CEMRACS'12

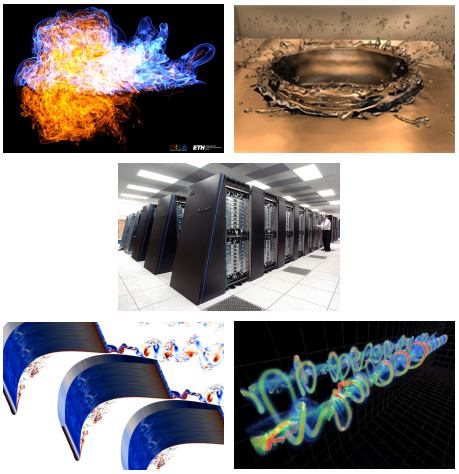
Centre d'Été de Mathématiques et de Recherche Avancée en Calcul Scientifique

Numerical Methods and Algorithms for High Performance Computing

CIRM, Marseille, France

July 16 - August 24, 2012

http://smai.emath.fr/cemracs/cemracs12/



Lectures (July 16 - July 20)

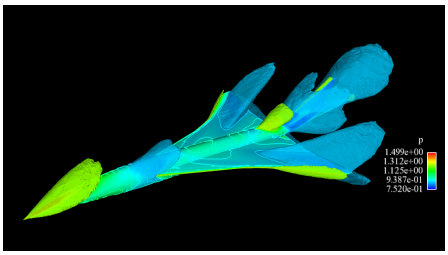
Linear Algebra	Multigrid Methods
Numerical Time Schemes	Domain Decomposition
Multiresolution	Adaptive Mesh Refinement
Uncertainty Propagation	

Research Session (July 23 - August 24)

Research Session (July 23 - August 24, 2012)

Project 1

COLARGOL / COmparaison des aLgorithmes dans AeRosol et aGhOra pour les fLuides compressibles



In this project, we propose to compare high order finite elements methods for compressible fluid flows, which have been implemented for one year : Aghora, developed at ONERA/DSNA, and Aerosol, developed at Inria Bordeaux Sud-Ouest (within the teams Bacchus and Cagire).

Main features of both software include
- arbitrary high order method on hybrid meshes.
- implementation of discontinuous Galerkin methods

Main differences are
- Residual distribution schemes (on continuous finite elements) are implemented within Aerosol
- the programming language (Fortran for Aghora, and C++ for Aerosol)

We propose in this project to compare implementations of local operations (local to a cell), and also strategies concerning parallelism and code factoring.

Comparisons will be led on two tests : isentropic vortex in two dimensions, and flow around a regular bump.

Collaboration
- Dragan Amenga (INRIA)
- Damien Genet (INRIA)
- Emeric Martin (ONERA)
- Vincent Perrier (INRIA)
- Florent Renac (ONERA)
- Mario Ricchiuto (INRIA)

Project 2

VOG : Vlasov On Gpu

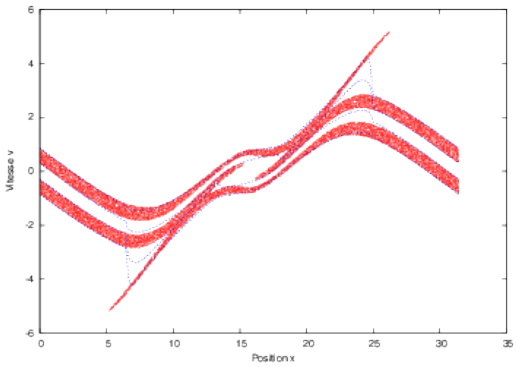
The Vlasov equation is a kinetic model that describes the evolution of a distribution function $f = f(x, v, t)$, where x is the space variable, v the velocity and t the time. The distribution function may, for instance, represent the electrons in a plasma. In this case, the Vlasov equation can be coupled with the Maxwell equations for computing the plasma evolution.
Two main families of numerical methods exist for simulating the Vlasov equation : the Particle-In-Cell (PIC) methods and the eulerian methods. This project is devoted to the eulerian methods : we will use a space-velocity grid for approximating the Vlasov equation.

