APPENDIX A: Real Gas Models for Gamma

PAB3D has an improved model to handle the conservation of total enthalpy. The PAB3D code used the single ideal perfect gas (Air) assumption. In our modification, we changed the code to have a Variable Gamma. However, there may be a severe consequence in using this modification in preserving total enthalpy for internal flow calculation. We were not able to simulate flow at high temperature (1100 R) without using very small CFL (Courant-Fredrick-Lewy) number. Several cases do not converge with even small CFL. We have addressed the most important issue in preserving total enthalpy, which improves the convergence rate with a higher CFL number. We solved the enthalpy-energy equation as a function of temperature. However, the pressure and enthalpy used in the governing equations are not compatible with the real gas formulations. For ideal and real gas simulations enthalpy is related to internal energy through the following relation:

$$\text{e = internal energy = h(T) – RT} \quad \text{.....(1)}$$

where, h is the local enthalpy, R is the equivalent gas constant and T is the gas exact temperature.

Additionally, we also know that

$$\begin{aligned} R &= \sum_{m=1}^{nspec} R_m \\ h(T) &= \sum_{m=1}^{mspec} h_m = e + RT \end{aligned} \quad \text{.....(2)}$$

$$\begin{aligned} e &= \frac{E - 0.5\rho(u^2 + v^2 + w^2)}{\rho} \\ e(T) &= h(T) - RT \end{aligned} \quad \text{.....(3)}$$

where, nspec is the number of species that we are simulating. We have used McBride[§] formulation for perfect gases to evaluate total enthalpy as:

$$h_m = h_m^f + R_m \{b_1 + a_2 \ln T + \sum_{n=1, n\neq 2} \frac{a_n}{n-2} T^{n-2}\}_m \quad \text{.....(4)}$$

Where, h_m^f is heat of formation of 298.15 K, J/mol, R_m is the Gas Constant for each species, a_2 and a_n are polynomial constants, b_1 is the integration constant of the C polynomial:

$$\begin{aligned} \{C_P\}_m &= \left\{ \sum_{n=1}^{7} a_n T^{n-2} \right\}_m \\ C_v(T) &= \sum_{m=1}^{nspes} \{C_p\}_m - R \end{aligned} \quad \text{.....(5)}$$

[§] Bonnie J. McBride and Sanford Gordon, "Computer Program for Calculation of Complex Chemical Equilibrium Compositions and Applications", NASA LeRC TP-1311, June 1996.

For most of the elements, McBride obtained the coefficients in the above equations by means of a least-squares fit. The gas table has three intervals that are 200 to 1000k, 1000 to 6000 K and 6000 to 20000 K for all the above coefficients. From the PAB3D solution at specific time step, we can evaluate the value of T that satisfies the above 4 equations. Using Newton-Raphson iteration technique, we can find the root for the e(T) equation as

$$T(k)=T(k-1)-(e(T)-e)/C_v(T) \quad \text{.....(5a)}$$

or,

$$T(k)=T(k-1)-(h(T)-e-RT)/C_p(T) \quad \text{.....(5b)}$$

where, k is the iteration number. We stop the iterations when (e(T)-e)/C_v is less than 1K, evaluate C_v from the above equation and γ

$$\gamma = \frac{C_v + R}{C_v} \quad \text{.....(6)}$$

We have originally proposed the following approach to evaluate enthalpy and pressure in the governing equations

1. Use the correct form of the heat conductive term in the energy equation:

$$H_d = \frac{\mu}{P_r}\left(\frac{\partial h}{\partial x_i}\right), \qquad h=H(T)$$

In the original code, the enthalpy (h) takes the following form:

$$h = C_p T = \frac{\gamma RT}{\gamma - 1} \text{ and } \mathrm{R} = \sum_{i=1}^{nspec} C_i R_i$$

$$\{C_p\}_m = \{\sum_{n=1} a_n T^{n-3}\}_m$$
$$C_v(T) = \sum_{m=1}^{nspec} \{C_p\}_m - R \quad \text{.....(7)}$$

2. Use the correct form in evaluating the pressure as:

$$P = \rho RT$$

In the original code, the pressure takes the following form:

$$P=\rho(\gamma-1)e \quad \text{.....(8)}$$

This is based on the assumptions that $e=C_vT$. We can then combine equations 2 & 3 to get $e+RT = e+P/\rho = h$, which is valid for Real and Ideal Gases

Let's now introduce a new variable Γ not to be confused with the specific heat ratio γ.

$$h=\Gamma e \quad \text{.....(9)}$$

Thus,

$$P=\rho(\Gamma-1)e=\rho RT \quad \text{.....(10)}$$

and

$$h=\frac{\Gamma R}{(\Gamma-1)}T \quad \text{.....(11)}$$

From equation 2 and the value of e, we can evaluate $\Gamma=h/e$ and return it to the main code. We have used equations 10 and 11 to evaluate both P and h. This approach will not require any change of Ideal Gas CFD code as Γ replaces γ through out the entire code.

