

# MAE 267 – Project 3

## Serial, Multi-Block, Finite-Volume Methods For Solving 2D Heat Conduction

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### 1 Statement of Problem

This analysis details the solution of the steady-state temperature distribution on a 1m x 1m block of steel with Dirichlet boundary conditions (Eqn 2). Single-processor solutions were previously performed on a square, non-uniform grids rotated in the positive z-direction by  $rot = 30^\circ$ . Two grids of 101x101 points and 501x501 points were used to solve the equation of heat transfer. Temperature was uniformly initialized to a value of 3.5 and the solution was iterated until the maximum residual found was less than  $1.0 \times 10^{-5}$ . The equation for heat conduction (Eqn 1) was solved using an explicit, node-centered, finite-volume scheme, with an alternative distributive scheme for the second-derivative operator. Steady-state temperature distribution was saved in a PLOT3D unformatted file, and CPU wall time of the solver was recorded.

Now, the code has been modified to decompose the domain into sub-domains referred to as blocks. Boundary and neighbor information for each block is stored so that connectivity can be accurately assessed when communication between blocks is required. The block domain, associated meshes, and initial temperature distribution are initialized and then saved to restart files. These are read in at the beginning of the solver.

### 2 Equations and Algorithms

The solver developed for this analysis utilizes a finite-volume numerical solution method to solve the transient heat conduction equation (Eqn 1).

$$\rho c_p \frac{\partial T}{\partial t} = k \left[ \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right] \quad (1)$$

The solution is initialized with the Dirichlet boundary conditions (Eqn 2).

$$T = \begin{cases} 5.0 [\sin(\pi x_p) + 1.0] & \text{for } j = j_{max} \\ |\cos(\pi x_p)| + 1.0 & \text{for } j = 0 \\ 3.0 y_p + 2.0 & \text{for } i = 0, i_{max} \end{cases} \quad (2)$$

Grids were generated according to the following (Eqn 3)

$$\begin{aligned} rot &= 30.0 \frac{\pi}{180.0} \\ x_p &= \cos \left[ 0.5\pi \frac{i_{max} - i}{i_{max} - 1} \right] \\ y_p &= \cos \left[ 0.5\pi \frac{j_{max} - j}{j_{max} - 1} \right] \\ x(i, j) &= x_p \cos(rot) + (1.0 - y_p) \sin(rot) \\ y(i, j) &= y_p \cos(rot) + x_p \sin(rot) \end{aligned} \quad (3)$$

To solve Eqn 1 numerically, the equation is discretized according to a node-centered finite-volume scheme, where first-derivatives at the nodes are found using Green's theorem integrating around the secondary control volumes. Trapezoidal, counter-clockwise integration for the first-derivative in the x-direction is achieved with Eqn 4.

$$\begin{aligned} \frac{\partial T}{\partial x} &= \frac{1}{2Vol_{i+\frac{1}{2}, j+\frac{1}{2}}} [(T_{i+1, j} + T_{i+1, j+1}) Ayi_{i+1, j} \\ &\quad - (T_{i, j} + T_{i, j+1}) Ayi_{i, j} \\ &\quad - (T_{i, j+1} + T_{i+1, j+1}) Ayi_{i, j+1} \\ &\quad - (T_{i, j} + T_{i+1, j}) Ayi_{i+1, j}] \end{aligned} \quad (4)$$

A similar scheme is used to find the first-derivative in the y-direction.

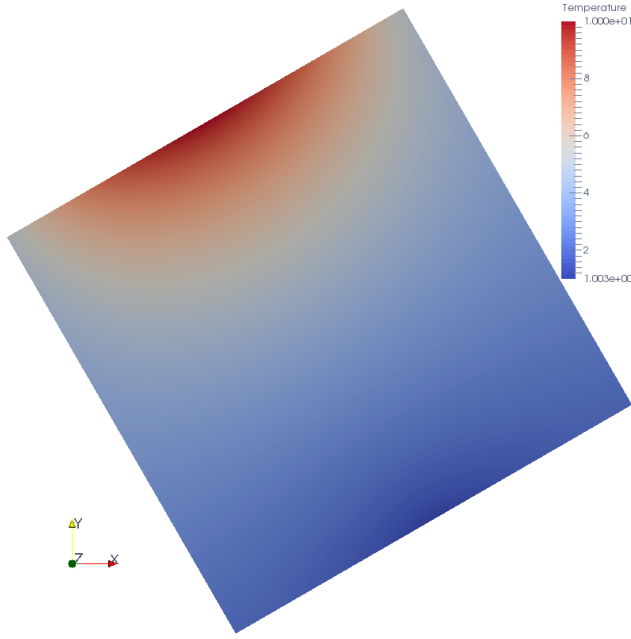


Fig. 1: Steady-state temperature solution for 501x501 grid decomposed into 10x10 blocks

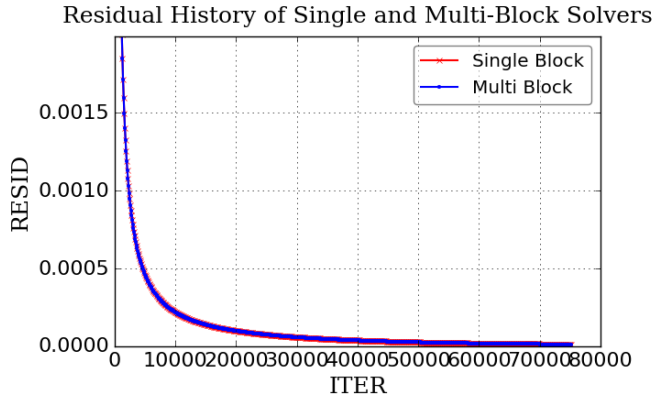


Fig. 2: Residual history for solving a 501x501 grid with a single block solver and a 10x10 multi-block solver

### 3 Results and Discussion

All simulations in this analysis were run on a 501x501 point grid, once with a single block solver and once with at 10x10 multi-block solver. Fig 1 portrays the multi-block solution, which is comparable to that of the single block solver. Convergence histories of the two solvers are compared in Fig 2. It can be seen that the two solvers are comparable in performance, both following a similar convergence path and converging at almost the same iteration.

Actual solver times are compared in Appendix A. The multi-block solver was found to be approximately 11 seconds (2.6%) faster than the single block solver. This may be due to more code streamlining in the later project. It can be expected that the speed of the multi-block solver will improve even further when linked-lists are employed to navigate neighbor boundary actions (this capability is currently

functional in the code, but does not work on HPC1, so a logic-based approach was used for this project.)

### 4 Conclusion

Decomposing the domain introduced unforeseen complications in adapting the single block solver. In some cases, it was as simple as adding a third loop for the block number, but in others (especially in updating the ghost nodes) considerable thought and error-checking was required. This implies that adapting the code for parallel processing will be an equally complicated step, so it is beneficial that we are adapting our codes modularly in stages.

## Appendix A: Solver Performance Comparison

```
1 Running a      501 by      501 grid took:
2      75128 iterations
3      428.74140000343323      seconds (Total CPU walltime)
4      428.61560106277466      seconds (Solver CPU walltime)
5
6 Found max residual of      9.9999670980684130E-006
7 At ij of      191      242
```

Listing 1: Single block solver performance

```
1 Running a      501 by      501 grid,
2 With NxM:      10 x      10 blocks took:
3      75128 iterations
4      417.04543089866638      seconds (Total CPU walltime)
5      415.74189305305481      seconds (Solver CPU walltime)
6
7 Found max residual of      9.9999670985857943E-006
8 on block id      44
9 At ij of      41      42
```

Listing 2: Multi block solver performance

## Appendix B: Multi-Block Grid Decomposition Code

```
1 ! MAE 267
2 ! PROJECT 3
3 ! LOGAN HALSTROM
4 ! 03 NOVEMBER 2015
5
6 ! DESCRIPTION: Modules used for solving heat conduction of steel plate.
7 ! Initialize and store constants used in all subroutines.
8
9 ! CONTENTS:
10 ! CONSTANTS --> Initializes constants for simulation. Sets grid size.
11 ! CLOCK --> Calculates clock wall-time of a process.
12 ! MAKEGRID --> Initialize grid with correct number of points and rotation,
13 !               set boundary conditions, etc.
14 ! CELLS --> Initialize finite volume cells and do associated calculations
15 ! TEMPERATURE --> Calculate and store new temperature distribution
16 !               for given iteration
17
18 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
19 !!!!! CONSTANTS MODULE !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
20 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
21
22 MODULE CONSTANTS
23   ! Initialize constants for simulation. Set grid size.
24   IMPLICIT NONE
25   ! CFL number, for convergence (D0 is double-precision, scientific notation)
26   REAL(KIND=8), PARAMETER :: CFL = 0.95D0
27   ! Material constants (steel): thermal conductivity [W/(m*K)],
28   !                               density [kg/m^3],
29   !                               specific heat ratio [J/(kg*K)]
30   !                               initial temperature
31   REAL(KIND=8), PARAMETER :: k = 18.8D0, rho = 8000.D0, cp = 500.D0, T0 = 3.5D0
32   ! Thermal diffusivity [m^2/s]
33   REAL(KIND=8), PARAMETER :: alpha = k / (cp * rho)
34   ! Pi, grid rotation angle (30 deg)
35   REAL(KIND=8), PARAMETER :: pi = 3.141592654D0, rot = 30.D0*pi/180.D0
36   ! ITERATION PARAMETERS
37   ! Minimum Residual
38   REAL(KIND=8) :: min_res = 0.00001D0
39   ! Maximum number of iterations
40   INTEGER :: max_iter = 1000000
41   ! CPU Wall Times
```

```

42 REAL(KIND=8) :: wall_time_total, wall_time_solve, wall_time_iter(1:5)
43 ! read square grid size, Total grid size, size of grid on each block (local)
44 INTEGER :: nx, IMAX, JMAX, IMAXBK, JMAXBK
45 ! Dimensions of block layout, Number of Blocks,
46 INTEGER :: M, N, NBLK
47 ! Block boundary condition identifiers
48 ! If block face is on North,east,south,west of main grid, identify
49 !   INTEGER :: NBND = 1, SBND = 2, EBND = 3, WBND = 4
50 INTEGER :: NBND = -1, EBND = -2, SBND = -3, WBND = -4
51 ! Output directory
52 CHARACTER(LEN=18) :: casedir
53 ! Debug mode = 1
54 INTEGER :: DEBUG
55 ! Value for constant temperature BCs for debugging
56 REAL(KIND=8), PARAMETER :: TDEBUG = T0 - T0 * 0.5
57
58 CONTAINS
59
60 SUBROUTINE read_input()
61   INTEGER :: I
62   CHARACTER(LEN=3) :: strNX
63   CHARACTER(LEN=1) :: strN, strM
64
65   ! READ INPUTS FROM FILE
66   ! (So I don't have to recompile each time I change an input setting)
67   !   WRITE(*,*) ''
68   !   WRITE(*,*) 'Reading input...'
69   OPEN (UNIT = 1, FILE = 'config.in')
70   DO I = 1, 3
71     ! Skip header lines
72     READ(1,*)
73   END DO
74   ! READ GRIDSIZE (4th line)
75   READ(1,*) nx
76   ! READ BLOCKS (6th and 8th line)
77   READ(1,*)
78   READ(1,*) M
79   READ(1,*)
80   READ(1,*) N
81   ! DEBUG MODE (10th line)
82   READ(1,*)
83   READ(1,*) DEBUG
84
85   ! SET GRID SIZE
86   IMAX = nx
87   JMAX = nx
88   ! CALC NUMBER OF BLOCKS
89   NBLK = M * N
90   ! SET SIZE OF EACH BLOCK (LOCAL MAXIMUM I, J)
91   IMAXBK = 1 + (IMAX - 1) / N
92   JMAXBK = 1 + (JMAX - 1) / M
93
94   ! OUTPUT DIRECTORIES
95   ! write integers to strings
96   WRITE( strNX, '(I3)') nx
97   ! IF ( N - 10 < 0 ) THEN
98   !   ! N is a single digit (I1)
99   !   WRITE( strN, '(I1)') N
100  ! ELSE
101  !   ! N is a tens digit
102  !   WRITE( strN, '(I2)') N
103  ! END IF
104  ! IF ( M - 10 < 0 ) THEN
105  !   WRITE( strM, '(I1)') M
106  ! ELSE
107  !   WRITE( strM, '(I2)') M
108  ! END IF
109  ! case output directory: nx_NxM (i.e. 'Results/101_5x4')
110  ! casedir = 'Results/' // strNX // '_' // strN // 'x' // strM // '/'

