Multi-scale geometric numerical methods: Program

Tuesday, June 12th

Afternoon

- Xavier Antoine : *On the numerical solution and dynamical laws of Schrödinger/Gross-Pitaevskii equations*
- Weizhu Bao : *Multiscale methods and analysis for the Dirac equation in the nonrelativistic limit regime*
- Lukas Einkemmer : *From Eulerian Vlasov simulation to dynamic low-rank integrators*

Wednesday, June 13th

Morning

- Yongyong Cai : *Numerical methods for Klein-Gordon equation in the non-relativistic limit*
- Eric Cances : *Computing the conductivity of multilayer 2D materials - A multiscale method based on non-commutative geometry*
- Fernando Casas : *Explicit exponential representations of linear and nonlinear flows*

Afternoon

- Alina Chertock : *An Asymptotic Preserving scheme for kinetic chemotaxis models in two space dimensions*
- Stéphane Descombes : *Locally implicit discontinuous Galerkin time domain method for electromagnetic wave propagation in dispersive media*

Thursday, June 14th

Morning

- Giacomo Dimarco : *Uncertainty quantification for kinetic equations*
- Francis Filbet : *Asymptotically stable Particle-In-Cell methods for the Vlasov-Poisson system with a strong external magnetic field*
- Philippe Helluy : *Implicit discontinous Galerkin algorithms without linear system inversion*

Afternoon

- Sonia Fliss : *Enriched homogenization in presence of boundaries or interfaces*
- Olivier Le Maitre : *Global sensitivity analysis in stochastic systems*

Friday, June 15th

Morning

- Qin Li : *Optical tomography and the Calderon problem : stability deterioration of inverse radiative transfer equation*
- Jesus Maria Sanz Serna : *A stroboscopic averaging algorithm for highly oscillatory delay problems*

Abstracts

— **Xavier Antoine** : *On the numerical solution and dynamical laws of Schrödinger/Gross-Pitaevskii equations*
Abstract : The purpose of this talk is to discuss some recent developments concerning the numerical simulation of space and time fractional Schrödinger and Gross-Pitaevskii equations. In particular, we address some questions related to the discretization of the models (order of accuracy and fast implementation) and clarify some of their dynamical properties. Some numerical simulations illustrate these points.

— **Weizhu Bao** : *Multiscale methods and analysis for the Dirac equation in the nonrelativistic limit regime*
Abstract : In this talk, I will review our recent works on numerical methods and analysis for solving the Dirac equation in the nonrelativistic limit regime, involving a small dimensionless parameter which is inversely proportional to the speed of light. In this regime, the solution is highly oscillating in time and the energy becomes unbounded and indefinite, which bring significant difficulty in analysis and heavy burden in numerical computation. We begin with four frequently used finite difference time domain (FDTD) methods and the time splitting Fourier pseudospectral (TSFP) method and obtain their rigorous error estimates in the nonrelativistic limit regime by paying particularly attention to how error bounds depend explicitly on mesh size and time step as well as the small parameter. Then we consider a numerical method by using spectral method for spatial derivatives combined with an exponential wave integrator (EWI) in the Gautschi-type for temporal derivatives to discretize the Dirac equation. Rigorous error estimates show that the EWI spectral method has much better temporal resolution than the FDTD methods for the Dirac equation in the nonrelativistic limit regime. Based on a multiscale expansion of the solution, we present a multiscale time integrator Fourier pseudospectral (MTI-FP) method for the Dirac equation and establish its error bound which uniformly accurate in term of the small dimensionless parameter. Numerical results demonstrate that our error estimates are sharp and optimal. Finally, these methods and results are then extended to the nonlinear Dirac equation in the nonrelativistic limit regime. This is a joint work with Yongyong Cai, Xiaowei Jia, Qinglin Tang and Jia Yin.

[1] W. Bao, Y. Cai, X. Jia and Q. Tang, Numerical methods and comparison for the Dirac equation in the nonrelativistic limit regime, J. Sci. Comput., 71 (2017), pp. 1094-1134.
[2] W. Bao, Y. Cai, X. Jia and Q. Tang, A uniformly accurate multiscale time integrator pseudospectral method for the Dirac equation in the nonrelativistic limit regime, SIAM J. Numer. Anal., 54 (2016), pp. 1785-1812.
[3] W. Bao, Y. Cai, X. Jia and J. Yin, Error estimates of numerical methods for the nonlinear Dirac equation in the nonrelativistic limit regime, Sci. China Math., 59 (2016), pp. 1461-1494.
[4] W. Bao and J. Yin, A fourth-order compact time-splitting Fourier pseudospectral method for the Dirac equation, arXiv : 1711.07193.

