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INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Team bacchus

Parallel tools for Numerical Algorithms and Resolution of essentially Hyperbolic problems

Bordeaux - Sud-Ouest

Theme : Computational models and simulation

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2. Overall Objectives

2.1. Overall Objectives

BACCHUS is a joint team of INRIA Bordeaux - Sud-Ouest, LaBRI (Laboratoire Bordelais de Recherche en Informatique – CNRS UMR 5800, University of Bordeaux and IPB) and IMB (Institut Mathématique de Bordeaux – CNRS UMR 5251, University of Bordeaux). BACCHUS has been created on the first of January, 2009 (http://bacchus.bordeaux.inria.fr).

The purpose of the BACCHUS project is to analyze and solve efficiently scientific computation problems that arise in complex research and industrial applications and that involve scaling. By scaling we mean that the applications considered require an enormous computational power, of the order of tens or hundreds of teraflops, and that they handle huge amounts of data. Solving these kinds of problems requires a multidisciplinary approach involving both applied mathematics and computer science.

Our major focus are fluid problems, and especially the simulation of *physical wave propagation problems* including fluid mechanics, inert and reactive flows, multimaterial and multiphase flows, acoustics, etc. BACCHUS intends to solve these problems by bringing contributions to all steps of the development chain that goes from the design of new high-performance, more robust and more precise numerical schemes, to the creation and implementation of optimized parallel algorithms and high-performance codes.

By taking into account architectural and performance concerns from the early stages of design and implementation, the high-performance software which will implement our numerical schemes will be able to run efficiently on most of today's major parallel computing platforms (UMA and NUMA machines, large networks of SMP nodes, production GRIDs).

2.2. Highlights

- The Scotch software, which is now fully 64-bit since its revision 5.1.10, has been able to partition graphs above 2 billion vertices on 2048 processors. Runs have been performed on up to 30.000 processing elements.
- RealfluiDS has been upgraded to hybrid meshes in 3D. We have been able to run an M6 wing mesh given by ONERA with 5.510^6 vertices with Q1 elements (256 procs) and a supersonic business jet configuration with the P2 third order version (128 procs, $8\ 10^5$ degrees of freedom).
- C. Dobrzynski, M. Ricchiuto and R. Abgrall, jointly with the MC2 team project, have participated in the organisation the CANUM 2010, june 2010, Carcans Maubuisson. see http://smai.emath.fr/canum2010/.

3. Scientific Foundations

3.1. Numerical schemes for fluid mechanics

Participants: Rémi Abgrall, Marc Duruflé, Mario Ricchiuto, Pietro Congedo.

A large number of industrial problems involve fluid mechanics. They may involve the coupling of one or more physical models. An example is provided by aeroelastic problems, which have been studied in details by other INRIA teams. Another example is given by flows in pipelines where the fluid (a mixture of air–water–gas) does not have well-known physical properties. One may also consider problems in aeroacoustics, which become more and more important in everyday life. In some occasions, one needs specific numerical tools to take into account *e.g.* a fluids' exotic equation of state, or because the amount of required computational resources becomes huge, as in unsteady flows. Another situation where specific tools are needed is when one is interested in very specific physical quantities, such as *e.g.* the lift and drag of an airfoil, a situation where commercial tools can only provide a very crude answer.

It is a fact that there are many commercial codes. They allow users to simulate a lot of different flow types. The quality of the results is however far from optimal in many cases. Moreover, the numerical technology implemented in these codes is often not the most recent. To give a few examples, consider the noise generated by wake vortices in supersonic flows (external aerodynamics/aeroacoustics), or the direct simulation of a 3D compressible mixing layer in a complex geometry (as in combustion chambers). Up to our knowledge, due to the very different temporal and physical scales need to be captured, a direct simulation of these phenomena is not in the reach of the most recent technologies because the numerical resources required are currently unavailable ! *We need to invent specific algorithms for this purpose.*

In order to efficiently simulate these complex physical problems, we are working on some fundamental aspects of the numerical analysis of non linear hyperbolic problems. *Our goal is to develop schemes that can adapt to modern computer architectures*.

More precisely, *we are working on a class of numerical schemes*, known in literature as Residual Distribution schemes, *specifically tailored to unstructured and hybrid meshes*. They have the most possible compact stencil that is compatible with the expected order of accuracy. This *accuracy is at least of second order, and it can go up to fourth order in practical applications.* Since the stencil is compact, the implementation on parallel machines becomes simple. These schemes are very flexible in nature, which is so far one of the most importat advantage over other techniques. This feature has allowed us to adapt the schemes to the requirements of different physical situations (*e.g.* different formulations allow either en efficient explicit time advancement for problems involving small time-scales, or a fully implicit space-time variant which is unconditionally stable and allows to handle stiff problems where only the large time scales are relevant). This flexibility has also enabled to devise a variant using the same data structure of the popular Discontinuous Galerkin schemes, which are also part of our scientific focus.

The compactness of the second order version of the schemes enables us to use efficiently the high performance parallel linear algebra tools developed by the team. However, the high order versions of these schemes, which are under development, require modifications to these tools taking into account the nature of the data structure used to reach higher orders of accuracy. This leads to new scientific problems at the border between numerical analysis and computer science. In parallel to these fundamental aspects, we also work on adapting more classical numerical tools to complex physical problems such as those encountered in interface flows, turbulent or multiphase flows, material science.

Within a few years, we expect to be able to deal with physical problems out of today's reach, such as aeroacoustics, unsteady aerodynamics, and compressible MHD (in relation with the ITER project). This will be achieved by means of a multi-disciplinary effort involving our research on compact distribution schemes, the parallel advances in algebraic solvers and partitioners, and the strong interactions with specialists in computer science and scientific computing.

Another topic of interest is the quantification of uncertainties in non linear problems. In many applications, the physical model is not known accurately. A typical example is the one of turbulent flows where, for a given turbulent model which depends on many coefficients, the coefficients themselves are not know accurately. A similar situation occur for real gas or multiphase flows where the equation of state form suffer from uncertainties. The dependency of the model with respect to these uncertainties can be studied by propagation of chaos techniques such as those developped during the recent years via polynomial chaos techniques. Different implementations exists, depending whether the method is intrusive or not. The accuracy of these methods is still a matter of research, as well how they can handle an as large as possible number of uncertainties or their versatility with respect to the structure of the random variable pdfs.

Our research in numerical algorithms has led to the development of the `RealfluiDS` platform which is described in section 5.2. This work is supported by the EU-Strep IDIHOM, various research contracts and in part by the ANR-CIS ASTER project (see section 4.3 also), and also by the ERC grant ADDECCO.

3.2. Algorithms and high-performance solvers

Participants: Cécile Dobrzynski, Pascal Hénon, François Pellegrini, Pierre Ramet.

3.2.1. High-performance direct solvers for distributed clusters

Solving large sparse systems $Ax = b$ of linear equations is a crucial and time-consuming step, arising in many scientific and engineering applications. Consequently, many parallel techniques for sparse matrix factorization have been studied and implemented.

