INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Project-Team Smash

Simulation, Modelling and Analysis of Heterogeneous Systems in mechanical engineering

Sophia Antipolis

THEME NUM

Activity Report

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2. Overall Objectives

2.1. Overall Objectives

SMASH is a common project between INRIA and the University of Provence. The main topic of our project focuses on problems related to mathematical and numerical modelling of heterogeneous flows such as multiphase media, granular materials or reactive flows with mass transfer. The scientific themes in concern are the design and improvements of models for these flows as well as the definition and analysis of discretization methods and schemes for their numerical simulation. The final aim is to implement the resulting algorithms on parallel machines for solving large scale problems of industrial or pre-industrial interest.

One of the main original feature of the SMASH researches on heterogeneous flows lies in the way we deal with multifluid flows (interface problems). We use an eulerian approach with a diffuse interface model. The two different media are not modelled separately (using adequate scheme for each phase) nor the interface needs to be defined explicitely. On the opposite, the diffuse interface zone is considered as a true multiphase region and described with a two-phase model. With such an Eulerian approach, numerical problems related to the discontinuities of the state equations through the interface, which occur when using separate models for each phase, do not appear anymore.

The domains in which two-phase flows are of interest are widespread in the industry (nuclear industry, oil company industry, car engine technology, food industry ...) but also in environmental studies (forest fire, coast erosion, ...), biomedical engineering, detonation theory or astrophysics research areas.

3. Scientific Foundations

3.1. Modelling of multiphase media

Keywords: *Hamilton principle*, *Homogenization*, *Mixture models*, *Two-phase models*.

The microcospic description of an heterogeneous medium has to take into account the specific physical properties of each material component. For both practical and numerical reasons, it may be impossible to take into account all those microscopic features. As an illustration, one m^3 of water mist typically contains a range of about 10^8 to 10^{12} droplets! Modelling such an heterogeneous medium consists in replacing it by an artificial mixture that ideally would have the same averaged properties. The resulting *multiphase* models are very far from the classical Euler or Navier-Stokes models.

The definition and setting of such multiphase models may be based on different techniques.

The first formalism [36], is very similar to the techniques involved in the definition of statistical models of turbulence with the use of averaging operators. It leads to an open set of equations (that is there are more unknowns than there are available equations). A way to close that system is to take into account some physical assumptions concerning the behaviour at the micro-scale level. This approach is certainly the most used in the industry but leads to difficult open questions in applied mathematics such as the hyperbolicity of the resulting models and the definition of non-conservative products. This methodology was the starting point of our studies in multiphase modelling and led us to promote the use of two-pressure, two-velocity *hyperbolic* models [7].

However, with this type of modelling, closure assumptions concerning the microscale behaviour have to be formulated. This is an extremely difficult task. Therefore, we are also investigating a modelling formalism based on the Hamilton principle of least action [39]. The advantage of this formalism is that the only assumptions are on the definition of the potential energy associated to the flow.

Using either technique results in a set of non linear partial differential equations (PDE). Then, we need to discretize it by some numerical scheme in order to get a set of algebraic equations that in turn will provide the discrete solution. We are therefore faced with mainly two classes of difficulties: the first class of difficuties consists in finding the good set of PDE's to model the multiphase flow we want to study; the second class comes from the choice of the discretization scheme.

To avoid this addition of difficulties, we have recently introduced an original modelling technique [1]. In this approach, we start with the continuous equations defined at the microscale level but instead of averaging it, we *first* discretize those microscale continuous equations *before* filtering the resulting set of discrete equations. With this technique, we end up directly with a macroscale discrete model.

3.2. Modelling of interface and multifluid problems

Keywords: *Diffuse interface*, *Eulerian Models*, *Front Capturing*, *Multifluid mixtures*.

An important part of CFD is to get a detailed description of the interaction between two different fluids at the scale of the interface between them. This is what we will call a *multifluid* problem. At the present time, tracking methods are certainly the most used technologies to treat this problem.

For compressible fluids, “capturing” or diffuse interface approach, where the interface is not defined explicitely as a discontinuity surface but as non-zero thickness mixing zone (where the physical quantities are continuously varying) are just begining to be used. Actually, before the original work of Abgrall [35] the capturing methods were pleagued by the difficulty of computing the pressure in the mixing zone. Abgrall shows the feasability of interface capturing methods provided that one partially gives up the conservative form of the equations. Improving upon this contribution, our project develops an original diffuse interface method where the artificial numerical zone is considered as a true two-phase flow region. Although seemingly artificial, this allows to consider a model that can handle huge density ratio and very different thermodynamics.

