Scalable Methods for Kinetic Equations

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Poster Titles and Abstracts

Multiscale and Multiphysics Simulations with GenASiS

Reuben D. Budiardja
University of Tennessee

Many computationally demanding problems in astrophysics and cosmology are multiphysics and multiscale in nature. One prime example of such problems is the elucidation of the explosion mechanism of core-collapse supernovae, whose physics includes magneto-hydrodynamics, self-gravity, nuclear burning, and kinetic theory for radiation transport. For a problem as rich as this, deploying all the necessary physics often requires a series of approximations of increasing sophistication, many of which have multiple formulations and solution methods to be tested. These challenges face the development of sophisticated multiphysics code. GenASiS is a new simulation system being developed to address these challenges using object-oriented paradigm.

An Arbitrary Order, Fully Implicit, Hybrid Kinetic Solver for Radiative Transport Using Integral Deferred Correction

Michael Crockatt
Michigan State University

An implicit, hybrid method for linear kinetic equations was recently proposed and an implementation using the implicit Euler method was studied. We present an arbitrarily high order solver based on this hybrid method using integral deferred corrections with respect to the implicit Euler method. The results of several convergence studies as well as several test problems are provided to show the efficacy of the hybrid method extends to implicit methods of higher order in both highly collisional and non-collisional regimes.

Fully non-linear multi-species Fokker-Planck-Landau collisions in gyrokinetic particle-in-cell simulations of fusion plasma

Rober Hager
Princeton Plasma Physics Laboratory

We describe the implementation and application of a time-dependent, fully non-linear multi-species Fokker-Planck-Landau collision operator based on the work of Yoon and Chang [Phys. Plasmas 21, 032503 (2014)] in the full-function gyrokinetic particle-in-cell codes XGC1 [Ku et al., Nucl. Fusion 49, 115021 (2009)] and XGCa. XGC simulations include pedestal and scrape-off layer region, where steep gradients and large fluctuations can cause significant deviations of the particle distribution function from a Maxwellian. Therefore, the use of a non-linear collision operator is advisable. For XGC simulations including gyrokinetic ions and drift-kinetic electrons, we generalized the single-species non-linear Fokker-Planck-Landau collision operator by Yoon and Chang to a multiple-species operator. This operator is based on a finite volume method using distribution functions sampled from the marker particles. The relative errors of mass, momentum, and energy conservation are limited to 10-6 through the convergence criterion of the implicit time stepping method used in the collision operator. After a collision operation, the updated distribution function is interpolated back to the particles. Due to the large number of configuration space grid points on which the collision operator is evaluated (XGCa: 104, XGC1: 106), the workload due to collisions can be comparable or larger than the workload due to particle motion. In order to keep the added computing time at a tolerable level we implemented a completely new load balancing algorithm that constantly adjusts particle and mesh decomposition to minimize run time. In addition, nested OpenMP parallelism is used that allows to evaluate the collision operator on several grid points at the same time in the outer thread level and accelerates the calculation for every single grid point in the inner level. Nested OpenMP threading also helps to meet memory constraints on computers like Mira that offers as little as 256 MB of memory per thread. Owing to all technical and algorithmic improvements, fully-nonlinear collisions are now used routinely in XGC simulations on leadership class supercomputers like Titan, Mira, and Edison. The computing time spent on collisions in a typical XGCa simulation using 700 compute nodes on Edison ranges between 5 and 30% depending on electron collisionality.

High-order energy conserving, (discontinuous) finite-element algorithms for (gyro) kinetic simulations of plasmas

Ammar Hakim
Princeton Plasma Physics Laboratory

Gkeyll aims to be a production quality code for the simulation of plasma edge turbulence with the gyrokinetic model. I will report on progress towards this goal, and also report on efforts to implement full kinetics (Vlasov-Maxwell system). A general class of high-order continuous/discontinuous Galerkin algorithms, based on discretizing the Poisson Bracket operator, have been implemented. A careful choice of basis function for representing the Hamiltonian and the distribution function yields a spatial scheme that conserves the quadratic invariants of the system. Combined with a finite-element solver for the potentials then yields a scheme which conserves the total energy (particles + fields) exactly. Momentum conservation, though not exact, is independent of velocity space resolution, and converges very rapidly with increasing spatial resolution. Self-adjoint smoothing operators have been developed to efficiently handle magnetic fluctuations.

For the Vlasov-Maxwell equations, an alternate scheme is implemented. This discretizes the E and B fields directly (rather than the electromagnetic potentials), and, with a proper choice of numerical fluxes, also yields an energy conserving scheme. A carefully constructed semi-implicit scheme to step over plasma frequency will be presented.

