Asymptotic Preserving and Multiscale Methods for Kinetic and Hyperbolic Problems

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University of Wisconsin-Madison
Mathematics

Abstracts

Christophe Berthon

Title. "An asymptotic preserving and well-balanced scheme for a chemotaxis model"

Abstract. This presentation concerns the numerical approximation of a PDE system which models cell movements according to a chemoattractant concentration. The system under consideration turns out to couple a hyperbolic system with a diffusive equation. The solutions of such a model satisfy several properties to be preserved at the numerical level. Indeed, the solutions may contain vacuum, satisfy steady regimes and asymptotic regimes. By deriving a judicious approximate Riemann solver, a finite volume method is designed in order to exactly preserve the steady regimes of particular physical interest. Moreover, the scheme is able to deal with vacuum regions and it preserves the asymptotic regimes.

Jose Carrillo

Title. "Non-local kinetic models for self-organised aggregations: Patterns Analysis via AP-Methods"

Abstract. The last two decades have seen a surge in kinetic and macroscopic models derived to investigate the multi-scale aspects of self-organised biological aggregations. Because the individual-level details incorporated into the kinetic models (e.g., individual speeds and turning rates) make them somewhat difficult to investigate, one is interested in transforming these models into simpler macroscopic models, by using various scaling techniques that are imposed by the biological assumptions of the models. However, not many studies investigate how the dynamics of the initial models are preserved via these scalings. Here, we consider two scaling approaches (parabolic and grazing collision limits) that can be used to reduce a class of non-local 1D and 2D models for biological aggregations to simpler models existent in the literature. Then, we investigate how some of the spatio-temporal patterns exhibited by the original kinetic models are preserved via these scalings. To this end, we focus on the parabolic scaling for non-local 1D models and

apply asymptotic preserving numerical methods, which allow us to analyse changes in the patterns as the scaling coefficient is varied. We show that some patterns (describing stationary aggregations) are preserved in the singular limit, while other patterns (describing moving aggregations) are lost. To understand the loss of these patterns, we construct bifurcation diagrams. This is a work in collaboration with R. Eftimie and F. Hoffmann.

Alina Chertock

Title. "Asymptotic preserving simulations of kinetic systems for chemotaxis "

Abstract. We consider numerical approximations of the kinetic equations describing a collective behavior of bacteria and theirinteraction with both nutrients and chemoattractant. We introduce a non-dimensional small parameter (epsilon=the ratio of the mean free paths corresponding to isotropic and chemotactic reorientation) and by choosing a diffusion scaling we obtain a transport equation in nondimensional form depending on this parameter. In [Chalub et al. (2004)] the conditions have been derived under which the drift-diffusion limit of this Fokker-Planck system yields the Keller-Segel model. With respect to this result our aim is to investigate asymptotic preserving schemes for the corresponding kinetic chemotaxis equations.

Frederic Coquel

Title. "TBA"

Abstract. TBA

Pierre Degond

Title. "Asymptotic-preserving schemes for complex fluids"

Abstract. We will review applications of Asymptotic Preserving schemes to various examples of complex fluids such as low Mach number flows, multiphase fluids, crowds and fluids with density constraints.

Bjorn Engquist

Title. "Coupling particle, kinetic and fluid models by HMM"

Abstract. The heterogeneous multiscale method (HMM) is a framework for coupling of macro and micro-scale models in order to have efficient and accurate computations of multiscale problems. Local micro-scale simulations give missing data to a macro-scale model. We will discuss some applications, for example, where local molecular dynamics or network simulations are used to generate data for

macro-scale fluid flow. Another example is the use of local kinetic Monte Carlo systems for macro-scale epitaxial growth.

