Self-Consistent Langevin Simulation of Coulomb Collisions in Charged-Particle Beams

Ji Qiang, Salman Habib, and Robert D. Ryne
Los Alamos National Laboratory

Work performed under the auspices of the
DOE Grand Challenge in Computational Accelerator Physics, Advanced Computing for 21st Century Accelerator Science and Technology Project, and Los Alamos Accelerator Code Group
using resources at the
Advanced Computing Laboratory and the
National Energy Research Scientific Computing Center

The Fokker-Planck Equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} = -\frac{\partial}{\partial \mathbf{v}} \cdot \mathbf{F_d} f + \frac{1}{2}\frac{\partial^2}{\partial \mathbf{v} \partial \mathbf{v}} : \mathbf{D} f$$

where

$$\begin{aligned} \mathbf{F} &= \mathbf{F}_{ext} + \mathbf{F}_{self} \\ \mathbf{F}_{self} &= -\nabla\phi \\ \nabla^2\phi(\mathbf{r}) &= -\frac{\rho(\mathbf{r})}{\epsilon_0} \end{aligned}$$

and

$$\begin{aligned} \rho(\mathbf{r}) &= \int \mathbf{d^3 v} f(\mathbf{r}, \mathbf{v}) \\ \phi(\mathbf{r}) &= \int G(\mathbf{r}, \mathbf{r}')\rho(\mathbf{r}')d\mathbf{r}' \end{aligned}$$

Here, ϕ is the electric potential, ρ is the charge density, and G is the Green's function of the Poisson's equation.

The Fokker-Planck Equation (Cont'd)

$$
\begin{aligned}
\mathbf{F_d} &= \frac{ne^4}{4\pi\epsilon_0^2 m^2}\lambda\frac{\partial H}{\partial \mathbf{v}} \\
\mathbf{D} &= \frac{ne^4}{4\pi\epsilon_0^2 m^2}\lambda\frac{\partial G}{\partial \mathbf{v}\partial \mathbf{v}} \\
\lambda &= ln(\frac{mv^2\lambda_D}{2e^2}) \\
H &= 2\int \mathbf{d}^3\tilde{\mathbf{v}}\frac{f(\mathbf{r},\tilde{\mathbf{v}})}{|\mathbf{v}-\tilde{\mathbf{v}}|} \\
G &= \int \mathbf{d}^3\tilde{\mathbf{v}} f(\mathbf{r},\tilde{\mathbf{v}})|\mathbf{v}-\tilde{\mathbf{v}}|
\end{aligned}
$$

Methods of Solution

- Direct PDE Solver:
  - Finite Difference
  - Eigenfunction Expansion
- Particle Based Methods:
  - Direct N-Body
  - Monte Carlo (DSMC)
  - Particle-In-Cell (PIC)

The Langevin Equations (Cont'd)

Previous studies:

- Use of velocity-independent Spitzer's dynamical friction
- Assumption of the isotropic distribution of field particles

This talk:

- Self-consistent calculation of dynamic friction and diffusion coefficient tensor from Rosenbluth potential (first principle approach).

The Langevin Equations

$$
\begin{aligned}
\mathbf{r}' &= \mathbf{v}, \\
\mathbf{v}' &= \frac{\mathbf{F}}{m} + \mathbf{F_d} + \mathbf{Q} \cdot \mathbf{\Gamma}(t),
\end{aligned}
$$

where $\mathbf{\Gamma}(t)$ are Gaussian random variables with

$$
\begin{aligned}
\langle \Gamma_i(t) \rangle &= 0, \\
\langle \Gamma_i(t) \Gamma_j(t') \rangle &= \delta_{ij} \delta(t - t').
\end{aligned}
$$

The matrix $\mathbf{Q}$ is related to the diffusion coefficient $\mathbf{D}$ by $D_{ij} = Q_{ik} Q_{jk}$.

The Langevin Equations (Cont'd)

$$(D + (\alpha_1\alpha_2 + \alpha_2\alpha_3 + \alpha_1\alpha_3)I)Q \quad = \quad (\alpha_1 + \alpha_2 + \alpha_3)D + \alpha_1\alpha_2\alpha_3 I$$

where $\alpha_i = \sqrt{\lambda_i}$ for $i = 1, 2, 3$, and λ_i is the eigenvalue of diffusion tensor D, which can be obtained from

$$det(D - \lambda I) \quad = \quad 0$$

The Leap-Frog Algorithm

$$
\begin{aligned}
\mathbf{r}^{i+1} &= \mathbf{r}^{i} + \mathbf{v}^{i+1/2}\Delta t \\
\mathbf{v}^{i+1/2} - \mathbf{v}^{i-1/2} &= \frac{q}{m}E^{i}\Delta t + \frac{q}{m}\frac{(\mathbf{v}^{i+1/2} + \mathbf{v}^{i-1/2})}{2} \times \mathbf{B}^{i}\Delta t \\
&\quad + \Delta\mathbf{v} \qquad (1)
\end{aligned}
$$

where $\mathbf{E}$ and $\mathbf{B}$ are the electric field and magnetic field, and the $\Delta\mathbf{v}$ are the contributions from collisions.

