

# Dynamic Load balancing and CFD Simulations on the MecaGRID and GRID5000

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*Dynamic Load balancing and CFD Simulations  
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\_\_\_\_\_ Thème NUM \_\_\_\_\_



*R*apport  
*de recherche*





## Dynamic Load balancing and CFD Simulations on the MecaGRID and GRID5000

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Thème NUM — Systèmes numériques  
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**Abstract:** CFD simulations on Clusters and GRIDS having mixed processor speeds present several challenges to achieve efficient load balancing. If both the fast and slow processors are given the same amount of work, the faster processors will finish their computations first and wait for the slower processors to finish. To achieve load balancing more work must be given to the faster processors so that all the processors finish their computations at the same time (work is proportional to the processor mesh size). Another complication is that for current Clusters and GRIDS in the near future, the user will not know in advance the mixture of fast and slow processors that will be assigned to their computation, thus the user cannot partition the mesh in advance of the CFD simulation. This difficulty is doubly complicated as the mesh partitioning step is usually performed on a workstation thus not directly linked to the parallel CFD code. For mesh partitioners executing on parallel computers, the complication arises in that the mesh partitioning code and the CFD code are separate MPI codes designed to be run independently of each other. As a result the two codes cannot simply be run back-to-back as each code may be assigned different mixtures of fast and slow processors resulting in a partitioned mesh not optimal for the CFD run.

In this study, in order to overcome the problems related to computing with arbitrary mixtures of fast and slow processors, the mesh generator has been integrated into the CFD code. Thus optimal size partitions are automatically created for different mixtures of fast and slow processors. The efficiency of this approach is demonstrated for Clusters, the MecaGRID and the GRID5000. Validation tests using the GRID5000, the MecaGRID, and the INRIA *nina-pf* cluster produced speedups on the order of 1.32 to 1.52 relative to the same run using the homogeneous partitioning which compares well with the theoretical speedup of 1.5.

Finally, we use the dynamic computing capability of the new CFD code to compute a 20 million vertices mesh using 256 processors at five different GRID5000 sites.

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**Key-words:** Computational fluid dynamics, GRID Computing, MecaGRID, GRID5000, F90, MPI, dynamic mesh creation and partitioning

## **Equilibrage de charge sur Clusters et GRILLES de calcul avec différents vitesses de processeurs**

**Résumé :** On s'intéresse à l'équilibrage de charge des simulations numériques en Mécanique des Fluides Numérique sur Clusters et Grilles de calcul comportant des processeurs de vitesses différentes. Pour réaliser cet équilibrage, il est nécessaire d'attribuer entre deux synchronisations/communications plus de calculs aux processeurs plus rapides qu'aux processeurs les plus lents, de manière à ne pas perdre de temps en attentes. Une difficulté supplémentaire réside dans l'impossibilité en pratique de savoir quel nombre de chaque type de processeur sera attribué à la tâche au moment de son démarrage, information dépendant de la charge instantanée du système. L'utilisateur est dans ce cas dans l'impossibilité de préparer une partition adéquate avant le lancement du calcul. Or en général les logiciels disponibles pour les deux étapes, partitionnement, simulation proprement dite, sont distincts et à lancer sur le système séparément. Dans ce cas ils ne tournent pas sur le même assortiment de processeurs. Dans cette étude, générateur de maillage et partitionneurs sont intégrés au solveur et seront donc lancés en une seule requête soumise au Cluster. Un partitionnement adapté au jeu de processeurs attribué peut donc être réalisé juste au moment du calcul. L'efficacité de cette approche est démontrée pour différentes configurations de grilles de calcul et de Clusters fortement hétérogènes.

**Mots-clés :** Mécanique des fluides numérique, Grille de calcul, F90, MecaGRID, GRID5000

## 1 Introduction

CFD simulations on Clusters and GRIDS using processors with different speeds present several major challenges in order to achieve efficient load balancing. We use the term cluster to denote a computer comprised of a collection of homogeneous processors and Cluster to refer to a computer comprised of several clusters at the same institution administered by the same system administrator. For example, the INRIA Cluster in Sophia Antipolis is comprised of two separate on-site clusters *nina* and *pf*. The term GRID refers to a Computational Grid composed of clusters belonging to different institutions, each having a different administrator. An example is the MecaGRID Project Funded by the French Ministry of Research<sup>1</sup> comprised of clusters belonging to INRIA<sup>2</sup> in Sophia Antipolis, the IUSTI<sup>3</sup> in Marseille and the CEMEF<sup>4</sup> in Sophia Antipolis. The GRID5000 is a Project funded by the French Ministry of INRIA, and the CNRS<sup>5</sup>. The goal of the GRID5000 is to create a GRID containing 5000 processors. The GRID is currently comprised of clusters in Sophia Antipolis, Toulouse, Orsay, Rennes, Bordeaux, Grenoble, Lyon, Nancy and Lille and involves 17 French research labs. The clusters forming a GRID are usually separated by large physical distances thus communication times between the different clusters of the GRID may be larger than those for Clusters.

The challenges that arise when simulations are assigned different types of processors relate to the different processor hardware characteristics (speeds, RAMs, and caches, ...etc). For example some processors may have 2 Ghz speed<sup>6</sup> with 1 GB of RAM and 512K cache while others have 1 Ghz with 1/2 GB of RAM with 256K cache with 256K cache. To achieve load balancing twice as much work must be given to the faster processors so that both the fast and slow processors finish their computations in approximately the same time. If both the fast and slower processors are given the same amount of work, the faster processors will finish their computations first and wait for the slower processors to finish.

