



KDMC development in Eiron

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Eiron

- To provide a path towards scalability for EIRENE
- ► C++
- Modular, extensible architecture
 - Simulator produces trajectories
 - Estimator estimates fields based on trajectories
 - Can be run separately or as one Simulator-Estimator
- End goal: parallel, scalable, domain decomposed simulations
- Principle developer: Oskar Lappi (Helsinki)









Current features

- 2D Cartesian slab geometry on structured grid
- Neutral particle tracing
- Velocity independent collision rates
- OpenMP and MPI parallelization
- Domain decomposition for estimation (not yet for simulation)
- JSON-based configuration and outputs









Roadmap

Current focus

Charon: Utility library for communication of particle streams

- Asynchronous request queues
- Sticky subdomain routing
- Variable sized messages
- Replayable message logs for performance profiling and debugging
- Full domain decomposition in Eiron using Charon
 - Each worker assigned one or more subdomains, for both simulation and estimation
 - Particles transfer particle stream when moving between workers
 - Load-balancing by assigning multiple workers to one subdomain

Backlog

Better physics models, current focus on parallelization









Kinetic equations

- ▶ Individual particles in position-velocity phase space (X_t, V_t, t)
- Evolution of distribution follows kinetic equation

$$\partial_t f(x,v,t) + \frac{v}{\epsilon} \partial_x f(x,v,t) = \frac{1}{\epsilon^2} Q(f(x,v,t))$$

Velocity jump process



$$dX_t = \frac{V_t}{\epsilon} dt, \quad V_t = \mathcal{V}^n, \quad t \in [t^n, t^{n+1}),$$
$$\mathcal{V}^n \sim \mathcal{M}(v), \quad t^{n+1} - t^n \sim \mathcal{E}(1/\epsilon^2)$$



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Kinetic equations

Velocity jump process

$$dX_t = \frac{V_t}{\epsilon} dt, \quad V_t = \mathcal{V}^n, \quad t \in [t^n, t^{n+1})$$

• $\epsilon \to 0$: Time between collisions $t^{n+1} - t^n \to 0$

Brownian motion

$$X^{n+1} = X^n + \sqrt{2\Delta t}\sqrt{D}\xi^n, \quad \xi^n \sim \mathcal{N}(0,1)$$

Output: Plasma source terms

$$S(x,t) = \int \Psi(x,v,t) f(x,v,t) dv$$



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Kinetic trajectory



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Kinetic-diffusion trajectory

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Kinetic-diffusion

- General idea: replace many kinetic steps with a diffusive step
- Advantage:
 - Less computational work
- Issues:
 - Different particle timestepping behavior
 - Loss of intermediate path information

B. Mortier, M. Baelmans, G. Samaey, A Kinetic-Diffusion Asymptotic-Preserving Monte Carlo Algorithm for the Boltzmann-BGK Model in the Diffusive Scaling. SIAM Journal on Scientific Computing 44(2) pp. A720–A744 (2022)

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Current status

- KDMC timestepping added to code base
- Developed comparison test-case
- Analysis: Both sets of trajectories should match as
 - $\Delta t \to 0$
 - Collision rate $\rightarrow \infty$
- Estimators for diffusive simulation
- Multilevel extension
 - Many trajectories with Δt large
 - Correction with fewer correlated pairs

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