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Multilevel Monte Carlo Asymptotic-Preserving Particle Method for Kinetic Equations

Emil Løvbak, Stefan Vandewalle and Giovanni Samaey
KU Leuven, Department of Computer Science, NUMA Section
July 3, 2018

Kinetic equations

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

$$\partial_t f(x, v, t) + v \partial_x f(x, v, t) = Q(f(x, v, t))$$

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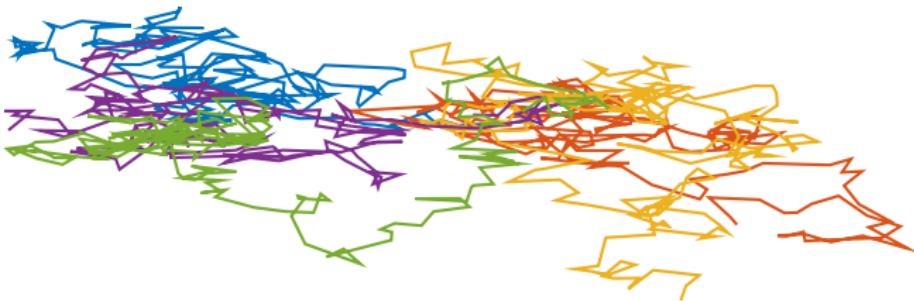
$$\varepsilon \partial_t f(x, v, t) + v \partial_x f(x, v, t) = \frac{1}{\varepsilon} Q(f(x, v, t))$$

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

- ▶ Velocity jump process



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

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

Kinetic equations

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

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- ▶ Brownian motion

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

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- ▶ Interested in moments $u(x, t) = \int m(v) f(x, v, t) dv$
- ▶ Examples: Density, Flux, Variance, ...

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

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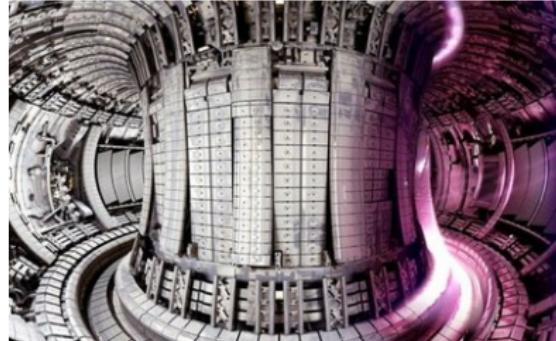
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$$\rho(x, t) = \int f(x, v, t) dv$$

- ▶ Limiting macroscopic equation for $\varepsilon \rightarrow 0$: $\partial_t \rho = \partial_{xx} \rho$

Kinetic equations

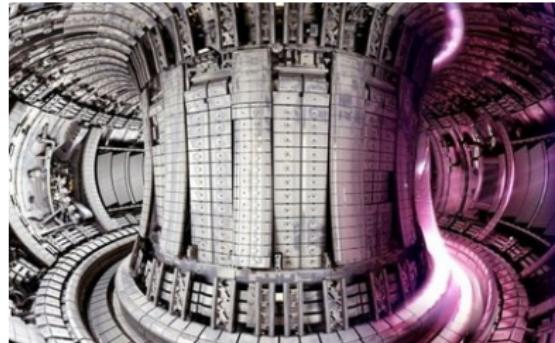
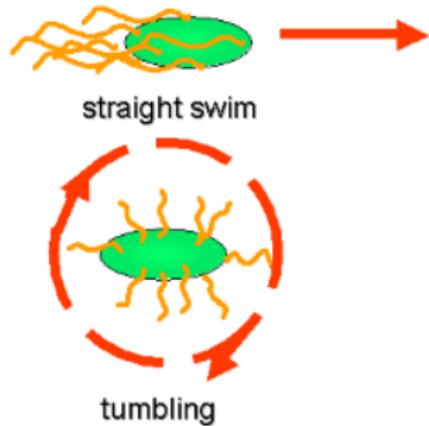
- ▶ Applications:
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Kinetic equations

► Applications:

