Scalable Methods for Kinetic Equations

Oak Ridge National Laboratory

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Presentation Titles and Abstracts

On some properties of the Landau kinetic equation

Alexander Bobylev
Karstad Univeristy and Keldysh Institute of Applied Mathematics

The talk is based on a joint paper with Irene Gamba and Irina Potapenko. We discuss some some general properties of the Landau kinetic equation. In particular, the difference between "true" Landau equation, which formally follows from classical mechanics, and "generalized" Landau equation, which is just an interesting mathematical object, is stressed. It is shown how to approximate the Landau equation by the Wild sum. It is the so-called quasi-Maxwellian approximation related to Monte Carlo methods. This approximation can be also useful for mathematical problems. A model equation which can be reduced to a "local" nonlinear parabolic equation is also constructed in connection with existence of the strong solution to the initial value problem. The self-similar asymptotic solution to the Landau equation for large v and t is discussed in detail. The solution, earlier confirmed by numerical experiments, describes a formation of Maxwellian tails for a wide class of initial data concentrated in the thermal domain. It is shown that the corresponding rate of relaxation (fractional exponential) is in exact agreement with recent mathematically rigorous estimates.

Simulation for Electron Impact Excitation/Deexcitation and Ionization/Recombination

Russel Caflisch
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We developed a kinetic model and a corresponding Monte Carlo simulation method for excitation/deexcitation and ionization/recombination by electron impact in a plasma free of external fields. The atoms and ions in the plasma are represented by continuum densities at a range of excitation levels and the electrons by an energy distribution function. A Boltzmann-type equation is formulated and a corresponding H-theorem is formally derived. An efficient Monte Carlo method is developed for an idealized analytic model of the excitation and ionization collision cross sections. To accelerate the simulation, a binary search method is used to overcome the singular rate in the recombination process. Numerical results are presented to demonstrate the efficiency of the method on spatially homogeneous problems. The evolution of the electron distribution function and atomic states is studied, revealing the possibility under certain circumstances of system relaxation towards stationary states that are not equilibrium states (i.e., not Gibbs distributions), due to non-ergodic behavior.

Scalable kinetic hybrid particle-in-cell method combined with continuum grid

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The Monte-Carlo particle-in-cell method and the continuum grid method have their own advantages and disadvantages. The particle-in-cell method has advantage in that it is less sensitive to the CFL condition, more flexible to complicated geometry, easier to render higher velocity space resolution, and superior to extreme scale computing for bigger physics problems. However, it has disadvantage in that it is subject to the Monte-Carlo noise and to the particle-grid interpolation error. In order to reduce these issues, a perturbative method, the so-called delta-f method, was invented with its own problem that the self-consistent multi-scale interaction of the perturbed quantities with the background profile is missing. The continuum grid method has advantage in that it is not subject to Monte-Carlo noise. However, it has disadvantage in that it is sensitive to the CFL condition and requires large memory for finer velocity space grid resolution at high dimensionality (plasma kinetic physics usually requires at least 5D simulations to contain the essential parallel Landau resonance physics and turbulence at first-principles level). We have developed a new hybrid method that can utilize the advantageous features of both methods by combining the particle-in-cell method for finer scale delta-f physics and a coarse-grained continuum grid to describe the larger scale physics. The particle-in-cell method gives the scalability, the insensitiveness to the CFL condition, and the flexibility to complex geometry; while the continuum grid reduces the Monte-Carlo noise and the interpolation error. The hybrid equation is mathematically identical to the full-function equation. The new hybrid scheme also enables easier incorporation of the nonlinear Fokker-Planck collision operator, atomic physics data, and sources and sinks. Remaining challenging issues for the long time simulation will also be discussed.

Nonlinearly implicit, energy- and charge-conserving multidimensional particle-in-cell algorithms for kinetic simulation of plasmas

Guangye Chen
Los Alamos National Laboratory

Particle-in-cell (PIC) simulation techniques have been widely successful in first-principles simulations of plasma dynamics. However, the fundamental algorithmic underpinnings of standard PIC algorithms have not changed in decades. The classical PIC method employs an explicit approach (e.g. leap-frog) to advance the Vlasov-Maxwell/Poisson system using particles coupled to a grid. Explicit PIC is subject to both temporal stability constraints (either light-wave CFL condition or resolving plasma-wave frequency) and spatial stability (so-called finite-grid instability) constraints, which makes it unsuitable for system-scale kinetic simulations, even with modern super-computers.

Implicit algorithms can potentially eliminate both spatial and temporal stability constraints, thus becoming orders of magnitude more efficient than explicit ones. This has motivated much exploration of these algorithms in the literature since the 1970s. However, the lack of efficient nonlinear solvers for a very large system of particle-field equations required approximations that resulted in intolerable accumulation of numerical errors in long-term simulations.

