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

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Presented at the IPAM Workshop on Mathematical and Computer Science Approaches to High Energy Density Physics, Univerity of California, Los Angeles CA, May 7, 2012
Work performed for U.S. DOE by LLNL under Contract DE-AC52-07NA27344, and by UCLA under grant DE-FG02-05ER25710

Main results

- We have developed a higher (Milstein)-order Coulomb-Langevin scheme
  - improved convergence demonstrated
  - correct mean behavior demonstrated
- A different approach was needed
  - recent Monte-Carlo approaches do not extend easily to higher order
- New method developed for sampling area integral terms
  - simple, accurate, efficient
- The method is being implemented as part of a multi-time-level scheme

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: Painter, Dettrick, ‘93, ‘99, 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 Euler(-Maruyama) method is the lowest in a hierarchy of methods for SDE's

$$Y^i_{n,j+1} - Y^i_{n,j} = \delta Y^i_{n,j} = a^i(t_{n,j}, \mathbf{Y}_{n,j})\delta t + b^i(t_{n,j}, \mathbf{Y}_{n,j})\delta W^i_{n,j}$$

- $t_{n,j} = t_n + j\delta t$, $t_n = t_0 + n\Delta t$, $\Delta t = N\delta t$
- $\delta W^i_{n,j}$ are independent normal random numbers with variance δt .
- Time discretization and limit: $\triangle \boldsymbol{Y}_N \equiv \lim_{N\to\infty} \sum_{k=1}^{N} \delta \boldsymbol{Y}_k$
  - $\Delta W \equiv W(t_{n+1}) - W(t_n) = \lim_{N\to\infty} \sum_{j=1}^{N} \delta W_{n,j}$
- Euler method:

$$\begin{aligned} \Delta Y^i_n &= a^i(t_n, \mathbf{Y}_n)\Delta t + b^i(t_n, \mathbf{Y}_n)\Delta W^i_n \\ &+ \begin{cases} O(\Delta t) & -\text{ strong} \\ O(\Delta t^2) & -\text{ weak} \end{cases} \rightarrow \begin{cases} O\left(\sqrt{T\Delta t}\right) & -\text{ strong} \\ O(T\Delta t) & -\text{ weak} \end{cases} \end{aligned}$$

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

$$Y^i_{n,j+1} - Y^i_{n,j} = \delta Y^i_{n,j} = a^i(t_{n,j}, \mathbf{Y}_{n,j})\delta t + b^i(t_{n,j}, \mathbf{Y}_{n,j})\delta W^i_{n,j}$$

- $t_{n,j} = t_n + j\delta t$, $t_n = t_0 + n\Delta t$, $\Delta t = N\delta t$
- $\delta W^i_{n,j}$ are independent normal random numbers with variance δt .
- Time discretization and limit: $\triangle \boldsymbol{Y}_N \equiv \lim_{N\to\infty} \sum_{k=1}^{N} \delta \boldsymbol{Y}_k$
  - $\Delta W \equiv W(t_{n+1}) - W(t_n) = \lim_{N\to\infty} \sum_{j=1}^{N} \delta W_{n,j}$
- Milstein method:

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

The Milstein method is of interest because it is represents a path to improved efficiency for Monte-Carlo methods

- The hierarchy of higher order schemes includes methods with improved weak convergence
- Significantly improves efficiency of multi-(time-)level schemes (Giles '07), which have lower computational complexity (cost) C for a given overall error than single-level Monte-Carlo schemes.
- Multi-level Milstein is optimal among MC schemes
  - Given rms error ϵ (MSE=ϵ^2), for MC integration up to a given time
    - ★ $C = O\left(\epsilon^{-3}\right)$ - single-level Euler-Maruyama
    - ★ $C = O\left(\epsilon^{-(2+1/n)}\right)$ - single-level, $O\left(\Delta t^n\right)$ weak MC
    - ★ $C = O\left(\epsilon^{-2}\left[\log\epsilon\right]^2\right)$ - multi-level, Euler
    - ★ $C = O\left(\epsilon^{-2}\right)$ - multi-level, Milstein

