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CHAPTER 1

Introduction

PUMA (for ***P***arallel ***U***nstructured ***M***aritime ***A***erodynamics) is a computer program for the analysis of internal and external non-reacting compressible flows over arbitrary complex geometries. PUMA is built on the MPI library of message-passing calls to ensure high portability as well as good performance.

PUMA is based on the finite-volume method and supports mixed-topology unstructured grids composed of tetrahedra, wedges, pyramids, and hexahedra. The code may be run so as to preserve time accuracy for unsteady problems, or may be run using a pseudo-unsteady formulation to enhance convergence to steady-state. Either explicit or implicit time integration may be used. Primitive flow quantities (density, velocity, and pressure) are computed at the cell centers and saved on exit.

Because PUMA uses dynamic memory allocation, problem size is limited only by the amount of memory available on the machine. Since PUMA is targeted for distributed-memory parallel computers, which usually have an abundance of memory, little effort has been expended on reducing PUMA's memory requirements. Currently, with double precision floating point variables used throughout the code, PUMA needs 582 bytes/cell and 634 bytes/face, not including message passing overhead. For tetrahedral grids, this amounts to about 2002 bytes/cell, or 250 words/cell. This requirement can be reduced significantly simply by using single-precision floating point variables; a flag in the Makefile is provided for this purpose.

This manual is organized as follows: Chapter 3 describes the utilities distributed with PUMA, Chapter 4 is a summary reference for input variables, file formats, etc.

CHAPTER 2

Description

CHAPTER 3

Utilities

Grid Translation Utilities

Note: For historical reasons, the grid files associated with PUMA usually have a `.sg` extension. Therefore, the PUMA-format grid files are sometimes called "sg-files".

fromp3d takes an ASCII multizone format PLOT3D file and makes an sg-file. Although multiple zones may be present in the PLOT3D file, the consolidation of coincident nodes (called "equivalencing") is not robust, especially for viscous grids. It is planned that `fromp3d` will be extended at some future date to use zonal connectivity information from the structured input files, obviating the need for a distance-based equivalencing step. However, since this utility is intended for use in comparing results with structured codes (for validation) and not for production work, this extension may never happen.

Usage:

```
fromp3d <plot3d_file>
```

fromVgrid produces an sg-file from VGRID project files. It combines the data in the `.int`, `.grd`, and `.bc` files; the `.mapbc` file is not used by this utility. Since the project name is used to construct the file names, the VGRID project files must all have the same root name.

Usage:

```
fromVgrid <project_name>
```

compactSurf consolidates all of the surface ID's from the VGRID system into groups by the surface name in the `.mapbc` file. Since VGRID assigns a different surface ID to each patch in a model, and the number of named surfaces is usually much smaller, this utility can make a tremendous reduction in the total number of surfaces in a grid.

Usage:

```
compactSurf
```

(this utility is interactive).

Grid Reordering Utilities

gps produces a minimum-bandwidth reordering of the cell connectivity matrix using the Gibbs-Poole-Stockmeyer algorithm. This matrix ordering minimizes the total number of messages between computational domains, but tends to produce long domain boundaries. If the matrix semibandwidth is larger than the total number of cells divided by the number of partitions, then only nearest-neighbor communication will occur. Note that the optimality of this ordering is independent of the number of partitions.

Usage:

```
gps <sg_grid>
```

makeGraph writes a file representing the graph of the cell connectivity matrix. This ASCII file is used by the METIS utility to produce an optimal decomposition of the grid. "Optimal" in this context implies minimization of the length of the inter-domain boundaries, and is dependent on the number of partitions.

Usage:

```
makeGraph <sg_grid>
```

metis is a domain decomposition code available through the University of Minnesota. See the documentation (cobra:~cwsb/metis.manual.ps) for details.

Usage:

```
pmetis <graph_file> <number_of_partitions>
```

partitionOrder processes the sg-grid file and partition file output from `pmetis` to produce a new sg-grid that is ordered according to the partition file.