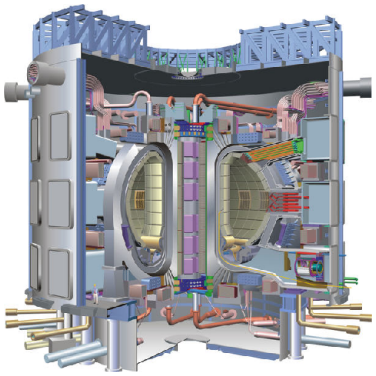
1 Semi-lagrangian methods on GPU

A first work has been done in [1] with the CUDA language. We will rely on this first work and also on a PIC code based on OpenCL [2]. The goal is to develop a semi-lagrangian program with OpenCL. We will implement several interpolation schemes : Lagrange, splines, Hermite type reconstruction. A preliminary work will be performed in 2D, but the final objective is to perform 4D or 5D numerical simulations, cf [3].

2 Hyperbolic methods

The EDP team at IRMA also develops a 3D general software for solving hyperbolic systems of conservation laws. It is based on the Discontinuous Galerkin (DG) method and uses MPI and OpenCL, which allows high performance computations on GPU clusters. It is applied to the Maxwell equations, but its general flux formulation allows other models. The semidiscretization of the Vlasov equation in the velocity space leads to a hyperbolic system in the (x, t) space. The number of variables is equal to the number of velocity discretization points. It is then possible to use the previously described solver to the Vlasov-Maxwell system. The goal is to program, test and validate this approach on 2D test cases described in [2]. An efficient implementation implies a special management of the memory access.





Collaboration
- Philippe Helluy (IRMA)
- Michel Mehrenberger (IRMA)

Young researchers
- Jonathan Jung (IRMA)
- Matthieu Kuhn (LSIIT)
- Luca Marradi (Université de Pise)
- Pham Thi Trang Nhung (IRMA)
- Christophe Steiner (IRMA)
- Chady Zaza (CEA)

Références

[1] Guillaume Latu, *Fine-grained parallelization of a Vlasov-Poisson application on GPU*, Europar'10, HPPC Workshop (2010).

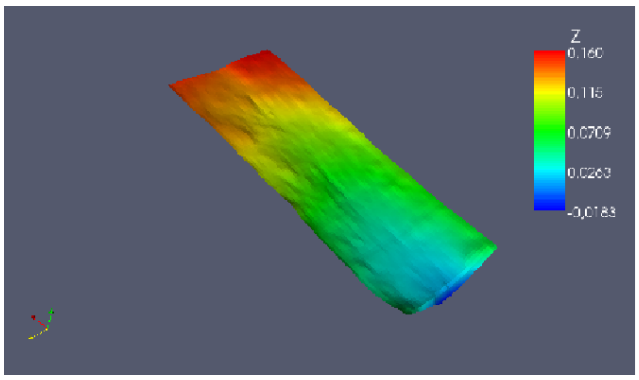
[2] A. Crestetto and P. Helluy, *Resolution of the Vlasov-Maxwell system by PIC Discontinuous Galerkin method on GPU with OpenCL*, soumis.

[3] A. Mangeney, F. Califano, C. Cavazzoni, P. Travnicek, *A Numerical Scheme for the Integration of the Vlasov-Maxwell System of Equations*, J. Comput. Phys. 179, 495–538 (2002).

Project 3
FullSWOFparal

In this project, we aim at developping a parallel version of FullSWOF_2D software. This software has been developped in the framework of the project ANR METHODE in order to simulate overland flow. Up to know this software based on the Shallow Water equations has only been used at small scales (parcel as illustrated on the figure below) on coarse meshes. We know aim at doing some flooding simulations at a bigger scale (watershed) on a high resolution topography. Thus it is necessary to parallelize the code using a domain decomposition strategy.

