Exactly Energy-Momentum-Conserving SDE and Algorithms for Nonlinear Landau-Fokker-Planck Equation

Yichen Fu[1], Justin R. Angus[1], Hong Qin[2], and Vasily I. Geyko[1]

1. Lawrence Livermore National Lab, Livermore, CA 94550
2. Princeton Plasma Physics Lab, Princeton University, Princeton, NJ 08543

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Outline

- Coulomb collisions: Fokker-Planck and Langevin approaches

- Restoring conservation laws in SDEs
  - Physical intuition
  - Mathematical derivation
  - Proof of conservation laws
  - From Itô to Stratonovich

- Exactly conservative numerical algorithms
  - Numerical algorithms for Coulomb collisions
  - Exactly conservative algorithm
  - Benchmark in relaxation processes
  - Complexity reduction

- Conclusions and discussions

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Coulomb collisions: the Fokker-Planck approach

- Collisional processes in fully ionized, weakly coupled plasmas are governed by cumulative small-angle Coulomb scattering. The collision between plasma species α and β can be described by the **Landau-Fokker-Planck (LFP) equation**:

$$\left(\frac{\partial f_\alpha}{\partial t}\right)_{\alpha\beta} = -\frac{\partial}{\partial \mathbf{v}} \cdot (\mu_{\alpha\beta} f_\alpha) + \frac{1}{2}\frac{\partial^2}{\partial \mathbf{v}\partial \mathbf{v}} : (D_{\alpha\beta} f_\alpha),$$

where the drag and diffusion coefficients are

$$\mu_{\alpha\beta} \doteq \lim_{\Delta t \to 0} \frac{\langle \Delta \mathbf{v} \rangle}{\Delta t} = \frac{L_{\alpha\beta}}{2m_\alpha}\left(\frac{1}{m_\alpha} + \frac{1}{m_\beta}\right) \int b(\mathbf{v} - \mathbf{v}') f_\beta(\mathbf{v}')\, \mathrm{d}\mathbf{v}',$$

$$D_{\alpha\beta} \doteq \lim_{\Delta t \to 0} \frac{\langle \Delta \mathbf{v} \Delta \mathbf{v} \rangle}{\Delta t} = \frac{L_{\alpha\beta}}{m_\alpha^2} \int a(\mathbf{v} - \mathbf{v}') f_\beta(\mathbf{v}')\, \mathrm{d}\mathbf{v}'.$$

Here, we have used:

$$a(\mathbf{v}) \doteq \frac{1}{|\mathbf{v}|}\left(\mathrm{I}_3 - \frac{\mathbf{v}\mathbf{v}^\intercal}{|\mathbf{v}|^2}\right), \quad b(\mathbf{v}) \doteq \partial_{\mathbf{v}} \cdot a(\mathbf{v}) = -2\mathbf{v}/|\mathbf{v}|^3, \quad L_{\alpha\beta} \doteq \frac{e_\alpha^2 e_\beta^2}{4\pi\epsilon_0^2} \ln \Lambda_{\alpha\beta}.$$

- The LFP equation conserves particle number, momentum, and energy of the system.

Coulomb collisions: the Langevin approach

- Coulomb collisions can also be described by the **Langevin equation** that focuses on the random movement of each particle:

$$\frac{\mathrm{d}\mathbf{v}^{\alpha,i}}{\mathrm{d}t} = \mu_{\alpha\beta}(\mathbf{v}^{\alpha,i}) + \sqrt{D_{\alpha\beta}(\mathbf{v}^{\alpha,i})}\,\boldsymbol{\eta}^i(t), \quad \langle \eta^i_m(t)\eta^i_n(t')\rangle = \delta_{mn}\delta(t-t'), \qquad i = 1, ..., N_\alpha, \quad m, n = 1, 2, 3.$$

  where $\boldsymbol{\eta}^i$ (t) is the random force on i-th particle, $\sqrt{D}$ is a matrix decomposition satisfying $\sqrt{D}\sqrt{D}^\intercal = D$.

- Mathematically, the Langevin equation is known as a **stochastic differential equation (SDE)** and is typically written in the following form of Itô SDE:

$$\mathrm{d}\mathbf{v}^{\alpha,i} = \mu_{\alpha\beta}(\mathbf{v}^{\alpha,i})\mathrm{d}t + \sqrt{D_{\alpha\beta}(\mathbf{v}^{\alpha,i})}\,\mathrm{d}\mathbf{W}^i,$$

  where $\mathbf{W}(t) \sim \mathcal{N}(0, \mathrm{I}_3 t)$ are independent 3-D Wiener processes.

- Although statistically equivalent to the LFP equation, the SDE for Coulomb collisions **does not** conserve energy and momentum of the system with finite number of particles. This is a major disadvantage of the Langevin approach describing Coulomb collisions.

- In this work, we derive new SDEs for Coulomb collisions that **naturally hold the conservation laws**. New algorithms are also developed to hold the exact conservation laws in discrete time.

