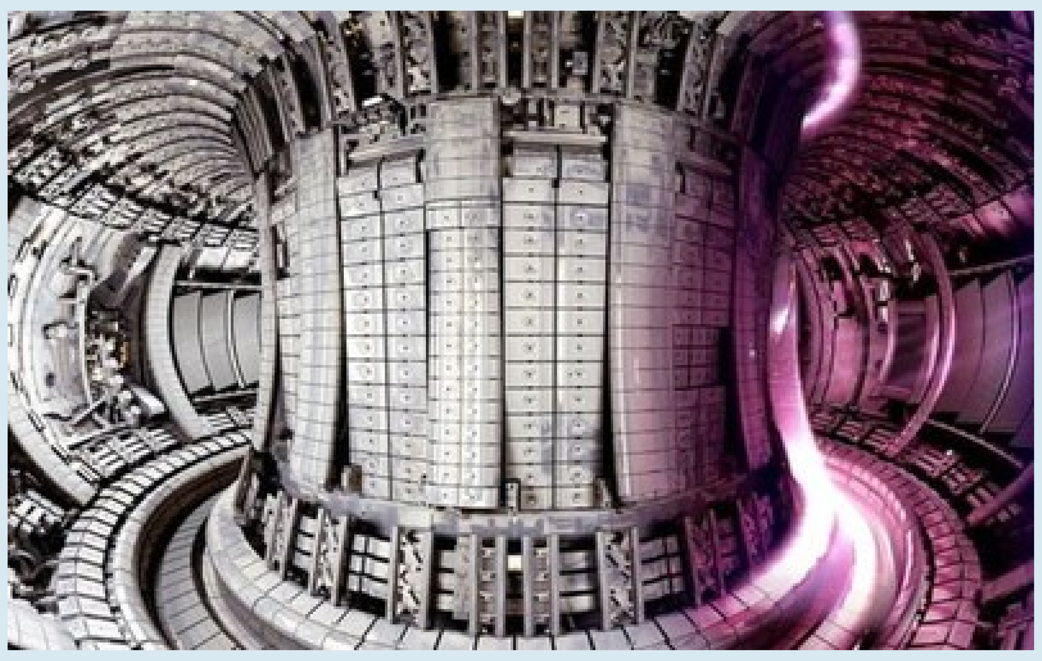
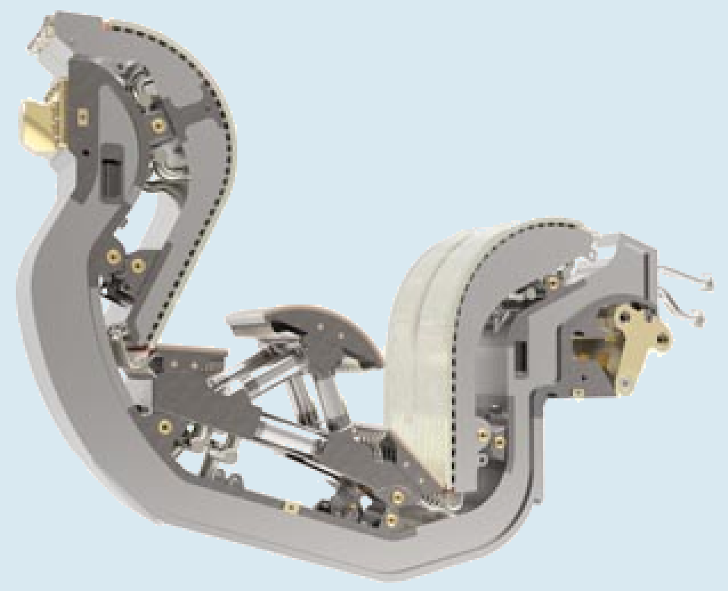
# Asymptotic-preserving multilevel Monte Carlo for neutral particle simulation in fusion reactors

Emil Løvbak, Stefan Vandewalle and Giovanni Samaey
KU Leuven, Department of Computer Science, NUMA Section
emil.loevbak@kuleuven.be