This front capturing - diffuse interface technique has proven its ability of solving interface flow problems more simply than usually and moreover offers the possibility to treat not only interface problems between pure fluids but also interfaces between mixtures (as for instance the boundaries of a cloud) in the same formalism.

3.3. Approximation methods

Keywords: *Finite Volume methods*, *Low Mach Compressible flows*, *Riemann Solvers*.

All the mathematical models considered and studied in SMASH consist in either a hyperbolic or parabolic system of PDE's. The discretization techniques applied to these PDE should respect the properties of the continuous model such as conservativity, positiveness preserving (e.g. pressure, density), jump conditions, maximum principle or entropy inequality. Most of our numerical methods are based on finite volume discretizations [37]. That indeed allows us to keep the full description of the physics of the media by solving local *Riemann problems* [40] corresponding to the evolution of the medium variables through a plane interface separating two physical states. SMASH focuses its efforts into the development of approximation methods using either exact or approximate Riemann solvers.

When the resulting model is non conservative, which occurs as a "mechanical" consequence when using an averaging process, additional mathematical and numerical difficulties arise. From a theoretical point of view, it is known since the works of Schwartz [38] that the product of two distributions is not defined. Therefore, the question of giving a sense to this product arises and as a consequence, the numerical approximation of non-conservative terms is unclear. For contact discontinuities, our discretization methods are based on the principle that both velocities and pressures should remain constant. The resulting discretization schemes respecting that principle appear to be both robust and efficient for interface flow problems compared to most existing methods. For shocks, we investigate formulations where the Rankine-Hugoniot relations are imposed via some physical analysis of the internal structure of the relaxation zone.

Another difficulty encountered in solving two-phase flow problems comes from the high disparity between the wave speeds of each existing fluid material. In particular, one of the fluids may be very close to the incompressibility limit. In that case, we face up the problem of very low Mach number flows. The numerical treatment of these flows is still a problem and involves non trivial modifications of the original upwind schemes [5], [4]. Our investigations in that domain concerns both acoustic and incompressible aspects in methodologies for setting up suitable numerical methods.

3.4. Solution algorithms

Keywords: *Grid Computing*, *Multigrid methods*, *Multilevel methods*, *Parallelism*.

The approximation step generates large algebraic systems that have to be solved. The problems that the team is studying can result in systems that can have several tenth of millions of unknowns. The choice of appropriate solution methods is therefore fundamental. The team concentrates its investigations on multi-level and multigrid methods. In this domain, since the meshes used for industrial applications can be totally non-structured, an important point is to be able to construct a hierarchy of meshes describing the problem with different levels of resolution. In this direction, the team studies both purely algebraic approaches as aggregation/agglomeration methods [6] as well as geometrical methods where a hierarchy of non-structured meshes is contructed by coarsening algorithms.

For the largest problems that we are currently considering, the use of modern parallel computers is mandatory. This requires a careful examination or adaptation of the numerical solvers. Nowadays, the usual way to parallelize large mesh-based scientific application relies on partitioning the computational domain. Then, a simple SPMD (Single Program Multiple Data) strategy using a message passing programming model (such as MPI "Message Passing Interface") can be used to parallelize these applications.

The SMASH team is also involved in some experiments in Grid computing using the same parallelization model (http://www-sop.inria.fr/smash/mecagrid/public/mainFrame.htm). Actually, the possibility to construct large scale computing platforms like the Grid5000 project is very attractive for solving some fundamental problems in engineering like multifluid applications or turbulence studies. However additional problems such as the heterogeneity of the computing nodes and of the interconnection networks or the multi-site localization of the computing or data storage ressources have to be solved to make the concept of Grid effective in high performance computing.

4. Application Domains

4.1. Panorama

With a large experience in working on numerical fluid mechanics problems, SMASH studies focuses its particular interests on compressible multiphase or multifuid flows; the application domains involves energy and transport industries: aeronautics, car engine combustion research, space research, oil company research, research on electricity and nuclear centers hazards, but involves also other various domains such as astrophysics and detonation studies.

4.2. Transport industry

Automotive industry : In Diesel engines, the new generation injection system technology use high pressure spray injection techniques. Our eulerian modelling techniques may be used to describe the first steps of atomization of the spray. These phenomena are preceded by a dynamic liquid-vapor transition phase during which the compressibility feature of the flow appears to be crucial. Figure 1 from [15] shows the vapor volume fraction in a two dimensional model of fuel injector The dark area represents the location where the vapor volume fraction is high. This study has been performed in the framework of an "ARC" (Action Concertée de Recherche) of CNRS, whose industrial partners were Peugeot and Renault.

