KU LEUVEN

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)

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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

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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

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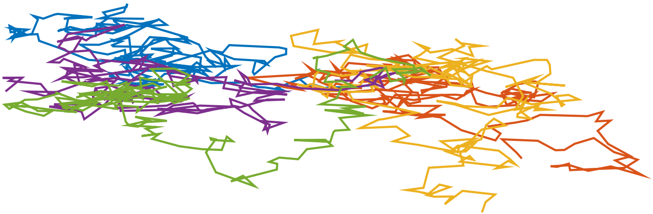
Kinetic equations

- 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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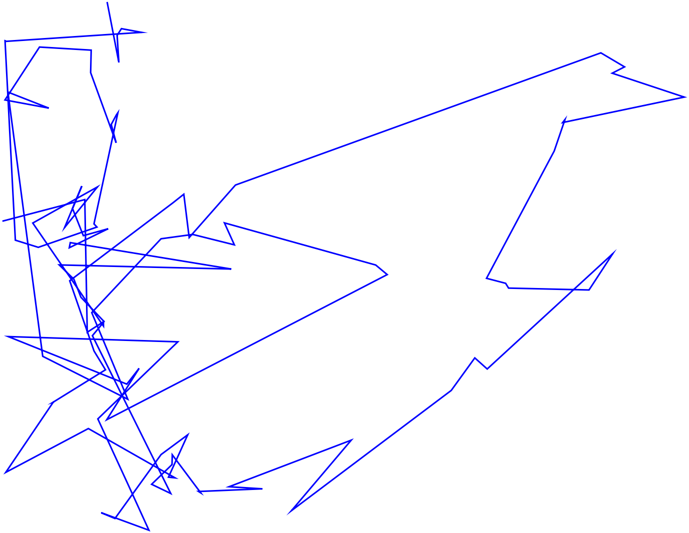
Kinetic trajectory



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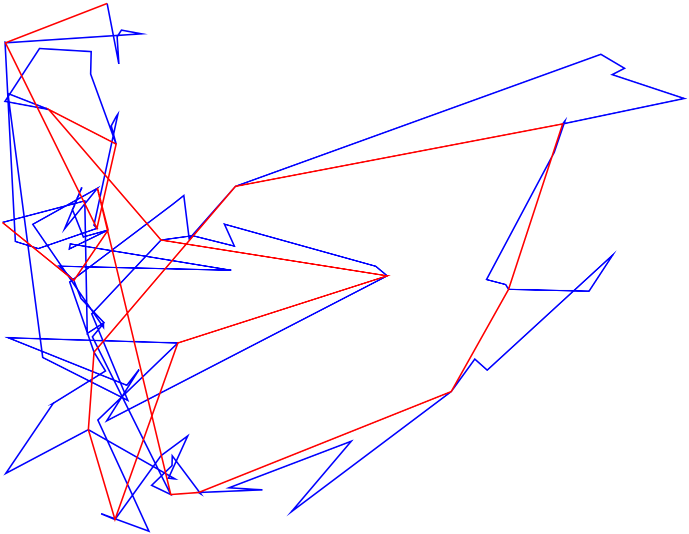
Kinetic-diffusion trajectory



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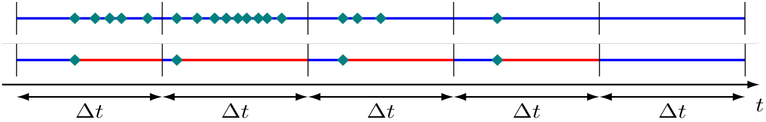
Kinetic-diffusion

- 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 $\to \infty$
- Estimators for diffusive simulation
- Multilevel extension
  - Many trajectories with Δt large
  - Correction with fewer correlated pairs

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