Convolution based particle solution to Fokker-Planck type equations

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A poster presentation at
19th European Fusion Theory Conference

October 12, 2021

Swiss
Plasma
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Consider the Fokker-Planck equation

$$\frac{\partial f}{\partial t} = \frac{\partial \left(A_i f\right)}{\partial v_i} + \frac{\partial^2 \left(D_{ij} f\right)}{\partial v_i \partial v_j} \tag{1.1}$$

with drift $\boldsymbol{A}$ and diffusion $\boldsymbol{D}$. Decompose distribution to control variate f_0 and remaining δf, i.e.,

$$f(\boldsymbol{v}, t) = \delta f(\boldsymbol{v}, t) + f_0(\boldsymbol{v}, t) \tag{1.2}$$

which leads to

$$\frac{\partial(\delta f)}{\partial t} = \frac{\partial \left(A_i \delta f\right)}{\partial v_i} + \frac{\partial^2 \left(D_{ij} \delta f\right)}{\partial v_i \partial v_j} \underbrace{+ \frac{\partial \left(A_i f_0\right)}{\partial v_i} + \frac{\partial^2 \left(D_{ij} f_0\right)}{\partial v_i \partial v_j}}_{S(f_0)} - \frac{\partial f_0}{\partial t}. \tag{1.3}$$

Taking f_0 as Gaussian distribution, it follows $S(f_0) = 0$ by construction.

Taking f_0 as a fixed Gaussian during collision, we need to solve for

$$\frac{\partial(\delta f)}{\partial t} = \frac{\partial\left(A_i \delta f\right)}{\partial v_i} + \frac{\partial^2\left(D_{ij}\delta f\right)}{\partial v_i \partial v_j}. \tag{1.4}$$

Consider an initial particle discretization

$$\delta f(\boldsymbol{v}, t_0) \approx \sum_{i=1}^{\infty} w^{(i)} \delta(\boldsymbol{v} - \boldsymbol{v}^{(i)}), \tag{1.5}$$

where we take the weights to be proportional to δf

$$w^{(i)} = \frac{\delta f(\boldsymbol{v}^{(i)}, t_0)}{\Omega_p}. \tag{1.6}$$

Goals:

1. Solve FP on random points without going to the underlying process!
2. Maintain proportionality of w to δf during collision!

Idea: evolve weights using method of fundamental solution (conv. sol.)

$$\delta f(\boldsymbol{v}, t+\tau) = \int \delta f(\boldsymbol{v}', t) P(\boldsymbol{v}, t+\tau | \boldsymbol{v}', t) d^N \boldsymbol{v}', \tag{2.1}$$

where $P(\boldsymbol{v}, t+\tau|\boldsymbol{v}', t)$ is the transition probability

$$P(\boldsymbol{v}, t+\tau|\boldsymbol{v}', t) = \frac{\exp\left(-\frac{1}{4\tau}\left[\boldsymbol{v} - \boldsymbol{v}' - A(\boldsymbol{v}, t)\tau\right]^T \boldsymbol{D}^{-1}(\boldsymbol{v}, t)\left[\boldsymbol{v} - \boldsymbol{v}' - A(\boldsymbol{v}, t)\tau\right]\right)}{(4\pi\tau)^{N/2}\sqrt{\mathrm{Det}[\boldsymbol{D}(\boldsymbol{v}, t)]}} \tag{2.2}$$

Hence discretizing δf on random points leads to

$$\delta f(\boldsymbol{v}, t+\tau) \approx \int \sum_{i=1}^{N_p} w^{(i)}(t)\delta(\boldsymbol{v}' - \boldsymbol{v}^{(i)}) P(\boldsymbol{v}, t+\tau|\boldsymbol{v}', t) d^N \boldsymbol{v}'$$

$$\implies w^{(j)}(t+\tau) = \sum_{i=1}^{N_p} w^{(i)}(t) P(\boldsymbol{v}^{(j)}, t+\tau|\boldsymbol{v}^{(i)}, t). \tag{2.3}$$

Challenge: P becomes singular as $\tau \to 0$!

Represent the markers with local Gaussians, instead of Diracs

$$\delta f(\boldsymbol{v}') = \sum_{i=1} w^{(i)} \overline{\delta}(\boldsymbol{v}^{(i)} - \boldsymbol{v}') \tag{2.4}$$

$$\overline{\delta}(\boldsymbol{v}) = \frac{\exp\left[-||\boldsymbol{v}||_2^2/(2s)\right]}{(2\pi s)^{N/2}} \tag{2.5}$$

for a finite variance s. Therefore

$$\overline{\delta f}(\boldsymbol{v}, t+\tau) = \int \left(\sum_{i=1} w^{(i)}(t) \overline{\delta}(\boldsymbol{v}^{(i)} - \boldsymbol{v}') \right) P(\boldsymbol{v}, t+\tau | \boldsymbol{v}', t) d^N \boldsymbol{v}' \tag{2.6}$$