The user can specify either using the fixed or the variable temperature model through IMODEL in the Spec Cont segment of the user Control file. If

- IMODEL = 0, use the fixed temperature to evaluate γ (old model)
- IMODEL = 1, use the variable temperature model in evaluating γ by solving the enthalpy and heat coefficient equations (5a).
- IMODEL = 2, use the variable temperature model in evaluating γ by the solving the enthalpy and heat coefficient equations (5b).
- IMODEL = 3, use the variable temperature model in evaluating Γ by solving the enthalpy heat coefficient equations and evaluate Γ (5b and 9).

A.1 Real Gas Supersonic Duct

This is a variable area duct of a ratio of 1.9. The grid geometry was given to AS&M Inc. by GEAE to evaluate the new Real gas model and compared with the theoretical values. We have fixed inflow pressure and velocity as well as the area ratio A2/A1. We have simulated two conditions at 685 and 840 K respectively. We have solved the Euler equations to avoid any viscous effect in the final solution. However the duct was not designed to avoid generating shocks inside the duct. **Table A–1** shows the conditions selected for the present simulations.

In general, all the models produce the same results qualitative. The real gas (1) generates much higher temperature as compared with the other models. **Table A–2** shows the comparisons between the predictions of the three models and the theoretical values. The real gas (3) predicted exit temperature, T2, and Mach # very close to the theoretical values for both flow conditions. The error was less than 0.5% that may be the contribution of the

Table A-1. Supersonic Duct Flow Conditions

	Condition 1	**Condition 2**
P1, N/m2	101235	101235
A2/A1	1.9	1.9
T1, K	685	840
U1, m/sec	600	600

Table A-2. Real Gas Predictions

	Ideal gas Theory	Ideal gas Pab3d	Real Gas Theory	Real Gas (1) PAB3D	Real Gas (3) PAB3D
T2, K (685)	448	450	458	494	460
M2 (685)	2.15	2.14	2.11	2.04	2.10
T2, K (840)	533	535	556	609	558
M2 (840)	2.14	2.13	2.074	2.002	2.08

shock wave generated inside the duct. The real gas (1) case was at least 10% of the theoretical values in both cases.

APPENDIX B: MPI Implementation

B.1 Cluster Machine Performance (more results will be forthcoming)

Tables B-1, B-2, and B-3 show samples of the cluster machine performance using MPI implementation of PAB3D for a balanced 3Block 3D Case with scalar diagonalization, Roe scheme, and single direction viscosities..

Table B-1. MPI PAB3D with Two-Equation Turbulence Model: 1,018,368 cells

Machine	CPU	MFLOPS	Total time/cell/itr (micro sec)	Percent speed up	Total time/cell/itr (× Single C-90)
Cray C-90 (f90)	1	360	12.0	NA	1
DEC Alpha 21164 533 MHz (Linux)	3	225	19.5	298	1.6
SGI Origin 2000 R10k 195 MHz	3	180	23.5	325	2.0
SGI R10k 195 MHz Octane	3	133	32.6	275	2.7
DEC Alpha 21164 533 MHz (Linux)	1	75	58.1	NA	4.8
SGI Origin 2000 R10k 195 MHz	1	56	76.4	NA	6.4
SGI R10k 195 MHz Octane	1	48	89.8	NA	7.5
Sun Ultra-2 200 MHz	1	43	99.2	NA	8.3

Table B-2. MPI PAB3D Two-Equation Turbulence Model: 127,296 cells (Table B–1 case, but with 1/8th the cells)

Machine	CPU	MFLOPS	Total time/cell/itr (micro sec)	Percent speed up	Total time/cell/itr (× Single C-90)
Cray C-90 (f90)	1	320	12	NA	1
DEC Alpha 533 MHz (Linux)	3	229	17	282	1.4
SGI Origin 2000 R10k 195 MHz	3	213	17.5	291	1.5
SGI R10k 195 MHz Octane	3	167	23	278	1.9
DEC Alpha 533 MHz (Linux)	1	80	48	NA	4.0
SGI Origin 2000 R10k 195 MHz	1	74	51	NA	4.3
SGI R10k 195 MHz Octane	1	60	64	NA	5.3
Sun Ultra-2 200 MHz	1	41	93	NA	7.8