Sparse direct solvers are mandatory when the linear system is very ill-conditioned; such a situation is often encountered in structural mechanics codes, for example. Therefore, to obtain an industrial software tool that must be robust and versatile, high-performance sparse direct solvers are mandatory, and parallelism is then necessary for reasons of memory capability and acceptable solving time. Moreover, in order to solve efficiently 3D problems with more than 50 million unknowns, which is now a reachable challenge with new SMP supercomputers, we must achieve good scalability in time and control memory overhead.

Solving a sparse linear system by a direct method is generally a highly irregular problem that induces some challenging algorithmic problems and requires a sophisticated implementation scheme in order to fully exploit the capabilities of modern supercomputers.

In the BACCHUS project, we focused first on the block partitioning and scheduling problem for high performance sparse LDL^T or LL^T parallel factorization without dynamic pivoting for large sparse symmetric positive definite systems. Our strategy is suitable for non-symmetric sparse matrices with symmetric pattern, and for general distributed heterogeneous architectures the computation and communication performance of which are predictable in advance. This has led to software developments (see sections 5.3, 5.5)

3.2.2. High-performance iterative and hybrid direct/iterative solvers

In addition to the project activities on direct solvers, we also study some robust preconditioning algorithms for iterative methods. The goal of these studies is to overcome the huge memory consumption inherent to the direct solvers in order to solve 3D problems of huge size (several million of unknowns). Our studies focus on the building of generic parallel preconditioners based on ILU factorizations. The classical ILU preconditioners use scalar algorithms that do not exploit well CPU power and are difficult to parallelize. Our work aims at finding some unknown orderings and partitioning that lead to a dense block structure of the incomplete factors. Then, based on the block pattern, some efficient parallel blockwise algorithms can be devised to build robust preconditioners that are also able to fully exploit the capabilities of modern high-performance computers.

In this context, we study two approaches.

- The first idea is to define an adaptive blockwise incomplete factorization that is much more accurate (and numerically more robust) than the scalar incomplete factorizations commonly used to precondition iterative solvers. Such incomplete factorization can take advantage of the latest breakthroughs in sparse direct methods and particularly should be very competitive in CPU time (effective power used from processors and good scalability) while avoiding the memory limitation encountered by direct methods. By this way, we expect to be able to solve systems in the order of hundred million of unknowns and even one billion of unknowns. Another goal is to analyze and justify the chosen parameters that can be used to define the block sparse pattern in our incomplete factorization.

  The driving rationale for this study is that it is easier to incorporate incomplete factorization methods into direct solution software than it is to develop new incomplete factorizations.

  Our main goal at this point is to achieve a significant diminution of the memory needed to store the incomplete factors (with respect to the complete factors) while keeping enough fill-in to make the use of BLAS3 (in the factorization) and BLAS2 (in the triangular solves) primitives profitable.

  In this approach, we focus on the critical problem to find approximate supernodes of ILU(k) factorizations. The problem is to find a coarser block structure of the incomplete factors. The "exact" supernodes that are exhibited from the incomplete factor non zero pattern are usually very small and thus the resulting dense blocks are not large enough for an efficient use of the BLAS3 routines. A remedy to this problem is to merge supernodes that have nearly the same structure. The benefits of this approach have been shown in [43]. These algorithms are implemented in the PaStiX library.

- The second technique makes use of a Schur complement approach.

  In recent years, a few Incomplete LU factorization techniques were developed with the goal of combining some of the features of standard ILU preconditioners with the good scalability features of multilevel methods. The key feature of these techniques is to reorder the system in order to extract parallelism in a natural way. Often a number of ideas from domain decomposition are utilized and mixed to derive parallel factorizations.

  Under this framework, we developed in collaboration with Yousef Saad (University of Minnesota) algorithms that generalize the notion of "faces" and "edge" of the "wire-basket" decomposition. The interface decomposition algorithm is based on defining a "hierarchical interface structure" (HID).

This decomposition consists in partitioning the set of unknowns of the interface into components called connectors that are grouped in "classes" of independent connectors [44].

In the context of robust preconditioner technique, we have developed an approach that uses the HID ordering to define a new hybrid direct-iterative solver. The principle is to build a decomposition of the adjacency matrix of the system into a set of small sub-domains (the typical size of a sub-domain is around a few hundreds or thousand nodes) with overlap. We build this decomposition from the nested dissection separator tree obtained using a sparse matrix reordering software as `Scotch`. Thus, at a certain level of the separator tree, the sub-trees are considered as the interior of the sub-domains and the union of the separators in the upper part of the elimination tree constitutes the interface between the sub-domains.

The interior of these sub-domains are treated by a direct method. Solving the whole system is then equivalent to solve the Schur complement system on the interface between the sub-domains which has a much smaller dimension. We use the hierarchical interface decomposition (HID) to reorder and partition this system. Indeed, the HID gives a natural dense block structure of the Schur complement. Based on this partition, we define some efficient block preconditioners that allow the use of BLAS routines and a high degree of parallelism thanks to the HID properties.

We propose several algorithmic variants to solve the Schur complement system that can be adapted to the geometry of the problem: typically some strategies are more suitable for systems coming from a 2D problem discretisation and others for a 3D problem; the choice of the method also depends on the numerical difficulty of the problem. In the `HIPS` library, we provide full iterative methods (very low memory consumption) as well as hybrid methods that mixes a direct factorization inside the domain and an iterative method in the Schur complement. The library provides many options that allow one to deal with real or complex arithmetic, and symmetric or unsymmetric matrices. In particular, the very interesting feature of `HIPS` is that it allows one to find some good trade-off between memory, robustness and time consumption in almost every case.

Details can be found in sections 5.4 and 6.3.

These works are also supported by the ANR-CIS project "SOLSTICE".

3.2.3. Meshes and graph partitioning

3.2.3.1. Parallel graph partitioning and static mapping

Finding vertex separators for sparse matrix ordering is only one of the many uses of generic graph partitioning tools. For instance, finding balanced and compact domains in problem graphs is essential to the efficiency of parallel iterative solvers. Here again, because of the size of the problems at stake, parallel graph partitioning tools are mandatory to provide good load balance and minimal communication cost.

The execution of parallel applications implies communication between processes executed on the different cores. On NUMA architectures which are strongly heterogeneous in terms of latency and capacity, communication cost strongly depends on the repartition of tasks among cores. Architecture-aware load balancing must take into account both the characteristics of the parallel applications (including for instance task processing costs and the amount of communication between tasks) and the topology of the target architecture (providing the powers of cores and the costs of communication between all of them). When processes are assumed to coexist simultaneously for all the duration of the program, this optimization problem is called mapping. A mapping is called static if it is computed prior to the execution of the program and is never modified at run-time.

The sequential `Scotch` tool was able to perform static mapping since its first version, but this feature was not widely known nor used by the community. With the increasing need to map very large problem graphs onto very large and strongly heterogeneous parallel machines (whether hierarchical NUMA clusters or GPU-based systems), there is an increasing demand for parallel static mapping tools.