<u>Francis Filbet</u>

Title. "High order semi-implicit schemes for kinetic equations"

Abstract. We consider a new formulation of implicit-explicit (IMEX) Runge-Kutta (R-K) methods for the numerical discretization of time dependent partial differential equations. The approach is based on identifying the (linear) dependence on the unknown of the system which generates the stiffness. Only the stiff dependence is treated implicitly, then making the whole method much simpler than fully implicit ones. This approach generalizes classical IMEX methods based on additive and partitioned R-K, and allows a novel application of semi-implicit schemes. We adopt several semi- implicit R-K methods up to order three. We illustrate the effectiveness of the new approach with many applications to reaction-diffusion, convection diffusion and nonlinear diffusion system of equations.

<u>Martin Frank</u>

Title. "Non-Classical Transport, Fractional Diffusion, and Radiation in Clouds"

Abstract. We investigate a kinetic equation that describes non-classical particle transport in media with correlated scattering centers. An example is water droplets in clouds. This equation is a time-dependent linear kinetic equation, whose initial values are given by a functional of its solution. We discuss the model's connection to particle billards. An asymptotic analysis in the limit of small mean free paths reveals a fractional diffusion equation.

<u>Thierry Goudon</u>

Title. "Some problems and simulation methods motivated by the modeling of particles laden flows"

Abstract. The mathematical modeling of particulate flows naturally lead to multi-scale problems. In turn, a wide variety of PDEs systems can be considered. Such systems can couple kinetic and hydrodynamic systems, or adopt a fully hydrodynamic viewpoint. Furthermore, in the incompressible framework the problem is complemented by constraint on a combination of fluid and particles velocities. To handle the difficulty we introduce a new family of schemes working on staggered grids, with a kinetic flavor in the design of the numerical fluxes.

<u>Jingwei Hu</u>

Title. "A numerical scheme for the Boltzmann equation with uncertainty efficient in the fluid regime"

Abstract. We develop a stochastic Galerkin method for the nonlinear Boltzmann equation with uncertainty. The method is based on the generalized polynomial chaos (gPC) and can handle random inputs from collision kernel, initial data or boundary data. We show that a simple singular value decomposition of gPC related coefficients combined with the Fourier-spectral method (in velocity space) allows one to compute the collision operator efficiently. When the Knudsen number is small, we propose a new technique to overcome the stiffness. The resulting scheme is uniformly stable in both kinetic and fluid regimes, which offers a possibility of solving the compressible Euler equation with random inputs. This is joint work with Shi Jin.

Song Jiang

Title. "An asymptotic preserving unified gas kinetic scheme for grey radiative transfer equations"

Abstract. The solutions of radiative transport equations can cover both optical thin and optical thick regimes due to the large variation of photon's mean-free path and its interaction with the material. In the small mean free path limit, the nonlinear time-dependent radiative transfer equations can converge to an equilibrium diffusion equation due to the intensive interaction among radiation and material. In the optical thin limit, the photon free transport mechanism will emerge. In this paper, we are going to develop an accurate and robust asymptotic preserving unified gas kinetic scheme (AP-UGKS) for the grey radiative transfer equations, where the radiation transport equation is coupled with the material thermal energy equation. The current work is based on the UGKS framework for the rarefied gas dynamics [K. Xu and J.C. Huang, J. Comput. Phys. 229 (2010), 7747-7764], and is an extension of a recent work [L. Mieussens, J. Comput. Phys. 253(2013), 138-156] from a one-dimensional linear radiation transport equation to a nonlinear two-dimensional grey radiative system. The newly developed scheme has the asymptotic preserving (AP) property in the optically thick regime in the capturing of diffusive solution without using a cell size being smaller than the photon's mean free path and time step being less than the photon collision time. Besides the diffusion limit, the scheme can capture the exact solution in the optical thin regime as well. The current scheme is a finite volume method. Due to the direct modeling for the time evolution solution of the interface radiative intensity, a smooth transition of the transport physics from optical thin to optical thick can be accurately recovered. Many numerical examples are included to validate the current approach. Finally, an extension of the proposed AP UGKS scheme to the frequency-dependent radiative transfer system will be discussed. (joint work with Wenjun Sun and Kun Xu)

Christian Klingenberg

Title. "Progress in well-balanced methods for the Euler equations"

Abstract. For the Euler equations with gravity we seek well-balanced methods. We describe a numerical discretization of the compressible Euler equations with a gravitational potential. A pertinent feature of the solutions to these inhomogeneous equations is the special case of stationary solutions with zero velocity, described by a nonlinear PDE, whose solutions are called hydrostatic equilibria. We present a well-balanced method for all hydrostatic equilibria. For this method we can ensure robustness, accuracy and stability, since it satisfies discrete entropy inequalities. This is joint work with Christophe Berthon, Vivien Desveaux and Markus Zenk.