System Kinetic Energy and Momentum Conservation

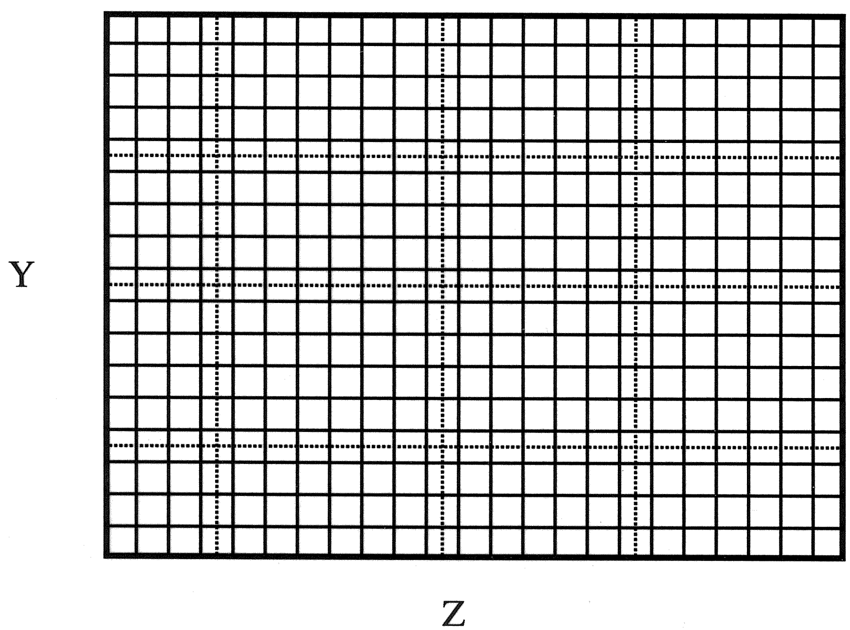
$$\Delta v_i \quad = \quad \gamma_i(\mathbf{F_d}_i \Delta t + \mathbf{Q}_{ij}\sqrt{\Delta t}\mathbf{W}_j + \mu_i)$$

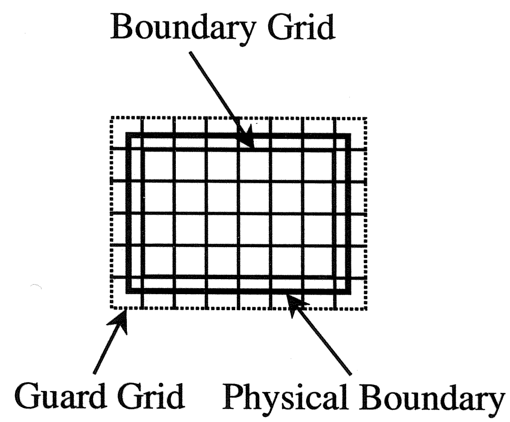
where

$$\begin{aligned}
\mu_i \quad &= \quad -\frac{\Delta t}{M}\sum_{n=1}^{M}\mathbf{F_d}_i^n - \frac{\sqrt{\Delta t}}{M}\sum_{n=1}^{M}\mathbf{Q}_{ij}^n\mathbf{W}_j^n \\
\gamma_i \quad &= \quad -2\frac{\sum_{n=1}^{M}(\sum_{i=1}^{3} v_i^n(\mathbf{F_d}_i^n\Delta t + \mathbf{Q}_{ij}^n\sqrt{\Delta t}\mathbf{W}_j^n))}{\sum_{n=1}^{M}(\sum_{i=1}^{3}(\mathbf{F_d}_i^n\Delta t + \mathbf{Q}_{ij}^n\sqrt{\Delta t}\mathbf{W}_j^n)^2)}
\end{aligned}$$

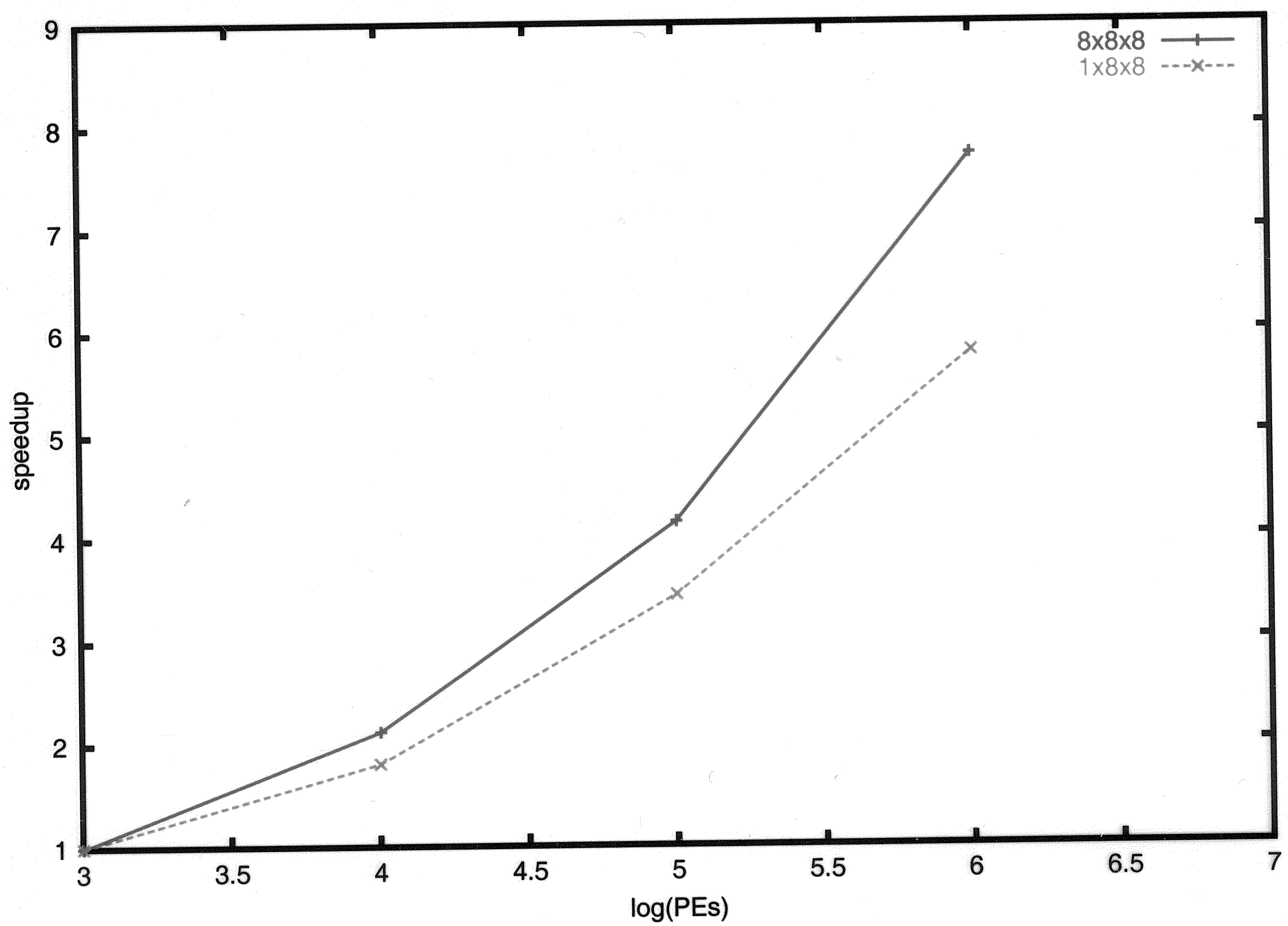
where the **W** are Gaussian random variables with mean zero and standard deviation one.