```

```

111 !           ! MAKE DIRECTORIES (IF THEY DONT ALREADY EXIST)
112 !           CALL EXECUTE_COMMAND_LINE ("mkdir -p " // TRIM(casedir) )
113
114 ! OUTPUT TO SCREEN
115 WRITE(*,*) ''
116 WRITE(*,*) 'Solving Mesh of size ixj:', IMAX, 'x', JMAX
117 WRITE(*,*) 'With MxN blocks:', M, 'x', N
118 WRITE(*,*) 'Number of blocks:', NBLK
119 WRITE(*,*) 'Block size ixj:', IMAXBK, 'x', JMAXBLK
120 IF (DEBUG == 1) THEN
121     WRITE(*,*) 'RUNNING IN DEBUG MODE'
122 END IF
123 WRITE(*,*) ''
124 END SUBROUTINE read_input
125 END MODULE CONSTANTS
126
127 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
128 !!!!! BLOCK GRID MODULE !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
129 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
130
131 MODULE BLOCKMOD
132 ! Initialize grid with correct number of points and rotation,
133 ! set boundary conditions, etc.
134 USE CONSTANTS
135
136 IMPLICIT NONE
137 PUBLIC
138
139 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
140 !!!!! DERIVED DATA TYPES !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
141 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
142
143 ! DERIVED DATA TYPE FOR GRID INFORMATION
144
145 TYPE MESHTYPE
146 ! Grid points, see coordinate rotaion equations in problem statement
147 REAL(KIND=8), ALLOCATABLE, DIMENSION(:, :) :: xp, yp, x, y
148 ! Temperature at each point, temporary variable to hold temperature sum
149 REAL(KIND=8), ALLOCATABLE, DIMENSION(:, :) :: T, Ttmp
150 ! Iteration Parameters: timestep, cell volume, secondary cell volume,
151 ! equation constant term
152 REAL(KIND=8), ALLOCATABLE, DIMENSION(:, :) :: dt, V, V2nd, term
153 ! Areas used in alternative scheme to get fluxes for second-derivative
154 REAL(KIND=8), ALLOCATABLE, DIMENSION(:, :) :: Ayi, Axi, Ayj, Axj
155 ! Second-derivative weighting factors for alternative distribution scheme
156 REAL(KIND=8), ALLOCATABLE, DIMENSION(:, :) :: yPP, yNP, yNN, yPN
157 REAL(KIND=8), ALLOCATABLE, DIMENSION(:, :) :: xNN, xPN, xPP, xNP
158 END TYPE MESHTYPE
159
160 ! DATA TYPE FOR INFORMATION ABOUT NEIGHBORS
161
162 TYPE NBRTYPE
163 ! Information about face neighbors (north, east, south, west)
164 ! And corner neighbors (Northeast, southeast, southwest, northwest)
165 INTEGER :: N, E, S, W, NE, SE, SW, NW
166 END TYPE NBRTYPE
167
168 ! DERIVED DATA TYPE WITH INFORMATION PERTAINING TO SPECIFIC BLOCK
169
170 TYPE BLKTYPE
171 ! DER. DATA TYPE STORES LOCAL MESH INFO
172 TYPE(MESHTYPE) :: mesh
173 ! IDENTIFY FACE AND CORNER NEIGHBOR BLOCKS AND PROCESSORS
174 TYPE(NBRTYPE) :: NB, NP
175 ! BLOCK NUMBER
176 INTEGER :: ID
177 ! GLOBAL INDICIES OF MINIMUM AND MAXIMUM INDICIES OF BLOCK
178 INTEGER :: IMIN, IMAX, JMIN, JMAX
179 ! LOCAL ITERATION BOUNDS TO AVOID UPDATING BC'S + UTILIZE GHOST NODES

```

```

180     INTEGER :: IMINLOC, JMINLOC, IMAXLOC, JMAXLOC, IMINUPD, JMINUPD
181     ! BLOCK ORIENTATION
182     INTEGER :: ORIENT
183 END TYPE BLKTYPE
184
185 ! LINKED LIST: RECURSIVE POINTER THAT POINTS THE NEXT ELEMENT IN THE LIST
186
187 TYPE LNKLIST
188     ! Next element in linked list
189     TYPE(LNKLIST), POINTER :: next
190     ! Identify what linked list belongs to
191     INTEGER :: ID
192 END TYPE LNKLIST
193
194 ! Collection of linked lists for faces and corners
195
196 TYPE NBRLIST
197     TYPE(LNKLIST), POINTER :: N, E, S, W, NE, SE, SW, NW
198 END TYPE NBRLIST
199
200 CONTAINS
201
202 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
203 !!! INITIALIZE GRID AND WRITE TO FILE !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
204 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
205
206 SUBROUTINE init_blocks(b)
207     ! BLOCK DATA TYPE
208     TYPE(BLKTYPE), TARGET :: b(:)
209     ! Neighbor information pointer
210     TYPE(NBRTYPE), POINTER :: NB
211     ! COUNTER VARIABLES
212     ! IM, IN COUNT BLOCK INDICIES
213     ! (IBLK COUNTS BLOCK NUMBERS, INBR IS BLOCK NEIGHBOR INDEX)
214     INTEGER :: I, J, IBLK, INBR
215
216     ! STEP THROUGH BLOCKS, ASSIGN IDENTIFYING INFO
217     !
218     !           |           |
219     !           |   North   |
220     !       NW| (IBLK + N) |NE
221     ! (IBLK + N - 1)| | (IBLK + N + 1)
222     ! -----
223     !           |           |
224     !       West |   Current   |   East
225     ! (IBLK - 1) |   (IBLK)   | (IBLK + 1)
226     !           |           |
227     ! -----
228     !           |           |
229     ! (IBLK - N - 1)|   South   | (IBLK - N + 1)
230     !           | (IBLK - N) |
231     !           |           |
232     !
233
234     ! START AT BLOCK 1 (INCREMENT IN LOOP)
235     IBLK = 0
236
237     DO J = 1, M
238         DO I = 1, N
239             ! INCREMENT BLOCK NUMBER
240             IBLK = IBLK + 1
241
242             ! Neighbor information pointer
243             NB => b(IBLK)%NB
244
245             ! ASSIGN BLOCK NUMBER
246             b(IBLK)%ID = IBLK
247             ! ASSIGN GLOBAL MIN/MAX INDICIES OF LOCAL GRID
248             b(IBLK)%IMIN = 1 + (IMAXBK - 1) * (I - 1)

```

```

249      b(IBLK)%JMIN = 1 + (JMAXBLK - 1) * (J - 1)
250      b(IBLK)%IMAX = b(IBLK)%IMIN + (IMAXBLK - 1)
251      b(IBLK)%JMAX = b(IBLK)%JMIN + (JMAXBLK - 1)
252
253      ! ASSIGN NUMBERS OF FACE AND CORNER NEIGHBOR BLOCKS
254      !if boundary face, assign bc later
255      NB%N = IBLK + N
256      NB%S = IBLK - N
257      NB%E = IBLK + 1
258      NB%W = IBLK - 1
259      NB%NE = IBLK + N + 1
260      NB%NW = IBLK + N - 1
261      NB%SW = IBLK - N - 1
262      NB%SE = IBLK - N + 1
263
264      ! Assign faces and corners on boundary of the actual
265      ! computational grid with number corresponding to which
266      ! boundary they are on.
267      ! Corners on actual corners of the computational grid are
268      ! ambiguously assigned.
269      IF ( b(IBLK)%JMAX == JMAX ) THEN
270          ! NORTH BLOCK FACE AND CORNERS ARE ON MESH NORTH BOUNDARY
271          ! AT ACTUAL CORNERS OF MESH, CORNERS ARE AMBIGUOUS
272          NB%N = NBND
273          NB%NE = NBND
274          NB%NW = NBND
275      END IF
276      IF ( b(IBLK)%IMAX == IMAX ) THEN
277          ! EAST BLOCK FACE IS ON MESH EAST BOUNDARY
278          NB%E = EBND
279          NB%NE = EBND
280          NB%SE = EBND
281
282      END IF
283      IF ( b(IBLK)%JMIN == 1 ) THEN
284          ! SOUTH BLOCK FACE IS ON MESH SOUTH BOUNDARY
285          NB%S = SBND
286          NB%SE = SBND
287          NB%SW = SBND
288      END IF
289      IF ( b(IBLK)%IMIN == 1 ) THEN
290          ! WEST BLOCK FACE IS ON MESH WEST BOUNDARY
291          NB%W = WBND
292          NB%SW = WBND
293          NB%NW = WBND
294      END IF
295
296      ! BLOCK ORIENTATION
297      ! same for all in this project
298      b(IBLK)%ORIENT = 1
299
300      END DO
301  END DO
302  END SUBROUTINE init_blocks
303
304  SUBROUTINE write_blocks(b)
305      ! WRITE BLOCK CONNECTIVITY FILE
306
307      ! BLOCK DATA TYPE
308      TYPE(BLKTYPE) :: b(:)
309      INTEGER :: I, BLKFILE = 99
310
311      11 format(3I5)
312      22 format(33I5)
313
314      ! OPEN (UNIT = BLKFILE , FILE = TRIM(casedir) // "blockconfig.dat", form='formatted')
315      OPEN (UNIT = BLKFILE , FILE = "blockconfig.dat", form='formatted')
316      ! WRITE AMOUNT OF BLOCKS AND DIMENSIONS
317      WRITE(BLKFILE, 11) NBLK, IMAXBLK, JMAXBLK

