number of elements for each macro element
C TMacBCType() The b.c. to be applied to the element
C 'ESS','NAT','CRNT','BV','LIN','TAFa','TAFC'
C TMacBCVal() The b.c. value for the element
C Value of the potential in the node I if BCType(i)=0
C Value of the potential derivative if BCType(i)=1
C TMacIndx(.) The first index is the macro element number,
C If the macro element is a line then the contents for
C second index=1 is the index number of the macro vertex
C at the start of the line segment.
C second index=2 is the index number of the macro vertex
C at the end of the line segment.
C TMacPar(.) Parameters used for various macro element types.
C 'SINE' $Y=Y_0+A*\sin(\text{MacPar}(I,1)*X+\text{MacPar}(I,2))$
C TMacShape() The type of macro-element. Currently, the only type allowed
C is 'LINE','SINE'
C TMacSpac() The spacing for the macro-element. (LOG, CHEB, EQU)
C TMacRatio() The spacing parameter for LOG spacing.

C ----- Declarations

COMMON /ECBTMac/ TMacShape,TNoOfMicElems,TMacBCType,TMacBCVal,
& TMacIndx,TMacPar,TMacSpac,TMacRatio

INTEGER TNoOfMicElems(MaxNoOfMacVert),
& TMacIndx(MaxNoOfMacVert,2)
REAL*8 TMacBCVal(MaxNoOfMacVert),TMacPar(MaxNoOfMacVert,3),
& TMacRatio(MaxNoOfMacVert)

CHARACTER*4 TMacShape(MaxNoOfMacVert),TMacBCType(MaxNoOfMacVert),
& TMacSpac(MaxNoOfMacVert)

C Include File: ECGaus.INC

C Written by: Ken Jordan

Date: 3/18/88

C Contains declarations for the common block containing gaussian quadrature
C variables. The Gauss Points and Weights may be obtained by calling
C subroutine GauLeg()

C ----- Parameters

C MaxNoOfGauss The maximum number of gauss points and weigths allowed by
C the program.

C ----- Variables

C NoOfGaussPts The number of gauss points specified by the user.

C GaussWts(*) The gauss weights to use (interval 0->1)

C GaussPts(*) The Gauss points to use (interval 0->1)

C ----- Declarations

PARAMETER MaxNoOfGauss=20

INTEGER NoOfGaussPts

REAL *8 GaussWts(MaxNoOfGauss),GaussPts(MaxNoOfGauss)

COMMON/ECGaus/ NoOfGaussPts,GaussPts,GaussWts

C Include File: ECGLOG.INC

C Written by: Ken Jordan

Date: 3/18/88

C Contains declarations for the common block containing gaussian quadrature
C variables. The Gauss Points and Weights may be obtained by calling
C subroutine GauLOG(). Points and weights are for integrating from 0 to
C 1, $f(x)*LN(1/x)$.

C ----- Parameters

C MaxNoOfGauLog The maximum number of gauss points and weights allowed by
C the program.

C ----- Variables

C NoOfGauLogPts The number of gauss points specified by the user.

C GauLogWts(*) The gauss weights to use (interval 0->1)

C GauLogPts(*) The GauLog points to use (interval 0->1)

C ----- Declarations

PARAMETER MaxNoOfGauLog=20

INTEGER NoOfGauLogPts

REAL*8 GauLogWts(MaxNoOfGauLog),GauLogPts(MaxNoOfGauLog)

COMMON/ECGaus/ NoOfGauLogPts,GauLogPts,GauLogWts

C I/O Subroutines

```

c   SUBROUTINE Center(String,TWidth,Centered)
c   SUBROUTINE WriteCenter(Lun,Width,Line)
c   SUBROUTINE ClrScr

c   SUBROUTINE ChInp(PROMPT,VAR)           (Obtains Ch,DP,Dt,I, or R
c   SUBROUTINE DPInp(Prompt,Var)         from the user. If a <CR>
c   SUBROUTINE DtInp(Prompt,Date$,Date) is pressed, 0 or ' ' is
c   SUBROUTINE IInp(Prompt,Var)         stored in the variable)
c   SUBROUTINE RInp(Prompt,Var)
C   SUBROUTINE GetFileName(Prompt,FileName)

c   SUBROUTINE EditCh(Prompt,Var)         (Obtains Ch,DP,Dt,I, or R
c   SUBROUTINE EditI(Prompt,Var)         from the user. If a <CR>
c   SUBROUTINE EditR(Prompt,Var)         is pressed, the previous
c   SUBROUTINE EditDP(Prompt,Var)         value of the variable remains
c   SUBROUTINE EditDtCh(Prompt,Date$,Date) in the variable)
c   SUBROUTINE EditDl(Prompt,Date$,Date)

c   SUBROUTINE PauseCrt
c   SUBROUTINE Menu(MenuTitle,MenuTxt,NTxt,MenuPrompt,MenuResps,NResps,
c   & DefResp,UsrResp)
c   SUBROUTINE Yorn(Prompt$,Yes)

```

C Special I/O Conversion routines. (e.g. 1 line of data to a matrix/
C matrix to 1 line of data)

```

c   SUBROUTINE CodeI(List,NoOfElems,String)
c   SUBROUTINE CodeR(List,NoOfElems,String)

c   SUBROUTINE DecodeCh(String,Delimiter,List,NoOfElems,MaxNoOfElems)
c   SUBROUTINE DecodeI(String,List,NoOfElems,MaxNoOfElems)
c   SUBROUTINE DecodeR(String,List,NoOfElems,MaxNoOfElems)
C   SUBROUTINE DecodeDP(String,List,NoOfElems,MaxNoOfElems)

```

C Matrix Manipulation subroutines

```

c   SUBROUTINE CompareListI(List1,NoOfElems1,
c   & List2,NoOfElems2,Matches,NoOfMatches)
c   SUBROUTINE CompareListR(List1,NoOfElems1,
c   & List2,NoOfElems2,Matches,NoOfMatches)

c   SUBROUTINE FindMaxCh(Matrix,NoOfElems,MaxCh,MaxLoc)
C   SUBROUTINE FindMaxDt(Dates,NoOfDates,MaxDt,MaxLoc)
c   SUBROUTINE FindMaxI(Matrix,NoOfElems,MaxI,MaxLoc)

c   SUBROUTINE FindMinCh(Matrix,NoOfElems,MinCh,MinLoc)
c   SUBROUTINE FindMinDt(Matrix,NoOfElems,MinDt,MinLoc)
c   SUBROUTINE FindMinI(Matrix,NoOfElems,MinI,MinLoc)

c   SUBROUTINE FindMatchesDP(Matrix,NElements,MatchElement,
c   & MatchLocs,Found,NoLocs)
c   SUBROUTINE FindMatchesI(Matrix,NElements,MatchElement,
c   & MatchLocs,Found,NoLocs)
c   SUBROUTINE FindMatchesR(Matrix,NElements,MatchElement,
c   & MatchLocs,Found,NoLocs)

```

```

c     SUBROUTINE MatDateBend(DateCh,NoOfElems,DateN)
c     SUBROUTINE MatExtremaR(Matrix,NoOfPts,Maxi,Mini)
c     SUBROUTINE MatExtremaDP(Matrix,NoOfPts,Maxi,Mini)

c     SUBROUTINE SearchCh(Matrix,NElements,MatchElement,Location,Found,
c & NoLocs)
c     SUBROUTINE SearchChSub(Matrix,NElements,StartLoc,EndLoc,
c & MatchElement,Location,Found,NoLocs)
c     SUBROUTINE SearchDP(Matrix,NElements,MatchElement,Location,Found,
c & NoLocs)
c     SUBROUTINE SearchI(Matrix,NElements,MatchElement,Location,Found,
c & NoLocs)
c     SUBROUTINE SearchL(Matrix,NElements,MatchElement,Location,Found,
c & NoLocs)
c     SUBROUTINE SearchR(Matrix,NElements,MatchElement,Location,Found,
c & NoLocs)

c     SUBROUTINE SortCh(Matrix,NoElems,Pointer)
c     SUBROUTINE SortDP(Matrix,NoElems,Pointer)
c     SUBROUTINE SortI(Matrix,NoElems,Pointer)
c     SUBROUTINE SortR(Matrix,NoElems,Pointer)

```

C Single Variable Character/Date Manipulation subroutines

```

c     SUBROUTINE UpperCaseCh(String)
c     SUBROUTINE LowerCaseCh(String)
c     SUBROUTINE ConvertChToI(String2,Int)
c     SUBROUTINE ConvertChToR(String2,Re)
c     SUBROUTINE ConvertChToDP(String2,Re)
c     SUBROUTINE ConvertDtToI(Date$,Mo,Da,Yr)
c     SUBROUTINE ConvertDPToWords(Number,Words)

c     SUBROUTINE DateBend(Date$,Date)           (converts MM/DD/YY to YYMMDD)
c     SUBROUTINE DateUnBend(TDate,Date$)       (converts YYMMDD to MM/DD/YY)

c     SUBROUTINE TrimCh(String)                 (Places first non-blank char
c                                               in String(1:). Sets all
C                                               trailing blanks to nuls CHAR(0))

c     SUBROUTINE RemoveBlanksFromCh(String)     (Places all non-blank chars
C                                               next to each other starting
C                                               in String(1:). E.g.
C                                               'This is a test' becomes
C                                               'Thisisatest'

c     SUBROUTINE RemoveCharFromCh(String,Blank)
c     SUBROUTINE StringLength(String,Length)
c     SUBROUTINE RptString(Repeat,NoOfTimes,String)

```

C File Manipulation Subroutines

```

c     SUBROUTINE FileRename(OldName,NewName)
c     SUBROUTINE FileDelete(FileName)
c     SUBROUTINE FilePurge(FileName)

```

C Numeric Manipulation Subroutines

```

c     Subroutine PRoundDP(Number,PowerOfTen,Rounded)
c     SUBROUTINE IXCHNG(I1,I2)

```

C Plotting Routines

```
c    SUBROUTINE SetPlotter(TermType)
c    SUBROUTINE GetPlotter(TermType)
c    SUBROUTINE SetUpImagen
c    SUBROUTINE SetUpTalaris
c    SUBROUTINE SetUpVT240
```

C ***** Center

```

SUBROUTINE Center(String,TWidth,Centered)

CHARACTER*(*) STRING,CENTERED
INTEGER WIDTH,TWidth
INTEGER BlankColumns,l,Length

Width=TWidth
IF (Width.GT.LEN(Centered)) Width=LEN(Centered)

CALL TrimCh(String)

Length=LEN(String)
DO L=Length,1,-1
  IF (String(L:L).NE.' ') GOTO 100
END DO

Centered(1:)= ' '
RETURN

100  IF (L.GT.Width) L=Width
    BlankColumns=(Width-L)/2

    Centered(1:BlankColumns)= ' '

    IF (BlankColumns.NE.0) THEN

      Centered(BlankColumns:)=String(1:
& MIN(LEN(CENTERED)-BlankColumns,L))

    ELSE
      Centered(1:)=String(1:)
    END IF

    RETURN
  END

```

C ***** ChInp

```

SUBROUTINE ChInp(PROMPT,VAR)

C This subroutine prints the PROMPT and obtains a character response in VAR

COMMON /EDITSUBS/DataEntered

CHARACTER*(*) PROMPT,VAR
INTEGER Apostrophe,Length
LOGICAL DataEntered

CALL StringLength(Prompt,Length)
WRITE(*,*) PROMPT(1:Length)
READ(*,100) VAR
100  FORMAT(A)

IF (Var.EQ.' ') THEN
  DataEntered=.FALSE.
ELSE

```

```

        DataEntered=.TRUE.
    END IF

200   Apostrophe=INDEX(Var,')')
    IF (Apostrophe.NE.0) THEN
        Var(Apostrophe:Apostrophe)=''
        GOTO 200
    END IF

    RETURN
    END

```

c ***** ClrScr

```

SUBROUTINE ClrScr

```

C This subroutine clears the digital terminal's screen

```

        BYTE ESCAPE/27/
        WRITE(*,100) ESCAPE
100   FORMAT (' ',A1,'[2J')

        RETURN
        END

```

C ***** CodeI

```

SUBROUTINE CodeI(List,NoOfElems,String)

```

```

CHARACTER*(*) String
CHARACTER*80 Dummy
INTEGER List(*)
INTEGER NoOfElems,Length,I,Comma
LOGICAL Zeros

```

```

        Length=0
        DO I=1,NoOfElems
            Dummy(1:)= ' '
10       write(unit=Dummy(1:),FMT=10) List(I)
            FORMAT (I,',')
            CALL RemoveBlanksFromCh(Dummy)

            Comma=INDEX(Dummy,',')

            String(Length+1:Length+Comma)=Dummy(1:Comma)
            Length=Length+Comma
        END DO

        IF (Length.GT.0) THEN
            String(Length:)= ' '
        ELSE
            String=' '
        END IF

        RETURN
        END

```

C ***** CodeR

```

SUBROUTINE CodeR(List,NoOfElems,String)

CHARACTER*(*) String
REAL List(*)
CHARACTER*80 Dummy
INTEGER NoOfElems,Length,I,Comma,Dot,ELoc,J,NewELoc
LOGICAL Zeros

Length=0
DO I=1,NoOfElems
  Dummy(1:)= '
  write(unit=Dummy(1:),FMT=10) List(I)
10  FORMAT (G,',')
  CALL RemoveBlanksFromCh(Dummy)

  Comma=INDEX(Dummy,',')
  Dot=INDEX(Dummy, '.')
  ELoc=INDEX(Dummy, 'E')
  IF (ELoc.EQ.0) THEN
    DO J=Comma-1, Dot+1, -1
      IF (Dummy(J:J).NE.'0') THEN
        Comma=J+1
        GOTO 20
      END IF
    END DO
    Comma=Dot
    Dummy(Comma:)= ','
20  ELSE
    NewELoc=ELoc
    DO J=ELoc-1, Dot+1, -1
      IF (Dummy(J:J).NE.'0') THEN
        NewELoc=J+1
        GOTO 30
      END IF
    END DO
    NewELoc=Dot
30  Dummy(NewELoc:)=Dummy(ELoc:)
    Comma=INDEX(Dummy,',')
  END IF

  String(Length+1:Length+Comma)=Dummy(1:Comma)
  Length=Length+Comma

END DO

IF (Length.GT.0) THEN
  String(Length:)= '
ELSE
  String= '
END IF

RETURN
END

```

C ***** CompareListI

```

SUBROUTINE CompareListI(List1,NoOfElems1,
& List2,NoOfElems2,Matches,NoOfMatches)

```

```

INTEGER NoOfElems1,NoOfElems2,NoOfMatches
INTEGER List1(*),List2(*),Matches(*),I,J

```

```

NoOfMatches=0
DO I=1,NoOfElems1
  DO J=1,NoOfElems2
    IF (List1(I).EQ.List2(J)) THEN
      NoOfMatches=NoOfMatches+1
      Matches(NoOfMatches)=List1(I)
    END IF
  END DO
END DO

```

```

RETURN
END

```

C ***** CompareListR

```

SUBROUTINE CompareListR(List1,NoOfElems1,
& List2,NoOfElems2,Matches,NoOfMatches)

```

```

INTEGER NoOfElems1,NoOfElems2,NoOfMatches,I,J
REAL List1(*),List2(*),Matches(*)

```

```

NoOfMatches=0
DO I=1,NoOfElems1
  DO J=1,NoOfElems2
    IF (List1(I).EQ.List2(J)) THEN
      NoOfMatches=NoOfMatches+1
      Matches(NoOfMatches)=List1(I)
    END IF
  END DO
END DO

```

```

RETURN
END

```

C ***** ConvertChToDP

```

SUBROUTINE ConvertChToDP(String2,Re)

```

```

CHARACTER*(*) String2
CHARACTER*80 String
INTEGER StringLength,NoCharacters,NoDots,NoSigns,NoE,ErrNo,I,J
LOGICAL Quit
DOUBLE PRECISION Re

```

```

String=String2
CALL UpperCaseCh(String)

```

```

NoE=0
NoSigns=0
NoDots=0
NoCharacters=0
StringLength=LEN(String)

```

```

I=0
QUIT=.FALSE.
DO WHILE (.NOT.QUIT)
  I=I+1
  IF (I.GT.StringLength) GOTO 3

  IF (((String(I:I).GE.'0').AND.(String(I:I).LE.'9'))
& .OR.(String(I:I).EQ.' ').OR.(String(I:I).EQ.'+'))
& .OR.(String(I:I).EQ.'-').OR.(String(I:I).EQ.'E')) THEN

    IF ((String(I:I).EQ.'-').OR.(String(I:I).EQ.'+')) THEN
      NoSigns=NoSigns+1
      IF (NoSigns.GE.2) GOTO 5
    END IF

    IF (String(I:I).EQ.'.') THEN
      NoDots=NoDots+1
      IF (NoDots.GE.2) goto 5
    END IF

    IF (String(I:I).EQ.'E') THEN
      NoE=NoE+1
      IF (NoE.GE.2) GOTO 5
      NoSigns=0
      IF ((String(I+1:I+1).EQ.'-')
& .OR.(String(I+1:I+1).EQ.'+')) THEN
        StringLength=MIN(I+3,StringLength)
      ELSE
        StringLength=MIN(I+2,StringLength)
      END IF
      IF (NoDots.EQ.0) THEN

        DO J=StringLength,I,-1
          String(J+1:J+1)=String(J:J)
        END DO
        StringLength=StringLength+1
        NoCharacters=NoCharacters+1
        String(NoCharacters:NoCharacters)='.'
        NoDots=NoDots+1
        I=I+1

      END IF
    END IF

    NoCharacters=NoCharacters+1
    String(NoCharacters:NoCharacters)=String(I:I)

  END IF
3  IF (I.GE.StringLength) QUIT=.TRUE.
  END DO

5  DO I=StringLength,NoCharacters+1,-1
    String(I:I)=CHAR(0)
  END DO

  IF (NoCharacters.EQ.0) THEN
    Re=0.
    RETURN
  
```



```

      END IF

      IF ((String(NoCharacters:NoCharacters).EQ.'+') .OR.
& (String(NoCharacters:NoCharacters).EQ.'-')) THEN
        NoCharacters=NoCharacters-1
      END IF

      IF (NoCharacters.EQ.0) THEN
        Re=0.
        RETURN
      END IF

      IF (NoDots.EQ.0) THEN
        NoDots=NoDots+1
        NoCharacters=NoCharacters+1
        String(NoCharacters:NoCharacters)='.'
      END IF

      IF (String(1:1).EQ.'') THEN
        DO J=NoCharacters,1,-1
          String(J+1:J+1)=String(J:J)
        END DO
        NoCharacters=NoCharacters+1
        String(1:1)='0'
      END IF

      IF (((String(1:1).EQ.'-') .OR. (String(1:1).EQ.'+'))
& .AND.(String(2:2).EQ.'')) THEN
        DO J=NoCharacters,2,-1
          String(J+1:J+1)=String(J:J)
        END DO
        NoCharacters=NoCharacters+1
        String(2:2)='0'
      END IF

      IF (NoE.EQ.1) THEN

        IF (String(1:1).EQ.'E') THEN
          DO I=NoCharacters,1,-1
            String(I+2:I+2)=String(I:I)
          END DO
          String(1:1)='1'
          String(2:2)='.'
          NoCharacters=NoCharacters+2
        END IF

        IF (String(NoCharacters:NoCharacters).EQ.'E') THEN
          NoCharacters=NoCharacters-1
          NoE=NoE-1
        END IF

      END IF

      DECODE(NoCharacters,10,String,IOSTAT=ErrNo,ERR=20) Re
10  FORMAT(G)
20  IF (ErrNo.GT.0) Re=1.E+37

      RETURN

```

END

C ***** ConvertChToI

SUBROUTINE ConvertChToI(String2,Int)

CHARACTER*(*) String2

CHARACTER*80 String

INTEGER Int,StringLength,NoCharacters,Sighn,I

String=String2

NoCharacters=0

StringLength=LEN(String)

Sighn=1

DO I=1,StringLength

IF (String(I:I).EQ.'-') Sighn=-Sighn

IF ((String(I:I).GE.'0').AND.(String(I:I).LE.'9')) THEN

NoCharacters=NoCharacters+1

String(NoCharacters:NoCharacters)=String(I:I)

END IF

IF (String(I:I).EQ.'.') GOTO 5

END DO

5 DO I=StringLength,NoCharacters+1,-1

String(I:I)=CHAR(0)

END DO

IF (NoCharacters.GT.9) NoCharacters=9

DECODE(NoCharacters,10,String) Int

10 FORMAT(I<NoCharacters>)

Int=Sighn*Int

RETURN

END

C ***** ConvertChToR

SUBROUTINE ConvertChToR(String,Re)

CHARACTER*(*) String

REAL Rc

REAL*8 Dp

CALL ConvertChToDP(String,Dp)

Re=Dp

RETURN

END

C ***** ConvertDPToWords

SUBROUTINE ConvertDPToWords(Number,Words)

C Include file: Numwords.inc

C Written by: Ken Jordan Date: 7/12/85
 C Approved by: Date:

C This file contains declarations and data statements for variables
 C useful for converting numbers to words.