Two-Dimensional Domain Decomposition

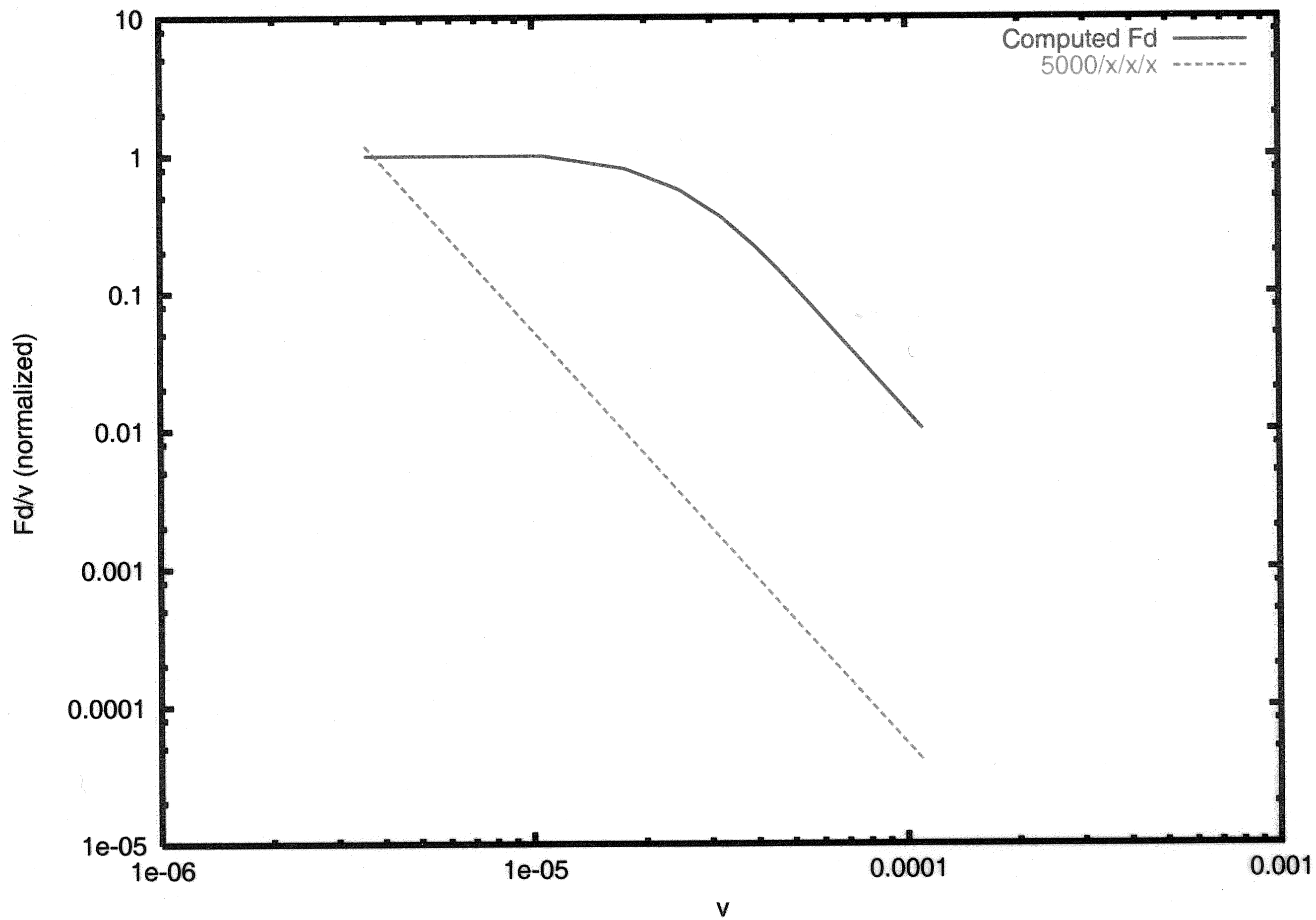




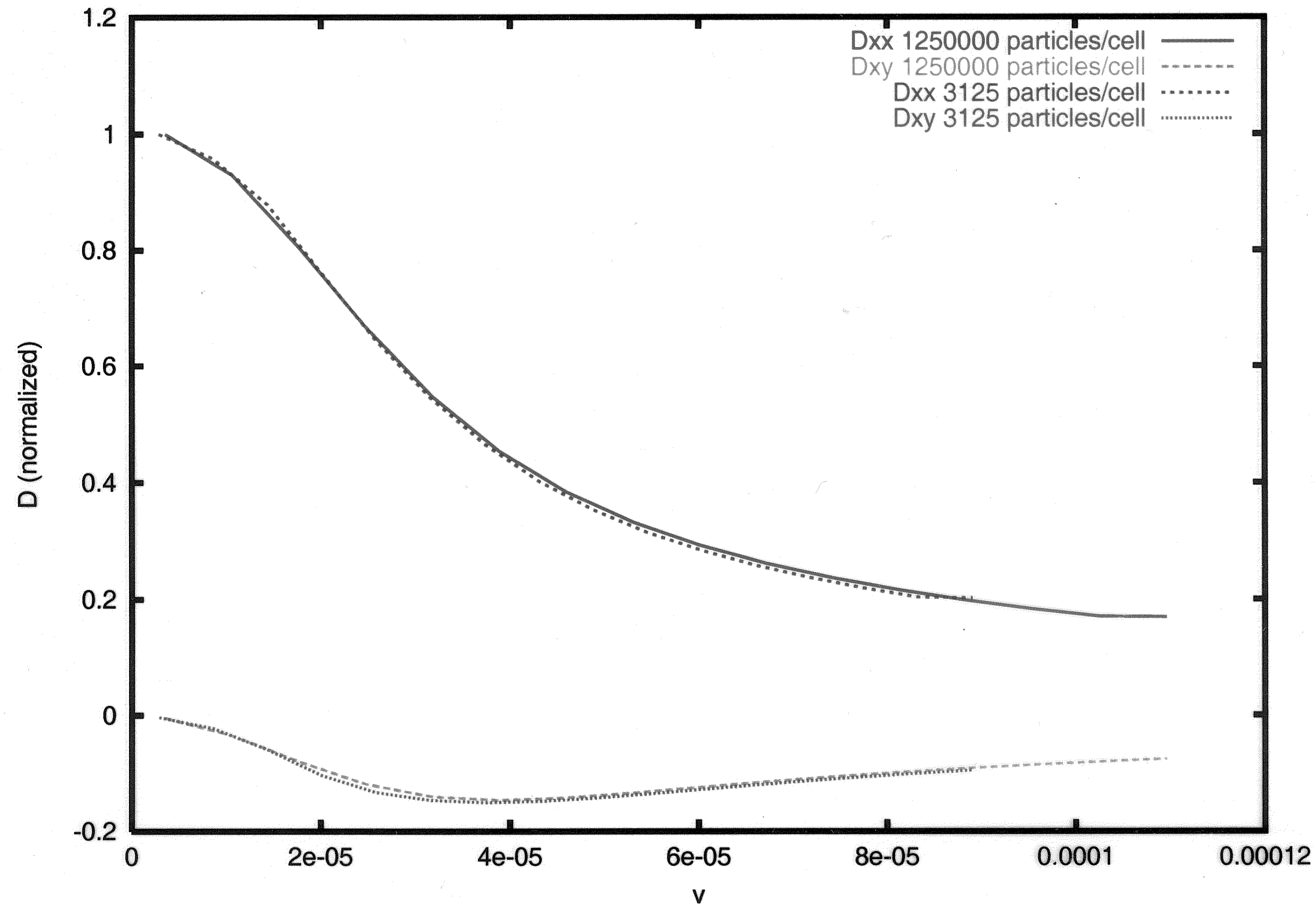
Performance Test II