```

```

318 DO I = 1, NBLK
319     ! FOR EACH BLOCK, WRITE BLOCK NUMBER, STARTING/ENDING GLOBAL INDICES.
320     ! THEN BOUNDARY CONDITION AND NEIGHBOR NUMBER FOR EACH FACE:
321     ! NORTH EAST SOUTH WEST
322     WRITE(BLKFILE, 22) b(I)%ID, &
323         b(I)%IMIN, b(I)%JMIN, &
324         b(I)%NB%N, &
325         b(I)%NB%NE, &
326         b(I)%NB%E, &
327         b(I)%NB%SE, &
328         b(I)%NB%S, &
329         b(I)%NB%SW, &
330         b(I)%NB%W, &
331         b(I)%NB%NW, &
332         b(I)%ORIENT
333 END DO
334 CLOSE(BLKFILE)
335 END SUBROUTINE write_blocks
336
337 SUBROUTINE read_blocks(b)
338     ! READ BLOCK CONNECTIVITY FILE
339
340     ! BLOCK DATA TYPE
341     TYPE(BLKTYPE) :: b(:)
342     INTEGER :: I, BLKFILE = 99
343     ! READ INFOR FOR BLOCK DIMENSIONS
344     INTEGER :: NBLKREAD, IMAXBKREAD, JMAXBKREAD
345
346     11 format(3I5)
347     22 format(33I5)
348
349 !     OPEN (UNIT = BLKFILE , FILE = TRIM(casedir) // "blockconfig.dat", form='formatted')
350 OPEN (UNIT = BLKFILE , FILE = "blockconfig.dat", form='formatted')
351 ! WRITE AMOUNT OF BLOCKS AND DIMENSIONS
352 READ(BLKFILE, 11) NBLK, IMAXBK, JMAXBK
353 DO I = 1, NBLK
354     ! FOR EACH BLOCK, WRITE BLOCK NUMBER, STARTING/ENDING GLOBAL INDICES.
355     ! THEN BOUNDARY CONDITION AND NEIGHBOR NUMBER FOR EACH FACE:
356     ! NORTH EAST SOUTH WEST
357     READ(BLKFILE, 22) b(I)%ID, &
358         b(I)%IMIN, b(I)%JMIN, &
359         b(I)%NB%N, &
360         b(I)%NB%NE, &
361         b(I)%NB%E, &
362         b(I)%NB%SE, &
363         b(I)%NB%S, &
364         b(I)%NB%SW, &
365         b(I)%NB%W, &
366         b(I)%NB%NW, &
367         b(I)%ORIENT
368 END DO
369 CLOSE(BLKFILE)
370 END SUBROUTINE read_blocks
371
372 SUBROUTINE init_mesh(b)
373     ! BLOCK DATA TYPE
374     TYPE(BLKTYPE), TARGET :: b(:)
375     TYPE(MESHTYPE), POINTER :: m
376     INTEGER :: IBLK, I, J
377
378 DO IBLK = 1, NBLK
379
380     m => b(IBLK)%mesh
381
382     ! ALLOCATE MESH INFORMATION
383     ! ADD EXTRA INDEX AT BEGINNING AND END FOR GHOST NODES
384     ALLOCATE( m%xp( 0:IMAXBK+1, 0:JMAXBK+1) )
385     ALLOCATE( m%yp( 0:IMAXBK+1, 0:JMAXBK+1) )
386     ALLOCATE( m%x( 0:IMAXBK+1, 0:JMAXBK+1) )

```



```

387     ALLOCATE( m%y( 0:IMAXBLK+1, 0:JMAXBLK+1) )
388     ALLOCATE( m%T( 0:IMAXBLK+1, 0:JMAXBLK+1) )
389     ALLOCATE( m%Ttmp(0:IMAXBLK+1, 0:JMAXBLK+1) )
390     ALLOCATE( m%dt( 0:IMAXBLK+1, 0:JMAXBLK+1) )
391     ALLOCATE( m%V2nd(0:IMAXBLK+1, 0:JMAXBLK+1) )
392     ALLOCATE( m%term(0:IMAXBLK+1, 0:JMAXBLK+1) )
393     ALLOCATE( m%Ayi( 0:IMAXBLK+1, 0:JMAXBLK+1) )
394     ALLOCATE( m%Axi( 0:IMAXBLK+1, 0:JMAXBLK+1) )
395     ALLOCATE( m%Ayj( 0:IMAXBLK+1, 0:JMAXBLK+1) )
396     ALLOCATE( m%Axj( 0:IMAXBLK+1, 0:JMAXBLK+1) )
397     ALLOCATE( m%V( 0:IMAXBLK, 0:JMAXBLK ) )
398     ALLOCATE( m%yPP( 0:IMAXBLK, 0:JMAXBLK ) )
399     ALLOCATE( m%yNP( 0:IMAXBLK, 0:JMAXBLK ) )
400     ALLOCATE( m%yNN( 0:IMAXBLK, 0:JMAXBLK ) )
401     ALLOCATE( m%ypN( 0:IMAXBLK, 0:JMAXBLK ) )
402     ALLOCATE( m%xNN( 0:IMAXBLK, 0:JMAXBLK ) )
403     ALLOCATE( m%xPN( 0:IMAXBLK, 0:JMAXBLK ) )
404     ALLOCATE( m%xPP( 0:IMAXBLK, 0:JMAXBLK ) )
405     ALLOCATE( m%xNP( 0:IMAXBLK, 0:JMAXBLK ) )
406
407     ! STEP THROUGH LOCAL INDICIES OF EACH BLOCK
408     DO J = 0, JMAXBLK+1
409         DO I = 0, IMAXBLK+1
410             ! MAKE SQUARE GRID
411             ! CONVERT FROM LOCAL TO GLOBAL INDEX:
412             ! Iglobal = Block%IMIN + (Ilocal - 1)
413             m%xp(I, J) = COS( 0.5D0 * PI * DFLOAT(IMAX - ( b(IBLK)%IMIN + I - 1) ) / DFLOAT(IMAX - 1) )
414             m%yp(I, J) = COS( 0.5D0 * PI * DFLOAT(JMAX - ( b(IBLK)%JMIN + J - 1) ) / DFLOAT(JMAX - 1) )
415             ! ROTATE GRID
416             m%x(I, J) = m%xp(I, J) * COS(rot) + (1.D0 - m%yp(I, J) ) * SIN(rot)
417             m%y(I, J) = m%yp(I, J) * COS(rot) + ( m%xp(I, J) ) * SIN(rot)
418         END DO
419     END DO
420 END DO
421 END SUBROUTINE init_mesh
422
423 SUBROUTINE init_temp(blocks)
424     ! Initialize temperature across mesh
425     ! BLOCK DATA TYPE
426     TYPE(BLKTYPE), TARGET :: blocks(:)
427     TYPE(BLKTYPE), POINTER :: b
428     TYPE(MESHTYPE), POINTER :: m
429     TYPE(NBRTYPE), POINTER :: NB
430     INTEGER :: IBLK, I, J
431
432     DO IBLK = 1, NBLK
433         b => blocks(IBLK)
434         m => blocks(IBLK)%mesh
435         NB => blocks(IBLK)%NB
436         ! FIRST, INITIALIZE ALL POINT TO INITIAL TEMPERATURE (T0)
437         m%T(0:IMAXBLK+1, 0:JMAXBLK+1) = T0
438         ! THEN, INITIALIZE BOUNDARIES DIRICHLET B.C.
439         IF (DEBUG /= 1) THEN
440
441             ! DIRICHLET B.C.
442             ! face on north boundary
443             IF (NB%N == NBND) THEN
444                 DO I = 1, IMAXBLK
445                     m%T(I, JMAXBLK) = 5.D0 * (SIN(PI * m%xp(I, JMAXBLK)) + 1.D0)
446                 END DO
447             END IF
448             IF (NB%S == SBND) THEN
449                 DO I = 1, IMAXBLK
450                     m%T(I, 1) = ABS(COS(PI * m%xp(I, 1))) + 1.D0
451                 END DO
452             END IF
453             IF (NB%E == EBND) THEN
454                 DO J = 1, JMAXBLK
455                     m%T(IMAXBLK, J) = 3.D0 * m%yp(IMAXBLK, J) + 2.D0

```

```

456         END DO
457     END IF
458     IF (NB%W == WBND) THEN
459         DO J = 1, JMAXBLK
460             m%T(1, J) = 3.D0 * m%yp(1, J) + 2.D0
461         END DO
462     END IF
463
464     ELSE
465
466         ! DEBUG BCS
467         IF (NB%N < 0) THEN
468             DO I = 1, IMAXBLK
469                 m%T(I, JMAXBLK) = TDEBUG
470             END DO
471         END IF
472         IF (NB%S < 0) THEN
473             DO I = 1, IMAXBLK
474                 m%T(I, 1) = TDEBUG
475             END DO
476         END IF
477         IF (NB%E < 0) THEN
478             DO J = 1, JMAXBLK
479                 m%T(IMAXBLK, J) = TDEBUG
480             END DO
481         END IF
482         IF (NB%W < 0) THEN
483             DO J = 1, JMAXBLK
484                 m%T(1, J) = TDEBUG
485             END DO
486         END IF
487     END IF
488 END DO
489 END SUBROUTINE init_temp
490
491
492
493 ! WRITE GRID HERE!!!!!!!!!!!!!!!!!!!!!!
494
495 ! WRITE TEMPERATURE HERE!!!!!!!!!!!!!!!!!!!!!!
496
497
498 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
499 !!! INITIALIZE SOLUTION AFTER RESTART FILE READ IN !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
500 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
501
502
503 ! READ BLOCKS HERE!!!!!!!!!!!!!!!!!!!!!!
504
505
506
507
508
509 SUBROUTINE set_block_bounds(blocks)
510     ! Calculate iteration bounds for each block to avoid updating BCs.
511     ! Populate block ghost nodes from initial temperature distribution
512     ! call after reading in mesh data from restart file
513     TYPE(BLKTYPE), TARGET :: blocks(:)
514     TYPE(BLKTYPE), POINTER :: b
515     TYPE(NBRTYPE), POINTER :: NB
516     INTEGER :: IBLK, I, J
517
518     DO IBLK = 1, NBLK
519         b => blocks(IBLK)
520         NB => b%NB
521
522         ! Set iteration bounds of each block to preserve BCs
523         ! south and west boundaries:
524         ! interior: iminloc, jminloc = 0 (use ghost)