Table B-3. MPI PAB3D with Laminar Model. 127,296 cells (Table B–2 case, but without Turbulence)

Machine	CPU	MFLOPS	Total time/cell/itr (micro sec)	Percent speed up	Total time/cell/itr (× Single C-90)
Cray C-90 (f90)	1	350	8	NA	1
DEC Alpha 533 MHz (Linux)	3	241	11.6	293	1.45
SGI Origin 2000 R10k 195 MHz	3	227	12.3	292	1.54
SGI R10k 195 MHz Octane	3	175	16	287	2
DEC Alpha 533 MHz (Linux)	1	81	34	NA	4.3
SGI Origin 2000 R10k 195 MHz	1	78	36	NA	4.5
SGI R10k 195 MHz Octane	1	60	46	NA	5.8
Sun Ultra-2 200 MHz	1	48	58	NA	7.2

B.2 Introduction and Approach for Distributed Computers (MPI) in the PAB3D Code

The MPI prototype of the PAB3D code has the following characteristics.

- A communication interface (Buffer)

- Global-iteration gathering
- Message passing interface using either LAM/MPI 6.1 or MPICH
- Single source code for distributed or single computer compatibility

In order to understand the MPI implementation and the use of a communication interface (Buffer) in the PAB3D code, we need to discuss its communication data base structure. Each block contains six faces as:

J_{min}, ===== Face 1 J_{max}, ===== Face 2

K_{min}, ===== Face 3 K_{max}, ===== Face 4

I_{min}, ===== Face 5 I_{max}, ===== Face 6

One or more sub-faces may present each of these faces. This defines the local ID of each sub-face as Block 1, Face 3 and sub-face 4. Each of these sub-faces is assigned a global ID (Patch #). This is only done for Block communication sub-faces. **Fig. B–1** shows the example of transforming from local to global and back to local.

The database allows the communications across cells, faces and blocks with a universal set of information. The information is written as an unstructured list of cell correspondences over the block interface. Each entry contains four items; the address of

A-Cell (Destination, NB1) and B-Cells (Sources, NB2), the value of the contact area as a fraction of the total cell face area of A-Cell (Frc), and the total area of A-Cell. This information is collected at the fine grid level. This database provides cell area information sufficient for any level of grid density reduction. The NB1, NB2 and Frc have a fixed number of items (NITM) for the corresponding patch.

Similar to the database structure, we created for each patch a buffer with a size equal to:

`2*NVAR*NITM,` where,
`NVAR=5+NT+NS`

NT, number of turbulent equations

NS, number of multi-species

Each of the source blocks is assigned a number of patches with their global Ids. Each of these blocks sends the Q, QT and QS to the corresponding patch location in the buffer. The blocking send is used to fill the buffer. We have used the MP_BARRIER till all the needed variables are sent to the buffer. Then, the destination block collects all the variables from the global locations and put them in the related local location (face and sub-face). A non-blocking receive (IRECIEVE) is used to collect the data. This is very fast receiving MPI operation. However, we found that DEC Alpha computers have problems using the IRECIEVE. The entire operation is done without the need of the source block to know what is the receiving block or vice versa. Basically, there is no need for synchronize send and receive operations (very expensive send or receive MPI operations).

Fig. B-1, shows the BC, Gathering and Broadcasting in the PAB3D MPI prototype. The N processors (computers) are numbered from P0 to PN-1. The main job of the P0 processor is the I/O and data manipulations. The P0, then, broadcasts all the necessary information to the rest of the processors. This is a one-time operation at the beginning of a new solution. At the end of each global iteration (# local iterations), the P0 processor gathers the data from the other processors. Each processor solves one or more than one block. After one or more block