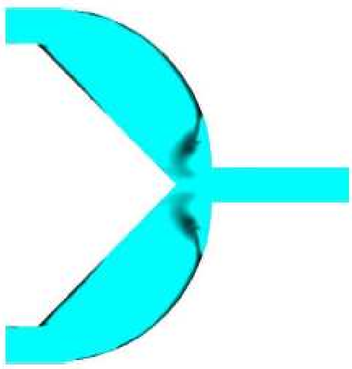

Figure 1. Vapor volume fraction in a two dimensional model of fuel injector

Aeronautics : The main needs in that area concern external aerodynamics, where turbulence has to be taken into account to model external complex flows around a complete geometry profile since the numerical simulations are still too costly to be a true part of the optimization process. SMASH is interested in defining suitable multigrid solvers for the Navier Stokes equations using unstructured finite volume discretization grids. In addition, the unsteady feature of turbulent flow problems encountered e.g. in vibration of some material structure and damaged material problems requires the need of LES type models ("Large Eddy Simulation" techniques).

Space industry : Another application area we are concerned with is the behaviour of a space launcher engine using liquid fuel or powder propellents. Since the media involve very heterogeneous ingredients, two-phase modellings as well as the study of free surface problems are needed

4.3. Energy industry

The needs in numerical modelling are concerned with thermohydraulics for nuclear energy production centers (CEA and EDF), flow problems in pipe lines for oil company industry (extraction, oil transport and refining) and all other industries related to energy production or chemical engineering.

In these industrial domains, turbines, boilers and pipes involve very complex flows which often evolve either violently and/or at high speed, or on the contrary evolve very slowly with a large stabilization time. Describing those phenomena which are intrinsically two-phase type flow problems appears to be fundamental in studies of security issues against hazards (nuclear industry, oil-chemical industry or chemical engineering industry). When dealing with very low Mach number flows, the numerical complexities and difficulties are even higher. The ability of a CFD code to treat efficiently and accurately the different phase flow regimes (gaz/liquid flows, bubbling flows, packet flows, liquid film and droplet flows, supersonic, very subsonic) is still problematic. These difficulties are amplified in some research program on controlled Fusion like ITER, where the generated heat flux can be as high as $20MW/m^2$. To cope with such high fluxes, the design of relevant two-phase models and of the associated numerical methods is of primary importance.

4.4. Examples of other application issues

Multiphase modelling techniques may also find a place in other various application domains. That is for instance the case in astrophysics for modelling keplerian type flows in a proto-planetary system composed of gas and particles. This type of study is currently done in the team in collaboration with astrophysicists to validate some assumptions on the process of planet formation in accretion disks. Figure 2 taken from [12] shows for instance the development of a non-linear instability in a gas flow around a star leading to the formation of vortices. The formation of such vortices is involved in some scenarii of planet formation.

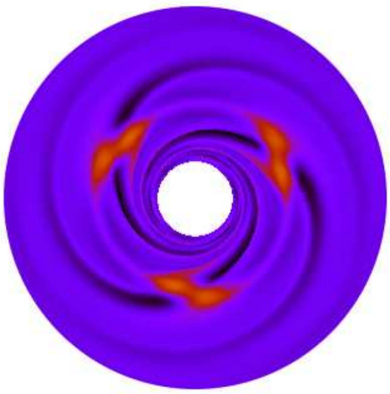

Figure 2. Pressure field after 2.7 orbital revolution

Another interesting application domain concerns multiphase flow problems in highly energy-giving granular media. Most of the existing CFD codes that aim to simulate those types of multiphase flows uses the Euler equation model closed by an equation of state defined for the fluid mixture. That necessarily implies that the phase temperatures (or phase density ...) equilibrium holds without making sure that such assumption remains relevant to this type of flow problems. The project-team works on the definition of two-temperature models in which the physics is more accurately described for such media.

5. New Results

5.1. Mathematical Modelling of two-phase and multi-fluid flows

5.1.1. Shock relations for multiphase mixtures with stiff mechanical relaxation

Participants: Sergey Gavrilyuk, Olivier Le Metayer [IUSTI], Jacques Massoni, Richard Saurel.