- Nuclear fusion
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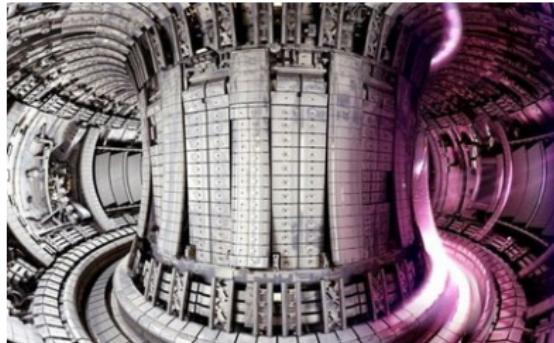
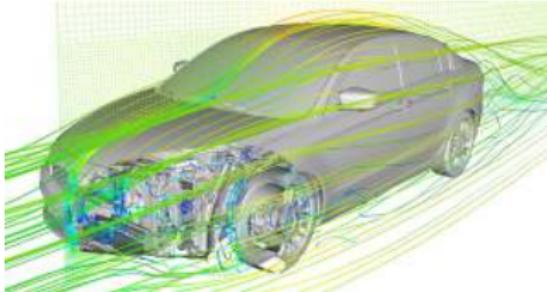
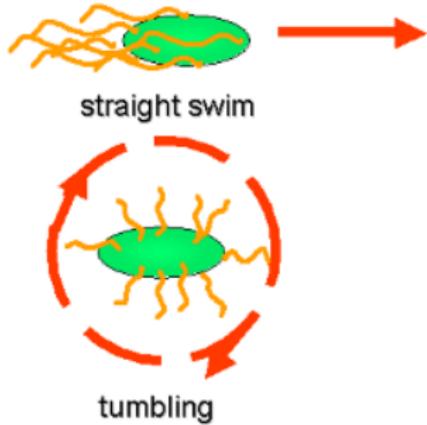


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Kinetic equations

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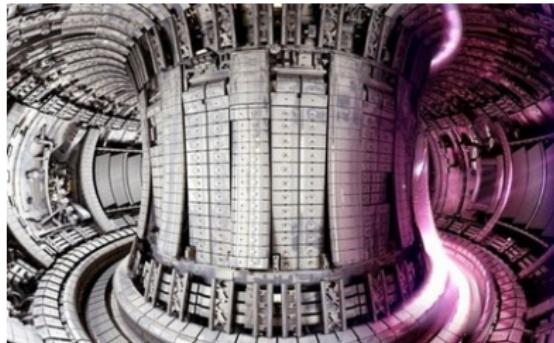
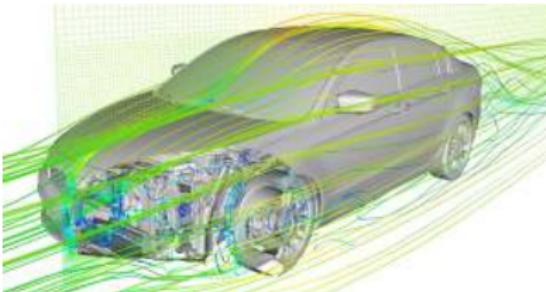
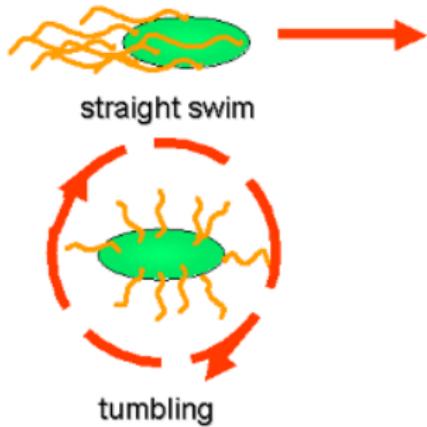
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► Often multiscale in nature

- Short mean free path
- Slow macroscopic dynamics



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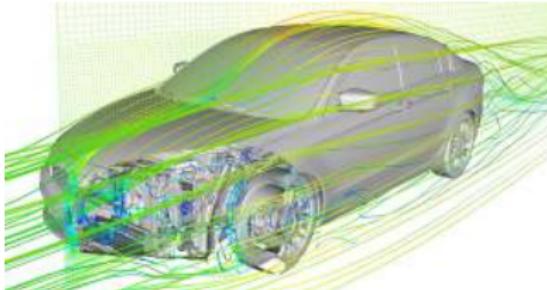
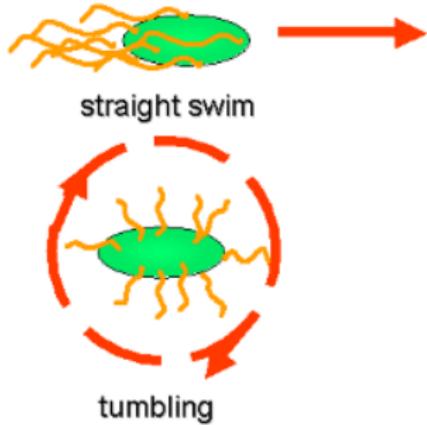
► Applications:

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► Often multiscale in nature

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⇒ computationally expensive



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Background: Asymptotic-Preserving Particle Schemes

- Goldstein-Taylor model:

$$\begin{cases} \partial_t f_+ + \frac{1}{\varepsilon} \partial_x f_+ = \frac{1}{\varepsilon^2} \left(\frac{\rho}{2} - f_+ \right) \\ \partial_t f_- - \frac{1}{\varepsilon} \partial_x f_- = \frac{1}{\varepsilon^2} \left(\frac{\rho}{2} - f_- \right) \end{cases}$$

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- In density flux representation:

$$\rho = f_+ + f_-, \quad j = \frac{f_+ - f_-}{\varepsilon}$$

$$\begin{cases} \partial_t \rho + \partial_x j = 0 \\ \partial_t j + \frac{1}{\varepsilon^2} \partial_x \rho = -\frac{1}{\varepsilon^2} j \end{cases}$$

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- Under limit $\varepsilon \rightarrow 0$:

$$\partial_t \rho = \partial_{xx} \rho$$

Background: Asymptotic-Preserving Particle Schemes

- ▶ A conventional Monte Carlo scheme with operator splitting:
 - Transport step:

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- ▶ Time step restriction $\Delta t = \mathcal{O}(\varepsilon)$

Outline

- ① Asymptotic-Preserving Particle Scheme
- ② Multilevel Monte Carlo
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- ▶ Modified equation via IMEX method:
[Dimarco, Pareschi, Samaey, 2018]

$$\begin{cases} \partial_t f_+ + \frac{\varepsilon}{\varepsilon^2 + \Delta t} \partial_x f_+ = \frac{\Delta t}{\varepsilon^2 + \Delta t} \partial_{xx} f_+ + \frac{1}{\varepsilon^2 + \Delta t} \left(\frac{\rho}{2} - f_+ \right) \\ \partial_t f_- - \frac{\varepsilon}{\varepsilon^2 + \Delta t} \partial_x f_- = \frac{\Delta t}{\varepsilon^2 + \Delta t} \partial_{xx} f_- + \frac{1}{\varepsilon^2 + \Delta t} \left(\frac{\rho}{2} - f_- \right) \end{cases}$$

- ▶ Model bias $\mathcal{O}(\Delta t)$
- ▶ $\varepsilon \rightarrow 0 \Rightarrow$ Diffusion

Asymptotic-Preserving Particle Schemes

- ▶ Transport-diffusion step:

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⇓

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

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Background: Multilevel Monte Carlo

- ▶ Monte Carlo for Quantity of Interest $Y(t^*) = f(X(t^*))$:

$$\hat{Y}(t^*) = \frac{1}{P} \sum_{p=1}^P f(X_{\Delta t, p}^n), \quad t^* = n\Delta t$$

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- ▶ In this case moments: $f(x) = x, x^2, x^3, \dots$
- ▶ Error:
 - Systematic:
 - Small Δt : Small bias, high cost
 - Large Δt : Large bias, low cost
 - Statistical:

$$\mathbb{V}[\hat{Y}(t^*)] = \frac{1}{P} \mathbb{V}[f(X_{\Delta t}^n)]$$

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- ▶ Fixed cost trade-off: Many samples or expensive samples?

Background: Multilevel Monte Carlo

- ▶ Multilevel Monte Carlo [Giles, 2015]:

- Many cheap samples:

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

- Correction with increasingly fewer correlated pairs of expensive samples:

$$\hat{Y}_l(t^*) = \frac{1}{P_l} \sum_{p=1}^{P_l} \left(f(X_{\Delta t_l, p}^{Mn}) - f(X_{\Delta t_{l-1}, p}^n) \right), \quad l = 1 \dots L, \quad M = \frac{\Delta t_{l-1}}{\Delta t_l}$$