In this presentation, we discuss a multi-dimensional, nonlinearly implicit, nonlinear electromagnetic PIC algorithm using a Jacobian-Free-Newton-Krylov method [1]. The approach delivers both accuracy and efficiency for multi-scale plasma kinetic simulations, and extends previous proof-of- principle studies on 1D electrostatic [2, 3, 4, 5] and electromagnetic systems [6]. To eliminate noise issues associated with numerical Cherenkov radiation [7], we focus our implementation on the Dar- win approximation to Maxwells equations. The formulation conserves exactly total energy, local charge, ignorable canonical momentum, and the Coulomb gauge. Linear momentum is not exactly conserved, but errors are kept small by an adaptive particle sub-stepping orbit integrator. Key to the performance of the algorithm is a moment-based preconditioner, featuring the correct asymptotic limits. The formulation can be extended with a mapped mesh, which opens the possibility of accurate spatially adaptive PIC simulations. The superior accuracy and efficiency properties of the scheme will be demonstrated with challenging numerical examples.

Implicit-Explicit linear multistep methods for kinetic equations

Giacomo Dimarco
University of Ferrara

We consider the development of high order asymptotic preserving linear multistep methods for kinetic equations and related problems. The methods are first presented for the BGK-like kinetic models and then extended to the case of the full Boltzmann equation. The behavior of the scheme in the Navier-Stokes regime is also studied and compatibility conditions derived. We show that compared to the IMEX Runge-Kutta methods, the IMEX multistep methods present several advantages due to the absence of coupling conditions and the greater computational efficiency.

Towards New Computational Methods for Neutrino Transport in Core-Collapse Supernovae

Eirik Endeve
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A core-collapse supernova is the explosive death of a massive star. On a time scale of about one second, its iron core collapses to nuclear densities and launches an outward-propagating shock wave, which eventually disrupts the star in a supernova enriching the Universe with heavy elements, and leaving behind a compact object. Central to supernova theory, and associated models, is computing the energy transfer from an intense neutrino radiation field to the stellar fluid behind the supernova shock wave. The neutrinos emanate from the surface of the forming compact object, and are a major driver of the explosion. The energy transfer occurs under non-equilibrium conditions, and a description of neutrinos based on the Boltzmann equation is warranted. The computational cost associated with neutrino transport has necessitated approximations which are a major source of uncertainty in current simulations. Modern algorithms and computing hardware will allow for relaxation of these approximations. Here we discuss our recent progress towards new methods for simulation of neutrino transport in core-collapse supernovae. We focus on methods for phase space advection, but also discuss preliminary work on conservation and inclusion of neutrino-matter interactions.

Computational issues for the Vlasov-Poisson/Maxwell Landau systems for plasmas

Irene Gamba
University of Texas at Austin

We discuss a hybrid numerical approach to Vlasov-Poisson-Landau for plasma systems. We propose a time splitting computational scheme that allows for a conservative approach for the whole system, where the Landau operator is computed by an spectral based solver, and both, the Vlasov-Poisson and Vlasov- Maxwell systems, are computed by a conservative Discontinuous Galerkin approach. Implementations of rough boundary conditions will be discussed. This lecture is based on different works in collaboration with Chenglong Zhang and with Jose Morales Escalante, as well as with Yingda Cheng, Fengyan Li and Phil Morrison.

Strategies and Algorithms for Hybrid Shared-Memory/Message-Passing Parallelism in Monte Carlo Radiation Transport Codes

David Griesheimer
Bettis Laboratory

Presently, most high-performance Monte Carlo (MC) radiation transport solvers use a hybrid message-passing and shared-memory approach to parallelism, which enables the codes to utilize available computing resources, both between and within compute nodes on a cluster. In this paper we review several strategies, algorithms, and best practices for improving efficiency and scalability of hybrid shared-memory/message-passing parallelism within a MC radiation transport code. The code-design strategies and best-practices presented within are largely based on experience obtained while developing MC21, an in-house, continuous-energy MC solver specifically designed for large-scale reactor analysis simulations on massively-parallel computing systems. In addition, the paper provides details on three novel parallel algorithms for operations that play a fundamental role in MC transport simulations: random number generation, fission source renormalization, and fixed-source sampling. The parallel efficiency and scalability of these methods is established through a series of scaling studies, performed with MC21, which cover a variety of representative scenarios for large-scale reactor analysis simulations. Results from these studies demonstrate that MC21, using the methods described in this paper, is able to handle extremely large problem sizes (up to 1 TB of memory, including 1.1E11 depletable nuclides) and scales well through thousands of processors.

