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# Higher-order Time Integration of Stochastic Differential Equations and Application to Coulomb Collisions


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# Main results

- We have developed a higher (Milstein)-order Coulomb-Langevin scheme
  - improved convergence demonstrated
  - correct mean behavior demonstrated
- A new approach was needed
  - existing approach does not extend easily to higher order
- New method developed for sampling area integral terms
  - simple, accurate, efficient

# Coulomb collisions are important in many plasma applications

- Any sufficiently dense plasma
  - Magnetic fusion (MFE), inertial fusion (ICF), plasma processing, near-earth (or planetary) space plasma
- Long history of study of Coulomb collisions in plasmas
  - Analytical results
    - ★ Landau ‘36-7; Rosenbluth et. al.; ‘57, Trubnikov‘65
  - Monte-Carlo (SDE) methods
    - ★ Langevin (+ field-term) methods - of interest in the present work: Manheimer et. al., ‘97; Lemons et. al., ‘09; Cohen et. al., ‘10
    - ★ Binary-collision methods - used in our hybrid work: Takizuke and Abe ‘77; Nanbu ‘97; Dimits et. al., ‘09
  - Continuum (PDE) methods
    - ★ e.g., Xiong, et. al., ‘08; Abel et. al., ‘08

# Coulomb collisions are long-range, unlike neutral-atomic/molecular collisions

- Dominated by many small-angle scattering “events”
  - large-angle scattering events are subdominant
- Appropriate description is a Fokker-Planck (forward Kolmogorov) equation (Landau, 1936/7 - not a Boltzmann equation):

$$\left.\frac{\partial f_\alpha}{\partial t}\right|_{\mathrm{coll}} = \frac{\partial}{\partial \mathbf{v}} \cdot \left[ \pi q_\alpha^2 L \sum_\beta q_\beta^2 \int d\tau' \left( f_\alpha \frac{\partial f_\beta'}{\partial \mathbf{v}'} - f_\beta' \frac{\partial f_\alpha}{\partial \mathbf{v}} \right) \frac{(u^2 \mathbf{I} - \mathbf{u}\mathbf{u})}{u^3} \right]$$

# The Milstein method is the first in a hierarchy of higher-order methods for SDE's

$$\delta Y^i_{n,j} = a^i(t_{n,j}, \mathbf{Y}_{n,j})\delta t + b^i(t_{n,j}, \mathbf{Y}_{n,j})\delta W^i_{n,j}$$

- $t_{n,j} = t_n + j\delta t$, $t_n = t_0 + n\Delta t$, $\Delta t = N\delta t$
- $\delta W^i_{n,j}$ are independent normal random numbers with variance $\delta t$ .
- $\Delta W \equiv W\left(t_{n+1}\right) - W\left(t_n\right) = \lim_{N\to\infty}\sum_{j=1}^{N}\delta W_{n,j}$ - Wiener increment
- First-order (in $\triangle t$) approximation to $\triangle \boldsymbol{Y}_N \equiv \lim_{N\to\infty}\sum_{k=1}^{N}\delta \boldsymbol{Y}_k$

$$\begin{aligned}
\Delta Y^i_n &= a^i(t_n, \mathbf{Y}_n)\Delta t + b^i(t_n, \mathbf{Y}_n)\Delta W^i_n \\
&+ b^i_{,j}(t_n, \mathbf{Y}_n) b^j(t_n, \mathbf{Y}_n)\int_0^{\Delta t} dW^i(t_n + s)\int_0^{s} dW^j(t_n + \eta) \\
&+ \begin{cases} O\left(\Delta t^{3/2}\right) & -\text{strong} \\ O\left(\Delta t^{2}\right) & -\text{weak}\end{cases} \to \begin{cases} O\left(T\Delta t\right) & -\text{strong} \\ O\left(T\Delta t\right) & -\text{weak}\end{cases}
\end{aligned}$$

# The Milstein method is of interest because it is the first in a hierarchy of higher-order methods for SDE's

- This hierarchy includes schemes with improved (higher-order) weak convergence
- Significantly improves efficiency of multi-(time-)level schemes (Giles '07), which have lower computational complexity for a given overall error than single-level Monte-Carlo schemes.

