Efficiency of micro-macro acceleration for scale-separated SDEs

Hannes Vandecasteele[1], Przemysław Zieliński[1] and Giovanni Samaey[1]
[1]KU Leuven
Hannes.Vandecasteele@cs.kuleuven.be

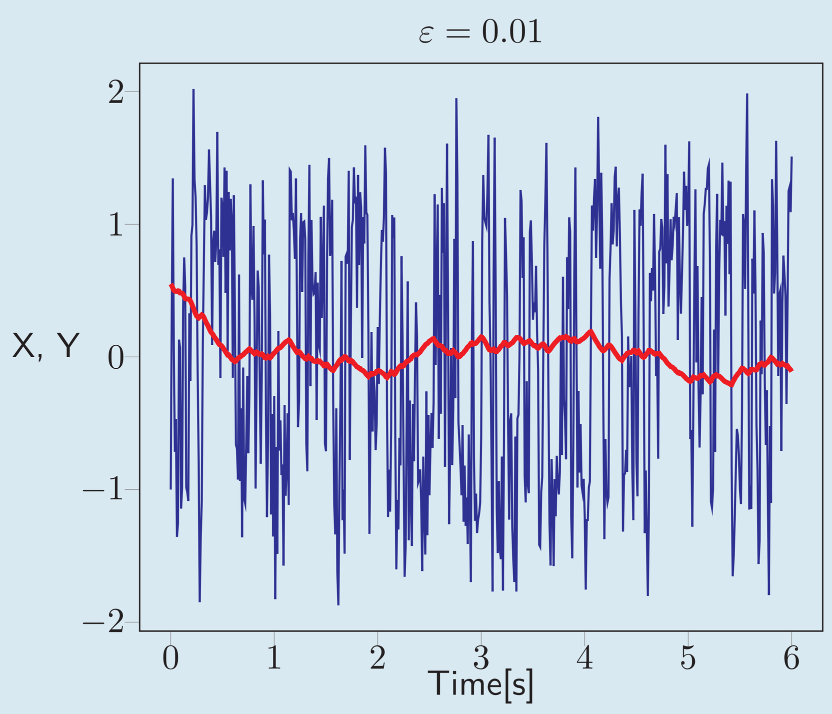
Problem Statement

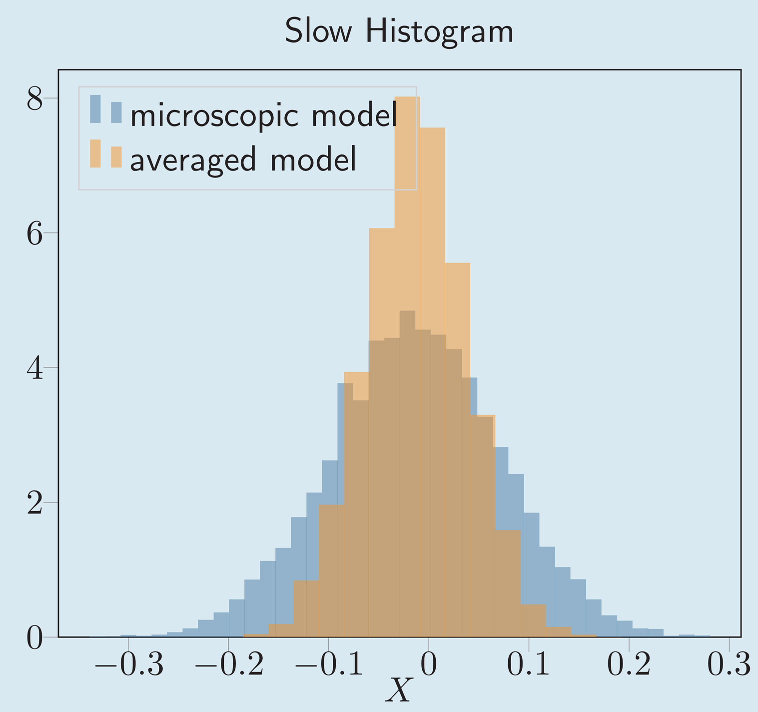
Many stochastic systems have an inherent multiscale nature due to a time-scale separation ε

$$dX = -(2X+Y)dt + AdW_x$$
$$dY = -\frac{1}{\varepsilon}(Y^3 - Y)dt + \frac{1}{\sqrt{\varepsilon}}dW_y$$