3.2.3.2. Adaptive dynamic mesh partitioning

Many simulations which model the evolution of a given phenomenon along with time (turbulence and unsteady flows, for instance) need to re-mesh some portions of the problem graph in order to capture more accurately the properties of the phenomenon in areas of interest. This re-meshing is performed according to criteria which are closely linked to the undergoing computation and can involve large mesh modifications: while elements are created in critical areas, some may be merged in areas where the phenomenon is no longer critical.

Performing such re-meshing in parallel creates additional problems. In particular, splitting an element which is located on the frontier between several processors is not an easy task, because deciding when splitting some element, and defining the direction along which to split it so as to preserve numerical stability most, require shared knowledge which is not available in distributed memory architectures. Ad-hoc data structures and algorithms have to be devised so as to achieve these goals without resorting to extra communication and synchronization which would impact the running speed of the simulation.

Most of the works on parallel mesh adaptation attempt to parallelize in some way all the mesh operations: edge swap, edge split, point insertion, etc. It implies deep modifications in the (re)mesher and often leads to bad performance in term of CPU time. An other work [38] proposes to base the parallel re-meshing on existing mesher and load balancing to be able to modify the elements located on the frontier between several processors.

In addition, the preservation of load balance in the re-meshed simulation requires dynamic redistribution of mesh data across processing elements. Several dynamic repartitioning methods have been proposed in the literature [46], [45], which rely on diffusion-like algorithms and the solving of flow problems to minimize the amount of data to be exchanged between processors. However, integrating such algorithms into a global framework for handling adaptive meshes in parallel has yet to be done.

4. Application Domains

4.1. Panorama

The main objective of the BACCHUS project is to analyze and solve scientific computing problems coming from complex research and industrial applications that require a scalable approach. This allows us to validate the numerical schemes, the algorithms and the associated software that we develop. We have today three reference application domains which are fluid mechanics, material physics and the MHD simulation dedicated to the ITER project.

In these three domains, we study and simulate phenomena that are by nature multiscale and multiphysics, and which require enormous computing power. A major part of these works leads to industrial collaborations in particular with the CNES, ONERA, and with the french CEA/CESTA, CEA/Ile-de-France and CEA/Cadarache centers.

4.2. Fluid mechanics

Participants: Rémi Abgrall [Corresponding member], Marc Duruflé, Mario Ricchiuto, Pietro Congedo.

The numerical simulation of steady and unsteady flows is still a challenge since efficient schemes and efficient implementations are needed. The accuracy of schemes is still a problem nowadays. This challenge is even higher if large size problems are considered, and if the meshes are not regular. The schemes developed in for fluid mechanics problems use Scotch, HIPS and PaStiX when the type of problems and the CPU requirements make this useful.

4.2.1. Steady transonic and supersonic flows

One of our application fields is the one of steady subsonic, transonic and supersonic flow problems when the equation of state is for example the one of air in standard conditions, or a more general one as in real gases and multiphase flows. This class of physical problems corresponds to “standard” aerodynamics and the models are those of the Euler equations and the Navier Stokes ones, possibly with turbulent effects. Here we consider the residual distribution and SUPG schemes.

4.2.2. Unsteady transonic flows

Another field of application is the one of *unsteady* problems for the same physical models. Depending on the applications, the physical models considered involve the Navier-Stokes equations, or the non-linear or linearized linearized Euler equations. The schemes we develop are the Residual distribution schemes 5.2 and Discontinuous Galerkin schemes 5.7. Specific modifications, with respect to their steady counter parts, are done in order to reduce dramatically the computational time, while maintaining the desired accuracy.

4.3. High performance simulation dedicated to ITER project

Participants: Rémi Abgrall, Pierre Ramet [Corresponding member].

Numerical simulation has become a major tool for the study of many physical phenomena involving charged particles, in particular beam physics, space and laboratory plasmas including fusion plasmas. Moreover, it is a subject of interest to figure out and optimize physics experiments in the present fusion devices and also to design future reactors like in the ITER project. Parallelism is required to carry on numerical simulations for realistic test cases.

We have established a collaboration with the physicists of the CEA/DRFC group in the context of the ANR CIS 2006 project called ASTER (Adaptive MHD Simulation of Tokamak Elms for iteR). The magneto-hydrodynamic instability called ELM for Edge Localized Mode is commonly observed in the standard tokamak operating scenario. The energy losses the ELM will induce in ITER plasmas are a real concern. However, the current understanding of what sets the size of these ELM induced energy losses is extremely limited. No numerical simulations of the complete ELM instability, from its onset through its non-linear phase and its decay, are referenced in literature. Recently, encouraging results on the simulation of an ELM cycle have been obtained with the `JOREK` code developed at CEA but at reduced toroidal resolution. The `JOREK` code uses a fully implicit time evolution scheme in conjunction with the `PaStiX` sparse matrix library.

5. Software

5.1. Introduction

We develop two kinds of software. The first one consists in generic libraries that are used within application codes. These libraries comprise a sequential and parallel partitioner for large irregular graphs or meshes (`Scotch`), and high performance direct or hybrid solvers for very large sparse systems of equations (`PaStiX` and `HIPS`). The second kind of software corresponds to dedicated software for fluid mechanics (`RealfluiDS`).

For these parallel software developments, we use the message passing paradigm (basing on the MPI interface), sometimes combined with threads so as to exploit multi-core architectures at their best: in some computation kernels such as solvers, when processing elements reside on the same compute node, message buffer space can be saved because the aggregation of partial results can be performed directly in the memory of the receiving processing element. Memory savings can be tremendous, and help us achieve problem sizes which could not be reached before (see Section 5.3).

5.2. RealfluiDS

Participant: Rémi Abgrall [corresponding member].

`RealfluiDS` is a software dedicated to the simulation of inert or reactive flows. It is also able to simulate multiphase, multimaterial and MHD flows. There exist 2D and 3D dimensional versions. The 2D version is used to test new ideas that are later implemented in the 3D one. Two classes of schemes have been implemented: classical finite volume schemes and the more recent residual distribution schemes. Several low Mach preconditioning techniques are also implemented. The code has been parallelized with and without overlap of the domains. Recently, the `PaStiX` solver has been integrated in `RealfluiDS` . A partitioning tool exists in the package, which uses `Scotch`.

5.3. PaStiX

Participant: Pierre Ramet [corresponding member].

This work is supported by the French "Commissariat à l'Énergie Atomique CEA/CESTA" in the context of structural mechanics and electromagnetism applications.

PaStiX (http://pastix.gforge.inria.fr) (Parallel Sparse matriX package) is a scientific library that provides a high performance parallel solver for very large sparse linear systems based on block direct and block ILU(k) iterative methods. Numerical algorithms are implemented in single or double precision (real or complex): LLt (Cholesky), LDLt (Crout) and LU with static pivoting (for non symmetric matrices having a symmetric pattern). This latter version is now used in RealfluiDS (see Section 5.2). The PaStiX library is released under INRIA CeCILL licence.

