Master Thesis – 3 Week Presentation

The Langevin Approach to Discretise the Collision Operator

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Outline

Vlasov Equation

Describes the evolution of phase space including long-range interactions

$$\frac{\partial f(\boldsymbol{r}, \boldsymbol{v})}{\partial t} + \boldsymbol{v} \cdot \frac{\partial f}{\partial \boldsymbol{r}} + \frac{\boldsymbol{F}}{m} \cdot \frac{\partial f}{\partial \boldsymbol{v}} = \left(\frac{\partial f}{\partial t} \right)_{\text{coll}} \tag{1}$$

Use Fokker-Planck (FP) equation to define the collision dependent term.

From a Markov Process to Fokker-Planck

- Markovian assumption holds if $t_c \ll \Delta t$

- By Taylor expansion of density change we arrive at

$$\left(\frac{\partial f(\boldsymbol{v})}{\partial t}\right)_{\text{coll}} = -\frac{\partial}{\partial v} \cdot (f \underbrace{\langle \Delta \mathbf{v} \rangle}_{\boldsymbol{F_d}}) + \frac{1}{2} \frac{\partial^2}{\partial \mathbf{v} \partial \mathbf{v}} : (f \underbrace{\langle \Delta \mathbf{v} \Delta \mathbf{v}^{\mathbf{T}} \rangle}_{\boldsymbol{D}}) \qquad (2)$$

  Doesn't require the system to be in thermal equilibrium

- Compute the Dynamical Friction $\boldsymbol{F_d}$ and Diffusion coefficients $\boldsymbol{D}$ by describing the scattering mechanism.

Elastic collisions

Simplifying assumptions:

- Single species medium
- Consider collisions as binary events (in particle frame)
- Ignore small angle deflections by defining a minimum scattering angle $\theta_{\text{min}} = \theta(\lambda_D)$ (Debye Shielding)

$$\boldsymbol{F_d} = \langle \Delta \mathbf{v} \rangle = \int f(\boldsymbol{v}) \int u \Delta \boldsymbol{v} \sigma(u, \Omega) d\Omega d\boldsymbol{v} \tag{3}$$

Use Rutherford cross-section for Coulomb interactions:

$$\sigma(u, \Omega) = \left(\frac{q^2}{8\pi\epsilon_0 m u^2} \right)^2 \frac{1}{sin^4(\theta/2)}$$

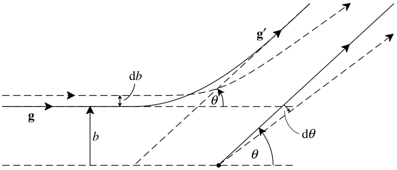

Figure: Binary Scattering
[Boyd and Sanderson, 2003]

Rosenbluth Potentials [Rosenbluth et al., 1957]

Potentials on velocity space only [Callen, 2018]:

$$\Gamma = \frac{q^4 \ln(\Lambda)}{4\pi\epsilon_0^2 m^2} \tag{4}$$

$$H(\boldsymbol{v}) = 2 \int d^3v' \frac{f(\boldsymbol{v'})}{|\boldsymbol{v} - \boldsymbol{v'}|} \tag{5}$$

$$G(\boldsymbol{v}) = \int d^3v' f(\boldsymbol{v'}) |\boldsymbol{v} - \boldsymbol{v'}| \tag{6}$$

$$\langle \Delta \mathbf{v} \rangle = \Gamma \frac{\partial H}{\partial \boldsymbol{v}} = \boldsymbol{F_d} \tag{7}$$

$$\langle \Delta \mathbf{v} \Delta \mathbf{v}^T \rangle = \Gamma \frac{\partial^2 G}{\partial \boldsymbol{v} \partial \boldsymbol{v}} = \boldsymbol{D} \tag{8}$$

Resulting Elliptic Identities:

$$\nabla_{\boldsymbol{v}}^2 \nabla_{\boldsymbol{v}}^2 G(\boldsymbol{v}) = -8\pi f(\boldsymbol{v}) \tag{9}$$

$$\nabla_{\boldsymbol{v}}^2 G(\boldsymbol{v}) = H(\boldsymbol{v}) \tag{10}$$

Resulting Scheme [Stoel, 2015]

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \frac{\partial f}{\partial \boldsymbol{r}} + \frac{\boldsymbol{F}}{m} \cdot \frac{\partial f}{\partial \boldsymbol{v}} = -\frac{\partial}{\partial v} \cdot (f \boldsymbol{F_d}) + \frac{1}{2} \frac{\partial^2}{\partial \mathbf{v} \partial \mathbf{v}} : (f \boldsymbol{D}) \tag{11}$$

Langevin type formulation of the Vlasov equation with the FP collisional term [Risken, 1984]:

$$\begin{cases} \dfrac{d\boldsymbol{r}}{dt} = \boldsymbol{v} \\ \dfrac{d\boldsymbol{v}}{dt} = \dfrac{\boldsymbol{F}}{m} + \boldsymbol{F}_d + \boldsymbol{Q} \cdot d\boldsymbol{W}_t \\ \boldsymbol{D} = \boldsymbol{Q}\boldsymbol{Q}^T \end{cases} \tag{12}$$

Disorder Induced Heating

- Cold coasting electron beam
- Collisions cause beam temparature to rise (undesired)
  - Beam widens
  - Emittance increases

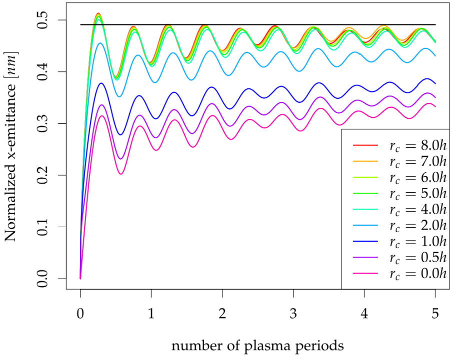

Figure: DIH resolved with P^{3}M [Ulmer, 2016]

Timeline I

Date	Target Goals
30/01	Assist Severin and ensure correctness of current implementation
20/02	Find Order of convergence / accuracy and compare whether really much better than P3M (even though it might still run only on single core)
20/02	Ensure Performance Portability (MPI, OpenMP and GPU)
06/03	Benchmarking of accuracy, runtime and scalability
27/03	Start improving most pressing bottlenecks
03/04	Easter Holidays
01/05	Research on better integrators / explore Multi-Level Monte-Carlo approach

Table: Timeline with approximate milestones

Timeline II

Date	Target Goals
08/05	Implement algorithmic improvements and compare accuracy / performance to previous implementation
29/05	(Potential Implementation into OPAL via IPPL-1 implementation)
12/06	Start writing and code clean-up
03/07	Submission

Table: Timeline with approximate milestones

References I

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