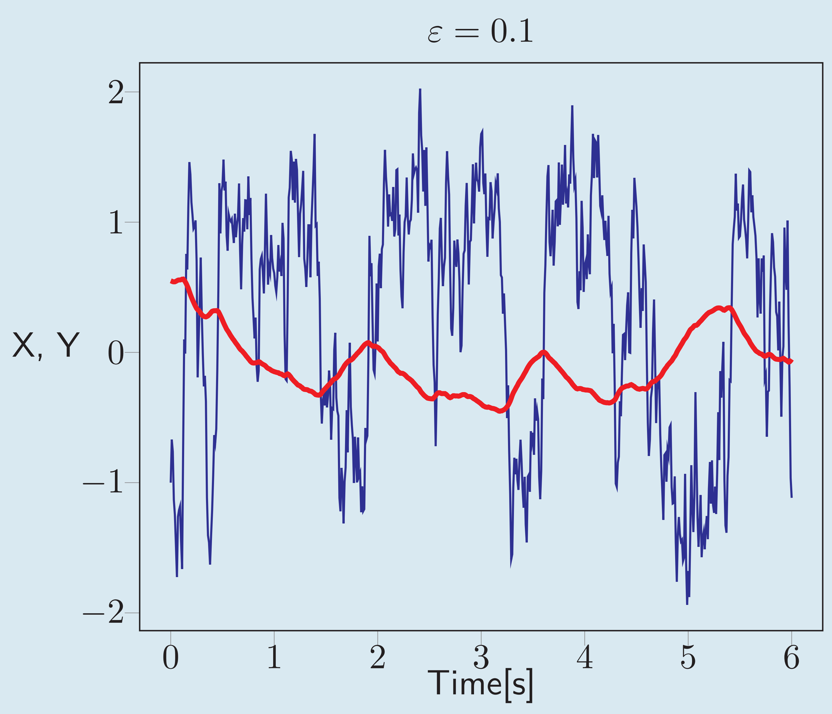
- When $\varepsilon \ll 1$, explicit methods are very inefficient. Averaging out the fast mode Y yields an approximate model for the slow mode X[2]