```

```

525         ! boundary: iminloc, jminloc = 2 (1st index is BC)
526         ! north and east boundaries:
527         ! interior: imaxloc, jmaxloc = maxblk (use ghost)
528         ! boundary: imaxloc, jmaxloc = maxblk-1 (max index is BC)
529
530     ! NORTH
531     IF (NB%N > 0) THEN
532         ! Interior faces have positive ID neighbors
533         b%JMAXLOC = JMAXBLK
534     ELSE
535         ! At North Boundary
536         b%JMAXLOC = JMAXBLK - 1
537     END IF
538
539     ! EAST
540     IF (NB%E > 0) THEN
541         ! Interior
542         b%IMAXLOC = IMAXBLK
543     ELSE
544         ! At east Boundary
545         b%IMAXLOC = IMAXBLK - 1
546     END IF
547
548     ! SOUTH
549     IF (NB%S > 0) THEN
550         ! Interior
551         b%JMINLOC = 0
552     ELSE
553         ! At south Boundary
554         b%JMINLOC = 1
555         ! boundary for updating temperature (dont update BC)
556         b%JMINUPD = 2
557     END IF
558
559     ! WEST
560     IF (NB%W > 0) THEN
561         ! Interior
562         b%IMINLOC = 0
563     ELSE
564         ! At west Boundary
565         b%IMINLOC = 1
566         b%IMINUPD = 2
567     END IF
568 END DO
569
570 SUBROUTINE set_block_bounds
571
572 SUBROUTINE init_linklists(blocks, nbrlists)
573     ! Create linked lists governing block boundary communication
574     ! BLOCK DATA TYPE
575     TYPE(BLKTYPE), TARGET :: blocks(:)
576     ! Neighbor information pointer
577     TYPE(NBRTYPE), POINTER :: NB
578     ! Linked lists of neighbor communication instructions
579     TYPE(NBRLIST) :: nbrlists
580     TYPE(NBRLIST) :: nbrl
581     INTEGER :: IBLK
582
583     DO IBLK = 1, NBLK
584         NB => blocks(IBLK)%NB
585
586         ! NORTH
587         ! If block north face is internal, add it to appropriate linked list
588         ! for north internal faces.
589         IF (NB%N > 0) THEN
590
591             IF ( .NOT. ASSOCIATED(nbrlists%N) ) THEN
592                 ! Allocate linked list if it hasnt been accessed yet
593                 ALLOCATE(nbrlists%N)
594                 ! Pointer linked list that will help iterate through the

```

```

594         ! primary list in this loop
595         nbrl%N => nbrlists%N
596     ELSE
597         ! linked list already allocated (started).  Allocate next
598         ! link as assign current block to it
599         ALLOCATE(nbrl%N%next)
600         nbrl%N => nbrl%N%next
601     END IF
602
603     ! associate this linked list entry with the current block
604     nbrl%N%ID = IBLK
605     ! break link to pre-existing pointer target.  We will
606     ! allocated this target later as the next item in the linked list
607     NULLIFY(nbrl%N%next)
608 END IF
609
610 ! SOUTH
611 IF (NB%S > 0) THEN
612     IF ( .NOT. ASSOCIATED(nbrlists%S) ) THEN
613         ALLOCATE(nbrlists%S)
614         nbrl%S => nbrlists%S
615     ELSE
616         ALLOCATE(nbrl%S%next)
617         nbrl%S => nbrl%S%next
618     END IF
619     nbrl%S%ID = IBLK
620     NULLIFY(nbrl%S%next)
621 END IF
622
623 ! EAST
624 IF (NB%E > 0) THEN
625     IF ( .NOT. ASSOCIATED(nbrlists%E) ) THEN
626         ALLOCATE(nbrlists%E)
627         nbrl%E => nbrlists%E
628     ELSE
629         ALLOCATE(nbrl%E%next)
630         nbrl%E => nbrl%E%next
631     END IF
632     nbrl%E%ID = IBLK
633     NULLIFY(nbrl%E%next)
634 END IF
635
636 ! WEST
637 IF (NB%W > 0) THEN
638     IF ( .NOT. ASSOCIATED(nbrlists%W) ) THEN
639         ALLOCATE(nbrlists%W)
640         nbrl%W => nbrlists%W
641     ELSE
642         ALLOCATE(nbrl%W%next)
643         nbrl%W => nbrl%W%next
644     END IF
645     nbrl%W%ID = IBLK
646     NULLIFY(nbrl%W%next)
647 END IF
648
649 ! NORTH EAST
650 IF (NB%NE > 0) THEN
651     IF ( .NOT. ASSOCIATED(nbrlists%NE) ) THEN
652         ALLOCATE(nbrlists%NE)
653         nbrl%NE => nbrlists%NE
654     ELSE
655         ALLOCATE(nbrl%NE%next)
656         nbrl%NE => nbrl%NE%next
657     END IF
658     nbrl%NE%ID = IBLK
659     NULLIFY(nbrl%NE%next)
660 END IF
661
662 ! SOUTH EAST

```

```

663     IF (NB%SE > 0) THEN
664         IF ( .NOT. ASSOCIATED(nbrlists%SE) ) THEN
665             ALLOCATE(nbrlists%SE)
666             nbrl%SE => nbrlists%SE
667         ELSE
668             ALLOCATE(nbrl%SE%next)
669             nbrl%SE => nbrl%SE%next
670         END IF
671         nbrl%SE%ID = IBLK
672         NULLIFY(nbrl%SE%next)
673     END IF
674
675     ! SOUTH WEST
676     IF (NB%SW > 0) THEN
677         IF ( .NOT. ASSOCIATED(nbrlists%SW) ) THEN
678             ALLOCATE(nbrlists%SW)
679             nbrl%SW => nbrlists%SW
680         ELSE
681             ALLOCATE(nbrl%SW%next)
682             nbrl%SW => nbrl%SW%next
683         END IF
684         nbrl%SW%ID = IBLK
685         NULLIFY(nbrl%SW%next)
686     END IF
687
688     ! NORTH WEST
689     IF (NB%NW > 0) THEN
690         IF ( .NOT. ASSOCIATED(nbrlists%NW) ) THEN
691             ALLOCATE(nbrlists%NW)
692             nbrl%NW => nbrlists%NW
693         ELSE
694             ALLOCATE(nbrl%NW%next)
695             nbrl%NW => nbrl%NW%next
696         END IF
697         nbrl%NW%ID = IBLK
698         NULLIFY(nbrl%NW%next)
699     END IF
700 END DO
701
702 SUBROUTINE init_linklists
703
704     ! Update ghost nodes of each block based on neighbor linked lists
705
706     ! BLOCK DATA TYPE
707     TYPE(BLKTYPE), TARGET :: b(:)
708     ! temperature information pointers for ghost and neighbor nodes
709     REAL(KIND=8), POINTER, DIMENSION(:, :) :: Tgh, Tnb
710     ! Linked lists of neighbor communication instructions
711     TYPE(NBRLIST) :: nbrlists
712     TYPE(NBRLIST) :: nbrl
713     ! iteration parameters, index of neighbor
714     INTEGER :: I, J, INBR
715
716     !!! FACES !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
717
718     ! NORTH FACE GHOST NODES
719     nbrl%N => nbrlists%N
720     ! Step through linked list of north faces with ghosts until end of list
721     DO
722         ! If next link in list doesnt exist (end of list), stop loop
723         IF ( .NOT. ASSOCIATED(nbrl%N) ) EXIT
724
725         ! Otherwise, assign neighbor values to all ghost nodes:
726
727         ! TEMPERATURE OF CURRENT BLOCK (CONTAINS GHOST NODES)
728         ! (identified by linked list id)
729         Tgh => b( nbrl%N%ID )%mesh%T
730
731         ! index of north neighbor

```

```

732     INBR = b( nbrl%N%ID )%NB%N
733     ! TEMPERATURE OF NEIGHBOR BLOCK (UPDATE GHOSTS WITH THIS)
734     Tnb => b( INBR )%mesh%T
735
736     DO I = 1, IMAXBLK
737         ! NORTH FACE GHOST NODE TEMPERATURE IS EQUAL TO TEMPERATURE OF
738         ! SECOND-FROM-SOUTH FACE OF NORTH NEIGHBOR
739         ! (Remember face nodes are shared between blocks)
740         Tgh(I, JMAXBLK+1) = Tnb(I, 2)
741     END DO
742     ! switch pointer to next link in list
743     nbrl%N => nbrl%N%next
744 END DO
745
746 ! SOUTH FACE GHOST NODES
747 nbrl%S => nbrlists%S
748 DO
749     IF ( .NOT. ASSOCIATED(nbrl%S) ) EXIT
750     Tgh => b( nbrl%S%ID )%mesh%T
751     INBR = b( nbrl%S%ID )%NB%S
752     Tnb => b( INBR )%mesh%T
753
754     DO I = 1, IMAXBLK
755         ! ADD NORTH FACE OF SOUTH NEIGHBOR TO CURRENT SOUTH FACE GHOSTS
756         Tgh(I, 0) = Tnb(I, JMAXBLK-1)
757     END DO
758     nbrl%S => nbrl%S%next
759 END DO
760
761 ! EAST FACE GHOST NODES
762 nbrl%E => nbrlists%E
763 DO
764     IF ( .NOT. ASSOCIATED(nbrl%E) ) EXIT
765     Tgh => b( nbrl%E%ID )%mesh%T
766     INBR = b( nbrl%E%ID )%NB%E
767     Tnb => b( INBR )%mesh%T
768
769     DO J = 1, JMAXBLK
770         ! ADD WEST FACE OF EAST NEIGHBOR TO CURRENT WEST FACE GHOSTS
771         Tgh(IMAXBLK+1, J) = Tnb(2, J)
772     END DO
773     nbrl%E => nbrl%E%next
774 END DO
775
776 ! WEST FACE GHOST NODES
777 nbrl%W => nbrlists%W
778 DO
779     IF ( .NOT. ASSOCIATED(nbrl%W) ) EXIT
780     Tgh => b( nbrl%W%ID )%mesh%T
781     INBR = b( nbrl%W%ID )%NB%W
782     Tnb => b( INBR )%mesh%T
783
784     DO J = 1, JMAXBLK
785         ! ADD EAST FACE OF WEST NEIGHBOR TO CURRENT EAST FACE GHOSTS
786         Tgh(0, J) = Tnb(IMAXBLK-1, J)
787     END DO
788     nbrl%W => nbrl%W%next
789 END DO
790
791 !!! CORNERS !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
792
793 ! NORTH EAST CORNER GHOST NODES
794 nbrl%NE => nbrlists%NE
795 DO
796     IF ( .NOT. ASSOCIATED(nbrl%NE) ) EXIT
797     Tgh => b( nbrl%NE%ID )%mesh%T
798     INBR = b( nbrl%NE%ID )%NB%NE
799     Tnb => b( INBR )%mesh%T
800     ! ADD SW CORNER OF NE NEIGHBOR TO CURRENT NE CORNER GHOSTS