Examples of multiphase mixtures for which velocity and pressure relaxation is a stiff phenomenon are involved in many practical applications dealing with condensed phase mixtures, solid alloys, propellant and solid explosives, specific composite materials, micro- and nanostructured mixtures etc. Shock relations for the mixture require the determination of the volume fraction jump or the jump of any other thermodynamic variable. Examination of the shock dispersion mechanism suggests such jump relations. These relations are the phase Hugoniots which are compatible with the mixture energy equation. The corresponding model is conservative and symmetric. It fulfils the single-phase limit and guarantees volume fraction positivity. The shock relations are validated over a large set of experimental data and provide a remarkable agreement.

5.1.2. Stability conditions of multiphase detonations and resolution of their internal structure

Participants: Marie-Helene Lallemand, Richard Saurel.

The stability conditions and the structure of single phase detonation waves have been known for more than one century. Nevertheless, those of multiphase detonation waves are still unknown. The main reasons lie in the lack of knowledge of appropriate flow model and shock jump conditions. On the basis of a single pressure, single velocity flow model, but with different temperatures, and appropriate jump conditions, the determination of the multiphase detonation wave structure is now possible. In this work, a new methodology for analysing and resolving this structure is proposed. In the particular case of a fluid that obeys the equation of state of an ideal gas, we give the explicit expression of the analytic solution and we propose a numerical algorithm for the approximate solution. This algorithm is the basis for elaborating the algorithm that we use for a multiphase model. We propose the determination of the internal structure of multiphase detonation waves. Numerical tests are performed, allowing the validation and the evaluation of both our model and solver [29].

5.1.3. Modelling of bubbly flows

Participants: Fabien Duval [IRSN], Hervé Guillard, Jean-Claude Latché [IRSN], Roxanna Panescu.

The simulation of disperse bubbly flows is very often done with the use of the so-called “drift flux” model where the slip velocity between the dispersed and the continuous phases is specified by an algebraic relationship. This simple approach suffers from a severe drawback : Depending on the flow regime, the slip relationship can change and with it, the mathematical nature of the model that can switch from an hyperbolic to a non-hyperbolic system. Using a Chapman-Enskog asymptotic analysis, we have derived a model for bubbly flow where the slip velocity is expressed by a Darcy type relation. This model is always hyperbolic with a clear mathematical structure. Numerical approximation for this model have been devised and applications to several test cases have been realized. This work have been presented at the conferences Applied Math 05 and "Trends in Numerical and Physical Modeling for Industrial Multiphase Flows, 2005", [21], [19].

5.1.4. Modelling of two-phase protoplanetary disks

Participants: Pierre Barge [Laboratoire d’Astrophysique de Marseille], Eric Daniel, Hervé Guillard, Satoshi Inaba [Dept of earth and Planetary sciences, Tokyo Institute of Technology].

A 2-D hydrodynamical code has been developed to study the interaction of gas and dust in protoplanetary disks [12]. Gas is considered as a compressible fluid while solid particles are treated as a pressureless gas.

Due to the interaction between the two phases, solid particles lose angular momentum and energy and migrate toward the central star. This code has been used to study the so-called lifetime problem and has shown that taking into account the full coupling of the solid and gaseous phases, particles can survive 16 times longer than in the uncoupled case. This opens interesting perspectives in the continuous growth scenario for the formation of planetesimals. This code will be used for the study of other scenarii (for instance the vortex scenario of Barge and Sommeria).

5.1.5. Interface and multi-fluid computations

Participants: Alain Dervieux, Anne-Cecile Lesage, Olivier Basset, Hervé Guillard.

SMASH has developed a 3-D multi-fluid research code based on one pressure, one velocity model [16]. This code is continuously improved and extended. New computational results obtained with it are described in [33]. In parallel with these studies that uses a multiphase modelling of the numerical mixing zone at the interface, the team also develops several activities where the level set technique is used to capture the interface zone. These studies are done in collaboration with Cemef for incompressible models [18] where they are mainly used as benchmark computations for parallel and grid computing. In partnership with Société Lemma, new Level Set methods are also studied for capillarity low gravity applications with small contact angle. In this framework, in partnership with Lemma, CNES and EADS, a thesis is started by Damien Guegan for interface phenomena in which thermal effects are important.

5.1.6. Large Eddy Simulation (LES)

Participants: Simone Camarri [U. Pisa], Charbel Farhat [U Stanford], Alain Dervieux, Bruno Koobus [Montpellier2], Maria-Vittoria Salvetti [U. Pisa], Vanessa Mariotti [U. Pisa], Eric Schall [U. Pau], K. El Omari [U. Pau], Y Benthaleb [U. Pau].

