New trends in complex flows

September 19-21 2022, Institut Henri Poincaré, Paris

	Monday 19th	Tuesday 20th	Wednesday 21st
09:00 - 09:45		Antoine Gerschenfeld	
09:45 - 10:30		Session poster	Sergey Gavrilyuk
10:30 - 11:00		Pause	Pause
11:00 - 11:45		Paola Allegrini	Henri Gouin
11:45 - 12:30		Charlotte Perrin	Louis Reboul
12:30 - 14:00	Accueil - café	Pause repas	Pause repas
14:00 - 14:45	Laurent Navoret	Session libre	Claire Chainais-Hillairet
14:45 - 15:30	Marica Pelanti	Katia Aït-Ameur	Clôture
15:30 - 16:00	Pause	Pause	
16:00 - 16:45	Frédérique Laurent-Nègre	Jerôme Bonelle	
16:45 - 17:30	Cocktail	Session poster	

Plenary speakers

Katia Aït-Ameur (CMAP, Ecole Polytechnique, Institut Polytechnique)

An acoustic/transport splitting method for the isentropic Baer-Nunziato two-phase flow model

We are interested in the computation of compressible two-phase flows with the isentropic Baer-Nunziato two-phase flow model [1, 4] by using a finite volume methods that decouples acoustic and transport phenomena. This approach is well-suited to many industrial applications like the simulation of flows in nuclear reactors when the material velocities are low compared to the sound velocities.

For the Euler system, the classic Lagrange-Projection method allows to per- form such decoupling by solving the flow equations in Lagrangian coordinates. Unfortunately, the Baer-Nunziato model involves three different material waves that do not allow to exhibit a simple expression of the system using Lagrangian coordinates. Using similar ideas as in [2, 4], we consider an operator splitting strategy that allows to separate an acoustic subsystem and a transport subsystem for the Baer-Nunziato model.
This operator splitting allows to design a numerical scheme with a time- implicit treatment of the (fast) acoustic waves, in order to get rid of a too restrictive CFL condition, and an explicit treatment of the (slow) mate- rial waves in order to preserve accuracy, for the isentropic Baer-Nunziato model.

[1] M. R. Baer and J. W. Nunziato. A two-phase mixture theory for the deflagration-to-detonation transition (DDT) in reactive granular ma- terials. Int. J. Multiphase Flow, 12(6):861–889, 1986.

[2] C. Chalons, S. Kokh, and N. Spillane. Large time-step numeri- cal scheme for the seven-equation model of compressible two-phase flows. In Springer, editor, Proceedings in Mathematics, FVCA 6, volume 4, pages pp. 225–233, 2011.

[3] F. Coquel, Q. L. Nguyen, M. Postel, and Q. H. Tran. Entropy-satisfying relaxation method with large time-steps for Euler IBVPs. 79(271):1493– 1533, 2010.

[4] J.-M. Coquel, F. and Hérard and K. Saleh. A splitting method for the isentropic Baer-Nunziato two-phase flow model. ESAIM: Proceedings, 38:241–256, 2012.

Paola Allegrini (Institut de Mathématiques de Toulouse, UT3-Paul Sabatier)

Un schéma numérique préservant l'asymptotique bas Mach pour les équations d'Euler

Ce travail est réalisé en collaboration avec Marie-Hélène Vignal, Institut de Mathématiques de Toulouse, UT3-Paul Sabatier.

Dans cet exposé je m'intéresse au développement et à l'étude d'un schéma asymptotiquement préservant (AP) pour les équations d'Euler compressible dans la limite bas Mach.
Pour les écoulements hautement subsoniques, les ondes acoustiques étant très rapides par rapport à la vitesse du fluide, le gaz peut être considéré comme incompressible. D'un point de vue numérique, lorsque le nombre de Mach tend vers zéro, les schémas classiques explicites présentent deux inconvénients majeurs : ils perdent en consistance et imposent une contrainte sur le pas de temps très restrictive.
Nous avons développé un schéma asymptotiquement stable, c'est-à-dire soumis à une CFL indépendante du nombre de Mach, et asymptotiquement consistant, c'est-à-dire consistant avec le modèle incompressible à la limite bas Mach.
Ce type de schéma a été très étudié dans la littérature, notamment pour Euler isentropique [6, 5, 4, 7] mais aussi pour Euler complet [3, 2] avec diverses méthodes : schémas Lagrangiens, maillages décalés ou colocalisés.
Dans ce travail, nous proposons un schéma AP basé sur une discrétisation IMEX (Implicite-Explicite) pour la partie en temps et volumes finis colocalisés pour la partie spatiale.
Je présenterai notre schéma AP, son extension à l'ordre 2 et la procédure MOOD utilisée pour réduire les oscillations (problème classique de la montée en ordre). Enfin, je finirai mon exposé avec la présentation de quelques résultats préliminaires pour les équations de Navier-Stokes.