```

```

801      Tgh(IMAXBK+1, JMAXBK+1) = Tnb(2, 2)
802      nbrl%NE => nbrl%NE%next
803  END DO
804
805  ! SOUTH EAST CORNER GHOST NODES
806  nbrl%SE => nbrlists%SE
807  DO
808      IF ( .NOT. ASSOCIATED(nbrl%SE) ) EXIT
809      Tgh => b( nbrl%SE%ID )%mesh%T
810      INBR = b( nbrl%SE%ID )%NB%SE
811      Tnb => b( INBR )%mesh%T
812      ! ADD NW CORNER OF SE NEIGHBOR TO CURRENT SE CORNER GHOSTS
813      Tgh(IMAXBK+1, 0) = Tnb(2, JMAXBK-1)
814      nbrl%SE => nbrl%SE%next
815  END DO
816
817  ! SOUTH WEST CORNER GHOST NODES
818  nbrl%SW => nbrlists%SW
819  DO
820      IF ( .NOT. ASSOCIATED(nbrl%SW) ) EXIT
821      Tgh => b( nbrl%SW%ID )%mesh%T
822      INBR = b( nbrl%SW%ID )%NB%SW
823      Tnb => b( INBR )%mesh%T
824      ! ADD NE CORNER OF SW NEIGHBOR TO CURRENT SW CORNER GHOSTS
825      Tgh(0, 0) = Tnb(IMAXBK-1, JMAXBK-1)
826      nbrl%SW => nbrl%SW%next
827  END DO
828
829  ! NORTH WEST CORNER GHOST NODES
830  nbrl%NW => nbrlists%NW
831  DO
832      IF ( .NOT. ASSOCIATED(nbrl%NW) ) EXIT
833      Tgh => b( nbrl%NW%ID )%mesh%T
834      INBR = b( nbrl%NW%ID )%NB%NW
835      Tnb => b( INBR )%mesh%T
836      ! ADD SE CORNER OF NW NEIGHBOR TO CURRENT NW CORNER GHOSTS
837      Tgh(0, JMAXBK+1) = Tnb(IMAXBK-1, 2)
838      nbrl%NW => nbrl%NW%next
839  END DO
840  END SUBROUTINE update_ghosts
841
842  SUBROUTINE update_ghosts_debug(b)
843      ! Update ghost nodes of each block using logical statements.
844      ! used to debug linked lists
845
846      ! BLOCK DATA TYPE
847      TYPE(BLKTYPE), TARGET :: b(:)
848      TYPE(NBRTYPE), POINTER :: NB
849      ! temperature information pointers for ghost and neighbor nodes
850      REAL(KIND=8), POINTER, DIMENSION(:, :) :: Tgh, Tnb
851      ! iteration parameters, index of neighbor
852      INTEGER :: I, J, INBR, IBLK
853
854
855      DO IBLK = 1, NBLK
856          NB => b(iblk)%NB
857
858
859          !!! FACES !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
860
861          IF ( NB%N > 0 ) THEN
862              ! TEMPERATURE OF CURRENT BLOCK (CONTAINS GHOST NODES)
863              Tgh => b( IBLK )%mesh%T
864              ! index of north neighbor
865              INBR = NB%N
866              ! TEMPERATURE OF NEIGHBOR BLOCK (UPDATE GHOSTS WITH THIS)
867              Tnb => b( INBR )%mesh%T
868
869              DO I = 1, IMAXBK

```

```

870 !
871     Tgh(I, JMAXBLK+1) = Tnb(I, 2)
872     b(iblk)%mesh%T(I, JMAXBLK+1) = b(NB%N)%mesh%T(I, 2)
873 END DO
874 END IF
875
876 !south
877 IF ( NB%S > 0 ) THEN
878     Tgh => b( IBLK )%mesh%T
879     INBR = NB%S
880     Tnb => b( INBR )%mesh%T
881
882     DO I = 1, IMAXBLK
883         ! ADD NORTH FACE OF SOUTH NEIGHBOR TO CURRENT SOUTH FACE GHOSTS
884         Tgh(I, 0) = Tnb(I, JMAXBLK-1)
885     END DO
886 END IF
887
888 !EAST
889 IF ( NB%E > 0 ) THEN
890     Tgh => b( IBLK )%mesh%T
891     INBR = NB%E
892     Tnb => b( INBR )%mesh%T
893     DO J = 1, JMAXBLK
894         ! ADD WEST FACE OF EAST NEIGHBOR TO CURRENT WEST FACE GHOSTS
895         Tgh(IMAXBLK+1, J) = Tnb(2, J)
896     END DO
897 END IF
898
899 ! WEST FACE GHOST NODES
900 IF ( NB%W > 0 ) THEN
901     Tgh => b( IBLK )%mesh%T
902     INBR = b( IBLK )%NB%W
903     Tnb => b( INBR )%mesh%T
904     DO J = 1, JMAXBLK
905         ! ADD EAST FACE OF WEST NEIGHBOR TO CURRENT EAST FACE GHOSTS
906         Tgh(0, J) = Tnb(IMAXBLK-1, J)
907     END DO
908 END IF
909
910 !!! CORNERS !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
911
912 ! NORTH EAST CORNER GHOST NODES
913 IF ( NB%NE > 0 ) THEN
914     Tgh => b( IBLK )%mesh%T
915     INBR = b( IBLK )%NB%NE
916     Tnb => b( INBR )%mesh%T
917     ! ADD SW CORNER OF NE NEIGHBOR TO CURRENT NE CORNER GHOSTS
918     Tgh(IMAXBLK+1, JMAXBLK+1) = Tnb(2, 2)
919 END IF
920
921 ! SOUTH EAST CORNER GHOST NODE
922 IF ( NB%SE > 0 ) THEN
923     Tgh => b( IBLK )%mesh%T
924     INBR = b( IBLK )%NB%SE
925     Tnb => b( INBR )%mesh%T
926     ! ADD NW CORNER OF SE NEIGHBOR TO CURRENT SE CORNER GHOSTS
927     Tgh(IMAXBLK+1, 0) = Tnb(2, JMAXBLK-1)
928 END IF
929
930 ! SOUTH WEST CORNER GHOST NODES
931 IF ( NB%SW > 0 ) THEN
932     Tgh => b( IBLK )%mesh%T
933     INBR = b( IBLK )%NB%SW
934     Tnb => b( INBR )%mesh%T
935     ! ADD NE CORNER OF SW NEIGHBOR TO CURRENT SW CORNER GHOSTS
936     Tgh(0, 0) = Tnb(IMAXBLK-1, JMAXBLK-1)
937 END IF
938
939 ! NORTH WEST CORNER GHOST NODES

```



```

939     IF ( NB%NW > 0 ) THEN
940         Tgh => b( IBLK )%mesh%T
941         INBR = b( IBLK )%NB%NW
942         Tnb => b( INBR )%mesh%T
943         ! ADD SE CORNER OF NW NEIGHBOR TO CURRENT NW CORNER GHOSTS
944         Tgh(0, JMAXBLK+1) = Tnb(IMAXBLK-1, 2)
945     END IF
946 END DO
947 END SUBROUTINE update_ghosts_debug
948
949 SUBROUTINE calc_cell_params(blocks)
950     ! calculate areas for secondary fluxes. ! Call after reading mesh data
951     ! from restart file
952     ! BLOCK DATA TYPE
953     TYPE(BLKTYPE), TARGET :: blocks(:)
954     TYPE(MESHTYPE), POINTER :: m
955     INTEGER :: IBLK, I, J
956     ! Areas used in counter-clockwise trapezoidal integration to get
957     ! x and y first-derivatives for center of each cell (Green's thm)
958     REAL(KIND=8) :: Ayi_half, Axi_half, Ayj_half, Axj_half
959
960     DO IBLK = 1, NBLK
961         m => blocks(IBLK)%mesh
962
963         DO J = 0, JMAXBLK
964             DO I = 0, IMAXBLK
965                 ! CALC CELL VOLUME
966                 ! cross product of cell diagonals p, q
967                 ! where p has x,y components px, py and q likewise.
968                 ! Thus, p cross q = px*qy - qx*py
969                 ! where, px = x(i+1,j+1) - x(i,j), py = y(i+1,j+1) - y(i,j)
970                 ! and    qx = x(i,j+1) - x(i+1,j), qy = y(i,j+1) - y(i+1,j)
971                 m%V(I,J) = ( m%x(I+1,J+1) - m%x(I, J) ) &
972                     * ( m%y(I, J+1) - m%y(I+1,J) ) &
973                     - ( m%x(I, J+1) - m%x(I+1,J) ) &
974                     * ( m%y(I+1,J+1) - m%y(I, J) )
975             END DO
976         END DO
977
978         ! CALC CELL AREAS (FLUXES) IN J-DIRECTION
979         DO J = 0, JMAXBLK+1
980             DO I = 0, IMAXBLK
981                 m%Axi(I,J) = m%x(I+1,J) - m%x(I,J)
982                 m%Ayj(I,J) = m%y(I+1,J) - m%y(I,J)
983             END DO
984         END DO
985
986         ! CALC CELL AREAS (FLUXES) IN I-DIRECTION
987         DO J = 0, JMAXBLK
988             DO I = 0, IMAXBLK+1
989                 ! CALC CELL AREAS (FLUXES)
990                 m%Axi(I,J) = m%x(I,J+1) - m%x(I,J)
991                 m%Ayi(I,J) = m%y(I,J+1) - m%y(I,J)
992             END DO
993         END DO
994
995         ! Actual finite-volume scheme equation parameters
996         DO J = 0, JMAXBLK
997             DO I = 0, IMAXBLK
998
999                 Axi_half = ( m%Axi(I+1,J) + m%Axi(I,J) ) * 0.25D0
1000                 Axj_half = ( m%Axi(I,J+1) + m%Axi(I,J) ) * 0.25D0
1001                 Ayi_half = ( m%Ayi(I+1,J) + m%Ayi(I,J) ) * 0.25D0
1002                 Ajj_half = ( m%Ayi(I,J+1) + m%Ayi(I,J) ) * 0.25D0
1003
1004                 ! (NN = 'negative-negative', PN = 'positive-negative',
1005                 ! see how fluxes are summed)
1006                 m%xNN(I, J) = ( -Axi_half - Axj_half )
1007                 m%xPN(I, J) = ( Axi_half - Axj_half )
1008                 m%xPP(I, J) = ( Axi_half + Axj_half )