Building a better BGK

Jeff Haack
Los Alamos National Laboratory

In this talk, I will present joint work with C. Hauck (ORNL) and M. Murillo (LANL) on a new multi-species BGK model for dense plasmas. This model conserves mass, momentum, and kinetic energy and allows for a more clear connection to the underlying cross sections and inter-species collision rates.

Properties of Gyrokinetic Turbulence in Tokamaks, and Discontinuous Galerkin Methods for (Gyro)Kinetics

Greg Hammett
Princeton Plasma Physics Laboratory

We begin with a summary of key properties of turbulence in tokamaks and the 5-D gyrokinetic equations that are used in computer simulations of this. A lot of progress has been made in developing comprehensive gyrokinetic simulations of turbulence in the main core region of tokamaks, but much work remains to understand the more challenging edge region and to develop codes that can handle all of the important effects believed important there. We will discuss some interesting features of Discontinuous Galerkin algorithms and our work towards developing a new DG-based code in the Gkeyll framework for handling the edge region. Gkeyll is also being developed for other problems including Vlasov-Poisson, Vlasov-Maxwell, and multi-fluid-Maxwell. Versions of DG can conserve energy exactly for Hamiltonian systems. Versions of DG can also conserve energy when using efficient Maxwellian-weighted basis functions. Some of the challenges of including magnetic fluctuations in gyrokinetics will be discussed, including subtleties in the choice of basis functions for electromagnetic potentials

Uncertainty quantification for multiscale hyperbolic and kinetic equations with uncertain coefficients

Shi Jin
University of Wisconsin-Madison

In this talk we will study the generalized polynomial chaos (gPC) approach to kinetic equations with uncertain coefficients/inputs, and multiple time or space scales, and show that they can be made asymptotic-preserving or well-balanced, in the sense that the gPC scheme preserves various asymptotic limits in the discrete space. This allows the implemention of the gPC methods for these problems without numerically resolving (by space, time, and gPC modes) the small scales. We also give a fast gPC algorithm for the Boltzmann equation with uncertainties in its collision kernel, initial or boundary data.

Kinetic Modeling Efforts in the AFRL In-Space Propulsuon Branch

Robert Martin
Air Force Research Laboratory

The talk will first briefly outline the design and ongoing verification of AFRL/RQRS's new spacecraft propulsion modeling framework. Recent algorithm development work will then be presented on topics including VDF reconstruction for dynamic particle weights, extended BGK and DSMC collision models, and a new weakly magnatized particle push.

New Approaches for Residual Monte Carlo

Jim Morel
Texas A & M University

Residual Monte Carlo methods can result in exponential convergence of the solution with the number of histories executed rather than the usual inverse of the square root of that number. Although residual Monte Carlo was developed in the 60s and received considerable attention from the radiation transport community in the late 90s, it has yet to become a practical method. We believe the primary difficulty with previous methods has been cancellation errors in the projection of the Monte Carlo solution onto global polynomial trial spaces to compute a residual. We describe recent results based upon the use of finite-element trial spaces for this purpose. In addition we describe hybrid Monte Carlo/FEM methods that are particularly well suited to extreme-scale computing.

Recent Progress in High-Order, Low-Order methods for Thermal Radiative Transfer Problems

Ryosuke Park
Los Alamos National Laboratory

Recently, we have developed a moment-based, scale-bridging algorithm for solving thermal radiative transfer problems. High-order, low-order (HOLO) method accelerates the solution of Boltzmann transport equation using discretely-consistent low-order, continuum system. In this talk, we discuss recent progress in the algorithmic development, including stability improvements, multiphysics extension, and preliminary parallel performance study.

A simple and effective limiter for DG-FEM with application to a micro-macro decomposition of Boltzmann-BGK

James Rossmanith
Iowa State University

In this work we develop a novel shock-capturing limiter that combines key ideas from the limiter of Barth and Jespersen [AIAA-89-0366 (1989)] and the maximum principle preserving (MPP) framework of Zhang and Shu [Proc. R. Soc. A, 467 (2011), pp. 2752–2776]. The limiting strategy is based on traversing the mesh element-by-element in order to (1) find local upper and lower bounds on user-defined variables by sampling these variables on neighboring elements, and (2) to then enforce these local bounds by minimally damping the high-order corrections. The main advantages of this limiting strategy is that it is simple to implement, effective at shock capturing, and retains high-order accuracy of the solution in smooth regimes. The resulting numerical scheme is applied to a micro-macro decomposition of the Boltzmann-BGK equation.The kinetic (micro) part of the equations are solved using a high-order semi-Lagrangian DG-FEM and the fluid (macro) part of the equations are solved using a DG-FEM with the newly proposed limiter.

