Overview of Accelerated Simulation Methods for Plasma Kinetics

R.E. Caflisch

In collaboration with: J.L. Cambier, B.I. Cohen, A.M. Dimits, L.F. Ricketson, M.S. Rosin, B. Yann

1 UCLA Math Dept 2 AFRL 3 LLNL 4 Courant Institute 5 Pratt Institute

AFRL Program Review
January 20, 2015

Work performed under funding from AFOSR and DOE.
Introduction
Phase space particle number density $f(\vec{x}, \vec{v}, t)$

Boltzmann Equation:

$$\partial_t f + \vec{v} \cdot \nabla_x f + \vec{a} \cdot \nabla_v f = C(f, f)$$  \hspace{1cm} \text{(1)}$$

$C(f, f)$ is:

- Boltzmann collision operator for rarefied gas dynamics (RGD)
- Landau-Fokker-Planck operator for Coulomb collisions
- Operator for excitation/deexcitation, ionization/recombination for collisional/radiative (CR) kinetics

This talk omits spatial variation and mean fields.
Collisions are simulated directly as in DSMC, with

- Distribution function is represented by set of discrete particles
- For short range interactions (RGD and CR kinetics), each particle has $\nu \Delta t$ collisions in time step $\Delta t$ for collision rate $\nu$.
  - Collision partners and parameters are randomly chosen.
- For long range interactions (Coulomb), each numerical collision is an aggregate of grazing collisions over time step.
  - Every particle collides once in every time step
  - Collisions are aggregates depending on $\Delta t$
Computational Obstacles for Monte Carlo Simulation

- Computational complexity for high collisionality (near continuum limit)
  - Hybrid method for RGD and Coulomb collisions
  - Negative particle method
- Many time steps
  - Multi-Level Monte Carlo (MLMC)
- Multiscale features
  - CR kinetics
Hybrid Schemes for Binary Collision Methods
Hybrid Scheme

Combine fluid and particle simulation methods\(^1\):

- Separate \( f \) into Maxwellian and non-Maxwellian components: \( f = m + f_p \)
- Treat \( m \) as fluid \( \rightarrow \) solves Euler equations
- Simulate \( f_p \) by Monte Carlo algorithm
- Interaction of \( m \) and \( f_p \): sample particles from \( m \) and collide them with particles from \( f_p \).

\(^1\)Caflisch et. al, Multiscale Model. Simul. 7 (2008) 865-887.
Hybrid scheme is efficient because collisions between $m$ and $m$ need not be simulated. Efficiency increased by thermalization:

- Collisions drive particles into equilibrium
- Move particles from $f_p$ to $m$ when they have collided enough (thermalization)
- Move sampled particles from $m$ into $f_p$ if the collision is strong enough (dethermalization)
- (De)Thermalization criterion using entropy\(^2\)
- Alternative criterion based on scattering angle\(^3\)

Generalization to spatial inhomogeneities is nontrivial

\(^3\)Dimits et. al., private communication
Bump-on-Tail

Russel Caflisch  Accelerated Simulation for Plasma Kinetics
Bump–on–Tail Test Problem

Improvement Factor vs. PIC

Relative $L^1$ Error

- Entropy Scheme
- Entropy + Dethermalization
- Scattering Angle Scheme
- Scattering Angle + Dethermalization

Russel Caflisch
Accelerated Simulation for Plasma Kinetics
Negative Particles
Hybrid methods need negative particles

The hybrid method presented above, assumes that $f \geq m$, This may be inefficient if there is a “defect” in the Maxwellian.
The hybrid method presented above, assumes that \( f \geq m \), This may be inefficient if there is a “defect” in the Maxwellian.

If \( f = m + f_p \) (with \( f_p > 0 \) so that \( f_p \) can be represented by particles) then \( m \) will be small.
Hybrid methods need negative particles

The hybrid method presented above, assumes that \( f \geq m \), This may be inefficient if there is a “defect” in the Maxwellian.

Better:

\[
f = m + f_p - f_n
\]

with \( f_p \geq 0, f_n \geq 0 \). Represent the defect by “negative particles”!
A negative particle $w_-$ (in $f_m$) cancels a particle in $m$ (or in $f_p$) which should not be present.

A collision $P - N$ between a positive particle $v_+$ and a negative particle $w_-$ cancels a collision $P - P$ between $v_+$ and a positive particle $w_+$ that should not have occurred.

- The $P - P$ collision removes $v_+$ and $w_+$ and adds $v'_+$ and $w'_+$:

  $$\text{P-P: } v_+, w_+ \rightarrow v'_+, w'_+$$

- So the $P - N$ collision should add a $v_+$, remove $w_-$ (equivalent to adding $w_+$) and add negative particles to cancel $v'_+$ and $w'_+$:

  $$\text{P-N: } v_+, w_- \rightarrow 2v_+, v'_-, w'_-$$

This can be derived from the Boltzmann equation (Hadjiconstantinou 2005).
General rules for collisions with negative particles

- **P-P:** $v_+, w_+ \rightarrow v'_+, w'_+$
- **P-N:** $v_+, w_- \rightarrow 2v_+, v'_-, w'_-$
- **N-N:** $v_-, w_- \rightarrow 2v_-, 2w_-, v'_+, w'_+$
- **P-M:** $m, v_+ \rightarrow m, w_-, v'_+, w'_+$
- **N-M:** $m, v_- \rightarrow m, w_+, v'_-, w'_-$

Particle number increases!