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

- Finance
- Chemical Physics
- See, e.g., Kloeden and Platen. '92
- Most all published Monte-Carlo treatments of Coulomb collisions have used the lowest-order Euler-Maruyama method.
- Exceptions:
  - Painter '93; Dettrick, H. J. Gardner and S. L. Painter '99
    - second-order weak scheme
  - Lemons et. al., '09,
    - Added higher order (Milstein) term for v, but not for angular scattering part of evolution
    - Did not do tests that might have shown a difference

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:

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

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

Milstein-order velocity step for Approach 1

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

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

- 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

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

2. Second vector othogogonal to fixed plane

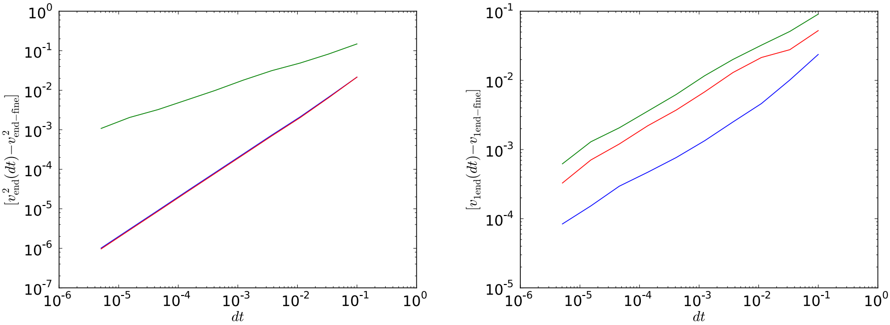
$$
\begin{aligned}
\hat{\boldsymbol{x}}_0 &= \hat{\boldsymbol{y}}_{\text{lab}} \times \hat{\boldsymbol{v}}_0 / \left| \hat{\boldsymbol{y}}_{\text{lab}} \times \hat{\boldsymbol{v}}_0 \right| \\
\hat{\boldsymbol{y}}_0 &= \hat{\boldsymbol{v}}_0 \times \hat{\boldsymbol{x}}_0
\end{aligned}
$$

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 $O(\triangle t)$ strong convergence for v, but not for angular component of the evolution

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

$$\left|v^2_{\text{end}}(dt) - v^2_{\text{end}-\text{fine}}\right| \qquad \left|v^x(dt) - v^x_{\text{fine}}\right|$$



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

- Coordinates: v, $\mu = \cos\theta$, ϕ; $\theta =$ 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

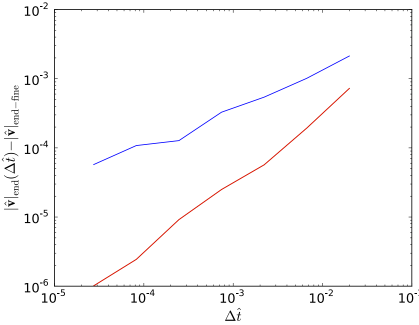
$$
\begin{aligned}
\Delta v &= F_{d0}\Delta t + \sqrt{2D_{v0}}\Delta W_v + \kappa_{\mathrm{M}} D'_{v0}\frac{1}{2}\left(\Delta W_v^2 - \Delta t\right), \\
\Delta \mu &= -2D_{a0}\mu_0\Delta t + \sqrt{2D_{a0}\left(1-\mu_0^2\right)}\Delta W_\mu, \\
&\quad + \kappa_{\mathrm{M}}\left[-2D_{a0}\mu_0\frac{1}{2}\left(\Delta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

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

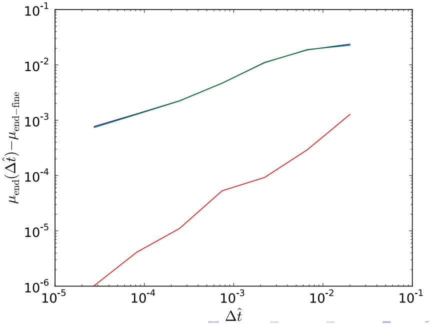
Approach 2 achieves $O(\triangle t)$ strong convergence for v and for angular component

- 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 $\nu(v_{\text{th}})\, t_{\text{end}} = 0.1$
- Blue-Euler, Green-Milstein diagonal, Red-full Milstein