— **Yongyong Cai** : *Numerical methods for Klein-Gordon equation in the non-relativistic limit*
Abstract : Klein-Gordon (KG) equation describes the motion of spinless particle. In the non-relativistic limit $\varepsilon \to 0^+$ (ε inversely proportional to the speed of light), the solution to the KG equation propagates waves with amplitude at O(1) and wavelength at $O(\varepsilon^2)$ in time and O(1) in space, which causes significantly numerical burdens due to the high oscillation in time. By the analysis of the non-relativistic limit of the KG equation, the KG equation can be asymptotically reduced to the nonlinear Schroedinger equations (NLS) with wave operator (NLSW) perturbed by the wave operator with strength described by a dimensionless parameter $\varepsilon \in (0, 1]$. Starting with the error analysis of finite difference methods for NLSW and the uniform bounds w.r.t. ε, we will show the error analysis of an exponential wave integrator sine pseudospectral method for NLSW, with improved uniform error bounds. Finally, a uniformly accurate multi scale time integrator

method will be constructed for solving the KG equation in the non-relativistic limit based on the NLSW expansion, and rigorous error bounds are established.

— **Eric Cances** : *Computing the conductivity of multilayer 2D materials - A multiscale method based on non-commutative geometry*
Abstract : 2D materials such as graphene have fascinating electronic and optical properties. Multilayer 2D materials are obtained by stacking several layers of possibly different 2D materials. Their study is one of the current hottest topics in physics and materials science. The numerical simulation of such systems is made difficult by incommensurabilities originating from lattice mismatches and twisting angles. In this talk, I will first present the most common framework, based on Kubo formula, for deriving the frequency-dependent electrical conductivity tensor of a given material from its molecular structure. For periodic systems (perfect crystals), Bloch theory allows one to numerically compute the conductivity from Kubo formula in an efficient way. The situation is much more involved for aperiodic systems such as incommensurate multilayer 2D materials. However, it can be handled by relying on tools from non-commutative geometry introduced in the 80's and 90's by Jean Bellissard and co-workers following ideas of Alain Connes.

— **Fernando Casas** : *Explicit exponential representations of linear and nonlinear flows*
Abstract : Differential equations involving non-autonomous vector fields, both linear and nonlinear, appear in many different areas of science, ranging from nuclear, atomic and molecular physics to quantum electrodynamics and control theory. Obtaining approximate exponential representations of the corresponding flow has several advantages, especially when the differential equation possesses qualitative (very often geometric) properties. In this talk we present some recent results in this area and show some interesting connections with the Hopf algebra of permutations, thus providing a new illustration of this abstract algebraic structure.

— **Alina Chertock** : *An Asymptotic Preserving scheme for kinetic chemotaxis models in two space dimensions*
Abstract : In this talk, I will present a two-dimensional multiscale chemotaxis model based on a combination of the macroscopic evolution equation for chemoattractant and the microscopic model for cell evolution. The latter is governed by a Boltzmann-type kinetic equa- tion with a local turning kernel operator which describes the velocity change of the cells. The parabolic scaling yields a non-dimensional kinetic model with a small parameter, which represents the mean free path of the cells. We propose a new asymptotic preserving numerical scheme that reflects the convergence of the studied micro-macro model to its macroscopic counterpart—the Patlak-Keller-Segel system—in the singular limit. The method is based on the operator splitting strategy and a suitable combination of the higher-order implicit and explicit time discretizations. In particular, we use the so-called even-odd decoupling and approximate the stiff terms arising in the singular limit implicitly. We prove that the resulting scheme satisfies the asymptotic preserving property. More precisely, it yields a consistent approximation of the Patlak-Keller-Segel system as the mean-free path tends to 0. The performance of the proposed scheme is illustrated on a number of numerical experiments.