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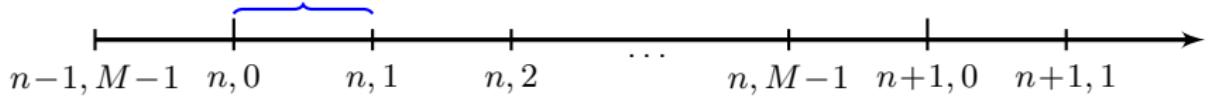
- If $\mathbb{E}[Y_l]$ and $\mathbb{V}[Y_l]$ decrease in absolute value with $l \Rightarrow$ Convergence

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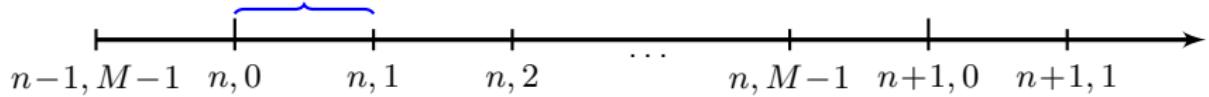
Correlating Particle Pairs: Transport-diffusion Step

$$X_{\Delta t_l}^{n,1} = X_{\Delta t_l}^{n,0} \pm \frac{\varepsilon}{\varepsilon^2 + \Delta t_l} + \sqrt{2\Delta t_l} \sqrt{\frac{\Delta t_l}{\varepsilon^2 + \Delta t_l}} \xi_l^{n,0}, \quad \xi_l^{n,0} \sim \mathcal{N}(0, 1)$$



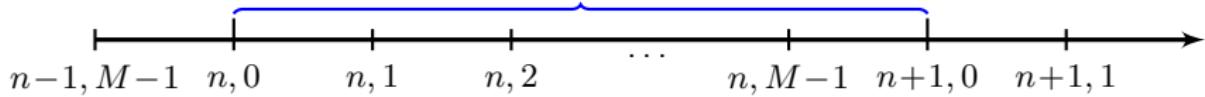
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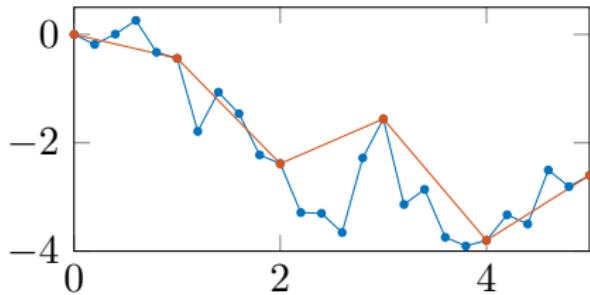
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► $\sqrt{M} \xi_{l-1}^n = \sum_{m=1}^M \xi_l^{n,m} \sim \mathcal{N}(0, \sqrt{M})$

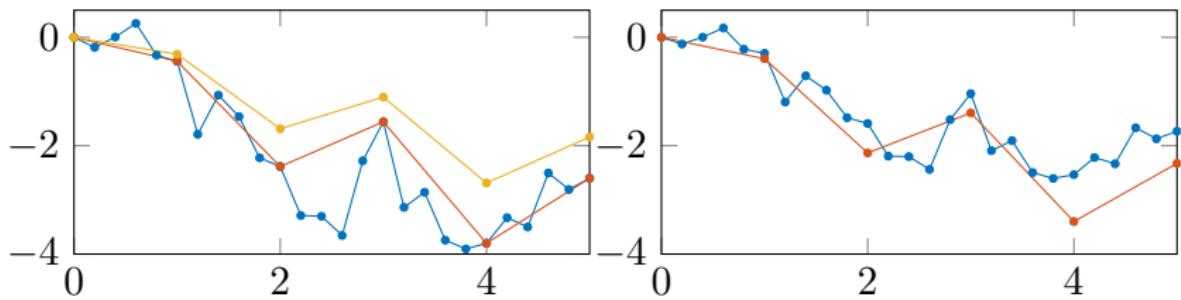


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- ▶ Different $\Delta t \Rightarrow$ different diffusion coefficient
- ▶ Variance rescaling: $\xi_{l-1}^n = \frac{1}{\sqrt{M}} \sum_{m=1}^M \xi_l^{n,m} \sim \mathcal{N}(0, 1)$



Correlating Particle Pairs: Collision Step

- ▶ Probability of collision is different for different Δt
- ▶ Implementation: If $\alpha_l^n > \frac{\varepsilon^2}{\varepsilon^2 + \Delta t_l}$, $\alpha_l^n \in \mathcal{U}[0, 1]$ then collision