The purpose of our works in LES/LNS is to develop new approaches for industrial applications of LES-based analyses on non-structured meshes [2], [30],[13]. In the mean term foreseen applications (aeronautics), the Reynolds number is several tenth millions, a too large number for pure LES models. However, certain regions in the flow can be much better predicted with LES than with usual statistical RANS (Reynolds averaged Navier-Stokes) models. These are mainly vortical separated regions as assumed in one of the most popular hybrid models, the DEtached Eddy Simulation model. It is hybrid in the sense that a blending is applied between LES and RANS. The approach which the french-italian team considers is the one of Batten-Golberg-Chakravarthy, the LNS (Limited Numerical Scale) method. A paper has been published in Wind and Structures [8].

Concerning statistical turbulence models, cubic low Reynolds extensions are studied in cooperation with University of Pau. Studies of large geometries such as airships are currently done with statistical models [32], [31]. A new investigation of combustion chambers of turbo-machines is also begining.

5.1.7. Acoustics in high speed flows

Participants: Ilya Abalakin [IMM-Moscow], Alain Dervieux, Tatiana Kozubskaya [IMM-Moscow].

Previous works of this troika addressed the developement of a new version of NLDE, and of superconvergent techniques for noise propagation with linear and nonlinear hyperbolic models. We want to mention that the high quality of the works of Tatyana Kozubskaya, leader of the team at Moscow in partnership with SMASH has been recognized by several invitations to present conferences and to be editor of a special issue of International Journal of Acoustics. The interest of the Russian-French team is concentrating on nonlinear phenomena in a resonance-type liner. This means in particular that the numerical scheme adapts to very different situations including propagation without dissipation and nonlinear interactions with entropy-related dissipation.

5.2. Approximation

5.2.1. Non conservative projection method

Participants: Richard Saurel, Erwin Franquet, Eric Daniel.

A new numerical method able to solve single phase and multiphase compressible flow models has been proposed. It uses two main ingredients. The first one is the Rankine Hugoniot conditions used for the building of an approximate Riemann solver. In the multiphase context where the equations are not conservative these relations are provided using the results of the study performed in 5.1.1 for mixtures where stiff mechanical relaxation is present. The second ingredient is a new projection method different from the conventional average done with Godunov type schemes. It consists in the resolution of a relaxation problem between the various sub-volumes present in a computational cell. These sub-volumes correspond to the ones swept by the various waves. For the sake of simplicity and efficiency the method is developed in a Lagrange - Projection context in order that a maximum of three sub-volumes be present in the computational cell. It is first detailed and validated for the single phase Euler equations and is shown to give a cure to anomalous computations of some basic problem such as sliding lines and fluids governed by real gas equations of state (Mie Gruneisen for example). It is then extended to the computation of a compressible five equation multiphase model able to deal with interface problems and shock propagation into mixtures of compressible materials. Although the model is non conservative the present numerical method provides conservative results, thanks to the multiphase Rankine Hugoniot conditions and conservative projection method. The method is validated over exact solutions and experimental ones and provides excellent agreement. [20]

5.2.2. Well balanced schemes for Keplerian flows

Participants: Hervé Guillard, Eric Daniel.

This study deals with the improvment of the numerical method used in the 2-D hydrodynamical code described in [12]. This code developed to study the interaction of gas and dust in protoplanetary disks require an extremely accurate approximation of the balance between the gravitational force, the centrifugal acceleration and the pressure gradient. However, finite volume methods are generally unable to guarantee that this balance is realized at the discrete level. This will only be true in the asymptotic limit of zero mesh step. In practice, this means that accurate results require a prohibitively large number of mesh points. In this study [20], we have derived a well balanced scheme that is able to realize at the discrete level the balance between the gravitational force, the centrifugal acceleration and the pressure gradient in cylindrical geometry. This is done by using the concept of hydrostatic reconstruction of the variables at the cell interfaces.

5.3. Solution Algorithms, Parallelism and Grid Computing

5.3.1. Mesh coarsening for anisotropic non-structured meshes

Participants: Hervé Guillard, Youssef Mesri.

