A micro-macro acceleration method for stiff stochastic differential equations (SDEs)

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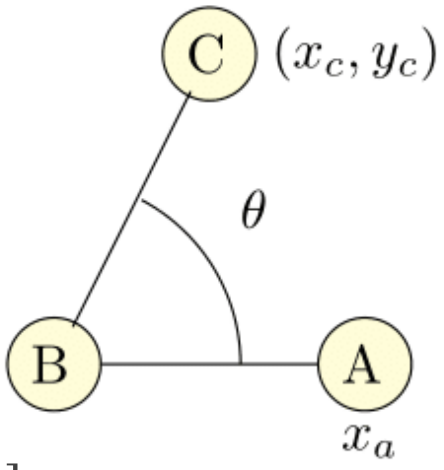
Stiff SDEs are ubiquitous

Stochastic differential equations of the form

$$dX(t) = a(X, t; \varepsilon)dt + b(X, t; \varepsilon)dW(t)$$

with ε a small-scale parameter and $W(t) \sim N(0, t)$ Brownian motion.

- Solve for the probability distribution of $X(t) \sim p(x, t)$
- High dimensional → Monte Carlo
- Individual paths vary fast $\mathrm{X}(\mathrm{t}; \omega, \varepsilon)$, $\omega \in \Omega$
- Mostly interested in slow *macroscopic state variables* $m_l(t) = \mathrm{E}\left[R_l\big(X(t)\big)\right]$



Applications in molecular dynamics

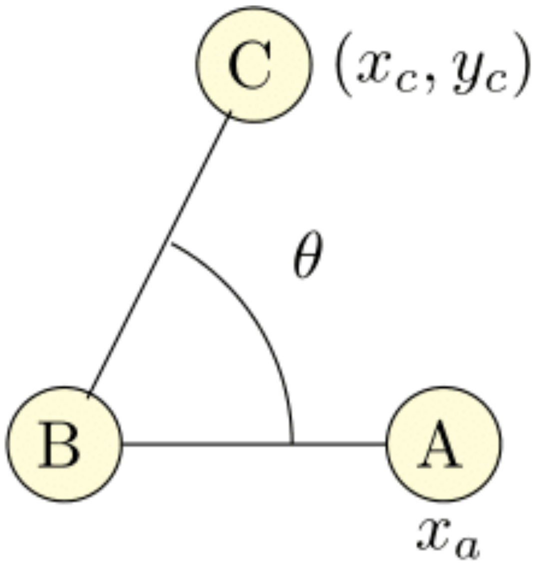
Important applications in molecular dynamics

$$dX(t) = -\nabla V(X(t))\,dt + \sqrt{2\beta^{-1}}\,\mathrm{dW(t)},$$

- $X = (x_a, x_c, y_c)$ positions of the atoms
- The potential energy $V(X)$ models interactions between atoms