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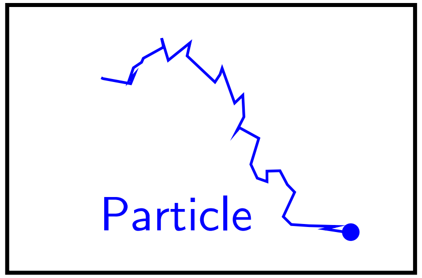
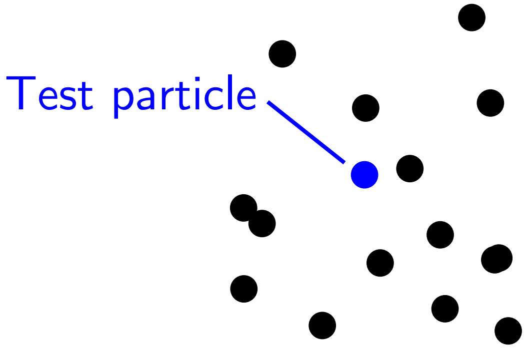
Intuition of conservation laws in SDE

- Consider the simplest system described by SDEs, the Brownian motion.
  - The energy and momentum of the small particle is clearly not conserved.
  - It is perfectly fine because the energy and momentum are absorbed by the background media, which we are not interested.



Background media

- In the Coulomb collisions in plasmas, the situation is different.
  - The particle being considered is usually denoted as "test particle", and all other particles are denoted as the "field particles"[1].
  - The energy and momentum of the test particle is not conserved due to its interaction with field particles.
  - However, the energy and momentum absorbed into field particles can not be ignored, because every particle is both test and field particles.
  - Therefore, the energy and momentum transfer between test and field particles has to be considered to order to hold the conservation law.



Field particles

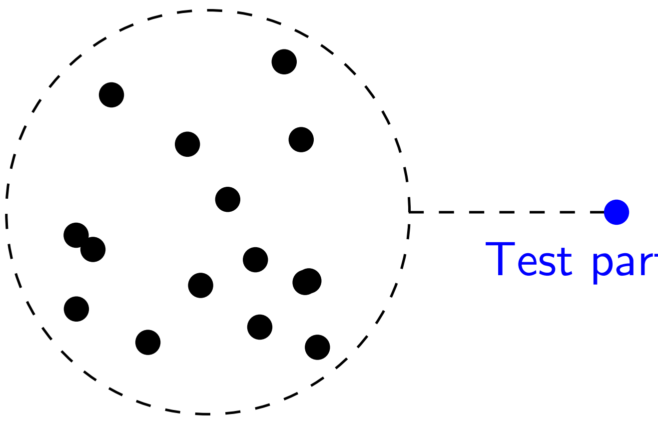
[1] R. Cohen, L. Spitzer, and P. Routly., Phy.s Rev., 1950.

Interaction between test and field particles

- Unfortunately, the energy and momentum transfer between test and field particles are difficult to analyze because test particle interacts with the **collective effect of field particles**.

- Consider intra-species collision between N particles, $f(\mathbf{v},t) \doteq w \sum_{i=1}^{N} \delta[\mathbf{v}-\mathbf{v}^i(t)]$. Let $\mathbf{u}^{ij} \doteq \mathbf{v}^i - \mathbf{v}^j$, the SDE for each particle is written as:

$$\mathrm{d}\mathbf{v}^i = \underbrace{\frac{wL}{m^2}\sum_{j,\, j\neq i} b(\mathbf{u}^{ij})\mathrm{d}t}_{\text{Deterministic force}} + \underbrace{\sqrt{\frac{wL}{m^2}\sum_{j,\, j\neq i} a(\mathbf{u}^{ij})}\,\mathrm{d}\mathbf{W}^i}_{\text{Stochastic force}}, \qquad i = 1, ..., N.$$



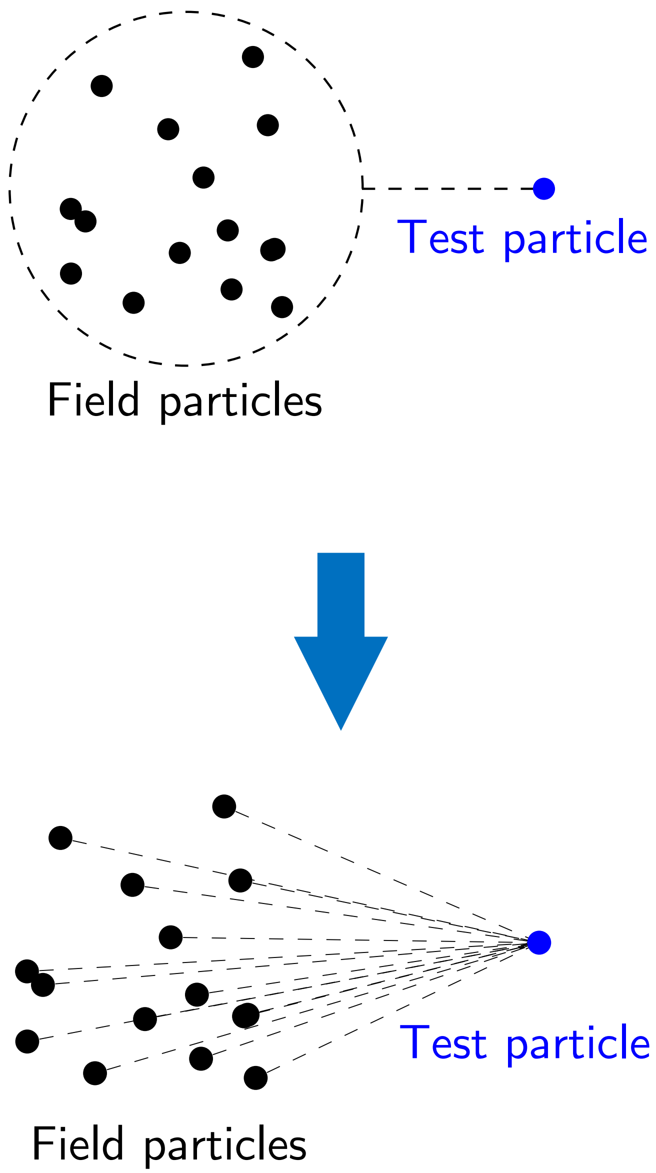
  - The deterministic force represents the interaction between each individual particles and satisfies Newton's third law.
  - The stochastic force, however, represents the collective effect from field particle to the test particle.
  - In fact, the stochastic force on each particle has no correlation because of the independency of the Wiener processes $\mathbf{W}^i$ and $\mathbf{W}^j$.
  - This is the origin of the breakdown of conservation laws.