Alexander Kurganov

Title. "TBA"

Abstract. TBA

Mohammed Lemou

Title. "A class of numerical schemes for kinetic equations in the anomalous diffusion scaling"

Abstract. A class of numerical schemes is presented to efficiently solve kinetic equations in the anomalous diffusion scaling. Such scaling is relevant for many models in kinetic theory and essentially appears in two important situations: the case of heavy-tailed equilibria and the case of singular collision frequency. Standard Asymptotic Preserving (AP) schemes for the diffusion limit do not work in the case of anomalous diffusion scaling since they are not able to undertake the effect of (too) large or (too) small velocities. We present three different numerical schemes in this case, which are all AP: a modified time-implicit scheme, a time-explicit micro/macro numerical scheme and a Duhamel formulation based scheme. The last strategy enjoys the stronger property of being uniformly accurate with respect to the scaling parameter. Numerical tests will be presented to show the efficiency of these strategies.

Fengyan Li

Title. "High order asymptotic preserving IMEX-RK DG methods for some kinetic models"

Abstract. In this talk, I will present our progress in developing high order asymptotic preserving methods for some kinetic models, including discrete-velocity models in a diffusive scaling and the BGK model in a hyperbolic scaling. The three main ingredients of the proposed methods are: macro-micro decomposition of the equations, discontinuous Galerkin (DG) spatial discretizations, stiffly accurate implicit-explicit Runge-Kutta (IMEX-RK) temporal discretizations. The performance of the methods will be illustrated by some theoretical results, complemented by

numerical experiments. This is a joint work with J. Jang (University of California Riverside), J.-M. Qiu and T. Xiong (University of Houston).

Qin Li

Title. "Numerical methods for linear half-space kinetic equations"

Abstract. Half-space kinetic equation is the model problem to understand the boundary layer emerging at the interface in the kinetic-fluid coupling. In this talk, we report our recent progress on analysis and algorithm development for general linear kinetic equations with general boundary conditions. Applications include neutron transport equation with multi-frequencies, linearized 2D Boltzmann equations with Maxwell boundary conditions etc. The coupled system (heat equation coupling with neutron transport equation) will also be shown.

Jian-Guo Liu

Title. "TBA"

Abstract. TBA

Jianfeng Lu

Title. "Bloch dynamics and Berry phase"

Abstract. In this talk, we will discuss mathematical derivation for the first and second order Berry phase correction to Bloch dynamics for effective electron dynamics in crystals. (joint work with Zhennan Zhou)

Maria Lukacova

Title. "Well-balanced asymptotic preserving schemes for singular limits in some geophysical flows"

Abstract. We will present some recent results on the asymptotic preserving FV and/or DG evolution Galerkin schemes for the shallow water and/or Euler equations. We will show theoretically as well as by numerical experiments that the resulting methods yield consistent approximations with respect to a singular parameter. The main idea is to use a suitable splittting of the whole nonlinear problem into a linear singular operator (describing fast linear waves) and a nonlinear nonsingular one (describing slow nonlinear waves). Moreover, suitable approximation of the source terms will yield a well-balanced method uniformly with respect to the singular parameter, as well. The present work has been done in cooperation with G. Bispen, L. Yelash (University of Mainz) and S. Noelle (RWTH Aachen

Sebastian Noelle

Title. "Asymptotic preserving numerical schemes for singular hyperbolic PDE's"