The PaStiX library uses the graph partitioning and sparse matrix block ordering package Scotch (see Section 5.5). PaStiX is based on an efficient static scheduling and memory manager, in order to solve 3D problems with more than 50 million of unknowns. The mapping and scheduling algorithm handles a combination of 1D and 2D block distributions. This algorithm computes an efficient static scheduling of the block computations for our supernodal parallel solver which uses a local aggregation of contribution blocks. This can be done by taking into account very precisely the computational costs of the BLAS 3 primitives, the communication costs and the cost of local aggregations. We also improved this static computation and communication scheduling algorithm to anticipate the sending of partially aggregated blocks, in order to free memory dynamically. By doing this, we are able to reduce the aggregated memory overhead, while keeping good performance.

Another important point is that our study is suitable for any heterogeneous parallel/distributed architecture when its performance is predictable, such as clusters of SMP nodes. In particular, we now offer a high performance version with a low memory overhead for SMP node architectures, which fully exploits the advantage of shared memory by using an hybrid MPI-thread implementation.
Direct methods are numerically robust methods, but the very large three dimensional problems may lead to systems that would require a huge amount of memory despite any memory optimization. A studied approach consists in defining an adaptive blockwise incomplete factorization that is much more accurate (and numerically more robust) than the scalar incomplete factorizations commonly used to precondition iterative solvers. Such incomplete factorization can take advantage of the latest breakthroughs in sparse direct methods and particularly should be very competitive in CPU time (effective power used from processors and good scalability) while avoiding the memory limitation encountered by direct methods.

5.4. HIPS

Participant: Pascal Hénon [corresponding member].

HIPS (Hierarchical Iterative Parallel Solver) is a scientific library that provides an efficient parallel iterative solver for very large sparse linear systems.

The key point of the methods implemented in HIPS is to define an ordering and a partition of the unknowns that relies on a form of nested dissection ordering in which cross points in the separators play a special role (Hierarchical Interface Decomposition ordering). The subgraphs obtained by nested dissection correspond to the unknowns that are eliminated using a direct method and the Schur complement system on the remaining of the unknowns (that correspond to the interface between the sub-graphs viewed as sub-domains) is solved using an iterative method (GMRES or Conjugate Gradient at the time being). This special ordering and partitioning allows for the use of dense block algorithms both in the direct and iterative part of the solver and provides a high degree of parallelism to these algorithms. The code provides a hybrid method which blends direct and iterative solvers. HIPS exploits the partitioning and multistage ILU techniques to enable a highly parallel scheme where several subdomains can be assigned to the same process. It also provides a scalar preconditioner based on the multistage ILUT factorization.

HIPS can be used as a standalone program that reads a sparse linear system from a file ; it also provides an interface to be called from any C, C++ or Fortran code. It handles symmetric, unsymmetric, real or complex matrices. Thus, HIPS is a software library that provides several methods to build an efficient preconditioner in almost all situations.

Since august 2008, HIPS is publicly available at http://hips.gforge.inria.fr under the INRIA CeCILL licence.

5.5. Scotch

Participant: François Pellegrini [corresponding member].

Scotch (http://www.labri.fr/~pelegrin/scotch/) is a software package for parallel and sequential sparse matrix ordering, parallel and sequential graph partitioning, as well as sequential static mapping, and mesh and hypergraph partitioning.

The initial purpose of Scotch was to compute high-quality partitions and static mappings of valuated graphs representing parallel computations and target architectures of arbitrary topologies. The original contribution consisted in developing a "*divide and conquer*" algorithm in which processes are recursively mapped onto processors by using graph bisection algorithms that are applied both to the process graph and to the architecture graph. This allows the mapper to take into account the topology and heterogeneity of the valuated graph which models the interconnection network and its resources (processor speed, link bandwidth). As new multicore, multinode parallel machines tend to be less uniform in terms of memory latency and communication bandwidth, this feature is regaining interest.

The software has then been extended in order to produce vertex separators instead of edge separators, using a multilevel framework. Recursive vertex separation is used to compute orderings of the unknowns of large sparse linear systems, which both preserve sparsity when factorizing the matrix and exhibit concurrency for computing and solving the factored matrix in parallel.

Version 5.0 of Scotch, released on August 2007, was the first version to comprise parallel routines. This extension, called PT-Scotch (for "*Parallel Threaded* Scotch"), is based on a distributed memory model, and makes use of the MPI and, optionally, Posix thread APIs. A distributed graph structure has been defined, which allows users to reserve vertex indices on each processor for future local adaptive refinement. Its parallel graph ordering routine provides orderings which are of the same quality as the ones yielded by the sequential Scotch ordering routine, while competing software ParMETIS experiences a severe loss of quality when the number of processors increase. Scotch 5.0 was released under the CeCILL-C free/libre software license, and has been registered at APP ("Agence pour la Protection des Programmes").

Version 5.1 of Scotch, released on September 2008, extended the parallel features of PT-Scotch, which can now compute graph partitions in parallel by means of a parallel recursive bipartitioning framework. Release 5.1.10 had made Scotch the first full 64-bit implementation of a general purpose graph partitioner, so that PT-Scotch has been able to successfully break the "32-bit" barrier and partition a graph above 2 billion vertices, spread across 2048 processors, at the French CCRT computer center.

Scotch has been integrated in numerous third-party software, which indirectly contribute to its diffusion. For instance, it is used by the ZOLTAN module of the TRILINOS software (SANDIA Labs), by CODE_ASTER LIBRE, a GPLed thermal and mechanical analysis software developed by French state-owned electricity producer EDF, by the parallel solvers MUMPS (ENSEEITH/IRIT, LIP and LaBRI), SuperLUDist (U.C. Berkeley), PaStiX (LaBRI) and HIPS (LaBRI), as well as by several other scientific computing software.

5.6. MMG3D

Participant: Cécile Dobrzynski [corresponding member].

MMG3D is a tetrahedral fully automatic remesher. Starting with a tetrahedral mesh, it produces quasi-uniform meshes with respect to a metric tensor field. This tensor prescribes a length and a direction for the edges, thus the resulting meshes will be anisotropic meshes. The software is based on local mesh modifications and an anisotropic version of Delaunay kernel is implemented to insert vertex on the mesh. Moreover, MMG3D allows to deal with rigid body motion and moving meshes. When a displacement is prescribed on a part of the boundary, a final mesh is generated such as the surface points will be moved according this displacement. MMG3Dis used in particular in GAMMA for their mesh adaptation developments, but also at EPFL (maths department), Dassault Aviation, Lemma (a french SME), etc. MMG3D can be used in FreeFem++ (http://www.freefem.org), a free software which it enables you to solve Partial Differential Equations (PDE) easily. More details can be found on http://www.math.u-bordeaux1.fr/~dobj/logiciels/mmg3d.php.

5.7. Montjoie

Participant: Marc Duruflé [corresponding member].

Montjoie is a finite element code initially handling only quadrilateral/hexahedral elements. Because of the tensorization of these elements, efficient algorithms can be written for the computation of finite element matrices. It can handle tetrahedra, prisms, pyramids, hexahedra with continuous finite element, edge elements and discontinuous Galerkin formulations. A local order of approximation can be used in each element of the mesh.

