INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Project-Team Smash

Simulation, Modeling and Analysis of Heterogeneous Systems in Continuum Mechanics

Sophia Antipolis - Méditerranée

THEME NUM

Activity Report

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2. Overall Objectives

2.1. Overall Objectives

SMASH is a common project between INRIA and Aix-Marseille University. Its main topic is related to the mathematical and numerical modeling of heterogeneous flows such as multiphase media, granular materials and interface problems.

The first issue deals with the design and improvements of theoretical models for these flows. Particular attention is paid to well posedness issues and systems' hyperbolicity. The second issue deals with the design of appropriate numerical schemes. These models are not well known as conventional single fluid models and pose numerical challenges such as, for example, the numerical approximation of non–conservative terms. These numerical issues pose theoretical ones such as, shock wave existence in multiphase mixture, cell average of non–conservative variables, Chapman–Jouguet conditions for heterogenous explosives etc.

The final aim is to implement the resulting algorithms on parallel machines for solving large scale problems for the design of advanced technology systems in Space, Defense and Nuclear energy.

One of the main original features of the SMASH researches on heterogeneous flows lies in the way we deal with multiphase mixtures. Our aim is to solve the *same equations* everywhere with the *same numerical* method :

- in pure fluid,
- in multi-velocity mixtures,
- in artificial smearing zones at material interfaces or in mixture cells,
- in shocks, phase transition fronts, detonation waves,
- in elastic-plastic materials.

An example of such computations is given in the Figure 1.

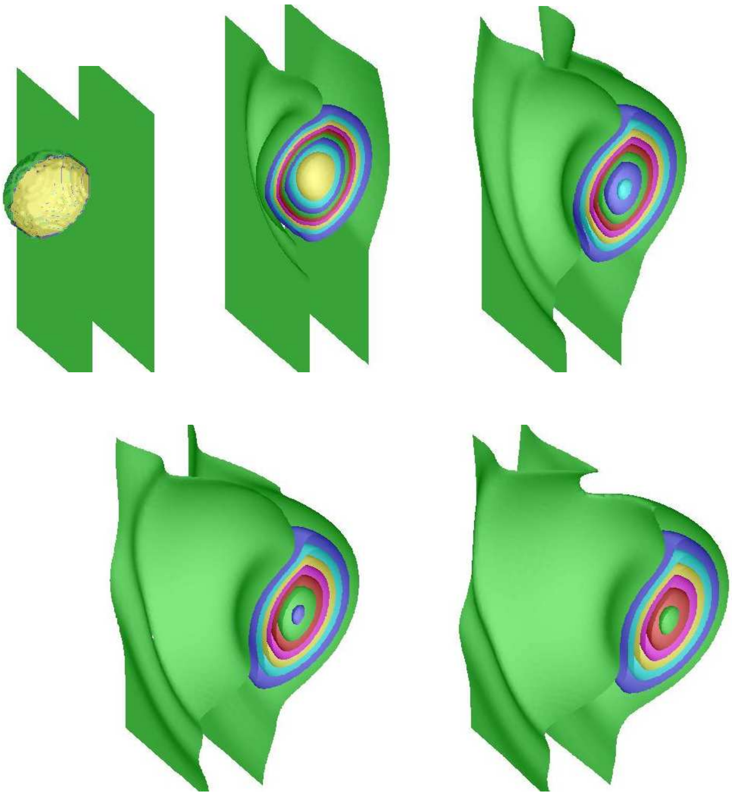

Figure 1. Numerical simulation of the impact under incidence of a copper projectile at 3 km/s onto a steel plate. Density contours. The various shock waves and crater formation are visible. Three materials are present : copper, steel and air. The difficulty with mixture cells and large density ratios is solved easily by a variant of the method given in [9].

There are some advantages with this approach :

- The most obvious relies in the coding simplicity and robustness as a unique algorithm is used,
- Conservation principles are guarantied for the mixture. Conventional algorithms are able to preserve mass conservation only when dealing with interfaces.
- Interface conditions are perfectly matched even for the coupling of complex media (granular flows, capillary fluids, transition fronts) even in the presence of shocks.

- This approach is the only one able to deal with dynamic appearance of interfaces (cavitation, spallation).
- Our method allows the coupling of multi-velocities, multi-temperatures mixtures to macroscopic interfaces where a single velocity must be present. To illustrate this capability consider the example of a cloud of bubbles rising in a liquid up to the surface where a free boundary is present. Two velocities have to be considered for the bubbles rising while a single velocity must be present just after their crossing through the interface. This is also the only method able to deal with such situations.

Our approach rises increasing attention from the scientific community as well as the industry. As will be detailed further, many projects are currently under development with french oriented research centers (DGA, CNES, Airbus) as well as foreign ones (Idaho National Laboratory - USA, Agency for Defense Development - South Korea).

3. Scientific Foundations

3.1. Modeling of Multiphase Media

Keywords: *Discrete Homogenization Method (DHM)*, *Hamilton Principle*, *Hyperbolic Models*.

Conventional models of two-phase mixtures having several velocities present under the form of partial differential systems with six equations: two mass, two momentum and two energy equations. These models are not hyperbolic and are consequently ill posed. It means that initial data and boundary conditions do not fully determine the solution at the next instant. In other words, wave propagation may have no physical sense, as the square sound speed may become negative.

This issue has been understood by [69] and subtle remedy was given by [51]. They proposed an extended model with seven equations. The extra differential equation replaced the pressure equilibrium assumption in the mixture. Thanks to this new equation, the model was correctly posed, unconditionnaly hyperbolic.

This model had little diffusion as it was presented in the context of a specific problem of detonation physics. Also, the model was difficult to solve at the numerical level, in particular with modern algorithms based on the Riemann problem solution. In [65] we developed the first Godunov type method for this model and derived accurate approximation formulas for the non-conservative terms. Moreover, a specific relaxation method was built in order to solve these equations in the presence of stiff relaxation terms. This issue was particularly important as,

- this model was involving two pressure and two velocities,
- at an interface the jump condition corresponds to continuous normal velocities and continuous pressures,
- in order to fulfill this condition it was necessary to relax the two pressures and velocities to unique equilibrium variables.

Such an issue was reached by using specific relaxation solvers, using infinite relaxation parameters like in [63]. With this solver, the model was able to solve interface problems (air/water for example) and multiphase mixtures with two velocities. Important applications of fundamental and applied physics were possible to solve. Financial supports from DGA and CEA helped us to pursue the investigations.