Restoring conservation laws

- As we understand the reason why conservation laws break down, we seek to modify the SDEs to achieve two objectives:
    1. The total energy and momentum of the system are conserved exactly;
    2. The statistics of particles should not change, i.e., the first and second moments, $\langle \Delta \mathbf{v} \rangle$ and $\langle \Delta \mathbf{v} \Delta \mathbf{v} \rangle$, should give the same LFP equation;

- We achieve the two objectives above through the following constructs:
    1. Factorize the collective interaction between test and field particles into direct, individual interactions between each particle;
    2. Add correlation to the stochastic force between each particle pair, so that Newton's third law is satisfied.

- With Newton's third law, one may expect that only momentum is conserved. However, as to be shown soon, energy is also conserved with the construction above.



Construction 1: Factorizing the collective interaction

- Consider three independent 3-D Gaussian random variables, $\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3 \sim \mathcal{N}(0, \mathrm{I}_3)$, and two positive semi-definite 3×3 matrices, M_1 and M_2. Define two random variables:

$$\mathbf{Y}_1 \doteq \sqrt{M_1}\,\mathbf{X}_1 + \sqrt{M_2}\,\mathbf{X}_2, \quad \mathbf{Y}_2 \doteq \sqrt{M_1 + M_2}\,\mathbf{X}_3.$$

- We observe that $\mathbf{Y}_1 \sim \mathbf{Y}_2 \sim \mathcal{N}(0, M_1 + M_2)$:

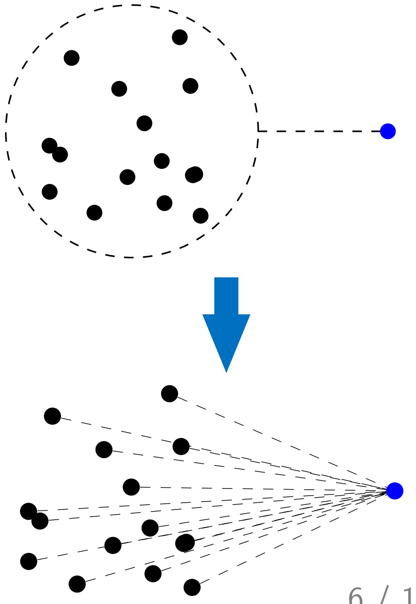
$$\langle \mathbf{Y}_1 \mathbf{Y}_1^\intercal \rangle = \sqrt{M_1}\sqrt{M_1}^\intercal \langle \mathbf{X}_1 \mathbf{X}_1^\intercal \rangle + \sqrt{M_2}\sqrt{M_2}^\intercal \langle \mathbf{X}_2 \mathbf{X}_2^\intercal \rangle + \text{cross terms} = M_1 + M_2 = \langle \mathbf{Y}_2 \mathbf{Y}_2^\intercal \rangle.$$

- Therefore, $\mathbf{Y}_1$ can be regarded as a **factorization** of $\mathbf{Y}_2$. Since Wiener processes are also Gaussian, we can factorize the stochastic force as:

$$\sqrt{\sum_{j,\, j\neq i} a(\mathbf{u}^{ij})}\,\mathrm{d}\mathbf{W}^i = \sum_{j,\, j\neq i} \sqrt{a(\mathbf{u}^{ij})}\mathrm{d}\mathbf{W}^{ij},$$

where $\mathbf{W}^i$ and $\mathbf{W}^{ij}$ are independent Wiener processes. In addition, $\sqrt{a(\mathbf{u})}$ can also be readily calculated:

$$\sigma(\mathbf{u}) \doteq \sqrt{a(\mathbf{u})} = \frac{1}{\sqrt{|\mathbf{u}|}}\left(\mathrm{I}_3 - \frac{\mathbf{u}\mathbf{u}^\intercal}{|\mathbf{u}|^2}\right).$$



Construction 2: Add correlation between interactions

- After factorizing the stochastic force, the SDE now reads:

$$\mathrm{d}\mathbf{v}^i = \sum_{\substack{j=1 \\ j\neq i}}^{N} \left[\frac{wL}{m^2} b(\mathbf{u}^{ij})\mathrm{d}t + \frac{\sqrt{wL}}{m}\sigma(\mathbf{u}^{ij})\mathrm{d}\mathbf{W}^{ij} \right] \sim \sum_{\substack{j=1 \\ j\neq i}}^{N} \mathbf{F}^{ij}.$$