The goal of this study is to achieve efficient simulations using the MPI CFD software, *AERO3D*, developed through a collaboration between the University

<sup>1</sup><http://www.recherche.gouv.fr/recherche/aci/grid.htm>

<sup>2</sup><http://www.inria.fr>

<sup>3</sup>Institut Universitaire des Systèmes Thermiques et Industriels

<sup>4</sup>Ecole des Mines de Paris à Sophia-Antipolis

<sup>5</sup><http://www.cnrs.fr>

<sup>6</sup>2 Ghz is an approximation to the actual value of 2.2 Ghz.

of Colorado at Boulder, the University of Montpellier, and INRIA Sophia Antipolis - see Fezoui et al [6], Farhat and Lanteri [5], and Lanteri [8]. The *AERO3D* software is intensively used, in particular by the universities of Montpellier, Pisa and Pau in several CFD research studies (see for example Camarri et al [3], El Omari et al [4], and Koobus and Farhat [7]).

The parallelization strategy in *AERO3D* uses mesh partitioning to subdivide a global mesh into smaller partitions<sup>7</sup>; each partition being computed by a different processor. The message-passing programming model of Fezoui et al [6], Farhat and Lanteri [5], and Lanteri[8] using the Message Passing Interface (MPI) communication library ensures software portability from one parallel system to another. The mesh partitioning algorithms and the generation of the corresponding communication data structures are computed in a PREPROCESSING step.

Mesh partitioners are often non-parallel codes executed on desktop computers. For the *AERO3D* code, the preferred mesh partitioners are METIS<sup>8</sup> and TopDomDec<sup>9</sup>, both non-parallel codes. Other mesh partitioners that execute on parallel machines using MPI will be discuss later. The usual procedure is to run the mesh partitioner first (PREPROCESSING) to create the partitions to be used by the CFD run. This is followed by the execution of the CFD software.

In general, when running on a Cluster (or future GRIDS), the user will not know in advance the mixture of processors that will be assigned to the computation. This is currently true for the INRIA *nina-pf* cluster which has both 2 Ghz and 1 Ghz processors; the user requests the total number or processors to be used and the job manager assigns the processors according to availability. Thus, if a user requests 32 processors on the INRIA Cluster<sup>10</sup>, *32-nina* and *0-pf*, *24-nina* and *8-pf*, *8-nina* and *24-pf*, *0-nina* and *32-pf* ... etc. are various possible allocations the user could receive. Note that for runs on the INRIA Cluster, all the requested processors must be available before any processors are assigned to the job. This is very efficient and the INRIA Cluster is an excellent example of how the future generation of GRIDS will function.

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<sup>7</sup>Also called subdomains or blocks

<sup>8</sup><http://www-users.cs.umn.edu/karypis/metis/>

<sup>9</sup>University of Colorado at Boulder

<sup>10</sup>The INRIA Cluster as of January 13, 2006 has 64 processors, *32-nina* and *32-pf*

As of the date of this report, this is not true neither for the MecaGRID or the GRID5000<sup>11</sup> where the user specifies which clusters of the GRID are to be used and the number of processors on each cluster.

In contrast to the INRIA Cluster, the MecaGRID assign processors on the individual clusters as soon as they become available at any site requested. Thus if the user requests 128 processors and 120 are immediately available, the 120 are assigned to the simulation and will start execution. However, the job will wait at the first MPI barrier until the remaining eight processors are assigned and reach the same barrier. This may be hours or days away effectively blocking the 120 processors that remain assigned but inactive from being used by other users. This is extremely inefficient as the cluster(s) on which the processors were requested may be totally saturated while other clusters on the GRID have immediate processors available. Future GRIDS will function like the INRIA *nina-pf* Cluster, that is, the user requests the total number of processors and the GRID job manager will assign the processors according to availability on all the clusters of the GRID.

What are the consequences of not knowing, in advance, the mixture of fast and slow processors that will be assigned to a computation? The major consequence is that the user cannot partition a mesh as a PREPROCESSING step. If we assume that the mesh partitioner is also an MPI code, this difficulty is doubly complicated as the mesh partitioner code and the CFD code are separate MPI codes designed to be run independently of each other. However this is not possible as different mixtures of fast and slow processors may be assigned to the two runs thus, the partitioned mesh will not be optimal for the CFD run.

In this study, to overcome the difficulties related to simulations involving fast and slow processors, the mesh generator has been integrated into the CFD software. This approach assures that the mesh partitions will be optimal for different combinations of fast and slow processors assigned to the CFD execution.

## 2 Dynamic memory allocation

In order to achieve load balancing on Clusters and GRIDS with mixed processor speeds, two conditions must be met. First, the CFD software must have

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<sup>11</sup>Both first generation GRIDS

dynamic memory allocation. To achieve this, an F90 version of the *AERO3D* software was created - see Wornom [10], the original code was programmed in F77. As a consequence the size of the F77 executable is determined at compile time based on the mesh data of the largest partition and the same executable is used on all the processors. This leads to situations where the RAM for slower processors is too small to run the executable. F90 permits dynamic memory allocation thus the executable size for each processor is proportional to the local processor mesh size.

The second condition is dynamic mesh partitioning. This is achieved in this study by integrating the mesh generator into the CFD software.

### 3 Mesh generators and mesh partitioners

#### 3.1 Standard procedure

In the standard procedure there are three independent software involved in a CFD simulation: a mesh generator, a mesh partitioner, and the CFD software.

The first step is to generate a mesh for the simulation. There are several commercial software available. An example is GSH3D developed at INRIA. In this study we prefer the simpler free open source software MeshCanale developed at the University of Pisa by Dr. Simone Camarri. Mesh generators may be non-parallel codes or parallel codes. GSH3D<sup>12</sup> and MeshCanale are both non parallel codes executed on desktop workstations.