5.8. PLATO

Participants: Hervé Guillard [PUMAS], Laure Combe [PUMAS,contact], Cédric Lachat, Pierre Ramet [corresponding member].

The developement of PLATO (A platform for Tokamak simulation) (http://www-sop.inria.fr/pumas/plato.php) is being supported by an ADT action of the D2T. PLATO is a suite of data and softwares dedicated to the geometry and physics of Tokamaks and its main objective is to provide the Inria large scale initiative "FUSION" teams working with plasma fluid models with a common development tool. The construction of this platform will integrate the following developments.

1. A (small) database corresponding to axi-symmetrical solutions of the equilibrium plasma equations for realistic geometrical and magnetic configurations (ToreSupra, JET and ITER). The construction of meshes is always an important time consuming task. Plato will provide meshes and solutions corresponding to equilibrium solutions that will be used as initial data for more complex computations.
2. A set of tool for the handling, manipulation and transformation of meshes and solutions using different discretisations (P1, Q1, P3, etc)
3. Numerical templates allowing the use of 3D discretization schemes using finite element schemes in the poloidal plane and spectral Fourier or structured finite volume representations in the toroidal one.
4. Several applications (Ideal MHD and drift approximation) used in the framework of the Inria large scale initiative "FUSION".

This year, after a definition of the PLATO architecture, the points 1. and 2. have been developped.

5.9. PaMPA

Participants: Cécile Dobrzynski, Hervé Guillard [PUMAS], Laurent Hascoët [Tropics], Cédric Lachat, François Pellegrini [Corresponding member].

PaMPA(Parallel Mesh Partitioning and Adaptation) is a middleware library dedicated to the management of distributed meshes. Its purpose is to relieve solver writers from the tedious and error prone task of writing again and again service routines for mesh handling, data communication and exchange, remeshing, and data redistribution. An API of the future platform has been devised, and the coding of the mesh handling and redistribution routines is in progress. PaMPAwill be used as a base module of the PLATO solver, to balance dynamically, refine and coarsen its distributed mesh.

6. New Results

6.1. Numerical schemes and algorithms for fluid mechanics.

Participants: Rémi Abgrall [Corresponding member], Guilaume Baurin, Pietro-Marco Congedo, Cécile Dobrzynski, Marc Duruflé, Dante De Santis, Algyane Froehly, Gianluca Geraci, Robin Huart, Arnaud Krust, Pascal Jacq, Cédric Lachat, Mario Ricchiuto, Christelle Wervaecke.

6.1.1. Residual distribution schemes

This year, many developments have been conducted and implemented in the `RealfluiDS` software after [36] which has opened up many doors.

A three dimensional and parallel version of the second order RD scheme on hybrid meshes (tetrahedral-hexahedral) for the steady Euler equation is now working. It has been validated on several M6 wing meshes given by ONERA. The largest mesh has $5.5\,10^6$ vertices and the simulation has been done on 256 processors. Meanwhile the third order version of the same scheme (for tetrahedrons) was run succesfully on a busines jet configuration in supersonic conditions. The mesh was given by GAMMA3. This last version is also able to run the Navier Stokes equation, but the approximation is not fully satisfactory.

For this reason, we have put a lot of effort in understanding the correct way of approximation advection-diffusion like problems that degenerate to standard RD scheme when the viscous term disapear. The main difficulty was to have a scheme that work well in the largest possible range of Peclet numbers. This goal has been achieved, ane we have two versions of the method (one using a gradient reconstruction and one using a relaxation interpretation of the steady advection diffusion.) These methods will be implemented in `RealfluiDS` in the coming months for IDIHOM.

Mario Ricchiuto has conducted work on more efficient RD discretizations for time dependent problems. This has led to two formulations. The first is a genuinely explicit variant of the method based on high order mass lumping and on a temporally shifted stabilization (upwinding) operator [7], [22]. This formulation is well suited for problems where the time scales of interest are small. The higher order variant of the methodology, currently limited to second order, is under development. In parallel, in collaboration with M. Hubbard of the university of Leeds, an unconditionally stable space-time formulation has been proposed [18], [32]. This variant allows arbitrarily large time steps to be taken while preserving the accuracy and monotonicity of the results. Further work is under way to extend the accuracy to more than second order. The PhD of Guillaume Baurin has started to implement the third order version of our methods in a real industrial platform (SAFRAN). He has started the implementation of the RD scheme for the Navier Stokes equation in that platform.

Results on curved meshes and non-Lagrangian elements (Bézier and NURBS) have been obtained by Algiane Froehly. The method is now third and fourth order accurate in 2D. Cécile Dobrzynski has worked on the construction of "high order" meshes using Bézier and Nurbs elements. Numerical results using these meshes and A. Froehly's development has been obtained in 2D for subsonic, transonic and hypersonic problems. Extension in 3D is underway, one of the main difficulty is to generate meshes.

6.1.2. A Stabilized Finite Element Method for Compressible Turbulent Flows.

C. Waervaecke's PhD thesis has been a collaborative work between BACCHUS, MC2 (Héloise Beaugendre) and PUMAS (Boniface Nkonga). The main weakness of the classical finite element method (Galerkin) is its lack of stability for advection dominated flows. We consider in this work a compressible Navier-Stokes equations combined with the one equation Spalart-Allmaras turbulence model. These equations are solved in a coupled way. The numerical stability is achieved thanks to the Streamline Upwind Petrov-Galerkin (SUPG) formulation. Within the framework of SUPG method, artificial viscosity is anisotropic and the principal component is aligned with streamlines. The aim is to put sufficient viscosity to get rid of instability and unphysical oscillations without damaging the accuracy of the method. The amount of artificial viscosity is controlled by a stabilization tensor. Since an optimal way to choose this tensor is still unknown, several ways have been investigated. Beside SUPG method is also used in combination with a shock-parameter term which

supplied additional stability near shock fronts. Numerical results show that the method is able to reproduce good turbulent profiles with less numerical diffusion than a finite volume method. Even in the case of almost incompressible flow, the numerical strategy is robust and gives good results.

6.1.3. Uncertainty quantification

S. Galéra, P. Congedo and R. Abgrall have made a detailed comparison between the semi-intrusive method developed last year with more classical non intrusive polynomial chaos methods, and Monte Carlo results. These results have been presented in part during the ECCOMAS CFD conference in June 2010. We have also adapted the SUPG method for turbulent flows to this method, so that we are able to produce turbulent simulations including one and two uncertainties (here on the inflow mach number and the velocity angle).

During E. Mbinki's internship, we have tried to understand the algorithms behind the Smoliak algorithm and how they can be adapted to the semi intrusive method using local conditional expectancy.

G. Geraci has started his PhD and one of the goals is to handle as many as possible uncertainties for fluid problems.

6.1.4. Discontinuous Galerkin schemes, New elements in DG schemes

Explicit schemes may become very expensive because of a restrictive stability condition (small CFL), especially when the computational mesh comprises some very small elements. A solution, known as local time-stepping, consists of considering different time steps for each element of the mesh. These kinds of solutions can be applied to continuous finite element but are more natural when applied to Discontinuous Galerkin methods. Marc Duruflé with S. Imperiale (PhD at project POEMS) have proposed a new local time-stepping strategy and validated the approach for wave problems.