Multigrid methods needs a hierarchy of meshes able to filter the components of the solution at different levels of resolution. On the other hand the accurate computations of aerodynamical problems including turbulence modelling have to use extremely anisotropic meshes in the boundary layers where the ratio of the mesh size in the direction perpendicular and parallel to the wall can be as small as 10^{-5}. For this type of anisotropic meshes, an efficient use of multigrid techniques requires a semi-coarsening strategy where the fine grids are progressively coarsened in the direction perpendicular to the wall. In this work, we study such semi-coarsening strategies using the notion of metrics to normalize the mesh size specification. Specifically, at each node of the fine mesh is associated a metric in which the elements are equilateral, then a new metric field is defined corresponding to a semi-coarsening in the direction perpendicular to the wall and a new mesh optimizing this new metric field is generated. This strategy implied to solve difficult problems related to the interpolation and smoothing of a metric field. The current work aims at validating this approach on industrial test cases.

5.3.2. Mesh partitioning for computational grids

Participants: Hervé Guillard, Youssef Mesri, Olivier Basset, Hughes Digonnet [ENSMP].

The goal of this work was to improve the efficiency of a parallel mesh partition tool taking into account heterogeneous processors speed and communication time. In a previous work, we had devised a mesh partition algorithm that achieves load balancing with heterogeneous CPU while trying to minimize the communication time on an non-homogeneous network. However, this algorithm, was based on local mesh transformations. For very large meshes, this results in large CPU time to achieve the partition of a mesh. The new algorithm uses global operations to partition the mesh and reduces the CPU time in a significant manner. Application of this partitioning strategy to large test-cases have shown a significant improvment in CPU time versus standard homogenous strategies [27], [28], [26].

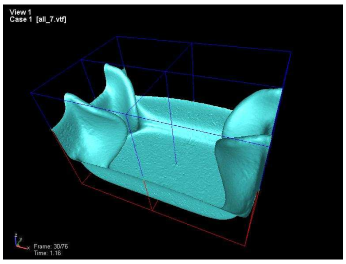

Figure 3. Liquid surface after refection on the boundaries

Figure 3 illustrates the efficiency of this partitioning algorithm on the computation of a 3-D dam break problem. On this problem, a water column is enclosed within a closed vessel. At time t=0, the walls of the vessel are removed and the water column collapses under the effect of gravity. The mathematical method and numerical method used for this study are described in [18]. The mesh contains 1.5Millions of nodes and 8.7 Millions of elements. An implicit time stepping method was used where at each time step 2 linear systems with respectively 6 millions and 1.5 millions of unknowns have to be solved. Six hundred time steps were used generating $4.5 \quad 10^9$ of data numbers. Table 5.3.2 gives the CPU time used for this computation on the MecaGrid (http://www-sop.inria.fr/smash/mecagrid/public/mainFrame.htm) composed of two clusters in Sophia-Antipolis and one cluster in Marseille. It can be seen that the use of the new heterogeneous partition strategy has lead to a significant reduction of the CPU time of more than 45%.

Clusters(39 procs used)	CPU time
Sop1-Sop2-MRS(homogeneous partitioning scheme)	5 days and 6 hours
Sop1-Sop2-MRS (heterogeneous partitioning scheme)	3 days and 1 hour

5.3.3. Grid-enabled application codes

Participants: Alain Dervieux, Bruno Koobus, Steve Wornom.

In the context of the MecaGRID initiative, the SMASH team develops a set of computational tools for demonstrations in Grid Computing. The central kernel is a CFD code (AERO) derived from the synthesis of research developed by the SMASH Team in collaboration with the University of Colorado at Boulder. This code executes in parallel using MPI and is natually suited for MPI Grid computing. However, the absence of dynamic memory allocation penalizes FORTRAN 77 codes in an environmment made of heterogeneous computing ressoures. A re-writing of the code using F95 has therefore been performed [34] and has shown significant improvment on the previous version of the code. A new kernel, AEDIF derived from AERO, computes two-phase flows using a new diphasic models developed in the project ([16]). AEDIF solves the discrete equations on unstructured meshes using tetrahedras with an MPI parallel mode based on mesh partitioning. This code has been ported on the MecaGRID (http://www-sop.inria.fr/smash/mecagrid/public/mainFrame.htm) and experiments with up to 64 processors localized on the three sites have been performed [33]. Figure 4 for instance represents the interaction of an air bubble with a shock wave. The computation realized on three different sites illustrates the interest of the concept of Grid computing, allowing different institutions to share their computing ressources and making possible large scale numerical experiments.