We want to compare two approaches : the first one, a « classical »based on a master-slave architecture using MPI and the second one using skeletal algorithms (OSL, Orléans Skeleton Libray and SkelGIS Skeletons for Geographical Information Systems which has been developped in the context of a CIFRE PhD thesis with the society Géo-Hyd). These approaches will be compared both in terms of performance and scalability. They will be first tested on a toy model : the heat equation.



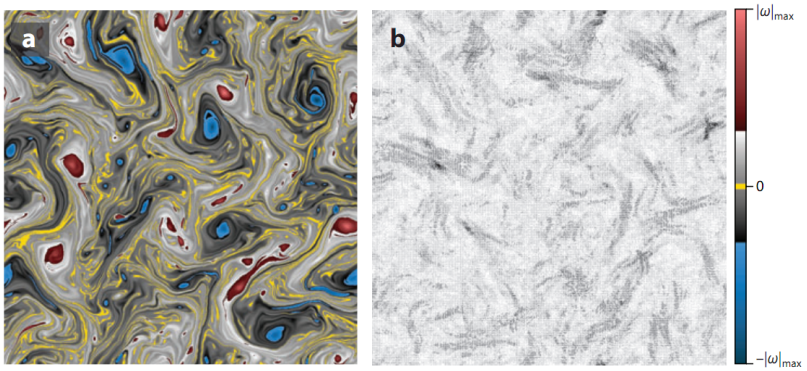
Collaboration
- Stéphane Cordier (MAPMO)
- Olivier Delestre (LJAD & EPU - Université de Nice - Sophia Antipolis)

Young researchers
- Hélène Coullon (Géo-Hyd)
- Guillaume Gourlaouen (EDF et CMAP)
- Minh-Hoang Le (MAPMO)
- Romain Serra (Polytech'Nice-Sophia)
- Chang Yang (Université lyon 1)

Project 4

POAM2-AHyMaHT : Parallelization and optimization of adaptive multiresolution methodologies : application to hydrodynamic and magnetohydrodynamic turbulence

The aim of the project is to make further progress on the development and parallelization of adaptive multiresolution methods (MR) for modeling and computing fully developed turbulent flows, for either electrically neutral (hydrodynamic) or electrically conducting (magneto-hydrodynamic) fluids. Different data structures, pointer based octrees (and binary trees) or patch based approaches will be examined, in particular also with respect to parallelization. The coherent vorticity simulation approach will be further developed using fully adaptive solvers. The comparison of MR with adaptive mesh refinement (AMR) methods is planned to asses the precision and the computational performance of both methods. Data analyses, including wavelet techniques, of turbulent shear flow will be performed in order to understand the acceleration statistics and the influence of body forces, e.g. the Coriolis force. Finally, we plan to implement the volume penalization approach into a classical Fourier pseudo-spectral code to impose no-slip boundary conditions and to simulate a 3d channel flow with imposed pressure gradient using a particular forcing technique.



Collaboration

- Kai Schneider (Aix Marseille U, France)
- Marie Farge (ENS Paris, France)
- Ralf Deiterding (Oak Ridge Nat. Lab., USA) Margarte Domingues (INPE, Brazil)
- Sonia Gomes (Campinas, Brazil)
- Frank Jacobitz (U San Diego, USA)

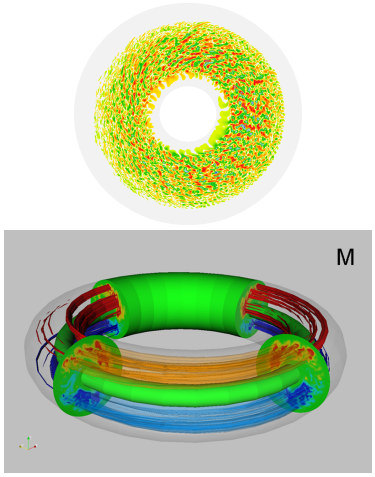
- Odim Mendes (INPE, Brazil)
- Katsunori Yoshimatsu (Nagoya U, Japan)
- Romain Nguyen Van Yen (FU Berlin, Germany)
- Julius Reiss (TU Berlin, Germany)
- Malcolm Roberts (U Edmonton, Canada)
- Thomas Engels (Aix Marseille U/TU Berlin, France/Germany)
- Youichi Sawamura (Nagoya U, Japan)

