Multilevel Monte Carlo Asymptotic-Preserving Particle Method for Kinetic Equations

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Kinetic equations

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

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

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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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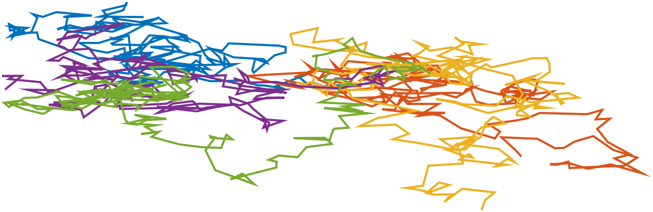
- Evolution of distribution follows kinetic equation

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

- 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

- Velocity jump process

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

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

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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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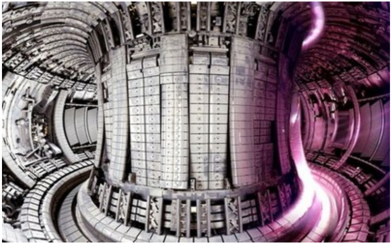
- Examples: Density, Flux, Variance, ...

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

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

Kinetic equations

- Applications:
  - Nuclear fusion



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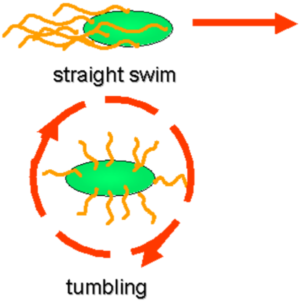
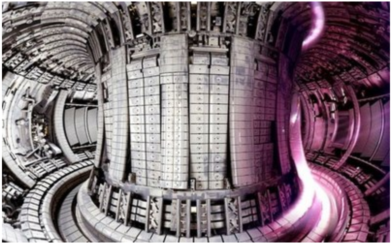
Kinetic equations

- Applications:
  - Nuclear fusion
  - Chemotaxis





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  - Nuclear fusion
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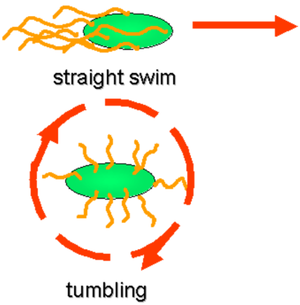

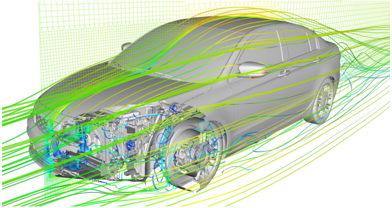

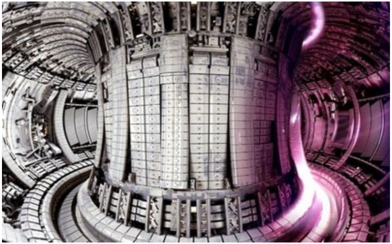

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Kinetic equations

- Applications:
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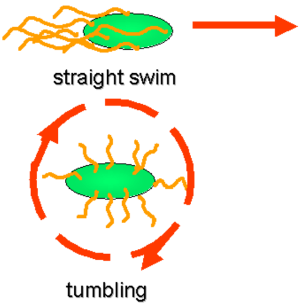
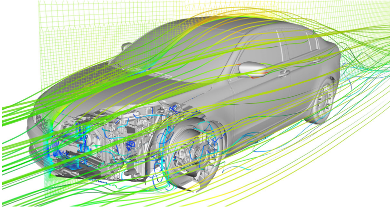
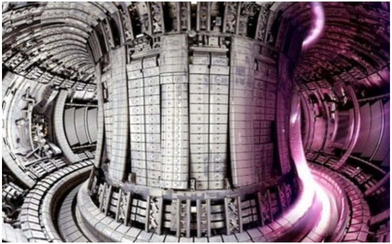
  - ...
- Often multiscale in nature
  - Short mean free path
  - Slow macroscopic dynamics