C -----
 C VARIABLES

C One_to_20\$0 The words for one to twenty.
 C Tea\$0 The words for ten to ninety.
 C Hundred\$ 'Hundred'
 C Thousand\$ 'Thousand'

C -----
 C Declarations

CHARACTER*10 One_to_20\$(19)/' One',' Two',' Three',' Four',
 & ' Five',' Six',' Seven',' Eight',' Nine',' Ten',' Eleven',
 & ' Twelve',' Thirteen',' Fourteen',' Fifteen',' Sixteen',
 & ' Seventeen',' Eighteen',' Nineteen'/

CHARACTER*8 Tea\$(9)/' Ten',' Twenty',' Thirty',' Forty',
 & ' Fifty',' Sixty',' Seventy',' Eighty',' Ninety'/

CHARACTER*7 Hundred\$/' Hundred'/
 CHARACTER*9 Thousand\$/' Thousand'/

INTEGER WordLoc,I,Space
 DOUBLE PRECISION Number,Amt
 CHARACTER*80 WordList(10)
 CHARACTER*(*) Words
 LOGICAL Thou_flag

Thou_flag=.FALSE.
 WordLoc=0

DO I=1,10
 , WordList(I)=' '
 END DO

Amt=Number
 IF (Amt.GE.1E5) THEN
 WordLoc=INT(Amt/1E5)
 WordList(10)=One_to_20\$(WordLoc)
 WordList(9)=Hundred\$
 Amt=Amt-WordLoc*1E5
 Thou_flag=.TRUE.
 END IF

IF (Amt.GE.20000) THEN
 WordLoc=INT(Amt/1E4)
 Thou_flag=.TRUE.
 WordList(8)=Tea\$(WordLoc)
 Amt=Amt-WordLoc*1E4
 END IF

IF (Amt.GE.1000) THEN

```

    Thou_flag=.TRUE.
    WordLoc=INT(Amt/1000)
    WordList(7)=One_to_20$(WordLoc)
    Amt=Amt-WordLoc*1000
  END IF

```

```

  IF (Thou_flag) WordList(6)=Thousand$

```

```

  IF (Amt.GE.100) THEN
    WordLoc=INT(Amt/100)
    WordList(5)=One_to_20$(WordLoc)
    WordList(4)=Hundred$
    Amt=Amt-WordLoc*100
  END IF

```

```

  IF (Amt.GE.20) THEN
    WordLoc=INT(Amt/10)
    WordList(3)=Ten$(WordLoc)
    Amt=Amt-WordLoc*10
  END IF

```

```

  IF (Amt.GE.1) THEN
    WordLoc=INT(Amt)
    WordList(2)=One_to_20$(WordLoc)
    Amt=Amt-WordLoc
  END IF

```

C Print out the pay in words

```

    CALL PRoundDP(Amt*100,0,Amt)

    WRITE(UNIT=Words,FMT=10) INT(Amt)
10  FORMAT(' and ',I2,'/100 Dollars')

    DO I=2,10
      IF (WordList(I).NE.' ') THEN
        CALL RemoveBlanksFromCh(WordList(I))
        Space=INDEX(WordList(I),' ')
        Words(1:)=WordList(I)(1:Space)//Words(1:)
      END IF
    END DO

    RETURN
  END

```

C ***** ConvertDtToI

```

SUBROUTINE ConvertDtToI(Date$,Mo,Da,Yr)

  CHARACTER*(*) Date$
  INTEGER Mo,Da,Yr

  CALL ConvertChToI(Date$(1:2),Mo)
  CALL ConvertChToI(Date$(4:5),Da)
  CALL ConvertChToI(Date$(7:8),Yr)

  RETURN
END

```

C ***** DPInp

SUBROUTINE DPInp(Prompt,Var)

C This subroutine prints the Prompt and obtains a double precision Var
C from the user

COMMON /EDITSUBS/DataEntered

CHARACTER*(*) PROMPT
DOUBLE PRECISION Var
CHARACTER*80 Response
LOGICAL DataEntered

CALL ChInp(Prompt,Response)
IF (Response.EQ.' ') THEN
 DataEntered=.FALSE.
ELSE
 DataEntered=.TRUE.
END IF
CALL ConvertChToDP(Response,Var)

RETURN
END

C ***** DateBend

SUBROUTINE DateBend(Date\$,Date)

INTEGER Date,Year,Month,Day
CHARACTER*8 Date\$,Temp

Temp=Date\$(7:8)
CALL ConvertChToI(Temp,Year)
Temp=Date\$(1:2)
CALL ConvertChToI(Temp,Month)
Temp=Date\$(4:5)
CALL ConvertChToI(Temp,Day)
Date=Year*10000+Month*100+Day

RETURN
END

C ***** DateUnBend

SUBROUTINE DateUnBend(TDate,Date\$)

INTEGER Year,Date,Month,Day,Tdate
CHARACTER*8 Date\$

IF (TDate.GT.999999) THEN
 DATES='99/99/99'
 RETURN
END IF

Date=Tdate
Year=Date/10000
Date=Date-Year*10000

```

Month=Date/100
Day=Date-Month*100

10 WRITE(Unit=Date$(1:),FMT=10) Month
   FORMAT(I2)
   WRITE(Unit=Date$(4:),FMT=10) Day
   WRITE(UNIT=Date$(7:),FMT=10) Year

Date$(3:3)='/'
Date$(6:6)='/'

RETURN
END

```

C ***** DecodeCh

```

SUBROUTINE DecodeCh(String,Delimiter,List,NoOfElems,MaxNoOfElems)

CHARACTER*(*) String,Delimiter,List(*)
INTEGER NoOfElems,MaxNoOfElems,NoOfParans,Length,MaxLength
INTEGER I,NoOfChar,MaxLen2
LOGICAL Spaces,Word,Quotes,Skip

Spaces=(Delimiter.EQ.' ')
NoOfElems=0
NoOfChar=0
NoOfParans=0

MaxLength=LEN(List(1))
CALL StringLength(String,Length)
MaxLen2=LEN(String)

Word=.FALSE.
Quotes=.FALSE.
Skip=.FALSE.

DO I=1,MaxNoOfElems
  List(I)(1:)' '
END DO

DO I=1,Length
  IF ((String(I:MIN(I+1,MaxLen2)).EQ.'''')
& .OR.(String(I:MIN(I+1,MaxLen2)).EQ.'''')) THEN
    Skip=.TRUE.
  ELSE IF ((String(I:I).EQ.'''').OR.(String(I:I).EQ.'''')) THEN
    IF (.NOT.Skip) Quotes=.NOT.Quotes
    Skip=.FALSE.
  ELSE IF (.NOT.Quotes) THEN
    IF (String(I:I).EQ.'(') NoOfParans=NoOfParans+1
    IF (String(I:I).EQ.')') NoOfParans=NoOfParans-1
  END IF

  IF (Word) THEN
    IF ((String(I:I).EQ.Delimiter(1:1)).AND.
& (.NOT.Quotes).AND.(NoOfParans.LE.0)) THEN
      Word=.FALSE.
    ELSE

```

```

        NoOfChar=NoOfChar+1
    IF (NoOfChar.LE.MaxLength) THEN
        List(NoOfElems)(NoOfChar:NoOfChar)=String(I:I)
    ELSE

        WRITE(*,*) 'Warning: too many characters. The'
        WRITE(*,*) 'following was ignored:'
        WRITE(*,*) String(I:)
        WRITE(*,*) 'The following was kept:'
        WRITE(*,*) List(NoOfElems)
        WRITE(*,*) ' '
        RETURN

    END IF

    END IF
ELSE
    IF (String(I:I).NE.Delimiter(1:1)) THEN

        Word=.TRUE.
        NoOfChar=1
        IF (NoOfElems.GE.MaxNoOfElems) THEN
            WRITE(*,*) 'WARNING, TOO MANY ELEMENTS IN LIST'
            WRITE(*,*) 'THE FOLLOWING WAS IGNORED:',String(I:)
            GOTO 100
        END IF
        NoOfElems=NoOfElems+1
        List(NoOfElems)(NoOfChar:NoOfChar)=String(I:I)

    ELSE

        IF (.NOT.Spaces) THEN
            IF (NoOfElems.GE.MaxNoOfElems) THEN
                WRITE(*,*) 'WARNING, TOO MANY ELEMENTS IN LIST'
                WRITE(*,*) 'THE FOLLOWING WAS IGNORED:',String(I:)
                GOTO 100
            END IF
            NoOfElems=NoOfElems+1
            List(NoOfElems)=' '
        END IF

    END IF
END IF
END DO
100 DO I=1,NoOfElems
    CALL RemoveBlanksFromCh(List(I))
END DO

RETURN
END

```

C ***** DecodeDP

SUBROUTINE DdecodeDP(String,List,NoOfElems,MaxNoOfElems)

CHARACTER*(*) String

```

CHARACTER*80 Dummy
DOUBLE PRECISION List(*)
INTEGER NoOfElems,MaxNoOfElems
INTEGER CommaLoc,Length

NoOfElems=0
CommaLoc=1
CALL StringLength(String,Length)
String(Length+1:Length+1)=' '

DO WHILE (CommaLoc.GT.0)
  CommaLoc=INDEX(String,',')
  IF (CommaLoc.GT.0) THEN
    IF (NoOfElems.LT.MaxNoOfElems) THEN

      IF (CommaLoc.EQ.1) THEN
        Dummy='0'
      ELSE
        Dummy=String(1:CommaLoc-1)
      END IF

      String=String(CommaLoc+1:)
      NoOfElems=NoOfElems+1
      CALL ConvertChToDP(Dummy,List(NoOfElems))

    ELSE

      WRITE(*,*) 'Warning: the following information was'
      WRITE(*,*) 'lost:',String
      CALL PauseCrt
      RETURN

    END IF
  END IF
END DO

RETURN
END

```

C ***** DecodeI

```

SUBROUTINE DecodeI(String,List,NoOfElems,MaxNoOfElems)

PARAMETER MaxListLen=200
CHARACTER*(*) String
INTEGER List(*)
INTEGER NoOfElems,MaxNoOfElems,I
DOUBLE PRECISION ListDP(MaxListLen)

IF (MaxNoOfElems.GT.MaxListLen) THEN

  WRITE(*,*) 'Warning: Programming error. DecodeI has '
  WRITE(*,*) 'been called with MaxNoOfElems greater than'
  WRITE(*,*) 'MaxListLen. MaxListLen in subroutine DecodeI'
  WRITE(*,*) 'will have to be increased to ',MaxNoOfElems
  WRITE(*,*) 'and the accounting programs re-compiled'
  WRITE(*,*) '(Note: DecodeI is in file SUBS.FOR)'
  STOP

```


ELSE

```
CALL DecodeDP(String,ListDP,NoOfElems,MaxListLen)
DO I=1,NoOfElems
  List(I)=INT(ListDP(I))
END DO
```

END IF

```
RETURN
END
```

C ***** DecodeR

SUBROUTINE DecodeR(String,List,NoOfElems,MaxNoOfElems)

```
PARAMETER MaxListLen=200
CHARACTER*(*) String
REAL List(*)
INTEGER NoOfElems,MaxNoOfElems,I
DOUBLE PRECISION ListDP(MaxListLen)
```

IF (MaxNoOfElems.GT.MaxListLen) THEN

```
WRITE(*,*) 'Warning: Programming error. DecodeR has '
WRITE(*,*) 'been called with MaxNoOfElems greater than '
WRITE(*,*) 'MaxListLen. MaxListLen in subroutine DecodeR'
WRITE(*,*) 'will have to be increased to ',MaxNoOfElems
WRITE(*,*) 'and the accounting programs re-compiled'
WRITE(*,*) '(Note: DecodeR is in file SUBS.FOR)'
STOP
```

ELSE

```
CALL DecodeDP(String,ListDP,NoOfElems,MaxListLen)
DO I=1,NoOfElems
  List(I)=ListDP(I)
END DO
```

END IF

```
RETURN
END
```

C ***** DpXChng

SUBROUTINE DpXCHNG(Dp1,Dp2)

```
REAL*8 Dp1,Dp2,Dp3
```

```
Dp3 = Dp1
Dp1 = Dp2
Dp2 = Dp3
```

```
RETURN
END
```

C ***** DdInp

```

SUBROUTINE DtInp(Prompt,Date$,Date)

CHARACTER*(*) Prompt,Date$
INTEGER Date,Day,Month,Year,I
CHARACTER*2 Dummy
LOGICAL Err

6870 WRITE(*,*) 'Enter date as MM/DD/YY'
CALL ChInp(Prompt,Date$)
IF (Date$.EQ.' ') THEN
    Date=0
    RETURN
END IF

IF (LEN(Date$).EQ.8) GO TO 6820

WRITE (*,6760) Date$
6760 FORMAT (' Error: date is not 8 characters long: ',A)
GO TO 6870

6820 IF ((Date$(3:3).EQ.'/').AND.(Date$(6:6).EQ.'/')) GO TO 6890

WRITE (*,6830) Date$
6830 FORMAT (' Error: Invalid date: ',A/,
1 ' 3rd and 6th characters must be '/')
GO TO 6870

6890 Err=.FALSE.
DO I=1,8
    IF ((I.NE.3).AND.(I.NE.6)) THEN
        IF ((Date$(I:I).LT.'0').AND.(Date$(I:I).GT.'9')) THEN
            IF (.NOT.Err) THEN
                WRITE(*,*) 'Error: nonnumeric characters at positions:'
            END IF
            Err=.TRUE.
            WRITE(*,*) I
        END IF
    END IF
END DO

IF (Err) GO TO 6870

Dummy=Date$(1:2)
CALL ConvertChToI(Dummy,Month)
IF ((Month.GE.1).AND.(Month.LE.12)) GO TO 7080

WRITE (*,6990) Month
6990 FORMAT (' Error: impossible month: ',I5)

GO TO 6870

7080 Dummy=Date$(4:5)
CALL ConvertChToI(Dummy,Day)
IF ((Day.GE.1).AND.(Day.LE.31)) GO TO 7140
WRITE (*,7090) Day
7090 FORMAT (' Error: impossible day: ',I5)

GO TO 6870

```

```

7140 Dummy=Date$(7:8)
      CALL ConvertChToI(Dummy,Year)

      Date=10000*Year+100*Month+Day

      RETURN
      END

```

C ***** EditCh

```

      SUBROUTINE EditCh(Prompt,Var)

```

C This subroutine prints the Prompt and the old value of Var, and obtains
C a new value of Var from the user

```

      COMMON /EDITSUBS/DataEntered

      CHARACTER*(*) Prompt,Var
      CHARACTER*80 OVar
      INTEGER VarLen,Length
      LOGICAL DataEntered

      VarLen=LEN(Var)
      OVar=Var
      CALL StringLength(OVar,Length)
      IF (Length.GT.0) THEN
        WRITE(*,*) 'Old Value was:',OVar(1:Length)
        WRITE(*,*) '<cr> keeps old value'
      END IF

      CALL ChInp(Prompt,Var)
      IF (.NOT.DataEntered) Var=OVar(1:VarLen)

      RETURN
      END

```

C ***** EditDP

```

      SUBROUTINE EditDP(Prompt,Var)

```

C This subroutine prints the Prompt and the old value of Var, and obtains
C a new value of Var from the user

```

      COMMON /EDITSUBS/DataEntered

      CHARACTER*(*) Prompt
      DOUBLE PRECISION Var,OVar
      LOGICAL DataEntered

      OVar=Var
      IF (OVar.NE.0) THEN
        WRITE(*,*) 'Old Value was:',OVar
        WRITE(*,*) '<cr> keeps old value'
      END IF

      CALL DPInp(Prompt,Var)
      IF(.NOT.DataEntered) Var=OVar

```

RETURN
END

C ***** EditDtCh

SUBROUTINE EditDtCh(Prompt,Date\$,Date)

CHARACTER*(*) Prompt,Date\$
INTEGER Date,Day,Month,Year,I
CHARACTER Dummy*2,ODate\$*8
LOGICAL Err

ODate\$=Date\$

6870 WRITE(*,*) 'Enter date as MM/DD/YY'
Date\$=ODate\$
CALL EditCh(Prompt,Date\$)

IF (LEN(Date\$).EQ.8) GO TO 6820

6760 WRITE (*,6760) Date\$
6760 FORMAT (' Error: date is not 8 characters long: ',A)
GO TO 6870

6820 IF ((Date\$(3:3).EQ.'/').AND.(Date\$(6:6).EQ.'/')) GO TO 6890

6830 WRITE (*,6830) Date\$
6830 FORMAT (' Error: Invalid date: ',A/,
1 ' 3rd and 6th characters must be '/')
GO TO 6870

6890 Err=.FALSE.
DO I=1,8
IF ((I.NE.3).AND.(I.NE.6)) THEN
IF ((Date\$(I:I).LT.'0').AND.(Date\$(I:I).GT.'9')) THEN
IF (.NOT.Err) THEN
WRITE(*,*) 'Error: nonnumeric characters at positions:'
END IF
Err=.TRUE.
WRITE(*,*) I
END IF
END IF
END DO

IF (Err) GO TO 6870

Dummy=Date\$(1:2)
CALL ConvertChToI(Dummy,Month)
IF ((Month.GE.1).AND.(Month.LE.12)) GO TO 7080

6990 WRITE (*,6990) Month
6990 FORMAT (' Error: impossible month: ',I5)

GO TO 6870

7080 Dummy=Date\$(4:5)
CALL ConvertChToI(Dummy,Day)
IF ((Day.GE.1).AND.(Day.LE.31)) GO TO 7140

```

7090 WRITE (*,7090) Day
      FORMAT (' Error: impossible day: ',I5)

```

```

      GO TO 6870

```

```

7140 Dummy=Date$(7:8)
      CALL ConvertChToI(Dummy,Year)

```

```

      Date=10000*Year+100*Month+Day

```

```

      RETURN
      END

```

```

C ***** EditDtl

```

```

      SUBROUTINE EditDtl(Prompt,Date$,Date)

```

```

      CHARACTER*(*) Prompt,Date$
      INTEGER Date
      CHARACTER*2 Dummy

```

```

      CALL DateUnBend(Date,Date$)
      CALL EditDtCh(Prompt,Date$,Date)

```

```

      RETURN
      END

```

```

C ***** EditI

```

```

      SUBROUTINE EditI(Prompt,Var)

```

```

C This subroutine prints the Prompt and the old value of Var, and obtains
C a new value of Var from the user

```

```

      COMMON /EDITSUBS/DataEntered

```

```

      CHARACTER*(*) Prompt
      INTEGER Var,OVar
      LOGICAL DataEntered

```

```

      OVar=Var
      IF (OVar.NE.0) THEN
        WRITE(*,*) 'Old Value was:',OVar
        WRITE(*,*) '<cr> keeps old value'
      END IF

```

```

      CALL IInp(Prompt,Var)

```

```

      IF(.NOT.DataEntered) Var=OVar

```

```

      RETURN
      END

```

```

C ***** EditR

```

```

      SUBROUTINE EditR(Prompt,Var)

```

```

C This subroutine prints the Prompt and the old value of Var, and obtains
C a new value of Var from the user

```

```
COMMON /EDITSUBS/DataEntered
```

```
CHARACTER*(*) Prompt
REAL Var,OVar
LOGICAL DataEntered
```

```
OVar=Var
IF (OVar.NE.0) THEN
  WRITE(*,*) 'Old Value was:',OVar
  WRITE(*,*) '<cr> keeps old value'
END IF
```

```
CALL RInp(Prompt,Var)
IF(.NOT.DataEntered) Var=OVar
```

```
RETURN
END
```

```
C ***** EditYorN
```

```
SUBROUTINE EditYorM(Prompt$,Yes)
```

```
LOGICAL Yes,No
CHARACTER Prompt$*(*),Response*1
```

C This subprogram obtains a Y or N response from the user.