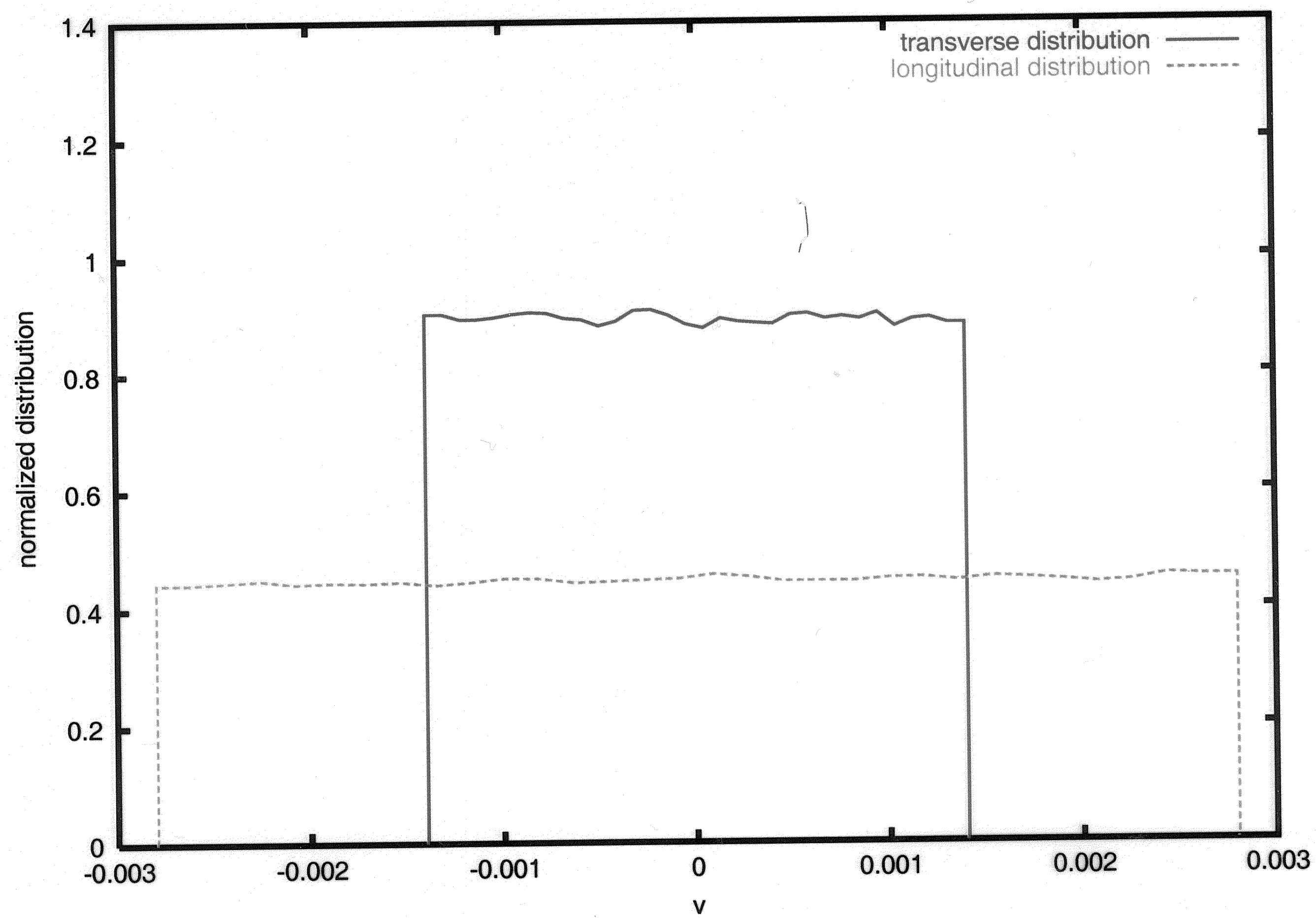
The Asymptotic Behavior of the Dynamic Friction Coefficient for a Maxwellian Distribution