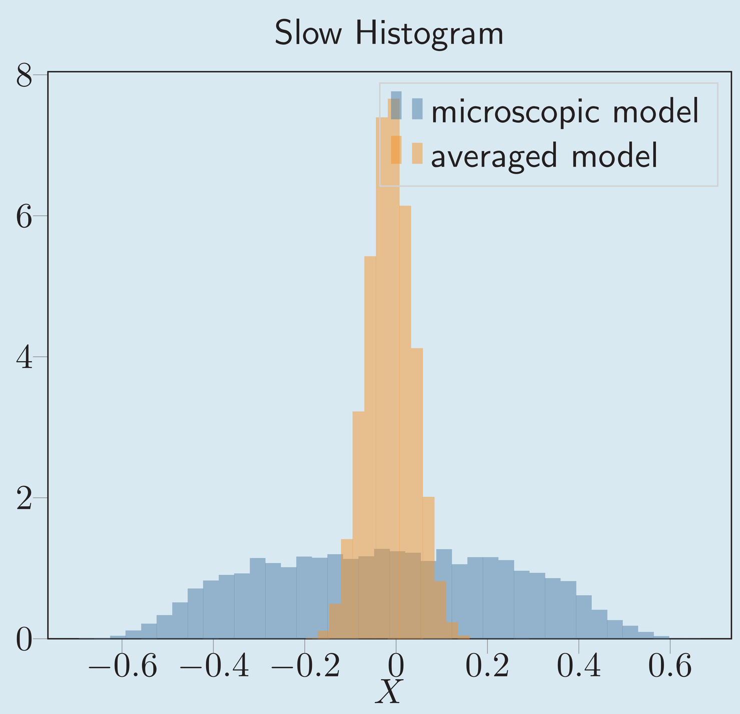
$$dX = -2Xdt + AdW$$





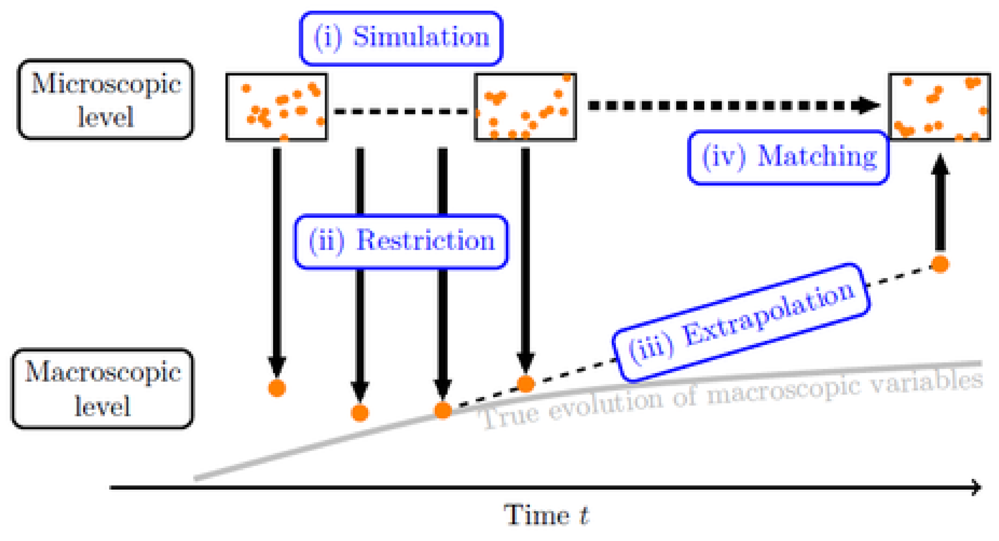
- For $\varepsilon \approx 1$ direct methods are accurate and efficient
- For intermediate ε, explicit methods are still expensive and the averaged model is inaccurate





Goal: remove the modelling error while dealing with the inherent multiscale nature

Micro-macro acceleration[1]

