Hybrid Methods with Negative Particles, for Accelerated Simulation of Plasma Kinetics

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Whitepaper for Topic D. Multiphysics and multiscale coupling.

Particle-based Monte Carlo methods (i.e., variants of DSMC such as [1]) are widely applicable and effective for kinetic simulation of plasma dynamics, including Coulomb collisions, as required for accurate computation of plasma boundary physics. For problems with small Knudsen number, however, the collision rate is large so that these simulations are intractable.

Our approach is a hybrid method that combines particle and continuum simulations. The distribution function f=f(x,v,t) is written as a combination f=M+k. The "thermal component" M=M(v,ρ,u,T) is a (local) Maxwellian distribution with fluid variables (ρ,u,T) that depend on (x,t) and solve continuum fluid equations. The "kinetic component" k is the deviation from Maxwellian and is represented as a collection of discrete particles, which undergo collisions as in DSMC. This representation is much more efficient (i.e., fewer particles are required), if the values of k can be both positive and negative; i.e., if the particles in k come with both positive and negative weights, so that $k = k_p - k_n$.

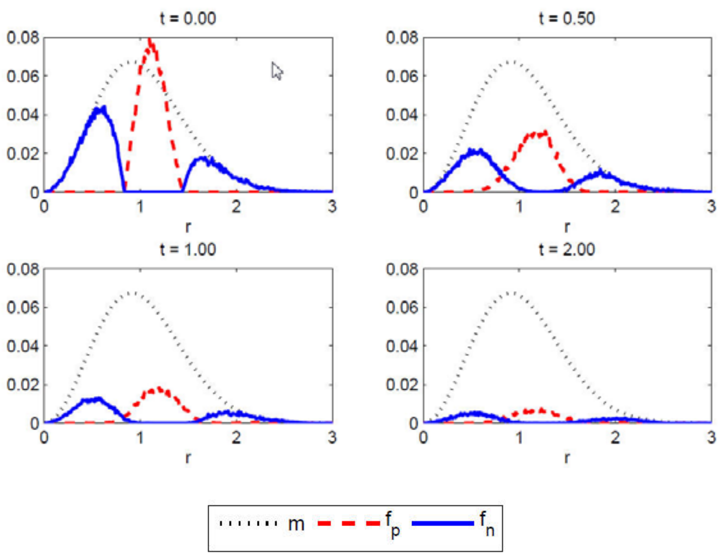
Negative particles have been difficult to include in nonlinear kinetic simulations, because accurate simulation of a collision between a positive particle and a negative particle (or two negative particles) involves the creation of new particle pairs, each consisting of a positive particle and a negative particle [2]. For Coulomb collisions this results in exponential growth of particle number on the numerical time scale. This whitepaper describes development of a new approach [3] to inclusion of negative particles which overcomes this growth in particle number.

The new method involves three steps. The first and most novel step is the use of a "coarse scaled" distribution function $\tilde{f}$, coming from simulation with a small number of particles. By construction, $\tilde{f}$ is an unbiased approximation to the original distribution function f, even though it is not very accurate. Some of the collisions between k_n and f are replaced by collisions between k_n and $\tilde{f}$, which are simulated without creation of additional particles.

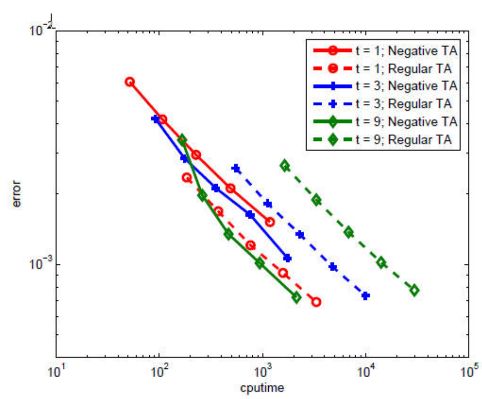
The second step is direct sampling of collisions between $k_p - k_n$ and M which is performed in a way that produces a small number of new particles, but is computationally intensive. The third is resampling step that reduces the number of particles by cancellation of particles that are nearby in phase space. Figures 1 and 2 show results of this method applied to a spatially homogeneous problem (Roseunbluth's test problem [4]), with excellent results.

We plan to implement this method in the hybrid framework of Lee et al. [5], which involves a thermalization/dethermalization (T/D) step to mediate the interaction between k and M. In [5], a relative entropy quantity was used as a criterion for T/D. This method works quite well for spatially homogeneous problems, but has two limitations: The first is that it only involves positive particles so that the deviation from Maxwellian must be positive. Another way of saying this is that the Maxwellian component must be chosen with a small density ρ, so that it lies below f. The second limitation is that spatial variation is complicated to include, since it is dethermalizing. Inclusion of negative particles using the method described above directly overcomes the first limitation. We expect that negative particles will also overcome the second limitation, since their use significantly simplifies the inclusion of spatial convection.

The expected impact of this method is that it could enable fast and accurate simulation of plasma kinetics in nonlinear, non-equilibrium regions, such as plasma boundaries. In particular, it should extend the range of applicability of previous simulation methods, such as δf methods.



1. Snapshots of the evolution of the components in Rosenbluth's test problem.



2. The efficiency test on Rosenbluth's problem.

References

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