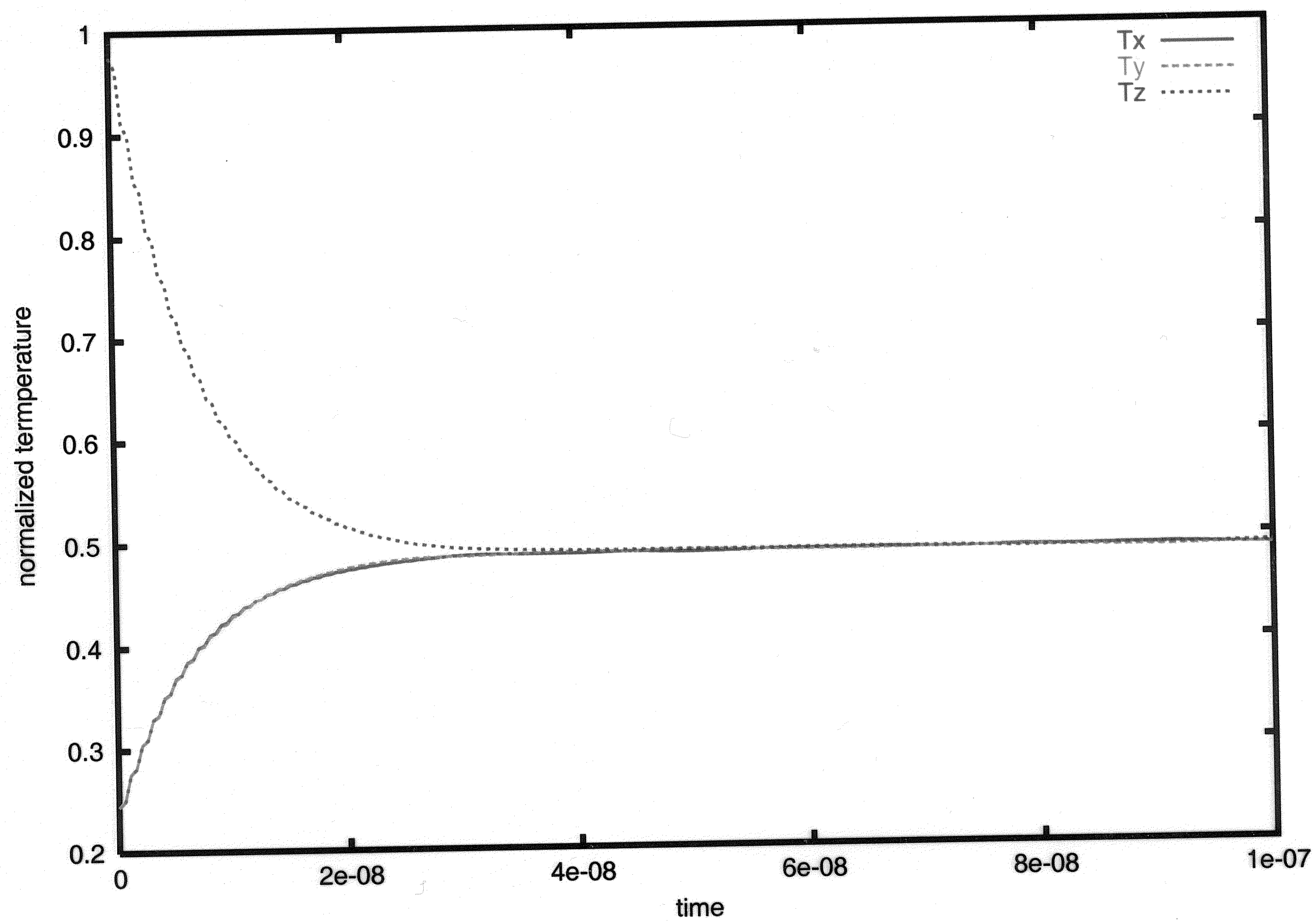
Diagonal and Off-Diagonal Diffusion Coefficients for a Maxwellian Distribution