Abstract. I will discuss systems of conservation laws where some wave speeds become singular. The classic example is the low Mach number limit in gas dynamics. In the singular limit, hyperbolicity gets lost, and near the limit, explicit time discretizations become either inefficient or unstable, both due to the CFL conditions. The established concept to design efficient and stable algorithms near the singular limit is a time-Implicit-Explicit splitting, called IMEX. The recent asymptotic preserving (AP) IMEX schemes follow the singular limit. A key question is the asymptotic stability of these schemes. I discuss two examples: a well-known, but unstable, scheme, and an also well-known, but stable scheme. Then I present a new stability analysis for IMEX schemes, which explains the outcomes of these experiments. I also give an outlook to a new concept of splittings, and a first application.

Lorenzo Pareschi

Title. "Implicit-explicit linear multistep methods for kinetic equations"

Abstract. We consider the development of high order asymptotic-preserving linear multistep methods for kinetic equations and related problems. The methods are first developed for BGK-like kinetic models and then extended to the case of the full Boltzmann equation. Compared to IMEX Runge-Kutta methods they have several advantages due to the absence of coupling conditions and the greater computational efficiency.

Gabriella Puppo

Title. "Asymptotic preserving boundary conditions for kinetic models"

Abstract. In this work we propose asymptotic preserving boundary conditions for kinetic problems. We concentrate on BGK type models, and illustrate with several examples why and how the asymptotic limit must be preserved also when imposing boundary conditions. Next, we illustrate the robustness of the method with examples involving rarefied flow at several regimes on non trivial geometries. Recently there has been great attention to the study of Asymptotic Preserving (AP) schemes (see for instance the recent review by Dimarco-Pareschi on ActaNumerica 2014 or Shi-Jin, 2012), but the same care has not been bestowed on the enforcement of boundary conditions. However, the numerical experiments we will present show clearly that, if proper boundary conditions are not imposed, spurious effects are to be expected, which prevent convergence to the correct asymptotic limit. We start from illustrating the problem, and proposing a solution. Next we discuss how to implement kinetic BGK and ES-BGK models preserving the correct asymptotic limits up to the boundary. The talk will also illustrate applications. In particular, we will

consider the passive transport of a set of particles on a rarefied flow in a nozzle. These simulations provide useful data for the study of the behaviour of pollutants, composed of unburnt particles, ejected from satellite thrusters.

<u>Friedrich Roepke</u>

Title. "Modeling low Mach number flows in astrophysical systems with preconditioned compressible schemes"

Abstract. Many astrophysical systems feature flows at low Mach numbers. These are modeled by the Euler equations in three space dimensions. Conventional finite volume discretizations, however, show excessive dissipation in this regime. We identify inconsistent scaling with low Mach number of numerical flux function as the origin of this problem. Inspired by the work of Turkel, we propose a new flux preconditioner that ensures the correct scaling. We demonstrate that our new method is capable of representing flows down to Mach numbers of 10e-10. We analyze the asymptotic behavior and the stability of our new scheme. For selected examples, we demonstrate that the low condition number of a time-implicit scheme holds promise for an efficient numerical treatment of astrophysical problems. This is joint work with WasilijBarsukow, Philipp Edelmann and Christian Klingenberg. We shall discuss the qualitative difference between the two estimates, which is particularly effective when the dissipative or relaxation terms displays an explicit and significant dependence in the space variable.

<u>Giovanni Russo</u>

Title. "Semi-implicit IMEX schemes for evolutionary partial differential equations"

Abstract. New formulation of implicit-explicit (IMEX) Runge-Kutta (R-K) methods for the numerical discretization of time dependent partial differential equations. The approach is based on identifying the (linear) dependence on the unknown of the system, which generates the stiffness. Only the stiff dependence is treated implicitly, then making the whole method much simpler than fully implicit ones. This approach generalizes classical IMEX methods based on additive and partitioned R-K, and allows a novel application of semi-implicit schemes. Several applications will be presented to a variety of systems. In particular, application to a class of degenerate convection-diffusion problems, for which the new semi-implicit approach allows, is more cost-effective when compared to IMEX schemes with fully implicit treatment. There are cases which require fully-implicit treatment of the stiff term, such as the case of low Mach-number flow for Euler equations of gas dynamics.