Young researchers

- Thomas Engels (Aix Marseille U/TU Berlin, France/Germany)
- Malcolm Roberts (U Edmonton, Canada)

Project 5

High performance solvers for Tokamak Physics



Understanding and control of turbulent transport in thermonuclear plasmas in magnetic confinement devices is a major goal. This aspect of first principle physics plays a key role in achieving the level of performance expected in fusion reactors. In the ITER design (http ://www.itercad.org/), the latter was estimated by extrapolating an empirical law. Computer simulation is and will continue to be a key tool for investigating several aspects of Fusion energy technology, because right now there is no burning plasma experiments like ITER.

This CEMRACS project targets to improve the performance of three parallel applications that mimic a part of the Tokamak, namely : GYSELA, TIM (kinetic descriptions) and TOKAM (fluid approach). Each code is not at the same level of development concerning : at the first hand, the number of physics features included, and at the other hand, parallel performance and scalability. Each code focuses on specific time and spatial scales in order to study peculiar physics phenoma. This project aims at : optimizing the GYSELA code for Bluegene/P and Bluegene/Q machines to scale to thousands of cores, improving parallelization of TIM code by using OpenMP in addition to MPI, improve the accuracy of the numerical scheme in TOKAM code and also the integration of the sparse parallel solver.

Collaboration

- Edouard Audit, permanent (CEA/Maison Simulation)
- Julien Bigot, postdoc (CEA/Maison Simulation)
- Thomas Cartier-Michaud, thèse (CEA/IRFM)
- Virginie Grandgirard, permanent (CEA/IRFM)
- Xavier Lacoste (INRIA/Bacchus)
- Guillaume Latu, permanent (CEA/IRFM)

- Chantal Passeron, permanent (CEA/IRFM)
- Pierre Ramet (INRIA/Bacchus)
- Fabien Rozar, stage (CEA/IRFM)
- Patrick Tamain, permanent (CEA/IRFM)
- Olivier Thomine, postdoc (CEA/IRFM)

Young researchers

- Julien Bigot (CEA/Maison Simulation)
- Thomas Cartier-Michaud (CEA/IRFM)
- Fabien Rozar(CEA/IRFM)

Project 6

Quantify cloud elasticity depending on the demand variation modeled as a turbulent flow

Context

The Cloud can be summarized as a model of on demand provisioning of resources (servers, networks and storage). This model is supposed to lower costs, resources being switched off when there is no need activated if requested. This cloud attribute is commonly called the elasticity.

Challenge

There is no study to my knowledge or modeling of the elasticity of the Cloud. In the best case, the elasticity is assumed as an intrinsic virtue of the Cloud. It is difficult to set quantitative values to define the elasticity, let alone metrics that can lead to the conclusion if a cloud is 10% -50% -100% or 1000% elastic. The mission is to use math to improve the current situation.

Proposal

Prelimary study

- Make an inventory of existing research on modeling the elasticity of the Cloud
- Criticize and suggest possible improvements

Mathematical modeling

- Use students' knowledge and information from the first week
- Model demand (for simplicity assume they are HTML requests) as turbulent flows (sales or events like Rolland Garros)
- Model the processing that can either be simple or complex (e.g. : datamining ou clash computing)
- Define quantitatively what elasticity may be. The ideal is to have a simple value style beta coefficient or stiffness of the spring.
- Illustrate how the modeling may apply in some typical cloud providers such as Amazon style, SFR, OVH ...

Option (if time permits)

Suggest an automation to trigger « just in time » IT resources provisioning to absorb demands and thus better optimize IT usage without compromising on customer satisfaction.