The two-phase flow model presents under the form (1) :

$$
\begin{aligned}
&\frac{\partial \alpha_1}{\partial t} + u_I \, \frac{\partial \alpha_1}{\partial x} = \mu \, (p_1 - p_2) \ , \\
&\frac{\partial \alpha_1 \, \rho_1}{\partial t} + \frac{\partial (\alpha_1 \, \rho_1 \, u_1)}{\partial x} = 0 \ , \\
&\frac{\partial \alpha_1 \, \rho_1 \, u_1}{\partial t} + \frac{\partial (\alpha_1 \, \rho_1 \, u_1^2 + \alpha_1 \, p_1)}{\partial x} = p_I \, \frac{\partial \alpha_1}{\partial x} + \lambda \, (u_2 - u_1) \ , \\
&\frac{\partial \alpha_1 \, \rho_1 \, E_1}{\partial t} + \frac{\partial (\alpha_1 \, \rho_1 \, E_1 \, u_1 + \alpha_1 \, p_1 \, u_1)}{\partial x} = p_I \, u_I \, \frac{\partial \alpha_1}{\partial x} - \mu \, p_I^{'} \, (p_1 - p_2) + \lambda \, u_I^{'} \, (u_2 - u_1) \ .
\end{aligned}
\tag{1}
$$

The equations for phase 1 only are written, those of phase 2 being symmetric. General closure relations for this system need :

- the interface velocity u_I and pressure p_I that represents the velocity and pressure that exert at the boundary of a cloud of bubbles or dropplets,
- the average interface velocity $u_I^{'}$ and pressure $p_I^{'}$ that exert in the bulk of a two-phase control volume,
- the relaxation parameters λ and μ that control the rate at which velocities and pressure relax to mechanical equilibrium respectively.

These relations where unknown, or estimated in limit cases, or determined by experimental means. In order to determine these closure relations a new homogenization method has been built in [1].

This new averaging method considers the mixture at the discrete level, with a stencil composed of three computational cells. In each cell, at each cell boundary and at each internal boundary separating the phases, the Riemann problem (RP) is solved. The RP solution provides all local interfacial information. These RP solutions are then averaged in the computational cell as done originally with the first version of the Godunov method, derived originally for the Euler equations. In our context, extra difficulties appear due to the presence of internal material interfaces, material discontinuities at cell boundaries and variable sub-volumes due to the phase presence in the cells. But the philosophy was the same as with the Godunov method: average RP solutions and not discretized partial differential equations.

The resulting system of this averaging procedure is a quite complicated discrete system in algebraic form. It corresponds to the result of the Discrete Equations Method (DEM). The closure relations for the various interface variables have been obtained by reaching the continuous limit of these discrete equations [10], [53] that provide information easier to interprete than discrete formulas.

With this strong modelling foundations, it was possible to consider problems with extended physics : turbulence, phase transition, ions and electrons in plasmas mixtures, granular materials, chemical reactions, continuum media with elastic-plastic effects. An example is shown in the Figure 2.

Most of these extensions have been or are currently done with the help of the Hamilton principle of least action [67], [3]. Sophisticated single phase material models have been built with the help of the Hamilton principle. They are then combined with the DEM to form a multiphase flow model.

3.2. Modeling of Interface and Multi-Fluid Problems

Keywords: *Diffuse Interface*, *Eulerian Models*, *Front Capturing*, *Mixture Cells*, *Multi-Fluid Mixtures*.

In order to solve interfaces separating pure fluids or pure materials, two approaches have been developped. The first one has been described previously. It consits in solving a non-equilibrium flow model with two pressures and two velocity and then relax instantaneously these variables to equilibrium ones. Such a method allows a perfect fulfillment of interface conditions in mixture cells that appear as a result of numerical diffusion at material interfaces.

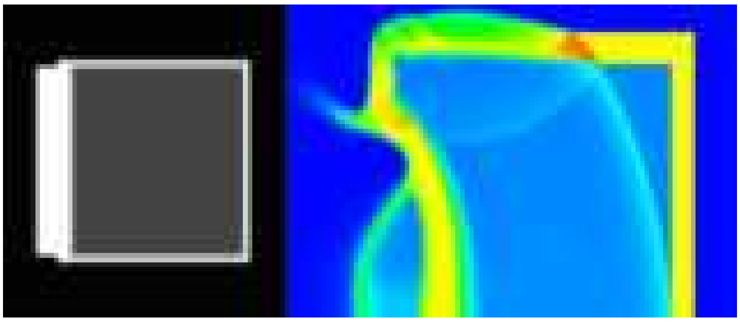

Figure 2. Impact of a projectile at 5 km/s on a copper tank filled with an heterogenous explosive. Initial situation on the left, and during the detonation regime on the right. A shock to detonation transition is observed. An extended multiphase formulation is used for the treatment of the energetic material and material interfaces. A solid shell appears in the projectile after impact (spallation effect). The method developed in [30] is used.

The second option consists in determining the asymptotic model that results of stiff mechanical relation. In the context of two fluids, it consists in a set of five partial differential equations [4] : two mass, one mixture momentum, one mixture energy and one volume fraction equations. Such a system is obviously less general than the previous non-equilibrium system, but it is particularly interesting to solve interface problems, where a single velocity is present. More precisely, it is more appropriate and simpler to include extra physics such as, phase transition, capillary effects, elastic-plastic effects, in this model.

Contrarily to conventional methods, there is no need to use a front tracking method, nor level set [55], nor interface reconstruction etc. The interface is solved as any point of the flow [61], [62] with the 5 equations model. This model provides correct thermodynamic variables in artificial mixture zones. Although seemingly artificial, this model can handle huge density ratio and materials governed by very different equations of state, in multi-dimensions. It is also able to describe multiphase mixtures where stiff mechanical relaxation effects are present, as for example high speed flows in porous media, reactive powders, solid alloys, composite materials etc.

Several extentions have been done during recent years by our project team SMASH :

- A model involving capillary, compressibility and viscous effects [64]. This is the first time such effects are introduced in a hyperbolic model. Validations with experiments done at IUSTI (the laboratory where the group of Marseille is located) have shown its excellent accuracy (see Figure 3 where the simulation results from [64] are shown with light lines and the experiments done at IUSTI are shown in grey contours.).
- Phase transition in metastable liquids [33]. This is the first time a model solves the ill-posedness problem of spinodal zone in van der Waals fluids.

The combination of capillary and phase transition effects is under study in the PhD thesis of Fabien Petitpas in order to build a model to perform direct numerical simulation (DNS) of phase transition at interfaces, to study explosive evaporation of liquid drops, or bubble growth in severe heat flux conditions. This topic has important applications in nuclear engineering and future reactors (ITER for example). A collaboration is starting with the Idaho National Laboratory, General Electrics, and MIT (USA) in order to build codes and experiments on the basis of our models and numerical methods.

In the presence of shocks, fundamental difficulties appear with multiphase flow modeling. Indeed, the volume fraction equation (or its variants) cannot be written under divergence form. It is thus necessary to determine appropriate jump relations.

Figure 3. Comparison of the drop shape during formation. No interface tracking nor interface reconstruction method are used. The same equations are solved at each mesh point. The model accounts for compressible, viscous and capillary effects. The compressible effects are negligible in the present situation, but they become fundamental in other situations (phase transition for example) where the full thermodynamics of each fluid is mandatory. The method treats in a routinely manner both merging and fragmentation.

In the limit of *weak* shocks, such relations have been determined by analysing the dispersive character of the shock structure in [36], [22] and [57]. Contrarily to single phase shocks backward information is able to cross over the shock front in multiphase flows. Such phenomenon renders the shocks smooth enough so that analytical integration of the energy equations is possible. They provide the missing jump condition.

These shock conditions have been validated against all experimental data available in the various American and Russian databases, for *weak* and *very strong* shocks.