# Higher-order methods for SDE's have been applied in a variety of fields

- Finance
- Chemical Physics
- See, e.g., Kloeden and Platen. '92
- Almost all published Monte-Carlo treatments of Coulomb collisions have used the low-order Euler-Maruyama method.
  - One exception: Lemons et. al., '09
    - ★ Added higher order (Milstein) term for $v$, but
    - ★ Did not do tests that might have shown a difference
    - ★ Did not include higher order terms for angular scattering

# Approach 1: Apply collisional drag and scattering in a frame aligned with particle velocity

- Manheimer et al, ‘97; Lemons et. al., ‘09; Cohen et. al., ‘10
- Basic underlying equation:

$$
\begin{aligned}
d\boldsymbol{v}(t) &= \left[F_d(v)\,dt + Q_{\shortparallel}(v)\,dW^{\shortparallel}(t)\right]\hat{\boldsymbol{v}}(t) + Q_{\perp}(v)\,d\boldsymbol{W}(t), \\
d\boldsymbol{W}^{\perp}(t) &= dW^{x}(t)\,\hat{\boldsymbol{x}}(t) + dW^{y}(t)\,\hat{\boldsymbol{y}}(t).
\end{aligned}
$$

- Here
  - interpret in Ito sense
  - $\triangle\boldsymbol{v}(t) \equiv \int_t^{t+\Delta t} d\boldsymbol{v}(t)$
  - $(\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}, \hat{\boldsymbol{v}})$ - frame aligned with $\boldsymbol{v}$
    - e.g., $\hat{\boldsymbol{x}} = \hat{\boldsymbol{y}}_0 \times \hat{\boldsymbol{v}} / |\hat{\boldsymbol{y}}_0 \times \hat{\boldsymbol{v}}|$, $\hat{\boldsymbol{y}} = \hat{\boldsymbol{v}} \times \hat{\boldsymbol{x}}$

# Milstein-order velocity step for Approach 1

- First-order accurate (in $\triangle t$) approximation to $\triangle \boldsymbol{v}(t) \equiv \int_t^{t+\Delta t} d\boldsymbol{v}(t)$

$$
\begin{aligned}
\triangle \boldsymbol{v} \;=\;& Q_{\shortparallel 0}\, \Delta t^{1/2} \triangle W^{\shortparallel}\, \hat{\boldsymbol{v}}_0 + Q_{\perp 0}\, \Delta t^{1/2} \left(\triangle W^{x}\, \hat{\boldsymbol{x}}_0 + \triangle W^{y}\, \hat{\boldsymbol{y}}_0\right) \\
+\;& \left\{ \triangle t\, F_d\left(v_0\right) + \frac{1}{2} Q_{\shortparallel 0} Q'_{\shortparallel 0}\, \Delta t \left( \left[\triangle W^{\shortparallel}\right]^2 - 1 \right) \right. \\
-\;& \left. \frac{Q_{\perp 0}^2}{2 v_0}\, \Delta t \left[ \left( \left[\triangle W^{x}\right]^2 - 1 \right) + \left( \left[\triangle W^{y}\right]^2 - 1 \right) \right] \right\} \hat{\boldsymbol{v}}_0 \\
+\;& Q_{\shortparallel 0} Q'_{\perp 0}\, \Delta t \left[ A^{x \shortparallel} \hat{\boldsymbol{x}}_0 + A^{y \shortparallel} \hat{\boldsymbol{y}}_0 \right] + O\left( \triangle t^{3/2} \right)
\end{aligned}
$$

- After applying $\triangle \boldsymbol{v}$, to get new $\boldsymbol{v}_{0\,\mathrm{new}} \equiv \boldsymbol{v}_{0\,\mathrm{old}} + \Delta \boldsymbol{v}$, apply next $\triangle \boldsymbol{v}$ using a frame aligned with $\boldsymbol{v}_{0\,\mathrm{new}}$