The second step is to partition the mesh created by the mesh generator. If none exists, the user must write an interface so that the global mesh file created by the mesh generator can be read by the mesh partitioner. For the mesh partitioners used with *AERO3D*, the global mesh file is named *fluid.sinus* - see Appendix A for details. This interface already existed MeshCanale and was written for GSH3D by the author. The user specifies the number of partitions and the mesh partitioner partitions the global mesh file.

Next, if none exists, the *AERO3D* user must write an interface so that the partitioned data created by the mesh partitioner is written in a format readable by the *AERO3D* software. These files are named *flu-00001*, *flu-00002*, where 1 and 2 refer to partitions 1 and 2, ..., and the *flu.glob* file that contains the mesh global parameters - see Appendix B for additional details. Writing

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<sup>12</sup>The 1999 sequential version of GSH3D is installed at INRIA Sophia Antipolis.

this interface is not a trivial step and is a major reason why the PARmetis<sup>13</sup> mesh partitioner is not presently used at INRIA to partition meshes for the *AERO3D* software. At the present time, the partitions created with the mesh partitioners developed at the CEMEF<sup>14</sup>, TopDomDec<sup>15</sup>, METIS\_Stanford<sup>16</sup>, and MeshCanaleMP (see section 3.2) are directly readable by the *AERO3D* software. The CEMEF, PARmetis and MeshCanaleMP are mesh partitioning codes that execute on parallel computers. TopDomDec and METIS\_Stanford are non-parallel codes executed on workstations. The third step is the execution of the CFD software that reads the partition data created by the mesh partitioner.

In summary, the standard procedure consists of executing three independent codes, the mesh generator, the mesh partitioner and the CFD software.

### 3.2 Integrated parallel procedure

The meshes used in the MecaGRID study of Wornom [11] were generated using the F77 non-parallel mesh generator MeshCanale run on a workstation. For this reason and the availability of the source code, MeshCanale was selected as the first mesh generator to be transformed into a F90 parallel MPI code and integrated into the *AERO3D* software.

We started by creating an F90 version of the MeshCanale code in order to have dynamic memory allocation. Next the adaptation to running in parallel using MPI was accomplished. The major effort was in writing subroutines to identify the different processors assigned to the simulation and a load balancing algorithm to define the partitions. The complication arises due to the English-Flag design (see section 4 used in MeshCanale. The English-Flag design involves eight hexagonal and the partitioning must result in a correct English-Flag design.

In MeshCanaleMP the mesh is generated simultaneously for all partitions. Therefore the notion of partitioning a global mesh created by a mesh generation code is no longer valid. Generating the mesh directly on each partition has several advantages over the standard approach<sup>17</sup>, in particular for large meshes.

<sup>13</sup><http://www-users.cs.umn.edu/~karypis/memis/>

<sup>14</sup>Centre de mise en forme des matériaux de l'Ecole des Mines de Paris-Sophia Antipolis

<sup>15</sup>University of Colorado at Boulder

<sup>16</sup>*AERO3D* interface written by Professor Farhat, University of Stanford, Palo Alto, CA

<sup>17</sup>Generating the global mesh with a grid generator and partitioning the global mesh using a mesh partitioning code

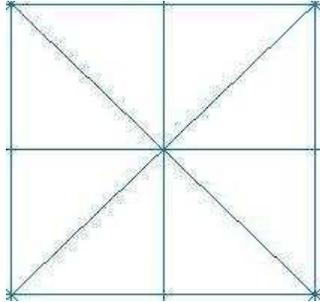


Figure 1: MeshCanale English-Flag design

Executing the mesh partitioner separately requires additional memory to store the global mesh. This additional memory is in addition to the memory needed to create the partitions. By integrating the mesh generator into the CFD software, this additional memory is avoided here as there is no global mesh file. The memory saved permits much larger mesh partitions to be created than would be otherwise possible. This effectively allows us to create partitions for very large meshes would not be possible using the standard approach.

## 4 Mesh generator - MeshCanale

MeshCanale is composed of three parts. First, MeshCanale creates a structured hexahedra mesh and then divides each hexahedra into six tetrahedra using the English-Flag design shown in Figure 1 for a plane. The third part writes the *fluid.sinus* file containing the number of vertices, tetrahedra, and external faces, the Cartesian coordinates, the tetrahedra connectivity, and the connectivity for the external faces and the type of boundary conditions to be applied.

### 4.1 Partitioning options

The MeshCanaleMP code was developed to study blast waves interacting with a high density fluid of spherical shape in a rectangular channel - see Figure 3 (from Wornom et al [9]) shows the solution after the blast wave has passed through the bubble. The blast wave is moving from the lower left to the upper

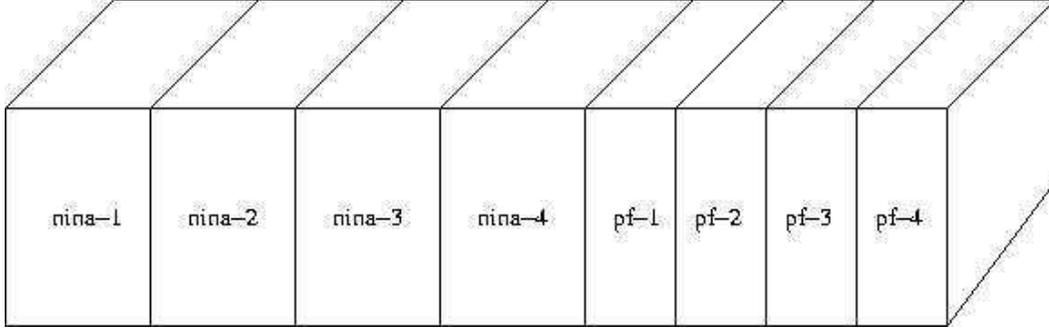


Figure 2: Partitioning by slicing

right of the figure. For this example a simple rectangular mesh,  $i = 1, \dots, I_{max}$ , ... with  $I_{max}$ ,  $J_{max}$ , and  $K_{max}$  equal to 51, 51, 97 ( $51 \times 51 \times 97$ ) was used.