Hai Le
University of California, Los Angeles

Monte Carlo simulation of atomic collisions with complexity reduction Kinetic simulation of excitation and ionization collisions in nonequilibrium plasmas is particularly challenging due to the multitude of processes involved and the multiscale features of the collision rates. We propose a complexity reduction method based on level grouping of atomic states within the framework of Monte Carlo methods. High order of accuracy of the reduction method is realized by allowing an internal distribution within each group. The stiffness of the collisional kinetics can be significantly reduced with minimal loss in accuracy. This is joint work with B. Yan, R. Caflisch and J.-L. Cambier.

Positive Filtered P_N Closures for Linear Kinetic Transport Equations, with Consistency Results

Paul Laiu
University of Maryland

We propose a modification to the standard spherical harmonic closure, known as PN closure, for kinetic equations. The modification produces a smooth, nonnegative polynomial ansatz by applying two-step filtering on the oscillatory, partially negative PN solutions, and integrates the closed mo- ment system with filtered moments. Such closure preserves nonnegativity of the solution and prevents breaking stability of nonlinear kinetic systems. We also prove consistency properties for the proposed closure, and report numerical results on the line source benchmark.

An Asymptotic-Preserving Stochastic Galerkin method for Semiconductor Boltzmann Equation with Random Inputs and Diffusive Scalings.

Liu Liu
University of Wisconsin-Madison

We consider a linear semi-conductor Boltzmann equation with diffusive scalings and uncertainties, which may come from the collision kernel, initial or boundary conditions. We design a stochastic asymptotic-preserving scheme and employ the generalized polynomial chaos (gPC) expansion with a stochastic Galerkin approach. The spectral convergence analysis, the stability for the scheme, as well as the numerical examples is to be implemented.

Reflection Boundary Conditions in DG Methods for Boltzmann - Poisson models of Electronic Transport in Semiconductors

Jose Morales
University of Texas at Austin

We shall discuss the implementation of Discontinuous Galerkin (DG) methods on Boltzmann - Poisson (BP) systems of electron transport in semiconductor devices at nano scales. We consider the mathematical and numerical modeling of Reflective Boundary Conditions in 2D devices and their implementation in DG-BP schemes. We study the specular, diffusive and mixed reflection BC on physical boundaries of the device for the modeling of surface roughness, comparing the influence of these different reflection cases in the computational prediction of moments close to the boundaries and their associated scale.

Modeling of non-uniform heating of laser-produced plasmas by DSMC-base method

Irina Potapenko
Keldysh Institute of Applied Mathematics

Kinetic treatment of plasma systems plays an important role in a description of macroscopic plasma properties that cannot be learned under hydrodynamic approach. The Boltzmann kinetic equation (BKE) is a cornerstone for the study of transport phenomena in gases and plasmas, as well as the photon.

Multilevel Monte Carlo simulation of kinetic plasma dynamics

Lee Ricketson
Courant Institute of Mathematical Sciences

Particle-based simulation methods are prevalent in the study of both plasma and rarefied gas dynamics. They are usually called particle-in-cell (PIC) schemes in the former context, and direct-simulation Monte Carlo (DSMC) in the latter. Despite the naming discrepancies, the mathematical structure of the underlying equations and the numerical methods have much in common. In particular, many instances of each may be viewed as a system of particles undergoing stochastic motion through interaction with some mean-field determined by the particles themselves. Mathematically, this takes the form of a McKean-Vlasov equation. We present a generalization of the multilevel Monte Carlo (MLMC) method - popular in financial applications - to McKean-Vlasov equations. The resulting efficiency improvements are demonstrated on problems from plasma physics.

Numerical solution of the quantum Lenard-Balescu equation

Christian Scullard
Lawrence Livermore National Laboratory

I present a spectral solution of the quantum Lenard-Balescu equation for a one-component plasma. This method perfectly conserves particles and energy, and the difficult dielectric function integrals can be accurately computed on the fly. I give a solution of the temperature equilibration problem in a one-component plasma. I also discuss the generalizations that are possible, such as multi-component and inhomogeneous systems.

Differential Approximation to RTEs and Its Applications to Inverse Problems

Qiwei Sheng
University of Tennessee, Knoxville

We present a family of differential approximations (RT/DA) to the radiative transfer equation (RTE) and explore its applications to an inverse problem based on RTE that reconstructs the scattering coefficients under a highly forward-peaked scattering setting. When solving the inverse problem, the RT/DA equation is employed as the forward model instead of RTE. An iterative numerical scheme for the RT/DA and a formulation of the reconstruction problem are introduced. Numerical experiments illustrate the reliability and accuracy of the numerical results using the proposed methods in a highly forward-scattering setting.

Recent Results from the Gkeyll Discontinuous Galerkin Kinetic Code

Eric Shi
Princeton University

Gkeyll is a continuum code under development with the aim of simulating electromagnetic plasma turbulence in the tokamak edge region with a gyrokinetic model. We will present benchmarks of Gkeyll for linear and nonlinear simulations of ETG/ITG turbulence in 2d axisymmetric and 3d slab geometries. We will also discuss plans and initial results for Maxwellian-weighted basis functions for velocity-space discretization.