At this point, the theory of multiphase mixtures with single velocity was closed. Thanks to this model we are currently :

- Determining the Chapman–Jouguet conditions for the detonation of multiphase explosives. They have been obtained during the PhD thesis of Erwin Franquet. Their analysis is under study with Prof. Liapidievski of the Lavrentiev Institute of Hydrodynamics, at Novosibirsk (Russia);
- Extending the approach to deal with fluid-structure interactions. A non-linear elastic model for compressible materials has been built [21]. It extends the preceding approach of Godunov to describe continuum media with conservative hyperbolic models. When embedded in our multiphase framework, fluid solid interactions are possible to solve in highly non-linear conditions (hypervelocity impacts, detonations) with a single system of partial differential equations and a single algorithm. This is the aim of Nicolas Favrie thesis;
- Extending the approach to deal with the dynamics of multiple fronts. This is important for example in Inertial Confined Fusion, as shown in the Figure 4.

Obviously, all these models are very different from the well studied gas dynamics equations. The building of numerical schemes requires special attention as detailed hereafter.

3.3. Approximation methods

Keywords: *Discrete Equations Methods*, *Finite Volume Methods*, *Relaxation Methods*, *Riemann Solvers*.

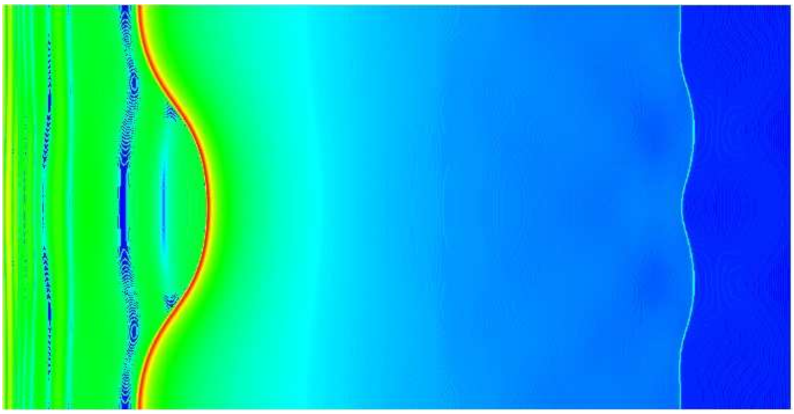

Figure 4. Numerical simulation of the coupled dynamics of the laser ablation front (on the left in red) and the laser absorption front (on the right in light blue) in Inertial Confined Fusion. The presence of rugosities on the target surface results in amplification of complex hydrodynamic instabilities. The difficulty comes from the presence of two fronts with coupled dynamics. These computations have been done by Dr. Olivier Le Métayer (SMASH) during a collaboration with Prof. Paul Clavin (IRPHE, Marseille) and CEA Bruyeres le Chatel.

All the mathematical models considered and studied in SMASH consist in hyperbolic systems of PDE's. Most of the attention is focused on the 7 equations model for non-equilibrium mixtures and the 5 equations model for mechanical equilibrium mixtures. The main difficulty with these models is that they cannot be written under divergence form. Obviously, the conservation principles and the entropy inequality are fulfilled, but some equations (the volume fraction equation for example) cannot be cast under conservative form. From a theoretical point of view, it is known since the works of Schwartz [66] 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 [54], [58]. Aware of this difficulty, we have developed two specific methods to solve such systems.

The first one is the discrete equations method (DEM) presented previously as a new homogenisation method. It is also a numerical method that solves non-conservative products for the 7 equations model in the presence of shocks. With this method, Riemann problem solutions are averaged in each sub-volume corresponding to the phase volumes in a given computational cell. When a shock propagates inside a cell, each time it interacts with an interface, that corresponds to the location where non-conservative products are undefined, a diffraction process appears. The shock discontinuity splits in several waves : a left facing reflected wave, a right facing transmitted wave and a contact wave. The interface position now corresponds to the one of the contact wave. Along its trajectory, the velocity and pressure are now continuous : this is a direct consequence of the diffraction process. The non-conservative products that appear in these equations are precisely those that involve velocity, pressure and characteristic function gradient. The characteristic function gradient remains discontinuous at each interface (it corresponds to the normal) but the other variables are now continuous. Corresponding non-conservative products are consequently perfectly defined: they correspond to the local solution of the Riemann problem with an incoming shock as initial data. This method has been successfully developed and validated in many applications ranging from interfaces, shocks in multiphase mixtures, detonation waves, phase transition fronts (cavitation) [1], [10], [7], [53].

The second numerical method deals with the numerical approximation of the five equations model. Thanks to the shock relations previously determined, there is no difficulty to solve the Riemann problem. However, the next step is to average (or to project) the solution on the computational cell. Such a projection is non trivial when dealing with a non-conservative variable. Form example, it is well known that a pressure, a temperature of a volume average has no physical sense. The same remark holds for the *cell average* of a volume fraction or an internal energy. To circumvent this difficulty a new relaxation method has been built. Let us present the basic ideas. The incoming waves in a computational cell produce different states out of equilibrium. In other words, during a time step, several waves are entering a cell. They propagate over a certain distance or volume and produce a fluid with a certain state (pressure, density, velocity). This is the same for single phase and multiphase flows. The computational cell now contains several sub-volumes with different states. Determining the *cell averaging* analog consists in determining the relaxed state when all these sub-volumes reach pressure and velocity equilibrium. Such equilibrium has to be reached at the end of each time step. During this relaxation process, the various sub-volumes change size, as the pressures and velocities are evolving. This is the same for the volume fractions. To describe these interactions and relaxation phenomenon a relaxation system is built expressing the various interactions with the sub-volumes. Its asymptotic solution is determined by solving a simple algebraic system that provides the set of equilibrium variables.

This method has been first developed in the context of the Euler equations and has been shown equivalent to the conventional Godunov method when the fluid is governed by the ideal gas or stiffened gas equation of state (EOS) [31]. When more sophisticated convex EOS are under consideration, the Godunov method produces spurious pressure and velocity oscillations while the new relaxation method is oscillation free. It has then been extended to the numerical approximation of the multiphase flow model with 5 equations. The *cell average* of the volume fraction was obtained following the same relaxation method. Excellent results were obtained, except regarding strong shock propagation into mixtures, for which it has been necessary to develop a specific method to deal with the partition of the energies or entropies among the various phases. Artificial heat exchanges inside the shock layer have been used [30].

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 concern both acoustic and incompressible aspects in methodologies for setting up suitable numerical methods.

3.4. Solution algorithms

Keywords: *Grid Computing*, *Multi-grid 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 multi-grid 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 constructed 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 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 multi-fluid 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 resources have to be solved to make the concept of Grid effective in high performance computing.

4. Application Domains

4.1. Panorama

About 15 years ago, working on the physics of detonation waves in highly energetic materials, we discovered a domain where flow conditions were extreme. Numerical simulations in detonation conditions are a true challenge. The mathematical models as well as numerical methods must be particularly well built. The presence of material interfaces was posing considerable difficulties.

During the years 90–95, we have investigated open and classified litterature in the domain of multimaterial shock-detonation physics codes. We came to the conclusion that nothing was clear regarding *mixture cells*. These *mixture cells* are a consequence of the numerical diffusion or cell projection of flow variables at contact discontinuites.

We thus have developed our own approach. On the basis of multiphase flow theory, revisited for a correct treatment of waves dynamics, we have proposed to solve mixture cells as true multiphase mixtures. This mixture, initially out of equilibrium, was going to relax to mechanical equilibrium with a single pressure and velocity.