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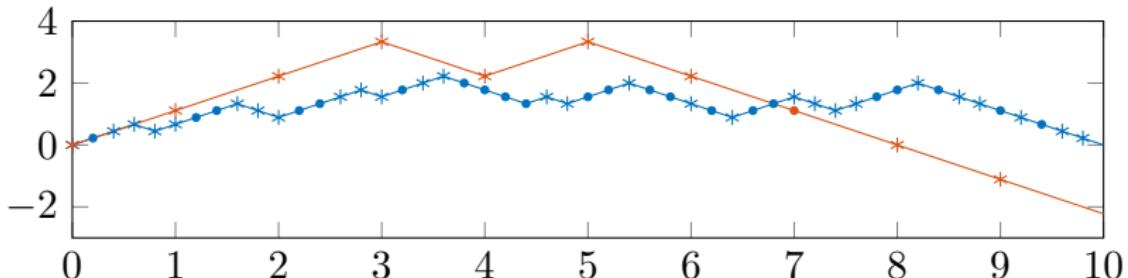
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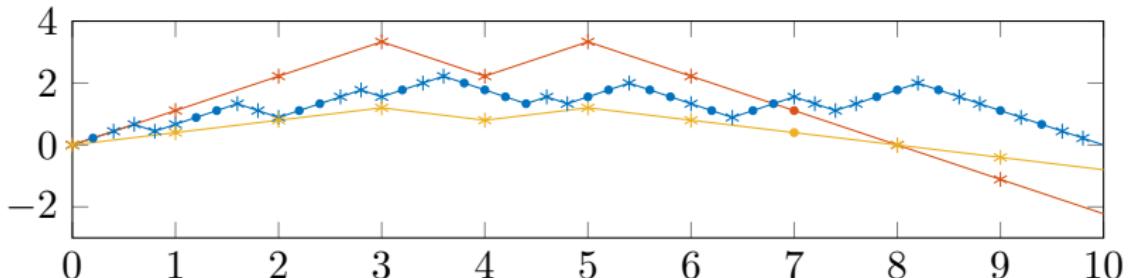
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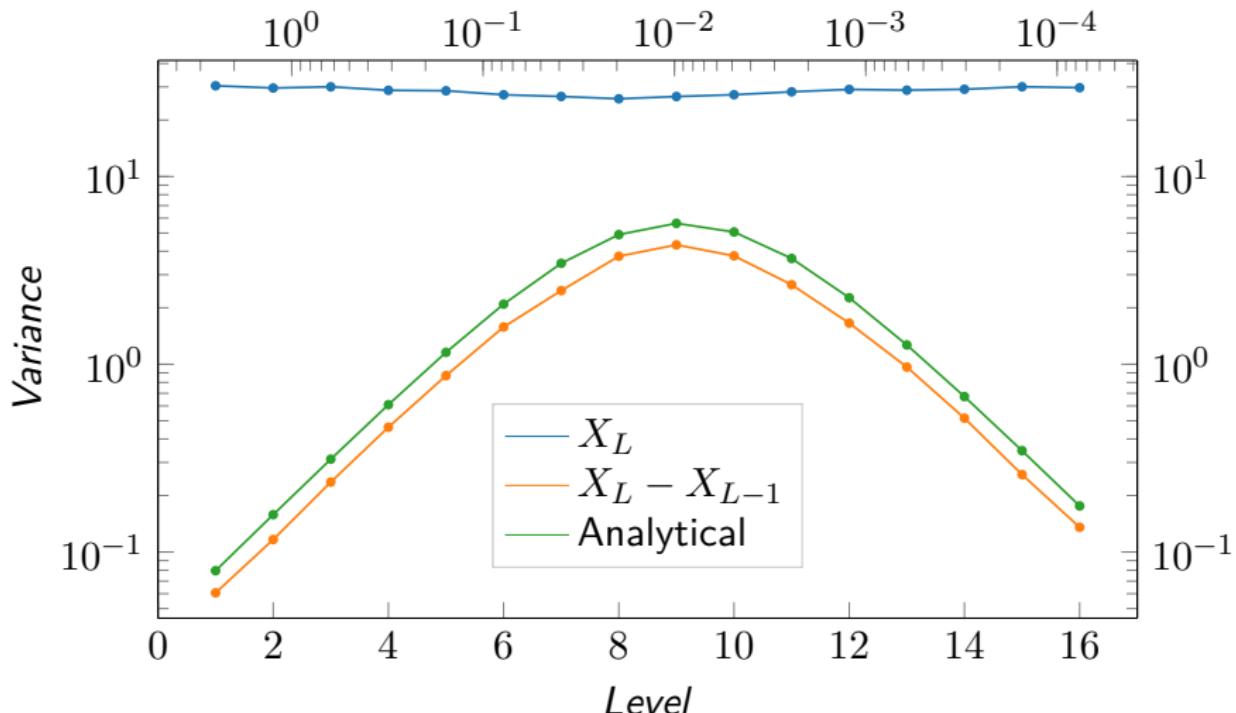
Outline