- Notice that $b(-\mathbf{u}) = b(\mathbf{u}),\ \sigma(-\mathbf{u}) = \sigma(\mathbf{u}),$ the force between particles satisfies Newton's third law, $\mathbf{F}^{ij} = -\mathbf{F}^{ji}$, if we impose the following correlation[2,3]:

$$\mathbf{W}^{ij}(t) = -\mathbf{W}^{ji}(t).$$

- Similarly, we can derive the SDEs for collision between species α and β:

$$\mathrm{d}\mathbf{v}^{\alpha,i} = \sum_{j=1}^{N_\beta} \left[\frac{wL_{\alpha\beta}}{2m_\alpha}\left(\frac{1}{m_\alpha} + \frac{1}{m_\beta}\right) b(\mathbf{u}^{ij})\mathrm{d}t + \frac{\sqrt{wL_{\alpha\beta}}}{m_\alpha}\sigma(\mathbf{u}^{ij})\mathrm{d}\mathbf{W}^{ij} \right],$$

$$\mathrm{d}\mathbf{v}^{\beta,j} = -\sum_{i=1}^{N_\alpha} \left[\frac{wL_{\alpha\beta}}{2m_\beta}\left(\frac{1}{m_\alpha} + \frac{1}{m_\beta}\right) b(\mathbf{u}^{ij})\mathrm{d}t + \frac{\sqrt{wL_{\alpha\beta}}}{m_\beta}\sigma(\mathbf{u}^{ij})\mathrm{d}\mathbf{W}^{ij} \right],$$

where $\mathbf{u}^{ij} \doteq \mathbf{v}^{\alpha,i} - \mathbf{v}^{\beta,j}$, so $\mathbf{u}^{ij} \neq -\mathbf{u}^{ji}$.

[2] J. Fontbona, et al., *Probab. Theory Relat. Fields*, 2009. [3] K. Carrapatoso, *Kinet. Relat. Models*, 2016.

Demonstration of exact conservation laws

- The energy and momentum of the system are:

$$E \doteq \sum_{s}^{\{\alpha,\beta\}} \sum_{i=1}^{N_s} \frac{1}{2} w m_s |\mathbf{v}^{s,i}|^2, \quad \mathbf{P} \doteq \sum_{s}^{\{\alpha,\beta\}} \sum_{i=1}^{N_s} w m_s \mathbf{v}^{s,i}.$$

  The momentum conservation, $\mathrm{d}\mathbf{P} = 0$, is a direct result of Newton's third law, but the energy conservation is not straightforward.

- Consider a given 1-D process $X(t)$ and a smooth function of it $f(X)$.
  - In deterministic case, $\mathrm{d}X = \mu\,\mathrm{d}t$, the chain rule reads:

$$\mathrm{d}f(X) = f'\,\mathrm{d}X = \mu f'\,\mathrm{d}t.$$

  - However, in stochastic case, $\mathrm{d}X = \mu\,\mathrm{d}t + \sigma\,\mathrm{d}W$, the chain rule becomes:

$$\mathrm{d}f(X) = f'\,\mathrm{d}X + \frac{\sigma}{2} f''\mathrm{d}t = \left(\mu f' + \frac{\sigma}{2} f''\right)\mathrm{d}t + \sigma f'\mathrm{d}W. \qquad \textbf{(Itô's lemma)}$$

- After carry out a long algebra using Itô's lemma, we can prove[4] the energy conservation $\mathrm{d}E = 0$.

[4] Y. Fu, J. R. Angus, H. Qin, V. I. Geyko, arXiv:2410.12079.

A few more mathematics: from Itô to Stratonovich

- All the SDEs discussed previously were understood as the **Itô SDE**. They can be understood as Itô stochastic integral, is defined in "forward Euler" type:

$$\mathrm{d}X_t = \sigma(X_t, t)\,\mathrm{d}W_t \quad \Rightarrow \quad X_t - X_0 = \int_0^t \sigma(X_{t'}, t')\,\mathrm{d}W_{t'} \doteq \lim_{N\to\infty} \sum_{i=1}^{N-1} \sigma(X_{t_i}, t_i)(W_{t_{i+1}} - W_{t_i}).$$

  The benefit of Itô integral is that it is a martingale: $\langle X_t \rangle - X_0 = \left\langle \int_0^t \sigma(X_{t'}, t')\,\mathrm{d}W_{t'} \right\rangle = 0.$

- Another widely-used definition is the **Stratonovich SDE**, which is defined in "midpoint" type:

$$\mathrm{d}X_t = \sigma(X_t, t) \circ \mathrm{d}W_t \quad \Rightarrow \quad X_t - X_0 = \int_0^t \sigma(X_{t'}, t') \circ \mathrm{d}W_{t'} \doteq \lim_{N\to\infty} \sum_{i=1}^{N-1} \sigma(X_{t_{i+1/2}}, t_{i+1/2})(W_{t_{i+1}} - W_{t_i}).$$

  It has the advantage of following the usual chain rule: $\mathrm{d}f(X_t) = f'(X_t) \circ \mathrm{d}X_t$.

- 1-D Itô and Stratonovich SDEs can be transformed as

$$\sigma(X) \circ \mathrm{d}W = \frac{1}{2}\sigma(X)\sigma'(X)\,\mathrm{d}t + \sigma(X)\,\mathrm{d}W,$$

  whose difference is a nonlinear deterministic term.