C Prompt\$ is the prompt to be used.

C Yes is the logical variable

```
IF (Yes) THEN
  Response='Y'
ELSE
  Response='N'
END IF
```

```
Yes=.FALSE.
No=.FALSE.
DO WHILE(.NOT.(Yes.OR.No))
```

```
WRITE (*,*) Prompt$
CALL EditCh('(Y or N)?',Response)
```

```
Yes=(Response.EQ.'Y').OR.(Response.EQ.'y')
No=(Response.EQ.'N').OR.(Response.EQ.'n')
```

```
IF (.NOT.(Yes.OR.No)) THEN
```

```
100   WRITE(*,100) Response
      FORMAT (' ','Error: response ',A,' is not Y or N.')
```

```
END IF
```

```
END DO
```

```
RETURN
END
```

C ***** FileDelete

```

SUBROUTINE FileDelete(FileName)

CHARACTER*(*) FileName
CHARACTER*80 DFile
LOGICAL FExist

DFile=FileName
CALL RemoveBlanksFromCh(DFile)
INQUIRE(FILE=DFile,EXIST=FEexist)

IF (FEexist) THEN
  CALL LIB$DELETE_FILE(DFile//';*')
D ELSE
D WRITE(*,*) 'Warning: Attempt to delete a non-existent file.'
D WRITE(*,*) 'File name:',FileName
END IF

RETURN
END

```

C ***** FilePurge

```

SUBROUTINE FilePurge(FileName)

CHARACTER*(*) FileName
LOGICAL FExist

INQUIRE(FILE=FileName,Exist=FEexist)

IF (FEexist) THEN
  CALL FileRename(FileName,'TEMP_'//FileName)
  CALL FileDelete(FileName)
  CALL FileRename('TEMP_'//FileName,FileName)
D ELSE
D WRITE(*,*) 'Warning: Attempt to Purge a nonexistent file.'
D WRITE(*,*) 'File name:',FileName
END IF

RETURN
END

```

C ***** FileRename

```

SUBROUTINE FileRename(OldName,NewName)

CHARACTER*(*) OldName,NewName
CHARACTER*80 DOld,DNew
LOGICAL FExist

DOld=OldName
CALL RemoveBlanksFromCh(DOld)
DNew=NewName
CALL RemoveBlanksFromCh(DNew)

INQUIRE(FILE=DOld,EXIST=FEexist)

```

```

IF (FExist) THEN
  CALL LIB$RENAME_FILE(DOld,DNew)
ELSE
  WRITE(*,*) 'Warning: attempting to rename a nonexistent file.'
  WRITE(*,*) 'Old Name:',OldName
  WRITE(*,*) 'New Name:',NewName
  CALL PauseCrt
END IF

RETURN
END

```

C ***** FindMatchesCh

```

SUBROUTINE FindMatchesCh(Matrix,NElements,MatchElement,
& MatchLocs,Found,NoLocs)

```

```

  CHARACTER*(*) Matrix(*),MatchElement
  INTEGER NElements,MatchLocs(*),Length,NoLocs,I
  LOGICAL Found

```

```

  Found=.FALSE.
  NoLocs=0

```

```

  IF (LEN(Matrix(1)).GT.LEN(MatchElement)) THEN
    Length=LEN(MatchElement)
  ELSE
    Length=LEN(Matrix(1))
  END IF

```

```

  DO I=1,NElements
    IF (Matrix(I)(1:Length).EQ.MatchElement(1:Length)) THEN
      Found=.TRUE.
      NoLocs=NoLocs+1
      MatchLocs(NoLocs)=I
    END IF
  END DO

```

```

  RETURN
END

```

C ***** FindMatchesDP

```

SUBROUTINE FindMatchesDP(Matrix,NElements,MatchElement,
& MatchLocs,Found,NoLocs)

```

```

  DOUBLE PRECISION Matrix(*),MatchElement
  INTEGER NElements,MatchLocs(*),NoLocs,I
  LOGICAL Found

```

```

  Found=.FALSE.
  NoLocs=0

```

```

  DO I=1,NElements
    IF (Matrix(I).EQ.MatchElement) THEN
      Found=.TRUE.
      NoLocs=NoLocs+1
      MatchLocs(NoLocs)=I
    END IF
  END DO

```



```

    END IF
  END DO

```

```

  RETURN
  END

```

C ***** FindMatchesI

```

  SUBROUTINE FindMatchesI(Matrix,NElements,MatchElement,
& MatchLocs,Found,NoLocs)

```

```

    INTEGER Matrix(*),MatchElement
    INTEGER NElements,MatchLocs(*),NoLocs,I
    LOGICAL Found

```

```

    Found=.FALSE.
    NoLocs=0

```

```

    DO I=1,NElements
      IF (Matrix(I).EQ.MatchElement) THEN
        Found=.TRUE.
        NoLocs=NoLocs+1
        MatchLocs(NoLocs)=I
      END IF
    END DO

```

```

  RETURN
  END

```

C ***** FindMatchesR

```

  SUBROUTINE FindMatchesR(Matrix,NElements,MatchElement,
& MatchLocs,Found,NoLocs)

```

```

    REAL Matrix(*),MatchElement
    INTEGER NElements,MatchLocs(*),NoLocs,I
    LOGICAL Found

```

```

    Found=.FALSE.
    NoLocs=0

```

```

    DO I=1,NElements
      IF (Matrix(I).EQ.MatchElement) THEN
        Found=.TRUE.
        NoLocs=NoLocs+1
        MatchLocs(NoLocs)=I
      END IF
    END DO

```

```

  RETURN
  END

```

C ***** FindMaxCh

```

  SUBROUTINE FindMaxCh(Matrix,NoOfElems,MaxCh,MaxLoc)

```

```

    CHARACTER(*) Matrix(*),MaxCh
    INTEGER MaxLoc,NoOfElems,I

```

```

IF (NoOfElems.LT.1) THEN
  MaxLoc=0
  MaxCh=' '
  RETURN
END IF

MaxLoc=1
MaxCh=' '

DO I=2,NoOfElems
  IF (Matrix(I).GT.MaxCh) THEN
    MaxLoc=I
    MaxCh=Matrix(I)
  END IF
END DO

RETURN
END

```

C ***** FindMaxDt

```

SUBROUTINE FindMaxDt(Dates,NoOfDates,Date,Loc)

```

```

  CHARACTER*8 Dates(*)
  INTEGER NoOfDates,Date,Loc,TDate,I

```

```

  IF (NoOfDates.LE.0) THEN
    Date=0
    Loc=0
    RETURN
  END IF

```

```

  CALL DateBend(Dates(1),Date)
  Loc=1

```

```

  DO I=2,NoOfDates
    CALL DateBend(Dates(I),TDate)
    IF (TDate.GT.Date) THEN
      Loc=I
      Date=TDate
    END IF
  END DO

```

```

  RETURN
END

```

C ***** FindMaxI

```

SUBROUTINE FindMaxI(Matrix,NoOfElems,MaxI,MaxLoc)

```

```

  INTEGER MaxLoc,NoOfElems,Matrix(*),MaxI,I

```

```

  IF (NoOfElems.LT.1) THEN
    MaxLoc=0
    MaxI=0
    RETURN
  END IF

```

```

MaxLoc=1
MaxI=Matrix(1)

DO I=2,NoOfElems
  IF (Matrix(I).GT.MaxI) THEN
    MaxLoc=I
    MaxI=Matrix(I)
  END IF
END DO

RETURN
END

```

C ***** FindMinCh

```

SUBROUTINE FindMinCh(Matrix,NoOfElems,MinCh,MinLoc)

CHARACTER*(*) Matrix(*),MinCh
INTEGER MinLoc,NoOfElems,I

IF (NoOfElems.LT.1) THEN
  MinLoc=0
  MinCh=' '
  RETURN
END IF

MinLoc=1
MinCh=' '

DO I=2,NoOfElems
  IF (Matrix(I).LT.MinCh) THEN
    MinLoc=I
    MinCh=Matrix(I)
  END IF
END DO

RETURN
END

```

C ***** FindMinDt

```

SUBROUTINE FindMinDt(Matrix,NoOfElems,MinDt,MinLoc)

CHARACTER*(*) Matrix(*),MinDt
INTEGER MinLoc,NoOfElems,Elem1,Elem2,I

IF (NoOfElems.LT.1) THEN
  MinLoc=0
  MinDt='00/00/00'
  RETURN
END IF

MinLoc=1
MinDt=Matrix(1)
CALL DateBend(MinDt,Elem2)

DO I=2,NoOfElems
  CALL DateBend(Matrix(I),Elem1)

```

```

        IF (Elem1.LT.Elem2) THEN
            MinLoc=I
            MinDt=Matrix(I)
            Elem2=Elem1
        END IF
    END DO

```

```

RETURN
END

```

C ***** FindMinI

```

SUBROUTINE FindMinI(Matrix,NoOfElems,MinI,MinLoc)

```

```

    INTEGER MinLoc,NoOfElems,Matrix(*),MinI,I

```

```

    IF (NoOfElems.LT.1) THEN

```

```

        MinLoc=0

```

```

        MinI=0

```

```

        RETURN

```

```

    END IF

```

```

    MinLoc=1

```

```

    MinI=Matrix(1)

```

```

    DO I=2,NoOfElems

```

```

        IF (Matrix(I).LT.MinI) THEN

```

```

            MinLoc=I

```

```

            MinI=Matrix(I)

```

```

        END IF

```

```

    END DO

```

```

RETURN

```

```

END

```

C ***** FraDP

```

SUBROUTINE FraDP(Number,Fraction)

```

```

    DOUBLE PRECISION Number,Fraction

```

```

    Fraction=Number-INT(Number)

```

```

RETURN

```

```

END

```

C ***** GetAxis

```

SUBROUTINE GetAxis(AxisName,AxisLabel,AxisMin,AxisMax,AxisLog)

```

```

    CHARACTER(*) AxisName,AxisLabel

```

```

    LOGICAL AxisLog

```

```

    REAL AxisMin,AxisMax

```

```

    WRITE(*,*) 'If you don''t enter an axis label, axis will NOT'

```

```

    WRITE(*,*) 'be plotted!'

```

```

    CALL EditCh(AxisName//' Axis Label?',AxisLabel)

```

```
CALL EditR(AxisName// ' Minimum',AxisMin)
CALL EditR(AxisName// ' Maximum',AxisMax)
```

```
IF ((AxisMin.LE.0).OR.(AxisMax.LE.0)) AxisLog=.FALSE.
```

```
IF (AxisLog)
& CALL EditYorN('Take Log of '//AxisName// ' Values?',AxisLog)
```

```
IF (AxisLog) THEN
  AxisMin=LOG(AxisMin)
  AxisMax=LOG(AxisMax)
END IF
```

```
RETURN
END
```

```
C ***** GetFileName
```

```
SUBROUTINE GetFileName(Prompt,FileName)
```

```
INCLUDE 'IO.INC'
```

```
INTEGER Length
CHARACTER*(*) Prompt,FileName
LOGICAL FileExist
```

```
IF (LunO.EQ.0) LunO=6
```

```
FileExist=.FALSE.
DO WHILE (.NOT.FileExist)
```

```
  CALL EditCh(Prompt,FileName)
```

```
  CALL TrimCh(FileName)
  CALL StringLength(FileName,Length)
  IF (Length.EQ.0) RETURN
```

```
  INQUIRE(FILE=FileName,EXIST=FileExist)
  IF (.NOT.FileExist) WRITE(LunO,20) FileName
END DO
```

```
RETURN
20  FORMAT(X,'Warning: Filename ',A<Length>,' doesn't exist.',/,
& X,'      Please try again.',/)
```

```
END
```

```
C ***** GetPlotter
```

```
SUBROUTINE GetPlotter(TermType)
```

```
CHARACTER*80 TermTitle/'Plotting Device Selection',
& TermTxt(8)/
1 'Code Plotting Device',
2 ', ',
3 ' IMA Imagen Printer',
4 ' TAL Talaris Printer',
5 ' TEK Tektronics 4010 Terminal',
```

```

6 ' VT VT240 Terminal',
7 ' SEL Selanar 100 Terminal',
8 ' LAS Apple Laserwriter',
& TermPrompt/'Plotting Device Code?'/
  CHARACTER*3 TermResps(6)/'IMA','TAL','VT','TEK','SEL','LAS'/,
& TermDefResp/'VT'/,TermType

```

```

  INTEGER TermNTxt/8/,TermNResps/6/

```

```

  CALL Menu(TermTitle,TermTxt,TermNTxt,TermPrompt,
& TermResps,TermNResps,TermDefResp,TermType)

```

```

  RETURN
  END

```

```

C ***** HeapSortDP

```

```

  SUBROUTINE HeapSortDP(N,Matrix)

```

```

C This subroutine will use the Heap Sort technique to sort Matrix in ascending
C numerical order. This subroutine is taken from Numerical Recipes: The
C Art of Scientific Computing by Press, Flannery, Teukolsky, and Vetterling,
C p. 231.

```

```

  INTEGER N,L,I,J,IL,IR
  REAL*8 Matrix(*),RRA

```

```

  IF (N.EQ.1) RETURN

```

```

  L=N/2+1
  IR=N

```

```

C The index L will be decremented from its initial value down to 1 during
C the "hiring" (heap creation) phase. Once it reaches 1, the index IR will
C be decremented from its initial value down to 1 during the "retirement
C and promotion" (heap selection) phase.

```

```

10  CONTINUE
    IF (L.GT.1) THEN

```

```

C This section of the IF-THEN-ELSE block is executed if we are still
C in the hiring phase.

```

```

      L=L-1
      RRA=Matrix(L)
    ELSE

```

```

C This section of the IF-THEN-ELSE block is executed if we are in the retirement
C and promotion phase. First we clear a space at the top of the array,
C and retire the top of the heap into it. Then we decrease the size
C of the corporation.

```

```

      RRA=Matrix(IR)
      Matrix(IR)=Matrix(1)
      IR=IR-1

```

```

    IF (IR.EQ.1) THEN

```

C This IF-THEN block is executed if the last promotion has been made.

```

      Matrix(1)=RRA
      RETURN
    END IF

```

```

  END IF

```

C Whether we are in the hiring phase or promotion phase, we here set up to
C sift down element RRA to its proper level.

```

    I=L
    J=L+L

```

```

  DO WHILE(J.LE.IR)

```

```

    IF (J.LT.IR) THEN
      IF (Matrix(J).LT.Matrix(J+1)) J=J+1
    END IF

```

```

    IF (RRA.LT.Matrix(J)) THEN
      Matrix(I)=Matrix(J)
      I=J
      J=J+J
    ELSE
      J=IR+1
    END IF

```

```

  END DO

```

```

    Matrix(I)=RRA

```

```

  GOTO 10

```

```

END

```

C ***** HeapSortIndexCh

```

  SUBROUTINE HeapSortIndexCh(N,Matrix,Index)

```

C This subroutine will use the Heap Sort technique to sort Matrix in ascending
C numerical order. This subroutine is taken from Numerical Recipes: The
C Art of Scientific Computing by Press, Flannery, Teukolsky, and Vetterling,
C p. 233.

```

    INTEGER N,L,I,J,IL,IR,Index(*),Indx
    CHARACTER*(*) Matrix(*)

```

```

    DO I=1,N
      Index(I)=I
    END DO

```

```

    IF (N.EQ.1) RETURN

```

```

    L=N/2+1
    IR=N

```

C The index L will be decremented from its initial value down to 1 during

C the "hiring" (heap creation) phase. Once it reaches 1, the index IR will
 C be decremented from its initial value down to 1 during the "retirement
 C and promotion" (heap selection) phase.

```
10 CONTINUE
   IF (L.GT.1) THEN
```

C This section of the IF-THEN-ELSE block is executed if we are still
 C in the hiring phase.

```
      L=L-1
      Indx=Index(L)
      Matrix(N+1)=Matrix(Indx)
    ELSE
```

C This section of the IF-THEN-ELSE block is executed if we are in the retirement
 C and promotion phase. First we clear a space at the top of the array,
 C and retire the top of the heap into it. Then we decrease the size
 C of the corporation.

```
      Indx=Index(IR)
      Matrix(N+1)=Matrix(Indx)
      Index(IR)=Index(1)
      IR=IR-1
```

```
    IF (IR.EQ.1) THEN
```

C This IF-THEN block is executed if the last promotion has been made.

```
      Index(1)=Indx
      RETURN
    END IF
```

```
  END IF
```

C Whether we are in the hiring phase or promotion phase, we here set up to
 C sift down element RRA to its proper level.

```
  I=L
  J=L+L
```

```
  DO WHILE(J.LE.IR)
```

```
    IF (J.LT.IR) THEN
      IF (Matrix(Index(J)).LT.Matrix(Index(J+1))) J=J+1
    END IF
```

```
    IF (Matrix(N+1).LT.Matrix(Index(J))) THEN
      Index(I)=Index(J)
      I=J
      J=J+J
    ELSE
      J=IR+1
    END IF
```

```
  END DO
```

```
  Index(I)=Indx
```


GOTO 10

END

C ***** HeapSortIndexDP

SUBROUTINE HeapSortIndexDP(N,Matrix,Index)

C This subroutine will use the Heap Sort technique to sort Matrix in ascending
C numerical order. This subroutine is taken from Numerical Recipes: The
C Art of Scientific Computing by Press, Flannery, Teukolsky, and Vetterling,
C p. 233.

INTEGER N,L,I,J,IL,IR,Index(*),Indx
REAL*8 Matrix(*),RRA

DO I=1,N
Index(I)=I
END DO

IF (N.EQ.1) RETURN

L=N/2+1
IR=N

C The index L will be decremented from its initial value down to 1 during
C the "hiring" (heap creation) phase. Once it reaches 1, the index IR will
C be decremented from its initial value down to 1 during the "retirement
C and promotion" (heap selection) phase.

10 CONTINUE
IF (L.GT.1) THEN

C This section of the IF-THEN-ELSE block is executed if we are still
C in the hiring phase.

L=L-1
Indx=Index(L)
RRA=Matrix(Indx)
ELSE

C This section of the IF-THEN-ELSE block is executed if we are in the retirement
C and promotion phase. First we clear a space at the top of the array,
C and retire the top of the heap into it. Then we decrease the size
C of the corporation.

Indx=Index(IR)
RRA=Matrix(Indx)
Index(IR)=Index(1)
IR=IR-1

IF (IR.EQ.1) THEN

C This IF-THEN block is executed if the last promotion has been made.

Index(1)=Indx
RETURN
END IF

END IF

C Whether we are in the hiring phase or promotion phase, we here set up to
C sift down element RRA to its proper level.

I=L
J=L+L

DO WHILE(J.LE.IR)

IF (J.LT.IR) THEN
IF (Matrix(Index(J)).LT.Matrix(Index(J+1))) J=J+1
END IF

IF (RRA.LT.Matrix(Index(J))) THEN
Index(I)=Index(J)
I=J
J=J+J
ELSE
J=IR+1
END IF

END DO

Index(I)=Indx

GOTO 10

END

C ***** HeapSortIndexR

SUBROUTINE HeapSortIndexR(N,Matrix,Index)

C This subroutine will use the Heap Sort technique to sort Matrix in ascending
C numerical order. This subroutine is taken from Numerical Recipes: The
C Art of Scientific Computing by Press, Flannery, Teukolsky, and Vetterling,
C p. 233.

INTEGER N,L,I,J,IL,IR,Index(*),Indx
REAL Matrix(*),RRA

DO I=1,N
Index(I)=I
END DO

IF (N.EQ.1) RETURN

L=N/2+1
IR=N

C The index L will be decremented from its initial value down to 1 during
C the "hiring" (heap creation) phase. Once it reaches 1, the index IR will
C be decremented from its initial value down to 1 during the "retirement
C and promotion" (heap selection) phase.