- ① Asymptotic-Preserving Particle Scheme
- ② Multilevel Monte Carlo
- ③ Correlating Particle Pairs
- ④ Practical Results

Applying MLMC to AP scheme: Results

Maximum variance of mean position per level, $\varepsilon = 0.1$

Rough time step



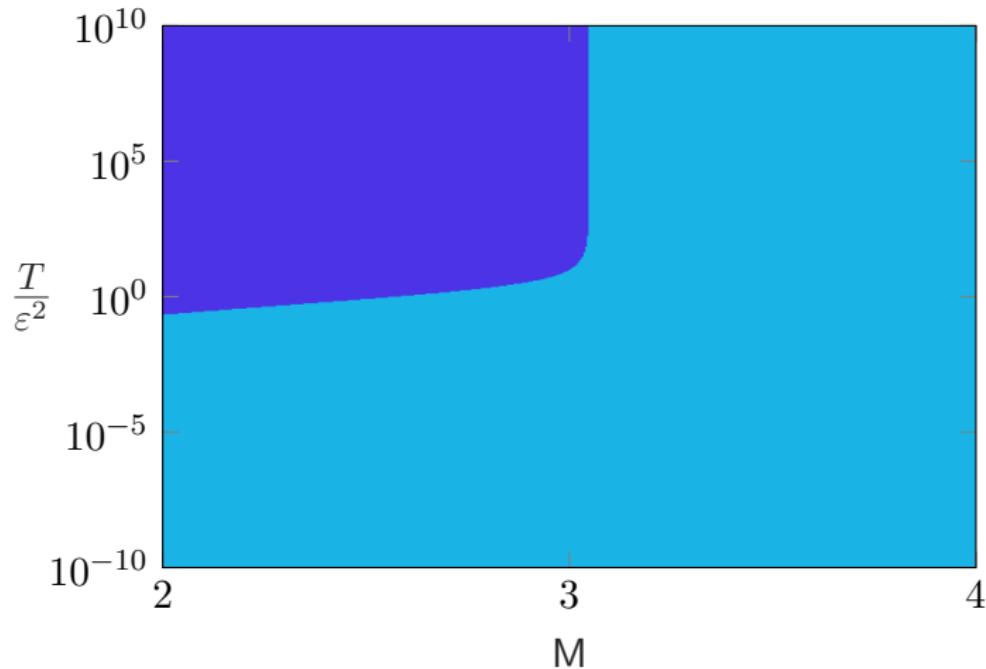
Applying MLMC to AP scheme: Results

Slide removed due to containing wrong results. We refer to future publications on this topic for a correction.

Applying MLMC to AP scheme: Results

$$4V_{l+1}C_{l+1} > \tilde{V}_{l+1}\tilde{C}_{l+1} \quad [\text{Giles, 2015}]$$

Dark region = where we can increase the geometric factor



Applying MLMC to AP scheme: Results

- ▶ Variance increases for $\Delta t \gg \varepsilon^2$ and decreases for $\Delta t \ll \varepsilon^2$
- ▶ For small Δt , general theory behind MLMC applies
- ▶ For large Δt , it seems that extra levels increase overall cost
- ▶ Proposed strategy:
 - Level 0 at roughest possible time step
 - Level 1 correlates roughest time step with ε^2
 - Levels 2 ... L are a geometric series of time steps
 - Optimal geometric factor $\in 2, 3, 4$ and depends on ε and the simulation length
- ▶ Experimental verification of strategy in progress

References

-  G. Dimarco, L. Pareschi and G. Samaey (2018)
Asymptotic-Preserving Monte Carlo methods for transport equations in the diffusive limit
SIAM J. Sci. Comput. 40, pp. A504–A528
-  M. B. Giles (2015)
Multilevel Monte Carlo methods
Acta Numerica 24, pp. 259–328