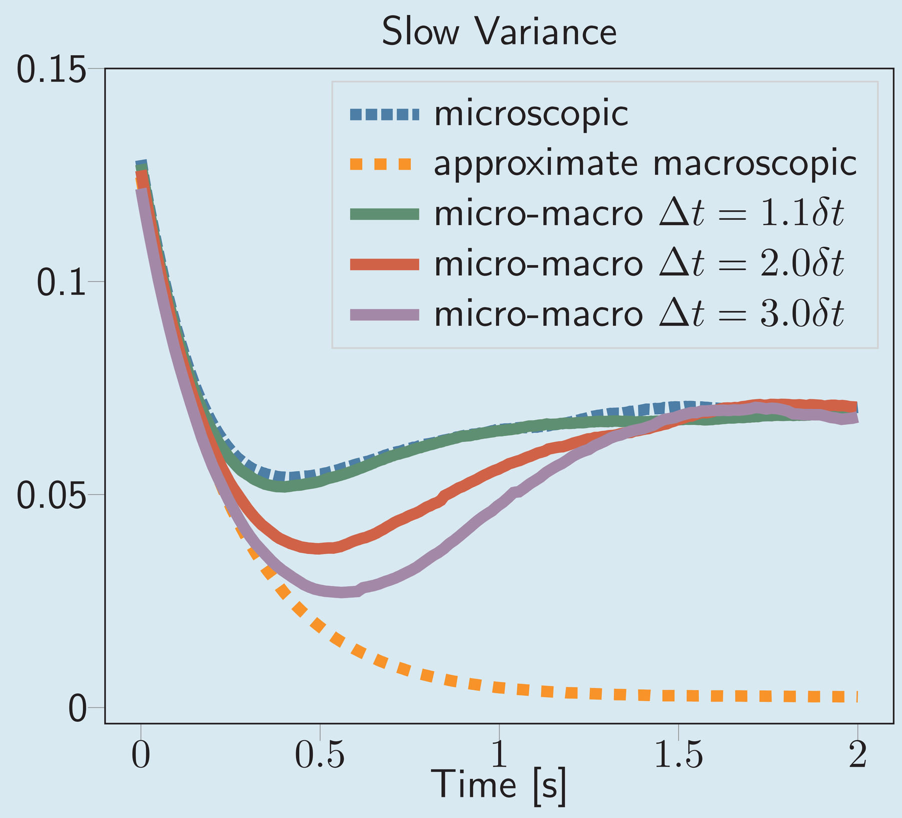


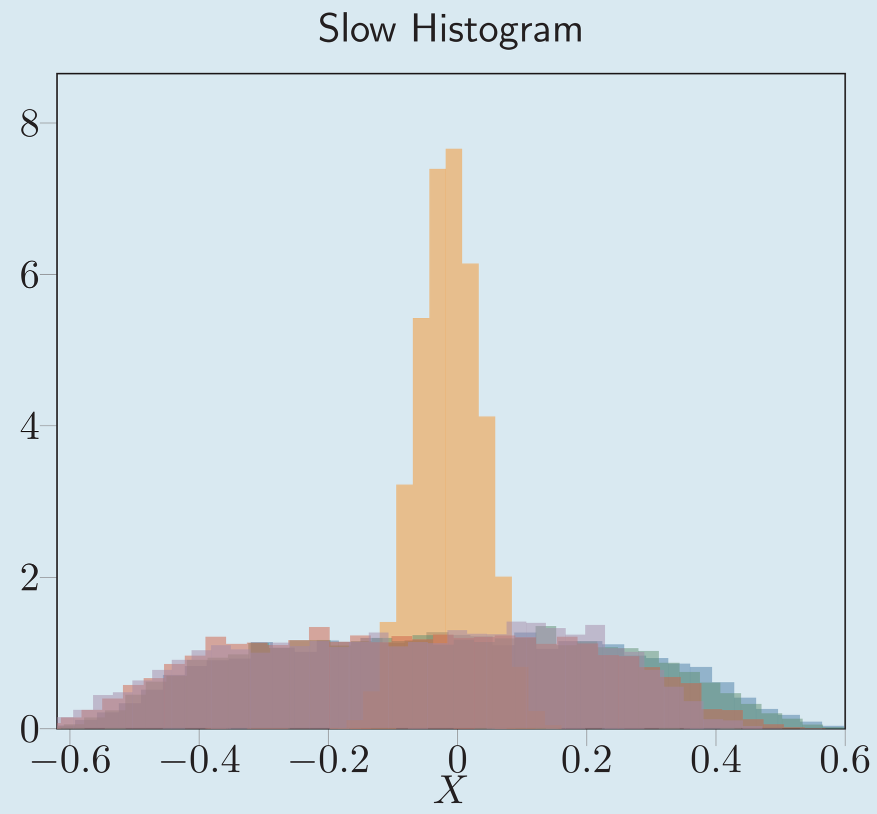
1. Simulate the Monte Carlo ensemble $(X_j^n)_j$ at time t^n over K microscopic steps of small step size δt
$$dX_j^{n,k+1} = X_j^{n,k} + a(X_j^{n,k})\delta t + b(X_j^{n,k})\delta W$$
2. Record the slow state funtions of interest R_l at every time step
$$m_l^{n,k} = \mathbb{E}[R_l(x)], \ l = 1, \ldots, L$$
3. Extrapolate these states over a larger time step Δt
$$\mathbf{m^{n+1}} = \mathbf{m^n} + \frac{\Delta t}{K\delta t}(\mathbf{m^{n,K}} - \mathbf{m^n})$$
4. Find a new distribution at time $t^{n+1} = t^n + \Delta t$, consistent with $\mathbf{m^{n+1}}$, minimizing the relative entropy
$$\varphi(x) = \underset{\varphi(x)}{\arg\min} \int_G \varphi(x) \ln\left(\frac{\varphi(x)}{\pi(x)}\right) dx.$$

This method converges to the exact dynamics when $\delta t, \Delta t \to 0$ and $L \to \infty$, and that the extrapolation stability bound is independent of δt and ε[3]

Numerical Results

For moderate ε, micro-macro acceleration removes the modelling error, while taking larger time steps than the microscopic integrator δt