Two obvious partitioning options exist: 1) Slicing and 2) Dicing. Figure 2 illustrates slicing using 8 processors, 4-*nina* and 4-*pf*; the 4-*nina* partitions are two times larger than the 4-*pf* partitions reflecting the faster speed of the *nina* processors. Message passing occurs between the partition interfaces. Note the only messages passed between the fast cluster (*nina*) and the slow cluster (*pf*) occur between processor 4 of *nina* and processor 1 of *pf*.

Using the slicing option, one can easily show that the minimum message passing occurs if the mesh is sliced in the counter direction opposite to the

$$\min(I_{max} \times J_{max}, I_{max} \times K_{max}, J_{max} \times K_{max}). \quad (1)$$

Therefore the  $51 \times 51 \times 97$  mesh was sliced in the  $k$ -direction.

The partitions created by slicing should be optimal for VPN (Virtual Private Network) GRIDS like the MecaGRID. For VPN GRIDS the processors have private IPAs and only one processor is used to exchange information between processors on different clusters of the GRID using tunneling between the frontend machines of the clusters comprising the GRID. Using the slicing method, only one *nina* processor exchanges information with one *pf* processor. If many processors are trying to pass data at the same time as will occur if 100 or more processors are involved, the VPN will experience greater transfer slowdowns when non-slicing partitioning methods are used. For GRIDS with public IPAs, such as GRID5000, the partitioning method will be less important.

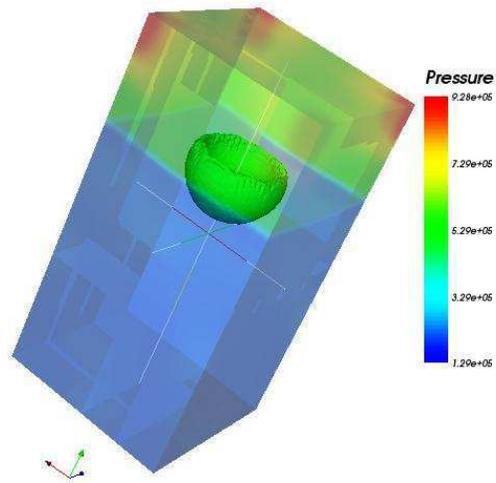


Figure 3: Blast wave pressure contours after 720 time steps

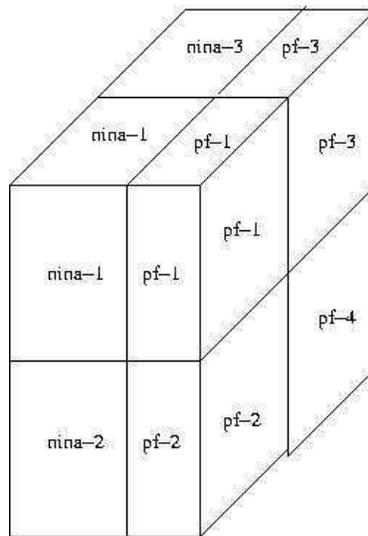


Figure 4: Partitioning by dicing

A alternative to slicing would be "dicing" where the mesh is divided into blocks. Figure 4 illustrates dicing with 8 processors, 4-*nina* and 4-*pf*. As can be seen, the message passing between the different processors is more complicated than that shown in Figure 2 where the slicing option is used. With 8 processors one can see that each *nina* CPU exchanges messages with a *pf* processor in addition to its *nina* neighbors. Thus there are four messages passed between the *nina* cluster and the *pf* cluster, likewise for the *pf* processors. The complexity increases as the total number of processors increases.

## 5 Heterogeneous partitioning

Consider the blast wave problem with a rectangular global mesh of 51x51x97 (*I*<sub>max</sub>, *J*<sub>max</sub>, *K*<sub>max</sub>) with *I*<sub>min</sub> = *J*<sub>min</sub> = *K*<sub>min</sub> = 1. Application of equation 1 shows that the minimum message passing occurs when the slicing method is applied in the k-direction.

Suppose we have two clusters with different processors speeds, one with 2.2 Ghz and the other with 0.999 Ghz. For illustration purposes we take the ratio of the fast processors to the slow processors equal to 2. For the heterogeneous partitioning we want the fast processors to compute twice as many tetrahedra as the slower processors.

The mesh is generated in two steps. First, we determine how many tetrahedra will be computed on the fast cluster and how many on the slow cluster.

The general expressions to be used when defining the hexagonal input (*i*,*j*,*k* values for each partition) to the MeshCanaleMP code are given by

$$\Delta k^{fast} = \frac{Kmax - 1}{1 + \frac{N^{slow}}{2 \times N^{fast}}} \quad (2)$$

$$\Delta k^{slow} = (Kmax - 1) - \Delta k^{fast} \quad (3)$$

Equations 2-3 returns an integer value only for equal number of fast and processors or only *nina* or *pf* processors are used - see Table 1 which shows an example for 32 total processors for *K*<sub>max</sub> = 97 with different mixtures of fast and slow processors.

When the number of fast processors is not an integer, and extra k-plane is given to the faster cluster (column Code).