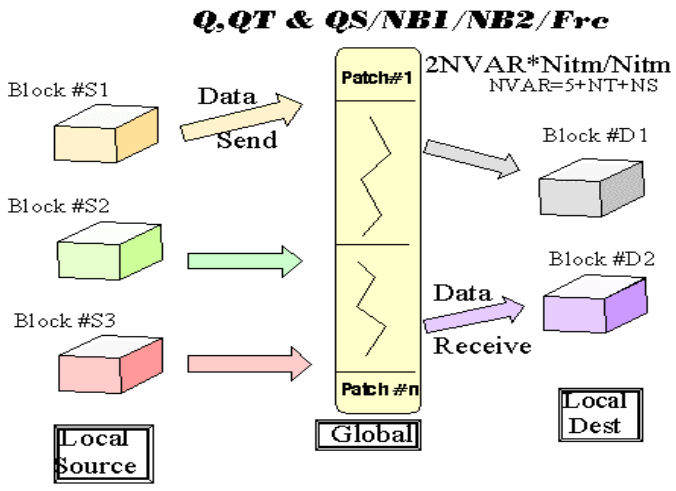

Figure B-1. Structure of General Data

iteration, the boundary conditions are sent to the buffer. Later, each block will collect the boundary conditions from the buffer using the global ID.

B.3 Test Cases using PAB3D MPI

The R10000 195 MHz SGI computers at the Configuration Aerodynamic Branch are used in the present simulations. Each of these computers has a speed close to $1/6^{th}$ of the Cray C90 computer. We have selected two test cases for the evaluation of the PAB3D MPI. First case represents a two-dimensional real gas simulation. The second case is three-dimension flow simulation. The second problem is a million grids 3D flow. Each case uses the standard two-equation turbulence model to simulate the viscous effect. These cases are not designed for efficient load balance using MPI.

Case 1: Five (5) Blocks 2D Nozzle with Real Gas Simulation (50,000 Grid Points)

A 50,000 grids and two-dimensional flow simulation of 3 gases flow is the first test case. We have used single and up to 3 processors in the evaluation of the PAB3D prototype. Using more than three processors will not add any speed because there are two blocks with sizes more than 33%.

Single processor performance: 57μs/grid point

MPI Performance

BCT 3%

GT 0.65%

Speed Increase 250%

Efficiency 83%

Multi processor performance 22.75 μs/grid point

BCT is the Boundary Conditions Time as ratio of total time.

GT is the Gathering Time as ratio to total time

Speed increase is the ratio between a single processor to the multiprocessors time

Efficiency is the (single processor time/(# processor * multiprocessor time)

Table B-4. Case 1 Grid distribution

Block #	%
1	3.7
2	35.9
3	38.4
4	20.1
5	1.9

Table B-5. Case 1 Load Distribution

P	Blocks	Load %
0	2	35.9
1	3	38.4
2	1 4 5	25.7

Case 2: Nine (9) Blocks 3D Nozzle Simulation (1,000,000 Grid Points)

A 1,000,000 grids and three-dimensional flow simulation of Nozzle/Jet Plume flow is the second test case. We have used single and up to 4 processors in the evaluation of the PAB3D prototype.