```

```

1008         m%xNP(I, J) = ( -Ax_i_half + Ax_j_half )
1009         m%yPP(I, J) = (  Ay_i_half + Ay_j_half )
1010         m%yNP(I, J) = ( -Ay_i_half + Ay_j_half )
1011         m%yNN(I, J) = ( -Ay_i_half - Ay_j_half )
1012         m%yPN(I, J) = (  Ay_i_half - Ay_j_half )
1013     END DO
1014 END DO
1015 END DO
1016 END SUBROUTINE calc_cell_params
1017
1018 SUBROUTINE calc_constants(blocks)
1019     ! Calculate constants for a given iteration loop. This way,
1020     ! they don't need to be calculated within the loop at each iteration
1021     TYPE(BLKTYPE), TARGET :: blocks(:)
1022     TYPE(MESHTYPE), POINTER :: m
1023     INTEGER :: IBLK, I, J
1024     DO IBLK = 1, NBLK
1025         m => blocks(IBLK)%mesh
1026         DO J = 0, JMAXBLK + 1
1027             DO I = 0, IMAXBLK + 1
1028                 ! CALC TIMESTEP FROM CFL
1029                 m%dt(I,J) = ((CFL * 0.5D0) / alpha) * m%V(I,J) ** 2 &
1030                     / ( (m%xp(I+1,J) - m%xp(I,J))**2 &
1031                         + (m%yp(I,J+1) - m%yp(I,J))**2 )
1032                 ! CALC SECONDARY VOLUMES
1033                 ! (for rectangular mesh, just average volumes of the 4 cells
1034                 ! surrounding the point)
1035                 m%V2nd(I,J) = ( m%V(I,  J) + m%V(I-1,  J) &
1036                     + m%V(I,J-1) + m%V(I-1,J-1) ) * 0.25D0
1037                 ! CALC CONSTANT TERM
1038                 ! (this term remains constant in the equation regardless of
1039                 ! iteration number, so only calculate once here,
1040                 ! instead of in loop)
1041                 m%term(I,J) = m%dt(I,J) * alpha / m%V2nd(I,J)
1042             END DO
1043         END DO
1044     END DO
1045 END SUBROUTINE calc_constants
1046
1047 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
1048 !!!! SOLVER !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
1049 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
1050
1051 SUBROUTINE calc_temp(b)
1052     ! Calculate first and second derivatives for finite-volume scheme
1053     TYPE(BLKTYPE), TARGET :: b(:)
1054     TYPE(MESHTYPE), POINTER :: m
1055     ! First partial derivatives of temperature in x and y directions
1056     REAL(KIND=8) :: dTdx, dTdy
1057     INTEGER :: IBLK, I, J
1058
1059     DO IBLK = 1, NBLK
1060         m => b(IBLK)%mesh
1061
1062         ! RESET SUMMATION
1063         m%Ttmp = 0.D0
1064
1065         ! PREVIOUSLY SET ITERATION LIMITS TO UTILIZE GHOST NODES ONLY
1066         !ON INTERIOR FACES
1067         DO J = b(IBLK)%JMINLOC, b(IBLK)%JMAXLOC
1068             DO I = b(IBLK)%IMINLOC, b(IBLK)%IMAXLOC
1069                 ! CALC FIRST DERIVATIVES
1070                 dTdx = + 0.5d0 &
1071                     * (( m%T(I+1,J) + m%T(I+1,J+1) ) * m%Ayi(I+1,J) &
1072                     - ( m%T(I,  J) + m%T(I,  J+1) ) * m%Ayi(I,  J) &
1073                     - ( m%T(I,J+1) + m%T(I+1,J+1) ) * m%Ayj(I,J+1) &
1074                     + ( m%T(I,  J) + m%T(I+1,  J) ) * m%Ayj(I,  J) &
1075                     ) / m%V(I,J)
1076                 dTdy = - 0.5d0 &

```

```

1077      * ( ( m%T(I+1,J) + m%T(I+1,J+1) ) * m%Axi(I+1,J) &
1078      -   ( m%T(I, J) + m%T(I, J+1) ) * m%Axi(I, J) &
1079      -   ( m%T(I,J+1) + m%T(I+1,J+1) ) * m%Axi(I,J+1) &
1080      +   ( m%T(I, J) + m%T(I+1, J) ) * m%Axi(I, J) &
1081      ) / m%V(I,J)
1082
1083      ! Alternate distributive scheme second-derivative operator.
1084      m%Ttmp(I+1, J) = m%Ttmp(I+1, J) + m%term(I+1, J) * ( m%yNN(I,J) * dTdx + m%xPP(I,J) * dTdy )
1085      m%Ttmp(I, J) = m%Ttmp(I, J) + m%term(I, J) * ( m%yPN(I,J) * dTdx + m%xNP(I,J) * dTdy )
1086      m%Ttmp(I, J+1) = m%Ttmp(I, J+1) + m%term(I, J+1) * ( m%yPP(I,J) * dTdx + m%xNN(I,J) * dTdy )
1087      m%Ttmp(I+1,J+1) = m%Ttmp(I+1,J+1) + m%term(I+1,J+1) * ( m%yNP(I,J) * dTdx + m%xPN(I,J) * dTdy )
1088
1089      END DO
1090      ! SAVE NEW TEMPERATURE DISTRIBUTION
1091      ! (preserve Ttmp for residual calculation in solver loop)
1092
1093      ! Previously set bounds, add one to lower limit so as not to
1094      ! update BC. (dont need to for upper limit because explicit scheme)
1095      DO J = b(1BLK)%JMINLOC + 1, b(1BLK)%JMAXLOC
1096          DO I = b(1BLK)%IMINLOC + 1, b(1BLK)%IMAXLOC
1097              m%T(I,J) = m%T(I,J) + m%Ttmp(I,J)
1098          END DO
1099      END DO
1100
1101      END SUBROUTINE calc_temp
1102
1103  END MODULE BLOCKMOD

```

Listing 3: Grids are decomposed into blocks and information pertaining to neighbors is stored using the GRIDMOD module

## Appendix C: Multi-Block Solver Subroutines

```

1  ! MAE 267
2  ! PROJECT 3
3  ! LOGAN HALSTROM
4  ! 03 NOVEMBER 2015
5
6  ! DESCRIPTION: Subroutines used for solving heat conduction of steel plate.
7  ! Subroutines utilizing linked lists are here so that linked lists do not need
8  ! to be function inputs.
9  ! Utilizes modules from 'modules.f90'
10 ! CONTENTS:
11 ! init --> Initialize the solution with dirichlet B.C.s
12 ! solve --> Solve heat conduction equation with finite volume scheme
13 ! output --> Save solution parameters to file
14
15 MODULE subroutines
16     USE CONSTANTS
17     USE BLOCKMOD
18     USE IO
19
20     IMPLICIT NONE
21
22 CONTAINS
23     SUBROUTINE init_gridsystem(blocks)
24         ! Initialize the solution with dirichlet B.C.s. Save to restart files.
25         TYPE(BLKTYPE) :: blocks(:)
26
27         ! INITIALIZE BLOCKS
28         CALL init_blocks(blocks)
29         ! WRITE BLOCK CONNECTIVITY FILE
30         CALL write_blocks(blocks)
31         ! INITIALIZE MESH
32         CALL init_mesh(blocks)
33         ! INITIALIZE TEMPERATURE WITH DIRICHLET B.C.
34         CALL init_temp(blocks)

```

```

35      ! WRITE GRID AND INITIAL TEMPERATURE TO PLOT3D RESTART FILES
36      CALL plot3D(blocks)
37
38  END SUBROUTINE init_gridsystem
39
40  SUBROUTINE init_solution(blocks, nbrlists)
41      ! Read initial conditions from restart files. Then calculate parameters
42      ! used in solution
43      TYPE(BLKTYPE) :: blocks(:)
44      ! LINKED LISTS STORING NEIGHBOR INFO
45      TYPE(NBRLIST) :: nbrlists
46
47      ! READ BLOCK CONFIGURATION INFORMATION FROM CONFIG FILE
48      CALL read_blocks(blocks)
49
50      ! READ GRID AND INITIAL TEMPERATURE FROM PLOT3D RESTART FILE
51      CALL readPlot3D(blocks)
52
53
54      ! CALC LOCAL BOUNDARIES OF CELLS
55      write(*,*) 'set local bounds'
56      CALL set_block_bounds(blocks)
57
58
59
60      ! INITIALIZE LINKED LISTS CONTAINING BOUNDARY INFORMATION
61      ! write(*,*) 'make linked lists'
62      ! CALL init_linklists(blocks, nbrlists)
63      ! POPULATE BLOCK GHOST NODES
64      ! write(*,*) 'update ghosts'
65      ! CALL update_ghosts(blocks, nbrlists)
66
67      CALL update_ghosts_debug(blocks)
68
69      ! CALC AREAS FOR SECONDARY FLUXES
70      write(*,*) 'calc solution stuff'
71      CALL calc_cell_params(blocks)
72      ! CALC CONSTANTS OF INTEGRATION
73      CALL calc_constants(blocks)
74
75  END SUBROUTINE init_solution
76
77
78  SUBROUTINE solve(blocks, nbrlists, iter, res_hist)
79      ! Solve heat conduction equation with finite volume scheme
80      TYPE(BLKTYPE) :: blocks(:)
81      ! LINKED LISTS STORING NEIGHBOR INFO
82      TYPE(NBRLIST) :: nbrlists
83      ! Residual history linked list
84      TYPE(RESLIST), POINTER :: res_hist
85      ! pointer to iterate linked list
86      TYPE(RESLIST), POINTER :: hist
87      ! Minimum residual criteria for iteration, actual residual
88      REAL(KIND=8) :: res = 1000.D0, resloc, resmax
89      ! iter in function inputs so it can be returned to main
90      INTEGER :: iter, IBLK, IBLKRES
91
92      INCLUDE "mpif.h"
93      REAL(KIND=8) :: start_solve, end_solve
94      WRITE(*,*) 'Starting clock for solver...'
95      start_solve = MPI_Wtime()
96
97      ! residual history
98      ALLOCATE(res_hist)
99      hist => res_hist
100
101      iter_loop: DO WHILE (res >= min_res .AND. iter <= max_iter)
102          ! Iterate FV solver until residual becomes less than cutoff or
103          ! iteration count reaches given maximum