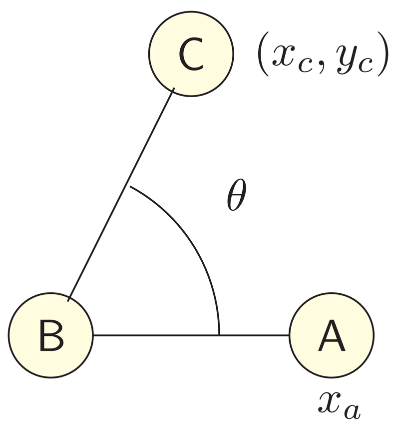




A tri-atom molecule

Consider a simple slow-fast molecule

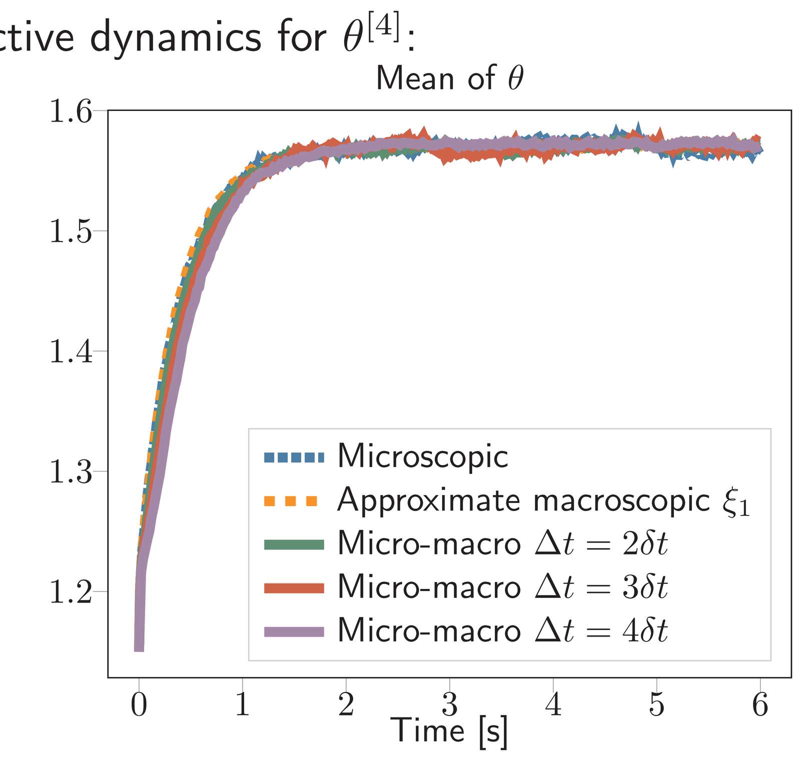
$$dx_a = -\frac{\partial V}{\partial x_a}dt + \sqrt{2\beta^{-1}}dW_{x_a}$$
$$dx_c = -\frac{\partial V}{\partial x_c}dt + \sqrt{2\beta^{-1}}dW_{x_c}$$
$$dy_c = -\frac{\partial V}{\partial y_c}dt + \sqrt{2\beta^{-1}}dW_{y_c}$$



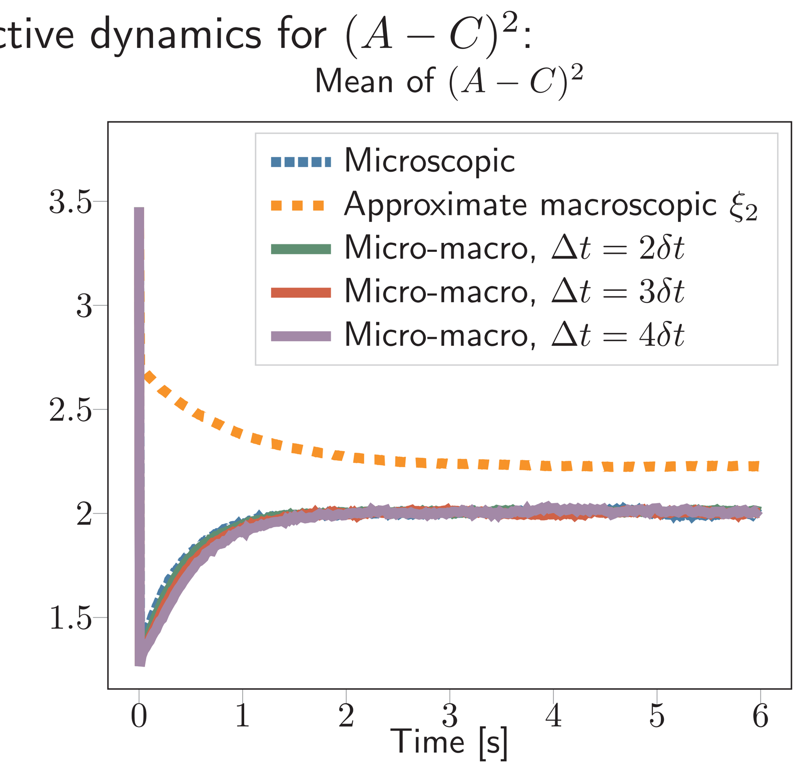
With a bimodal potential energy function

$$V = \frac{1}{2\varepsilon}\left((x_a-1)^2 + (r_c-1)^2\right) + \frac{k}{2}\left(\left(\theta - \frac{\pi}{2}\right)^2 - \delta\theta^2\right)$$

Effective dynamics for θ[4]:



Effective dynamics for $(A-C)^2$:



References

[1] DEBRABANT, Kristian; SAMAEY, Giovanni; ZIELINSKI, Przemysław. A micro-macro acceleration method for the Monte Carlo simulation of stochastic differential equations. SIAM Journal on Numerical Analysis, 2017, 55.6: 2745-2786.
[2] PAVLIOTIS, Grigoris; STUART, Andrew. Multiscale methods: averaging and homogenization. Springer Science & Business Media, 2008.
[3] DEBRABANT, Kristian; SAMAEY, Giovanni; ZIELINNSKI, Przemysław; Study of micro-macro acceleration schemes for linear slow-fast stochastic differential equations with additive noise , In preparation.
[4] LEGOLL, Frédéric; LELIEVRE, Tony. Effective dynamics using conditional expectations. Nonlinearity, 2010, 23.9: 2131.

KU Leuven
Department of Computer Science
Celestijnenlaan 200A box 2402
3001 Leuven, Belgium