# Several possible choices for other unit vectors

1. Second vector along line of constant longitude in lab frame

$$\begin{aligned} \hat{\boldsymbol{x}}_0 &= \hat{\boldsymbol{\theta}}_{\rm lab} \\ \hat{\boldsymbol{y}}_0 &= \hat{\boldsymbol{v}}_0 \times \hat{\boldsymbol{x}}_0 \end{aligned}$$

2. Second vector othogogonal to fixed plane

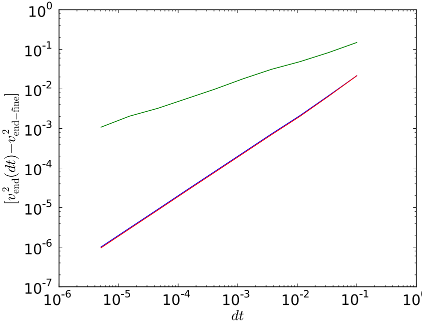
$$\begin{aligned} \hat{\boldsymbol{x}}_0 &= \hat{\boldsymbol{y}}_{\rm lab} \times \hat{\boldsymbol{v}}_0 / \left| \hat{\boldsymbol{y}}_{\rm lab} \times \hat{\boldsymbol{v}}_0 \right| \\ \hat{\boldsymbol{y}}_0 &= \hat{\boldsymbol{v}}_0 \times \hat{\boldsymbol{x}}_0 \end{aligned}$$

3. Rotate unit vector system as a rigid body about the single axis that gives the change in $\hat{\boldsymbol{v}}_0$

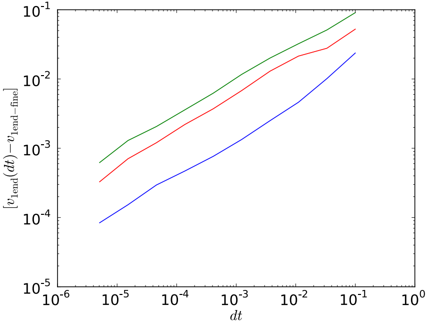
# Approach 1 achieves $O\left(\triangle t\right)$ strong convergence for $v$, but not for angular component of the evolution

- 400 realizations; time step range = $3^{10}$; end time $\nu\left(v_{\rm th}\right)t_{\rm end} = 0.1$
- Green-Euler, red-Milstein fixed-plane, blue-Milstein rigid rot.

$$\left|v^2_{\rm end}(dt) - v^2_{\rm end-fine}\right|$$




$$\left|v^x(dt) - v^x_{\rm fine}\right|$$



# (better) Approach 2: formulate whole problem as SDE's for spherical coordinates wrt a fixed (lab.) frame

- Coordinates: $v$, $\mu = \cos\theta$, $\phi$; $\theta =$ polar angle, $\phi =$ azimuthal angle
- From Rosenbluth et. al., '57,

$$\frac{1}{\Gamma_{tf}}\left(\frac{\partial f_t}{\partial t}\right)_c = -\frac{1}{v^2}\frac{\partial}{\partial v}\left[\left(v^2\frac{\partial h}{\partial v}+\frac{\partial g}{\partial v}\right)f_t\right]+\frac{1}{2v^2}\frac{\partial^2}{\partial v^2}\left(v^2\frac{\partial^2 g}{\partial v^2}f_t\right) + \frac{1}{2v^3}\frac{\partial g}{\partial v}\left\{\frac{\partial}{\partial \mu}\left[\left(1-\mu^2\right)\frac{\partial f_t}{\partial \mu}\right]+\frac{1}{\left(1-\mu^2\right)}\frac{\partial^2 f_t}{\partial \phi^2}\right\}.$$

$$\Gamma_{tf} = \frac{4\pi q_t^2 q_f^2 \lambda}{m_t^2}.$$

- For a Maxwellian field-particle plasma, have analytical expressions for $g\left(v\right)$ and $h\left(v\right)$ (Trubnikov, '65).