Scaling Deterministic Solution of the Boltzmann Transport Equation on Heterogeneous Computing Platforms

Karl Rupp
Vienna University of Technology

We revisit a domain-specific parallel preconditioning scheme for spherical harmonics expansions of the Boltzmann transport equation. The scheme, which has been initially developed for graphics processing units, is refined and extended to distributed memory architectures. Numerical experiments demonstrate the suitability of the proposed scheme for moderately sized compute clusters. Finally, we outline future research directions aimed at further improving scalability.

Higher Moment Models for Multi-Fluid Plasmas

Uri Shumlak
University of Washington

Moments of the Boltzmann equation produce the multi-fluid plasma model. A plasma model has at least two-fluids, representing electron and ion species. Additional fluids can include neutrals, impurities, or excited ions. Moment equations are truncated, e.g. after five, ten, thirteen, or twenty equations, and are closed with expressions that relate higher moment variables to lower moment variables. Higher moment models extend the region of validity to plasmas with lower collisionality. Large mass differences between electrons and ions in the multi-fluid plasma model introduce disparate temporal and spatial scales and require numerical algorithms with sufficient accuracy to capture the multiple scales. Source terms couple the fluids to themselves (interspecies interactions) and to the electromagnetic fields. Interspecies interactions also occur through collisional source terms that account for the direct transfer of momentum and energy. In addition to plasma and electrodynamic physics, the multi-fluid plasma model can capture atomic physics in the form of reaction rate equations for ionization and recombination, which introduce new temporal scales to the plasma dynamics. The numerical algorithm must treat the inherent stiffness introduced by the multiple physical effects of the model and tightly couple the source terms of the governing equations. The governing equations are expressed in a balance law form. A discontinuous Galerkin method with an approximate Riemann solver is developed for the spatial discretization and Runge-Kutta methods perform the temporal advance. Numerically solving this large equation system requires parallelizing at several levels of granularity to fully utilize modern compute architectures.

iFP: An Optimal, Fully Implicit, Fully Conservative, 1D2V Vlasov-Rosenbluth-Fokker-Planck Code for Spherical ICF Simulations

Will Taitano
Los Alamos National Laboratory

Contrary to predictions of radiation-hydrodynamics design codes, the National Ignition Facility has not succeeded in achieving ignition. Recent experimental evidence suggests that plasma kinetic effects may play an important role during Inertial Confinement Fusion (ICF) capsules implosion. Consequently, kinetic models and simulations may need to be used to better understand experimental results and design ICF targets. We present a new, optimal, fully implicit, and fully conservative 1D2V Vlasov-Fokker-Planck (VFP) code, iFP, which simulates ICF implosions kinetically. Such simulations are difficult to perform because of the disparate time and length scales involved. The challenge in obtaining a credible solution is further complicated by the need to enforce discrete conservation properties. In our studies, we employ the Rosenbluth formulation for the Fokker-Planck collision operator. Our approach uses a fully implicit temporal advance to step over stiff collision- time scales. For the solver, we use a Jacobian-free Newton-Krylov method with an optimal multigrid-based preconditioning technology. To address the issues of velocity disparity between various species as well as those associated with temporal and spatial temperature variations, we have developed: 1) a velocity space meshing scheme, which adapts to the species local thermal velocity; and 2) an asymptotic expansion of the Rosenbluth potentials based on the large ratio of thermal speeds of the fast-to-slow species (vth,f/vth,s ¿¿ 1). We have also implemented a Lagrangian mesh, which allows the physical space mesh to move as the capsule compresses. Finally, we enforce discrete conservation of mass, momentum, and energy by solving a set of discrete nonlinear constraints, which are derived from continuum symmetries present in the VFP equations. Herein, we present some results testing the code capabilities and show preliminary simulations of a plasma shock.

An asymptotic-preserving scheme for linear kinetic equation with fractional diffusion limit

Li Wang
University of California

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. Such an addition is essential to drive the solution to the correct asymptotic limit.

Hybrid Methods with Deviational Particles for Inhomogeneous Plasma

Bokai Yan
University of California, Los Angeles

We propose a Hybrid method with Deviational Particles (HDP) for a plasma modeled by the inhomogeneous Vlasov-Poisson-Landau system. We split the distribution into a Maxwellian part evolved by a grid based fluid solver and a deviation part simulated by numerical particles. These particles, named deviational particles, could be both positive and negative. The Coulomb collisions between charged particles are simulated by the Monte Carlo method proposed in an early work, while the advection of deviational particles in an electric field is solved by applying a Macro-Micro projection. Furthermore, coarse particles employed to accelerate the simulation of Coulomb collision are simulated by a traditional PIC-MCC method (Particle-In-Cell method for the advection and Monte Carlo method for Collisions). The particle resampling techniques on both deviational particles and coarse particles are investigated and improved, which further improves the efficiency of this HDP method. Various numerical tests are performed to demonstrate the accuracy and efficiency of this method.