10 CONTINUE
IF (L.GT.1) THEN

C This section of the IF-THEN-ELSE block is executed if we are still
C in the hiring phase.

```

      L=L-1
      Indx=Index(L)
      RRA=Matrix(Indx)
    ELSE

```

C This section of the IF-THEN-ELSE block is executed if we are in the retirement
C and promotion phase. First we clear a space at the top of the array,
C and retire the top of the heap into it. Then we decrease the size
C of the corporation.

```

      Indx=Index(IR)
      RRA=Matrix(Indx)
      Index(IR)=Index(1)
      IR=IR-1

```

```

    IF (IR.EQ.1) THEN

```

C This IF-THEN block is executed if the last promotion has been made.

```

      Index(1)=Indx
      RETURN
    END IF

```

```

  END IF

```

C Whether we are in the hiring phase or promotion phase, we here set up to
C sift down element RRA to its proper level.

```

    I=L
    J=L+L

```

```

  DO WHILE(J.LE.IR)

```

```

    IF (J.LT.IR) THEN
      IF (Matrix(Index(J)).LT.Matrix(Index(J+1))) J=J+1
    END IF

```

```

    IF (RRA.LT.Matrix(Index(J))) THEN
      Index(I)=Index(J)
      I=J
      J=J+J
    ELSE
      J=IR+1
    END IF

```

```

  END DO

```

```

    Index(I)=Indx

```

```

  GOTO 10

```

```

END

```

C ***** HeapSortR

SUBROUTINE HeapSortR(N,Matrix)

C This subroutine will use the Heap Sort technique to sort Matrix in ascending
 C numerical order. This subroutine is taken from Numerical Recipes: The
 C Art of Scientific Computing by Press, Flannery, Teukolsky, and Vetterling,
 C p. 231.

```
INTEGER N,L,I,J,IL,IR
REAL Matrix(*),RRA
```

```
IF (N.EQ.1) RETURN
```

```
L=N/2+1
IR=N
```

C The index L will be decremented from its initial value down to 1 during
 C the "hiring" (heap creation) phase. Once it reaches 1, the index IR will
 C be decremented from its initial value down to 1 during the "retirement
 C and promotion" (heap selection) phase.

```
10 CONTINUE
   IF (L.GT.1) THEN
```

C This section of the IF-THEN-ELSE block is executed if we are still
 C in the hiring phase.

```
     L=L-1
     RRA=Matrix(L)
   ELSE
```

C This section of the IF-THEN-ELSE block is executed if we are in the retirement
 C and promotion phase. First we clear a space at the top of the array,
 C and retire the top of the heap into it. Then we decrease the size
 C of the corporation.

```
     RRA=Matrix(IR)
     Matrix(IR)=Matrix(1)
     IR=IR-1
```

```
   IF (IR.EQ.1) THEN
```

C This IF-THEN block is executed if the last promotion has been made.

```
     Matrix(1)=RRA
     RETURN
   END IF
```

```
END IF
```

C Whether we are in the hiring phase or promotion phase, we here set up to
 C sift down element RRA to its proper level.

```
I=L
J=L+L
```

```
DO WHILE(J.LE.IR)
```

```
  IF (J.LT.IR) THEN
```

```

      IF (Matrix(J).LT.Matrix(J+1)) J=J+1
    END IF

```

```

      IF (RRA.LT.Matrix(J)) THEN
        Matrix(I)=Matrix(J)
        I=J
        J=J+J
      ELSE
        J=IR+1
      END IF

```

```

    END DO

```

```

    Matrix(I)=RRA

```

```

  GOTO 10

```

```

END

```

```

C ***** IInp

```

```

  SUBROUTINE IInp(Prompt,Var)

```

```

C This subroutine prints the Prompt and obtains an Integer from the user

```

```

  COMMON /EDITSUBS/DataEntered

```

```

  CHARACTER*(*) Prompt
  INTEGER Var
  CHARACTER*80 Response
  LOGICAL DataEntered

```

```

  CALL ChInp(Prompt,Response)
  IF (Response.EQ.' ') THEN
    DataEntered=.FALSE.
  ELSE
    DataEntered=.TRUE.
  END IF
  CALL ConvertChToI(Response,Var)

```

```

  RETURN
END

```

```

C ***** IXChng

```

```

  SUBROUTINE IXCHNG(I1,I2)

```

```

  INTEGER I1,I2,I3

```

```

  I3=I1
  I1=I2
  I2=I3

```

```

  RETURN
END

```

```

C ***** IncrementI

```

```
SUBROUTINE IncrementI(I,Ip1,Inc,Limit)
```

```
C This subroutine returns I+Inc in Ip1 (or I+Inc-Limit if I+Inc is over  
C Limit)
```

```
INTEGER I,Ip1,Inc,Limit
```

```
Ip1=I+Inc  
IF (Ip1.GT.Limit) Ip1=Ip1-Limit  
IF (Ip1.LE.0) Ip1=Limit+Ip1
```

```
RETURN  
END
```

```
C ***** LowerCaseCh
```

```
SUBROUTINE LowerCaseCh(String)
```

```
CHARACTER*(*) String  
INTEGER StringLength,NoCharacters,Char,I
```

```
NoCharacters=0  
StringLength=LEN(String)
```

```
DO I=1,StringLength  
  IF ((String(I:I).GE.' ').AND.(String(I:I).LE.'-')) THEN  
    NoCharacters=NoCharacters+1  
  IF ((String(I:I).GE.'A').AND.(String(I:I).LE.'Z')) THEN  
    String(NoCharacters:NoCharacters)=CHAR(ICHAR(String(I:I))+32)  
  ELSE  
    String(NoCharacters:NoCharacters)=String(I:I)  
  END IF  
END IF  
END DO
```

```
DO I=StringLength,NoCharacters+1,-1  
  String(I:I)=' '  
END DO
```

```
RETURN  
END
```

```
C ***** MatDPToR
```

```
SUBROUTINE MatDPToR(DP,NoOfElems,R)
```

```
REAL*8 DP(*)  
REAL R(*)  
INTEGER NoOfElems,I
```

```
DO I=1,NoOfElems  
  R(I)=DP(I)  
END DO
```

```
RETURN  
END
```

```
C ***** MatDateBend
```

```
SUBROUTINE MatDateBend(DateCh,NoOfElems,DateN)
```

```
CHARACTER*(*) DateCh(*)
INTEGER NoOfElems,DateN(*),I
```

```
DO I=1,NoOfElems
  CALL DateBend(DateCh(I),DateN(I))
END DO
```

```
RETURN
END
```

C ***** MatExtremaDP

```
SUBROUTINE MatExtremaDP(Matrix,NoOfPts,Maxi,Mini)
```

C This subroutine locates the minimum and maximum elements in a REAL matrix.

```
REAL*8 Matrix(*),Maxi,Mini
INTEGER NoOfPTS,I
```

```
IF (Maxi.EQ.Mini) THEN
  Maxi=Matrix(1)
  Mini=Matrix(1)
END IF
```

```
DO I=1,NoOfPts
  Maxi=MAX(Maxi,Matrix(I))
  Mini=MIN(Mini,Matrix(I))
END DO
```

```
RETURN
END
```

C ***** MatExtremaR

```
SUBROUTINE MatExtremaR(Matrix,NoOfPts,MaxI,MinI)
REAL Matrix(*),Maxi,Mini
INTEGER NoOfPTS,I
WRITE(*,*) 'Error: incorrect routine. Use VecExtremaR'
STOP
END
```

C ***** MatSumI

```
SUBROUTINE MatSumI(Matrix,Start,End,Sum)
```

C This subroutine finds the sum of values in Matrix(*) from item Start to C item End. The sum is returned in variable Sum.

```
INTEGER Matrix(*),Start,End,Sum,I
```

```
Sum=0
DO I=Start,End
  Sum=Sum+Matrix(I)
END DO
```

```
RETURN
```

END

C ***** Menu

SUBROUTINE Menu(MenuTitle,MenuTxt,NTxt,MenuPrompt,MenuResps,NResps,
& DefResp,UsrResp)

C This subroutine prints a menu title, menu text, and a menu prompt, and
C obtains the response from the user. If the user merely presses return,
C the DEFRESP is used. If MENUTITLE is passed as blanks, only the prompt
C is used. Special Response codes are:
C date - the computer checks the input for a valid date
C # - the computer checks each character to verify it is a digit, comma
C E, +, -, period, or space.

INTEGER NTxt,NResps,I,J,Length

CHARACTER*(*) MenuTxt(NTxt)
CHARACTER*(*) MenuResps(NResps),DefResp,UsrResp
CHARACTER*(*) MenuTitle,MenuPrompt

LOGICAL Match,NumMatch,DateMatch

IF (MenuTitle.NE.' ') THEN
CALL StringLength(MenuTitle,Length)
Length=MAX(1,Length)
WRITE(*,*) MenuTitle(1:Length)

DO I=1,NTxt
CALL StringLength(MenuTxt(I),Length)
Length=MAX(1,Length)
WRITE(*,*) MenuTxt(I)(1:Length)
END DO
WRITE(*,*) ' '
END IF

Match=.FALSE.
DO WHILE (Match.EQ..FALSE.)

WRITE(*,*) 'Default Response:',DefResp
CALL ChInp(MenuPrompt,UsrResp)
CALL UpperCaseCh(UsrResp)
IF (UsrResp.EQ.' ') THEN
UsrResp=DefResp
WRITE(*,*) UsrResp
END IF

DO I=1,NResps
IF (MenuResps(I).EQ.'#') THEN
NumMatch=.TRUE.
DO J=1,LEN(UsrResp)
IF (INDEX(' .+-1234567890E',UsrResp(J:J)).LE.0)
& NumMatch=.FALSE.
END DO
Match=Match.OR.NumMatch
ELSE IF (MenuResps(I).EQ.'date') THEN
DateMatch=.TRUE.
IF (UsrResp(3:3).NE.'/') DateMatch=.FALSE.


```

        IF (UsrResp(6:6).NE.'') DateMatch=.FALSE.
        DO J=1,8
            IF (INDEX(' /0123456789',UsrResp(J:J)).LE.0)
& DateMatch=.FALSE.
            END DO
            Match=Match.OR.DateMatch
        ELSE
            CALL UpperCaseCh(MenuResps(I))
            CALL StringLength(MenuResps(I),Length)
            Length=MAX(1,Length)
            IF (UsrResp(1:Length).EQ.MenuResps(I)(1:Length)) Match=.TRUE.
        END IF
    END DO

    IF (Match.EQ..FALSE.) THEN
        WRITE(*,*) 'Warning: ',UsrResp,' is an invalid response.'
    END IF

END DO

RETURN
END

```

C ***** PowerRound

```

REAL*8 FUNCTION PowerRound(Number,PowerOfTen)

INTEGER PowerOfTen,NoOfDigits,Sign
REAL*8 Number,Rounded,Divisor,Ten/10.0/
CHARACTER*80 Test

IF (Number.LT.0) THEN
    Sign=-1
    Number=-Number
ELSE
    Sign=1
END IF

IF (Number.GT.0) THEN
    NoOfDigits=LOG(Number)/LOG(Ten)-PowerOfTen+1

    IF (NoOfDigits.LE.0) THEN
        Rounded=0.0
    ELSE
        Divisor=Ten**PowerOfTen
        WRITE(UNIT=Test(1:),FMT=10)
& Number/Divisor
10    FORMAT(F<NoOfDigits+2>.0)
        CALL ConvertChToDP(Test,Rounded)
        Rounded=Rounded*Divisor
    END IF

    IF (Sign.LT.0) THEN
        Rounded=-Rounded
    END IF

ELSE
    Rounded=0.0

```

```

END IF

PowerRound=Rounded
RETURN
END

```

C ***** PRoundDP

```

Subroutine PRoundDP(Number,PowerOfTen,Rounded)

DOUBLE PRECISION Number,TenRaised,Ten/10.0/,Rounded,Intermediate
INTEGER PowerOfTen
INTEGER*4 BigInt

TenRaised=(Ten)**(PowerOfTen)
BigInt=Number/TenRaised
Intermediate=BigInt

Rounded=Intermediate*TenRaised

RETURN
END

```

C ***** PauseCRT

```

SUBROUTINE PauseCrt

CHARACTER*1 DummyVar

CALL ChInp('Press Return to Continue',DummyVar)

RETURN
END

```

C ***** QInp

```

SUBROUTINE QInp(Prompt,Var16)

```

C This subroutine prints the Prompt and obtains a quadruple precision Var
C from the user

```

CHARACTER*(*) PROMPT
DOUBLE PRECISION Var8
REAL*16 Var16

CALL DPInp(Prompt,Var8)
Var16=Var8

RETURN
END

```

C ***** RInp

```

SUBROUTINE RInp(Prompt,Var)

COMMON /EDITSUBS/DataEntered

```

C This subroutine prints the Prompt and obtains a real Var from the user

```

CHARACTER*(*) PROMPT
REAL Var
CHARACTER*80 Response
LOGICAL DataEntered

CALL ChInp(Prompt,Response)
IF (Response.EQ.' ') THEN
  DataEntered=.FALSE.
ELSE
  DataEntered=.TRUE.
END IF
CALL ConvertChToR(Response,Var)

RETURN
END

```

C ***** RXChng

```

SUBROUTINE RXChng(R1,R2)

```

C This subroutine is called by Bub2Sort to exchange two real numbers

```

REAL R1,R2,T

```

```

T=R1
R1=R2
R2=T

```

```

RETURN
END

```

C ***** ReOrderDP

```

SUBROUTINE ReOrderDP(Matrix,NoElems,Pointer)

```

```

PARAMETER MaxNoOfElems=2000
REAL*8 Matrix(*),Temp(MaxNoOfElems)
INTEGER NoElems,Pointer(*),I

```

```

IF (NoElems.GT.MaxNoOfElems) THEN
  WRITE(*,*) 'Error: Number of elements in Matrix is larger '
  WRITE(*,*) '      than the maximum number of elements allowed.'
  WRITE(*,*) '      NoElems=',NoElems
  WRITE(*,*) '      MaxNoOfElems=',MaxNoOfElems
  STOP 'In Routine: ReOrderDP'
END IF

```

```

DO I=1,NoElems
  Temp(I)=Matrix(I)
END DO

```

```

DO I=1,NoElems
  Matrix(I)=Temp(Pointer(I))
END DO

```

```

RETURN
END

```

C ***** ReOrderR

```

SUBROUTINE ReOrderR(Matrix,NoElems,Pointer)

PARAMETER MaxNoOfElems=2000
REAL Matrix(*),Temp(MaxNoOfElems)
INTEGER NoElems,Pointer(*),I

IF (NoElems.GT.MaxNoOfElems) THEN
  WRITE(*,*) 'Error: Number of elements in Matrix is larger '
  WRITE(*,*) '      than the maximum number of elements allowed.'
  WRITE(*,*) '      NoElems=',NoElems
  WRITE(*,*) '      MaxNoOfElems=',MaxNoOfElems
  STOP 'In Routine: ReOrderR'
END IF

DO I=1,NoElems
  Temp(I)=Matrix(I)
END DO

DO I=1,NoElems
  Matrix(I)=Temp(Pointer(I))
END DO

RETURN
END

```

C ***** RemoveBlanksFromCh

```

SUBROUTINE RemoveBlanksFromCh(String)

CHARACTER*(*) String
CHARACTER*1 Blank/' '/

CALL RemoveCharFromCh(String,Blank)

RETURN
END

```

C ***** RemoveCharFromCh

```

SUBROUTINE RemoveCharFromCh(String,Blank)

CHARACTER*(*) String,Blank
INTEGER Length,Char,I

Length=LEN(String)
Char=0
DO I=1,Length
  IF (String(I:I).NE.Blank(1:1)) THEN
    Char=Char+1
    String(Char:Char)=String(I:I)
  END IF
END DO
DO I=Char+1,Length
  String(I:I)= ' '
END DO

```

```
RETURN
END
```

```
C ***** RptString
```

```
  SUBROUTINE RptString(Repeat,NoOfTimes,String)
```

```
  CHARACTER*(*) Repeat,String
  INTEGER NoOfTimes,SLen,RLen,I
```

```
  SLen=0
  RLen=LEN(Repeat)
```

```
  DO I=1,NoOfTimes
    String(SLen+1:)=Repeat
    SLen=SLen+RLen
    IF (SLen.GE.LEN(String)) RETURN
  END DO
```

```
  RETURN
  END
```

```
C ***** SearchCh
```

```
  SUBROUTINE SearchCh(Matrix,NElements,MatchElement,Location,Found,
& NoLocs)
```

```
  CHARACTER*(*) Matrix(*),MatchElement
  INTEGER NElements,Location,NoLocs,I,MatchLength
  LOGICAL Found
```

```
  Location=0
  Found=.FALSE.
  NoLocs=0
```

```
  IF (NElements.GT.0) THEN
    MatchLength=MIN(LEN(Matrix(1)),LEN(MatchElement))
  END IF
```

```
  DO I=1,NElements
    IF (Matrix(I)(1:MatchLength).EQ.
& MatchElement(1:MatchLength)) THEN
      Found=.TRUE.
      Location=I
      NoLocs=NoLocs+1
    END IF
  END DO
```

```
  RETURN
  END
```

```
C ***** SearchChSub
```

```
  SUBROUTINE SearchChSub(Matrix,NElements,StartLoc,EndLoc,
& MatchElement,Location,Found,NoLocs)
```

```
  CHARACTER*(*) Matrix(*),MatchElement
  INTEGER NElements,Location,NoLocs,I,StartLoc,EndLoc
```

LOGICAL Found

Location=0
Found=.FALSE.
NoLocs=0

DO I=1,NElements
 IF (Matrix(I)(StartLoc:EndLoc).EQ.MatchElement) THEN
 Found=.TRUE.
 Location=I
 NoLocs=NoLocs+1
 END IF
END DO

RETURN
END

C ***** SearchDP

SUBROUTINE SearchDP(Matrix,NElements,MatchElement,Location,Found,
& NoLocs)

INTEGER NElements,Location,NoLocs,I
DOUBLE PRECISION Matrix(*),MatchElement
LOGICAL Found

Location=0
Found=.FALSE.
NoLocs=0

DO I=1,NElements
 IF (Matrix(I).EQ.MatchElement) THEN
 Found=.TRUE.
 Location=I
 NoLocs=NoLocs+1
 END IF
END DO

RETURN
END

C ***** SearchI

SUBROUTINE SearchI(Matrix,NElements,MatchElement,Location,Found,
& NoLocs)

INTEGER Matrix(*),MatchElement
INTEGER NElements,Location,NoLocs,I
LOGICAL Found

Location=0
Found=.FALSE.
NoLocs=0

DO I=1,NElements
 IF (Matrix(I).EQ.MatchElement) THEN
 Found=.TRUE.
 Location=I

```

        NoLocs=NoLocs+1
    END IF
END DO

```

```

RETURN
END

```

C ***** SearchL

```

SUBROUTINE SearchL(Matrix,NElements,MatchElement,Location,Found,
& NoLocs)

```

```

    LOGICAL Matrix(*),MatchElement
    INTEGER NElements,Location,NoLocs,I
    LOGICAL Found

```

```

    Location=0
    Found=.FALSE.
    NoLocs=0

```

```

    DO I=1,NElements
        IF (Matrix(I).EQ.MatchElement) THEN
            Found=.TRUE.
            Location=I
            NoLocs=NoLocs+1
        END IF
    END DO

```

```

RETURN
END

```

C ***** SearchLEI

```

SUBROUTINE SearchLEI(Matrix,NElements,MatchElement,Location)

```

```

    INTEGER Matrix(*),MatchElement,NElements,Location,I

```

```

    Location=0

```

```

    DO I=1,NElements
        IF (Matrix(I).LE.MatchElement) THEN
            Location=I
            RETURN
        END IF
    END DO

```

```

RETURN
END

```

C ***** SearchR

```

SUBROUTINE SearchR(Matrix,NElements,MatchElement,Location,Found,
& NoLocs)

```

```

    REAL Matrix(*),MatchElement
    INTEGER NElements,Location,NoLocs,I
    LOGICAL Found

```

```

Location=0
Found=.FALSE.
NoLocs=0

DO I=1,NElements
  IF (Matrix(I).EQ.MatchElement) THEN
    Found=.TRUE.
    Location=I
    NoLocs=NoLocs+1
  END IF
END DO

RETURN
END