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



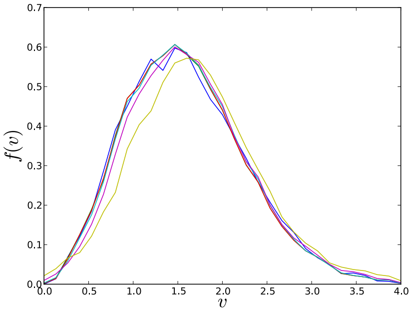
$$|\mu_{\text{end}}(\Delta t) - \mu_{\text{end-fine}}|$$

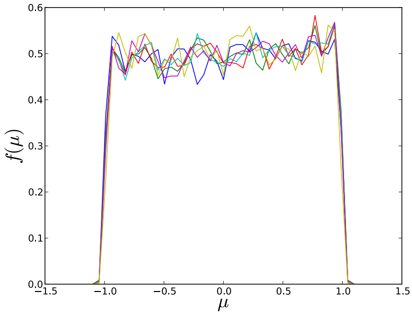


Approach 2 gives correct dependences for velocity-space density functions (“distributions”)

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

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





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

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

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

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

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

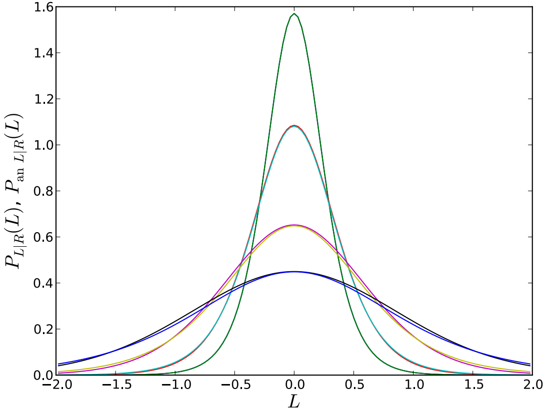
$$\begin{aligned} P_{0L}(L) &\equiv P_{cL}(L|R=0) = \frac{\pi}{2}\frac{1}{\cosh^2(L/2)} \quad - \quad \text{exact} \\ s(R) &= P_{cL}(L=0|R) \end{aligned}$$

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

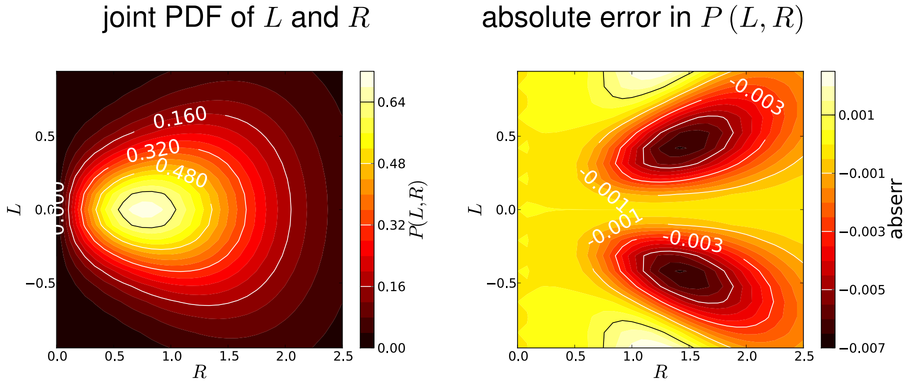
$$L_R(R) = \frac{s(R)}{2\pi}\log\left(\frac{u}{1-u}\right).$$

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 Δt
- 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 $\Delta t = n\delta t$

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

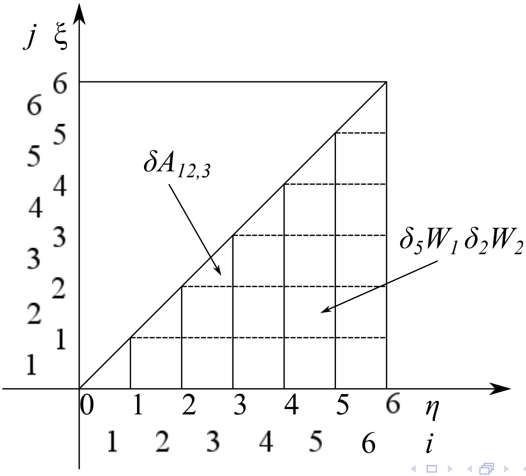
- Compounding area integrals:

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

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

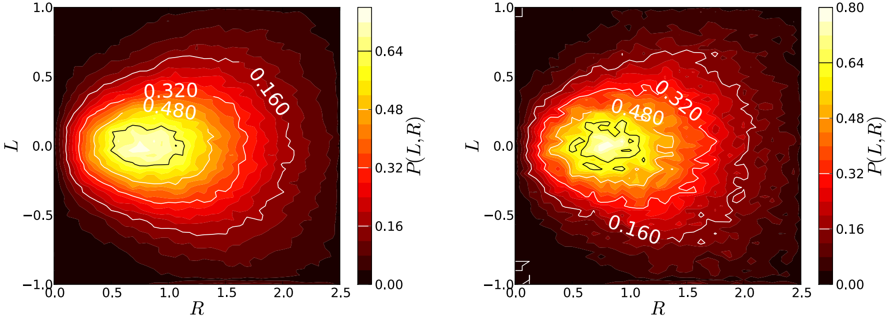
Compounding of area integrals

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



Our sampling and compounding algorithms and implementations work

PDF for 9×10^4 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

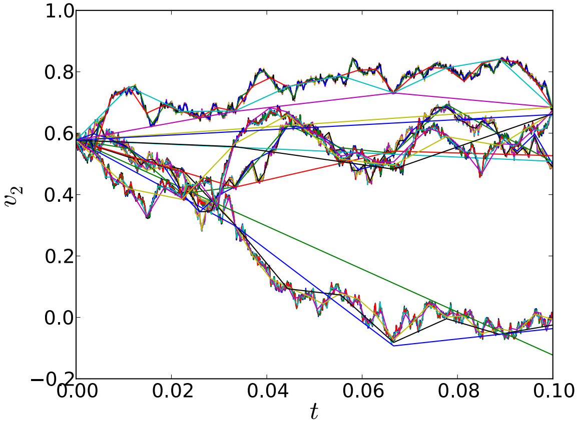
- We have developed a higher (Milstein)-order Coulomb-Langevin scheme
  - improved convergence demonstrated
  - correct mean behavior demonstrated
- A new approach was needed
  - existing approach does not extend easily to higher order
- New method developed for sampling area integral terms
  - simple,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

backup slides

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



Giles' multi-level Monte-Carlo schemes

- Given want to construct the most efficient estimator Θ with a given error ϵ of an ensemble average $\langle P[\mathbf{Y}]\rangle$ of some (generally nonlinear) functional of $\mathbf{Y}(t)$
  - simplest example $\langle P(\mathbf{Y}(T))\rangle$
  - more generally, P can depend on history
- Use, e.g., $\Theta(P[\mathbf{Y}]) = \sum_{l=0}^{L} S_l[\mathbf{Y}]$ different weightings also possible
- $S_l[\mathbf{Y}] = \frac{1}{N_l}\sum_{j=1}^{N_l} \Delta_l P[\mathbf{Y}_j]$
- Δ_l is a difference between computations using the same underlying trajectorydone using two successive time step levels $k = l-1, l$ $\Delta_k t = T.M^{-k}$
- The underlying trajectories used for the differences for different l are independent

Why are Giles' multi-level Monte-Carlo schemes efficient?

- $\mathrm{MSE} = \mathrm{bias}^2 + \mathrm{variance}$
  - bias is the part that depends on time step only
  - variance is the part that depends on the quality of the statistical sampling
- Optimal cost achieved when $\mathrm{bias}^2 \approx \mathrm{variance}$
- bias is determined by finest time step used (and weak order of underlying scheme)
- variance is determined mainly by the number of particles used
- Multilevel schemes achieve optimal efficiency by using more particles at coarser time levels
  - this minimizes variance
  - higher difference terms
    - ★ reduce bias error
    - ★ can be computed with fewer particles

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