— **Stéphane Descombes** : *Locally implicit discontinuous Galerkin time domain method for electromagnetic wave propagation in dispersive media*
Abstract : We are concerned with the numerical simulation of electromagnetic wave propagation in dis- persive media i.e. when the electromagnetic material characteristics depend of the frequency. In the time-domain, this translates in a time dependency of these parameters that can be taken into account through an additional differential equation for, e.g, the electric polarization, which is coupled to the Maxwell's equations which is a PDE system.
We propose and analyze different efficient time integration methods for dealing with grid induced stiffness when using non-uniform (locally refined) meshes and use these methods to study the interaction of electromagnetic waves with biological tissues.

— **Giacomo Dimarco** : *Uncertainty quantification for kinetic equations*
Abstract : In this talk we will survey some recent results concerning the construction of efficient numerical methods for uncertainty quantification (UQ) in kinetic equations. There are many sources of uncertainties that can arise in these models : such as the incomplete knowledge of the interaction mechanism between particles or the imprecise measurements of the initial and boundary data or for instance the uncertainty in the geometry and many others.
Recently we developed novel approaches to UQ of kinetic equations based on micro-macro Monte Carlo techniques which using control variate estimators based on the local equilibrium are capable to accelerate the slow statistical convergence of Monte Carlo methods. We will discuss these techniques and we will give examples of the improvements one can achieve in comparisons with other methods for UQ.

— **Lukas Einkemmer** : *From Eulerian Vlasov simulation to dynamic low-rank integrators*
Abstract : Many phenomena in both space and laboratory plasmas require a kinetic description. However, these equations are posed in a high dimensional phase space and the corresponding solutions exhibit small-scale oscillations. In addition, traditional numerical methods suffer from a restrictive CFL condition. In this talk, we will present strategies that are able to overcome these difficulties. This will lead us from time splitting based semi-Lagrangian discontinuous Galerkin schemes to the recently introduced dynamic low-rank algorithm for the Vlasov equation. The latter, in particular, has the potential to dramatically reduce the computational cost associated with kinetic simulations. An overarching topic of this talk will be the preservation of physical properties of the continuous model. We will show that even for relatively short times this is an important consideration. Unfortunately, this is particularly challenging for low-rank algorithms. We will discuss some recently proposed strategies to alleviate this deficiency.

— **Francis Filbet** : *Asymptotically stable Particle-In-Cell methods for the Vlasov-Poisson system with a strong external magnetic field*
Abstract :

— **Sonia Fliss** : *Enriched homogenization in presence of boundaries or interfaces*
Abstract : This work is motivated by the fact that classical homogenization theory poorly takes into account interfaces (or boundaries). It is particularly unfortunate when one is interested in phenomena arising at the interfaces (or boundaries) of the periodic media (the propagation of plasmonic waves at the surface of metamaterials for instance). To overcome this limitation, we have constructed an effective model which is enriched near the interfaces (or the boundaries). For now, we have treated the case of simple geometries : for instance a plane interface between a homogeneous and a periodic half spaces. By coupling the matched asymptotic expansion method and two scale expansions, we have derived a high order approximate model which consists in replacing the periodic media by an effective one but the transmission conditions are not classical. The obtained conditions involve Laplace- Beltrami operators at the interface and requires to solve cell problems in periodicity cell (as in classical homogenization) and in infinite strips (to take into account the phenomena near the interface). We establish well posedness for the approximate model and error estimates which justify that this new model is more accurate near the interface and in the bulk. From a numerical point of view, the only difficulty comes from the problems set in infinite strips (one half is homogeneous and the other is periodic). This is overcome using DtN operators corresponding to the homogeneous and the periodic media.The numerical results confirm the theoretical ones.

— **Philippe Helluy** : *Implicit Discontinous Galerkin Algorithms Without Linear System Inversion*
The Palindromic Discontinuous Galerkin (PDG) method is a general approach for solving hyperbolic systems of conservation laws. In many applications the time scale of the interesting phenomena is very different from the time scale imposed by the explicit CFL condition.

The PDG method is a general implicit (but matrix-free) high order method for approximating systems of conservation laws. It is unconditionally stable and has the complexity of an explicit scheme.
It relies on a relaxed vectorial kinetic interpretation of the conservation laws (proposed in [Aregba and Natalini, 2000]). The kinetic system is approximated with a high order DG method. The order does not decrease with the stiffness of the relaxation term.
We will present several theoretical and practical aspects of the PDG method.