```

C ***** SetPlotter

```

SUBROUTINE SetPlotter(TermType)

CHARACTER*(*) TermType
INTEGER IErr

IF (TermType.EQ.'VT') THEN
  CALL dev('dec_vt240_general',IErr)
ELSE IF (TermType.EQ.'SEL') THEN
  CALL dev('tektronix_4014_general',IErr)
ELSE IF (TermType.EQ.'TEK') THEN
  CALL dev('tektronix_4014_general',IErr)
ELSE IF (TermType.EQ.'LAS') THEN
  CALL dev('postscript_all_general',IErr)
  CALL HWROT('AUTO')
ELSE
  WRITE(*,*) 'Error: unknown terminal type.'
  WRITE(*,*) '  TermType=',TermType
  STOP 'In Routine: SetPlotter'
END IF

CALL Page(8.5,11.0)
CALL Area2D(5.0,5.0)

CALL HWSCAL('SCREEN')

RETURN
END

```

C ***** SgnDP

```

INTEGER FUNCTION SgnDP(Number)

DOUBLE PRECISION Number

IF (Number.LT.0) THEN
  SgnDP=-1
ELSE IF (Number.GT.0) THEN
  SgnDP=1
ELSE
  SgnDP=0
END IF

```



```
RETURN
END
```

```
C ***** SortCh
```

```
SUBROUTINE SortCh(Matrix,NoElems,Pointer)

INTEGER NoElems,Pointer(*)
CHARACTER*(*) Matrix(*)

CALL HeapSortIndexCh(NoElems,Matrix,Pointer)

RETURN
END
```

```
C ***** SortDP
```

```
SUBROUTINE SortDP(Matrix,NoElems,Pointer)
```

C This subroutine sorts the matrix to pointer. Upon return from the
C subroutine the elements of pointer(1),pointer(2),... are the locations
C in Matrix of the first element, second element, ...

```
INTEGER NoElems,Pointer(*),Top,Bottom,I
DOUBLE PRECISION Matrix(*),Elem1,Elem2
```

```
LOGICAL Exchanges
```

```
DO I=1,NoElems
  Pointer(I)=I
END DO
```

```
Bottom=1
Top=NoElems
```

```
Exchanges=.TRUE.
```

```
DO WHILE (Exchanges)
```

```
  Exchanges=.FALSE.
  DO I=Bottom,Top-1
    Elem1=Matrix(Pointer(I))
    Elem2=Matrix(Pointer(I+1))
    IF (Elem1.GT.Elem2) THEN
      CALL IXCHNG(Pointer(I),Pointer(I+1))
      Exchanges=.TRUE.
      Top=I
    END IF
  END DO
```

```
IF (Exchanges) THEN
  Exchanges=.FALSE.
  DO I=Top,Bottom+1,-1
    Elem1=Matrix(Pointer(I-1))
    Elem2=Matrix(Pointer(I))
    IF (Elem1.GT.Elem2) THEN
      CALL IXCHNG(Pointer(I-1),Pointer(I))
      Exchanges=.TRUE.
    END IF
  END DO
END IF
```

```

        Bottom=I
      END IF
    END DO
  END IF

END DO

RETURN
END

```

C ***** SortI

```

SUBROUTINE SortI(Matrix,NoElems,Pointer)

```

C This subroutine sorts the matrix to pointer. Upon return from the
C subroutine the elements of pointer(1),pointer(2),... are the locations
C in Matrix of the first element, second element, ...

```

  INTEGER NoElems,Pointer(*),Top,Bottom,I
  INTEGER Matrix(*),Elem1,Elem2

  LOGICAL Exchanges

  DO I=1,NoElems
    Pointer(I)=I
  END DO

  Bottom=1
  Top=NoElems

  Exchanges=.TRUE.

  DO WHILE (Exchanges)

    Exchanges=.FALSE.
    DO I=Bottom,Top-1
      Elem1=Matrix(Pointer(I))
      Elem2=Matrix(Pointer(I+1))
      IF (Elem1.GT.Elem2) THEN
        CALL IXCHNG(Pointer(I),Pointer(I+1))
        Exchanges=.TRUE.
        Top=I
      END IF
    END DO
    IF (Exchanges) THEN
      Exchanges=.FALSE.
      DO I=Top,Bottom+1,-1
        Elem1=Matrix(Pointer(I-1))
        Elem2=Matrix(Pointer(I))
        IF (Matrix(Pointer(I-1)).GT.Matrix(Pointer(I))) THEN
          CALL IXCHNG(Pointer(I-1),Pointer(I))
          Exchanges=.TRUE.
          Bottom=I
        END IF
      END DO
    END IF
  END DO

END DO

```

```
RETURN
END
```

```
C ***** SortR
```

```
  SUBROUTINE SortR(Matrix,NoElems,Pointer)
```

```
C This subroutine sorts the matrix to pointer. Upon return from the
C subroutine the elements of pointer(1),pointer(2),... are the locations
C in Matrix of the first element, second element, ...
```

```
  INTEGER NoElems,Pointer(*)
  REAL Matrix(*)
```

```
  CALL HeapSortIndexR(NoElems,Matrix,Pointer)
```

```
  RETURN
  END
```

```
C ***** StringLength
```

```
  SUBROUTINE StringLength(String,Length)
```

```
  CHARACTER*(*) String
  INTEGER Length
```

```
  Length=LEN(String)
  DO WHILE((String(Length:Length).EQ.' ').OR.
& (String(Length:Length).EQ.CHAR(0)))
    Length=Length-1
  IF (Length.EQ.0) RETURN
  END DO
```

```
  RETURN
  END
```

```
C ***** TrimCh
```

```
  SUBROUTINE TrimCh(String)
```

```
  CHARACTER*(*) String
  INTEGER Length,I
```

```
  Length=LEN(String)
```

```
  DO I=1,Length
    IF ((ICCHAR(String(I:I)).LT.32)
& .OR.(ICCHAR(String(I:I)).EQ.255)) String(I:I)=' '
  END DO
```

```
  IF (String.EQ.' ') RETURN
  IF (Length.LT.2) RETURN
```

```
  DO WHILE (String(1:1).EQ.' ')
    String(1:)=String(2:)
  END DO
```

```
  RETURN
```

END

C ***** UpperCaseCh

SUBROUTINE UpperCaseCh(String)

CHARACTER(*) String
INTEGER StringLength,NoCharacters,Char,I

NoCharacters=0
StringLength=LEN(String)

DO I=1,StringLength
 IF (ICHAR(String(I:I)).LT.32) String(I:I)= ' '
 IF ((String(I:I).GE.' ') .AND.(String(I:I).LE.'- ')) THEN
 NoCharacters=NoCharacters+1
 IF ((String(I:I).GE.'a') .AND.(String(I:I).LE.'z')) THEN
 String(NoCharacters:NoCharacters)=CHAR(ICHAR(String(I:I))-32)
 ELSE
 String(NoCharacters:NoCharacters)=String(I:I)
 END IF
 END IF
END DO

IF (NoCharacters+1.LE.StringLength) String(NoCharacters+1:
& StringLength)=' '

RETURN
END

C ***** VecExtremaDP

SUBROUTINE VecExtremaDP(Matrix,NoOfPts,Maxi,Mini)

C This subroutine locates the minimum and maximum elements in a REAL array

REAL*8 Matrix(*),Maxi,Mini
INTEGER NoOfPts,I

Maxi=Matrix(1)
Mini=Matrix(1)

DO I=2,NoOfPts
 Maxi=MAX(Maxi,Matrix(I))
 Mini=MIN(Mini,Matrix(I))
END DO

RETURN
END

C ***** VecExtremaR

SUBROUTINE VecExtremaR(Matrix,NoOfPts,Maxi,Mini)

C This subroutine locates the minimum and maximum elements in a REAL array

REAL Matrix(*),Maxi,Mini
INTEGER NoOfPts,I

```

Maxi=Matrix(1)
Mini=Matrix(1)

DO I=2,NoOfPts
  Maxi=MAX(Maxi,Matrix(I))
  Mini=MIN(Mini,Matrix(I))
END DO

RETURN
END

```

C ***** WriteCenter

```

SUBROUTINE WriteCenter(Lun,Width,Line)

PARAMETER MaxWidth=108

INTEGER Lun,Width,TrueWidth
CHARACTER*(*) Line
CHARACTER*(MaxWidth) In,Out

IF (Width.GT.MaxWidth) THEN
  TrueWidth=MaxWidth
ELSE
  TrueWidth=Width
END IF

In=Line
CALL Center(In,TrueWidth,Out)

WRITE(Lun,10) Out
10  FORMAT(X,A<TrueWidth>)

RETURN
END

```

C ***** YorN

```

SUBROUTINE Yorn(Prompt$,Yes)

LOGICAL Yes,No
CHARACTER Prompt$*(*),Response*1

```

C This subprogram obtains a Y or N response from the user.

C Prompt\$ is the prompt to be used.

C Yes is the logical variable

```

Yes=.FALSE.
No=.FALSE.
DO WHILE(.NOT.(Yes.OR.No))

  WRITE (*,*) Prompt$
  CALL ChInp('Y or N)?',Response)

  Yes=(Response.EQ.'Y').OR.(Response.EQ.'y')
  No=(Response.EQ.'N').OR.(Response.EQ.'n')

```

```
IF (.NOT.(Yes.OR.No)) THEN
  WRITE(*,100) Response
100  FORMAT (' ', 'Error: response ', A, ' is not Y or N.')
  END IF
END DO
RETURN
END
```

c *

C ***** CalcCF

SUBROUTINE CalcCF(XI,C,N)

C This subroutine is from Conte and DeBoor, p.287

C Variables-----

C Input Variables

C XI(1),...,XI(N+1) strictly increasing sequence of breakpoints.

C C(1,I), C(2,I), VAlue and first derivative at XI(I), I=1,...,N+1

C of the piecewise function.

C Output Variables

C C(1,I), C(2,I), C(3,I), C(4,I) Polynomial coefficients of the function on the

C interval (XI(I),XI(I+1)), I=1,...,N.

INTEGER N,I

REAL*8 C(4,N+1),XI(N+1),dX,DivDF1,DivDF3

DO I=1,N

dX=XI(I+1)-XI(I)

DivDF1=(C(1,I+1)-C(1,I))/dX

DivDF3=C(2,I)+C(2,I+1)-2.0*DivDF1

C(3,I)=(DivDF1-C(2,I)-DivDF3)/dX

C(4,I)=DivDF3/(dX*dX)

END DO

RETURN

END

C ***** Compute1DPhis

SUBROUTINE Compute1DPhis(BasisDeg,Zeta,Phi,PhiZeta)

C This subroutine computes the values of the local 1D weighting functions, and

C the values of their slopes.

C Input Variables

C Zeta The value of the local variable at which to evaluate the

C functions. (Range: 0<Zeta<1)

C BasisDeg degree of basis functions, 3 are hermite cubics

C Output Variables

C Phi() Phi(1) is the first local weighting function evaluated at

C zeta. Phi(2) is the second.

C PhiZeta() These are the derivates (with respect to zeta) evaluated at

C zeta.

DOUBLE PRECISION Zeta

REAL*8 Phi(*),PhiZeta(*)

INTEGER BasisDeg

```

IF (BasisDeg.EQ.1) THEN

  Phi(1)=1.0D0-Zeta
  Phi(2)=Zeta

  PhiZeta(1)=-1.0D0
  PhiZeta(2)=1.0D0

ELSE IF (BasisDeg.EQ.2) THEN

  Phi(1)=1.0D0-3.0D0*Zeta+2.0D0*Zeta**2
  Phi(2)=4.0D0*Zeta-4.0D0*Zeta**2
  Phi(3)=Zeta*(2.0D0*Zeta-1.0D0)
  PhiZeta(1)=-3.0D0+4.0D0*Zeta
  PhiZeta(2)=4.0D0-8.0D0*Zeta
  PhiZeta(3)=-1.0D0+4.0D0*Zeta

ELSE IF (BasisDeg.EQ.3) THEN

  Phi(1)=1.0-3.0*Zeta**2+2.0*Zeta**3
  Phi(2)=Zeta-2.0*Zeta**2+Zeta**3
  Phi(3)=3.0*Zeta**2-2.0*Zeta**3
  Phi(4)=-Zeta**2+Zeta**3

  PhiZeta(1)=-6.0*Zeta+6.0*Zeta**2
  PhiZeta(2)=1.0-4.0*Zeta+3.0*Zeta**2
  PhiZeta(3)=6.0*Zeta*(1.0-Zeta)
  PhiZeta(4)=-2.0*Zeta+3.0*Zeta**2

END IF

RETURN
END

C ***** ComputeIntersection

SUBROUTINE ComputeIntersection(Xa1,Ya1,Xa2,Ya2,Xb1,Yb1,Xb2,Yb2,
& XInt,YInt,Error)

C   =0 => line segments intersect
C Error=1 => lines intersect, but segments do not.
C   =2 => lines are parallel
C Xa1 X or Y Coordinate, segment a or b, 1st or 2nd point.
C Yb2

INTEGER Error
LOGICAL Intersect
REAL*8 Xa1,Ya1,Xa2,Ya2,Xb1,Yb1,Xb2,Yb2,Ta,Tb
REAL*8 Denom,XInt,YInt,Temp,PowerRound
EXTERNAL PowerRound

Error=2

```



```
Denom=(Xa1-Xa2)*(Yb2-Yb1)-(Ya1-Ya2)*(Xb2-Xb1)
Intersect=(Denom.NE.0.0D0)
```

```
IF (Intersect) THEN
```

```
C The lines intersect. Compute the intersection point in parametric form
C (Y,X)=(Y(t),X(t)) for both segment a and b
```

```
Ta = ((Yb2-Yb1)*(Xa1-Xb1)+(xb1-xb2)*(ya1-yb1))/Denom
Tb = ((ya2-ya1)*(Xa1-Xb1)+(xa1-Xa2)*(Ya1-Yb1))/Denom
```

```
IF ((0.LE.Ta).AND.(Ta.LE.1).AND.(0.LE.Tb).AND.(Tb.LE.1)) THEN
  Error=0
ELSE
  Error=1
END IF
```

```
C Compute the location of the intersection.
```

```
XInt=Ta*(Xa2-Xa1)+Xa1
YInt=Ta*(Ya2-Ya1)+Ya1
```

```
C Round to the nearest -16 place
```

```
XInt=PowerRound(XInt,-16)
YInt=PowerRound(YInt,-16)
```

```
END IF
```

```
RETURN
END
```

```
C ***** EElliptic
```

```
REAL*8 FUNCTION EElliptic(M)
```

```
C Taken from Numerical Recipes, p. 187
C This function returns the complete elliptic integral with
C QQc=kc
```

```
REAL*8 M
```

```
REAL*8 QQc,Qc,A,B,P,F,E,Em,G,Q
```

```
C CA Square-root of desired accuracy.
```

```
PARAMETER CA=0.00000005
PARAMETER PIO2=1.570796326794896619231322
```

```
IF (ABS(M).GE.1) STOP 'Error in Routine EElliptic: M>=1.'
Qc=SQRT(1.0-ABS(M))
```

```
A=1.0
B=1-M
P=1.0
E=Qc
Em=1.0
```

```

1      F=A
      A=A+B/P
      G=E/P
      B=2*(B+F*G)
      P=G+P
      G=EM
      EM=QC+EM
      IF (ABS(G-QC).GT.G*CA) THEN
          QC=2*SQRT(E)
          E=QC*EM
          GOTO 1
      END IF

      EElliptic=PIO2*(B+A*EM)/(EM*(EM+P))
      RETURN
      END

```

C ***** EEIP

```

      REAL*8 FUNCTION EEIP(M)

```

C Polynomial Approximation for Complete Elliptic Integral E, from Abramowitz and C Stegun, p. 587

```

      REAL*8 M,M1,First,Second
      REAL*8 A(4)/0.44325141463,0.06260601220,0.04757383546,
& 0.01736506451/
      REAL*8 B(4)/0.24998368310,0.09200180037,0.04069697526,
& 0.00526449639/
      INTEGER I

      IF (M.GE.1.0) STOP 'In Routine: EEIP; Error, M>=1'
      M1=1.0-M

      First=1.0
      Second=0.0
      DO I=1,4
          First=First+A(I)*(M1**I)
          Second=Second+B(I)*(M1**I)
      END DO

      EelP=First-Second*LOG(M1)

      RETURN
      END

```

C ***** ErfCDP

```

      REAL*8 FUNCTION ErfCDP(X)

```

C This function returns the complementary errorf function of x. See C numerical recipes p. 164

```

      REAL*8 X,GammaQDP,GammaPDP
      EXTERNAL GammaQDP,GammaPDP

      IF (X.LT.0.0) THEN
          ErfCDP=1.0D0+GammaPDP(0.5,X**2)

```

```

ELSE
  ErfCDP=GammaQDP(0.5,X**2)
END IF

```

```

RETURN
END

```

```

C ***** ErfDP

```

```

REAL*8 FUNCTION ErfDP(x)

```

```

C This function from NUMERICAL RECIPES, p. 164

```

```

REAL*8 X,GammaPDP
EXTERNAL GammaPDP

```

```

IF (X.LT.0) THEN
  ErfDP=-GammaPDP(0.5,x**2)
ELSE
  ErfDP=GammaPDP(0.5,x**2)
END IF

```

```

RETURN
END

```

```

C ***** Factor

```

```

SUBROUTINE Factor(W,N,D,IPivot,IFlag,MaxDim)

```

```

C This subroutine, taken from Conte and DeBoor p165, computes the LU
C factorization of the Matrix W. The program follows Algorithm 4.2 in
C Conte and DeBoor using scaled partial pivoting.

```

```

C Input Variables

```

```

C W(N,N)    Contains the matrix to be factored.
C N         The order of the Matrix
C D(N)      Work Vector, holds row sizes.