Mixture		Theoretical		Code	
$N^{fast}$	$N^{slow}$	$\Delta k^{fast}$	$\Delta k^{slow}$	$\Delta k^{fast}$	$\Delta k^{slow}$
32	0	96.000	0.000	96	0
28	4	74.667	21.333	75	21
24	8	57.600	38.400	58	38
20	12	43.636	52.364	44	52
16	16	32.000	64.000	32	64
12	20	22.154	73.846	23	73
8	24	13.714	82.286	14	82
4	28	6.400	89.600	7	89
0	32	0.000	96.000	0	96

Table 1: Computation of intervals

The next step is defining the size of the partitions. These are given by the relation

$$\delta k^{fast} = \Delta k^{fast} / N^{fast} \quad (4)$$

$$\delta k^{slow} = \Delta k^{slow} / N^{slow} \quad (5)$$

For most mixtures,  $\delta k^{fast}$  and  $\delta k^{slow}$  will not be integers and adjustments are made similar to that for  $\Delta k^{fast}$  and  $\Delta k^{slow}$ .

### 5.1 Executing MeshCanaleMP separately of AERO3D

In this section we discuss features related to running MeshCanaleMP as a stand alone program. MeshCanaleMP reads its data from the file *CanaleMP.data*. Table 2 shows the different entries in the file *CanaleMP.data*

The LargeMesh flag was added for cases where very large meshes are used. The LargeMesh flag is independent of the MeshCanaleMP option - see section 5.3.

The flags *nWRTflu* and *nWRTsinus* control writing of the *flu-00001*, *flu-00002*, ..., *flu.glob* files and the *fluid.sinus* file. The flags are set to 1 to activate.

The number of mesh points in i, j, k are given by Imax, Jmax, and Kmax. The max/min values of x are given by xmax/xmin, similar for the y and z coordinates. The boundary condition types are set by the bcImax, bcImin, bcJmax, bcJmin, bcKmax, and bcKmin.

```

read (myunit,*) LargeMesh
read (myunit,*) nWRTsinus, nWRTflu
read (myunit,*) Imax,Jmax,Kmax
read (myunit,*) xmin,xmax
read (myunit,*) ymin,ymax
read (myunit,*) zmin,zmax
read (myunit,*) bcImax, bcImin
read (myunit,*) bcJmax, bcJmin
read (myunit,*) bcKmax, bcKmin

```

Table 2: *CanaleMP.data* file

Vertices	CPUs	fluid.sinus	flu-xxxx	Total	WRTsinus	WRTflu
252K	16	30 MB	3 MB	3.7 sec	1.4 sec	2 sec
2M	48	233 MB	9 MB	28.8 sec	10 sec	19 sec
16M	48	1.86 GB	69 MB	233 sec	90 sec	142 sec
117M	48	14.9 GB	505 MB	45 sec	-	-
117M	64	14.9 GB	378 MB	7 sec	-	-

Table 3: MeshCanaleMP examples

Table 3 gives examples of different runs using MeshCanaleMP for meshes up to 117 million vertices and 64 processors on the INRIA *nef* cluster<sup>18</sup>. The first four runs show the total time, the time to write the *fluid.sinus* file<sup>19</sup>, and the partition files *flu-00001*, *flu-00002*, ... etc and the *flu.glob* file. Note that the majority of the time is in writing these files. For a mesh with 16 million mesh vertices the *fluid.sinus* file is 1.86 GB and the 48-processor *flu-xxxx* files 69 MB, these files were written unformatted. The formatted files are approximately four times larger. It is obvious that for large simulations one must avoid writing these files.

## 5.2 Executing MeshCanaleMP from within *AERO3D*

The basic parameters and control flags for the *AERO3D* software are found in the *flu.data* file. These include the number of time steps, whether the run

<sup>18</sup>The *nef* cluster has 64 processors at 2.2 Ghz speed and was used for the development of the MeshCanaleMP code.

<sup>19</sup>*fluid.sinus* file is input to the mesh partitioner. It is also needed for graphics.

uses the explicit or implicit algorithm, whether the time scheme is 1st or 2nd order, ... etc.

To execute the MeshCanaleMP mesh partitioner within the *AERO3D* execution, four additional flags have been added; these flags are given for seven different examples in Table 4 (1=activate).

Run	LargeMesh	nMeshCanaleMP	nWRTflu	nWRTsinus
1	0	0	0	0
2	0	0	0	1
3	0	1	1	1
4	0	1	0	1
5	0	1	0	0
6	1	1	0	0
7	1	0	0	0

Table 4: Flags related to accessing MeshCanaleMP within *AERO3D* software

After the processors have been allocated for the *AERO3D* run, the MeshCanaleMP program is executed, if the parameter  $nMeshCanaleMP = 1$  to create the mesh and the partitions.

If  $nMeshCanaleMP = 0$ , the MeshCanaleMP is not used and the files with the data for each partition must already exist. Run 1 corresponds to the case where the user has existing partition data files<sup>20</sup>, *flu-00001*, *flu-00002*, ... etc and the *flu.glob* file. This is the standard procedure for the *AERO3D* code.

Several subroutines that have been written for the MeshCanaleMP are useful for runs where the MeshCanaleMP is not used. For example, the graphical program needs the *fluid.sinus* file containing the global mesh data in addition to the solution files. Normally the *fluid.sinus* is the input to the mesh partitioner and is available. Should it not be available, as sometimes occurs, the *AERO3D* code will write the *fluid.sinus* file if  $nWRTsinus = 1$ . Run 2 asks *AERO3D* to write the *fluid.sinus* file for the existing *flu-00001*, *flu-00002*, ... etc and the *flu.glob* file used.

Run 3 runs the MeshCanaleMP from within the *AERO3D* code and writes the *flu-00001*, *flu-00002*, ... etc and the *flu.glob* file and the *fluid.sinus* file.