Single processor performance: 90 ms/grid point

MPI Performance for 3 Processors

BCT 2.5%

GT 0.45%

Speed Increase 252%

Efficiency 84%

Multi processor performance 35.7 μs/grid point 50% of C90 Speed

MPI Performance for 4 Processors

BCT 2.3%

GT 0.46%

Speed Increase 330%

Efficiency 82%

Multi processor performance 27.7 μs/grid point 69% of C90 Speed

Table B-6. Case 2 Grid distribution

Block #	%
1	8.4
2	9.6
3	18.5
4	27.4
5	27.4
6	1.7
7	1.8
8	2.6
9	2.6

Table B-7. Case2 Load Distribution using 3 Processors

P	Blocks	Load %
0	1 2 3	36.5
1	5 6 8	31.7
2	4 7 9	31.8

Table B-8. Case2 Load Distribution using 4 Processors

P	Blocks	Load %
0	1 2 6 9	22.4
1	3 7 8	23.0
2	4	27.3
3	5	27.3

APPENDIX C: Example Problem

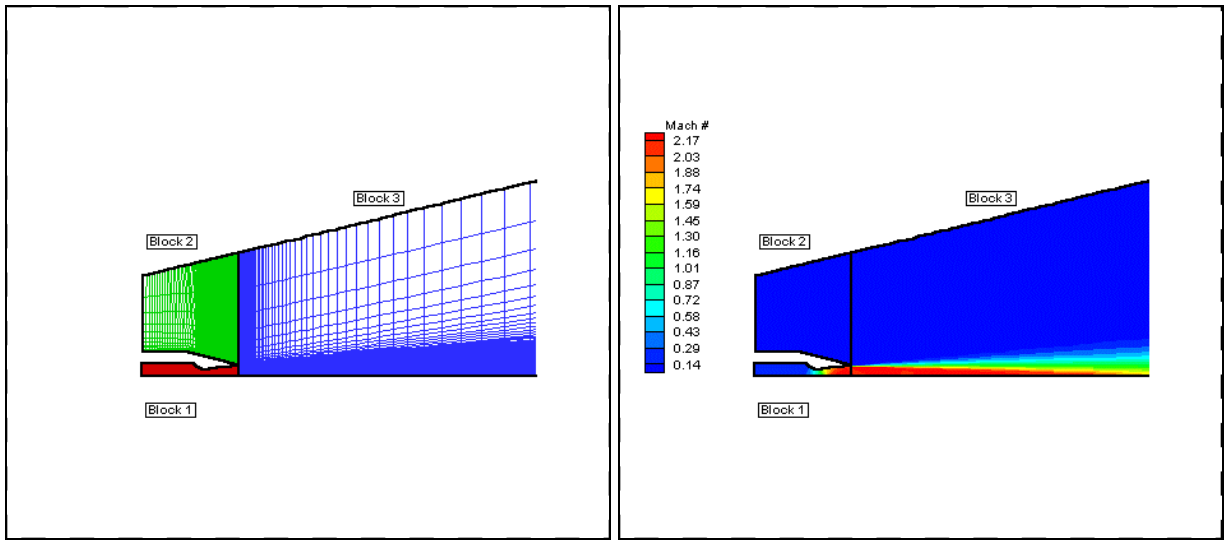

Figure C-1. Problem Definition

This case involves a "submerged" Supersonic jet emanating from an axisymmetric convergent-divergent Mach 2.2 nozzle. This nozzle was studied by J.M. Eggers in 1962. Velocity profiles and eddy viscosity distributions were obtained within the jet. The working fluid is air and the nozzle is operated at the pressure ratio corresponding to perfect expansion.

This case uses the grid and experimental data included in the NPARC code validation archive and the Wind validation archive.

C.1 Solver Control File

```
#!PAB3D 100
 "Grid File"
axinoz01.g
 "Restart File"
restart.d
 "INIT File"
'init.d' 'user.cont'
 nte    year  Flg Hr:Mnt
  0             98 '0 00:00'
   nzone    ichk ischeme
       1       3       4
    ngit   isafe   iauto
       2       0       0
nit
100  100
nitz
  1   1
#Blocks Block# idim jdim kdim nitb nseq  dt dtmb
       3
1     189      59       2       1     111    -1.0     0.0
```

```
2     189      25       2       1     111    -1.0     0.0
3     149     107       2       1     111    -1.0     0.0
 ####Block    1: (188,58,1)
   ivfxj  ivflux    irst   ivisc   kturb     ibs     ibf
       1       3       2      10       6       1     188
 i-order   i-lmt j-order   j-lmt k-order   k-lmt   ibias
       3       2       3       2       3       2       0
       ncut-Imin       ncut-Imax       Imin & Imax Faces
              1               1
    ibci      j1      j2      k1      k2
     -11       1      58       1       1
   10035       1      58       1       1
       ncut-Jmin       ncut-Jmax       Jmin & Jmax Faces
              1               1
   ibcjk      k1      k2      i1      i2
     -17       1       1       1     188
       0       1       1       1     188
       ncut-Kmin       ncut-Kmax       Kmin & Kmax Faces
              1               1
   ibcjk      j1      j2      i1      i2
     -17       1      58       1     188
     -17       1      58       1     188
 ####Block    2: (188,24,1)
   ivfxj  ivflux    irst   ivisc   kturb     ibs     ibf
       1       3       2      10       6       1     188
 i-order   i-lmt j-order   j-lmt k-order   k-lmt   ibias
       3       2       3       2       3       2       0
       ncut-Imin       ncut-Imax       Imin & Imax Faces
              1               1
    ibci      j1      j2      k1      k2
      -1       1      24       1       1
   10035       1      24       1       1
       ncut-Jmin       ncut-Jmax       Jmin & Jmax Faces
              1               1
   ibcjk      k1      k2      i1      i2
       0       1       1       1     188
      -1       1       1       1     188
       ncut-Kmin       ncut-Kmax       Kmin & Kmax Faces
              1               1
   ibcjk      j1      j2      i1      i2
     -17       1      24       1     188
     -17       1      24       1     188
 ####Block    3: (148,106,1)
   ivfxj  ivflux    irst   ivisc   kturb     ibs     ibf
       1       3       2      10       6       1     148
 i-order   i-lmt j-order   j-lmt k-order   k-lmt   ibias
       3       1       3       1       3       1       0
       ncut-Imin       ncut-Imax       Imin & Imax Faces
              3               1
    ibci      j1      j2      k1      k2
   10016       1      58       1       1
     -17      59      82       1       1
   10026      83     106       1       1
      -6       1     106       1       1
       ncut-Jmin       ncut-Jmax       Jmin & Jmax Faces
              1               1
   ibcjk      k1      k2      i1      i2
```

```
     -17       1       1       1     148
      -1       1       1       1     148
       ncut-Kmin       ncut-Kmax       Kmin & Kmax Faces
                1               1
   ibcjk      j1      j2      i1      i2
     -17       1     106       1     148
     -17       1     106       1     148
Axisymmetric Supersonic Nozzle
 rj  dt      iflagts     fmax  isym
 0.0254 -1.00  -4          5.00  2
 igrid  iriso inorm  kg1 kg2 iperf1 jkswp impvis
11     8     1      1   5   0      0     1
  ibc  i2d  itrp
 0    0    1
 ivrt istat sigl sigu gam  itre
 3    0     0.0  2.5  1.4  0
 nprfile
 0
```