From this starting point, many extensions have been done, most times initiated by applications connected to the Defense domain. Collaborations have never stopped with these specialized laboratories since 1993. Applications have also been done with Space, Automotive, Oil, Nuclear engineering domains. International projects are now starting with the US and South Korea.

From the technology developed in the Defense area, important applications are now coming for Space industry. The aim is to restart the Ariane cryogenic engine after taking out a satellite, in order to change orbit to take out another satellite. Restarting a cryogenic engine is very challenging as the temperature difference between cryogenic liquid and walls is about 300K. Stiff phase change, cavitation, flashing in ducts and turbopumps are expected. These phenomena have to be particularly well computed as it is very important to determine the state of the fluids at the injection chamber. This is crucial for the engine ignition and combustion stability.

From a modeling point of view, our models and methods are aimed to replace the technology owned by space laboratories, taken 10 years ago from nuclear laboratories.

To deal with all these industrial relations, the startup RS2N has been created in 2004 on the basis of the Innovation Law of the Minister Claude Allegre.

4.2. Defense Applications

Detonation physics

A contract with the Gramat Research Center (DGA) is under realisation for the modelling of nano-structured energetic materials. The total amount is 250 K€ for 3 years. It will end in 2008.

Explosions

Two contracts with the Gramat Research Center (DGA) are under realisation for the modelling of explosions with liquid tanks, granular materials, combustion of particle clouds, phase change etc. The total amount is 1.1M€ for 6 years work. It will end in 2011.

Underwater solid rocket motors

A contract is under discussion with Chugnam University (South Korea), interface of Korean defense agencies, to model flows in the wake of underwater solid rocket motors.

4.3. Transport Industry

Aeronautics

A contract with Airbus Industries is under realization. It consists in the building of a homogenized model of compressible fluid flowing and interacting with many solid obstacles. The aim is to model high pressure duct explosions in turboreactors in order to adapt security system to various kind of planes. The total amount is 200 K€ for 2 years work. It will end in 2007.

Space

As mentioned previously a big project is under discussion with CNES to model multiphase flows in space launcher cryogenic engines. A 6–9 years collaboration is envisaged. Three postdoc fellows have already been supported.

4.4. Energy Industry

A big project is under examination with Idaho National Laboratory (INL), General Electric and MIT for the direct numerical simulation of bubble growth and phase change at liquid-gas interfaces. The aim is to model ebullition crisis at critical heat flux. This is important for the next generation of nuclear power plants. A 2.5 M$ project has been submitted.

5. New Results

5.1. Mathematical Modeling

5.1.1. Shock Jump Relations for Multiphase Mixtures

Participants: Richard Saurel, Olivier Le Métayer, Jacques Massoni, Sergey Gavrilyuk.

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, propellants and solid explosives, specific composite materials, micro- and nano-structured mixtures etc. Shock relations for the mixture necessitate the determination of the volume fraction jump or any other thermodynamic variable jump. 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 fulfills the single-phase limit and guaranties volume fraction positivity. The shock relations are validated over a large set of experimental data and provide a remarkable agreement [36].

5.1.2. Rankine-Hugoniot relations for shocks in heterogeneous mixtures

Participants: Sergey Gavrilyuk, Richard Saurel.

The conservation of mass, momentum and energy are not sufficient to close the system of jump relations for shocks propagating in heterogeneous media. A closed set of relations corresponding to a two-stage structure of shock fronts is proposed. At the first stage, a *micro-kinetic energy* due to the relative motion of mixture components forms at shock front. At the second stage, this *micro-kinetic energy* disappears inducing strong variations of the thermodynamical states that reach mechanical equilibrium. The *micro-kinetic energy* produced at the shock front is estimated by using an idea described in the previous paragraph. The relaxation zone between the shocked state and the equilibrium state is integrated by a thermodynamic path whose justification is provided. Comparisons with experiments on shock propagation in a mixture of condensed materials confirm the proposed theory [22].

5.1.3. A dissipative multiphase isothermal system

Participants: Hervé Guillard, Fabien Duval [IRSN].

This work deals with the design and numerical approximation of an Eulerian mixture model for the simulation of two-phase isothermal dispersed flows. In contrast to the more classical two-fluid or Drift-flux models, the influence of the velocity disequilibrium is taken into account through dissipative second-order terms characterized by a Darcy law for the relative velocity. As a result, the convective part of the model is always unconditionally hyperbolic. We show that this model corresponds to the first-order equilibrium approximation of classical two-fluid models. A finite volume approximation of this system taking advantage of the hyperbolic nature of the convective part of the model and of the particular structural form of the dissipative part is proposed. Numerical applications are presented, to assess the capabilities of the model [23].

5.1.4. Traveling waves solutions in multiphase isothermal system

Participants: Hervé Guillard, Vincent Perrier [University of Bordeaux I].

To exhibit the inner structure of shock waves in two-phase flows, a traveling wave analysis of the two phase isothermal Euler model of [23] has been performed. The interest of this model comes from the fact that the dissipative regularizing terms are not of viscous type but instead comes from relaxation phenomena toward equilibrium between the phases. This gives an unusual structure to the diffusion tensor where dissipative terms appear only in the mass conservation equations. We show that this implies that the mass fractions are not constant inside the shock although the Rankine-Hugoniot relations give a zero jump of the mass fraction through the discontinuities. We also show that there exists a critical speed for the traveling waves above which no $\mathcal{C}$ solutions exist. Neverthless for this case, it is possible to construct traveling solutions involving single phase shocks [49].

5.1.5. A iso-pressure, iso-velocity dissipative system

Participants: Hervé Guillard, Mathieu Labois.

This work extends the results of [23] to two-temperature models. We have derived a five-equation dissipative model from the standard six-equation bifluid model using the Chapman-Enskog expansion technique. Developments to the first order lead to a hyperbolic system, and even if the model features only one velocity, dissipative second-order terms enable it to deal with velocity disequilibria. Indeed, terms that can be understood as differences between the phase velocities arise, which depend notably on the pressure gradient. They enable the model to obtain results closer to the seven-equation model that the reduced model without dissipative terms studied in [4].

Numerical methods are being developed to deal with these dissipative terms in one dimension [40].

The two-velocity, two-pressure model and the reduced model have been implemented in the parallel, three-dimensional code Num3sis. Pressure and velocity relaxation methods for the seven-equation model are included, which enables a return to the equilibrium of these variables in a finite time.

5.1.6. Modeling phase transition in metastable liquids

Participants: Richard Saurel, Fabien Petitpas, Remi Abgrall [University of Bordeaux, INRIA project team SCALAPPLIX].

A hyperbolic two-phase flow model involving five partial differential equations is built for liquid-gas interface modelling. The model is able to deal with interfaces of simple contact where normal velocity and pressure are continuous as well as transition fronts where heat and mass transfer occur, involving pressure and velocity jumps. These fronts correspond to extra waves into the system. The model involves two temperatures and entropies but a single pressure and a single velocity. The closure is achieved by two equations of state that reproduce the phase diagram when equilibrium is reached. Relaxation toward equilibrium is achieved by temperature and chemical potential relaxation terms whose kinetics is considered infinitely fast at specific locations only, typically at evaporation fronts. Doing so, metastable states are involved for locations far from these fronts. Computational results are compared to the experimental ones of [68] and show a good agreement. Situations involving complex wave patterns with up to 5 waves are reported. Moreover, the Chapman-Jouguet kinetic relation used to determine the evaporation front speed in cavitating system is recovered and explained as an expansion wave of the present model in the limit of stiff thermal and chemical relaxation [33].