[1] P. Allegrini, M.-H. Vignal, Study of a low oscillatory second order all Mach IMEX scheme for the full Euler equations, soumis, 2022.

[2] W. Boscheri, G. Dimarco, R. Loubère, M. Tavelli, M.-H. Vignal, A second order all Mach number IMEX finite volume solver for the three dimensional Euler equations, J. Comp. Phys. 415, 2020.

[3] M. Dumbser, V. Casulli, A conservative, weakly nonlinear semi-implicit finite volume scheme for the compressible Navier-Stokes equations with general equation of state, Applied Mathematics and Computation, vol. 272, issue P2, 479-497, 2016.

[4] G. Dimarco, R. Loubère, V. Michel-Dansac, M.-H. Vignal, Second order Implicit-Explicit Total Variation Diminishing schemes for the Euler system in the low Mach regime, J. Comput. Phys., 372, 178–201, 2018.

[5] G. Dimarco, R. Loubère, M.-H. Vignal, Study of a new asymptotic preserving scheme for the Euler system in the low Mach number limit, SIAM J. Sci. Comput., 39(5), A2099–A2128, 2017.

[6] P. Degond, M. Tang, All speed scheme for the low Mach number limit of the isentropic Euler equations. Commun. Comput. Phys. 10(1), 1–31, 2011.

[7] P. Bruel, S. Delmas, J. Jung, V. Perrier, A low Mach correction able to deal with low Mach acoustics, J. Comp. Phys. 378, 723-759, 2019.

Jérôme Bonelle (EDF R&D)

Polyhedral discretization in a industrial CFD code : case of CDO schemes in code_saturne

Compatible Discrete Operator" (CDO) schemes have been developed for a decade and integrated in code_saturne, the open-source and general-purpose CFD code of EDF.
The main goal of CDO schemes is to bring more robustness on distorted and/or polytopal meshes while preserving the efficiency requested by an industrial usage.
After having introduced the main features of CDO schemes, some V&V test cases will be presented along with two kinds of industrial applications : groundwater flows and solidification processes.

Claire Chainais-Hillairet (Université de Lille et Inria)

Corrosion of iron in an underground repository: modelling and mathematical analysis

The modelling and the numerical simulation of corrosion take part in the general description of the nuclear waste repository. The derivation of models that are accurate in the long-time regime is a challenge, especially in this context. In this talk, I will start by recalling the Diffusion Poisson Coupled Model introduced by Bataillon et al. en 2010. The derivation of the DPCM does not rely on energetic considerations, so that thermodynamic stability is not clear. Then I will show that some minor corrections lead to a thermodynamically consistent model. This new model has a variational structure and I will explain how we have established the existence of a global-in-time solution.
This is a joint work with Clément Cancès, Benoît Merlet, Federica Raimondi and Juliette Venel.

Antoine Gerschenfeld (CEA Saclay)

Développement de schémas numériques sur maillages généraux adaptés à la résolution d'écoulements multiphasiques