$$= \sum_{i=1} w^{(i)}(t) \underbrace{\left(\int \overline{\delta}(\boldsymbol{v}^{(i)} - \boldsymbol{v}') P(\boldsymbol{v}, t+\tau | \boldsymbol{v}', t) d^N \boldsymbol{v}' \right)}_{\overline{P}(\boldsymbol{v}, t+\tau | \boldsymbol{v}^{(i)}, t)} \tag{2.7}$$

where the integral can be computed analytically. For diagonal diffusion tensor

$$\overline{P}(\boldsymbol{v}, t+\tau | \boldsymbol{v}^{(i)}, t) = \prod_{k=1}^{N_d} \frac{\exp\left[-(v_k^{(i)} - v_k - A_k \tau)^2/(4\tau \mathcal{D}_k + 2s)\right]}{\sqrt{4\pi\tau\mathcal{D}_k + 2\pi s}}. \tag{2.8}$$

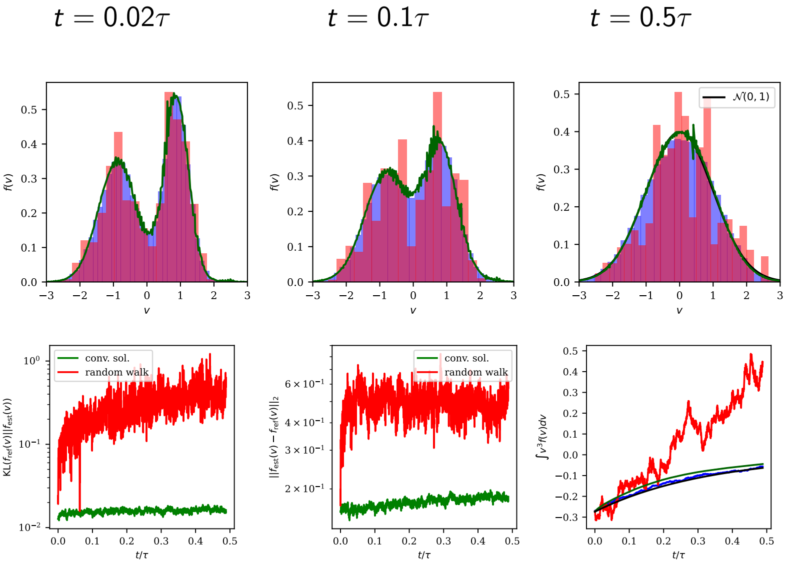

Figure: Evolution of distribution function $f(v)$ following FP with drift $A_i = (v_i - U_i)/\tau$, diffusion $D_{ij} = k_b T/m\delta_{ij}$, time step $\Delta t/\tau = 10^{-4}$ and $N_p = 500$ markers. Green: Conv. sol., red: rand. walk, blue: ref. rand. walk.

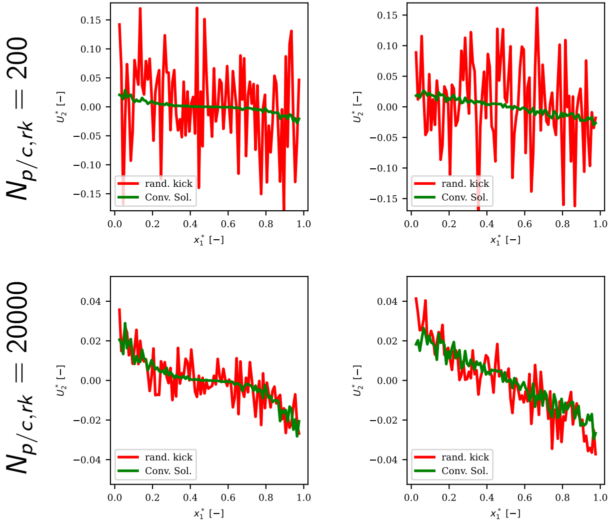

Figure: Couette flow with moving thermal walls $U_w = \pm 0.05 v_{\mathrm{th}}$ following FP $\frac{\partial f}{\partial t} + \frac{\partial (f v_i)}{\partial x_i} = S^{\mathrm{FP}}(f)$ with $N_{p/c} = 200$ shown in green for conv. sol.

Conclusion and outlook:

- We obtained a smooth δf solution to Fokker-Planck equation on random points.
- This scheme maintains $w \propto \delta f$ during collision.
- Next, implement this approach to treat FP collision models of ORB5.

Acknowledgements:

This work is part of the EUROfusion 'Theory, Simulation, Validation and Verification' (TSVV) Task and has received funding from the European research and training programme 2019-2020 under grant agreement No. 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission. This work is also supported by a grant from the Swiss National Supercomputing Centre (CSCS) under project ID s1067.