# Coulomb test-particle problem as SDE's for spherical coordinates wrt a fixed frame

- Write as Ito form drag-diffusion (forward Kolmogorov) equation:

$$\left(\frac{\partial \hat{f}_t}{\partial \hat{t}}\right)_c = -\frac{\partial}{\partial v}\left[F_d(v)\,\hat{f}_t\right] + \frac{\partial^2}{\partial v^2}\left[D_v(v)\,\hat{f}_t\right] + \frac{\partial}{\partial \mu}\left[2D_a(v)\mu\,\hat{f}_t\right]$$
$$+\frac{\partial^2}{\partial \mu^2}\left[D_a(v)\left(1-\mu^2\right)\,\hat{f}_t\right] + \frac{\partial^2}{\partial \phi^2}\left[\frac{D_a(v)}{(1-\mu^2)}\,\hat{f}_t\right],$$

where $\hat{f}_t = 2\pi v^2 f_t$

- Corresponding Ito-Langevin equations:

$$\begin{aligned} dv\,(t) &= F_d\,(v)\,dt + \sqrt{2D_v(v)}dW_v\,(t)\,, \\ d\mu\,(t) &= -2D_a(v)\mu dt + \sqrt{2D_a(v)\left(1-\mu^2\right)}dW_\mu\,(t)\,, \\ d\phi\,(t) &= \sqrt{\frac{2D_a(v)}{(1-\mu^2)}}dW_\phi\,(t)\,. \end{aligned}$$

# Milstein scheme for Coulomb test-particle problem

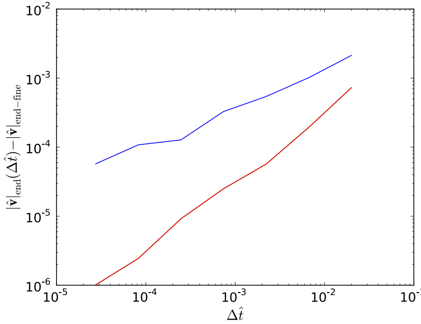
$$
\begin{aligned}
\Delta v &= F_{d0}\Delta t + \sqrt{2D_{v0}}\Delta W_v + \kappa_{\mathrm{M}} D'_{v0}\frac{1}{2}\left(\Delta W_v^2 - \Delta t\right), \\
\Delta\mu &= -2D_{a0}\mu_0\Delta t + \sqrt{2D_{a0}\left(1-\mu_0^2\right)}\Delta W_\mu, \\
&\quad +\kappa_{\mathrm{M}}\left[-2D_{a0}\mu_0\frac{1}{2}\left(\Delta W_\mu^2 - \Delta t\right) + \sqrt{\frac{D_{v0}}{D_{a0}}}\sqrt{\left(1-\mu_0^2\right)}D'_{a0}A_{v\mu}\right], \\
\Delta\phi &= \sqrt{\frac{2D_a(v)}{1-\mu_0^2}}\Delta W_\phi + \kappa_{\mathrm{M}}\left[\sqrt{\frac{D_{v0}}{D_{a0}}}\frac{D'_{a0}}{\sqrt{1-\mu_0^2}}A_{v\phi} + \frac{2D_{a0}\mu_0}{1-\mu_0^2}A_{\mu\phi}\right],
\end{aligned}
$$

$$
\begin{aligned}
\Delta\psi &= \psi\left(t_{i+1}\right) - \psi\left(t_i\right), \\
\psi_0 &= \psi\left(t_i\right), \\
A_{kl} &= \int_{t_i}^{t_{i+1}} dW_l\left(s\right)\int_{t_i}^{s} dW_k\left(\xi\right),
\end{aligned}
$$

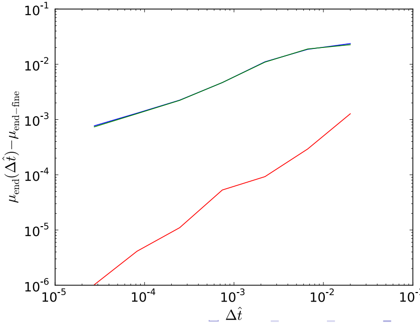
# New approach achieves $O(\triangle t)$ strong convergence for $v$ and for angular component