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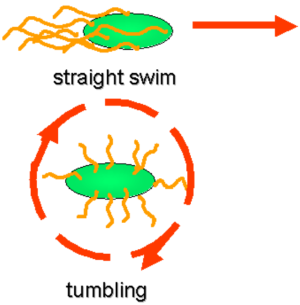
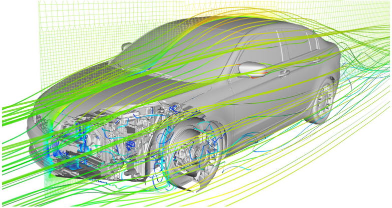
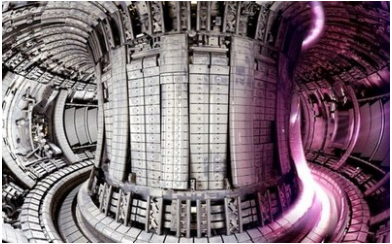
$\Rightarrow$ computationally expensive







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Background: Asymptotic-Preserving Particle Schemes

- Goldstein-Taylor model:

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

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- In density flux representation:

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

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

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- Under limit $\varepsilon \to 0$:

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

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- 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
3. Correlating Particle Pairs
4. Practical Results

Outline

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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 $\mathcal{O}(\Delta t)$
- $\varepsilon \to 0 \Rightarrow$ Diffusion

Asymptotic-Preserving Particle Schemes

- Transport-diffusion step:

$$\begin{cases} \partial_t f_+ + \dfrac{\varepsilon}{\varepsilon^2 + \Delta t} \partial_x f_+ = \dfrac{\Delta t}{\varepsilon^2 + \Delta t} \partial_{xx} f_+ \\ \partial_t f_- - \dfrac{\varepsilon}{\varepsilon^2 + \Delta t} \partial_x f_- = \dfrac{\Delta t}{\varepsilon^2 + \Delta t} \partial_{xx} f_- \end{cases}$$

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$$\Downarrow$$

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

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No collision: $\dfrac{\varepsilon^2}{\varepsilon^2 + \Delta t}$

Collision: $\dfrac{\Delta t}{\varepsilon^2 + \Delta t}$

Outline

Background: Multilevel Monte Carlo

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

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

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

$$\mathbb{V}[\hat{Y}(t^*)] = \frac{1}{P}\mathbb{V}\left[f(X^n_{\Delta t})\right]$$

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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:

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

  - Correction with increasingly fewer correlated pairs of expensive samples:

$$\hat{Y}_l(t^*) = \frac{1}{P_l} \sum_{p=1}^{P_l} \Big(f(X^{Mn}_{\Delta t_l, p}) - f(X^n_{\Delta t_{l-1}, p}) \Big)\,,\ l = 1 \ldots L,\ M = \frac{\Delta t_{l-1}}{\Delta t_l}$$

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  - Telescopic sum:

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

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  - Telescopic sum:

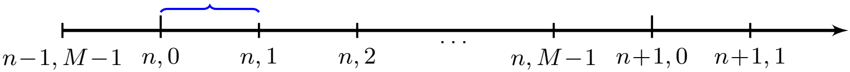
$$\hat{Y}(t^*) = \sum_{l=0}^{L} \hat{Y}_l(t^*)$$

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

Outline

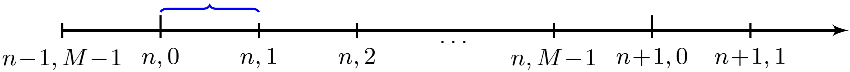
Correlating Particle Pairs: Transport-diffusion Step

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



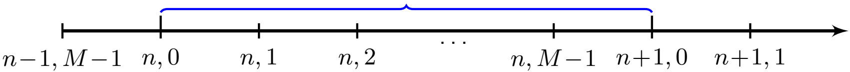
Correlating Particle Pairs: Transport-diffusion Step