Usage:

```
partitionOrder <sg_grid> <number_of_partitions>
```

partitions produces and EnSight geometry file from an sg-grid, a partition file, and (optionally) a `.mapbc` file. It is different from `toEnsightGrid` in that each partition is created as a separate part. It is intended for previewing a partitioning. WARNING: `partitionOrder` can produce very large files.

Usage:

```
partitionOrder <original_sg_file> <partition_file> [mapbc_file]
```

Post-processing Utilities

consolidate combines the separate restart files written in a parallel run into a single restart file. This must be done before a restart run can be started.

Usage:

```
consolidate <restart_base_name>
```

(this is the same as the `"restartTo"` name in the input file).

dump produces an ASCII file of solution data at every cell center. The data in each column of the file is given in Table 1 on page 8.

This utility uses boundary condition, reference quantity, and freestream data from the input file in addition to the restart file. Therefore, valid values for these quantities must be used in the input file. The easiest thing to do is take the input file from the analysis run and use it to produce dump data.

CAUTION: FOR USE BY TRAINED CFD PROFESSIONALS ONLY. CAN PRODUCE HUGE FILES.

Usage:

```
dump <puma_input_file>
```

toEnsightGrid produces an EnSight format geometry file from an sg-file. The `.mapbc` file may also be specified; this will give the parts meaningful names in EnSight.

TABLE 1. Columns in the Dump File

Column	Description
1	x
2	y
3	z
4	density
5	u-velocity
6	v-velocity
7	w-velocity
8	static pressure
9	speed
10	Mach number
11	entropy
12	speed of sound
13	temperature
14	stagnation density
15	stagnation pressure
16	stagnation temperature
17	pressure coefficient

Usage:

```
toEnsightGrid <sg_file> [mapbc_file]
```

toEnsightResults produces EnSight variable files and an EnSight results file from an sg-file and a restart file (the grid file must be available to perform the interpolation from cell centers to vertices). Either conservative or primitive variable sets may be written; the default is to use conservative variables.

Usage:

```
toEnsightResults [-cons || -prim] <sg_file> <restart_file>
```

walls is similar to `dump` except that data is written only for faces that have boundary conditions of type 8, 9, or 10. In addition to the variables written by the `dump` utility, the absolute value of the skin friction and the wall heat transfer, respectively, are written to the last two columns.

Usage:

```
walls <puma_input_file>
```

CHAPTER 4

Reference

Input File

Sample Input File

```
Gamma    Rgas     rhoRef   Vref             muRef
1.4      287.04   0.16036  343.13818        1.81297E-05
rho_inf  u_inf             v_inf    w_inf    p_inf            fsMult
0.16036  686.27635        0.0      0.0      13486.712        1.0
mu_inf           T_Suth   PrLam    PrTurb
1.81297E-05      110.0    0.72     0.9
numIts   maxMinutes       wrRestart        wrResid  relResid absResid
1500     3780             100              1        1.0e-6   1.0e-15
CFLconst CFLslope
20.0e+0  0.0
localStepping    spatial_order    inviscid_flux    integ_scheme     limiter
1                2                "roe"            "ssor"           "none"
innerIters       innerTol omega   stages   K       commScheme
100              1.0e-1   1.0     1        0.0e+2  "delta q"
gridName         restartFrom      restartTo        residName
"grid.p3da.sg.8""puma-8.rst"      "puma-8.rst"     "puma-8.rsd"
implicitBCs      viscousModel
1                "laminar"
Num_surfaces
8
surface  BC_type  value1   value2   value3   value4   value5
1        -1
2        -3
3        -8
4        -2       0.18132488 663.5140391 -36.00617594 0.0 15992.39212
5         0
6         0
7        -2       0.18132488 663.5140391 -36.00617594 0.0 15992.39212
8         9
```