## Tokamak Fusion Reactors



- Reaction takes place in a **plasma**:
  - Charged particles
  - Dense ⇒ fluid ⇒ finite volume code
- Collisions between plasma and **neutral particles**:
  - Low density ⇒ kinetic equation ⇒ high dimensional
  - High collision rate ⇒ small time steps
- **Goal: Divertor design** constrained by coupled plasma and neutral models



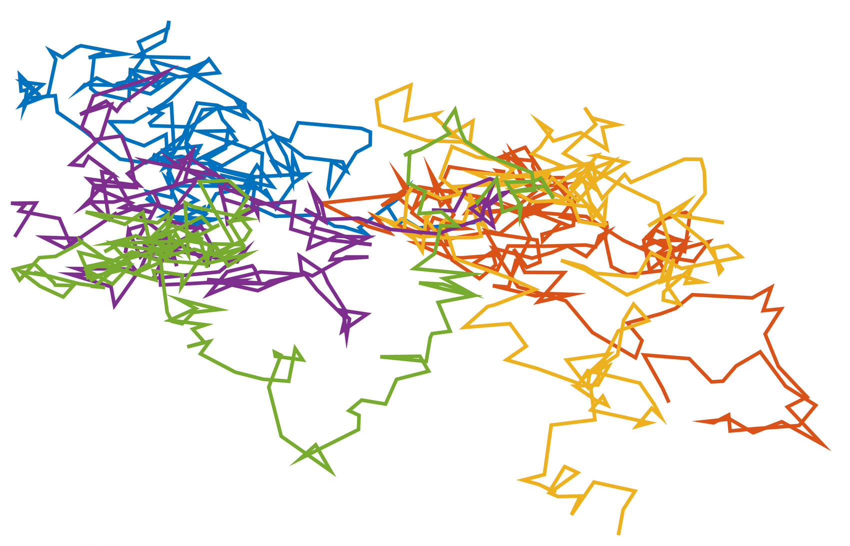
- **Challenge: Expensive neutral particles simulation**

## Diffusive Kinetic Equations

- We simulate the paths of **individual particles** in a position-velocity phase space

$$\left(\frac{v}{\varepsilon}\frac{\partial}{\partial x} + R_a\right) f(x,v) = S(x,v) + \frac{R_c}{\varepsilon^2}\left(\mathcal{M}(v)\rho(x) - f(x,v)\right)$$

- Particle trajectories follow a **velocity jump process**



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

$$\mathcal{V}^n \sim \mathcal{M}(v), \quad t^{n+1} - t^n \sim \mathcal{E}\left(\frac{R_c}{\varepsilon^2}\right),$$

where particles follow a straight trajectory between collisions and sample post-collisional velocities from $\mathcal{M}(v)$

- When $\varepsilon \to 0$, the time between collisions $t^{n+1} - t^n \to 0$ and this converges to **diffusion**

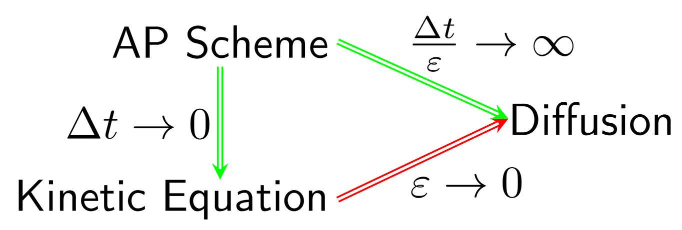
$$X^{n+1} = X^n + \sqrt{2\Delta t}\,\xi^n, \quad \xi^n \sim \mathcal{N}\left(\mu_{\mathcal{M}}, \sigma^2_{\mathcal{M}}\right)$$