Collaboration

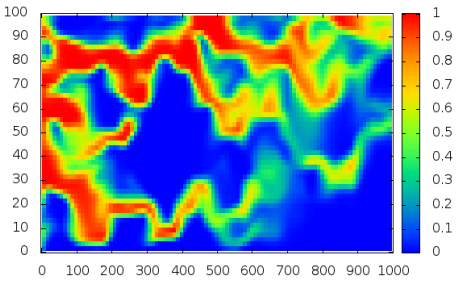
- Chuyen Huynh (CISCO)

Young researchers

- Jean-Matthieu Etancelin (LJK)
- Tony Février (LMO)
- Georges Sadaka (LAMFA)

Project 7

CoMPaS : Compositional Multiphase Parallel darcy flow Simulations



The objective of the project is to develop a parallel multiphase Darcy flow simulator adapted to general polyhedral meshes and to the implementation of advanced finite volume discretizations with various choices of the degrees of freedom (cell centers, vertices, face centers). The main targeted applications are the simulation of CO2 geological storage, nuclear waste repository and reservoir simulations.

The Cemracs is the starting point of the project and will focus on the implementation of basic tools such as the distributed polyhedral grid and the connection to a parallel linear solver library.

Collaboration

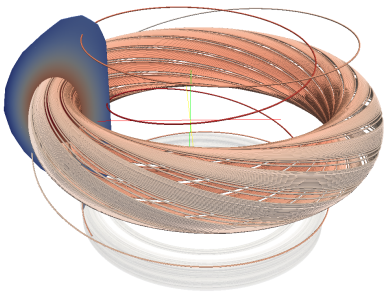
- Roland Masson (INRIA, Univ. Nice)
- Cindy Guichard (INRIA, Univ. Nice)

Young researchers

- Eric Dalissier (ICJ)
- Wei Zhang (LMO)

Project 8

Simulation of the parallel dynamics in Tokamaks



Tokamaks are experimental machines used in plasmas physics for the study of nuclear fusion by magnetic confinement. ITER presently under construction in Cadarache will be the largest of these machines ever built and intends to prove the feasibility of controlled fusion. The design of this machine relies largely on numerical simulation.

One of the bottleneck in the current understanding of magnetized plasmas concerns the perpendicular transport of matter and energy that destroys the confinement. This transport is essentially of turbulent nature and its correct simulation imposes the use of very fine three dimensional meshes that can currently only be considered on parallel architectures.

In this project, the study of the parallel dynamics in tokamaks will be considered in the framework of simplified MHD models : reduced MDH and/or Drift approximations. We shall concentrate on the resolution of some difficult problems, constituting at present bottlenecks for the current algorithms : resolution of large linear systems in parallel for implicit methods and the use of non-structured meshes allowing to describe zones where the solution presents locally strong variations.

Collaboration

- Hervé Guillard (INRIA)
- Boniface Nkonga (INRIA)
- Petr Vanek (University of Pilsen)

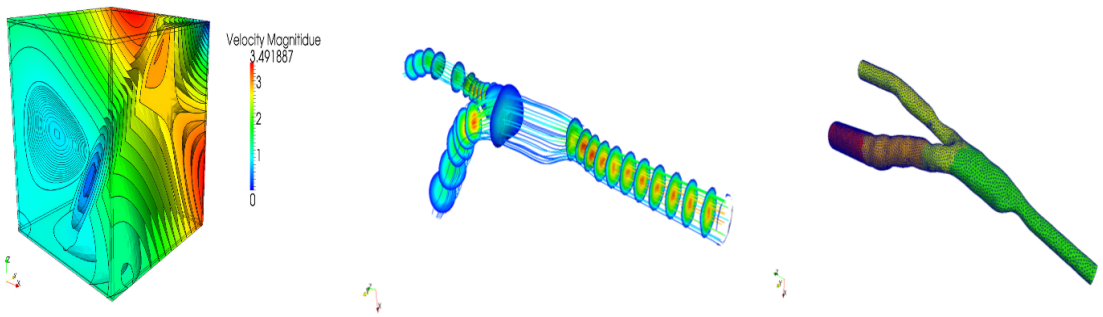
Young researchers

- Marco Bilanceri (INRIA Sophia-Antipolis)
- Tian Tian (POLYTECH NICE)
- Jeaniffer Vides (INRIA, Maison de la Simulation)