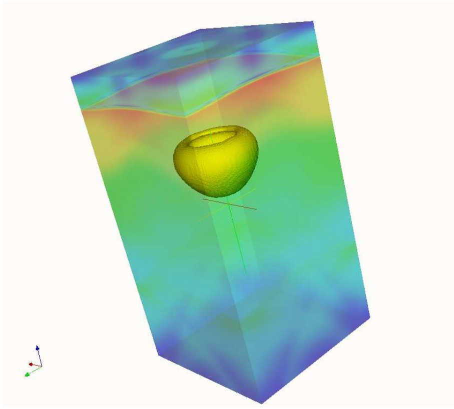

Figure 4. Air bubble and shock interaction

5.3.4. Large Eddy Simulation on a computational Grid

Participants: Alain Dervieux, Bruno Koobus, Vanessa Mariotti.

Progresses made on the use of the computational grid MecaGRID allow one to consider computations involving several millions of mesh points. During an internship, Vanessa Mariotti from the university of Pisa studies the turbulent interaction of a cross-jet with a pipe flow with LES/LNS turbulence models (see section 5.1.6 and [30]).

5.3.5. Distributed Mesh applications

Participants: Mohamed Essaidi, Hervé Guillard.

For current applications of metacomputing in CFD, the meshes can involve millions of points and elements and cannot anymore be stored in the memory of a single processor. In this framework, all the basic I/O operations, creation of data structures (e.g creation of the CSR format to store the mass and stiffness matrices) or geometrical operations associated to unstructured Finite Elements or Finite Volume methods have to be performed from the begining in a distributed context. This is the starting point of this study whose aim is to create an OO library for the handling of very large Finite Element unstructured meshes in a distributed environment.

6. Contracts and Grants with Industry

6.1. Analysis of closure relations for a two-fluid model

Participants: Richard Saurel, Olivier Le Metayer [IUSTI].

This work with CEA Bruyères le chatel was devoted to the analysis of closure relations for a two-fluid compressible multiphase model for modelling the mixing between two fluids by compression waves.

6.2. Modelling of bubbly flows

Participants: Hervé Guillard, Roxanna Panescu.

In the framework of a preliminary program to study convective pattern in bubbly flows, IRSN and SMASH have engaged a common initiative for the numerical modelling of bubbly flows.

6.3. Level-Set software

Participants: Alain Dervieux, Anne-Cécile Lesage.

The subject of this partnership with the technological company LEMMA is to develop a level-set based multi-fluid software for applications in the aerospace industry.

6.4. Multiphase Algorithms for high energy material

Participants: Jacques Massoni, Richard Saurel, Olivier Le Metayer [IUSTI], Eric Daniel.

This study realized with the support of DGA, deals with the development of multiphase algorithms to compute the dispersion of a multiphase mixture in air and its interaction with detonation products.

6.5. Coarsening Algorithms for Multigrid applications

Participants: Hervé Guillard, Youssef Mesri.

This contract with Dassault-Aviation supports a 18 month study devoted to the design of semi-coarsening algorithms for 3-D anisotropic meshes for multigrid applications.

6.6. Modelling of nano-structured explosives

Participants: Richard Saurel, Eric Daniel, Sergey Gavrilyuk, Olivier Le Metayer [IUSTI], Erwin Franquet, Jacques Massoni.

This work supported by DGA addresses the modelling of the micro-scale physics in nano-structured explosives.

7. Other Grants and Activities

7.1. National and Regional initiatives

7.1.1. Ministry Grant ACI-GRID "MECAGRID"

Participants: Olivier Basset, Thierry Coupez [Ecole des mines de Paris], Hughes Digonnet [Ecole des mines de Paris], Hervé Guillard, Olivier Basset [Ecole des mines de Paris], Jacques Massoni.

This initiative launched in November 2002 associates the CEMEF of Ecole de Mines de Paris, IUSTI of the University of Provence and INRIA in the construction of a computational grid from three PC clusters located in the PACA region (http://www-sop.inria.fr/smash/mecagrid/public/mainFrame.htm). This grid is devoted to massively parallel applications in multimaterial fluid mechanics.

7.1.2. Collaboration with University of Pisa

Participants: Maria-Vittoria Salvetti [University of Pisa], Francois Beux [University of Pisa], Vanessa Mariotti [University of Pisa], Simone Camarri [University of Pisa], Hervé Guillard, Alain Dervieux.

Through its support program for the development of regional research centers, the Conseil regional de la région PACA supports a collaboration with the University of Pisa on the development of numerical models for two-phase flows.

7.2. Bilateral international relation

- Scientific exchanges with IMM-Moscow (I. Abalakin, T. Kozubskaya) continue with common communications and papers on Acoustics.
- The project has an on-going common works with Stanford University (C. Farhat) for fluid-structure interaction and two-phase flow problems.