- **Problem:** Need small time steps to resolve collisions

## Asymptotic-preserving Scheme [1]

- **Solution:** An asymptotic-preserving scheme replaces collisions with diffusion

$$\left(\frac{v\varepsilon}{\varepsilon^2+\Delta t}\frac{\partial}{\partial x} + \frac{\Delta t}{\varepsilon^2+\Delta t}\frac{\partial^2}{\partial x^2} + R_a\right) f(x,v) = S(x,v) + \frac{R_c}{\varepsilon^2 + R_c\Delta t}\left(\mathcal{M}(v)\rho(x) - f(x,v)\right)$$




- **Transport-diffusion step**

$$X^{n+1} = X^n + \frac{\varepsilon}{\varepsilon^2+\Delta t}V^n\Delta t + \sqrt{2\Delta t}\sqrt{\frac{\Delta t}{\varepsilon^2+\Delta t}}\xi^n$$

- **Collision step**

No collision: $\exp\left(-\frac{R_c\Delta t}{\varepsilon^2 + R_c\Delta t}\right)$ ⇒ $\frac{\varepsilon^2}{\varepsilon^2 + R_c\Delta t}$

Collision: $\left(1 - \exp\left(-\frac{R_c\Delta t}{\varepsilon^2 + R_c\Delta t}\right)\right)$ ⇒ $\frac{R_c\Delta t}{\varepsilon^2 + R_c\Delta t}$

- **Absorption step**

No absorption: $\exp\left(-R_a\Delta t\right)$ ⇒ $1 - R_a\Delta t$

Absorption: $\left(1 - \exp\left(-R_a\Delta t\right)\right)$ ⇒ $R_a\Delta t$

## Multilevel Monte Carlo [2]

- A **Monte Carlo** estimator for a Quantity of Interest $Y(x) = \mathbb{E}[f(X,V)]$ has the form

$$\hat{Y}(x) = \frac{1}{P}\sum_{p=1}^{P}\sum_{n=0}^{N} f(X^n_{\Delta t,p}, V^n_{\Delta t,p})$$

- Error = Bias + Variance

$$\mathbb{E}[|\hat{Y}(x) - Y(x)|] \sim \Delta t, \quad \mathbb{V}[\hat{Y}(x)] = \frac{1}{P}\mathbb{V}\left[f(X^n_{\Delta t}, V^n_{\Delta t})\right]$$

- **Trade-off:** If computational cost is fixed, do we take many samples or expensive samples?
- **Multilevel Monte Carlo** many cheap samples and a sequence of increasingly expensive corrections

$$\hat{Y}_0(t^*) = \frac{1}{P_0}\sum_{p=1}^{P_0} f(X^n_{\Delta t_0,p})$$

$$\hat{Y}_l(t^*) = \frac{1}{P_l}\sum_{p=1}^{P_l}\left(f(X^{Mn}_{\Delta t_l,p}) - f(X^n_{\Delta t_{l-1},p})\right), \; l \geq 1$$

- Levels are combined with a **telescopic sum**

$$\hat{Y}(t^*) = \sum_{l=0}^{L}\hat{Y}_l(t^*)$$

## References

[1] G. Dimarco, L. Pareschi, G. Samaey, *Asymptotic-Preserving Monte Carlo methods for transport equations in the diffusive limit*, SISC, 40:A504–A528, 2018.

[2] M.B. Giles *Multilevel Monte Carlo Path Simulation*, Operations Research, 56(3):607–617, 2008.

[3] E. Løvbak, B. Mortier, G. Samaey, S. Vandewalle, *Multilevel Monte Carlo with Improved Correlation for Kinetic Equations in the Diffusive Scaling*, ICCS 2020, 374–388, 2020.

[4] E. Løvbak, G. Samaey, S. Vandewalle, *A multilevel Monte Carlo method for asymptotic-preserving particle schemes in the diffusive limit*, Numer. Math., 148:141–186, 2021.