Stratonovich SDE for Coulomb collisions

- After (another) long algebra, we can derive the Stratonovich SDEs for intra- and inter-species collision. Surprisingly, **the deterministic terms vanish completely** in Stratonovich SDEs.

- For intra-species collision between N particles, the Stratonovich SDE is:

$$\boxed{\mathrm{d}\mathbf{v}^i = \frac{\sqrt{wL}}{m} \sum_{\substack{j=1 \\ j \neq i}}^{N} \sigma(\mathbf{u}^{ij}) \circ \mathrm{d}\mathbf{W}^{ij}, \quad \mathbf{W}^{ij} = -\mathbf{W}^{ji}.}$$

- For inter-species collision between N_α and N_β particles in two species, the SDEs are:

$$\boxed{\mathrm{d}\mathbf{v}^{\alpha,i} = \frac{\sqrt{wL_{\alpha\beta}}}{m_\alpha} \sum_{j=1}^{N_\beta} \sigma(\mathbf{u}^{ij}) \circ \mathrm{d}\mathbf{W}^{ij}, \quad \mathrm{d}\mathbf{v}^{\beta,j} = -\frac{\sqrt{wL_{\alpha\beta}}}{m_\beta} \sum_{i=1}^{N_\alpha} \sigma(\mathbf{u}^{ij}) \circ \mathrm{d}\mathbf{W}^{ij}.}$$

- The conservation laws can be easily proved using those Stratonovich SDE with regular chain rules.

- When one species is infinitely heavy, the SDEs return to the case of pitch-angle scattering[5,6].

[5] X. Zhang, Y. Fu, and H. Qin, *Phys. Rev. E*, 2020. [6] Y. Fu, X. Zhang, and H. Qin, *J. Comput. Phys.*, 2022

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Numerical algorithms for Coulomb collisions

- In 6-D full-f particle-based simulations, algorithms for nonlinear LFP collision operators typically fall into the following two categories:
  - Binary collision algorithms[7-10], which mimic the Coulomb scattering process between binary pairs;
  - SDE-based algorithms[11-14], which explore the correspondence between LFP equation and SDEs.

- Other algorithms includes:
  - Particle-field methods[15], which map particles to grid, calculate collisions, and map grid back to particle;
  - Deterministic particle method[16-18] that transform LFP equation into ODEs;

- Here, we develop a numerical algorithms for our new SDEs in order to (i) verify that our SDE gives the correct collision physics; (ii) serve as a new method to calculate nonlinear LFP equation.

[7] T. Takizuka, and H. Abe., *J. Comput. Phys.*, 1977.
[8] W. X. Wang, *et al.*, *J. Comput. Phys.*, 1996.
[9] K. Nanbu, *Phys. Rev. E*, 1997.
[10] A. V. Bobylev, I. F. Potapenko, *J. Comput. Phys.*, 2013.
[11] W. M. Manheimer, *et al.*, *J. Comput. Phys.*, 1997.
[12] M. G. Cadjan, M. F. Ivanov. *J. Plasma Phys.*, 1999.
[13] F. L. Hinton, *Phys. Plasmas*, 2008.
[14] D. S. Lemons, *et al.*, *J. Comput. Phys.*, 2009.
[15] E. S. Yoon, C. S. Chang. *Phys. Plasmas*, 2014.
[16] J. A. Carrillo, *et al.*, *J. Comput. Phys. X*, 2020.
[17] E. Hirvijioki, *Plasma Phys. Control. Fusion*, 2021.
[18] F. Zonta, *et al.*, *Phys. Plasmas*, 2022.

Exact conservative algorithm for SDE: construction

- To construct an algorithm that holds conservation laws numerically, we notice that:

$$\sigma(\mathbf{u}) \circ \mathrm{d}\mathbf{W} = \frac{1}{\sqrt{|\mathbf{u}|}} \left(\mathrm{I}_3 - \frac{\mathbf{u}\mathbf{u}^{\intercal}}{|\mathbf{u}^2|} \right) \circ \mathrm{d}\mathbf{W} = \left(\frac{\mathbf{u} \times \mathrm{d}\mathbf{W}}{|\mathbf{u}|^{5/2}} \right) \times \mathbf{u}.$$

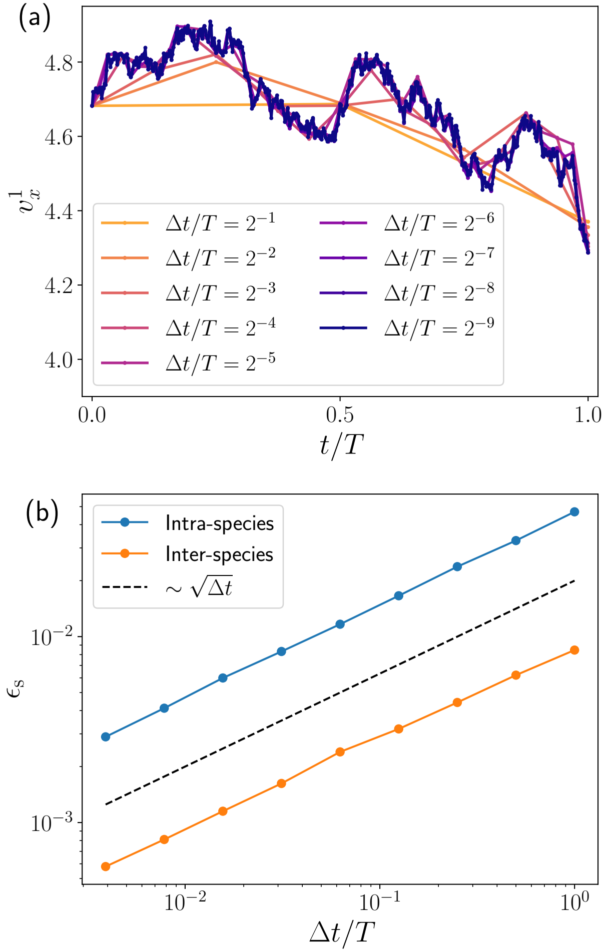
- Therefore, we can construct an algorithm for the Stratonovich SDE as