Rémi Abgrall and Pierre-Henri Maire, with François Vilar (PhD at CELIA funded by a CEA grant started in October 2009), have started to work on Lagrangian schemes within the Discontinuous Galerkin schemes. The idea is to start from the formulation of the Euler equation in full Lagrange coordinates: the spatial derivative are written in Lagrangian coordinates. This has led to a publication in Computers and Fluids where our results in 1D are described. Currently, we are developing the method in 2 dimensions. The main difficulty is to understand the role and the structure of the Geometric Conservation law.

6.1.5. Mesh adaptation

C. Dobrzynski has developed an efficient tool for handling moving 2D and 3D meshes. Here, contrarily to most ALE methods, the connectivity of the mesh is changing in time as the objects within the computational domain are moving. The objective is to guaranty a high quality mesh in terms of minimum angle for example. Other criteria, which depend on the physical problem under consideration, can also been handled. Currently this meshing tool is being coupled with `RealfluiDS` in order to produce CFD applications. One target example is the simulation of the 3D flow over helicopter blades.

A work on high order mesh generation has begun. We are modifying the classic mesh operators to take into account the curve edges. Beginning with a derefined valid curve mesh, we would to be able to generate an uniform refined curve mesh and also to adapt the mesh density in certain region (boundary layer). Moreover, starting with a P^1 (triangle) mesh and some information on the boundary, we are able to generate a valid three order curved mesh. The algorithm is based on edge swaps and is similar to a boundary enforcement procedures.

6.2. High performance simulation for plasma physics

Participants: Rémi Abgrall, Robin Huart, Pascal Hénon, Pierre Ramet [Corresponding member], Hocine Sellama.

We have been involved in two tasks: in the first one we work on novel numerical schemes for solving the compressible resistive MHD equations [37]. In the second one, in connecting with the JOREK code developped in CEA Cadarache, we work on adaptive mesh refinement problems and their connection with the solution of large linear systems to be solved in parallel.

The aim of our work in the ASTER project is to provide an efficient numerical method for solving the MHD equations, more especially in the form they are used for the ITER model. Here we want to improve the ability of Residual Distribution schemes to solve this hyperbolic system. Once fixed the choice of the full set of equations and the behavior of physical parameters, and with a validated numerical solver for these equations, we should be able to simulate plasma instabilities like those encountered in the ITER tokamak configuration. The step to ELMs simulations would then be achieved. This is a global view of the context, and it may be seen as a framework. However, one should notice that, contrarily to the work on JOREK at the CEA Cadarache, our purpose is a more general and academic code (`RealfluiDS`).

Due to the localized nature of the ELMs at the boundary of the plasma the use of mesh refinement is ideally suited to minimize the number of elements required for a given accuracy. The high resolution is only required where large gradients develop which is on a surface which is deforming in time. At a later stage during the ELM evolution, blobs of plasma are disconnected from the main plasma for which a mesh refinement also appears to be an optimal solution. We first adapt the mesh at the beginning of the simulation during the initialization phase, in order to guarantee the equilibrium, then we will apply the modifications on the mesh in order to get the adaptative mesh refinement procedure during the whole simulation.

The `JOREK` code is now able to use several hundred of processors routinely. Simulations of ELMs are produced taking into account the X-point geometry with both closed and open field lines. But a higher toroidal resolution is required for the resolution of the fine scale filaments that form during the ELM instability. The complexity of the tokamak's geometry and the fine mesh that is required leads to prohibitive memory requirements. In the current release, the memory scaling is not satisfactory: as one increases the number of processes for a given problem size, the memory footprint on each process does not reduce as much as one can expect. This will be one of the goals that motivate the partners involved in this project to present a new collaboration proposal.

6.3. Algorithms and high-performance solvers

Participants: Mathieu Faverge, Sébastien Fourestier, Damien Genêt, Hervé Guillard [(Pumas)], Laurent Hascoët [(Tropics)], Pascal Hénon [Corresponding member], Cédric Lachat, Xavier Lacoste, François Pellegrini, Pierre Ramet, Cécile Dobrynski.

6.3.1. Parallel domain decomposition and sparse matrix reordering

Like for the year before, the work carried out within the `Scotch` project (see section 5.5) focused on four main axes.

The first one regards the parallelization of the static mapping routines already available in the sequential version of `Scotch`. Since its version 5.1, `Scotch` provides parallel graph partitioning capabilities, but graph partitions are computed to date by means of a parallel multilevel recursive bisection framework. This framework provides partitions of very high quality for a moderate number of parts (about under 512), but load imbalance dramatically increases for larger numbers of parts. Also, the more parts the user wants, the more expensive it is to compute them, because of the recursive bisection process. In order to reduce load imbalance in the recursive bipartitioning process, a parallel load imbalance reduction algorithm has been devised for the bipartitioning case. This algorithm yields perfectly balanced subdomains, at almost no cost for mesh graphs compared to direct k-way methods, while it may significantly increase the cut for very irregular graphs. Load imbalance reduction algorithms for the k-way case are consequently mandatory, and are the objective of the year to come. In spite of these drawbacks, and thanks to the re-coding of some of its routines, `PT-Scotch` can now partition graphs of above 2 billion vertices, a barrier that many users wanted to be removed. For example, it has been able to provide perfectly balanced partitions of distributed meshes of 1.6 billion edges on 8096 processors at LLNL.

The second axis concerns dynamic repartitioning. Since graphs may now comprise more than one billion vertices, distributed on machines having more than one hundred thousand processing elements, it is important to be able to compute partitions which create as few data movements as possible with respect to a prior partition. The integration of repartitioning features into the sequential version of `Scotch` is now complete, with very good results, which are about to be published. The third year of the PhD of Sébastien Fourestier aims at transposing these results to the parallel case.

A third research axis regards the design of specific graph partitioning algorithms. Several applications, such as Schur complement methods for hybrid solvers (see Section 5.4), need k-way partitions where load balance should take into account not only vertices belonging to the sub-domains, but also boundary vertices, which lead to computations on each of the sub-domains which share them. A sequential version is now available as a prototype, thanks to the work of Jun-Ho Her in the context of the ANR project "PETAL", and has been successfully used in conjunction with the HIPS solver. A paper is in preparation. The transposition of these algorithms to the parallel case may prove difficult. A new directions for this research is the creation of other specific algorithms, in the context of a collaboration with Sherry Li at Berkeley.

The fourth axis is the design of efficient and scalable software tools for parallel dynamic remeshing. This is a joint work with Cécile Dobrzynski, in the context of the PhD of Cédric Lachat, funded by the PUMAS team. PaMPA ("Parallel Mesh Partitioning and Adaptation") is a middleware library dedicated to the management of distributed meshes. Its purpose is to relieve solver writers from the tedious and error prone task of writing again and again service routines for mesh handling, data communication and exchange, remeshing, and data redistribution. An API of the future platform has been devised, and the coding of the mesh handling and redistribution routines is in progress. As a direct application of PaMPA, Damien Genêt, who started his PhD this fall, will write a new generation fluid dynamics solver on top of this middleware.