5.1.7. *Studies of the shock accelerated heterogeneous bubbles motion*

Participants: Guillaume Layes [IUSTI, Aix Marseille University], Olivier Le Métayer.

This work deals with quantitative comparisons between experimental and numerical results over shock waves-bubbles interactions. The bubbles are filled with three different gases (Nitrogen, Krypton and Helium) surrounded by Air in order to investigate all kinds of density jumps across the Air/gas interface. For each case, three incident shock wave intensities are also studied. The experiments are leaded by using a shock tube coupled with a visualization diagnostic device : the T80 shock tube [59]. Considering the similar initial and geometrical conditions, the numerical results are obtained with the help of a recent method : the discrete equations method (DEM) [1], [10], [7], [53]. For each configuration, the quantitative comparisons are excellent showing the capability of both methods (numerical and experimental) to describe complex physical flows [28].

5.1.8. *Dispersive Nonlinear waves in two–layer flows with free surface*

Participants: Ricardo Barros, Sergey Gavrilyuk, Vladimir Teshukov [Lavrentiev Institute of Hydrodynamics, Novosibirsk], Ricardo Barros, Sergey Gavrilyuk.

Part I : Modelization

In [15], we derive an approximate multi-dimensional model of dispersive waves propagating in a two-layer fluid with free surface. This model is a *two-layer* generalization of the Green-Naghdi model. Our derivation is based on Hamilton’s principle. From the Lagrangian for the full-water problem we obtain an approximate Lagrangian with second order accuracy with respect to a small parameter representing the ratio of a typical vertical to a typical horizontal scale. This approach allows us to derive governing equations in a compact and symmetric form. Important properties of the model are revealed. In particular, we introduce the notion of generalized vorticity an derive analogs of integrals of motion, such as Bernoulli integrals, which are well known in ideal Fluid Mechanics. Conservation laws for the total momentum and total energy are also derived.

Part II : Large amplitude solitary waves Embedded into the continuous spectrum

In [14], we study the dispersive model derived in [15], for the description of long wave propagation in two-layer flows with free surface. As in the case of the full-water problem, this model reproduces the resonance between short waves and long waves. The resulting wave is a generalized solitary wave, characterized by ripples in the far field in addition to the solitary pulse. In this work we focus on particular members of this family resulting from vanishing ripples. These are called embeddded solitary waves and they correspond to true homoclinic orbits. Two wave regimes, characterized by elevation or depression of the interface between the layers, are presented. A critical depth ratio separates the two regimes. It is shown how this relates to a change of the global properties for the potential of the Hamilton system derived for traveling waves. In oceanic conditions, solitary waves are presented and their broadening is observed as the wave speed increases. We have observed that, for such waves to exist, their speed cannot exceed a certain limit value depending on the density ratio and thickness of each fluid. Finally, other sets of parameters were considered for which multibumped solitons exist, showing the richness and complexity of the Hamiltonian system considered here.

5.1.9. *Statistical description of a cloud of compressible bubbles*

Participants: Nouredine Chikhi, Sergey Gavrilyuk.

We use the methods of statistical mechanics to describe the interaction of N compressible gas bubbles in an incompressible, inviscid and irrotational liquid. The governing equations for bubble positions, radii and corresponding momenta form a Hamiltonian system depending on the virtual mass matrix. An explicit expression of the virtual mass matrix is presented which is calculated with accuracy $(b/d)^3$ where b and d are respectively the mean bubble radius and the mean inter-bubble distance. We study two limits cases : the limit of moving rigid spheres and the limit of immobile oscillating bubbles. In each case, we construct a canonical ensemble partition function. In the limit of rigid spheres, we improve results by Yurkovetsky and Brady (see reference in [17]). In particular, we derive an analytic expression for the *attractive* potential which may be responsible for the clustering effect, and show why the accuracy $(b/d)^3$ is not sufficient to characterize the *repulsive* potential. In the limit of immobile oscillating bubbles, we prove the existence of a long range repulsive potential which may be responsible for the stability of bubble clouds [17].

5.1.10. One-dimensional equations of fluids with internal inertia

Participants: A. Hematulin, S.V. Meleshko, S.L. Gavrilyuk.

One–dimensional flows of fluids with internal inertia are studied in [25]. The given equations include such models as the non-linear one-velocity model of a bubbly fluid (with incompressible liquid phase) at small volume concentration of gas bubbles (Iordanski (1960), Kogarko (1961), Wijngaarden (1968)), and the dispersive shallow water model (Green & Naghdi (1976), Salmon (1988)). The group classification separates these models in 10 different classes. Optimal systems of subalgebras are constructed for all models. The knowledge of optimal systems of admitted subalgebras allows constructing essentially different invariant solutions.

5.1.11. Shock wave propagation in condensed multiphase materials

Participants: Éric Daniel, Jacques Massoni.

We propose in [18], to find out numerical solutions of a traveling shock wave in condensed mixtures by using a direct numerical simulation (DNS). Condensed multiphase materials under shock wave conditions are mechanically characterized by a unique pressure and a unique velocity. In this study, the mixture is considered as a collection of grains separated by interface between each material : this problem of interfaces is solved by a diffuse interface method. The results are compared to existing one–dimensional numerical models, analytical solutions and also experimental data. The volume fraction (or the phase temperature) is not measured in experiments and it is therefore important to verify the behavior of a phase quantity through various methods. A non–monotonous evolution of the volume fraction is obtained with analytical solution as well as numerical simulation.

5.1.12. A conservative model for non linear elasticity

Participants: Sergey Gavrilyuk, Nicolas Favrie, Richard Saurel.

An Eulerian conservative hyperbolic model of elastic materials subjected to finite deformation is addressed in [21]. It is mainly based on the model developed by Godunov (1978). Some modifications are done concerning a more suitable form of the governing equations. They are evolution equations for a local cobasis which is naturally related with the Almansi deformation tensor. Such a tensor is convenient for the Eulerian description of flows. Another novelty is that the equation of state is given in terms of invariants of the Almansi tensor in a form which separates hydrodynamic from shear effects. This model is compared with another hyperbolic non–conservative model which is widely used in engineering sciences. We develop for this model a Riemann solver and determine some reference solutions which are compared with the new conservative model. The numerical results for different tests show a good agreement of both models for waves of very small and very large amplitudes. However, for waves of intermediate amplitudes, important discrepancies between results are clearly visible.

5.1.13. Modeling dynamic compaction of powders

Participants: Richard Saurel, Fabien Petitpas, Marie-Hélène Lallemand, Hervé Guillard, Sergey Gavrilyuk.