L'analyse de sûreté des réacteurs nucléaires nécessite dans de nombreux cas de résoudre la dynamique d'écoulements diphasiques liquide-vapeur, décrits par le modèle "Euler-Euler" à 6 équations (conservation de la masse, de la q.d.m. et de l'énergie de chacune des phases). La plupart des codes de thermohydraulique développés dans ce domaine (TRACE, RELAP, CATHARE… [2]) résolvent ce système à l'aide d'une discrétisation spatiale décalée de type MAC [5] et d'un schéma en temps semi-implicite de type ICE [6] : ce choix offre une robustesse importante (absence de modes parasites, faible sensibilité aux forces irrotationelles) et un coût numérique attractif (le système linéaire résolu à chaque itération de Newton ne porte que sur la pression), mais ne s'applique qu'aux maillages cartésiens structurés. Ainsi, les codes industriels capables de résoudre le modèle Euler-Euler sur des maillages plus généraux (Neptune_CFD, CUPID) ont recours à une discrétisation spatiale colocalisée : ils peuvent cependant souffrir d'une perte de robustesse, en particulier lorsque le rapport des densités des deux phases ρ_l/ρ_g est très élevé.
Afin de traiter des écoulements diphasiques de sodium ($\rho_l/\rho_g \sim 2000$), le CEA a entrepris de développer une famille de schémas numériques, dénommées "PolyMAC" applicables à des maillages généraux et compatibles avec une résolution de type ICE. Pour les équations scalaires, ces schémas, dénommés "P0P1nc", "P0" et "P1" se rapprochent respectivement des schémas "Hybrid Mixed Mimetic" [4], "MPFA-O" [1] et N-MFD [3]. Cette communication décrira ces trois schémas, détaillera les difficultés rencontrées pour les appliquer à l'échelle industrielle ($\gtrsim 10^6$ mailles, $\gtrsim 10^3$ cœurs), et enfin présentera les résultats obtenus sur quelques exemples applicatifs.

[1] I. Aavatsmark. An introduction to multipoint flux approximations for quadrilateral grids. Computational Geosciences, **6(3)**, 405–432, 2002. doi :10.1023/A :1021291114475.

[2] D. Bestion. 11 - the structure of system thermal-hydraulic (sys-th) code for nuclear energy appli- cations. In F. D'Auria, ed., Thermal-Hydraulics of Water Cooled Nuclear Reactors, pp. 639–727. Woodhead Publishing, 2017.

[3] Brezzi, Franco, Buffa, Annalisa, Lipnikov, Konstantin. *Mimetic finite differences for elliptic problems*. ESAIM : M2AN, **43(2)**, 277–295, 2009. doi :10.1051/m2an :2008046.

[4] J. Droniou, R. Eymard, T. Gallouët, C. Guichard, R. Herbin. *Hybrid mimetic mixed schemes*. In *The Gradient Discretisation Method*, pp. 353–375. Springer International Publishing, Cham, 2018.

[5] F. Harlow, J. Welch. Numerical calculation of time-dependent viscous incompressible flow of fluid with free surface. Physics of Fluids, **8**, 2182–2189, 1965.

[6] F. H. Harlow, A. A. Amsden. Numerical calculation of almost incompressible flow. Journal of Computational Physics, **3(1)**, 80 – 93, 1968.

Sergey Gavrilyuk (Université d'Aix-Marseille)

TBA

Henri Gouin (Université d'Aix-Marseille)

A theoretical model of Leidenfrost's temperature

The Leidenfrost effect is a phenomenon in which a liquid, poured onto a surface significantly hotter than the liquid's boiling point, produces a layer of vapor that prevents the liquid from rapid evaporation. Rather than making physical contact, a drop of water levitates above the surface.

The temperature above which the phenomenon occurs is called Leidenfrost's temperature. The reason for the existence of Leidenfrost's temperature, which is much higher than the boiling point of the liquid, is not fully understood and predicted. Here we prove that Leidenfrost's temperature corresponds to a bifurcation in the solutions of equations describing evaporation of a non-equilibrium liquid--vapor interface. For water, the theoretical values of obtained Leidenfrost's temperature, and that of the liquid bulk which is smaller than the boiling point of liquid, fit the experimental results found in the literature.

Frédérique Laurent-Nègre (EM2C, CentraleSupélec)

Quadrature based moment methods for the description of velocity and size polydispersion of particles

Many applications involve a disperse population of particles (droplets, bubbles, soots, ...), which need to be accurately simulated. In particular, their velocity dispersion may need to be considered for inertial particles, till the possibility of particle trajectory crossing. Moreover, most of the time, the size polydispersion is important to be taken into account.
These populations can usually be described by a kinetic type equation. Compared to other methods like Monte-Carlo, the moment methods are very attractive for solving this equation, considering the possibility of computational cost reduction for a fixed accuracy. In particular, the quadrature method of moments (QMOM) is an efficient moment method, widely used for the description of the size polydispersion. It uses a Gauss quadrature to compute the unclosed terms. However, it is rarely used for the velocity moments due to the weak hyperbolicity of the underlying system of equations and can also encounter some accuracy limitations in some cases, for size moments.
Here, we will focus on two recently developed quadrature based moment methods: the hyperbolic quadrature method of moments (HyQMOM) and the generalized quadrature method of moments (GQMOM). HyQMOM, first developed in 1D, is a globally hyperbolic velocity moment method, able to describe the velocity dispersion and the particle trajectory crossing. It also has a good behavior when the moment vector tends to the boundary of the moment space, which can append in applications, due to source terms. GQMOM is a generalization of QMOM, allowing the use of a larger number of quadrature points, without increasing the number of moments, thus providing a more accurate moment closure than QMOM at nearly the same computational cost. Both moment methods are based on the properties of the monic orthogonal polynomials Q_n that are uniquely defined by the moments up to order 2n-1.