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



Correlating Particle Pairs: Transport-diffusion Step

$$X_{\Delta t_l}^{\color{red}{n+1,0}} = X_{\Delta t_l}^{n,0} \cdots + \sqrt{2\Delta t_l}\sqrt{\frac{\Delta t_l}{\varepsilon^2 + \Delta t_l}} {\color{red}{\sum_{m=1}^{M} \xi_l^{n,m}}}, \quad \xi_l^{n,m} \sim \mathcal{N}(0,1)$$



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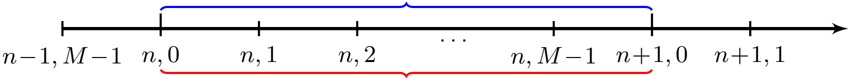

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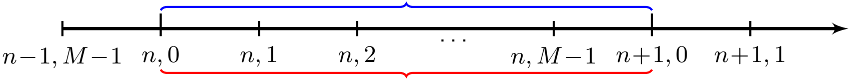
- Different $\Delta t \Rightarrow$ different diffusion coefficient



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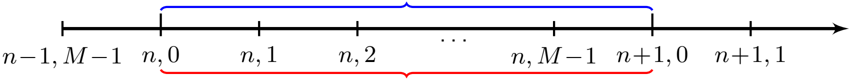

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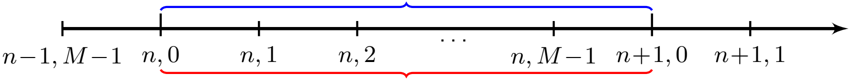
- Different $\Delta t \Rightarrow$ different diffusion coefficient



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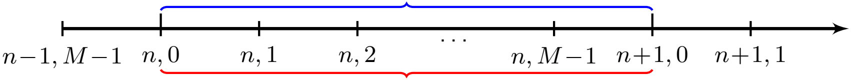

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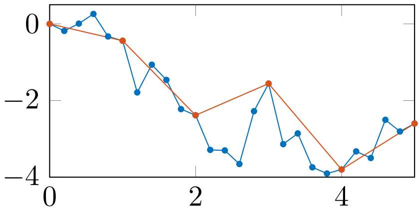
- Different $\Delta t \Rightarrow$ different diffusion coefficient
- $\sqrt{M}\xi_{l-1}^{n} = \sum_{m=1}^{M} \xi_l^{n,m} \sim \mathcal{N}\left(0, \sqrt{M}\right)$



Correlating Particle Pairs: Transport-diffusion Step

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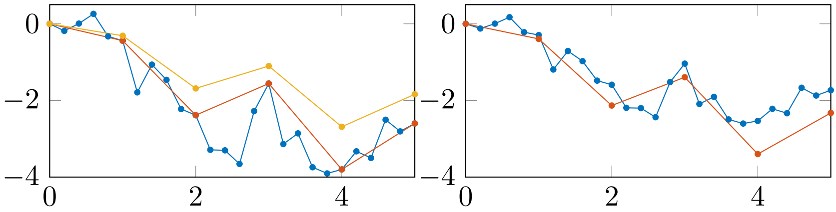
- Different $\Delta t \Rightarrow$ different diffusion coefficient
- Variance rescaling: $\xi_{l-1}^{n} = \frac{1}{\sqrt{M}} \sum_{m=1}^{M} \xi_l^{n,m} \sim \mathcal{N}(0,1)$



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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- Generate uniformly distributed α_{l-1}^n from $\alpha_{\mathsf{max}} = \max\limits_m \alpha_l^{n,m}$:

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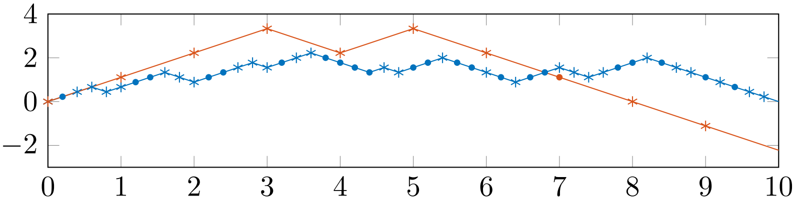
- New speed is $\beta_l^n \mathcal{V}_l$, $\beta_l^n = \pm 1$ with equal probability

$$\beta_{l-1}^n = \beta_l^{n,i}, \quad i = \underset{1\le m\le M}{\arg\max} \left(m \middle| \alpha_l^{n,m} \ge \frac{\varepsilon^2}{\varepsilon^2 + \Delta t_{l-1}} \right)$$