A hyperbolic model for the irreversible dynamic compaction of powders is built in [35]. The main difficulty with such modelling is related to irreversibility : a granular medium subjected to a pressure constraint decreases in volume but does not recover its initial volume when the pressure constraint is removed. To deal with such hysteresis phenomenon the model must involve dissipative effects. Such effects are modeled via a non-Newtonian fluid viscosity the explicit expression of which is obtained by an asymptotic analysis of a two–phase non–equilibrium model. Intergranular forces that come from both elastic and plastic contraints at the scale of each grain contact are then introduced with a consistent thermodynamic method. The resulting model accounts for granular effects and associated dissipation. It is free of any adjustable parameter. Its validation needs a modification of the method developed in [34] and the building of a specific code with an Arbitrary Lagrangian Eulerian multiphase method to reproduce the experiments of powder dynamic loading in presses.

5.1.14. Flows with interfaces

Keywords: *Level Set*, *compressible*, *incompressible*.

Participants: Alain Dervieux, Hervé Guillard, Bruno Koobus [université de Montpellier 2], Frédéric Alauzet [Projet Gamma, INRIA-Rocquencourt], Stephen Wornom [Lemma], Olivier Allain [Lemma], Damien Guégan.

Level Set methods are studied inside several partnerships. Cooperation with Cemef is reported in [52]. In partnership with Société Lemma, new Level Set methods are studied for the accurate prediction of capillary flows, [29] and to sloshing.
The thesis of Damien Guégan supported in partnership with Lemma, CNES and EADS, on mesh adaption methods for interface computation, in cooperation with Frédéric Alauzet, see [41]. A part of this work contributes to the ARC LNM entitled *Combiner efficacement techniques d'adaptation de maillages et méthodes de lignes de niveaux*.

5.1.15. Turbulence models

Keywords: *Large Eddy Simulation*, *Variational Multi-scale*, *hybrid models*, *unstructured meshes*, *vortex shedding*.

Participants: Bruno Koobus [University of Montpellier 2], Hilde Ouvrard [University of Montpellier 2], Alain Dervieux, Hervé Guillard, Stephen Wornom [Lemma], Charbel Farhat [Stanford University], Simone Camarri [University of Pise], Maria-Vittoria Salvetti [University of Pise], Éric Schall [University of Pau], Yacine Bentaleb [University of Pau].

The purpose of our works in hybrid RANS/LES is to develop new approaches for industrial applications of LES-based analyses. 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. After working on the LNS model of Batten-Golberg-Chakravarthy and produce several interesting results, [48], [47], the french-italian team has designed a novel type of hybrid model. It relies on a Variational Multiscale LES component and a low-Reynolds K-epsilon model. Although combined with several mechanisms of hybridisation and scale selection, the LES component remains important, in his thesis started end of 2006, Hilde Ouvrard compared our Smagorinsky model with new models, namely the WHALE model and Vreman's model. Applications to vortex flows around circular and square cylinder show the improvement with respect to previous versions.
A particular application addresses shapes involving edges for which the backscatter of small scales towards larger ones is important and well accounted for by the Variational Multiscale method, see [46]. Concerning statistics turbulence models, cubic low Reynolds extensions have been studied in cooperation with university of Pau. Also in relation with unsteady turbulence models, a cooperation with IMFT (Marianna Braza and Rémi Bourguet) has started on reduced order models, see [16], [37], [38].

5.1.16. Acoustics

Keywords: *LES*, *hybrid models*.

Participants: Bruno Koobus, Alain Dervieux, Tatyana Kozubskaya [IMM-Moscow], ILya Abalakin [IMM-Moscou].

Previous works in this cooperation addressed the development of a new version of NLDE, and of superconvergent techniques for noise propagation with linear and nonlinear hyperbolic models. Projects on coupling unstructured aerodynamics and cartesian 3D acoustics have been during the visit of Alain Dervieux at Moscow in order to build a contribution to an European proposal.

5.2. Approximation Methods

5.2.1. Relaxation-projection method for compressible flows

Participants: Richard Saurel, Erwin Franquet, Éric Daniel, Olivier Le Métayer, Fabien Petitpas, Erwin Franquet, Richard Saurel, Olivier Le Métayer.

Part I : The numerical equation of state for the Euler equations

A new projection method in [31], is developed for the Euler equations to determine the thermodynamic state in computational cells. It consists in the resolution of a mechanical relaxation problem between the various sub-volumes present in a computational cell. These sub-volumes correspond to the ones traveled by the various waves that produce states with different pressures, velocities, densities and temperatures. Contrarily to Godunov type schemes the relaxed state corresponds to mechanical equilibrium only and remains out of thermal equilibrium. The pressure computation with this relaxation process replaces the use of the conventional equation of state (EOS). A simplified relaxation method is also derived and provides a specific EOS (named the Numerical EOS). The use of the Numerical EOS gives a cure to spurious pressure oscillations that appear at contact discontinuities for fluids governed by real gas EOS. It is then extended to the computation of interface problems separating fluids with different EOS (liquid-gas interface for example) with the Euler equations. The resulting method is very robust, accurate, oscillation free and conservative. For the sake of simplicity and efficiency the method is developed in a Lagrange - Projection context and is validated over exact solutions [31]. In a companion paper [30] the method is extended to the numerical approximation of a non-conservative hyperbolic multiphase flow model for interface computation and shock propagation into mixtures.

Part II : Artificial heat exchanges for multiphase shocks

The relaxation-projection method developed in [31] is extended to the non-conservative hyperbolic multiphase flow model of [60]. This model has the ability to treat multi-temperatures mixtures evolving with a single pressure and velocity and is particularly interesting for the computation of interface problems with compressible materials as well as wave propagation in heterogeneous mixtures. The non-conservative character of this model poses however computational challenges in the presence of shocks. The first issue is related to the Riemann problem resolution that necessitates shock jump conditions. Thanks to the Rankine-Hugoniot relations proposed and validated in [36] exact and approximate 2-shocks Riemann solvers are derived. However, the Riemann solver is only a part of a numerical scheme and non-conservative variables pose extra difficulties for the projection or cell average of the solution. It is shown that conventional Godunov schemes are unable to converge to the exact solution for strong multiphase shocks. This is due to the incorrect partition of the energies or entropies in the cell averaged mixture. To circumvent this difficulty a specific Lagrangian scheme is developed. The correct partition of the energies is achieved by using an artificial heat exchange in the shock layer. With the help of an asymptotic analysis this heat exchange takes a similar form as the *pseudoviscosity* introduced by Von Neumann and Richtmyer (1950). The present Lagrangian numerical scheme thus combines Riemann solvers and artificial heat exchanges. An Eulerian variant is then obtained by using the relaxation-projection method developed earlier by the authors for the Euler equations. The method is validated against exact solutions based on the multiphase shock relations as well as exact solutions of the Euler equations in the context of interface problems. The method is able to solve interfaces separating pure fluids or heterogeneous mixtures with very large density ratio and with very strong shocks [30].

5.2.2. A Lagrangian numerical method for compressible multiphase flows

Participants: Richard Saurel, Jacques Massoni, François Renaud [CEA].

This paper is devoted to the numerical approximation of a hyperbolic non-equilibrium multiphase flow model with different velocities on moving meshes. Such a goal poses several difficulties. The presence of different flow velocities in conjunction with cell velocities poses difficulties for upwinding fluxes. Another issue is related to the presence of non conservative terms. To solve these difficulties the Discrete Equations Method [1], [10], [7], [53] is employed and generalized in the context of moving cells. The complementary conservation laws, available for the mixture, are used to determine the velocities of the cell boundaries. With these extensions an accurate and robust multiphase flow method on moving meshes is obtained and validated over several test problems with exact or experimental solutions [32].