TABLE 2. Description of Input File Parameters

Parameter	Description	Permissible Values	Typical Values (SI)
Gamma	Ratio of specific heats	>0.0	1.4
Rgas	Gas constant	>0.0	287.04
rhoRef	Reference value for density	>0.0	1.225
VRef	Reference speed	>0.0	freestream speed of sound
muRef	Reference molecular viscosity	>=0.0	1.813e-5
rho_inf	Freestream density (dimensional)	>0.0	same as rhoRef
u_inf, v_inf, w_inf	Freestream velocity components (dimensional)	any	
p_inf	Freestream pressure (dimensional)	>0.0	101,325
fsMult	Scalar multiplier of the initial freestream velocity components. Used in supersonic blunt-body problems	0.0-1.0	1.0
mu_inf	Freestream molecular viscosity (dimensional)	>=0.0	same as muRef
T_Suth	Temperature offset for Sutherland's law for viscosity	>0.0	110.0
PrLam	Laminar Prandtl number	>0.0	0.72
PrTurb	Turbulent Prandtl number	>0.0	0.9
numIts	Maximum number of iterations to perform in this run	>0	100-1000 for implicit, 1000-5000 for explicit
maxMinutes	Maximum number of minutes to run	>=0	maximum for queue minus 5-10 minutes
wrRestart	Restart files will be written every wrRestart iterations	>0	100 or numIts / 5
wrResid	Residual history file will be updated every wrResid iterations	>0	1 for implicit, 5-10 for explicit

TABLE 2. Description of Input File Parameters

Parameter	Description	Permissible Values	Typical Values (SI)
relResid	The run will end when the relative residual goes below this value	>=0.0	1.0e-4 to 1.0e-6
absResid	The run will end when the absolute residual goes below this value	>=0.0	1.0e-16
CFLconst	If CFLconst > 0.0, the value of the CFL number is computed using CFL=CFLconst + CFLslope * log10 (R0/Rn) at every iteration. If CFLconst < 0.0, then it is interpreted as a timestep, and CFLslope is ignored.	>0.0: CFL number entered <0.0: Timestep entered	$10\text{-}10^{21}$
CFLslope	See above.	>=0.0	0.0; CFLconst/4
localStepping	If 1, use local timestepping to improve convergence to steady state	0, 1	1
spatial_order	Order of the first neglected term in the Taylor series expansion of the spatial error	1, 2	2
inviscid_flux	Numerical flux scheme to use	"roe", "van leer"	"roe"
integ_scheme	Time integration scheme to use	"runge-kutta", "jacobi", "fsor", "rsor", "ssor"	"ssor"
limiter	Monotone limiter to use in second-order computations	"none", "venkat", "barth", "van albada", "superbee"	"van albada" or "none"

TABLE 2. Description of Input File Parameters

Parameter	Description	Permissible Values	Typical Values (SI)
innerIters	Maximum number of iterations to perform on the inner problem	>1	100
innerTol	Inner problem is converged when $\frac{\|Ax-b\|}{\|b\|} \le innerTol$	>=0.0	0.1
omega	Used in SOR schemes. No benefit. Shouldn't be in here.	0<omega<2	1.0
stages	Number of stages to perform in Runge-Kutta time integration	>1	1, 2, 4
K	Parameter in Venkatakrishnan and Van Albada limiters	>0.0	0.0-500.0
commScheme	Communications strategy to use for parallel solution of the inner problem	"ignore", "approximate", "diagonals", "delta q"	"delta q"
gridName	Filename (and path) of the grid file		"grids/<prob>.sg"
restartFrom	The name of the restart file used to initialize the solution. Freestream conditions are used if NULL.		"", "<prob>.rst"
restartTo	The name of the restart file to save the solution		Default is "restart.rst"
residName	File name to save residual history		If NULL (""), no residual history will be saved
implicitBCs	Boolean flag. If 1, then use implicit BC's	0, 1	1

TABLE 2. Description of Input File Parameters

Parameter	Description	Permissible Values	Typical Values (SI)
viscousModel	Treatment of viscous fluxes	"inviscid", "euler", "laminar", "spalart", "k-omega"	There is no difference between the "inviscid" and the "euler" model
Nsurfaces	Number of boundary surface ID's	>0	