```

```

104
105      ! CALC NEW TEMPERATURE AT ALL POINTS
106      CALL calc_temp(blocks)
107
108      ! UPDATE GHOST NODES WITH NEW TEMPERATURE SOLUTION
109      ! CALL update_ghosts(blocks, nbrlists)
110      CALL update_ghosts_debug(blocks)
111
112      ! CALC RESIDUAL
113      resmax = 0.D0
114      DO IBLK = 1, NBLK
115          ! Find max of each block
116          resloc = MAXVAL( ABS( blocks(IBLK)%mesh%Ttmp(2:IMAXBK-1, 2:JMAXBK-1) ) )
117          ! keep biggest residual
118          IF (resmax < resloc) THEN
119              resmax = resloc
120          END IF
121      END DO
122      ! FINAL RESIDUAL
123      res = resmax
124
125      ! SWITCH TO NEXT LINK
126      ! (skip first entry)
127      ALLOCATE(hist%next)
128      hist => hist%next
129      NULLIFY(hist%next)
130      ! STORE RESIDUAL HISTORY
131      hist%iter = iter
132      hist%res = res
133
134
135      ! INCREMENT ITERATION COUNT
136      iter = iter + 1
137
138  END DO iter_loop
139
140      ! there was an extra increment after final iteration we need to subtract
141      iter = iter - 1
142
143      ! CACL SOLVER WALL CLOCK TIME
144      end_solve = MPI_Wtime()
145      wall_time_solve = end_solve - start_solve
146
147      IF (iter > max_iter) THEN
148          WRITE(*,*) 'DID NOT CONVERGE (NUMBER OF ITERATIONS:', iter, ')'
149      ELSE
150          WRITE(*,*) 'CONVERGED (NUMBER OF ITERATIONS:', iter, ')'
151          WRITE(*,*) '          (MAXIMUM RESIDUAL      :', res, ')'
152      END IF
153  END SUBROUTINE solve
154
155  SUBROUTINE output(blocks, iter)
156      ! Save solution parameters to file
157      TYPE(BLKTYPE), TARGET :: blocks(:)
158      REAL(KIND=8), POINTER :: tmpT(:, :), tempTemperature(:, :)
159      REAL(KIND=8) :: resloc, resmax
160      INTEGER :: iter, I, J, IBLK, IRES
161
162      ! Temperature => mesh%T(2:IMAX-1, 2:JMAX-1)
163      ! tempTemperature => mesh%Ttmp(2:IMAX-1, 2:JMAX-1)
164
165      ! CALC RESIDUAL
166      resmax = 0.D0
167      DO IBLK = 1, NBLK
168          ! Find max of each block
169          resloc = MAXVAL( ABS( blocks(IBLK)%mesh%Ttmp(2:IMAXBK-1, 2:JMAXBK-1) ) )
170          ! keep biggest residual
171          IF (resmax < resloc) THEN
172              resmax = resloc

```

```

173         IRES = IBLK
174     END IF
175 END DO
176
177
178 ! Write final maximum residual and location of max residual
179 ! OPEN(UNIT = 1, FILE = casedir // "SteadySoln.dat")
180 ! DO i = 1, IMAX
181 !     DO j = 1, JMAX
182 !         WRITE(1,'(F10.7, 5X, F10.7, 5X, F10.7, I5, F10.7)', mesh%x(i,j), mesh%y(i,j), mesh%T(i,j))
183 !     END DO
184 ! END DO
185 ! CLOSE (1)
186
187 ! Screen output
188 tmpT => blocks(IRES)%mesh%Tmp
189 WRITE (*,*), "IMAX/JMAX", IMAX, JMAX
190 WRITE (*,*), "N/M", N, M
191 WRITE (*,*), "iters", iter
192 WRITE (*,*), "max residual", MAXVAL(tmpT(2:IMAXBK-1, 2:JMAXBK-1))
193 WRITE (*,*), "on block id", IRES
194 WRITE (*,*), "residual ij", MAXLOC(tmpT(2:IMAXBK-1, 2:JMAXBK-1))
195
196 ! Write to file
197 ! OPEN (UNIT = 2, FILE = TRIM(casedir) // "SolnInfo.dat")
198 OPEN (UNIT = 2, FILE = "SolnInfo.dat")
199 WRITE (2,*), "Running a", IMAX, "by", JMAX, "grid,"
200 WRITE (2,*), "With NxM:", N, "x", M, "blocks took:"
201 WRITE (2,*), iter, "iterations"
202 WRITE (2,*), wall_time_total, "seconds (Total CPU walltime)"
203 WRITE (2,*), wall_time_solve, "seconds (Solver CPU walltime)"
204 ! WRITE (2,*), wall_time_iter, "seconds (Iteration CPU walltime)"
205 WRITE (2,*)
206 WRITE (2,*), "Found max residual of ", MAXVAL(tmpT(2:IMAXBK-1, 2:JMAXBK-1))
207 WRITE (2,*), "on block id", IRES
208 WRITE (2,*), "At ij of ", MAXLOC(tmpT(2:IMAXBK-1, 2:JMAXBK-1))
209 CLOSE (2)
210 END SUBROUTINE output
211
212
213
214 END MODULE subroutines

```

Listing 4: Main subroutines used for solving heat transfer on a multi-block grid

## Appendix D: Multi-Block Plot3D Reader-Writer

```
1  ! MAE 267
2  ! PROJECT 3
3  ! LOGAN HALSTROM
4  ! 03 NOVEMBER 2015
5
6  ! DESCRIPTION: This module contains functions for information input and output.
7  ! Write grid and temperature files in PLOT3D format.
8  ! Write and read block grid configuration file
9
10 ! NOTE: How to Visualize Blocks in Paraview:
11 ! open unformatted PLOT3D file.
12 ! Change 'Coloring' from 'Solid' to 'vtkCompositeIndex'
13
14 MODULE IO
15   USE CONSTANTS
16   USE BLOCKMOD
17   IMPLICIT NONE
18
19   ! VARIABLES
20   INTEGER :: gridUnit = 30 ! Unit for grid file
21   INTEGER :: tempUnit = 21 ! Unit for temp file
22   INTEGER :: resUnit = 23
23   REAL(KIND=8) :: tRef = 1.D0 ! tRef number
24   REAL(KIND=8) :: dum = 0.D0 ! dummy values
25
26   ! LINKED LIST OF RESIDUAL HISTORY
27
28   TYPE RESLIST
29     ! Next element in linked list
30     TYPE(RESLIST), POINTER :: next
31     ! items in link:
32     REAL(KIND=8) :: res
33     INTEGER :: iter
34   END TYPE RESLIST
35
36   CONTAINS
37   SUBROUTINE plot3D(blocks)
38     IMPLICIT NONE
39
40     TYPE(BLKTYPE) :: blocks(:)
41     INTEGER :: IBLK, I, J
42
43     ! FORMAT STATEMENTS
44     ! I --> Integer, number following is number of sig figs
45     ! E --> scientific notation,
46     !       ! before decimal is sig figs of exponent?
47     !       ! after decimal is sig figs of value
48     ! number before letter is how many entries on single line
49     ! before newline (number of columns)
50     10   FORMAT(I10)
51     20   FORMAT(10I10)
52     30   FORMAT(10E20.8)
53
54     !!! FORMATTED !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
55
56     ! OPEN FILES
57     ! OPEN(UNIT=gridUnit,FILE= TRIM(casedir) // 'grid_form.xyz',FORM='formatted')
58     ! OPEN(UNIT=tempUnit,FILE= TRIM(casedir) // 'T_form.dat',FORM='formatted')
59     OPEN(UNIT=gridUnit,FILE= 'grid_form.xyz',FORM='formatted')
60     OPEN(UNIT=tempUnit,FILE= 'T_form.dat',FORM='formatted')
61
62     ! WRITE TO GRID FILE
63     WRITE(gridUnit, 10) NBLK
64     WRITE(gridUnit, 20) ( IMAXBLK, JMAXBLK, IBLK=1, NBLK)
65     ! WRITE(gridUnit, 20) ( blocks(IBLK)%IMAX, blocks(IBLK)%JMAX, IBLK=1, NBLK)
66     DO IBLK = 1, NBLK
67       WRITE(gridUnit, 30) ( (blocks(IBLK)%mesh%x(I,J), I=1,IMAXBLK), J=1,JMAXBLK), &
```

```

68          ( (blocks(IBLK)%mesh%y(I,J), I=1,IMAXBLK), J=1,JMAXBLK)
69
70 END DO
71
72 ! WRITE TO TEMPERATURE FILE
73 ! When read in paraview, 'density' will be equivalent to temperature
74 WRITE(tempUnit, 10) NBLK
75 WRITE(tempUnit, 20) ( IMAXBLK, JMAXBLK, IBLK=1, NBLK)
76 DO IBLK = 1, NBLK
77
78     WRITE(tempUnit, 30) tRef,dum,dum,dum
79     WRITE(tempUnit, 30) ( (blocks(IBLK)%mesh%T(I,J), I=1,IMAXBLK), J=1,JMAXBLK), &
80                          ( (blocks(IBLK)%mesh%T(I,J), I=1,IMAXBLK), J=1,JMAXBLK), &
81                          ( (blocks(IBLK)%mesh%T(I,J), I=1,IMAXBLK), J=1,JMAXBLK), &
82                          ( (blocks(IBLK)%mesh%T(I,J), I=1,IMAXBLK), J=1,JMAXBLK)
83
84 END DO
85
86 ! CLOSE FILES
87 CLOSE(gridUnit)
88 CLOSE(tempUnit)
89
90 !!! UNFORMATTED !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
91
92 ! OPEN FILES
93 ! OPEN(UNIT=gridUnit,FILE= TRIM(casedir) // 'grid.xyz',FORM='unformatted')
94 ! OPEN(UNIT=tempUnit,FILE= TRIM(casedir) // 'T.dat',FORM='unformatted')
95 OPEN(UNIT=gridUnit,FILE = 'grid.xyz',FORM='unformatted')
96 OPEN(UNIT=tempUnit,FILE = 'T.dat',FORM='unformatted')
97
98 ! WRITE TO GRID FILE (UNFORMATTED)
99 ! (Paraview likes unformatted better)
100 WRITE(gridUnit) NBLK
101 WRITE(gridUnit) ( IMAXBLK, JMAXBLK, IBLK=1, NBLK)
102 ! WRITE(gridUnit) ( blocks(IBLK)%IMAX, blocks(IBLK)%JMAX, IBLK=1, NBLK)
103 DO IBLK = 1, NBLK
104     WRITE(gridUnit) ( (blocks(IBLK)%mesh%x(I,J), I=1,IMAXBLK), J=1,JMAXBLK), &
105                     ( (blocks(IBLK)%mesh%y(I,J), I=1,IMAXBLK), J=1,JMAXBLK)
106
107 END DO
108
109 ! WRITE TO TEMPERATURE FILE
110 ! When read in paraview, 'density' will be equivalent to temperature
111 WRITE(tempUnit) NBLK
112 WRITE(tempUnit) ( IMAXBLK, JMAXBLK, IBLK=1, NBLK)
113 DO IBLK = 1, NBLK
114
115     WRITE(tempUnit) tRef,dum,dum,dum
116     WRITE(tempUnit) ( (blocks(IBLK)%mesh%T(I,J), I=1,IMAXBLK), J=1,JMAXBLK), &
117                     ( (blocks(IBLK)%mesh%T(I,J), I=1,IMAXBLK), J=1,JMAXBLK), &
118                     ( (blocks(IBLK)%mesh%T(I,J), I=1,IMAXBLK), J=1,JMAXBLK), &
119                     ( (blocks(IBLK)%mesh%T(I,J), I=1,IMAXBLK), J=1,JMAXBLK)
120
121 END DO
122
123 ! CLOSE FILES
124 CLOSE(gridUnit)
125 CLOSE(tempUnit)
126
127 END SUBROUTINE plot3D
128
129 SUBROUTINE readPlot3D(blocks)
130 IMPLICIT NONE
131
132 TYPE(BLKTYPE) :: blocks(:)
133 INTEGER :: IBLK, I, J
134 ! READ INFO FOR BLOCK DIMENSIONS
135 INTEGER :: NBLKREAD, IMAXBLKREAD, JMAXBLKREAD
136
137 ! FORMAT STATEMENTS
138 ! I --> Integer, number following is number of sig figs
139 ! E --> scientific notation,