Projects 9, 10 and 11

Feel++ for high performance computing

http ://www.feelpp.org



In the context of CEMRACS 2012, we propose three projects around Feel++ requiring high performance computing. A major objective of these three projects is to build on the development efforts of Feel++ (parallelization, domain specific language for partial differential equation and Galerkin methods, ...) in the past few months for some of our applications on supercomputers and in particular the TGCC (very large computing center). The description of these projects also presents the associated collaborations and the people who will attend the CEMRACS.

Project 9

ViVaBrain : Vascular blood flows

We are interested in the simulation of blood flows in complex geometries from 3D medical imaging. For example, the picture is a venous network in the brain with a little more than 30 inputs and 2 outputs (one can also consider this as an arterial network) is one of the geometries on which we will put our efforts. We are particularly interested in the problem of boundary conditions, the mesh generation both in the context of fluid flow only but also in the context of fluid-structure interaction and the effective resolution in parallel using Feel++.

Collaboration

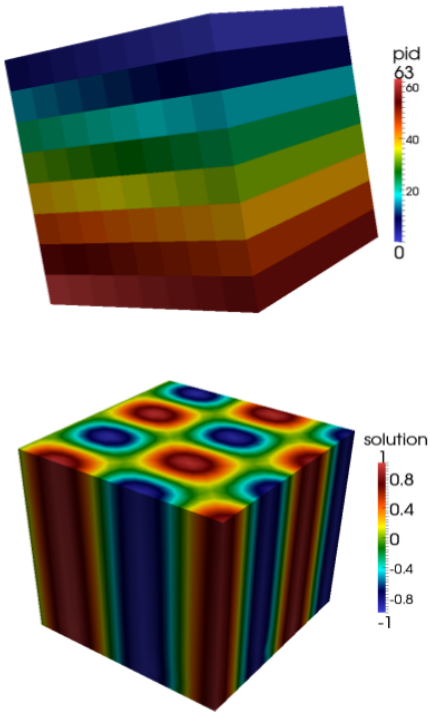
- University of Strasbourg, IRMA, EDP-TC team (R. Tarabay, Mr. Szopos, C. Prud'homme)
- University of Grenoble Laboratoire Jean Kuntzmann, EDP team (V . Chabannes)
- Interdisciplinary Laboratory of Physics, team DYFCOM (Ismail)

Young researchers

- Céline Caldini-Queiros (INRIA/LMB)
- Tarik Madani (LAMFA)
- Jussara Marandola Kofuji (Georgia Institute of Technology)

Project 10

HAMM : domain decomposition, coarse grid solver, application to nonlinear mechanics



We developed a code to test different methods of domain decomposition type Schwarz (DD, DN, NN, RR) on 2D and 3D linear problems. At the CEMRACS'12 we propose to implement in Feel++ new coarse grid preconditioners developed by the team around F. Nataf (UPMC / CNRS), which have already been tested on FreeFem++. We will also work on a 2D/3D preconditioner for the mortar method in parallel with S. Bertoluzza.
Finally we also propose to establish a benchmark for comparing solvers/preconditioners for nonlinear problems in solid mechanics. This benchmark will be implemented both in FreeFem++ and Feel++. Tests and comparisons will be made on the TGCC. The figures show a calculation on 128 processors.

