



ASYMPTOTIC METHODS AND NUMERICAL APPROXIMATIONS OF MULTI-SCALE EVOLUTIONS PROBLEMS, AND UNCERTAINTY QUANTIFICATION.

du 16 mai 2019 au 17 mai 2019

Workshop



Organisateurs :

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PROGRAMME

JEUDI 16/05

09:30-10.00 : Welcome

10:00-11:00 : **Shi Jin** (Shanghai Jiao Tong university, China)

11:00-12:00 : **Joackim Bernier** (Université de Rennes 1, France)
"Splitting of semigroups generated by quadratic operators"

The quadratic operators enjoy many algebraic properties. In particular, they naturally form a finite dimensional Lie algebra. Thus, the formal expansions associated with the splitting methods (based on the BCH formula) converge. On the one hand, we will use this fact to study the polar decompositions of the semigroups they generate. As a corollary, we will characterise the smoothing properties of these semigroups. On the other hand, we will consider the special case of the transport equation associated with a rotation in the plane. I will show how this later can be decomposed into a product of 3 shear transformations. I will explain why this decomposition is really efficient from a numerical point of view and I will present some applications to the resolution of the equations of Vlasov Maxwell and Vlasov HMF.

The first part of the talk is a joint work with Paul Alphonse and the second part is a joint work with Fernando Casas and Nicolas Crouseilles.

14:00-15:00 : **Giovanni Russo** (Università di Catania, Italy)

"Multi-scale numerical modeling of sorption kinetics"

The trapping of diffusing particles by either a single or a distribution of moving traps is an interesting topic that has been employed to model a variety of different real problems in chemistry, physics and biology. Here we study the dynamics of diffusing particles in a domain with an oscillating bubble. Laboratory experiments provide evidence of a non monotone behavior in time of the concentration of particles by a detector located behind the bubble, under suitable experimental condition. A comprehensive explanation of the phenomenon is not yet fully available.

The particles are attracted and trapped near the surface of the bubble. The basic mathematical model is a drift-diffusion model, where the particles diffuse and feel the potential of the bubble when they are near its surface. The numerical simulation of the system presents two multi-scale challenges. One is spatial: the range of the bubble potential is confined within a few microns at the bubble surface, while the bubble radius is of the order of a millimeter, so a fully resolved solution would be too expensive. The second challenge is on the time scale: the bubble oscillates with a frequency of the order of 100 Hz, while the diffusion time scale is of the order of 10³ seconds, this requiring at least 10⁶ time steps to fully resolve the problem in time.

A reduced model is derived to solve the multi-scale problem in space: the interaction with the bubble is modeled as a very thin layer, with a particle surface density proportional to the local density in the bulk, near the bubble. In the rest of the domain the particle density satisfies just a diffusion equation, with suitable boundary conditions on the bubble, deduced from conservation properties.

The model is carefully tested on problems in 1D, 2D planar and 3D axis-symmetric geometry. The equation is discretized on a regular Cartesian mesh, using a ghost-point approach, and solved by Crank-Nicolson scheme. The implicit step is efficiently solved by a suitably adapted multi-grid method.

The amplitude of the bubble oscillations is small compared to the bubble radius. We take advantage of this fact by replacing the time dependent position by imposing a suitable time dependent velocity at the bubble surface. Because of the low Reynolds number, the velocity distribution is computed by Stokes approximation.

The multi-scale challenge in time is still under investigation.

15:00-16:00 : **Gilles Vilmart** (Université de Genève, Switzerland)

"Multirevolution integrators for differential equations with fast stochastic oscillations"

We introduce new integrators for highly oscillatory stochastic differential equations in the situation where the fast oscillations themselves are driven by a Stratonovich noise.

The approach is based on the framework of multi-revolution composition methods previously introduced for deterministic and stochastic problems and it inherits its geometric features, in particular to design integrators preserving exactly quadratic first integrals.

Applications include highly-oscillatory Kubo oscillators and spatial discretizations of nonlinear Schrödinger equation with fast white noise dispersion.

Joint work with Adrien Laurent. Preprints available at <http://www.unige.ch/~vilmart>

16:00-16:30 : *Coffee Break*

16:30-17:30 : **Di Fang** (University Wisconsin-Madison, USA)

"Diabatic Surface Hopping, Marcus Rate and Ehrenfest dynamics"

Surface hopping algorithms are popular tools to study dynamics of the quantum-classical mixed systems.

In this talk, we will present a surface hopping algorithm in diabatic representations, in the view point of time dependent perturbation theory and semiclassical analysis. The algorithm is validated numerically in both weak coupling and avoided crossing regimes.