```

```

C Output Variables

```

```

C W(N,N)    The LU Factorization of P*W where W is the
C           original input matrix, and P is a permutation matrix
C           specified by IPivot.
C IPivot(N) The Row IPivot(K) was used to eliminate X(K), K=1,...,N
C IFlag     =1 if an even number of interchanges was carried out,
C           =-1 if an odd number of interchanges was carried out,
C           =0 if the upper triangular factor has one or more zero
C           diagonal entries.
C           Thus, the determinant is Iflag*W(1,N)

```

```

INTEGER IFlag,IPivot(*),I,IStar,J,K,MaxDim,N
REAL*8 D(*),W(MaxDim,MaxDim),Awikod,ColMax,Ratio,RowMax,Temp

```

```

IFlag=1

```

```

C Intialize IPivot,D

```

```

DO I=1,N
  IPivot(I)=I

  RowMax=0.0
  DO J=1,N
    RowMax=MAX(RowMax,ABS(W(I,J)))
  END DO

  IF (RowMax.EQ.0.0) THEN
    IFlag=0
    RowMax=1.0
  END IF

  D(I)=RowMax
END DO

IF (N.LE.1) RETURN

```

C Compute Factorization

```
DO K=1,N-1
```

C Determine Pivot Row, IStar

```

ColMax=ABS(W(K,K))/D(K)
IStar=K
DO I=K+1,N
  Awikod=ABS(W(I,K))/D(I)
  IF (Awikod.GT.ColMax) THEN
    ColMax=Awikod
    IStar=I
  END IF
END DO

IF (ColMax.EQ.0.0) THEN
  IFlag=0
ELSE
  IF (IStar.GT.K) THEN

```

C Make K the Pivot Row by Interchanging it with the chosen row IStar.

```

  IFlag=-IFlag

  I=IPivot(IStar)
  IPivot(IStar)=IPivot(K)
  IPivot(K)=I

  Temp=D(IStar)
  D(IStar)=D(K)
  D(K)=Temp

  DO J=1,N
    Temp=W(IStar,J)
    W(IStar,J)=W(K,J)
    W(K,J)=Temp
  END DO

END IF

```

C Eliminate X(K) from Rows K+1,...,N.

```

      DO I=K+1,N
        W(I,K)=W(I,K)/W(K,K)
        Ratio=W(I,K)
        DO J=K+1,N
          W(I,J)=W(I,J)-Ratio*W(K,J)
        END DO
      END DO
    END IF
  END DO

  IF (W(N,N).EQ.0.0) IFlag=0

  RETURN
  END

```

C ***** GammaPdp

```

  REAL*8 FUNCTION GammaPdp(A,X)

```

C This function returns the incomplete gamma function $P(a,x)$. See Numerical
C Recipes p. 160.

```

  REAL*8 A,X,GamSer,Gln,GammCF

  IF ((X.LT.0).OR.(A.LE.0)) THEN
    WRITE(*,*) 'Error: X<0 or A<=0'
    WRITE(*,*) ' X=',X, ' A=',A
    STOP 'In Function: GammaPdp'
  END IF

```

```

  IF (X.LT.A+1) THEN

```

C Use the series representation

```

    CALL GSerDP(GamSer,A,X,Gln)
    GammaPdp=GamSer

```

```

  ELSE

```

C Use the continued fraction representation and takes its complement

```

    CALL GCFDP(GammCF,A,X,Gln)
    GammaPdp=1.0-GammCF

```

```

  END IF

```

```

  RETURN
  END

```

C ***** GammaQDP

```

  REAL*8 FUNCTION GammaQDP(A,X)

```

C This function returns the incomplete gamma function $Q(a,x)=1-P(a,x)$ See
C Numerical Recipes p.162

```
REAL*8 A,X,GamSer,GlN,GammCF
```

```
IF ((X.LT.0).OR.(A.LE.0)) THEN
```

```
  WRITE(*,*) 'Error: improper A or X values. Proper Ranges are:'
```

```
  WRITE(*,*) '    0<=X, and 0<A'
```

```
  WRITE(*,*) '    X=',X
```

```
  WRITE(*,*) '    A=',A
```

```
  STOP 'In Function: GammaQDP'
```

```
END IF
```

```
IF (X.LT.A+1.) THEN
```

```
  CALL GSer(GamSer,A,X,GLN)
```

```
  GammaQdp=1.0D0-GamSer
```

```
ELSE
```

```
  CALL GCF(GammCF,A,X,GlN)
```

```
  GammaQDP=GammCF
```

```
END IF
```

```
RETURN
```

```
END
```

```
C ***** GammLNDP
```

```
REAL*8 FUNCTION GammLnDP(XX)
```

```
C Returns the value LOG(GAMMA(XX)) for XX>0. Full accuracy is obtained
```

```
C for XX>1. For 0<XX<1, the reflection formula (6.1.4) can be used first.
```

```
C See Numerical Recipes p.157
```

```
  REAL*8 Cof(6)/76.18009173D0,-86.50532033D0,24.01409822D0,  
& -1.231739516D0,0.120858003D-2,-0.536382D-5/  
& Stp/2.50662827465D0,Half/0.5D0/,One/1.0D0/,Fpf/5.5D0/  
& X,Tmp,Ser,XX
```

```
  INTEGER J
```

```
  X=XX-One
```

```
  Tmp=X+Fpf
```

```
  Tmp=(X+Half)*LOG(Tmp)-Tmp
```

```
  Ser=One
```

```
  DO J=1,6
```

```
    X=X+One
```

```
    Ser=Ser+Cof(J)/X
```

```
  END DO
```

```
  GammLnDP=Tmp+LOG(Stp*Ser)
```

```
RETURN
```

```
END
```

```
C ***** GCFDP
```

```
SUBROUTINE GCFDP(GammCF,A,X,GLN)
```

```
C Returns the incomplete gamma function Q(a,x) evaluated by its continued
```

```
C fraction representation as GammCF. Also returns LOG Gamma(A) as GLN.
```

```
C See Numerical Recipes p. 162
```

```

REAL*8 GammCF,A,X,Gln,G,GOld,A0,A1,B0,B1,Fac
REAL*8 An,Ana,Anf,GammLnDP
INTEGER N
EXTERNAL GammLnDP

```

```

PARAMETER ITMax=500
PARAMETER Eps=3.E-7

```

C Variables

C GOLD The previous value of G tested against for convergence.

```
Gln=GammLnDP(A)
```

```
GOld=0.
```

```
A0=1.
A1=X
```

```
B0=0.
B1=1.
```

```
Fac=1.
```

```

DO N=1,ITMax
  An=FLOAT(N)
  ANA=AN-A

```

C One step of the recurrence (5.2.5)

```

A0=(A1+A0*ANA)*Fac
B0=(B1+B0*ANA)*Fac

```

C The next step of the recurrence (5.2.5)

```

Anf=AN*Fac
A1=X*A0+Anf*A1
B1=X*B0+Anf*B1

```

C Shall we renormalize?

```

IF (A1.NE.0.0) THEN
  Fac=1./A1
  G=B1*Fac
  IF (ABS((G-GOld)/G).LT.Eps) THEN
    GammCF=EXP(-X+A*LOG(X)-Gln)*G
    RETURN
  END IF
  GOld=G
END IF
END DO

```

```

WRITE(*,*) 'Error: A too large or ITMax too small'
WRITE(*,*) '      A=',A
WRITE(*,*) '      X=',X
WRITE(*,*) '      ITMax=',ITMAX
STOP 'In Routine: GCFDP'

```

END

C ***** GSerDP

SUBROUTINE GSerDP(GamSer,A,X,Gln)

C Returns the incomplete Gamma Function $P(a,x)$ evaluated by its series
C representation as GamSer. Also returns LOG Gamma(a) as Gln.

INTEGER N
REAL*8 GamSer,A,X,Gln,Ap,Sum,Del,GammLnDP
EXTERNAL GammLnDP

PARAMETER ITMax=100
PARAMETER Eps=3.0E-7

Gln=GammLnDP(A)

IF (X.LT.0) STOP 'In Subroutine: GSerDP'

IF (X.EQ.0.0) THEN
GamSer=0.0
RETURN
END IF

AP=A
Sum=1.0/A
Del=Sum

DO N=1,ITMax
AP=AP+1.
Del=Del*X/AP
Sum=Sum+Del
IF (Abs(Del).LT.ABS(Sum)*Eps) THEN
GamSer=Sum*EXP(-X+A*LOG(X)-GLN)
RETURN
END IF
END DO

STOP 'In Routine: GSerDP, A too large or ITMax too small'
END

C ***** GauLeg

SUBROUTINE GauLeg(Np,Points,Weights)

C This subroutine returns the Gauss-Legendre integration points and weights for
C a Np-point gaussian quadrature integration over the interval $0 < x < 1$.
C The value of the integral is approximated by the
C $\text{sum}(F(\text{Points}(i))*\text{Weights}(i), i=1, Np)$

C (Modified from Press, Flannery, Teukolsky, and Vetterling,
C NUMERICAL RECIPES: The Art of Scientific Computing, 1986, Cambridge
C University Press, p. 125-126)

REAL*8 Points(*),Weights(*),Z,PP,Z1,Z2,P1,P2,P3
INTEGER Np,I,J

PARAMETER Eps=3.D-14

C Loop over the desired roots

```
DO I=1,(Np+1)/2
  Z=COS(3.141592654D0*(I-0.25D0)/(Np+0.5D0))
```

C Starting with the above approximation to the Ith root, we enter the main
C loop of refinement by Newton's method.

```
1 CONTINUE
  P1=1.D0
  P2=0.D0
  DO J=1,Np
    P3=P2
    P2=P1
    P1=((2.D0*J-1.D0)*Z*P2-(J-1.D0)*P3)/J
  END DO
```

C P1 is now the desired Legendre polynomial. We next compute PP, its
C derivative, by a standard relation involving also P2, the polynomial of
C one lower order.

```
PP=Np*(Z*P1-P2)/(Z*Z-1.D0)
Z1=Z
Z=Z1-P1/PP
IF (ABS(Z-Z1).GT.Eps) GOTO 1
```

```
Points(Np+1-I)=Z
Weights(Np+1-I)=2.D0/((1.D0-Z*Z)*PP*PP)
```

END DO

```
DO I=1,NP/2
  Points(I)=-Points(Np+1-I)
  Weights(I)=Weights(Np+1-I)
END DO
```

C The following DO-LOOP convert the gauss points and weights from an interval
C of -1 to 1 to an interval from 0.0 to 1.0

```
DO I=1,NP
  Points(I)=(Points(I)+1.0D0)/2.0D0
  Weights(I)=Weights(I)/2.0D0
END DO
```

```
RETURN
END
```

C ***** GauLog

SUBROUTINE GauLog(Np,Points,Weights)

```
INTEGER Np
REAL*8 Points(*),Weights(*)
```

C This subroutine returns the gauss points and weights for integrating
C $\ln(1/x) * f(x)$ from 0 to 1. The integral is the sum of
C $\text{Weights}(i) * f(\text{Points}(i))$ for $i=1$ to Np . The the values for points and
C weights come form GAUSSIAN QUADRATURE FORMULAS, A.H. Stroud and Don Secrest
C Prentice-Hall, Inc., Englewood Cliffs, N.J. C 1966

IF (Np.EQ.2) THEN

Points(1)=0.11200880616697618295
Points(2)=0.60227690811873810275

Weights(1)=0.71853931903038444066
Weights(2)=0.28146068096961555933

ELSE IF (Np.EQ.3) THEN

Points(1)=0.063890793087325404996
Points(2)=0.36899706371561876554
Points(3)=0.76688030393894145542

Weights(1)=0.51340455223236332512
Weights(2)=0.39198004120148755480
Weights(3)=0.094615406566149120064

ELSE IF (Np.EQ.4) THEN

Points(1)=0.041448480199383220803
Points(2)=0.24527491432060225193
Points(3)=0.55616545356027583718
Points(4)=0.84898239453298517464

Weights(1)=0.38346406814513512485
Weights(2)=0.38687531777476262733
Weights(3)=0.19043512695014241536
Weights(4)=0.039225487129959832452

ELSE IF (Np.EQ.5) THEN

Points(1)=0.029134472151972053303
Points(2)=0.17397721332089762870
Points(3)=0.41170252028490204317
Points(4)=0.67731417458282038070
Points(5)=0.89477136103100828363

Weights(1)=0.29789347178289445727
Weights(2)=0.34977622651322418037
Weights(3)=0.23448829004405241888
Weights(4)=0.098930459516633146976
Weights(5)=0.018911552143195796489

ELSE IF (Np.EQ.6) THEN

Points(1)=0.021634005844116948995
Points(2)=0.12958339115495079613
Points(3)=0.31402044991476550879
Points(4)=0.53865721735180214454
Points(5)=0.75691533737740285216
Points(6)=0.92266885137212023733

Weights(1)=0.23876366257854756972
 Weights(2)=0.30828657327394679296
 Weights(3)=0.24531742656321038598
 Weights(4)=0.14200875656647668542
 Weights(5)=0.055454622324886290015
 Weights(6)=0.010168958692932275886

ELSE IF (Np.EQ.7) THEN

Points(1)=0.016719355408258515941
 Points(2)=0.10018567791567512158
 Points(3)=0.24629424620793059904
 Points(4)=0.43346349325703310583
 Points(5)=0.63235098804776608846
 Points(6)=0.81111862674010557652
 Points(7)=0.94084816674334772176

Weights(1)=0.19616938942524820752
 Weights(2)=0.27030264424727298214
 Weights(3)=0.23968187300769094830
 Weights(4)=0.16577577481043290656
 Weights(5)=0.088943227137657964435
 Weights(6)=0.033194304356571067025
 Weights(7)=0.0059327870151259239991

ELSE IF (Np.EQ.8) THEN

Points(1)=0.013320244150892465012
 Points(2)=0.079750429013894938409
 Points(3)=0.19797102932618805379
 Points(4)=0.35415399435190941967
 Points(5)=0.52945857523491727770
 Points(6)=0.70181452993909996383
 Points(7)=0.84937932044110667604
 Points(8)=0.95332645005635978876

Weights(1)=0.16441660472800288683
 Weights(2)=0.23752561002330602050
 Weights(3)=0.22684198443191912636
 Weights(4)=0.17575407900607024498
 Weights(5)=0.11292403024675905185
 Weights(6)=0.057852210717782072398
 Weights(7)=0.020979073742132978043
 Weights(8)=0.0036864071040276190133

ELSE IF (Np.EQ.9) THEN

Points(1)=0.010869336084175477113
 Points(2)=0.064983666338007939406
 Points(3)=0.16222939802388293870
 Points(4)=0.29374990397167465807
 Points(5)=0.44663188190546803720
 Points(6)=0.60548166277612862084
 Points(7)=0.75411013715716356665
 Points(8)=0.87726582883583825317
 Points(9)=0.96225055941028184144

Weights(1)=0.14006843874813473426

Weights(2)=0.20977220520103044750
Weights(3)=0.21142714989660272853
Weights(4)=0.17715623393907998954
Weights(5)=0.12779922803329549588
Weights(6)=0.07847890261156217546
Weights(7)=0.039022504985399096847
Weights(8)=0.013867295549593023290
Weights(9)=0.0024080410363923115729

ELSE IF (Np.EQ.10) THEN

Points(1)=0.0090426309621996506369
Points(2)=0.053971266222500629504
Points(3)=0.13531182463925077487
Points(4)=0.24705241628715982422
Points(5)=0.38021253960933233397
Points(6)=0.52379231797184320116
Points(7)=0.66577520551642459722
Points(8)=0.79419041601196621735
Points(9)=0.89816109121900353816
Points(10)=0.96884798871863353939

Weights(1)=0.12095513195457051498
Weights(2)=0.18636354256407187032
Weights(3)=0.19566087327775998271
Weights(4)=0.17357714218290692084
Weights(5)=0.13569567299548420166
Weights(6)=0.093646758538110525987
Weights(7)=0.055787727351415874075
Weights(8)=0.027159810899233331145
Weights(9)=0.0095151826028485149992
Weights(10)=0.0016381576335982632548

ELSE IF (Np.EQ.11) THEN

Points(1)=0.0076439411746377066292
Points(2)=0.045541828256578918548
Points(3)=0.11452229745512458369
Points(4)=0.21037858122703353088
Points(5)=0.32669555322169284797
Points(6)=0.45545324692881343831
Points(7)=0.58764835635908440789
Points(8)=0.71396385001256144053
Points(9)=0.82545321780181180417
Points(10)=0.91419392161254313794
Points(11)=0.97386025627558615232

Weights(1)=0.10565225609910049130
Weights(2)=0.16657168060062904863
Weights(3)=0.18056321828775372476
Weights(4)=0.16727873677378417932
Weights(5)=0.13869705740163122050
Weights(6)=0.10383343336504406027
Weights(7)=0.069536697888735232346
Weights(8)=0.040541600803596329568
Weights(9)=0.019435402476218172780
Weights(10)=0.0067374293424500627021
Weights(11)=0.0011524869610574777832

ELSE IF (Np.EQ.12) THEN

Points(1)=0.0065487222790800587892
Points(2)=0.038946809560449959161
Points(3)=0.098150263106006628862
Points(4)=0.18113858159063157735
Points(5)=0.28322006766737255470
Points(6)=0.39843443516343664370
Points(7)=0.51995262679235266272
Points(8)=0.64051091671610645430
Points(9)=0.75286501205183057837
Points(10)=0.85024002416230220067
Points(11)=0.92674968322391410104
Points(12)=0.97775612968999747917

Weights(1)=0.093192691443931324491
Weights(2)=0.14975182757632236417
Weights(3)=0.16655745436459300532
Weights(4)=0.15963355943698765116
Weights(5)=0.13842483186483562106
Weights(6)=0.11001657063572116233
Weights(7)=0.079961821770828970264
Weights(8)=0.052406954824641770650
Weights(9)=0.030071088873761187123
Weights(10)=0.014249245587998279107
Weights(11)=0.0048999245823217609390
Weights(12)=0.00083402903805690336469

ELSE IF (Np.EQ.13) THEN

Points(1)=0.0056747662562426690299
Points(2)=0.033690108799032536748
Points(3)=0.085036754474175028089
Points(4)=0.15749755947788902873
Points(5)=0.24756957887684314613
Points(6)=0.35074431236085520042
Points(7)=0.46177374676161024622
Points(8)=0.57495946652556132074
Points(9)=0.68445988035043004253
Points(10)=0.78460256881034708051
Points(11)=0.87018642840788838882
Points(12)=0.93675782930675139337
Points(13)=0.98084345181159094850

Weights(1)=0.082900496793275787818
Weights(2)=0.13536867316574450040
Weights(3)=0.15377328439229220085
Weights(4)=0.15145815850998819062
Weights(5)=0.13604033653728306071
Weights(6)=0.11317682288163380335
Weights(7)=0.087374430480045258238
Weights(8)=0.062160230641804869517
Weights(9)=0.040087728934165851898
Weights(10)=0.022723844939972195328
Weights(11)=0.010671230412968444087
Weights(12)=0.0036464922759741400797
Weights(13)=0.00061827003485169707685

ELSE IF (Np.EQ.14) THEN

Points(1)=0.0049660035738685422439
Points(2)=0.029432540118885178286
Points(3)=0.074376292224535762610
Points(4)=0.13813849198918628179
Points(5)=0.21805564849895907807
Points(6)=0.31066208391810198317
Points(7)=0.41187247517775020720
Points(8)=0.51717930739865432972
Points(9)=0.62186485972851111970
Points(10)=0.72122074520810885373
Points(11)=0.81076598807158985635
Points(12)=0.88645403803443465718
Points(13)=0.94485913946181863892
Points(14)=0.98333102648567848004

Weights(1)=0.074291225067510412498
Weights(2)=0.12298877246932291429
Weights(3)=0.14219930656252335570
Weights(4)=0.14322929764126422201
Weights(5)=0.13234508377208520926
Weights(6)=0.11413587573667647525
Weights(7)=0.092283038079073613216
Weights(8)=0.069753673293937564550
Weights(9)=0.048830323600513564644
Weights(10)=0.031101796064416141117
Weights(11)=0.017462811950196093832
Weights(12)=0.0081424234298759361332
Weights(13)=0.0027684364185639373318
Weights(14)=0.00046793591404056013532

ELSE IF (Np.EQ.15) THEN

Points(1)=0.0043831101754754038348
Points(2)=0.025935898105330616102
Points(3)=0.065596095412316245254
Points(4)=0.12210193407333160332
Points(5)=0.19339526237400711598
Points(6)=0.27677283870610202439
Points(7)=0.36901512713974294381
Points(8)=0.46652432896470658267
Points(9)=0.56547347379181730642
Points(10)=0.66196291901245642138
Points(11)=0.75217888337878579878
Points(12)=0.83254803386618958925
Points(13)=0.89988205012089808432
Points(14)=0.95150618874340990272
Points(15)=0.98536446812213193892

Weights(1)=0.067009978916493713603
Weights(2)=0.11226415028670574182
Weights(3)=0.13176017703967990373
Weights(4)=0.13521764906193472513
Weights(5)=0.12788179864568037040
Weights(6)=0.11353290749021942129
Weights(7)=0.095205239784358658511
Weights(8)=0.075389314167395954339

```

Weights(9)=0.056078424492653717992
Weights(10)=0.038768295375018231110
Weights(11)=0.024451483268750075960
Weights(12)=0.013624630138238846905
Weights(13)=0.0063164475985907611998
Weights(14)=0.0021388899159444713478
Weights(15)=0.00036061381833540664685

```

```
ELSE IF (Np.EQ.16) THEN
```

```

Points(1)=0.0038978344871159159240
Points(2)=0.023028945616873239820
Points(3)=0.058280398306240412348
Points(4)=0.10867836509105403648
Points(5)=0.17260945490984393776
Points(6)=0.24793705447057849514
Points(7)=0.33209454912991715598
Points(8)=0.42218391058194860011
Points(9)=0.51508247338146260347
Points(10)=0.60755612044772872408
Points(11)=0.69637565322821406115
Points(12)=0.77843256587326540520
Points(13)=0.85085026971539108323
Points(14)=0.91108685722227190541
Points(15)=0.95702557170354215759
Points(16)=0.98704780024798447675

```

```

Weights(1)=0.060791710043591232851
Weights(2)=0.10291567751758214438
Weights(3)=0.12235566204600919355
Weights(4)=0.12756924693701598871
Weights(5)=0.12301357460007091542
Weights(6)=0.11184724485548572262
Weights(7)=0.096596385152124341252
Weights(8)=0.079356664351473138782
Weights(9)=0.061850494581965207095
Weights(10)=0.045435246507726668628
Weights(11)=0.031098974751581806409
Weights(12)=0.019459765927360842078
Weights(13)=0.010776254963205525645
Weights(14)=0.0049725428900876417125
Weights(15)=0.0016782011100511945150
Weights(16)=0.00028235376466843632177

```

```
ELSE
```

```

WRITE(*,*) 'Error: Np is too large or small!-',Np,'=Np'
STOP 'In Routine: GauLog'

```

```
END IF
```

```

RETURN
END

```

```
C ***** GaussPtsWts
```

```
SUBROUTINE GaussPtsWts(Np,Points,Weights)
```

C This subroutine returns the Gauss-Legendre integration points and weights for
 C a Np-point gaussian quadrature integration over the interval $0 < x < 1$.
 C The value of the integral is approximated by the
 C $\text{sum}(F(\text{Points}(i)) * \text{Weights}(i), i=1, Np)$

C (Modified from Conte and de Boor, ELEMENTARY NUMERICAL ANALYSIS, 3d ed.
 C McGraw Hill p.316)

C Input Variables

C Np The number of points approximating the interval

C Output Variables

C Points(NP) The points to use in approximating the integral

C Weights(NP) The weights to use.