$$\mathbf{v}^i_{k+1} - \mathbf{v}^i_k = \frac{\sqrt{wL}}{m} \sum_{\substack{j=1 \\ j\neq i}}^{N} \left(\frac{\mathbf{u}^{ij}_k \times \Delta\mathbf{W}^{ij}}{|\mathbf{u}^{ij}_k|^{5/2}} \right) \boxed{\times\, \mathbf{u}^{ij}_{k+1/2},} \quad \Delta\mathbf{W}^{ij} = -\Delta\mathbf{W}^{ji} \sim \mathcal{N}(0, \mathrm{I}_3\Delta t).$$

Here, $\mathbf{u}^{ij}_{k+1/2} \doteq (\mathbf{u}^{ij}_{k+1} + \mathbf{u}^{ij}_k)/2$, and $\mathbf{u}^{ij}_k \doteq \mathbf{v}^i_k - \mathbf{v}^j_k$. The key feature of the algorithm is that it is a mixture of explicit and midpoint methods.

- Furthermore, we can analytically prove that this algorithm converges to the SDE with a strong order of 1/2, i.e., the strong error comparing to exact solution $\tilde{\mathbf{v}}^i_k$ is:

$$\epsilon_{\mathrm{s}} \doteq \left\langle \sum_{i=1}^{N} |\mathbf{v}^i_k - \tilde{\mathbf{v}}^i_k| \right\rangle \sim \mathcal{O}(\sqrt{\Delta t}) \quad \text{for} \quad k = 1, 2, ..., N_t.$$



Exact conservative algorithm for SDE: properties

- The numerical method has the following properties:

$$\mathbf{v}^i_{k+1} - \mathbf{v}^i_k = \frac{\sqrt{wL}}{m} \sum_{\substack{j=1 \\ j \neq i}}^{N} \left(\frac{\mathbf{u}^{ij}_k \times \Delta \mathbf{W}^{ij}}{|\mathbf{u}^{ij}_k|^{5/2}} \right) \times \mathbf{u}^{ij}_{k+1/2}, \quad \Delta \mathbf{W}^{ij} = -\Delta \mathbf{W}^{ji} \sim \mathcal{N}(0, \mathrm{I}_3 \Delta t).$$

  - Though implicit, RHS only depends on $\mathbf{v}^i_{k+1}$ only linearly. So $\mathbf{v}^i_{k+1}$ are explicitly solvable.

  - The algorithm preserves momentum exactly due to the anti-symmetry $\Delta \mathbf{W}^{ij} = -\Delta \mathbf{W}^{ji}$:

$$\sum_{i=1}^{N} mw(\mathbf{v}^i_{k+1} - \mathbf{v}^i_k) = 0.$$

  - The algorithm preserves energy exactly:

$$\sum_{i=1}^{N} \frac{1}{2} mw\left(|\mathbf{v}^i_{k+1}|^2 - |\mathbf{v}^i_k|^2\right) = \sum_{i=1}^{N} mw\left(\mathbf{v}^i_{k+1} - \mathbf{v}^i_k\right) \cdot \mathbf{v}^i_{k+1/2} = 0.$$

  - Therefore, the algorithm holds all conservation laws of SDE in discrete time.

Benchmark in two relaxation processes

We benchmark our algorithm in two relaxation processes:

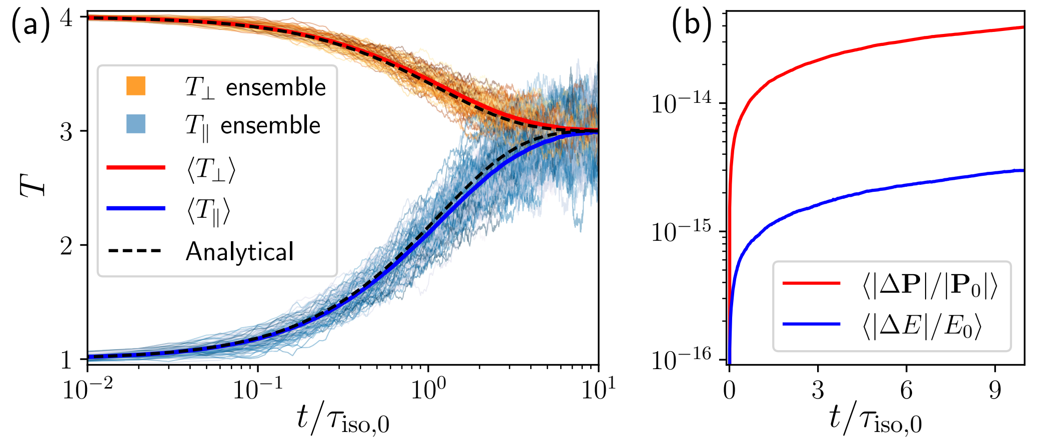
- **Temperature isotropization** along different directions in one species.