Runs 4-5 are for very large meshes (> 2 million vertices). For large meshes writing the *flu-00001*, *flu-00002*, ... etc and the *fluid.sinus* file should be

<sup>20</sup>See APPENDIX B for description

avoided as these files can be extremely disk space consuming<sup>21</sup>. Since the *flu-00001*, *flu-00002*, ... etc files are created doing the run there is no real reason to save them. Run 5 does not save the *fluid.sinus* thus assumes that the graphical files have been created within the *AERO3D* run.

### 5.3 *LargeMesh = 1*

For meshes on the order of 16 million vertices and larger, the *fluid.sinus* and the files containing the solutions at different time steps are too large to be viewed with ParaView<sup>22</sup> on a workstation with 4 GB of RAM. The solution files are named *solf.000100.data* where 000100 is the solution at the 100th time step.

When *LargeMesh = 1*, the *fluid.sinus* and the solution file *solf.000100.data* are written separately for each processor. The files are written as *fluid.sinus-00001*, *fluid.sinus-00002*, .. etc and *solf-00001.000100.data*, *solf-00002.000100.data*, ... etc. These smaller files are much smaller files than if all the processor solutions were written on a single file. As a consequence, they can be viewed using ParaView run sequentially or the MPI version of ParaView<sup>23</sup>.

Runs 6 and 7 show examples where the *LargeMesh* option is used with and without the *MeshCanaleMP* code.

### 5.4 *LargeMesh = 2*

When the option *LargeMesh = 2* is used, no 3D solution files are written.

## 6 Subroutines added to the *AERO3D* software

During this study six useful subroutines were added to the *AERO3D* code.

### 6.1 Subroutines used by *MeshCanaleMP*

The following subroutines have been added to the *AERO3D* software for the *MeshCanaleMP* option.

<sup>21</sup>The sysops is very appreciative when these extremely large files are not written

<sup>22</sup><http://www.kitware.com>

<sup>23</sup>Work in progress.

CanaleMP.f  
 GetHostNames.f  
 MeshCanaleMP\_F90.f

## 6.2 Useful subroutines with/without the MeshCanaleMP option

WRTflu.f  
 WRTsinus.f  
 WRTsinusPart.f  
 WRTsolPart.f

## 7 Results

### 7.1 Load balancing using mixed speed processors

In this section, the benefit of using heterogeneous mesh partitioning on Clusters and GRIDS mixed processor speeds is illustrated. The *nina-pf* Cluster, the MecaGRID, and the GRID5000 were chosen for these tests. Table 5 shows the processor speeds used in this analysis.

Cluster/GRID	cluster(Location)		Processor speed (Ghz)	
	Fast cluster	Slow cluster	Fast cluster	Slow cluster
INRIA Cluster	Sophia	Sophia	2.2	1.0
MecaGRID	Marseilles	Sophia	2.0	1.0
GRID5000	Sophia	Grenoble	2.0	0.9

Table 5: Processor speed for tests

The test case computed flow in a nozzle. Two meshes were studied; the first mesh contains 252K vertices with 1.44 million tetrahedra and the second 502K vertices with 2.88 million tetrahedra.

For the homogeneous mesh partitioning the partitions were of equal size. For the heterogeneous mesh partitioning the mesh was partitioned so that the fast-cluster partitions were twice as large as the slow-cluster partitions.

Table 6 shows the wall times for a simulation of 150 time steps for different size meshes and different mixtures of fast and slow processors for the different mesh sizes. From these tables, an important reduction in simulation time is

Cluster/GRID	Mesh	CPUs	wall time (sec)		speedup
			homo	hetero	
INRIA Cluster	252K	<i>8-nina 8-pf</i>	738	477	1.55
MecaGRID	252K	<i>8-iusti 8-pf</i>	780	588	1.33
GRID5000	252K	<i>8-sophia 8-icluster2</i>	1422	994	1.46
GRID5000	252K	<i>16-sophia 16-icluster2</i>	1050	794	1.32
INRIA Cluster	502K	<i>16-nina 16-pf</i>	843	553	1.52
INRIA Cluster	502K	<i>24-nina 8-pf</i>	738	529	1.39
GRID5000	502K	<i>16-sophia 16-icluster2</i>	1815	1319	1.38

Table 6: Homogeneous vs heterogenous partitioning

noted using the heterogeneous partitioning, 1.55<sup>24</sup> for the 252K vertices mesh and 1.52 for the 502 vertices mesh the theoretical speedup for these cases is 1.5. For the case where 24 fast and 8 slow processors were used, the reduction in simulation time was 1.39 (the theoretical value is 1.25)<sup>25</sup>. These reductions in simulation times indicate that good load balancing is achieved when heterogeneous partitions are used. Figure 5 shows the computational times for 16 processors to compute the fluxes in *AERO3D* for both the homogeneous and heterogeneous partitions using *8-nina* and *8-pf* processors for each processor. Note that the work/processor (time) for the heterogeneous partitions are approximately equivalent whereas for the homogeneous partitions the faster processors (P0-P7) spend 1/2 their time waiting for the slower processors (P8-P16) to finish.

## 7.2 Experiences using the MecaGRID and the GRID5000

Table 6 shows smaller computational times for the MecaGRID compared to the GRID5000. Considering that the MecaGRID communicates over the internet with a measured network bandwidth of approximately 5 Mbps (see Basset[1]-[2]) compared to the GRID5000 that uses a 1 Gbps bandwidth dedicated network, one would expect the opposite result.