- Since every particle collides in every time step, it’s much worse for Coulomb collisions!
- Bokai Yan will present a new method for overcoming this particle increase.
Multilevel Monte Carlo (MLMC) for Langevin Method
Langevin Formulation

Linear LFP equation for \( f(v, t) \) is equivalent to stochastic differential equations (SDEs) for \( v(t) \)

\[
dv_i = F_i \, dt + D_{ij} \, dW_j, \quad (2)
\]

where \( f \) is probability density of \( v \) and \( i, j \) are component indices

- \( W = W(t) \) is Brownian motion in velocity
- \( dW \) is white noise in velocity
- Direct extension to spatial dependence
- Valid for nonlinear LFP, if \( F \) and \( D \) are updated as needed
Euler-Maruyama discretization in time:

\[
\begin{align*}
    v_{i,n+1} &= v_{i,n} + F_{i,n} \Delta t + D_{ij,n} \Delta W_{j,n}, \\
    \Delta W_n &= W_{n+1} - W_n
\end{align*}
\] (3)

in which \( v_{i,n} = v_i(t_n) \) and \( F_n = F(v_n) \)

**Computational cost vs. error \( \varepsilon \):**

- Statistical error is \( O(N^{-1/2}) \)
- \( \Delta t \) error is \( O(\Delta t) \), since \( \Delta W = O(\sqrt{\Delta t}) \) and random
- Optimal choice is \( \varepsilon = N^{-1/2} = \Delta t \)
- Cost = \( N \Delta t^{-1} = \varepsilon^{-3} \)
MLMC Basics

- Introduce time step levels, $\Delta t_\ell = T2^{-\ell}$, for $\ell = 0, \ldots, L$

- Use computation at coarse level as a “control variate” for computation at finer level
- Optimally combine the different levels
- Motivated by multigrid methods

$\ell$

- Multilevel Schemes: How they work

- Statistical error converges with
  
- Like multi-grid method.

- Convergent sum, when using Milstein method

- $\hat{v}_{N_L} = E[v_0] + \sum_{l=1}^{L} E[(v_l - v_{l-1})]$

- Multilevel Monte Carlo – p. 10

- Russel Caflisch

- Accelerated Simulation for Plasma Kinetics
For RMSE < $\varepsilon$, the complexity now scales like\(^4\)

\[
\text{Cost} = \begin{cases} 
O\left(\varepsilon^{-2}(\log \varepsilon)^2\right) & \text{for Euler-Maruyama} \\
O\left(\varepsilon^{-2}\right) & \text{for Milstein}
\end{cases}
\]

(5)

Notes:

- MLMC-Euler-Maruyama scales better than standard MC
- MLMC-Milstein is even better
- $O\left(\varepsilon^{-2}\right)$ scaling is possible without Milstein, using antithetic sampling method \(^5\)


A Sample Plasma Problem

Rosin, Ricketson, et. al., J Comp Phys 2014

Russel Caflisch
Accelerated Simulation for Plasma Kinetics
Direct Simulation of CR Kinetics
Kinetic simulation of electron-impact excitation/deexcitation and ionization/recombination.\(^6\)

- **Plasma representation**
  - Discrete particles for electron energy distribution \(f(E)\)
  - Continuum densities \(\rho_k\) for atoms at \(k \leq m - 1\) levels of excitation and \(\rho_i\) for ions (Bohr model)

- **Cross-sections**
  - Semi-classical cross-sections for excitation and ionization.
  - Detailed balance yields cross-sections for deexcitation and recombination.

Closely related to work of Hai Le.

\(^6\)Yan et. al., J Comp Phys to appear
Boltzmann Equation

- Electrons

\[ \partial_t f(E) = Q_{IR}^e + Q_{ED}^e \]

- Atomic level \( k \)

\[ \partial_t \rho_k = Q_{IR}^k + Q_{ED}^k \]

- Ions

\[ \partial_t \rho_i = Q_{IR}^i \]

\( Q \) is the collision operator for ionization/recombination (IR) and excitation/deexcitation (ED).
Entropy Inequality

- Entropy $S$ is
  \[ S = -kN \log(N/G) - 1 \]

- $N =$ number density of particles
- $G =$ degeneracy of particles
- $k =$ Boltzmann constant

- Boltzmann $H$-theorem, for $H=-S$, is
  \[ \frac{dH}{dt} \leq 0 \]
  with equality only for equilibrium

- New(?) explicit formula for $S$ in terms of distribution functions.

- Multiple non-Maxwellian equilibria for excitation/deexcitation!
  $H$ theorem is always valid.
Multiscale and singular features are a bottleneck in Monte Carlo simulation

- Many processes
  - $m$ states ($m - 1$ levels + ion)
  - interactions between any two states $k$, $k'$ (including $k = i$)
  - $m(m - 1)/2$ different types of interactions

- Wide range of interaction rates
  - interaction $k \leftrightarrow (k - 1)$ has rate $O(k^6)!$

- Singularity in recombination rate for recombining electron energies $E_1$ and $E_2$

$$r_{rec} = O\left(\frac{1}{\sqrt{E_1 E_2}}\right)$$
Numerical Results

Evolution for ionization/recombination only

- Maxwellian equilibrium as expected
- Similar results if excitation/deexcitation is included
Evolution for ionization/recombination only

- Decrease in $H$ as expected
Numerical Results

Evolution for excitation/deexcitation only, with 2 atomic levels

- Equilibrium is clearly non-Maxwellian
- For 10 levels, equilibrium very close to Maxwellian
Decrease in $H$ as expected, in spite of non-Maxwellian
Summary: Accelerated Methods for Monte Carlo Simulation

- Hybrid method for RGD and Coulomb collisions
- Negative particle method
- Multi-Level Monte Carlo (MLMC)
- CR kinetics