<u>Benjamin Seibold</u>

Title. "Benefits of staggered grids and exponential time integrators in radiation moment methods"

Abstract. For the numerical approximation of linear moment models of radiative transfer (PN, SPN, FPN, DN), we demonstrate the structural advantages that come with using staggered grids and exponential time integrators. These include: second-order accuracy; the commutation of discretization with manipulation of the PDE and discrete systems, respectively; and most importantly: asymptotic preserving properties. The numerical approach is implemented in the free and open-source software StaRMAP, which allows the computation of moment models of arbitrary moment order.

Nicolas Seigun

Title. "Boundaries and interfaces in asymptotics from hyperbolic systems"

Abstract. In presence of boundaries or of spatial interfaces, hyperbolic equations with source terms lead to physical layers. In the case of some particular asymptotics as hyperbolic relaxation or parabolic limits, these layers vanish at the limit. The question we address is the design of numerical schemes which are able to accurately solve the limit problem, avoiding numerical layers.

Min Tang

Title. "An asymptotic preserving tailored finite point method for strongly anisotropic and discontinuous diffusivity"

Abstract. In magnetized plasma, the magnetic field confines the particles around the field lines. The anisotropy intensity in the viscosity and heat conduction may reach the order of \$10^{12}\$. Numerically, the error in the diffusion parallel to the magnetic field may pollute the small perpendicular diffusion. We propose a Tailored Finite Point method (TFPM) that can deal with strongly anisotropic tensor diffusivity even when the coefficients are discontinuous at the interfaces. On the one hand, the scheme is proved to be Asymptotic Preserving in the limit that the diffusion tensor becomes degenerate, even for non-aligned coordinates. Uniform convergence with respect to the anisotropy can be observed numerically. On the other hand, when the diffusivity is along the coordinates, the positivity and maximum principle can be proved, even for strong anisotropy. Compared with the TFPM introduced by Han and Huang for the advection diffusion equations with isotropic but small diffusion coefficients, we use the value as well as their derivatives at the grid points to construct the scheme, which makes it possible to deal with strongly anisotropic tensor diffusivity. We present numerical experiments to show the performance of the proposed scheme.

Li Wang

Title. "An asymptotic preserving scheme for linear kinetic equation with fractional diffusion limit"

Abstract. We present a new asymptotic-preserving scheme for the linear Boltzmann equation which, under appropriate scaling, leads to a fractional diffusion limit. Our scheme rests on novel micro-macro decomposition to the distribution function, which splits the original kinetic equation following a reshuffled Hilbert expansion. As opposed to classical diffusion limit, a major difficulty comes from the fat tail in the equilibrium which makes the truncation in velocity space depending on the small parameter. Our idea is, while solving the macro-micro part in a truncated velocity domain (truncation only depends on numerical accuracy), to incorporate an integrated tail over the velocity space that is beyond the truncation, and its major component can be precomputed once with any accuracy. Numerical experiments validate its efficiency in both kinetic and fractional diffusive regimes.

<u>Bokai Yan</u>

Title. "Monte Carlo methods with negative particles"

Abstract. Long range Coulomb collisions between charged particles (electrons and ions) dominate the nonequilibrium dynamics in plasma. However, numerical simulations of these non-equilibrium processes become challenging as the system approaches equilibrium, because the widely used particle methods mainly sample from the equilibrium part and hence are highly inefficient. In this talk I present a novel Monte Carlo method with "negative" particles, which represent defect in the equilibrium part. This is a hybrid type method, which saves the major cost in simulating near-equilibrium dynamics. This method is designed for the general bilinear collision operators and then applied to the Coulomb collisions. Various numerical simulations demonstrate the high accuracy and efficiency.