Multiscale Mathematics For Plasma Kinetics Spanning Multiple Collisionality Regimes

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Summary

This project is developing more efficient kinetic algorithms for the simulation of plasma systems that span a wide range of collisionality. Kinetic modeling of such plasmas is highly challenging, is in need of improved algorithms, and is key to understanding plasma systems that underlie controlled fusion (magnetic and inertial), semiconductor processing, and space plasmas. The new algorithms are being tested, optimized, and demonstrated on paradigm plasma physics problems, including a collisional electrostatic sheath and nonlocal kinetic electron thermal transport along magnetic field lines.

Kinetic modeling is needed to understand moderately collisional or "near-continuum" (NC) plasmas. In a NC plasma, collisions are frequent for most of the particles of one or more charged particle species, but sub populations of that species important to key phenomena are present for which collisions are sufficiently weak that a fluid description fails. NC plasmas are a key component in various laboratory and technological devices such as controlled fusion (both magnetic and inertial) and semiconductor processing, as well as in natural settings, e.g., space plasmas.

Many phenomena in NC plasmas are inaccessible to kinetic modeling for two reasons. The main dependent variable in kinetic modeling is a density defined on a position-velocity phase space. This phase space has roughly twice the number of dimensions of the configuration space on which fluid variables would be defined, thus requiring many more (by a factor ranging from 10 to more than 10^6) degrees of freedom (mesh nodes or simulation particles) when discretized than in a fluid model. Present kinetic models also require time steps significantly shorter than a typical collision time. This poses a difficulty since a significant fraction of the NC species particles have collision rates much more rapid than the phenomena of interest.

We are developing a class of new hybrid (fluid+particle) kinetic algorithms that are expected to greatly reduce the computational resources needed for and significantly expand the range of such problems accessible to kinetic modeling of NC plasmas. These algorithms are being implemented and tested on paradigm plasma physics problems that have sufficient physics to fully exercise the algorithms, enable comparison against present methods, and properly quantify their performance.

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Two new hybrid-kinetic schemes have been formulated. The first is similar to the interpolated-fluid Monte-Carlo (IFMC) scheme [1] successfully used in rarefied gas dynamics (RGD). The second scheme is a hybrid of a δf particle-in-cell (PIC) Monte-Carlo (MC) method with a fluid method.

The key kinetic and fluid equations have been derived for both schemes. The fluid equations are amenable to standard compressible fluid schemes, as they resemble the standard compressible Euler equations, albeit with additional sources that represent their closure by solutions of the associated kinetic equations. The kinetic equations are tailored to specific PIC-Monte-Carlo (MC) methods. The IFMC-like algorithm uses a full PIC-MC scheme, with fixed-weight particles. These may be created or destroyed both due to physical sources and sinks and through "thermalization/ dethermalization" (TDT), which passes their content (mass, momentum, energy) to/from the fluid part of the system. The TDT step limits the simulation particle population to those parts of phase space where it is needed, and gives correct behavior to those particles for which the change in velocity due to collisions is their most rapid change.

In the case of the δf-PIC scheme, the particles may either have time-dependent weights or particle populations with both positive and negative fixed weights. This enables the particles to represent the solution of optimized δf kinetic equations in which as much as possible of the phase-space distribution function content is put into the fluid portion of the system. A TDT step can be implemented either by damping or growing the particle weights or by removing or seeding simulation particles.

By late FY'06 we will complete implementation of the first of our hybrid algorithms and initiate simulations of two test problems: (a) a collisional electrostatic sheath and (b) nonlocal collisional electron thermal transport along magnetic field lines.

Even for these relatively simple settings, the implementation and demonstration of these algorithms has many components. Progress to date includes modernizing and porting to current computational platforms a legacy PIC-MC code ("ICEPIC") which is a suitable testbed for implementation of the new algorithms and for running test problems with both standard and new algorithms. In addition, we have implementated and tested an optimal Monte-Carlo Coulomb collision algorithm (due to K. Nanbu) and a field solver for the Poisson equation with a self-consistent nonlinear adiabatic electron response. Formulation work has been completed and implementation is underway for two candidate TDT criteria and algorithms, and for a suitable fluid algorithm and time-stepping scheme for synchronization between fluid and particle advances.

References:

[1] L. Pareschi and R.E. Caflisch, "An implicit Monte Carlo method for rarefied gas dynamics," J. Comput. Phys., **154**, 90-116, (1999).

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