5.2.3. *Eulerian relaxation method for interfaces in multiphase mixtures*

Participants: Richard Saurel, Fabien Petitpas, Ray. A Berry [Idaho National Laboratory].

Numerical approximation of the five-equations two-phase flow of [60] is examined. This model has shown excellent capabilities for the numerical resolution of interfaces separating compressible fluids as well as wave propagation in compressible mixtures [30]. However, its numerical approximation poses some serious difficulties. Among them, the non-monotonic behavior of the sound speed causes sonic transitions in the numerical diffusion zones at interfaces. Moreover, volume fraction variations across acoustic waves results in difficulties for the Riemann problem resolution, and in particular for the derivation of approximate solvers. To circumvent these difficulties, the pressure equilibrium assumption is relaxed and a pressure non-equilibrium model is developed. It results in a single velocity, non-conservative hyperbolic model with seven equations involving relaxation terms. This treatment satisfies the equation of state on both sides of an interface and guarantees correct and conservative transmission of shocks across interfaces. This model considerably simplifies numerical resolution. Following a strategy developed previously for another flow model [9], the hyperbolic part is first solved without relaxation terms and subsequently solved with a simple relaxation solver. The resulting method is easy to code, fast, valid for unstructured meshes, very robust and accurate. The algorithm and model are compared to exact solutions of the Euler equations as well as solutions of the five-equation model under severe flow conditions, for interface computation and cavitating flows [34]. By using artificial heat exchanges [30] the method is able to accurately compute shocks propagating in multiphase mixtures.

5.2.4. *Approximation of gas-particle system*

Participants: Hervé Guillard, Thibaud Kloczko.

The aim of this work has been to define a numerical model and the associated numerical methods that can be used to study dust explosion risks that can eventually occur in the vacum chamber of the future fusion reactor ITER. During the life of the plasma, dust (Beryllium, graphite) is accumulating at the bottom of the vacum chamber. If air enters the vacuum chamber, strong expansion waves and shock wave structures will be generated and will interact with the deposited dust, mobilize it into the atmosphere leading eventually to an explosion. The simulation of this scenario is a challenge for today numerical methods and models. The geometry of the vacum chamber is three dimensional and of large dimensions. This study therefore requires computational ressources that can only be found on large parallel platforms. On the other hand, the chamber is initially near vacum and the simulation of its pressurization by an accidental air entry requires robust numerical methods able to compute near vacum flows that will occur in a large range of Mach number from very supersonic to very subsonic ones. This work has studied numerical algorithms able to deal with the approximation of the convective part of the equations both for the gas and the particle phase as well as some implicit numerical methods (Rosenbrock implicit time schemes) able to compute stiff source terms that represent in these models the interaction between the continuous and dispersed phases.

5.3. Solution Algorithms

5.3.1. *Coarsening strategies for non-structured anisotropic meshes*

Participants: Hervé Guillard, Youssef Mesri, Thierry Coupez [Ecole des Mines de Paris].

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 computation of aerodynamical problems including turbulence modeling 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 multi-grid techniques requires a semi-coarsening strategy where the fine grids are progressively coarsened in the direction perpendicular to the wall. This work have proposed a semi-coarsening algorithm to construct in an automated way the meshes needed for these applications. This work has been validated on 3-D industrial test cases and is certainly the first published algorithm able to perform this task [50].

5.3.2. Mesh-partitioning for heterogeneous architectures

Participants: Hervé Guillard, Alexandre Moyer, Stéphane Lantéri [EPI Nachos].

In the context of the MecaGrid initiative
(http://www-sop.inria.fr/smash/mecagrid/public/mainFrame.htm),
the Smash project-team have developed a set of computational tools for Grid computing. In this work, the mesh partitioning strategies for heterogeneous architectures that have been studied during the MecaGrid initiative are revisited taking into account the hierarchical nature of grid architecture (clusters of clusters, themselves composed of multi-core processors). This work is performed in the framework of the DiscoGrid ANR action (http://www-sop.inria.fr/nachos/team_members/Stephane.Lanteri/DiscoGrid/).

5.3.3. Demonstration in Parallel and Grid Computing

Keywords: *LES*, *hybrid models*.

Participants: Bruno Koobus [Montpellier 2], Alain Dervieux, Hervé Guillard, Stephen Wornom [Lemma], Youssef Mesri.

The parallel codes of Smash which were developed for the project ACI-GRID and also used on the parallel SGI O3800 of CINES are now used for GRID-5000. See [26] for a recent summary.

6. Contracts and Grants with Industry

6.1. Contracts and Grants with Industry

6.1.1. DGA

6.1.1.1. Modelling detonation waves in nano-structured energetic materials

Participants: Richard Saurel, Olivier Le Métayer, Erwin Franquet, Fabien Petitpas, Éric Daniel.

This study realized under DGA grant deals with the development of models and computational tools for nano-structured explosives. Comparative experiments are done at Nuclear Federal Center, Sarov, Russia.

6.1.1.2. Modelling liquid and particle dispersion under explosion phenomena

Participants: Jacques Massoni, Richard Saurel, Olivier Le Métayer, Éric Daniel, Julien Verhaegen.

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

6.1.1.3. Multiphase modelling of fluid–solid interaction

Participants: Sergey Gavrilyuk, Nicolas Favrie, Richard Saurel.

A grant is under examination by DGA to support our fundamental investigations on interface modeling with fluid and elastic–plastic solids.

6.1.2. Airbus : Compressible flows in heterogenous media

Participants: Olivier Le Métayer, Nicolas Favrie, Richard Saurel.

This study realized under Airbus Industry grant, deals with the building of a homogenized model of compressible fluid flowing and interacting with many solid obstacles.

6.1.3. CNES : Multiphase flows in cryogenic space launcher engines

Participants: Olivier Le Métayer, Richard Saurel, Erwin Franquet, Vincent Deledicque, Éric Daniel, Jacques Massoni.

A big project is under discussion with CNES to model multiphase flows in space launcher cryogenic engines (Ariane).

6.1.4. Société technologique Lemma

Keywords: *Turbulence modeling*, *interfaces*, *mesh adaptation*.

Participants: Frédéric Alauzet [Projet Gamma, INRIA-Rocquencourt], Alain Dervieux, Damien Guégan [Boursier CNES-EADS/Lemma], Steve Wornom [Lemma].

In the terms of a grant between INRIA and Lemma on "Turbulence Modeling", Steve Wornom is made available for reaearch at INRIA and his hosting in Smash project-team is partly supported. The thesis of Damien Guégan is supported by CNES, EADS and Lemma.

7. Other Grants and Activities

7.1. Other Grants and Activities

7.1.1. International Grants

7.1.1.1. Korea : Underwater solid rocket motors

Participants: Éric Daniel, Jacques Massoni, Richard Saurel, Olivier Le Métayer.

A grant with Chungnam University (South Korea) is under discussion for the modelling of interface flows in the wake of hypervelocity underwater torpedos.