- $v$ evolution unaffected by angular evolution, and $\therefore$ by area terms
- Angular evolution has poor convergence without area terms
- 16 realizations; time step range = $3^8$; end time $\nu(v_{\rm th})\, t_{\rm end} = 0.1$
- Blue-Euler, Green-Milstein diagonal, Red-full Milstein

$$||v_{\rm end}(\Delta t)| - |v_{\rm end-fine}||$$



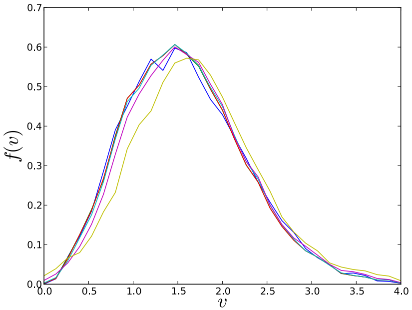

$$|\mu_{\rm end}(\Delta t) - \mu_{\rm end-fine}|$$

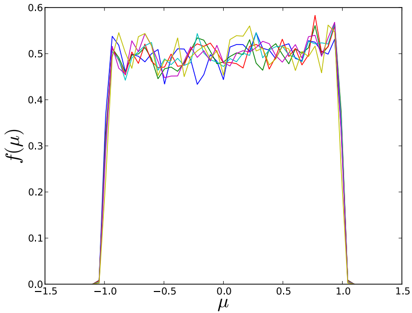


# New approach gives correct dependences for velocity-space density functions (“distributions”)

- Blue - initial; other curves at $t_{\text{end}}$; yellow - coarsest $\Delta t$
- 10000 particles; end time $\nu\left(v_{\text{th}}\right)t_{\text{end}} = 10$; $\Delta / t_{\text{end}} = 3^{-4}, 3^{-5}, 3^{-6}, 3^{-7}$

$f\left(v\right)$ $\qquad$ $f\left(\mu\right)$



# Theory and numerical implementations exist for the sampling of the stochastic integral terms

$$\int_0^{\Delta t} dW^i(t_n+s)\int_0^s dW^j(t_n+\eta) = \begin{cases} \frac{1}{2}\left[\left(\Delta W_n^i\right)^2 - \Delta t\right], & i=j \\ \frac{1}{2}\left[\Delta W_n^i \Delta W_n^j + L_n^{i,j}\right], & i\neq j \end{cases}$$

- Levy, '51

$$\begin{aligned} P_{cL}\left(L_n^{i,j}|\Delta W_n^i, \Delta W_n^j\right) &= \hat{P}_{cL}\left(L_n^{i,j}|R_n^{i,j}\right) \\ r_n^{i,j} &= \sqrt{\left(\Delta W_n^i\right)^2 + \left(\Delta W_n^j\right)^2} \end{aligned}$$

$$\begin{aligned} \phi_{cL}(k|R) &\equiv \langle \exp(-ikL)\rangle|_R \\ &= \frac{k/2}{\sinh(k/2)} \exp\left\{\frac{R^2}{2}\left[1 - \frac{(k/2)\cosh(k/2)}{\sinh(k/2)}\right]\right\}. \end{aligned}$$

# We have developed a simple accurate method for sampling area integrals

- Existing methods
  - Interpolation from 2D table based on Levy's results (Gaines and Lyons '94)
    - accurate and efficient
    - somewhat involved
    - challenging for conditional sampling - adaptive integration
  - Discrete approximations (Clark and Cameron '80; Kloeden and Platen '92; Gaines and Lyons '97)
    - simple to implement
    - straightforward for adaptive integration
    - expensive for good accuracy (many random numbers per $L$ sample)
- Our method is a simplification of that of Gaines and Lyons '94
  - based on an accurate approximation to Levy's PDF
  - can implement with 1D tables or analytical functions
  - can be used to significantly reduce memory and computation requirements for conditional sampling