$$\frac{\mathrm{d}T_\perp}{\mathrm{d}t} = -\frac{1}{2}\frac{\mathrm{d}T_\parallel}{\mathrm{d}t} = \tau_{\mathrm{iso}}^{-1}(T_\parallel - T_\perp).$$

Let $A \doteq T_\perp/T_\parallel - 1 > 0$, the isotropization time τ_{iso} is[19]:

$$\tau_{\mathrm{iso}}^{-1} \doteq \frac{e^4 n \ln\Lambda}{8\pi^{3/2}\epsilon_0^2\sqrt{m}\,T_\parallel^{3/2}} A^{-2}[(A+3)\tan^{-1}(\sqrt{A})/\sqrt{A} - 3].$$

$e = 1,\ m = 1,\ N = 256,\ \Delta t = 10^{-2}\,\tau_{\mathrm{iso},0}$



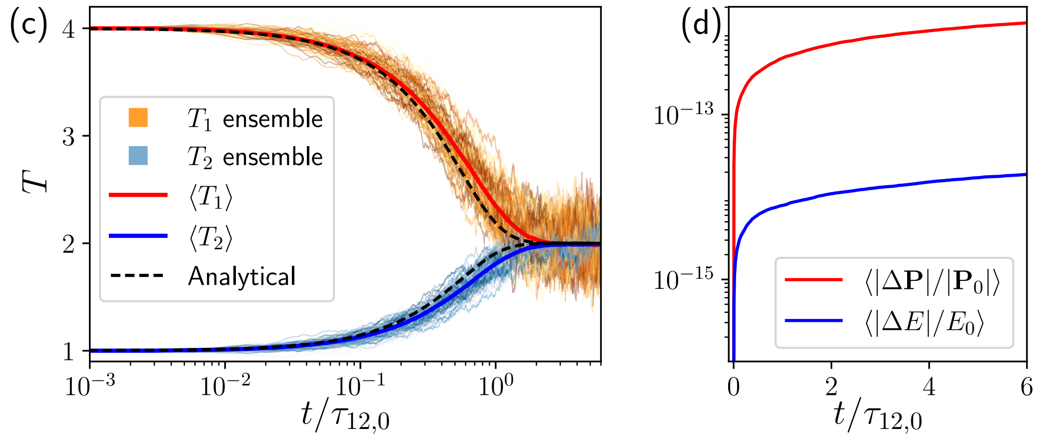
- **Temperature relaxation** between two isotropic species.

$$\frac{\mathrm{d}T_\alpha}{\mathrm{d}t} = \tau_{\alpha\beta}^{-1}(T_\beta - T_\alpha).$$

The relaxation time $\tau_{\alpha\beta}$ is[20]:

$$\tau_{\alpha\beta}^{-1} \doteq \frac{e_\alpha^2 e_\beta^2 n_\beta \ln\Lambda_{\alpha\beta}}{3\sqrt{2}\pi^{3/2}\epsilon_0^2 m_\alpha m_\beta}\left(\frac{T_\alpha}{m_\alpha} + \frac{T_\beta}{m_\beta}\right)^{-3/2}.$$

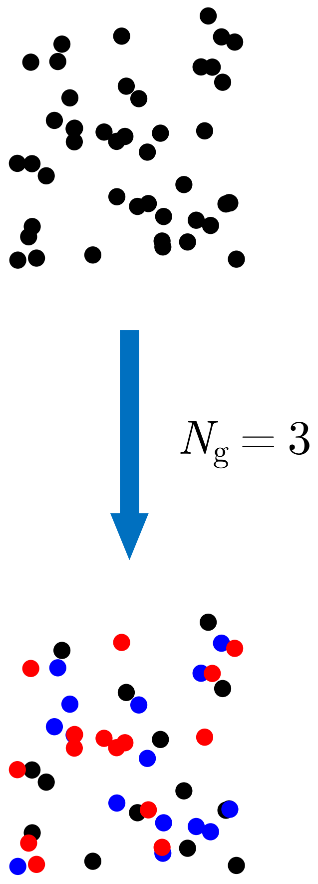
$\frac{e_1}{e_2} = \frac{2}{-1},\ \frac{m_1}{m_2} = \frac{1}{5},\ \frac{N_1}{N_2} = \frac{64}{128},\ \Delta t = 10^{-3}\tau_{11,0}$



[19] S. Ichimaru, and M. N.. Rosenbluth. *Phys. Fluids*, 1970. [20] J. Wesson and D. J. Campbell, *Tokamaks*, 2011.

Complexity reduction

- In our algorithm, every particle interact with each other, so the computational complexity is at least $\mathcal{O}(N^2)$. To reduce the complexity, we use a particle grouping technique as follows:
  1. In each step, divide all particles randomly into N_g groups with N/N_g particles in each group;
  2. Modify the weight of each particle as $w_\mathrm{g}{=}N_\mathrm{g}\,w$;
  3. Calculate the collision only among the same group.