C Internal Variables

C I Loop counter

DOUBLE PRECISION Points(*),Weights(*)
 INTEGER Np,I

IF (Np.EQ.1) THEN

Points(1)=0.0
 Weights(1)=2.0

ELSE IF (Np.EQ.2) THEN

Points(2)=0.577350269189626
 Weights(2)=1.0

ELSE IF (Np.EQ.3) THEN

Points(2)=0.0
 Points(3)=0.774596669241483
 Weights(2)=0.888888888888889
 Weights(3)=0.555555555555556

ELSE IF (Np.EQ.4) THEN

Points(3)=0.339981043584856
 Points(4)=0.861136311594053
 Weights(3)=0.652145154862546
 Weights(4)=0.347854845137454

ELSE IF (Np.EQ.5) THEN

Points(3)=0.0
 Points(4)=0.538469310105683
 Points(5)=0.906179845938664
 Weights(3)=0.568888888888889
 Weights(4)=0.478628670499366
 Weights(5)=0.236926885056189

ELSE IF (Np.EQ.6) THEN


```

Points(4)=0.238619186083197
Points(5)=0.661209386466265
Points(6)=0.932469514203152
Weights(4)=0.467913934572691
Weights(5)=0.360761573048139
Weights(6)=0.171324492379170

```

```
ELSE IF (Np.GT.6) THEN
```

```

        WRITE(*,600) NP
600    FORMAT(X,'The number of points ('I3,') is greater than 6.',
& /,X,'Please call this GaussPtsWts with Np <= 6.',
& /,X,'The GauLeg routine will compute the gauss points ',
& /,X,'for an Np')
        STOP 'In Routine GaussPtsWts'

```

```
END IF
```

```

DO I=1,NP/2
  Points(I)=-Points(Np+1-I)
  Weights(I)=Weights(Np+1-I)
END DO

```

C The following DO-LOOP convert the gauss points and weights from an interval
C of -1 to 1 to an interval from 0.0 to 1.0

```

DO I=1,NP
  Points(I)=(Points(I)+1.0D0)/2.0D0
  Weights(I)=Weights(I)/2.0D0
END DO

```

```

RETURN
END

```

C ***** GaussQuad

```
SUBROUTINE GaussQuad(NoOfGauss,Points,Weights,Funk,Sum)
```

C This subroutine will perform the gaussian quadrature tsummation.
C (Note, can be used for integration by gaussian quadrature of
C $f(x)$ or $\ln(1/x)f(X)$ by changing the weights passed to the subroutine

C Passed Variables

```

  INTEGER NoOfGauss
  REAL*8 Sum,Points(*),Weights(*)

```

C Passed Functions

```

  REAL*8 Funk
  EXTERNAL Funk

```

C Internal Variables

```

  INTEGER Gs

```

C Subroutine Code

```

Sum=0
DO Gs=1,NoOfGauss
  Sum=Sum+Funk(Points(Gs))*Weights(Gs)
END DO

RETURN
END

```

C ***** Interp1D

```

SUBROUTINE Interp1D(X1,F1,X2,F2,Xd,Fd)

REAL*8 X1,X2,Xd,F1,F2,Fd

IF (X2.EQ.X1) THEN
  Fd=F1
ELSE
  Fd=F1+(F2-F1)*(Xd-X1)/(X2-X1)
END IF

RETURN
END

```

C ***** Interp2D

```

SUBROUTINE Interp2D(X1,Y1,X2,Y2,F11,F12,F21,F22,Xd,Yd,Fd)

REAL*8 X1,Y1,X2,Y2,F11,F12,F21,F22,Xd,Yd,Fd
REAL*8 FX1,FX2,FD1,F1Y,F2Y,FD2

CALL Interp1D(X1,F11,X2,F21,XD,FX1)
CALL Interp1D(X1,F12,X2,F22,Xd,FX2)
CALL Interp1D(Y1,FX1,Y2,FX2,Yd,Fd1)

CALL Interp1D(Y1,F11,Y2,F12,Yd,F1Y)
CALL Interp1D(Y1,F21,Y2,F22,Yd,F2Y)
CALL Interp1D(X1,F1Y,X2,F2Y,Xd,Fd2)

FD=(Fd1+Fd2)/2.0

RETURN
END

```

C ***** Kelliptic

```

REAL*8 FUNCTION Kelliptic(M)

```

C Taken from Numerical Recipes, p. 187
C This function returns the complete elliptic integral with
C QQC=k

C CA Square-root of desired accuracy.

```

PARAMETER CA=0.00000005
PARAMETER PIO2=1.570796326794896619231322

```

```

REAL*8 M,PP,AA,BB

```

```

REAL*8 Qc,A,B,P,E,EM,F,G

IF (ABS(M).GE.1) THEN
  WRITE(*,*) 'Error: M>=1 ',M,'=M'
  STOP 'In-Routine: KElliptic'
END IF

QC=SQRT(1.0-ABS(M))

A=1
B=1
P=1
E=QC
EM=1.0

1  F=A
   A=A+B/P
   G=E/P
   B=2*(B+F*G)
   P=G+P
   G=EM
   EM=QC+EM
   IF (ABS(G-QC).GT.G*CA) THEN
     QC=2*SQRT(E)
     E=QC*EM
     GOTO 1
   END IF

KElliptic=PIO2*(B+A*EM)/(EM*(EM+P))
RETURN
END

C ***** KEIP

REAL*8 FUNCTION KEIP(M)
REAL*8 M

REAL*8 First,Second,M1

CALL KelPCoef(M,M1,First,Second)
KelP=First-Second*LOG(M1)

RETURN
END

C ***** KEIPCoef

SUBROUTINE KEIPCoef(M,M1,First,Second)

C Polynomial Approximation to Complete Elliptic Integral K, taken from
C Abramowitz and Stegun, p 587

REAL*8 M,M1,First,Second
REAL*8 A(5)/1.38629436112,0.09666344259,0.03590092383,
& 0.03742563713,0.01451196212/
REAL*8 B(5)/0.5,0.12498593597,0.06880248576,
& 0.03328355346,0.00441787012/
INTEGER I

```

```

IF (M.GE.1.0) THEN
  WRITE(*,*) 'Error: M>=1   M=',M
  M=M/0.0
  STOP 'In Routine: KEIP'
END IF

```

```

M1=1.0-M

```

```

First=0.0
Second=0.0
DO I=1,5
  First=First+A(I)*(M1**(I-1))
  Second=Second+B(I)*(M1**(I-1))
END DO

```

```

RETURN
END

```

```

C ***** LUBksbDP
C *****LUBksb

```

```

SUBROUTINE LUBksb(A,N,Np,Indx,B)

```

C This routine from Numerical Recipes, p. 37.

C Solves the set of N linear equations $A.x=B$. Here A is input, not
 C as the matrix A but rather as its LU decomposition, determined by the
 C routine LUDcmp. Indx is input as the permutation vector returned by
 C LUDcmp. B is input as the right-hand side vector B, and returns with
 C the solution vector X. A,N,Np and Indx are not modified by this routine
 C and can be left in place for successive calls with different right-hand
 C sides B. This routine takes into account the possibility that B will begin
 C with many zero elements, so it is efficient for use in matrix inversion.

```

INTEGER N,Np,Indx(Np),II,I,LL,J
REAL A(Np,Np),B(Np),Sum

```

C When II is set to a positive value, it will become the index of the first
 C nonvanishing element of B. We now do the forward substitution, equation
 C 2.3.6. The only new wrinkle is to unscramble the permutation as we go.

```

II=0

```

```

DO I=1,N
  LL=Indx(I)
  Sum=B(LL)
  B(LL)=B(I)
  IF (ii.NE.0) THEN
    DO J=ii,i-1
      Sum=Sum-A(I,J)*B(J)
    END DO
  ELSE IF (Sum.NE.0) THEN

```

C A nonzero element was encountered, so from now on we will have
 C to do the sums in the loop above.

```

  II=i
END IF

```

```
B(I)=Sum
```

```
END DO
```

C Now we do the backsubstitution, equation 2.3.7

```
DO I=N,1,-1
  Sum=B(I)
  IF (I.LT.N) THEN
    DO J=I+1,N
      Sum=Sum-A(I,J)*B(J)
    END DO
  END IF
```

C Store a component of the solution vector X.

```
B(I)=Sum/A(I,I)
END DO
```

```
RETURN
END
```

```
SUBROUTINE LUBksbDP(A,N,Np,Indx,B)
```

C This routine from Numerical Recipes, p. 37.

C Solves the set of N linear equations $Ax=B$. Here A is input, not
 C as the matrix A but rather as its LU decomposition, determined by the
 C routine LUDcmp. Indx is input as the permutation vector returned by
 C LUDcmp. B is input as the right-hand side vector B, and returns with
 C the solution vector X. A,N,Np and Indx are not modified by this routine
 C and can be left in place for successive calls with different right-hand
 C sides B. This routine takes into account the possibility that B will begin
 C with many zero elements, so it is efficient for use in matrix inversion.

```
INTEGER N,Np,Indx(Np),II,I,LL,J
REAL*8 A(Np,Np),B(Np),Sum
```

C When II is set at a positive value, it will become the index of the first
 C nonvanishing element of B. We now do the forward substitution, equation
 C 2.3.6. The only new wrinkle is to unscramble the permutation as we go.

```
II=0
```

```
DO I=1,N
  LL=Indx(I)
  Sum=B(LL)
  B(LL)=B(I)
  IF (ii.NE.0) THEN
    DO J=ii,i-1
      Sum=Sum-A(I,J)*B(J)
    END DO
  ELSE IF (Sum.NE.0) THEN
```

C A nonzero element was encountered, so from now on we will have
 C to do the sums in the loop above.

```

      II=i
      END IF
      B(I)=Sum
    END DO

```

C Now we do the backsubstitution, equation 2.3.7

```

      DO I=N,1,-1
        Sum=B(I)
        IF (I.LT.N) THEN
          DO J=I+1,N
            Sum=Sum-A(I,J)*B(J)
          END DO
        END IF
      END DO

```

C Store a component of the solution vector X.

```

      B(I)=Sum/A(I,I)
    END DO

    RETURN
  END

```

C ***** LUDcmp

```

      SUBROUTINE LUDcmp(A,N,Np,Indx,D)

```

C This routine from NUMERICAL RECIPES by W.H. Press, B.P. Flannery,
C S.A. Teukolsky, W.T. Vetterling.

C Given an NxN matrix A, with physical dimension Np, this routine replaces
C it by the LU decomposition of a row-wise permutation of itself. A and
C N are input. A is output, arranged as in equation (2.3.14); Indx is an
C output vector which records the row permutation effected by the partial
C pivoting; D is output as + or - 1 depending on whether the number of
C row interchanges was even or odd, respectively. This routine is used
C in combination with LUBKSB to solve linear equations or to invert a
C matrix.

C NMaxLargest expected N
C Tiny A small number
C VV() The implicit scaling of each row.

```

      PARAMETER NMax=100
      PARAMETER Tiny=1.0E-20

      INTEGER N,Np,Indx(Np),IJ,K,IMax
      REAL A(Np,Np),VV(NMax),AAMax,Sum,D,Dum

      IF (N.GT.NMax) THEN
        WRITE(*,*) 'Error: matrix dimension too large.'
        WRITE(*,*) '      N=',N
        WRITE(*,*) '      NMax=',NMax
        STOP 'In Routine: LUDcmp'
      END IF

      D=1

```

C The following DO-loop loops over rows to get the implicit scaling C information.

```

DO I=1,N
  AAMax=0.
  DO J=1,N
    AAMax=MAX(ABS(A(I,J)),AAMax)
  END DO

  IF (AAMax.EQ.0.0) THEN
    WRITE(*,*) 'Error: Singular Matrix.'
    STOP 'In Routine: LUDcmp'
  END IF

  VV(I)=1.0/AAMax
END DO

```

C The following DO-loop loops over the columns of Crout's method.

```

DO J=1,N

```

C The following DO-loop computes equation (2.3.12) except for $i=j$.

```

DO I=1,J-1
  Sum=A(I,J)

  DO K=1,I-1
    Sum=Sum-A(I,K)*A(K,J)
  END DO

  A(I,J)=Sum
END DO

```

C The following DO-loop searches for the largest pivot element

```

AAMax=0.0
DO I=J,N
  Sum=A(I,J)
  DO K=1,J-1
    Sum=Sum-A(I,K)*A(K,J)
  END DO
  A(I,J)=Sum

  Dum=VV(I)*ABS(Sum)
  IF (Dum.GT.AAMax) THEN
    IMax=I
    AAMax=Dum
  END IF
END DO

```

C The following IF-THEN block makes the row-exchange if it is required.

```

IF (J.NE.IMax) THEN

```

```

      DO K=1,N
        Dum=A(Imax,K)
        A(Imax,K)=A(J,K)
        A(J,K)=Dum
      END DO

      D=-D
      VV(IMax)=VV(J)

    END IF

    Indx(J)=IMax
    IF (A(J,J).EQ.0) A(J,J)=Tiny

    IF (J.NE.N) THEN
      Dum=1.0/A(J,J)
      DO I=J+1,N
        A(I,J)=A(I,J)*Dum
      END DO
    END IF
  END DO

  RETURN
  END

```

C ***** LUDcmpDP

SUBROUTINE LUDcmpDP(A,N,Np,Indx,D)

C This routine from NUMERICAL RECIPES by W.H. Press, B.P. Flannery,
C S.A. Teukolsky, W.T. Vetterling.

C Given an NxN matrix A, with physical dimension Np, this routine replaces
C it by the LU decomposition of a row-wise permutation of itself. A and
C N are input. A is output, arranged as in equation (2.3.14); Indx is an
C output vector which records the row permutation effected by the partial
C pivoting; D is output as + or - 1 depending on whether the number of
C row interchanges was even or odd, respectively. This routine is used
C in combination with LUBKSB to solve linear equations or to invert a
C matrix.

C NMaxLargest expected N
C Tiny A small number
C VV() The implicit scaling of each row.

```

  PARAMETER NMax=1000
  PARAMETER Tiny=1.0E-20

```

```

  INTEGER N,Np,Indx(Np),I,J,K,IMax
  REAL*8 A(Np,Np),VV(NMax),AAMax,Sum,D,Dum

```

```

  IF (N.GT.NMax) THEN
    WRITE(*,*) 'Error: matrix dimension too large.'
    WRITE(*,*) '      N=',N
    WRITE(*,*) '      NMax=',NMax
    STOP 'In Routine: LUDcmp'
  END IF

```


D=1

C The following DO-loop loops over rows to get the implicit scaling
C information.

```
DO I=1,N
  AAMax=0.
  DO J=1,N
    AAMax=MAX(ABS(A(I,J)),AAMax)
  END DO

  IF (AAMax.EQ.0.0) THEN
    WRITE(*,*) 'Error: Singular Matrix.'
    STOP 'In Routine: LUDcmp'
  END IF

  VV(I)=1.0/AAMax
END DO
```

C The following DO-loop loops over the columns of Crout's method.

```
DO J=1,N
```

C The following DO-loop computes equation (2.3.12) except for $i=j$.

```
DO I=1,J-1
  Sum=A(I,J)
  DO K=1,I-1
    Sum=Sum-A(I,K)*A(K,J)
  END DO

  A(I,J)=Sum
END DO
```

C The following DO-loop searches for the largest pivot element

```
AAMax=0.0
DO I=J,N
  Sum=A(I,J)
  DO K=1,J-1
    Sum=Sum-A(I,K)*A(K,J)
  END DO
  A(I,J)=Sum

  Dum=VV(I)*ABS(Sum)
  IF (Dum.GT.AAMax) THEN
    IMax=I
    AAMax=Dum
  END IF
END DO
```

C The following IF-THEN block makes the row-exchange if it is required.

```

IF (J.NE.IMax) THEN
    DO K=1,N
        Dum=A(Imax,K)
        A(Imax,K)=A(J,K)
        A(J,K)=Dum
    END DO

    D=-D
    VV(IMax)=VV(J)

END IF

Indx(J)=IMax
IF (A(J,J).EQ.0) A(J,J)=Tiny

IF (J.NE.N) THEN
    Dum=1.0/A(J,J)
    DO I=J+1,N
        A(I,J)=A(I,J)*Dum
    END DO
END IF
END DO

RETURN
END

```

C ***** MatInv

```

SUBROUTINE MatInv(A,Inv,Indx,Col,N,Np)

```

C This routine from Numerical Recipes p. 38

C Matrix A will be destroyed!

```

INTEGER N,Np,Indx(Np),I,J
REAL A(Np,Np),Inv(Np,Np),Col(Np),D

DO I=1,N
    Col(I)=0.0
END DO

CALL LUDcmp(A,N,Np,Indx,D)

DO I=1,N

    DO J=1,N
        Col(J)=0.0
    END DO

    Col(I)=1.0
    CALL LUBksb(A,N,Np,Indx,Col)

    DO J=1,N
        Inv(J,I)=Col(J)
    END DO

END DO

```

```

RETURN
END

```

C ***** MatVecMultDP

```

SUBROUTINE MatVecMultDP(MaxDim,Dim,Mat,Vec,Res)

```

```

INTEGER MaxDim,Dim,I,J
REAL*8 Mat(MaxDim,MaxDim),Vec(*),Res(*)

```

```

DO I=1,Dim
  Res(I)=0.D0
  DO J=1,Dim
    Res(I)=Res(I)+Mat(I,J)*Vec(J)
  END DO
END DO

```

```

RETURN
END

```

C ***** MatZeroDP

```

SUBROUTINE MatZeroDP(NoOfRows,NoOfColumns,Matrix)

```

```

INTEGER NoOfRows,NoOfColumns,I,J,RowDim
REAL*8 Matrix(RowDim,*)

```

```

DO I=1,NoOfRows
  DO J=1,NoOfColumns
    Matrix(I,J)=0.0
  END DO
END DO

```

```

RETURN
END

```

C ***** PCubic.

```

REAL*8 FUNCTION PCubic(XBar,Xi,C,N)

```

C This function is from Conte and DeBoor p.285. Returns the value at XBar of
C the piecewise cubic function on N intervals with breakpoint sequence Xi and
C coefficients C.

```

INTEGER N,I,J
REAL*8 C(4,N),XBar,Xi(N+1),dX
DATA I/1/

```

```

IF (I.GT.N+1) I=N+1

```

```

IF (XBar.GE.XI(I)) THEN
  DO J=I,N
    IF (XBar.LT.XI(J+1)) GOTO 30
  END DO
  J=N

```

```

ELSE
  DO J=I-1,1,-1
    IF (XBar.GE.XI(J)) GOTO 30
  END DO

```

```

        END DO
        J=1
    END IF

30    I=J
    dX=XBar-XI(I)
    PCubic=C(1,I)+dX*(C(2,I)+dX*(C(3,I)+dX*C(4,I)))

    RETURN
    END

C ***** PrintMatDP

SUBROUTINE PrintMatDP(MaxDim,Dim,Mat,Title)

    INTEGER Dim,MaxDim,Length,I,J,K
    REAL*8 Mat(MaxDim,*)
    CHARACTER*(*) Title
    LOGICAL FirstLine

    CALL StringLength(Title,Length)
    IF (Length.GT.0) THEN
        WRITE(*,*) ' '
        WRITE(*,*) Title(1:Length)
        WRITE(*,*) ' '
    END IF

C 12345678 1234567 1234567 1234567 1234567
C Row      Col 1   Col 2   Col 3   Col 4   Col 5
C 12312345123456789a
C iii      dddddddddd dddddddddd dddddddddd dddddddddd dddddddddd
C          dddddddddd dddddddddd dddddddddd dddddddddd dddddddddd

10    FORMAT(X,'Row',8X,'Col 1',7X,'Col 2',7X,'Col 3',7X,'Col 4',7X,
    & 'Col 5',/)
20    FORMAT(X,I3,3X,5(:,2X,G10.4))
30    FORMAT(X,3X,3X,5(:,2X,G10.4))

    WRITE(*,10)

    DO I=1,Dim
        FirstLine=.FALSE.
        DO J=0,Dim-5,5
            IF (.NOT.FirstLine) THEN
                WRITE(*,20) I,(Mat(I,J+K),K=1,5)
                FirstLine=.TRUE.
            ELSE
                WRITE(*,30) (Mat(I,J+K),K=1,5)
            END IF
        END DO

        IF (J+5.LT.Dim) J=J+5

        IF (.NOT.FirstLine) THEN
            WRITE(*,20) I,(Mat(I,K),K=J+1,Dim)
        ELSE
            WRITE(*,30) (Mat(I,K),K=J+1,Dim)
        END IF
    END IF