We then discuss some recent progress on the asymptotics of the algorithm in weak and large coupling regimes.

VENDREDI 17/05

09:00-10.00 : **Axel Klar**(University of Kaiserslautern, Germany)

"Asymptotic methods for kinetic and hyperbolic evolution problems on networks"

Networks with an evolution given by PDEs arise in many applications, e.g. modeling water- or gas-networks, road traffic or the human circulatory system.

In this talk a multi-scale approach for deriving coupling conditions for macroscopic equations from the underlying kinetic network problem is presented.

In particular, this requires the solution of kinetic half-space problems at the nodes of the network. Combining such half-space problems with half-Riemann solvers leads to coupling conditions for the corresponding macroscopic variables. We consider several linear and nonlinear problems including kinetic discrete velocity models and linear and nonlinear hyperbolic relaxation systems.

Finally, numerical investigations are presented.

10:00-10:30 : Coffee Break

10:30-11:30 : **Giacomo Dimarco**(University of Ferrara, Italy)

"Multi-scale control variate methods for uncertainty quantification in kinetic equations."

Kinetic equations play a major role in modeling large systems of interacting particles. Uncertainties may be due to various reasons, like lack of knowledge on the microscopic interaction details or incomplete informations at the boundaries. These uncertainties, however, contribute to the curse of dimensionality and the development of efficient numerical methods is a challenge. In this talk, we consider the construction of novel multi-scale methods for such problems which, thanks to a control variate approach, are capable to reduce the variance of standard Monte Carlo techniques.

11:30-12:30 : **Jingwei Hu**(Purdue University, USA)

14:00-15:00 : **Qin Li**(University Wisconsin-Madison, USA)

"PDE compression — asymptotic preserving, numerical homogenization and randomized solvers"

All classical PDE numerical solvers are deterministic. Grids are sampled and basis functions are chosen a priori. The corresponding discrete operators are then inverted for the numerical solutions. We study if randomized solvers could be used to compute PDEs. More specifically, for PDEs that demonstrate multiple scales, we study if the macroscopic behavior in the solution could be quickly captured via random sampling. The framework we build is general and it compresses PDE solution spaces with no analytical PDE knowledge required. The concept, when applied onto kinetic equations and elliptic equations with porous media, is equivalent to asymptotic preserving and numerical homogenization respectively.

15:00-16:00 : **Mattia Zanella** (Politecnico di Torino, Italy)

"Monte Carlo gPC methods for kinetic equations with uncertainties"

We introduce and discuss numerical schemes for the approximation of kinetic equations that incorporate uncertain quantities. In contrast to a direct application of stochastic Galerkin generalized polynomial chaos (SG-gPC) methods which are widely considered for uncertainty quantification of differential equations, this class of schemes make use of a Monte Carlo approach in the phase space coupled with a stochastic Galerkin expansion in the random space. The proposed methods naturally preserve the positivity of the statistical moments of the solution and are capable to achieve spectral accuracy in the random space. Several tests on kinetic models for collective phenomena validate the proposed methods both in the homogeneous and inhomogeneous setting, shading light on the influence of uncertainties in phase transition phenomena driven by noise such as their smoothing and confidence bands.

G. Dimarco, L. Pareschi, M. Zanella. Uncertainty quantification for kinetic models in socio-economic and life sciences. In Uncertainty Quantification for Hyperbolic and Kinetic Equations, Editors S. Jin, and L. Pareschi, SEMA SIMAI Springer Series, vol. 14, pp 151-191, 2017.

J. A. Carrillo, M. Zanella. Monte Carlo gPC methods for diffusive kinetic flocking models with uncertainties. Preprint arXiv:1902.04518, 2019.

J. A. Carrillo, L. Pareschi, M. Zanella. Particle based gPC methods for mean-field models of swarming with uncertainty. Communications in Computational Physics, 25(2): 508-531, 2019.

16:00-16:30 : Coffee Break

THÉMATIQUE(S)

Vie de l'École, Recherche - Valorisation

Mise à jour le 24 avril 2019

À TÉLÉCHARGER

[Programme Workshop - 16 & 17 mai 2019 \(PDF, 274 Ko\)](#)

À LIRE AUSSI

18th IMA Leslie Fox Prize in Numerical Analysis



Karine Beauchard, lauréate du prix Michel Montpetit - Inria 2017

DOCUMENTATION

Vous souhaitez recevoir plus d'information sur l'ENS Rennes, vous pouvez pour cela remplir [le formulaire de demande de documentation](#).

INFORMATIONS PRATIQUES

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