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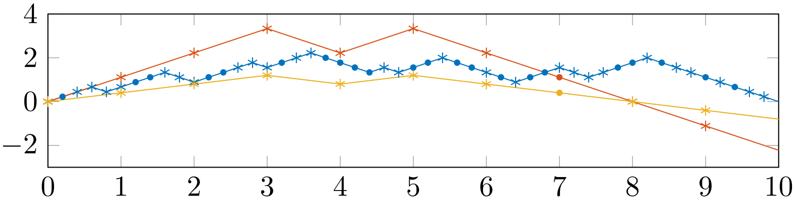
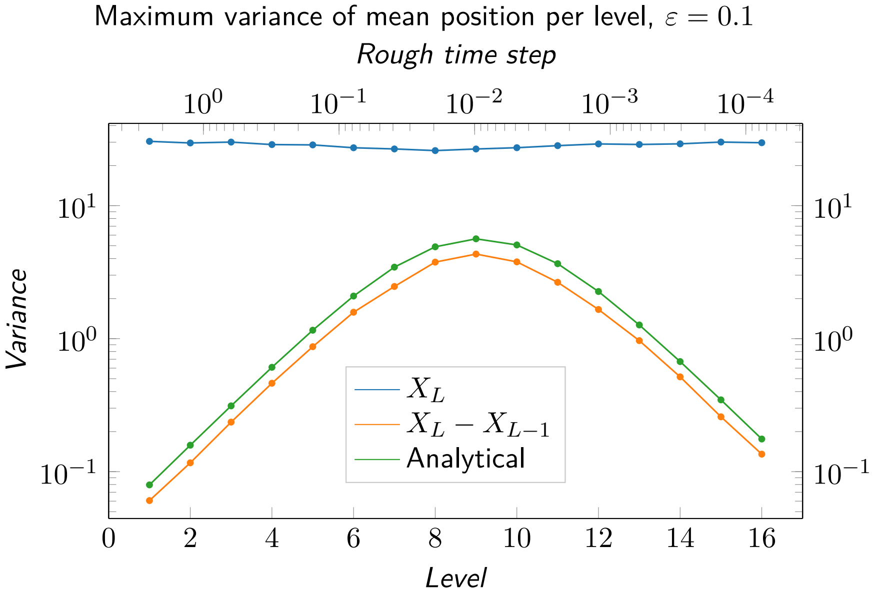


Outline

Applying MLMC to AP scheme: Results



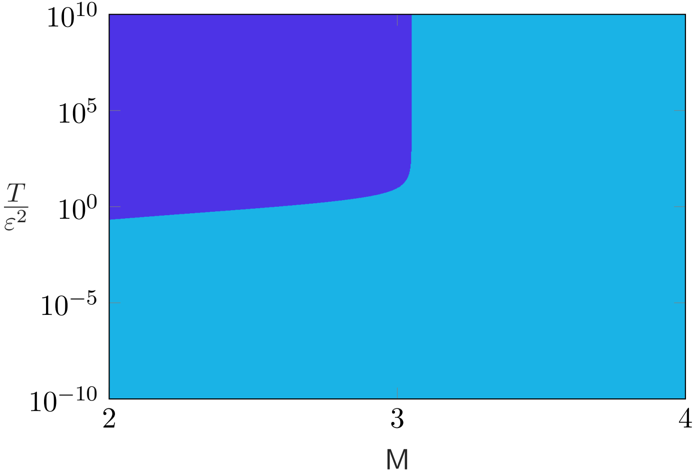
Applying MLMC to AP scheme: Results

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

Applying MLMC to AP scheme: Results

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

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