There are several reasons why this may have occurred. The most likely explanation is that the goal of the tests was to compare computational speedups with the theoretical speedup values, therefore no intermediate solutions were

<sup>24</sup>speedup = homogeneous time/ heterogeneous time

<sup>25</sup>The theoretical value of 1.25 was based on a speed ratio of 2 whereas the hardware speed ratio is approximately 2.2. This may explain why the real speedup was greater than the quoted theoretical value

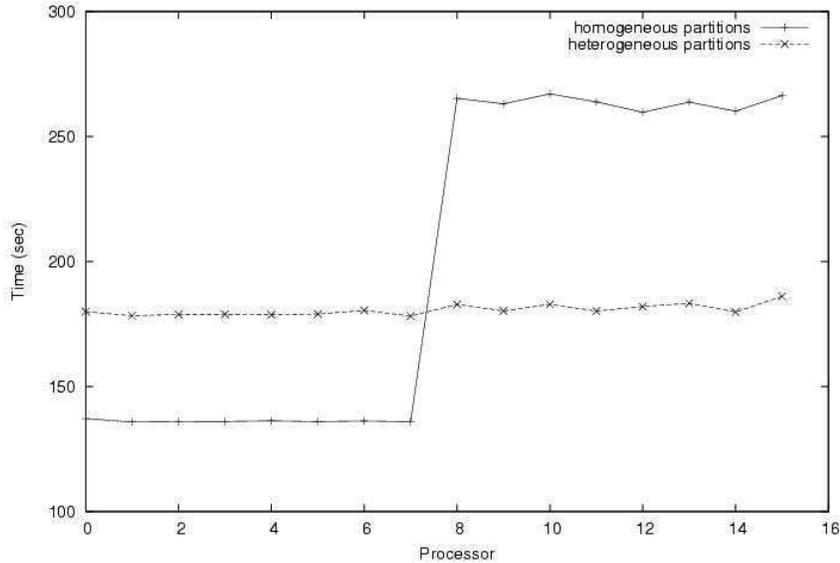


Figure 5: CPU time for each processor

safeguarded<sup>26</sup> As this was avoided, the superior bandwidth of the GRID5000 was not fully used. If safeguarding of the solution had been included in the simulation, the performance of the GRID5000 would have been superior to that of the MecaGRID. Unfortunately the GRID5000 calculations were made after the MecaGRID was retired from service. Therefore it was not possible to make new tests using the MecaGRID to verify this hypothesis.

A second factor may be the larger physical distances between the two GRID5000 clusters (404 km) compared to the MecaGRID clusters (237 km). GRID distances are not measured in km but in latency times<sup>27</sup> but the physical distance and the latency distances are related. Network latency can be estimated using a ping test. 100 ping tests between the *pf* cluster and a processor of the *iusti* cluster (MecaGRID) returns the following:

100 packets transmitted, 100 packets received, 0% packet loss  
 round-trip min/avg/max = 4.3/9.5/14.4 ms

<sup>26</sup> Typically a production simulation may require many thousands of time steps and the user will safeguard the solution every 500 or 1000 times steps. Safeguarding the solutions requires passing the 3D data from each processor to processor "0" and the network bandwidth becomes an important factor in the efficiency of the transfer.

<sup>27</sup> There are two important characteristics of GRIDS, network bandwidth and network latency.

The variability in the min/avg/max times is high because the MecaGRID clusters communicate over the internet which is non-dedicated.

A single ping test from the Sophia GRID5000 cluster frontend to the *icluster2* cluster in Grenoble returns: ping frontale.grenoble

rtt min/avg/max = 12.362/12.385/12.455

The low variability in the min/avg/max times between the GRID5000 sites is because the GRID5000 network is dedicated.

Recall that the slicing partitioning option was used here (section 4.1). Therefore only one processor from the fast-cluster passes messages to one processor of the slow-cluster and the size of the data being passed is very small compared to that required to safeguard the intermediate solutions; thus one could assume that latency plays the most important role in the test case.

Based on latency arguments alone, assuming that bandwidth plays a minor role, the transfer between the MecaGRID clusters should be 1.3 times faster than between the GRID5000 clusters. The computed ratios are 1.8 for the homogeneous case and 1.7 for the heterogeneous case, thus this argument seems to be invalid.

Another reason may be that the MecaGRID computations were made using the Globus 2.2.4 software<sup>28</sup>. Wornom [11] noted that runs on the *nina-pf* cluster using the Globus software were faster than the same computation using the *ch\_p4*; both are part of MPICH<sup>29</sup>. We have no way to evaluate this hypothesis.

Table 7 shows the characteristics for the different processors involved. We can only note the better performance of the MecaGRID relative to the GRID5000 but we cannot explain it.

Property	MecaGRID		GRID5000	
	Fast cluster	Slow cluster	Fast cluster	Slow cluster
Processor	Pentium IV	Pentium III	AMD Opteron	Itanium 2
speed	2.0 Ghz	0.937 Ghz	2.0 Ghz	0.900 Ghz
RAM	0.900 GB	0.512 GB	1.0 GB	1.5 GB
cache	512 KB	256 KB	1024 KB	256 KB

Table 7: GRID Processor Characteristics

<sup>28</sup><http://www.globus.org>

<sup>29</sup><http://www-unix.mcs.anl.gov/mpi/mpich/>

### 7.3 Large mesh simulations using the GRID5000

This section uses the large mesh options available in MeshCanaleMP<sup>30</sup> to perform large mesh simulation made possible with the large number of processors of the GRID5000. These simulations were made using clusters having all Opteron processors thus the load balancing feature discussed previously was not needed.

Recall that the standard CFD procedure is to partition the mesh in advance of the CFD execution. Thus is inefficient and avoided here. In fact the largest CFD runs presented here cannot be made using the standard procedure using the *AERO3D*. Here, the mesh is not partitioned in advance of the CFD execution but is created and partitioned during the CFD run; We refer to this as dynamic computing.