Collaboration

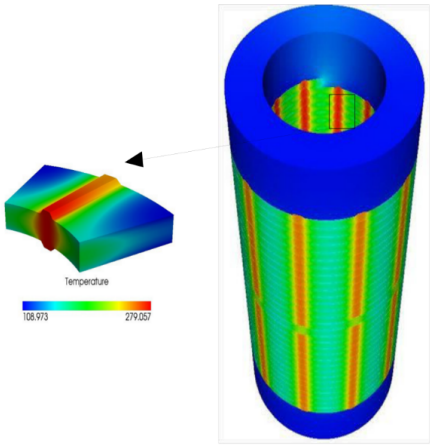
- University of Grenoble, Laboratoire Jean Kuntzmann, EDP team (A. Samake, V. Chabannes)
- Université Pierre et Marie Curie, Laboratoire Jacques Louis Lions & CNRS (Jolivet)
- University Strasbourg, IRMA, EDP-TC team (C. Prud'homme)
- IMATI CNR Pavia Italy (S. Bertoluzza)

Young researchers

- Abdoulaye Samake (LJK)
- Pierre Jolivet (LJK - LJLL)

Project 11

RB4FASTSIM : Massively parallel certified and non-intrusive reduced basis methods for simulating multi-physics nonlinear models



In this project we are interested in the reduced basis methods in their version intrusive (certified) and less intrusive (Y. Maday. R. Chakir) and their application to multiphysics problems nonlinear 3D requiring high performance computing resources. The models considered are those of LNCMI (thermal, electrostatic, magnetostatic, solid mechanics) and EADS-IW (Aerothermal). In particular, besides the parallelization of the underlying models, we will focus on the parallelization of reduced basis methods.

Collaboration

- University of Grenoble, Laboratoire Jean Kuntzmann, EDP team (S. Veys)
- University Pierre et Marie Curie, Laboratoire Jacques Louis Lions (R. Chakir)
- University of Strasbourg, IRMA, EDP-TC team (C. Prud'homme)
- CNRS, Laboratoire National High Magnetic Field (C. Trophime)

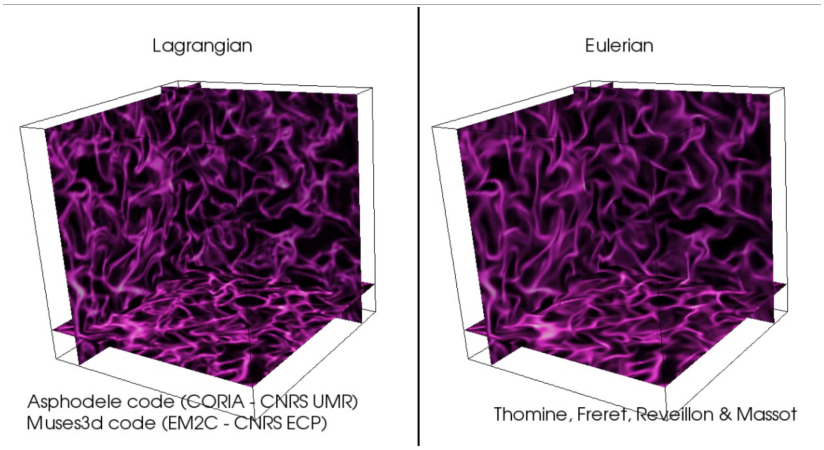
Young researchers

- Elisa Schenone (UPMC - INRIA-Rocquencourt)
- Stéphane Veys (LJK)

Project 12

On the development of high order realizable moments methods for the simulation of sprays : adaptation to GPU/hybrid architectures

Among the main difficulties on the way to accurate numerical simulation of multiphase combustion, one is the design of a high order accurate, realizability preserving, numerical method for the resolution of Eulerian models on unstructured grids in order to deal with very complex geometries such as that of a combustion chamber. The current project team is coming to the 2012 session of the CEMRACS with a two dimensional code within which the numerical method is high order accurate, total variation bounded in the mean and preserves a convex space of realizable state vectors. To achieve such hardly-combined properties, the method is rather expensive and has currently to deal with pretty high stability constraints, which means small time steps. On the other hand, the method is maximum compact and thus very suitable for parallelization. During this summer session, the team aims at experimenting the parallelization of the current numerical method and study its behavior on CPU, GPU and possibly hybrid clusters.



Collaboration

- Adam Larat (EM2C)
- Aymeric Vié (EM2C)

Financial Support