6.3.2. High-performance direct solvers on multi-platforms

New supercomputers incorporate many microprocessors which include themselves one or many computational cores. These new architectures induce strongly hierarchical topologies. These are called NUMA architectures. In the context of distributed NUMA architectures, a work has begun, in collaboration with the INRIA RUNTIME team, to study optimization strategies, and to improve the scheduling of communications, threads and I/O. Sparse direct solvers are a basic building block of many numerical simulation algorithms. We propose to introduce a dynamic scheduling designed for NUMA architectures in the PaStiX solver. The data structures of the solver, as well as the patterns of communication have been modified to meet the needs of these architectures and dynamic scheduling. We are also interested in the dynamic adaptation of the computation grain to use efficiently multi-core architectures and shared memory. Experiments on several numerical test cases have been performed to prove the efficiency of the approach on different architectures. M. Faverge defended his Ph.D. [39] on these aspects in the context of the NUMASIS ANR CIGC project.

6.3.3. Hybrid direct-iterative solver based on a Schur complement approach.

In HIPS, we propose several algorithmic variants to solve the Schur complement system that can be adapted to the geometry of the problem: typically some strategies are more suitable for systems coming from a 2D problem discretisation and others for a 3D problem; the choice of the method also depends on the numerical difficulty of the problem. We have a parallel version of HIPS that provides full iterative methods as well as hybrid methods that mixes a direct factorization inside the domain and an iterative method in the Schur complement.

In [41], we have presented an hybrid version of the solver where the Schur complement preconditioner was built using parallel scalar ILUT algorithm. This year we have also developed a parallel version of the algorithms where the Schur complement incomplete factorization is done using a dense block structure. That is to say that there is no additional term dropping in the Schur complement preconditioner other than the ones prescribed by the block pattern defined by the HID graph partitioning. This variant of the preconditioner is more expensive in term of memory but for some difficult test cases they are the only alternative to direct solvers. A general comparison of all the hybrid methods in HIPS has been presented in [42].
J. Gaidamour defended his Ph.D. [40] on the hybrid solver techniques developed in HIPS.

6.3.4. MURGE a common interface to sparse linear solvers.

This year we have also defined a general programming interface for sparse linear solvers. Our goal is to normalize the API of sparse linear solvers and to provide some very simple ways of doing some fastidious tasks such as parallel matrix assembly for instance. We have thus proposed a generic API specifications called MURGE (http://murge.gforge.inria.fr) for which we also provided some test programs and documentation.

This interface has been coded in `HIPS` and `PaStiX` . We have also tested this interface in `RealfluiDS` and `JOREK` for `HIPS` and `PaStiX`.

New supercomputers incorporate many microprocessors which include themselves one or many computational cores. These new architectures induce strongly hierarchical topologies. On one hand, we have introduced a dynamic scheduling designed for these architectures in the PaStiX solver. On the other hand, we have a parallel version of HIPS that provides full iterative methods as well as hybrid methods that mixes a direct factorization inside the domain and an iterative method in the Schur complement. Moreover, graphs or meshes partitioners (Scotch software for instance) are able to deal with problems that have more than several billion of unknowns. Solving linear systems is clearly the limiting step to reach this challenge in numerical simulations. An important aim for this work is the design and the implementation of a sparse linear solver that can exploit the power of this new supercomputers. We will have to propose solutions for the following problems:

- full parallel and scalable preprocessing steps (ordering and symbolic factorization);
- efficient algorithmic coupling of direct and iterative methods that allow a powerful management of whole the levels of parallelism;
- adapted scheduling of computation tasks to take advantage of the runtime that operates on mixed architectures with multi-cores and GPUs.

7. Contracts and Grants with Industry

7.1. SNECMA

Participants: Guillaume Baurin, Rémi Abgrall, Mario Ricchiuto [Corresponding member].

Dates: 2008-2011

Transfer and development of the Residual Distribution schemes in the Natur code (in collaboration with INCKA).

7.2. DASSAULT

Participants: Rémi Abgrall [Corresponding member], Pierre-Elie Normand [PhD student, DGA grant, Dassault-Aviation].

Dates: 2008-2011

Study and validation of very high order SUPG schemes in AETHER.

8. Other Grants and Activities

8.1. National initiatives

8.1.1. ASTER: Adaptive MHD Simulation of Tokamak Elms for iteR

Participants: Rémi Abgrall, Robin Huart, Pascal Hénon, Pierre Ramet [Corresponding member], Hocine Sellama.

Grant: ANR-06-CIS
Dates: 2006 – 2010
Partners: CEA Cadarache.

Overview: The magneto-hydrodynamic instability called ELM for Edge Localized Mode is commonly observed in the standard tokamak operating scenario. The energy losses the ELM will induce in ITER plasmas are a real concern. However, the current understanding of what sets the size of these ELM induced energy losses is extremely limited. No numerical simulations of the complete ELM instability, from its onset through its non-linear phase and its decay, exist in literature. Recently, encouraging results on the simulation of an ELM cycle have been obtained with the `JOREK` code developed at CEA but at reduced toroidal resolution. The `JOREK` code uses a fully implicit time evolution scheme in conjunction with the `PaStiX` sparse matrix library. In this project it is proposed to develop and implement methods to improve the MHD simulation code to enable high-resolution MHD simulations of ELMs. The ELM simulations are urgently needed to improve our understanding of ELMs and to evaluate possible mechanism to control the energy losses. The improvements include adaptive mesh refinement, a robust numerical MHD scheme and refinable cubic Hermite finite elements. These developments need to be consistent with the implicit time evolution scheme and the `PaStiX` solver. The implicit scheme is essential due to the large variety of time scales in the MHD simulations. The new methods will be implemented and evaluated in the code `RealfluiDS` , developed by the BACCHUS team and the `JOREK` code to optimize the exchange of expertise on numerical methods and MHD simulations.

The project is a collaboration between the Departement de Recherche sur la Fusion Controlée (DRFC, CEA/Cadarache) and the Laboratoire Bordelais de Recherche en Informatique (LaBRI) and Mathématiques Appliquées de Bordeaux (IMB) at the University of Bordeaux 1.
Web: http://aster.gforge.inria.fr/

8.1.2. PETAL: PETascaling ALgorithms for preconditioning used in scientific applications

Participants: Pascal Hénon [Corresponding member], Jun-Ho Her, François Pellegrini, Pierre Ramet.