```



```

137         ! before decimal is sig figs of exponent?
138         ! after decimal is sig figs of value
139         ! number before letter is how many entries on single line
140         ! before newline (number of columns)
141     10     FORMAT(I10)
142     20     FORMAT(10I10)
143     30     FORMAT(10E20.8)
144
145     !!! FORMATTED !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
146
147     ! OPEN FILES
148     ! OPEN(UNIT=gridUnit,FILE= TRIM(casedir) // 'grid_form.xyz',FORM='formatted')
149     ! OPEN(UNIT=tempUnit,FILE= TRIM(casedir) // 'T_form.dat',FORM='formatted')
150     OPEN(UNIT=gridUnit,FILE= 'grid_form.xyz',FORM='formatted')
151     OPEN(UNIT=tempUnit,FILE= 'T_form.dat',FORM='formatted')
152
153     ! READ GRID FILE
154     READ(gridUnit, 10) NBLKREAD
155     READ(gridUnit, 20) ( IMAXBKREAD, JMAXBKREAD, IBLK=1, NBLKREAD)
156     ! WRITE(gridUnit, 20) ( blocks(IBLK)%IMAX, blocks(IBLK)%JMAX, IBLK=1, NBLK)
157     DO IBLK = 1, NBLKREAD
158         READ(gridUnit, 30) ( (blocks(IBLK)%mesh%x(I,J), I=1,IMAXBK), J=1,JMAXBK), &
159                             ( (blocks(IBLK)%mesh%y(I,J), I=1,IMAXBK), J=1,JMAXBK)
160     END DO
161
162
163     ! READ TEMPERATURE FILE
164     ! When read in paraview, 'density' will be equivalent to temperature
165     READ(tempUnit, 10) NBLKREAD
166     READ(tempUnit, 20) ( IMAXBKREAD, JMAXBKREAD, IBLK=1, NBLKREAD)
167     DO IBLK = 1, NBLKREAD
168
169         READ(tempUnit, 30) tRef,dum,dum,dum
170         READ(tempUnit, 30) ( (blocks(IBLK)%mesh%T(I,J), I=1,IMAXBK), J=1,JMAXBK), &
171                             ( (blocks(IBLK)%mesh%T(I,J), I=1,IMAXBK), J=1,JMAXBK), &
172                             ( (blocks(IBLK)%mesh%T(I,J), I=1,IMAXBK), J=1,JMAXBK), &
173                             ( (blocks(IBLK)%mesh%T(I,J), I=1,IMAXBK), J=1,JMAXBK)
174     END DO
175
176     ! CLOSE FILES
177     CLOSE(gridUnit)
178     CLOSE(tempUnit)
179 END SUBROUTINE readPlot3D
180
181 SUBROUTINE write_res(res_hist)
182     TYPE(RESLIST), POINTER :: res_hist
183     ! pointer to iterate linked list
184     TYPE(RESLIST), POINTER :: hist
185
186     ! open residual file
187     ! OPEN(UNIT=resUnit,FILE= TRIM(casedir) // 'res_hist.dat')
188     OPEN(UNIT=resUnit,FILE = 'res_hist.dat')
189     ! column headers
190     WRITE(resUnit,*) 'ITER      RESID'
191
192     ! point to residual linked list
193     hist => res_hist
194     ! skip first link, empty from iteration loop design
195     hist => hist%next
196     ! write residual history to file until list ends
197     DO
198         IF ( .NOT. ASSOCIATED(hist) ) EXIT
199         ! write iteration and residual in two columns
200         WRITE(resUnit,*) hist%iter, hist%res
201         hist => hist%next
202     END DO
203
204     CLOSE(resUnit)
205 END SUBROUTINE write_res

```

```

206
207
208 END MODULE IO

```

Listing 5: Code for saving formatted multiblock PLOT3D solution files and reading restart files

## Appendix E: Other Relevant Codes

```

1  ! MAE 267
2  ! PROJECT 3
3  ! LOGAN HALSTROM
4  ! 03 NOVEMBER 2015
5
6
7  ! DESCRIPTION: Solve heat conduction equation for single block of steel.
8  ! To compile: mpif90 -o main -O3 modules.f90 plot3D_module.f90 subroutines.f90 main.f90
9  ! makes executable file 'main'
10 ! 'rm *.mod' afterward to clean up unneeded compiled files
11 ! To run: ./main or ./run.sh or sbatch run.sh on hpc1
12
13
14 PROGRAM heatTrans
15 !   USE CLOCK
16   USE CONSTANTS
17   USE subroutines
18   USE IO
19
20   IMPLICIT NONE
21
22   !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
23   !!! INITIALIZE VARIABLES !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
24   !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
25
26   ! BLOCKS
27   TYPE(BLKTYPE), ALLOCATABLE :: blocks(:)
28   ! LINKED LISTS STORING NEIGHBOR INFO
29   TYPE(NBRLIST) :: nbrlists
30   ! ITERATION PARAMETERS
31   ! Residual history linked list
32   TYPE(RESLIST), POINTER :: res_hist
33   ! Maximum number of iterations
34   INTEGER :: iter = 1, IBLK
35
36   INCLUDE "mpif.h"
37   REAL(KIND=8) :: start_total, end_total
38   REAL(KIND=8) :: start_solve, end_solve
39   ! CLOCK TOTAL TIME OF RUN
40   start_total = MPI_Wtime()
41
42   !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
43   !!! INITIALIZE !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
44   !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
45
46   ! READ INPUTS FROM FILE
47   CALL read_input()
48   ALLOCATE( blocks(NBLK) )
49   ! INITIALIZE GRID SYSTEM
50   WRITE(*,*) 'Making mesh...'
51   CALL init_gridsystem(blocks)
52
53   !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
54   !!! SOLVER !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
55   !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
56
57   ! INITIALIZE SOLUTION
58   CALL init_solution(blocks, nbrlists)

```

```

59  ! SOLVE
60  WRITE(*,*) 'Solving heat conduction...'
61  CALL solve(blocks, nbrlists, iter, res_hist)
62
63  !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
64  !!! SAVE RESULTS !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
65  !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
66
67  WRITE(*,*) 'Writing results...'
68  ! SAVE SOLUTION AS PLOT3D FILES
69  CALL plot3D(blocks)
70  ! CALC TOTAL WALL TIME
71  end_total = MPI_Wtime()
72  wall_time_total = end_total - start_total
73
74  ! SAVE RESIDUAL HISTORY
75  CALL write_res(res_hist)
76  ! SAVE SOLVER PERFORMANCE PARAMETERS
77  CALL output(blocks, iter)
78
79  !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
80  !!! CLEAN UP !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
81  !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
82
83  DO IBLK = 1, NBLK
84      DEALLOCATE( blocks(IBLK)%mesh%xp )
85      DEALLOCATE( blocks(IBLK)%mesh%yp )
86      DEALLOCATE( blocks(IBLK)%mesh%x )
87      DEALLOCATE( blocks(IBLK)%mesh%y )
88      DEALLOCATE( blocks(IBLK)%mesh%T )
89      DEALLOCATE( blocks(IBLK)%mesh%Ttmp )
90      DEALLOCATE( blocks(IBLK)%mesh%dt )
91      DEALLOCATE( blocks(IBLK)%mesh%V )
92      DEALLOCATE( blocks(IBLK)%mesh%V2nd )
93      DEALLOCATE( blocks(IBLK)%mesh%term )
94      DEALLOCATE( blocks(IBLK)%mesh%yPP )
95      DEALLOCATE( blocks(IBLK)%mesh%yNP )
96      DEALLOCATE( blocks(IBLK)%mesh%yNN )
97      DEALLOCATE( blocks(IBLK)%mesh%yPN )
98      DEALLOCATE( blocks(IBLK)%mesh%xNN )
99      DEALLOCATE( blocks(IBLK)%mesh%xPN )
100     DEALLOCATE( blocks(IBLK)%mesh%xPP )
101     DEALLOCATE( blocks(IBLK)%mesh%xNP )
102 END DO
103
104 WRITE(*,*) 'Done!'
105
106 ! MOVE OUTPUT FILE TO OUTPUT DIRECTORY
107 ! CALL EXECUTE_COMMAND_LINE ("mv a.out " // casedir // '.')
108
109
110 END PROGRAM heatTrans

```

Listing 6: Wrapper program