7.1.1.2. Idaho National Laboratory : DNS of multiphase flows and ebullition crisis

Participants: Fabien Petitpas, Richard Saurel.

A project has been submitted by the Idaho National Laboratory (INL), General Electrics (GE), the Massachuset Institute of Technology (MIT) and the SMASH project team to develop models, codes and experiments for DNS of boiling flows.

7.1.2. Bilateral Scientific Relations

7.1.2.1. Institute of Mathematical Modeling, Moscou : Acoustics

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

The long-term scientific collaboration with IMM on acoustics focusses now on superconvergent techniques for noise propagation with linear and nonlinear hyperbolic models. Projects on coupling unstructured aerodynamics and cartesian 3D acoustics have been initiated during the visit of Alain Dervieux at Moscow in order to build a contribution to an European proposal.

7.1.2.2. North Dakota University : Nanofluids Modelling

Participants: Sergey Gavrilyuk, I. Akhatov.

A scientific collaboration with North Dakota University on nanofluids modelling have been initiated with I. Akhatov. A paper has been published in 2006 [56], another one is in preparation.

7.1.2.3. Idaho National Laboratory : Numerical Methods for DNS

Participants: Richard Saurel, Fabien Petitpas, Ray A. Berry.

A scientific collaboration with Idaho National Laboratory (Dr. Ray A. Berry) on numerical methods for DNS has been initiated [34].

7.1.2.4. DFG/CNRS : Liquid-Vapor Flows

Participants: François Coquel, Thierry Gallouët, Philippe Helluy, Jean–Marc Hérard, P. Josserand, Stéphane Zaleski, Rémi Abgrall, Christophe Berthon, Boniface Nkonga, Richard Saurel, Sylvie Benzoni-Gavage, Didier Jamet, Alain Dervieux, Philippe Le Floch, Vincent Perrier, Christian Rohde, Mario Ohlberger, Stefan Müller, Ballman, Werner Lauterborn, Wilfried Kurz, Norbert Peters, Binninger, Richard Warnecke, Dietmar Kröner, W. Dreyer, M. Hermann, J. Haink, C. Kraus, R. Dahms, M. Ferch, C. Merkle.

The French-German collaboration DFG/CNRS on micro and macro modeling and simulation of liquid-vapor flows (FOR 563), aims to improve two-phase flow models and associated numerical methods.

8. Dissemination

8.1. Dissemination

8.1.1. Teaching

In the academic year 2006–2007, project members have taught the following courses :

Olivier Le Métayer : Aix-Marseille I University : 192 h,
First and second years of Polytech Engineering School (mathematics, fluid mechanics).

Sergey Gavrilyuk : Aix-Marseille III University : 192h,

Master M1 : *Mechanics, Physics and Modeling*
(mathematics-physics, continuum media);

Master M2 : *Energetics and Combustion*
(two-phase flows modeling).

Éric Daniel : Aix-Marseille I University : 20h,
(in delegation at INRIA) in :

Master M2 : *Energetics and Combustion*
(two-phase flows modeling).

Jacques Massoni : Aix-Marseille I University : 192 h,

First and second years of Polytech Engineering School
(programming languages, fluid mechanics);

Master M2 : *Energetics and Combustion*
(scientific programming with parallel machines).

Richard Saurel : Aix-Marseille I University : 100h,
(in delegation at the University Institute of France)

Second year of Polytech Engineering School;

Master M1 : *Analysis and numerical resolution of unsteady flows*;

Master M2 : *Energetics and Combustion*
(Multiphase flows modeling, Interface problems, Numerical methods).

8.1.2. Conference organization

Hervé Guillard has organized from 16 to 20 April 2007 the Numerical Flow Models for Controlled Fusion conference that has gathered around 50 physicists, applied mathematicians and specialists of computer sciences to review the main flow models used for controlled fusion.

8.1.3. Responsabilities

Éric Daniel : is Director of the Master M2 *Energetics and Combustion*. The preceding director was R. Saurel, also member of project team SMASH.

Richard Saurel : has been elected as Director of the Doctoral School in Engineering Sciences, including all research units of Marseille in *Mechanics*, *Acoustics*, *Energetics*, *Macroscopic Physics*, *Micro and Nanoelectronics*. The laboratories are all CNRS UMR and UPR units: LMA, IUSTI, IRPHE, M2P2, L2MP. It involves more than 300 researchers and about 180 PhD students.

8.1.4. Ph.D and Master Thesis

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

Ricardo Barros : Aix-Marseille University, Portugal, Ministry of Research Grant,
Modeling bubbly liquids;

Nicolas Favrie : Aix-Marseille University, MRE-AMN Grant,
Multiphase modeling of interfaces separating fluids and elastic-plastic solids;

Damien Guégan : University of Nice-Sophia-Antipolis,
Adaptation de maillages pour la simulation d'écoulements instationnaires multi-fluides en level-set;

Youssef Mesri : University of Nice-Sophia Antipolis, Dassault and European contact,
Gestion et contrôle de maillages non-structurés anisotropes; Applications à l'aérodynamique;

Mathieu Labois : Aix-Marseille University,
Développement de modèles diphasiques en non-équilibre;

Laurent Munier : Aix-Marseille University and DGA Gramat, DGA financial support,
Experimental and numerical study of liquid and solid dispersion under explosion conditions.

Fabien Petitpas : Aix-Marseille University, MRE Grant,
DNS models and methods for liquid-vapor phase change;

Julien Verhaegen : Aix-Marseille University, DGA grant support,
Modeling multiphase explosions and dispersion phenomena.

8.1.5. Invited Conferences

Members of the project team SMASH have delivered invited lectures in the following conferences and seminars :

S. Gavrilyuk :

IX Kharitons Readings Extreme States of Matter,
March 2007, Sarov, Russia;

O. Le Métayer :

IX Kharitons Readings Extreme States of Matter,
March 2007, Sarov, Russia;

R. Saurel :

- Second Workshop DFG-CNRS : Micro-Macro modelling and simulation of liquid-vapour flows,
  Institut de Mathématiques de Bordeaux, 10–12 january 2007 ;
- Moving Interface Problems and Application in Fluid Dynamics,
  Institute for Mathematical Sciences,

National University of Singapore, March 2007;

- 6th International Congress on Industrial and Applied Mathematics (ICIAM 07),
  Zurich, July 2007,
  Session Interface Methods and Applications in Multi-phase Problems;
- 3eme Congrès National de Mathématiques Appliquées et Industrielles, SMAI 2007,
  Praz sur Arly, France, 4-8 juin 2007;
- Computational Science and Engineering Conference (CESC 2007) :
  Nuclear energy and reactor simulations,
  Washington DC, April 2007.

8.1.6. Special Awards

The following members of the team have been elected for the following awards for their scientific work :

- **O. Le Métayer** has been elected for the prize *Pierre Yves Hervé* of the French Pyrotechnic Association in regards of his work in detonation physics. It will be awarded during the Europyro 2007 conference to be held at Beaune, October 2007.
- **R. Saurel** has been elected for the *Science and Defense 2006* Prize in regards of his work on the multiphase theory of diffuse interfaces. A jury, composed of French Academy of Sciences members, directed by the Fields Medal Professor Pierre Louis Lions elected him. This prize will be awarded during a ceremony at Defense Ministry on December 17th, 2007.

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