The GRID5000 is an experimental and performance evaluation GRID at this time thus the simulations are not full scale. There 13 clusters currently comprising the GRID5000 involving 17 labs. The goal is to have 5000 processors on the GRID but as of date of this report there are less than 1000 processors active with 200 users competing for these resources. The user can see the status of the different clusters on the GRID5000 using the web site <https://frontal38.imag.fr/cgi-bin/oagridmonika.cgi>. The status is constantly changing. The user can reserve processors at a future time or seeing what processors are available, try to quickly reserved some processors before another user reserves them for a short period of time. Dynamic computing is well adapted to the latter approach. Some results are shown in Table 8. The largest case involves 20 million vertices using 256 processors at five different GRID5000 sites.

GRID	Mesh	CPUs	Distribution	CPU time
GRID5000	1/4 M	16	16- <i>sophia</i>	0.10 hrs
GRID5000	1 M	32	16- <i>sophia</i> 16- <i>bordeaux</i>	0.34 hrs
GRID5000	2 M	64	32- <i>sophia</i> 32- <i>bordeaux</i>	1.09 hrs
GRID5000	8 M	128	96- <i>sophia</i> 32- <i>bordeaux</i>	1.52 hrs
GRID5000	16 M	128	96- <i>sophia</i> 32- <i>bordeaux</i>	4.77 hrs
GRID5000	20 M	256	96- <i>sophia</i> 80- <i>orsay</i> 16- <i>bordeaux</i> 32- <i>rennes</i> 32- <i>nancy</i>	2.11 hrs

Table 8: Dynamic mesh results

<sup>30</sup>LargeMesh = 2, nWRTflu = 0, and nWRTsinus = 0

## 8 Conclusions

In this study, in order to overcome the problems related to computing with arbitrary mixtures of fast and slow processors occurring on clusters and GRIDS with different speed processors, the mesh generator and the mesh partitioner (called MeshCanaleMP) have been integrated into the CFD code. Thus optimal load balancing partitions based on processor speed are automatically created for different mixtures of fast and slow processors.

Validation tests using the GRID5000, the MecaGRID, and the the INRIA *nina-pf* cluster produced speedups on the order of 1.32 to 1.52 relative to the same run using the homogeneous partitioning which compares well with the theoretical speedup of 1.5.

Finally we presented CFD tests for meshes involving up to 20 Million vertices made possible with the large mesh options in the code and the processors available with the GRID5000.

## 9 Acknowledgements

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<sup>31</sup><http://www.recherche.gouv.fr/recherche/aci/grid.htm>

<sup>32</sup><http://www.grid5000.org/>

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## APPENDIX A

*fluid.sinus* Formats

Table 9 shows various formats for the *fluid.sinus* mesh file where *ns*, *nt*, *nfac* are the number of vertices, tetrahedra, and external faces, *coor*, the Cartesian coordinates, *nu* the tetrahedra connectivity, *logfac* the boundary conditions to be applied at the external faces, and *nsfac*, the connectivity for the triangular external faces.

```
write(myunit,*) ns, nt, nfac
write(myunit,*) (coor(1,i), coor(2,i), coor(3,i), i=1,ns)
write(myunit,*) (nu(1,i), nu(2,i), nu(3,i), nu(4,i), i=1,nt)
write(myunit,*) (logfac(i), i=1,nfac)
write(myunit,*) (nsfac(1,i), nsfac(2,i), nsfac(3,i), i=1,nfac)
```

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```
write(myunit) ns, nt, nfac
write(myunit) (coor(1,i), coor(2,i), coor(3,i), i=1,ns)
write(myunit) (nu(1,i), nu(2,i), nu(3,i), nu(4,i), i=1,nt)
write(myunit) (logfac(i), i=1,nfac)
write(myunit) (nsfac(1,i), nsfac(2,i), nsfac(3,i), i=1,nfac)
```

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Table 9: *fluid.sinus* formats: Top) formatted Bottom) unformatted

## APPENDIX B

Description of the *flu-0000n* files.

In the *flu-0000n* we find successively:

ipd = subdomain number (involved by this file *flu-xxxxx*)  
 ns, nt, nfac = local number of nodes, tetrahedra and boundary facets  
 (local means associated with the considered subdomain)  
 nghd = number of neighboring subdomains

For  $i=1, nghd$  we read:

ishd( $i$ ) = identification (number) of the  $i$ th neighboring subdomain  
 insghd(ishd( $i$ )) = number of nodes located on the common interface between  
 the considered subdomain and its  $i$ th neighboring subdomain

For  $ii=1, insghd(ishd(i))$  we read:

isghd( $ii, ishd(i)$ ) = local number of these common nodes  
 EndFor  $ii$

EndFor  $i$

For  $is=1, ns$  we read:

coor(1, $is$ ), coor(2, $is$ ), coor(3, $is$ ) = x-, y- and z-coordinate of node  $is$   
 EndFor  $is$

For  $jt=1, nt$  we read:

nu(1, $jt$ ), nu(2, $jt$ ), nu(3, $jt$ ), nu(4, $jt$ ) = local number of the 4 vertices  
 of tetrahedron  $jt$   
 EndFor  $jt$

For  $ifac=1, nfac$  we read

logfac( $ifac$ ) = boundary identification for each boundary facet  $ifac$   
 nsfac(1, $ifac$ ), nsfac(2, $ifac$ ), nsfac(3, $ifac$ ) = local number of the 3 vertices  
 of boundary facet  $ifac$

EndFor ifac

For is=1,ns

irefd(is) = 1 if node "is" is an internal node for the considered subdomain,  
0 else

(by internal node, we mean a node which does not belong to the common  
interfaces shared with neighboring subdomains)

EndFor is

For is=1,ns

igrefd(is) = global number (i.e. number in the global mesh) of node is

EndFor is

REMARK = all the previous variables are integer except `coor(,)` which is  
real.



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