```

```
IF (FirstLine) WRITE(*,*) ' '
```

```
END DO
```

```
RETURN
```

```
END
```

```
C ***** PrintMatR
```

```
SUBROUTINE PrintMatR(MaxDim,Dim,Mat,Title)
```

```
INTEGER Dim,MaxDim,Length,I,J,K
```

```
REAL Mat(MaxDim,*)
```

```
CHARACTER*(*) Title
```

```
LOGICAL FirstLine
```

```
CALL StringLength(Title,Length)
```

```
IF (Length.GT.0) THEN
```

```
WRITE(*,*) ' '
```

```
WRITE(*,*) Title(1:Length)
```

```
WRITE(*,*) ' '
```

```
END IF
```

```
C 12345678 1234567 1234567 1234567 1234567
```

```
C Row Col 1 Col 2 Col 3 Col 4 Col 5
```

```
C 12312345123456789a
```

```
C iii dddddddddd dddddddddd dddddddddd dddddddddd dddddddddd
```

```
C dddddddddd dddddddddd dddddddddd dddddddddd dddddddddd
```

```
10 FORMAT(X,'Row',8X,'Col 1',7X,'Col 2',7X,'Col 3',7X,'Col 4',7X,  
& 'Col 5',/)
```

```
20 FORMAT(X,I3,3X,5(:,2X,G10.4))
```

```
30 FORMAT(X,3X,3X,5(:,2X,G10.4))
```

```
WRITE(*,10)
```

```
DO I=1,Dim
```

```
FirstLine=.FALSE.
```

```
DO J=0,Dim-5,5
```

```
IF (.NOT.FirstLine) THEN
```

```
WRITE(*,20) I,(Mat(I,J+K),K=1,5)
```

```
FirstLine=.TRUE.
```

```
ELSE
```

```
WRITE(*,30) (Mat(I,J+K),K=1,5)
```

```
END IF
```

```
END DO
```

```
IF (J+5.LT.Dim) J=J+5
```

```
IF (.NOT.FirstLine) THEN
```

```
WRITE(*,20) I,(Mat(I,K),K=J+1,Dim)
```

```
ELSE
```

```
WRITE(*,30) (Mat(I,K),K=J+1,Dim)
```

```
END IF
```

```
IF (FirstLine) WRITE(*,*) ' '
```

```
END DO
```

```
RETURN
END
```

C ***** ReadSIMEQ

```
SUBROUTINE ReadSIMEQ(FileName)

CHARACTER*(*) FileNAme
INCLUDE 'SIMEQ.INC'
INTEGER I,J

OPEN(UNIT=1,FILE=FileNAme,STATUS='OLD',FORM='FORMATTED')
READ(1,*) N1,IFlag

DO I=1,N1
  READ(1,*) IPivot(I)
END DO

DO I=1,N1
  DO J=1,N1
    READ(1,*) W1(I,J)
  END DO
END DO

CLOSE(1)

RETURN
END
```

C ***** Slnpd

```
SUBROUTINE Slnpd(A,B,Determinant,N,Nx)
```

C Solution of linear systems of equations by the gauss elimination method
 C providing for interchanging rows when encountering a
 C zero diagonal coefficient

C A System Matrix ($Ax=B$)
 C B Originally contains the independent coefficients. After solution
 C it contains the values of the system unknowns.(x)
 C N Actual number of unknowns
 C Nx Row and Column dimension of A
 C Determinant The determinant of the matrix A
 C Tolerance Values below this are interpreted as zero.

```
INTEGER Nx,N
REAL*8 A(Nx,Nx),B(Nx),Determinant,Tolerance/0.000001/
```

```
INTEGER K,JLoc,J,L,I
REAL*8 C
```

```
Determinant=0.0
```

```
DO K=1,N-1
  IF (ABS(A(K,K)).LT.Tolerance) THEN
```

C Try to interchange rows to get non-zero diagonal coefficients

```

      JLoc=0
      DO J=K+1,N
        IF ((ABS(A(J,K)).GT.Tolerance).AND.(JLoc.NE.0)) THEN
          JLoc=J
        END IF
      END DO

      IF (JLoc.EQ.0) THEN

        WRITE(6,2) K
        FORMAT(X,'**** Singularity in row ',I5)
        RETURN

      END IF

      DO L=K,N
        CALL DPXchg(A(K,L),A(J,L))
      END DO
      CALL DPXchg(B(K),B(J))

```

```

      END IF

```

C Divide row by the diagonal coefficient

```

      DO J=K+1,N
        A(K,J)=A(K,J)/A(K,K)
      END DO
      B(K)=B(K)/A(K,K)

```

C Eliminate unknown X(K) from row i

```

      DO I=K+1,N
        C=A(I,K)
        DO J=K+1,N
          A(I,J)=A(I,J)-C*A(K,J)
        END DO
        B(I)=B(I)-C*B(K)
      END DO
    END DO

```

C Compute Last Unknown

```

      IF (ABS(A(N,N)).LT.Tolerance) THEN
        WRITE(6,2) N
        RETURN
      END IF

      B(N)=B(N)/A(N,N)

```

C Apply backsubstitution process to compute remaining unknowns

```

      DO L=1,N-1
        K=N-L
        DO J=K+1,N
          B(K)=B(K)-A(K,J)*B(J)
        END DO
      END DO

```

C Compute Determinant

```

Determinant=1.0
DO I=1,N
  Determinant=Determinant*A(I,I)
END DO

RETURN
END

```

C ***** SolveRelEq

```

SUBROUTINE SolveRelEq(B,X)

REAL*8 B(*),X(*)

INCLUDE 'SIMEQ.INC'

IF (IFlag.NE.0) THEN
  CALL Subst(W1,IPivot,B,N1,X,MaxNoOfEqus)
ELSE
  WRITE(*,200)
200  FORMAT(X,'Warning: the system of linear equations is',
& ' not solvable.')
  STOP 'In Routine: SolveRelEq'
END IF

RETURN
END

```

C ***** SolveSimEq

```

SUBROUTINE SolveSimEq(W,B,N,X,MaxDim)

C Variables

C W   The (N,N) matrix of coefficients.
C B   The (N) vector, WX=B
C X   The Solution (N)
C MaxDim The maximum dimension of the matrices.

INCLUDE 'SIMEQ.INC'

INTEGER N,MaxDim,I,J
REAL*8 W(MaxDim,MaxDim),D(MaxNoOfEqus),B(*),X(*)

IF (N.GT.MaxNoOfEqus) THEN
  WRITE(*,100) N,MaxNoOfEqus
100  FORMAT(X,'Warning: There are ',I4,'simultaneous equations',
& ',X,'This routine SolveSimEq can only solve up to ',I4,',')
  STOP 'In Routine: SolveSimEq'
END IF

```

C Copy the Maxtrix to a dummy matrix so that original matrix is not destroyed
C by call to Factor. Also, this allows a routine SolveRelEq to be used
C to solve for related problems $W.x=b$ #b

```

N1=N

```



```

      DO I=1,N
        DO J=1,N
          W1(I,J)=W(I,J)
        END DO
      END DO

      CALL Factor(W1,N1,D,IPivot,IFlag,MaxNoOfEqus)

      IF (IFlag.NE.0) THEN
        CALL Subst(W1,IPivot,B,N1,X,MaxNoOfEqus)
      ELSE
        WRITE(*,200)
200    FORMAT(X,'Warning: the system of linear equations is',
& ' not solvable.')
        STOP 'In Routine: SolveSimEq'
      END IF

      RETURN
      END

C ***** SolveTriDiag

      SUBROUTINE SolveTriDiag(Sub,Diag,Sup,B,N,X)

C This subroutine solves a tridiagonal linear system of equations:
C   Sub(I)*X(I-1) + Diag(I)*X(I) + Sup(I)*X(I+1) = B(I), I=1,...,N
C (With Sub(1) and Sup(N) taken to be zero) by factorization and
C substitution.

C (Taken from Conte and de Boor, ELEMENTARY NUMERICAL ANALYSIS, 3d. ed.
C McGraw Hill, p.155)

C Input Variables

C Sub(N)      The subdiagonal of the Matrix.
C Diag(N)     The diagonal of the Matrix
C Sup(N)      The superdiagonal of the matrix.
C B(N)        The load vector.
C N           The number of equations

C Output Variables

C X(N)        The solution

C Internal Variables

C I           Loop counter
C Beta(100)   The load vector after the elimination
C Gamma(100)  The diagonal after the elimination

      REAL*8 Sub(*),Diag(*),Sup(*),B(*),X(*)
      REAL*8 Beta(100),Gamma(100)
      INTEGER N,I

      IF (N.GT.100) THEN
        WRITE(*,100) N
100    FORMAT(X,'Warning: too many simultaneous equations.',
& /,X,'N=',I3,' and N must be <=100')

```

```

      STOP 'In Routine: SolveTriDiag'
    END IF

    IF (N.LE.1) THEN
      X(1)=B(1)/Diag(1)
      RETURN
    END IF

    Gamma(1)=Diag(1)
    Beta(1)=B(1)

    DO I=2,N
      Gamma(I)=Diag(I)-Sub(I)*Sup(I-1)/Gamma(I-1)
      Beta(I)=B(I)-Sub(I)*Beta(I-1)/Gamma(I-1)
    END DO

    X(N)=Beta(N)/Gamma(N)
    DO I=N-1,1,-1
      X(I)=(Beta(I)-Sup(I)*X(I+1))/Gamma(I)
    END DO

    RETURN
  END

```

C ***** Sparse

SUBROUTINE Sparse(B,N,X,Rsq)

C This subroutine solves the linear system $A.X=b$ for the vector X of length
 C N , given the right-hand vector B , and given two subroutines, $ASub(Xin,Xout)$
 C and $ATSub(XIn,XOut)$, which respectively calculate Ax and ATx for x given
 C as their first arguments, returning the result in their second arguments.
 C These subroutines should take every advantage of the sparseness of
 C the matrix A . On input, X should be set to a first guess of the desired
 C solution (all zero components is fine). On output, X is the solution
 C vector, and Rsq is the sum of the squares of the components of the residual
 C vector $A.X-b$. If this is not small, then the matrix is numerically singular
 C and the solution represents a least-squares best approximation.

C $NMax$ The maximum expected N
 C Eps RMS Accuracy desired
 C $Eps2$ Criterion for sum-squared residuals
 C $IRst$ The number of restarts attempted internally.

```

  PARAMETER NMax=700
  PARAMETER Eps=1.0E-6

```

```

  INTEGER N,IRst,J,Iter
  REAL*8 B(*),X(*),G(NMax),H(NMax),Xi(NMax),XJ(NMax)
  REAL*8 Eps2,Rp,Bsq,ANum,ADen,Rsq,GG,DGG,Gam

```

```

  Eps2=N*Eps*Eps

```

```

  Irst=0
1  IRst=IRst+1

```

```

  CALL ASub(X,XI)

```

```

Rp=0
Bsq=0
DO J=1,N
  Bsq=Bsq+B(J)**2
  Xi(J)=XI(J)-B(J)
  RP=RP+XI(J)**2
END DO

CALL ATSub(Xi,G)

DO J=1,N
  G(J)=-G(J)
  H(J)=G(J)
END DO

DO Iter=1,10*N

  CALL ASub(H,XI)

  ANum=0.
  ADen=0.

  DO J=1,N
    ANum=ANum+G(J)*H(J)
    ADen=ADen+XI(J)**2
  END DO

  IF (ADen.EQ.0.) THEN -----
    WRITE(*,*) 'Error: Singular Matrix'
    WRITE(*,*) '  Iteration number ',Iter
    WRITE(*,*) '  X Vector:'
    WRITE(*,*) (H(J),J=1,N)
    STOP 'In Routine: SPARSE'
  END IF

  ANum=ANum/ADen
  DO J=1,N
    XI(J)=X(J)
    X(J)=X(J)+ANum*H(J)
  END DO

  CALL ASub(X,Xj)

  Rsq=0.

  DO J=1,N
    XJ(J)=XJ(J)-B(J)
    Rsq=Rsq+XJ(J)**2
  END DO

```

C The following IF statement tests for convergence.

```
IF ((Rsq.EQ.RP).OR.(Rsq.LE.BSQ*Eps2)) RETURN
```

```
IF (Rsq.GT.Rp) THEN
```

C Not improving. Do a restart

```

DO J=1,N
  X(J)=XI(J)
END DO

```

C Return if too many restarts. This is the normal return when we run into
C roundoff error before satisfying the return above.

```

      IF (IRst.GE.3) RETURN

      GOTO 1
    END IF

    Rp=Rsq

    CALL ATSub(Xj,Xi)

    GG=0.
    Dgg=0.

    DO J=1,N
      GG=GG+G(J)**2
      DGG=DGG+(Xi(J)+G(J))*XI(j)
    END DO

```

C A Rare but normal return.

```

      IF (GG.EQ.0) RETURN

      Gam=Dgg/GG
      DO J=1,N
        G(J)=-Xi(j)
        H(J)=G(J)+Gam*H(J)
      END DO

    END DO

    WRITE(*,*) 'Error: too many iterations.'
    WRITE(*,*) '  Number of iterations=',10*N

    STOP 'In Routine: Sparse'

  END

```

C ***** Spline

```

SUBROUTINE Spline(Xi,C,N)

```

C This subroutine from Conte and DeBoor p.290

C Variables-----

C Input Variables

C XI(1),...,XI(N+1) Strictly increasing sequence of breakpoints
C C(1,I),C(2,I) Value and 1st derivative at XI(I), I=1,...,N+1
C of the cubic spline

C Output Variables

C C(1,I),C(2,I),C(3,I),C(4,I) Polynomial Coefficients of the spline
 C on the interval (XI(I),XI(I+1)), I=1,...,N.

```
PARAMETER Np1Max=1000
INTEGER N,M,Offset
REAL*8 C(4,N+1),XI(N+1),D(Np1Max),Diag(Np1Max),G
DATA Diag(1)/1.0/,D(1)/0.0/
```

```
IF (N+1.GT.Np1Max) THEN
  WRITE(*,*) 'Error: N is too large. N=',N
  WRITE(*,*) 'Maximum N Allowed=',Np1Max-1
  STOP 'In Routine: Spline'
END IF
```

```
Offset=0
DO M=2,N+1
  IF (XI(M)-XI(M-1).LE.0) THEN
    Offset=Offset+1
    WRITE(*,*) 'Warning: Sequence of breakpoints is',
    & ' not strictly increasing'
    WRITE(*,*) ' Used: XI(',M,')=',XI(M),C(1,M)
    WRITE(*,*) ' XI(',M-1,')=',XI(M-1),C(1,M-1)
  END IF
  XI(M-Offset)=XI(M)
  C(1,M-Offset)=C(1,M)
  C(2,M-Offset)=C(2,M)
  C(3,M-Offset)=C(3,M)
  C(4,M-Offset)=C(4,M)
END DO
N=N-Offset
```

```
DO M=2,N+1
  D(M)= XI(M)-XI(M-1)
  IF (D(M).LE.0) THEN
    END IF
  Diag(M)=(C(1,M)-C(1,M-1))/D(M)
END DO
```

```
DO M=2,N
  C(2,M)=3.0*(D(M)*Diag(M+1)+D(M+1)*Diag(M))
  Diag(M)=2.0*(D(M)+D(M+1))
END DO
```

```
DO M=2,N
  G=-D(M+1)/Diag(M-1)
  Diag(M)=Diag(M)+G*D(M-1)
  C(2,M)=C(2,M)+G*C(2,M-1)
END DO
```

```
DO M=N,2,-1
  C(2,M)=(C(2,M)-D(M)*C(2,M+1))/Diag(M)
END DO
```

```
RETURN
END
```

SUBROUTINE Subst(W,IPivot,B,N,X,MaxDim)

C This subroutine uses the factorization from FACTOR to solve the system
 C of linear equations $W*X=B$ (where W is the original matrix input to FACTOR.
 C Taken from Conte and DeBoor, p164.

C Input Variables

C W(N,N) The matrix output from FACTOR
 C IPivot(N) The pivoting matrix output from FACTOR
 C N The dimension of the matrix.
 C B(N) The right side of the system to be solved.

C Output Variables

C X(N) The vector satisfying $W*X=B$

```
INTEGER IPivot(*),I,IP,J,MaxDim,N
REAL*8 B(*),W(MaxDim,MaxDim),X(*),Sum
```

```
IF (N.LE.1) THEN
  X(1)=B(1)/W(1,1)
  RETURN
END IF
```

```
Ip=IPivot(1)
X(1)=B(IP)
DO I=2,N
  Sum=0.0
  DO J=1,I-1
    Sum=W(I,J)*X(J)+Sum
  END DO
  IP=IPivot(I)
  X(I)=B(IP)-Sum
END DO
```

```
X(N)=X(N)/W(N,N)
DO I=N-1,1,-1
  Sum=0.0
  DO J=I+1,N
    Sum=W(I,J)*X(J)+Sum
  END DO
  X(I)=(X(I)-Sum)/W(I,I)
END DO
```

```
RETURN
END
```

C ***** VecNormDP

```
REAL*8 FUNCTION VecNormDP(NoOfElem,Vec)
```

C This subroutine Computes the norm of Vec

```
INTEGER I,NoOfElem
REAL*8 Vec(*),Norm
```

```
Norm=0.0
```

```

DO I=1,NoOfElem
  Norm=Norm+Vec(I)*Vec(I)
END DO

```

```

VecNormDP=SQRT(Norm)

```

```

RETURN
END

```

C ***** VecScaMultDP

```

SUBROUTINE VecScaMultDP(Dim,Vec,Sca,Res)

```

```

INTEGER Dim,I,J
REAL*8 Vec(*),Res(*),Sca

```

```

DO I=1,Dim
  Res(I)=Vec(I)*Sca
END DO

```

```

RETURN
END

```

C ***** VecSumDP

```

REAL*8 FUNCTION VecSumDP(NoOfElems,Vector)

```

C This subroutine sums the elements from 1 to NoOfElems in Vector(*). The
C result is stored in Sum

```

REAL*8 Vector(*),Sum
INTEGER NoOfElems,I

```

```

Sum=0.0D0
DO I=1,NoOfElems
  Sum=Sum+Vector(I)
END DO

```

```

VecSumDP=Sum

```

```

RETURN
END

```

C ***** VecZeroDP

```

SUBROUTINE VecZeroDP(NoOfElems,Vector)

```

```

REAL*8 Vector(*)
INTEGER NoOfElems,I

```

```

DO I=1,NoOfElems
  Vector(I)=0.0D0
END DO

```

```

RETURN
END

```

C ***** WriteSIMEQ

```
SUBROUTINE WriteSIMEQ(FileName)

CHARACTER*(*) FileNAme
INCLUDE 'SIMEQ.INC'
INTEGER I,J

OPEN(UNIT=1,FILE=FileNAme,STATUS='UNKNOWN',FORM='FORMATTED')
WRITE(1,*) N1,', ',IFlag

DO I=1,N1
  WRITE(1,*) IPivot(I)
END DO

DO I=1,N1
  DO J=1,N1
    WRITE(1,*) W1(I,J)
  END DO
END DO

CLOSE(1)

RETURN
END
```

c *

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