TABLE 3. Boundary Condition Types

Type	Description	Value 1	Value 2	Value 3	Value 4	Value 5
0	Do nothing					
1	Fixed at freestream					
2	Fixed at given values	density	u	v	w	pressure
3	First-order extrapolation from the interior					
4	Second-order extrapolation from the interior					
5	Inflow/outflow (Riemann)					
6	Specified p0, T0	total pressure	total temperature			
7	Fixed back pressure	pressure				
8	Tangency					
9	No-slip adiabatic wall					
10	No-slip fixed-temperature wall	T_{wall}				
17	Zero u-velocity					
18	Zero v-velocity					
19	Zero w-velocity					

File Formats

Grid File (ASCII)

For the sake of portability, this is an ASCII file. The fields on each line are delimited by spaces; the lines may be up to 127 characters long, and may not be strung together.

The file format is given below:

```
header
nodeRecord[0]
nodeRecord[1]
.
.
.
nodeRecord[Nnodes - 1]
faceRecord[0]
faceRecord[1]
.
.
.
faceRecord[NbounFaces - 1]
faceRecord[NbounFaces]
.
.
.
faceRecord[Nfaces - 1]
```

Where the records are defined as follows:

```
header:
        Nnodes Nfaces Ncells NbounFaces
nodeRecord:
        x y z
faceRecord:
        cell[0] cell[1] surface Ncorners corner[0] ... corner[Ncorners - 1]
```

The parameters in the header are defined as follows: `Nnodes` is the total number of nodes in the grid; `Nfaces` is the total number of faces (boundary and interior) in the grid; `Ncells` is the total number of cells (interior only); and `NbounFaces` is the total number of boundary faces (or ghost cells) in the grid.

The first `NbounFaces` faces are boundary faces. The first cell (`cell[0]`) in each of these faces is a ghost cell. Its value in the first face is `Ncells`, and it is incremented by 1 for each boundary face. Therefore, the value is always ≥ Ncells, and the total size of the solution vector in the code is `Ncells + NbounFaces`.

The remainder of the faces are interior faces; the value of `surface` is zero for each of these records.

Residual History File (ASCII)

The residual history file contains the entire convergence history of an analysis. It is read upon initialization of every restart run. Since each plotting package seems to use a different convention for explanatory lines in the file, there are no comments, labels, titles, etc. in the file. This is a plain space-delimited ASCII file, and every line is identical.

TABLE 4. Columns of the Residual History File

Column	Description
1	Iteration number
2	Total elapsed wall clock time for this iteration
3	Absolute L_2-norm of the residual for this iteration (R_n)
4	Relative L_2-norm of the residual for this iteration (R_n / R_0)
5	Number of iterations required to converge inner problem on the previous iteration
6	Absolute convergence of the inner problem for the previous iteration $(\|Ax - b\|)$
7	Relative convergence of the inner problem for the previous iteration $\left(\frac{\|Ax - b\|}{\|b\|}\right)$
8	Total mass flux imbalance
9	Total x-momentum flux imbalance
10	Total y-momentum flux imbalance
11	Total z-momentum flux imbalance
12	Total energy flux imbalance
13	Normalized mass flux imbalance
14	Normalize x-momentum flux imbalance
15	Normalized y-momentum flux imbalance
16	Normalized z-momentum flux imbalance
17	Normalized energy flux imbalance
18	CFL number used for the current iteration

Restart File (Binary)

The restart file is a C binary file containing all of the data needed to reinitialize the solution to continue an analysis. There are also some addititional data on freestream and reference conditions as well as the residual norm for each cell; the residual data is useful for diagnosing incorrect boundary conditions, areas of inadequate grid resolution, and other analysis problems.

TABLE 5. Format of the Restart File

Type	Variables
int	Number of cells in restart file
double	Ratio of specific heats γ
double	Gas constant R
double	Reference density ρ_{ref}
double	Reference speed V_{ref}
double	Simulation time of this restart file (seconds)
double[5]	Freestream values $\left[\rho \ u \ v \ w \ p\right]^T$
double[Ncells][5]	Solution vector for each cell $\left[\rho \ u \ v \ w \ p\right]^T$
double[Ncells]	Residual norm for each cell