## Correlating AP simulations [3,4]

- **Goal:** Couple two discrete paths

$$\begin{cases} \Delta X^n_{\Delta t_{\ell-1}} = \tilde{v}_{\Delta t_{\ell-1}} V^n_{\Delta t_{\ell-1}}\Delta t_{\ell-1} + \sqrt{2\Delta t_{\ell-1}}\sqrt{D_{\Delta t_{\ell-1}}}\xi^n_{\Delta t_{\ell-1}} \\ \Delta X^n_{\Delta t_\ell} = \sum_{m=0}^{M-1}\left(\tilde{v}_{\Delta t_\ell} V^{n,m}_{\Delta t_\ell}\Delta t_\ell + \sqrt{2\Delta t_\ell}\sqrt{D_{\Delta t_\ell}}\xi^{n,m}_{\Delta t_\ell}\right) \end{cases}$$

with $\tilde{v}_{\Delta t} = \frac{\varepsilon}{\varepsilon^2 + \Delta t}$ and $D_{\Delta t} = \frac{\Delta t}{\varepsilon^2 + \Delta t}$

- **Diffusive increments: weighted** and **rescaled** sum

$$\xi^n_{l-1} = \sqrt{\theta_\ell}\frac{\sum_{m=1}^{M}\xi^{n,m}_l}{\sqrt{M}} + \sqrt{1-\theta_\ell}\frac{\sum_{m=0}^{M-1}V^{n,m}_{\Delta t_{\ell-1}}}{\sqrt{\mathbb{V}\left[\sum_{m=0}^{M-1}V^{n,m}_{\Delta t_{\ell-1}}\right]}}$$

- **Collision/absorption:** event with probability $p_e$ occurs in step $n,m$ if $1 - p_{e,\Delta t_\ell} < u^{n,m}_{e,\Delta t_\ell} \sim \mathcal{U}([0,1])$

$$u^n_{e,\Delta t_{\ell-1}} = \left(\max_m u^{n,m}_{e,\Delta t_\ell}\right)^M \sim \mathcal{U}([0,1])$$

- **Velocity** $V^n_{\Delta t_{\ell-1}}$ taken from last fine simulation collision