— **Olivier Le Maitre** : *Global Sensitivity Analysis in Stochastic Systems*
Abstract : Stochastic models are used in many scientific fields, including mechanics, physics, life sciences, queues and social-network studies, chemistry. Stochastic modeling is necessary when deterministic ones cannot capture features of the dynamics, for instance to represent effects of unresolved small-scale fluctuations, or when systems are subjected to important inherent noise. Often, stochastic models are not completely known and involve some calibrated parameters that should be considered as uncertain. In this case, it is critical to assess the impact of the uncertain model parameters on the stochastic model predictions. This is usually achieved by performing a sensitivity analysis (SA) which characterizes changes in a model output when the uncertain parameters are varied. In the case of stochastic model, one classically applies the SA to statistical moments of the prediction, estimating for instance the derivatives with respect of the uncertain parameters of the output mean and variance. In this presentation, we introduce new approaches of SA in stochastic system based on variance decomposition methods (ANOVA, Sobol). Compared to previous methods, our SA methods are global, with respect to both the parameters and stochasticity, and decompose the variance into stochastic, parametric and mixed contributions.
We consider first the case of uncertain Stochastic Differential Equations (SDE), that is systems with external noisy forcing and uncertain parameters. A polynomial chaos (PC) analysis with stochastic expansion coefficients is proposed to approximate the SDE solution. We first use a Galerkin formalism to determine the expansion coefficients, leading to a hierarchy of SDEs. Under the mild assumption that the noise and uncertain parameters are independent, the Galerkin formalism naturally separates parametric uncertainty and stochastic forcing dependences, enabling an orthogonal decomposition of the variance, and consequently identify contributions arising from the uncertainty in parameters, the stochastic forcing, and a coupled term. Non-intrusive approaches are subsequently considered for application to more complex systems hardly amenable to Galerkin projection. We also discuss parallel implementations and application to derived quantity of interest, in particular a novel sampling strategy for non-smooth quantities of interest but smooth SDE solution. Numerical examples are provided to illustrate the output of the SA and the computational complexity of the method.
Second, we consider the case of stochastic simulators governed by a set of reaction channels with stochastic dynamics. Reformulating the system dynamics in terms of independent standardized Poisson processes permits the identification of individual realizations of each reaction channel dynamic and a quantitative characterization of the inherent stochasticity sources. By judiciously exploiting the inherent stochasticity of the system, we can then compute the global sensitivities associated with individual reaction channels, as well as the importance of channel interactions. This approach is subsequently extended to account for the effects of uncertain parameters and we propose dedicated algorithms to perform the Sobol's decomposition of the variance into contributions from arbitrary subset of uncertain parameters and stochastic reaction channels. The algorithms is illustrated on simplified systems, including the birth-death, Schlögl, and Michaelis-Menten models. The sensitivity analysis output is also contrasted with a local derivative-based sensitivity analysis method.

— **Qin Li** : *Optical tomography and the Calderon problem : stability deterioration of inverse radiative transfer equation*
Abstract : Optical tomography (OT) amounts to reconstructing the scattering coefficient in the

radiative transfer equation (RTE) via boundary measurements. Calderon problem is about reconstructing the diffusive coefficient via the Dirichlet-to-Neumann map. On one hand, the two problems are asymptotically equivalent, but on the other, OT is proved to be Lipschitz stable while Calderon problem is logarithmic-ill. The stability deterioration is mainly caused by the scale of the Knudsen number, as will be presented in the talk in both nonlinear and the linearized settings. Algorithmically, both Tikhonov regularization and Bayesian approaches are taken.

— **Jesus Maria Sanz Serna** : *A stroboscopic averaging algorithm for highly oscillatory delay problems*

Abstract : We propose and analyze a heterogenous multiscale method for the efficient integration of constant-delay differential equations subject to fast periodic forcing. The stroboscopic averaging method (SAM) suggested here may provide approximations with $h^2 + \Omega^{-2}$ errors with a computational effort that grows like H^{-1} (the inverse of the stepsize), uniformly in the forcing frequency Ω.