# Our approximation for the Levy-area PDF is based on approximate shape invariance of $P_{cL}(L|R)$

- Approximation to conditional PDF of $L$ given $R$

$$
P_{cL}(L|R) \approx P_{\mathrm{c-an}\,L}(L|R) = s(R)\,P_{0L}(s(R)\,L)
$$

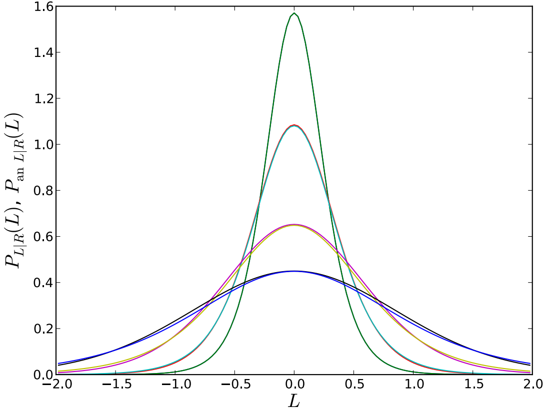
$$
\begin{aligned}
P_{0L}(L) &\equiv P_{cL}(L|R=0) = \frac{\pi}{2}\frac{1}{\cosh^2(L/2)} \quad - \quad \text{exact} \\
s(R) &= P_{cL}(L=0|R)
\end{aligned}
$$

- Can calculate $s(R)$ from 1D table or analytical fit
- Resulting algorithm for sampling $L$

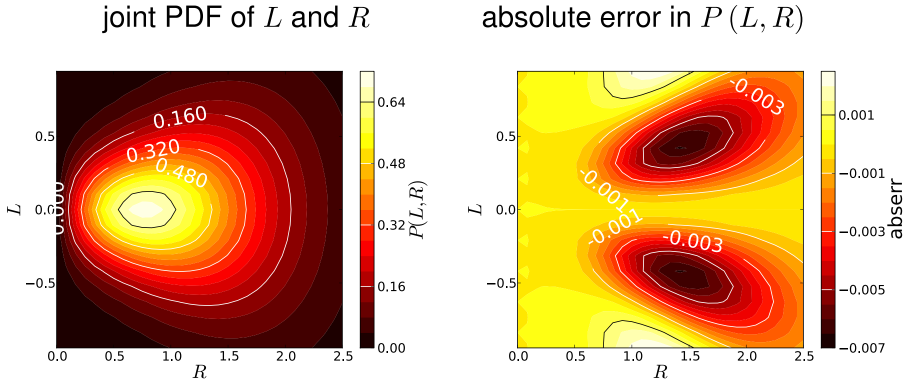
$$
L_R(R) = \frac{s(R)}{2\pi}\log\left(\frac{u}{1-u}\right).
$$

# Our approximation for the Levy-area PDF is accurate to $\sim 1\%$

Exact and approximate conditional PDF's
of $L$ given $R$ vs. $L$ for $R = 0,\ 1,\ 2,\ 3$



# Our approximation for the Levy-area PDF is accurate to $\sim 1\%$



# For strong convergence studies, Wiener increments and area integrals must be compounded

- Need to calculate trajectories representing a given underlying realization with different $\Delta t$
- Compounding is also needed for multilevel (Giles) schemes
- Compounding for Wiener increments: given $\delta_j W \equiv \int_{t_{j-1}}^{t_j} dW(s)$, where $t_j = t_{j-1} + \delta t$, and $\Delta t = n\delta t$

$$\Delta W \equiv \int_0^{\Delta t} dW(s) = \sum_{j=1}^{n} \delta_j W.$$

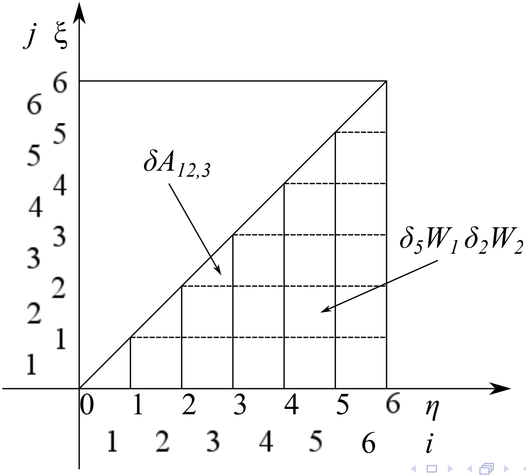
- Compounding area integrals:

$$\delta A_{12j} \equiv \int_{t_{j-1}}^{t_j} dW_1(\eta) \int_{t_{j-1}}^{\eta} dW_2(\xi),$$

$$\Delta A_{12} \equiv \int_0^{\Delta t} dW_1(\eta) \int_0^{\eta} dW_2(\xi),$$

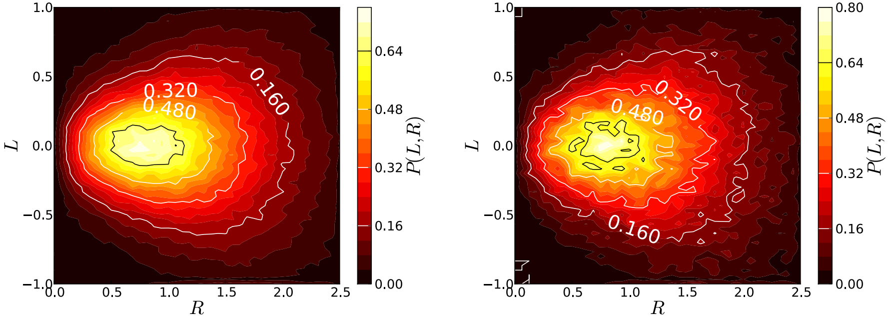
# Compounding of area integrals

$$\Delta A_{12} = \sum_{i=2}^{n} \delta_i W_1 \left( \sum_{j=1}^{i-1} \delta_j W_2 + \delta A_{12,j} \right) .$$



# Our sampling and compounding algorithms and implementations work

PDF for $9 \times 10^4$ samples | compounded by factor of 5




- Strong scaling results for 2D Milstein (e.g., above collision results) provide a demonstration

# Conditional sampling is needed for (time-) adaptive SDE integration

- Sample finer triplets $(\delta_j W_1, \delta_j W_2, \delta_j A_{12})$ given the coarser ones $(\Delta W_1, \Delta W_2, \Delta A_{12})$
- Reverse of compounding
- Existing methods are based on discrete representations
  - expensive because many (pseudo)random numbers needed per sample
- Direct conditional sampling can be done
  - construct $P_c\left(\delta L|\delta R, \Delta L, \Delta R\right)$ using Levy's result for $P_{cL}\left(L|R\right)$
  - store as 4D table
  - interpolate
- Our approximation $P_{\mathrm{c-an}\,L}\left(L|R\right) = s\left(R\right) P_{0L}\left(s\left(R\right) L\right)$ reduces dimensionality of conditional sampling PDF to 3
  - much more manageable memory requirement

# Summary

- We have developed a higher (Milstein)-order Coulomb-Langevin scheme
  - improved convergence demonstrated
  - correct mean behavior demonstrated
- A new approach was needed
  - existing approach does not extend easily to higher order
- New method developed for sampling area integral terms
  - simple, accurate, efficient
  - implemented (along with compounding)
- Future work in this direction
  - higher-order weak schemes
  - implement Giles' multilevel scheme
  - higher order adaptive SDE integrator

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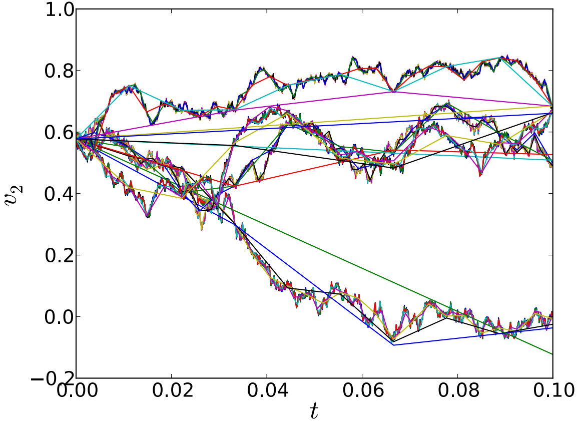
# Strong convergence results

- Convergence of trajectories (e.g., $v$ at a given time) as $\triangle t \to 0$.

4 trajectories compted with different time steps



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