- French-German collaboration DFG/CNRS: Micro and macro modelling and simulation of liquid - vapour flows (FOR 563). This collaboration aims to improve two-phase flows models and associated numerical methods. French participants: F. Coquel, T. Gallouet, P. Helluy, J.M. HÃÂ©rard, P. Josserand, S. Zaleski, R. Abgrall, C. Berthon, B. Nkonga, R. Saurel, S. Benzoni-Gavage, D. Jamet, A. Dervieux, P. Le Floch, V. Perrier. German Participants: C. Rohde, Ohlberger, S. Muller, Ballman, Lauterborn, Kurz, N. Peters, Binninger, Warnecke, D. Kroner, W. Dreyer, M. Hermann, J. Haink, C. Kraus, R. Dahms, M. Ferch, C. Merkle.
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8. Dissemination

8.1. Teaching

In the academic year 2004-2005, project members have taught the following courses :

Eric Daniel University of Provence : 200h, University of Provence, Second years of engineering school and mastère.

Jacques Massoni University of Provence : 200 h, First and second years of engineering school and mastère, second year.

Richard Saurel University of Provence : 100h, Second year of engineering school and mastère. Richard Saurel is also director of the Mastère “Energétique et Combustion”.

8.2. Ph. D thesis and Masters Thesis

This year, the project has harboured the following Ph. D Students :

ROXANNA PANESCU University of Nice-Sophia-Antipolis, "Méthodes de volumes-Eléments finis pour les écoulements de liquides à bulles"

ANNE-CÉCILE LESAGE University of Nice-Sophia-Antipolis, "Méhodes numériques pour les écoulements diphasiques"

OLIVIER BASSET ENSMP, "Simulation numérique d’écoulements diphasiques sur grille de calcul"

YOUSSEF MESRI, University of Nice-Sophia-Antipolis,"Adaptation for anisotropic non-structured meshes"

ERWIN FRANQUET, University of Provence, "Modelling of nano-structured explosives"

MATHIEU LABOIS, University of Provence, "Développement de modèles diphasiques à sept équations"

DAMIEN GUEGAN, University of Nice-Sophia-Antipolis, "Modèles pour les fluides capillaires en faible gravité"

8.3. Conferences and Seminar Organization

- In june 26, july 2nd, 2005, the team has organized the international spring school “Modelling of interface and front problems” that has gathered around forty physicists, mathematicians and numeriscists working on this topic.
- Richard Saurel and Hervé Guillard are members of the scientific committee of CFM2005 (Congrès Français de Mécanique that gathers this year 1100 participants). Richard Saurel was co-chairman of the multiphase flow session that gathers around sixty participants.

8.4. Conferences and workshops

Members of the team have delivered lectures in the following conferences and seminars (see the bibliography) :

- A. Dervieux, Invited seminar at Oxford university on mesh adaptation
- A. Dervieux, Invited seminar at Montreal university on mesh adaptation
- A. Dervieux, Invited conference at Collège de France "De la matière à l'ordinateur: modélisation des milieux continus et des interfaces", at the occasion of Marcel Dassault prize that was awarded by him.
- H. Guillard, Invited conference at the conference "Mathematical methods in Hydrodynamics", université des Sciences et Technologies de Lille, Villeneuve d'Ascq, June 27-29 th 2005,
- H. Guillard, Invited Lecturer at the spring school "Numerical Simulation of Complex and Multiphase Flows", 18th - 22nd April 2005, Porquerolles, organized by Université de Toulon et du Var, http://multiphase05.univ-tln.fr/
- R. Saurel, Invited conference at the technical workshop on source term characterisation, Centre d'Etude de Gramat, 14-15th of June 2005. Anglo-French technical arrangement. Assessment and control of chemical and biological risks.
- R. Saurel, Invited conference at the AWE Conference on Numerical methods for multi-material fluid flows, 5th-8th September 2005, St Catherine College, Oxford.
- R. Saurel, Invited Lecturer at the Advanced School on Fluid Dynamics of Cavitation and Cavitating Turbopumps, CISM, Udine (Italie), July 25-29.
- "Finite Volumes for complex applications IV", July 2005, Marrakech, Morocco(Y. Mesri, H. Guillard).
- "SMAI05, 2eme Congrès national de mathématiques appliquées et industrielles", Evian 2005, (Y. Mesri).
- International Conference on "Applied Mathematics and Scientific Computing, APPLMATH 05" Conference, June 2005, Brijuni, Croatia (H. Guillard).
- "Finite Element for Flow Problems" Conference, Swansea, Wales, UK, (A.-C. Lesage, A. Dervieux).

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