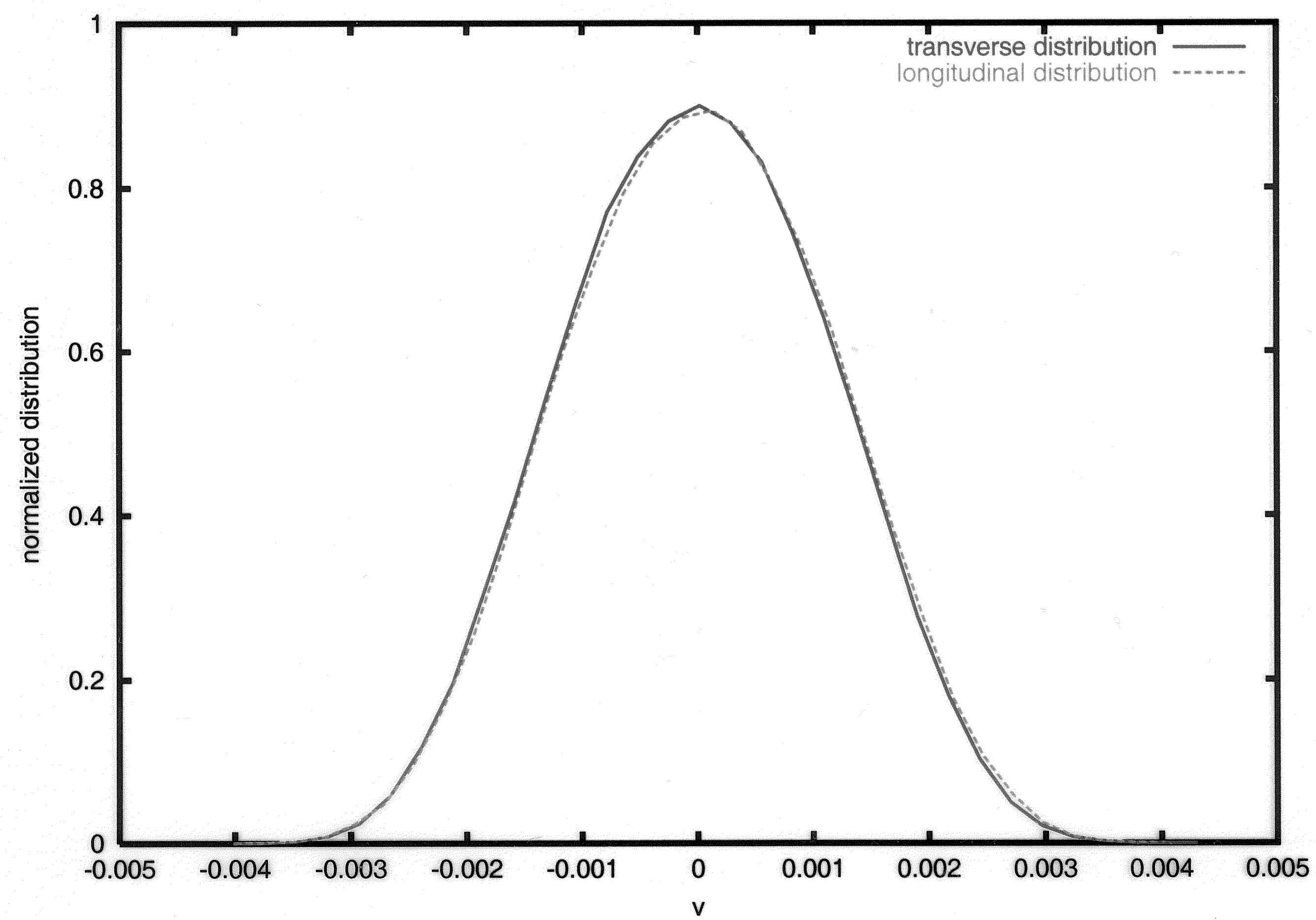
Transverse and Longitudinal Initial Velocity Distributions



Transverse and Longitudinal Temperature as a Function of Time



Transverse and Longitudinal Velocity Distributions after 60 Steps



A Second-Order Stochastic Leap-Frog Algorithm for Multiplicative Noise Brownian Motion

- To be published in *Phys. Rev. E, 2000*.
- Second-order convergence of moments in a finite time interval
- Sampling of only one uniformly distributed random variable per time step
- White and colored noise included

A Second-Order Stochastic Leap-Frog Algorithm for Multiplicative Noise Brownian Motion

$$
\begin{aligned}
\dot{x}_1 &= F_1(x_1, x_2, x_3, x_4, x_5, x_6) + \sigma_{11}(x_2, x_4, x_6)\xi_1(t) \\
\dot{x}_2 &= F_2(x_1) \\
\dot{x}_3 &= F_3(x_1, x_2, x_3, x_4, x_5, x_6) + \sigma_{33}(x_2, x_4, x_6)\xi_3(t) \\
\dot{x}_4 &= F_4(x_3) \\
\dot{x}_5 &= F_5(x_1, x_2, x_3, x_4, x_5, x_6) + \sigma_{55}(x_2, x_4, x_6)\xi_5(t) \\
\dot{x}_6 &= F_6(x_5)
\end{aligned}
$$

Leap-Frog Algorithm for White Multiplicative Noise

$$\bar{D}_i(h) = \bar{x}_i(0) + hF_i(\bar{x}_1^*, \bar{x}_2^*, \bar{x}_3^*, \bar{x}_4^*, \bar{x}_5^*, \bar{x}_6^*); \qquad \{i = 1, 3, 5\}$$

$$\bar{D}_i(h) = \bar{x}_i^* + \frac{1}{2}hF_i\left[x_{i-1} + hF_{i-1}(\bar{x}_1^*, \bar{x}_2^*, \bar{x}_3^*, \bar{x}_4^*, \bar{x}_5^*, \bar{x}_6^*)\right]; \{i = 2, 4, 6\}$$

$$\bar{S}_i(h) = \sigma_{ii}\sqrt{h}W_i(h) + \frac{1}{2}F_{i,k}\sigma_{kk}h^{3/2}\tilde{W}_i(h) + \frac{1}{2}\sigma_{ii,j}F_jh^{3/2}\tilde{W}_i(h) + \frac{1}{4}F_{i,kl}\sigma_{kk}\sigma_{ll}h^2\tilde{W}_i(h)\tilde{W}_i(h); \{i = 1, 3, 5;\ j = 2, 4, 6;\ k, l = 1, 3$$

$$\bar{S}_i(h) = \frac{1}{\sqrt{3}}F_{i,j}\sigma_{jj}h^{3/2}\tilde{W}_j(h) + \frac{1}{4}F_{i,jj}\sigma_{jj}^2h^2\tilde{W}_j(h)\tilde{W}_j(h) \quad \{i = 2, 4, 6;\ j = 1, 3, 5\}$$

$$\bar{x}_i^* = \bar{x}_i(0) + \frac{1}{2}hF_i(\bar{x}_1, \bar{x}_2, \bar{x}_3, \bar{x}_4, \bar{x}_5, \bar{x}_6)\{i = 1, 2, 3, 4, 5, 6\}$$