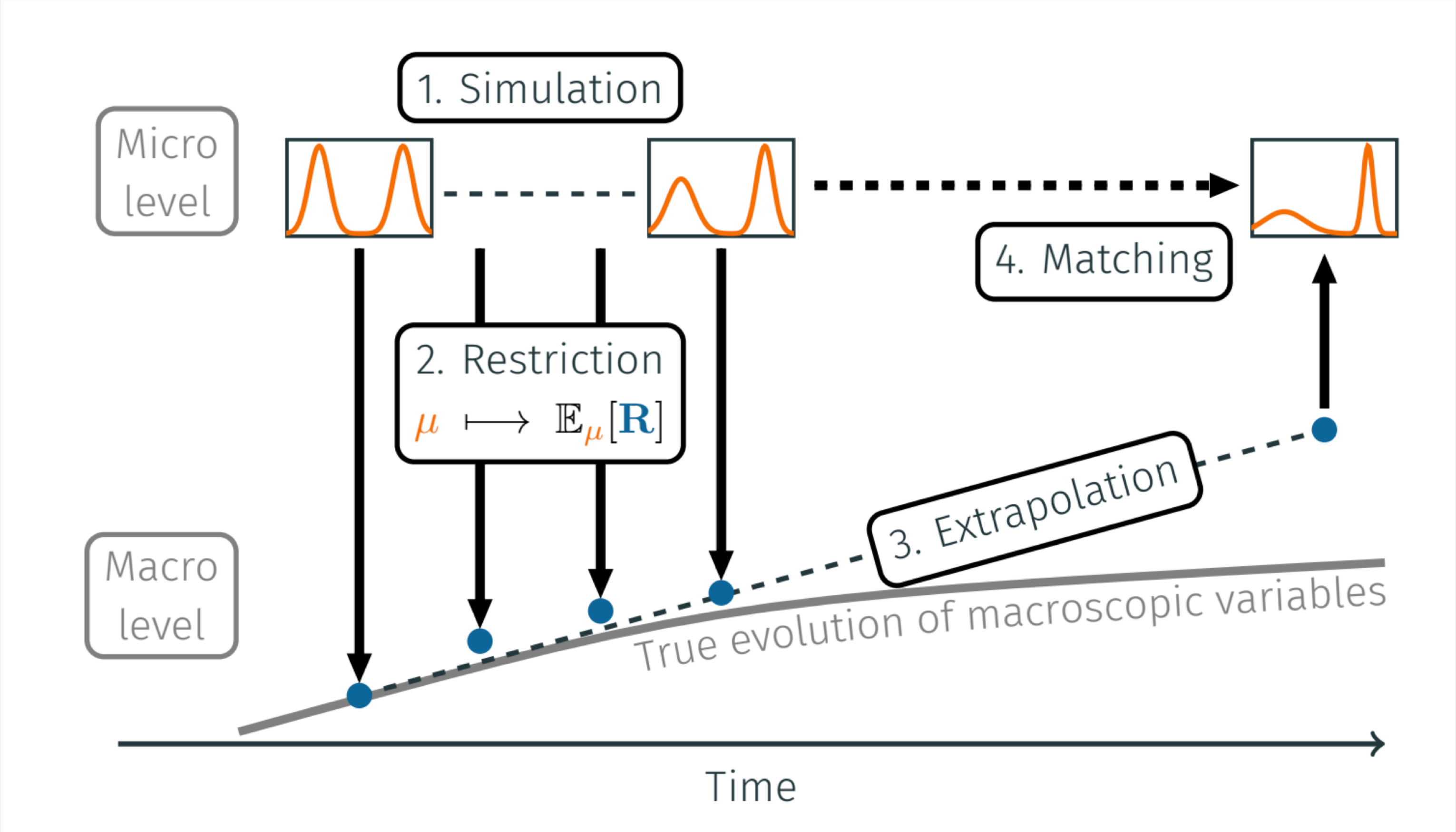
$$V(X) = \frac{1}{2\varepsilon}(x_a - 1)^2 + \frac{1}{2\varepsilon}\left(\sqrt{x_c^2 + y_c^2} - 1\right)^2 + \left(\theta - \frac{\pi}{2}\right)^2$$

- Brownian motion $W(t)$ models collisions with ambient solvent



A micro-macro acceleration method

Explicit methods have small stability domain, $\delta t = \mathcal{O}(\varepsilon)$



Efficiency of micro-macro acceleration

With micro-macro acceleration, we are able to *take larger time steps* than a microscopic method, while *attaining a good accuracy*