- Consider the inter-species collision with same number of particles in each species. In the limit of each group having one particle in both species, our method returns to pair-collision algorithms. Let θ be the scattering angle of each particle and define $\delta \doteq \tan(\theta/2)$, we can prove that:

$$\frac{\langle\delta^2\rangle}{\Delta t} = \frac{e_\alpha^2 e_\beta^2 n \ln\Lambda_{\alpha\beta}}{8\pi\epsilon_0^2 m_\mathrm{r}^2 |\mathbf{u}_k^{ij}|^3} + \mathcal{O}(\sqrt{\Delta t}),$$

which is the same as the Takizuka-Abe method[7] up to the lowest order.

[7] T. Takizuka, and H. Abe., *J. Comput. Phys.*, 1977.

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  - Physical intuition
  - Mathematical derivation
  - Proof of conservation laws
  - From Itô to Stratonovich
- Exactly conservative numerical algorithms
  - Numerical algorithms for Coulomb collisions
  - Exactly conservative algorithm
  - Benchmark in relaxation processes
  - Complexity reduction
- **Conclusions and discussions**

Conclusion and main takeaway

- Properties of Gaussian random variables allow us to factorize collective forces between field and test particles into individual forces between particle pairs, which might be useful in deriving SDEs for different processes.

$$\sqrt{\sum_{j,\, j\neq i} a(\mathbf{u}^{ij})}\,\mathrm{d}\mathbf{W}^i = \sum_{j,\, j\neq i} \sqrt{a(\mathbf{u}^{ij})}\mathrm{d}\mathbf{W}^{ij}.$$

- Upon enforcing Newton's third law on the stochastic force, we can describe the Coulomb collision as an exactly energy-momentum-conserving stochastic process. Its Stratonovich SDE has a particular simple form: a pure diffusion process without drag.

$$\mathrm{d}\mathbf{v}^i = \frac{\sqrt{wL}}{m}\sum_{\substack{j=1\\ j\neq i}}^{N} \sigma(\mathbf{u}^{ij}) \circ \mathrm{d}\mathbf{W}^{ij}, \quad \mathbf{W}^{ij} = -\mathbf{W}^{ji}.$$

- A numerical algorithm has been constructed for the SDEs that hold conservation laws exactly in discrete time. It is also benchmarked in relaxation processes against analytical solutions.

$$\mathbf{v}^i_{k+1} - \mathbf{v}^i_k = \frac{\sqrt{wL}}{m}\sum_{\substack{j=1\\ j\neq i}}^{N} \left(\frac{\mathbf{u}^{ij}_k \times \Delta\mathbf{W}^{ij}}{|\mathbf{u}^{ij}_k|^{5/2}}\right) \times \mathbf{u}^{ij}_{k+1/2}, \quad \Delta\mathbf{W}^{ij} = -\Delta\mathbf{W}^{ji} \sim \mathcal{N}(0, \mathrm{I}_3\Delta t).$$

Discussion

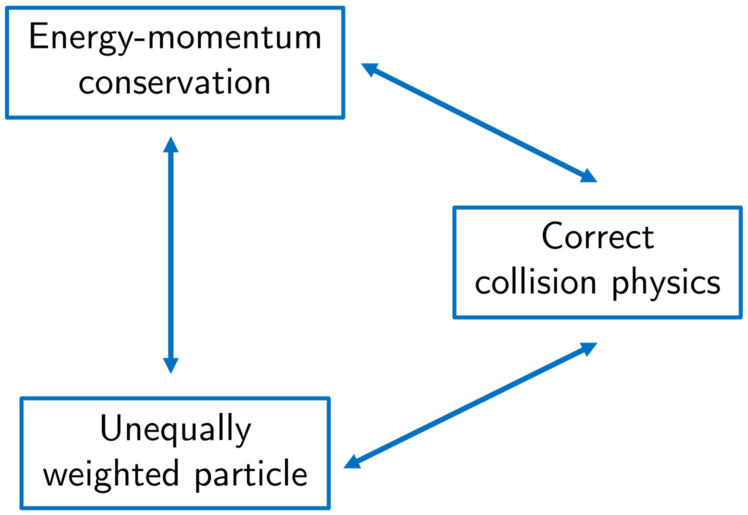
- In the current study, the SDEs are derived from LFP equations. However, we can also derive the SDE from microscopic description and then derive the LFP based on the SDE.

- Although the SDEs hold conservation laws exactly, **it does not work for unequally weighted particles** because the variances of the force are not equal.

$$\mathbf{F}^{ij} = m w_i \mathrm{d}\mathbf{v}^i \sim w_i \sqrt{w_j}\,\sigma(\mathbf{u}^{ij})\mathrm{d}\mathbf{W}^{ij} \quad \Rightarrow \quad \langle \mathbf{F}^{ij}(\mathbf{F}^{ij})^\intercal \rangle \neq \langle \mathbf{F}^{ji}(\mathbf{F}^{ji})^\intercal \rangle.$$

- Same difficulty exists in binary collision algorithms, whose conservation laws can only be addressed with predictor-corrector type of methods[14,21].

- On the other hand, Coulomb collisions in gyrokinetics can also be described by the FP equation[22,23]. Corresponding SDEs may be derived in a similar manner.



[14] D. S. Lemons, *et al.*, *J. Comput. Phys.*, 2009.
[21] J. R. Angus, Y. Fu, V. I. Geyko, D. Grote, D. Larson, arXiv:2407.19151
[22] A. J. Brizard, *Phys. Plasmas*, 2004.
[23] E. Hirvijoki, et al., *Phys. Plasmas*, 2013