Grant: ANR Cosinus 2008
Dates: 2009–2011
Partners: INRIA Saclay-Ile de France (leader of the project), Paris 6, IFP (Rueil-Malmaison), CEA Saclay
Overview: In this collaborative effort, we propose to develop parallel preconditioning techniques for the emergent hierarchical models of clusters of multi-core processors, as used for example in future petascale machines. The preconditioning techniques are based on recent progress obtained in combining the well known incomplete LU (ILU) factorization with the tangential filtering, another incomplete factorization where a filtering condition is satisfied. The goal of this project is to transform these preconditioners into black box parallel preconditioners that could be as usable as standard and popular methods such as ILU. For this, we address several issues related to the quality of the combined preconditioner. We also aim to make the connection of these methods with the domain decomposition methods. To obtain a preconditioner suitable for parallelism, we will study associated graph partitioning and reordering techniques.
Web: http://petal.saclay.inria.fr/

8.2. Actions Funded by the EC

8.2.1. IDIHOM: a European project on the development of adaptive higher order variational methods for aerospace applications

Participants: Rémi Abgrall [Corresponding member], Dante DeSantis, Damien Genêt, Pascal Hénon, Pascal Jacq, Cédric Lachat, François Pellegrini, Mario Ricchiuto.

Grant: European Commission
Dates: 2010-2013
Partners: DASSAULT, DLR, ONERA, NLR, ARA, VKI, INRIA, , Universities of Stuttgart, Bergame, Twente, Nottingham, Swansea, Charles (Prague), Varsovie, CENAERO, ENSAM Paris)

Overview: Computational Fluid Dynamics is a key enabler for meeting the strategic goals of future air transportation. However, the limitations of today numerical tools reduce the scope of innovation in aircraft development, keeping aircraft design at a conservative level. Within the 7th European Research Framework Programme, the strategic target research project IDHIOM has been initiated. The goal of IDHIOM is the industrialization of innovative adaptive higher-order methods for the compressible flow equations enabling reliable, mesh independent numerical solutions for large-scale aerodynamic applications in aircraft design. A critical assessment of the newly developed methods for industrial aerodynamic applications will allow the identification of the best numerical strategies for integration as major building blocks for the next generation of industrial flow solvers. In order to meet the ambitious objectives, a partnership of 22 organizations from universities, research organizations and aerospace industry from 10 countries with well proved expertise in CFD has been set up guaranteeing high level research work with a clear path to industrial exploitation.
Web: http://www.dlr.de/as/en/Desktopdefault.aspx/tabid-2035/2979_read-4582/

8.2.2. ADDECCO : ADaptive schemes for DEterministic and stoChastiC Flow PrOblems

Participant: Rémi Abgrall [Corresponding member].

Grant: European Commission
Dates: 2009-2014

The numerical simulation of complex compressible flow problem is still a challenge nowadays, even for the simplest physical model such as the Euler and Navier Stokes equations for perfect gases. Researchers in scientific computing need to understand how to obtain efficient, stable, very accurate schemes on complex 3D geometries that are easy to code and to maintain, with good scalability on massively parallel machines. Many people work on these topics, but our opinion is that new challenges have to be tackled in order to combine the outcomes of several branches of scientific computing to get simpler algorithms of better quality without sacrificing their efficiency properties. In this proposal, we will tackle several hard points to overcome for the success of this program.

We first consider the problem of how to design methods that can handle easily mesh refinement, in particular near the boundary, the locations where the most interesting engineering quantities have to be evaluated. CAD tools enable to describe the geometry, then a mesh is generated which itself is used by a numerical scheme. Hence, any mesh refinement process is not directly connected with the CAD. This situation prevents the spread of mesh adaptation techniques in industry and we propose a method to overcome this even for steep problems.

Second, we consider the problem of handling the extremely complex patterns that occur in a flow because of boundary layers: it is not always sufficient to only increase the number of degrees of freedom or the formal accuracy of the scheme. We propose to overcome this with class of very high order numerical schemes that can utilise solution dependent basis functions.

Our third item is about handling unsteady uncertainties in the model, for example in the geometry or the boundary conditions. This need to be done efficiently: the amount of computation increases a priori linearly with the number of uncertain parameters. We propose a non–intrusive method that is able to deal with general probability density functions (pdf), and also able to handle pdfs that may evolve during the simulation via a stochastic optimization algorithm, for example. This will be combined with the first two items of this proposal. Many random variables may be needed, the curse of dimensionality will be dealt thanks to multiresolution method combined with sparse grid methods.

The aim of this proposal is to design, develop and evaluate solutions to each of these challenges. Currently, and up to our knowledge, none of these problems have been dealt with for compressible flows with steep patterns as in many moderns aerodynamics industrial problems. We propose a work program that will lead to significant breakthroughs for flow simulations with a clear impact on numerical schemes and industrial applications. Our solutions, though developed and evaluated on flow problems, have a wider potential and could be considered for any physical problem that are essentially hyperbolic.

9. Dissemination

9.1. Participation to the Scientific Community

Rémi Abgrall is associate editor of the international journals “Mathematical of Computation”, “Computer and Fluids”, “Journal of Computational Physics”, “Journal of Scientific Computing” and “Journal of Computing Science and Mathematics”. He is member of the scientific committee of the international conference ICCFD, and of the “commission d’évaluation de la direction Simulation Numérique en aérodynamique” of ONERA. He is member of the CFD committee of ECOMAS. He is also member of the scientific committee of CERFACS. He is member of the GP1 group of Allistène. He is member of the Comité National du CNRS, section 01. He is member of the board of the GAMNI group of SMAI and is its current responsible. He is member of the board of Institut Polytechnique de Bordeaux.

Pierre Ramet and Rémi Abgrall are members of the GENCI scientific committee (Mathematics and Computer Sciences). R. Abgrall also belongs to the Fluid mechanics one.

Pascal Hénon, François Pellegrini and Pierre Ramet have been members of the “commission consultative” for the LaBRI in 2010.

Pascal Hénon was also in the decision board for the “Plafrim” project, and Pierre Ramet was in the decision board of the "MCIA" project (*Mésocentre Aquitain : un environnement Mutualisé de Calcul Intensif en Aquitaine*).

Mario Ricchiuto, Cécile Dobrzynski and Rémi Abgrall have, in collaboration with the team–project MC2, prepared the CANUM 2010 in Carcan Maubuisson (june 2010).

9.2. Teaching

Rémi Abgrall is responsible of the interim period (3rd year) of the MATMECA department of ENSEIRB-MATMECA.

Cécile Dobrzynski teached during the Summer School CEA/EDF/INRIA on the topic of Mesh generation.

In complement of the normal teaching activity of the university members and of IPB members, Pascal Hénon teaches at IPB (computer science engineering school).

François Pellegrini teaches every year a master 2 class at ENSEIRB-MATMÉCA on the architecture of high-performance systems and ways to exploit them, in the context of practical projects. This year, he also gave a tutorial on MPI parallel programming and graph partitioning with `Scotch`, during the “*Séminaire de l’école d’été CEMRACS’10 – Modèles numériques pour la fusion*” at Luminy.

Pierre Ramet gives a master 2 class on parallel numerical algorithms at IPB (computer science engineering school). He also teached on the topic of sparse linear solvers during the summer school at CEMRACS (Marseille), and during a workshop organized by the CNRS (Lyon).

Mario Ricchiuto has given lectures in the “Mastère Spécialisé en Ingénierie Aéronautique et Spatiale” organized by ENSAM, ENSEIRB-MATMÉCA, Institut de Cognitique and several local industrial partners. He also teaches at ENSEIRB-MATMÉCA.

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