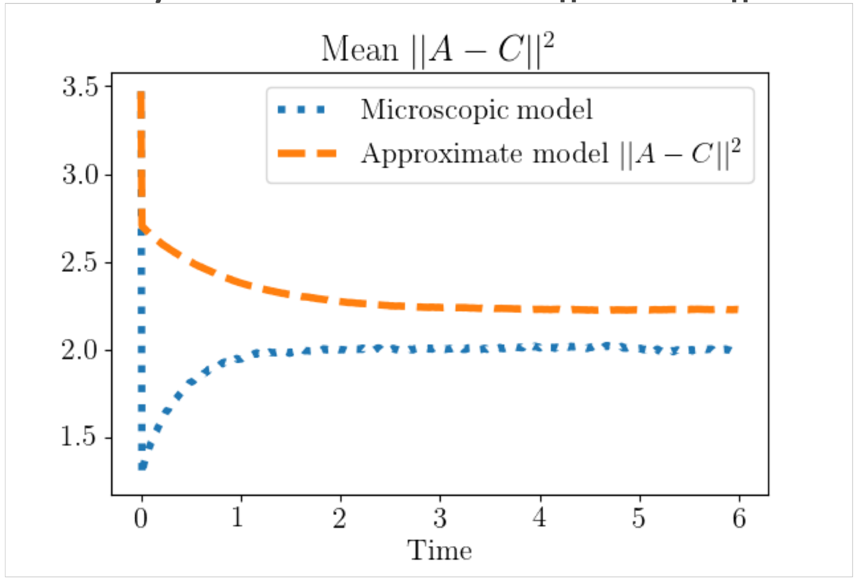
- Convergence to the microscopic dynamics as $\delta t, \Delta t \mapsto 0$
- Stability bound for extrapolation is independent of ε
- We have recently shown numerically that micro-macro acceleration can take larger $\Delta t \gg \delta t$ and attain accurate simulation results.

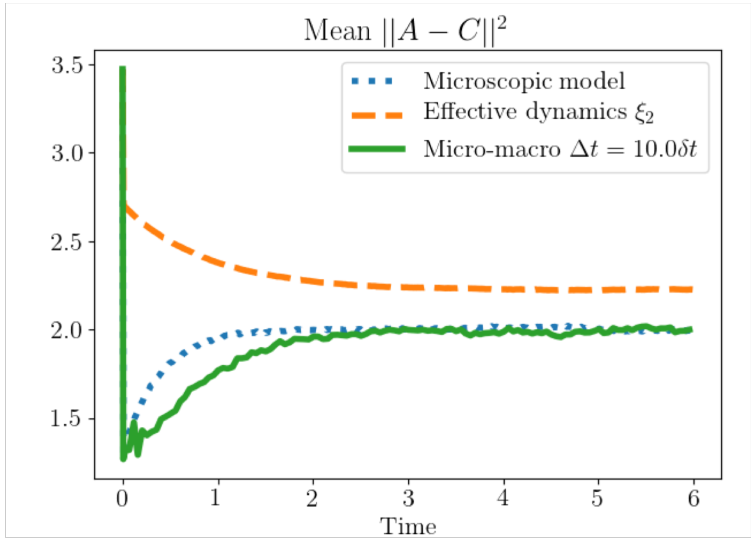
Efficiency of micro-macro acceleration

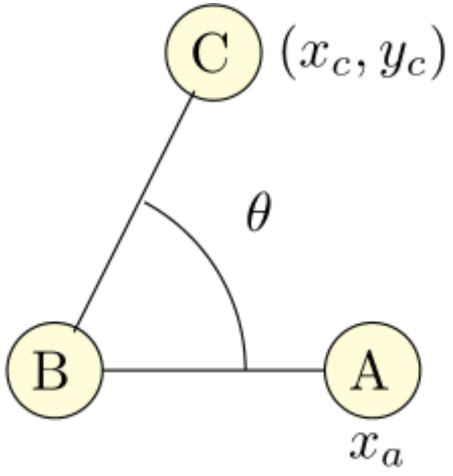
Consider again the three-atom molecule with

$$V(x_a, x_c, y_c) = \frac{1}{2\varepsilon}(x_a - 1)^2 + \frac{1}{2\varepsilon}\left(\sqrt{x_c^2 + y_c^2} - 1\right)^2 + \left(\theta - \frac{\pi}{2}\right)^2$$

We study the evolution of $\|A - C\|^2$







→ Extrapolation step is of the order of the time-scale separation

Thank you for your attention !