where $\tilde{W}_i(h)$ is a series of random numbers with the moments

$$\langle\tilde{W}_i(h)\rangle = \langle(\tilde{W}_i(h))^3\rangle = \langle(\tilde{W}_i(h))^5\rangle = 0 \qquad (1)$$

$$\langle(\tilde{W}_i(h))^2\rangle = 1, \quad \langle(\tilde{W}_i(h))^4\rangle = 3. \qquad (2)$$

where

$$\begin{aligned}
\bar{x}_i^* &= \bar{x}_i(0) + \frac{1}{2}h\left[F_i(\bar{x}_1,\bar{x}_2,\bar{x}_3,\bar{x}_4,\bar{x}_5,\bar{x}_6)\right. \\
&\quad \left. +\sigma_{ii}(\bar{x}_2,\bar{x}_4,\bar{x}_6)\xi_i\right]; \qquad \{i=1,3,5\} \\
\bar{x}_i^* &= \bar{x}_i(0) + \frac{1}{2}hF_i(\bar{x}_1,\bar{x}_2,\bar{x}_3,\bar{x}_4,\bar{x}_5,\bar{x}_6); \qquad \{i=2,4,6\} \\
\xi_i^* &= \xi_i(0)\exp(-\frac{1}{2}k_i h); \qquad \{i=1,3,5\}
\end{aligned}$$

$$\tilde{W}_i(h) = \begin{cases} -\sqrt{3}, & R < 1/6 \\ 0, & 1/6 \leq R < 5/6 \\ \sqrt{3}, & 5/6 \leq R \end{cases}$$

where R is a uniformly distributed random number on the interval (0,1).

Leap-Frog Algorithm for Colored Ornstein-Uhlenbeck Multiplicative Noise

$$
\begin{aligned}
\bar{D}_i(h) &= \bar{x}_i(0) + hF_i(\bar{x}_1^*, \bar{x}_2^*, \bar{x}_3^*, \bar{x}_4^*, \bar{x}_5^*, \bar{x}_6^*) + h\sigma_{ii}(\bar{x}_2^*, \bar{x}_4^*, \bar{x}_6^*)\xi_i^*; \\
&\quad \{i = 1, 3, 5\} \\
\bar{D}_i(h) &= \bar{x}_i^* + \frac{1}{2}hF_i\left[\bar{x}_{i-1} + hF_{i-1}(\bar{x}_1^*, \bar{x_2}^*, \bar{x}_3^*, \bar{x_4}^*, \bar{x}_5^*, \bar{x_6}^*)\right. \\
&\quad \left. + h\sigma_{i-1i-1}(\bar{x}_2^*, \bar{x}_4^*, \bar{x}_6^*)\xi_{i-1}^*\right]; \qquad \{i = 2, 4, 6\} \\
\bar{D}_{\xi_i}(h) &= \xi_i(0)\exp(-k_i h); \qquad \{i = 1, 3, 5\} \\
\bar{S}_i(h) &= \frac{1}{\sqrt{3}}\sigma_{ii}(\bar{x}_2, \bar{x}_4, \bar{x}_6)k_i h^{3/2}\tilde{W}_i(h); \qquad \{i = 1, 3, 5\} \\
\bar{S}_i(h) &= 0; \qquad \{i = 2, 4, 6\} \\
\bar{S}_{\xi_i} &= k_i\sqrt{h}\tilde{W}_i(h) - \frac{1}{2}k_i^2 h^{3/2}\tilde{W}_i(h); \qquad \{i = 1, 3, 5\}
\end{aligned}
$$

where

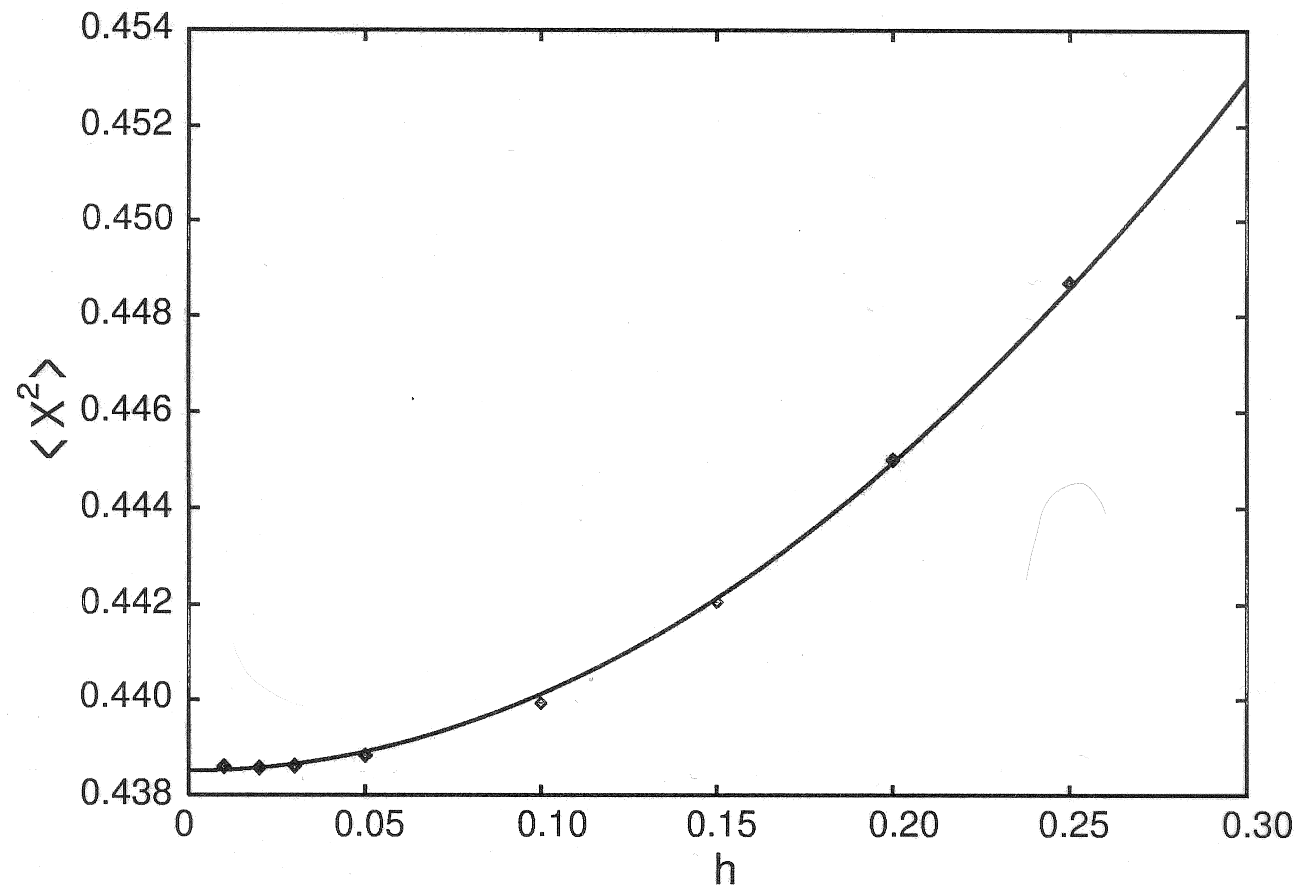
$$
\begin{aligned}
\bar{x}_i^* &= \bar{x}_i(0) + \frac{1}{2}h\left[F_i(\bar{x}_1, \bar{x}_2, \bar{x}_3, \bar{x}_4, \bar{x}_5, \bar{x}_6)\right. \\
&\quad \left. + \sigma_{ii}(\bar{x}_2, \bar{x}_4, \bar{x}_6)\xi_i\right]; \qquad \{i = 1, 3, 5\} \\
\bar{x}_i^* &= \bar{x}_i(0) + \frac{1}{2}hF_i(\bar{x}_1, \bar{x}_2, \bar{x}_3, \bar{x}_4, \bar{x}_5, \bar{x}_6); \qquad \{i = 2, 4, 6\} \\
\xi_i^* &= \xi_i(0)\exp(-\frac{1}{2}k_i h); \qquad \{i = 1, 3, 5\}
\end{aligned}
$$