C.2 User's Control File

```
'Begin Memo'
'End Memo'
'Begin Spec Cont'
 1.0   ,3  ,'CO2'  'N2'  'Air'          0
    0.1  0.9   0.
    0.1  0.9   0.
    0.0  0.0   1.
'End Spec Cont'
'Begin Ginit Cont'
   iunit  nblock    Ireg
       0       3       0
    ncut    jmin    jmax    kmin    kmax    iset
       1
               1      59       1       2       3
       1
               1      25       1       2       2
       1
               1     107       1       2       2
    nset   iinit
       3       1
      P0      T0    Mach     int  mut/mu   alpha    beta   gamma     iin
 162.000 525.000   0.300   0.000   0.000   0.000   0.000   1.400       0
      P0      T0    Mach     int  mut/mu   alpha    beta   gamma     iin
  14.700 525.000   0.010   0.000   0.000   0.000   0.000   1.400       0
      P0      T0    Mach     int  mut/mu   alpha    beta   gamma     iin
  14.700 525.000   0.300   0.000   0.000   0.000   0.000   1.400       0
'End Ginit Cont'
'Begin KE Cont'
 ibk ilhg iord       dtf itk icomp      comp       Int     ut/ul inl icu idmp
   1  -14    0       1.0   2     5         0     0.001     0.100   0   0    0
   2  -14    0       1.0   2     5         0     0.001     0.100   0   0    0
   3    3    0       1.0   2     5         0     0.001     0.100   0   0    0
'End KE Cont'
'Begin Surf Cont'
 ib,ifc1,ict,  bcf1,bcf2,bcf3,bcf4,bcf5
```

```
 2   1   1    0.145  0.15  90.  1.   0.4
'End'End Surf Cont'
'Beg'Begin Tran Cont'
 Number of Blocks with Trip Points & Trip K- Int
          2  5.0000001E-02
 Block Number  &  Number of I-Planes
    1               1
    Number of Points for Plane #1
          1
 Location J K I (for the finest grid)
          8           0           1
 Block Number  &  Number of I-Planes
 5               1
    Number of Points for Plane #1
          1
 Location J K I (for the finest grid)
          8           0           1
'End'End Tran Cont'
'Beg'Begin Bc Cont'
   iunit  nblock    Ireg
       0       3       0
    ncut    jmin    jmax    kmin    kmax    iset
       1
                1      59       1       2       1
       1
                1      25       1       2       2
       1
                1     107       1       2       2
    nset   iinit
       3       1
      P0      T0    Mach     int  mut/mu   alpha    beta   gamma     iin
 162.000 525.000   0.300   0.000   0.000   0.000   0.000   1.400       0
      P0      T0    Mach     int  mut/mu   alpha    beta   gamma     iin
  14.700 525.000   0.010   0.000   0.000   0.000   0.000   1.400       0
      P0      T0    Mach     int  mut/mu   alpha    beta   gamma     iin
  14.700 525.000   0.300   0.000   0.000   0.000   0.000   1.400       0
'End'End Bc Cont'
'Beg'Begin Perf Cont'
'End'End Perf Cont'
'Beg'Begin MPI Cont'
 prc# #nbl bl1-blnb
 0    2   2    4
 1    3   1    3   5
'End'End MPI Cont'
```

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