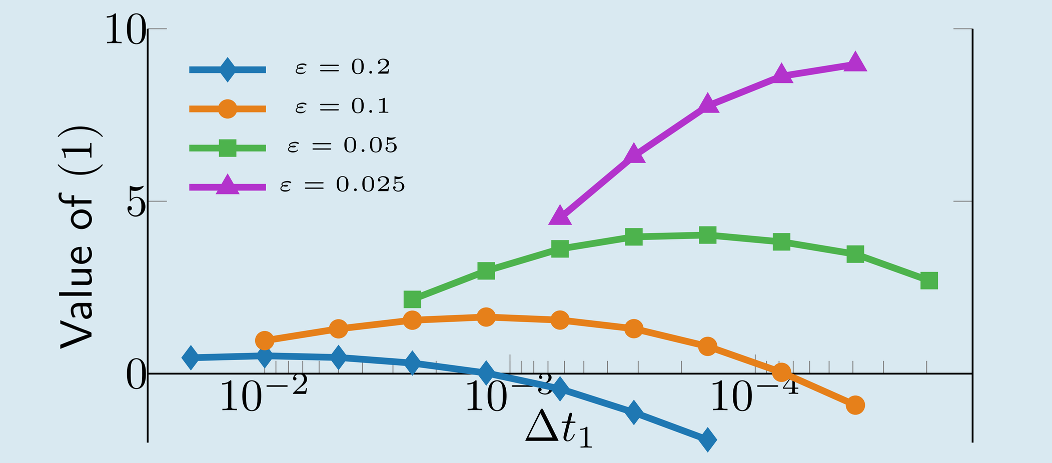
## Results

- **Particle displacement** after 0.5 s, $\mathcal{M}(v) = \mathcal{N}(v;0,1)$

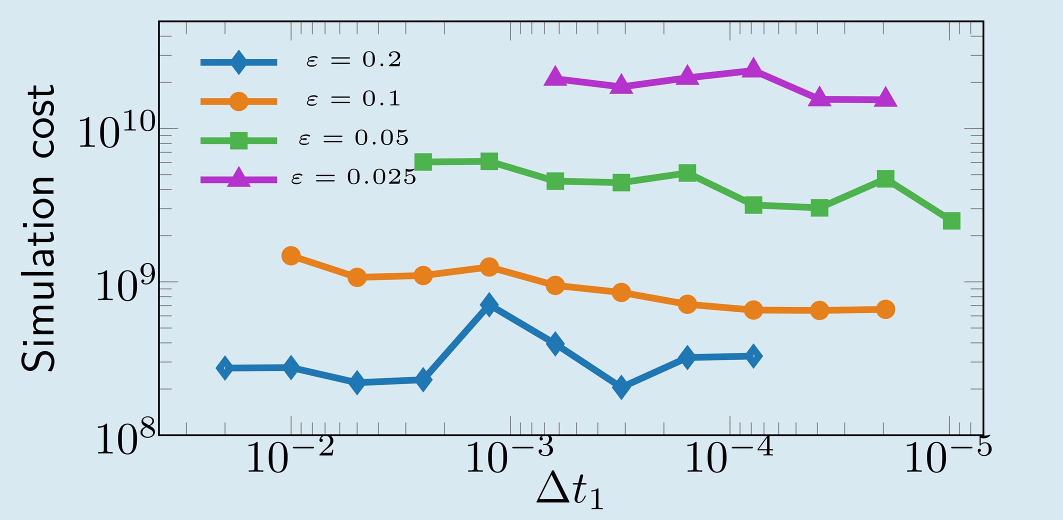
| $\ell$ | $\Delta t_\ell$ | $\mathbb{E}[\hat{F}_\ell - \hat{F}_{\ell-1}]$ | $\mathbb{V}[\hat{F}_\ell - \hat{F}_{\ell-1}]$ | $P_\ell C_\ell$ |
|---|---|---|---|---|
| 0 | $5.0\times10^{-1}$ | $9.9\times10^{-1}$ | $2.0\times10^{0}$ | $1.0\times10^{7}$ |
| 1 | $1.0\times10^{-2}$ | $-1.2\times10^{-1}$ | $1.7\times10^{-1}$ | $2.1\times10^{7}$ |
| 2 | $5.0\times10^{-3}$ | $1.0\times10^{-2}$ | $4.7\times10^{-1}$ | $6.1\times10^{7}$ |
| 3 | $2.5\times10^{-3}$ | $2.8\times10^{-2}$ | $4.4\times10^{-1}$ | $8.3\times10^{7}$ |
| ... | ... | ... | ... | ... |
| 11 | $9.8\times10^{-6}$ | $4.1\times10^{-4}$ | $4.7\times10^{-3}$ | $1.3\times10^{8}$ |
| 12 | $4.9\times10^{-6}$ | $3.3\times10^{-4}$ | $2.2\times10^{-3}$ | $1.5\times10^{8}$ |
| 13 | $2.4\times10^{-6}$ | $3.9\times10^{-4}$ | $1.8\times10^{-4}$ | $6.1\times10^{6}$ |
| $\sum$ | | $9.81\times10^{-1}$ | | $1.5\times10^{9}$ |

Single level cost ≈ $2.1 \times 10^{12}$, $P_0$ paths with $\Delta t_{13}$

- Optimal **level strategy**




$$\sqrt{\mathbb{V}\left[\Delta\hat{F}_\ell\right]C_\ell} + \sqrt{\mathbb{V}\left[\Delta\hat{F}_{\ell+1}\right]C_{\ell+1}} - \sqrt{\mathbb{V}\left[\Delta\hat{F}'_{\ell+1}\right]C'_{\ell+1}} \quad (1)$$




## Conclusions

- Asymptotic-preserving multilevel Monte Carlo produces multiple orders of magnitude speed-up on toy problems
- Ongoing verification work in fusion test-case
- Future work:
  - Boundaries
  - Non-homogenous plasma parameters