Numerical Convergence Tests

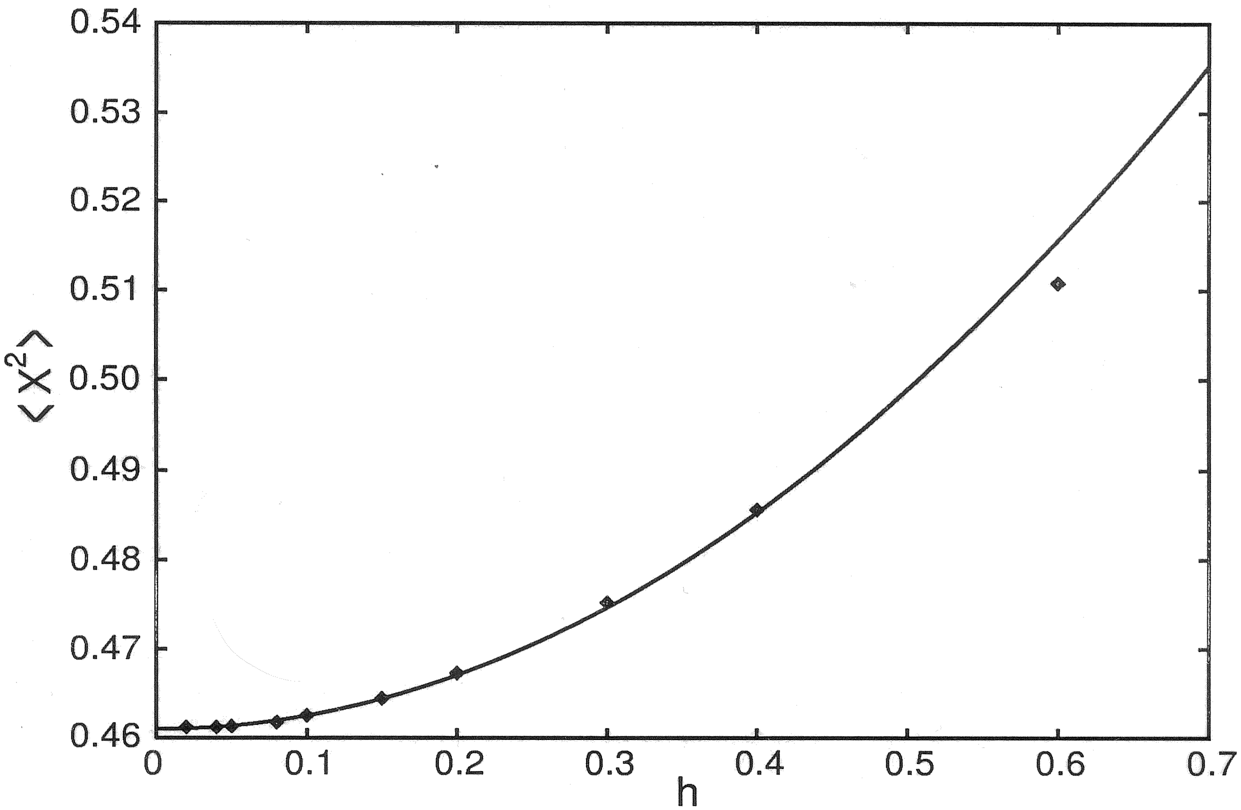
The equations of motion are:

$$\begin{aligned} \dot{p} &= -\gamma p - \eta^2 x - \alpha x \xi(t) \\ \dot{x} &= p \end{aligned}$$

Finite damping ($\gamma = 0.1$) Convergence Test: Colored Ornstein-Uhlenbeck Noise



Finite Damping ($\gamma = 0.1$) Convergence Test: White Gaussian Noise



Comparing Stochastic Leap-Frog and the Heun Algorithm