Laurent Navoret (Université de Strasbourg)

TBA

Marica Pelanti (ENSTA Paris, Institut Polytechnique de Paris)

A pressure-based method for low Mach number two-phase flows with phase change

We present a pressure-based method for the numerical solution of a four-equation two- phase compressible flow model with mass transfer [1]. The proposed methodology has the capability to simulate low Mach number multiphase flows with phase change such as boiling flows. The considered model assumes kinetic, mechanical and thermal equilibrium between the two phases, and in its primitive variable formulation it is composed of the equations for the volume fraction, the temperature, the velocity and the pressure. The model includes the effects of viscosity, surface tension, thermal conductivity and gravity. Mass transfer is modeled through a chemical potential relaxation term. We employ an operator splitting algorithm where we first solve the model equations with no mass transfer terms via a pressure-based method on a staggered Cartesian grid, and then we apply a relaxation procedure to integrate these transfer terms accounting for phase transition [2]. A key feature of the proposed pressure-based methodology is the use of high performance solvers for the solution of the Helmholtz equation for the pressure, which drastically reduces the computational cost. Several numerical tests are presented to demonstrate the effectiveness of the proposed method, including tests involving flows with large density ratios, flows at low Mach number, and a challenging three-dimensional nucleate boiling simulation. Preliminary work is also presented on the implementation on boundary conditions accounting for surface wettability effects, with simulations of a vapor bubble detaching from a heated wall with different contact angles.

[1] A. D. Demou, N. Scapin, M. Pelanti and L. Brandt, A pressure-based diffuse interface method for low-Mach multiphase flows with mass transfer. J. Comput. Phys., Vol. 448, 110730, 2022.

[2] M. Pelanti, Arbitrary-rate relaxation techniques for the numerical modeling of compressible two-phase flows with heat and mass transfer, Int. J. Multiphase Flow, Vol. 153, 104097, 2022.

Charlotte Perrin (Université d’Aix-Marseille)

Around an extended Aw-Rascle system

In this talk, I will present and analyse a one-dimensionnal fluid system similar to the famous Aw-Rascle-Zhang system where the offset function is the gradient of a singular function of the density.
These equations can be used for traffic or suspension flows where a maximal packing constraint is taken into account. This is a joint work with N. Chaudhuri, L. Navoret and E. Zatorska.

Louis Reboul CMAP, Ecole Polytechnique, Institut Polytechnique)

Second-order uniformly asymptotic-preserving ImEx schemes for hyperbolic balance laws with stiff relaxation and extension to plasma discharge applications

We introduce a new class of second-order in time and space numerical schemes, which are uniformly asymptotic preserving schemes. The proposed Implicit-Explicit (ImEx) approach, does not follow the usual path relying on the method of lines, either with multi-step methods or Runge-Kutta methods, or semi-discretized in time equations, but is inspired from the Lax-Wendroff approach with the proper level of implicit treatment of the source term.
We are able to rigorously show that both the second-order accuracy and the stability conditions are independent of the fast scales in every asymptotic regime, including the study of boundary conditions. The prototype system for the linear case is the hyperbolic heat equation, whereas Euler equations of gas dynamics with friction are the one for the nonlinear case. The method is also able to yield very accurate steady solutions in the nonlinear case when the source term depends on space. A thorough numerical assessment of the proposed strategy is provided by investigating smooth solutions, solutions with shocks and solutions leading to a steady state with variable source term in space. Our aim also includes plasma discharges with sheaths, where we have two small parameters related to Debye length and mass ratio, and we present some numerical simulations that assess and illustrate the potential of a method similar to the one we have introduced but applied to the isotherrmal Euler-Poisson equations. In particular, this last case can be regarded as a nonlinear low- Mach configuration coupled with a stiff source term. Numerical simulations assess and illustrate the potential of the method we have introduced.