A numerical study of a micro-macro MGRIT method for scale-separated SDEs

Ignace Bossuyt, Stefan Vandewalle, Giovanni Samaey

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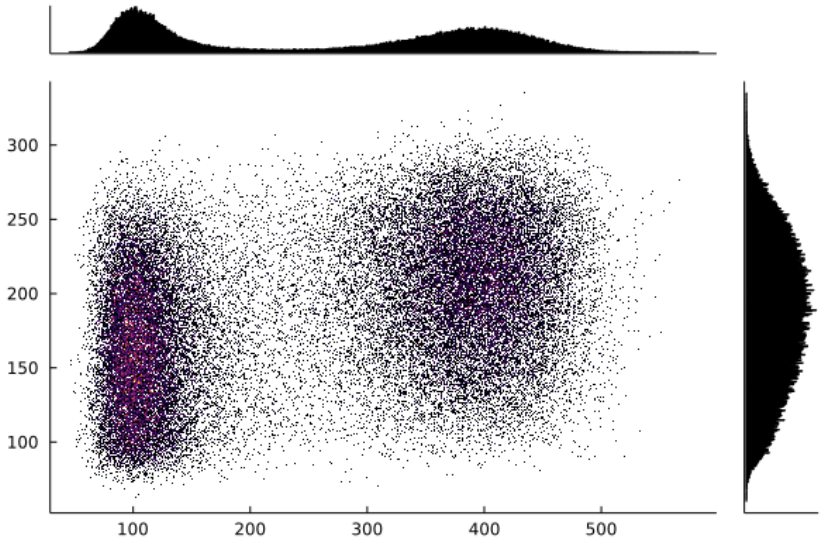
Context

(Multiscale) Molecular kinetics
Simulation of high-dimensional SDEs → Monte Carlo simulation

$$dX = a(X,Y)dt + s(X,Y)dW$$
$$dY = \frac{b(X,Y)}{\epsilon}dt + \frac{\tau(X,Y)}{\sqrt{\epsilon}}dZ$$

Quantity of Interest: moments/prob. density of slow variable $X(t)$



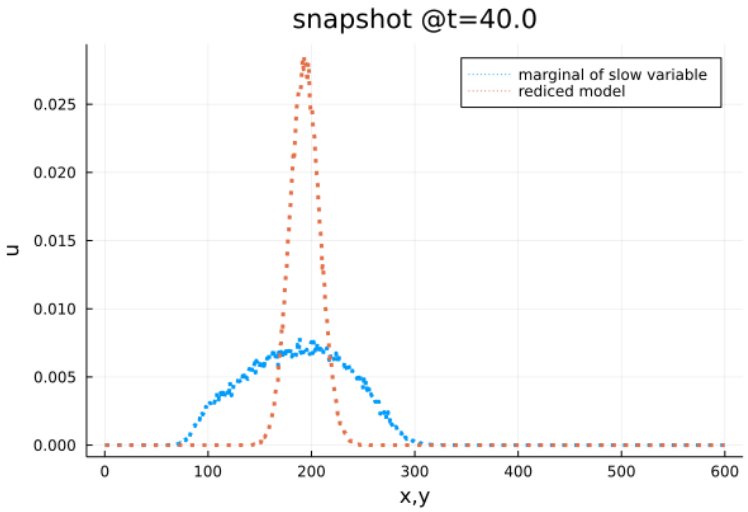
Context: reduced model

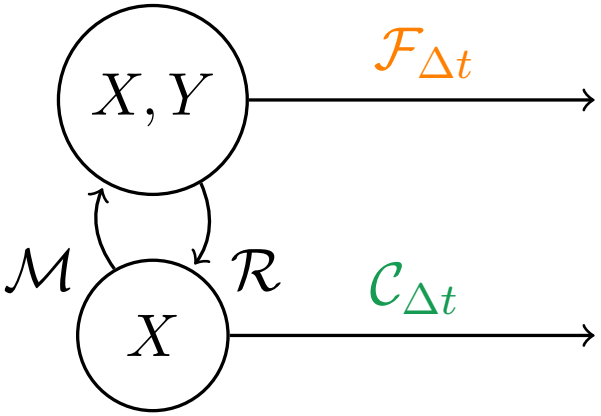
$\mathcal{F}_{\Delta t}$: High-dimensional slow-fast SDE:

$$\begin{aligned} dX &= a(X,Y)dt + s(X,Y)dW \\ dY &= \frac{b(X,Y)}{\epsilon}dt + \frac{\tau(X,Y)}{\sqrt{\epsilon}}dZ \end{aligned} \tag{1}$$

$\mathcal{C}_{\Delta t}$: We assume existence of formula for reduced model[1]

$$dX = A(X)dt + S(X)dW \tag{2}$$





[1] (Pavliotis and Stuart 2008)

Parareal [2]

Original parareal

$$u_{k+1}^{n+1} = \mathcal{C}_{\Delta t}(u_{k+1}^{n}) + \mathcal{F}_{\Delta t}(u_{k}^{n}) - \mathcal{C}_{\Delta t}(u_{k}^{n}) \tag{3}$$

Predictor:

$$u^{n-1} \xrightarrow{\mathcal{C}_{\Delta t}} u^{n} \xrightarrow{\mathcal{C}_{\Delta t}} u^{n+1} \xrightarrow{\mathcal{C}_{\Delta t}} u^{n+2}$$

Corrector (in parallel):

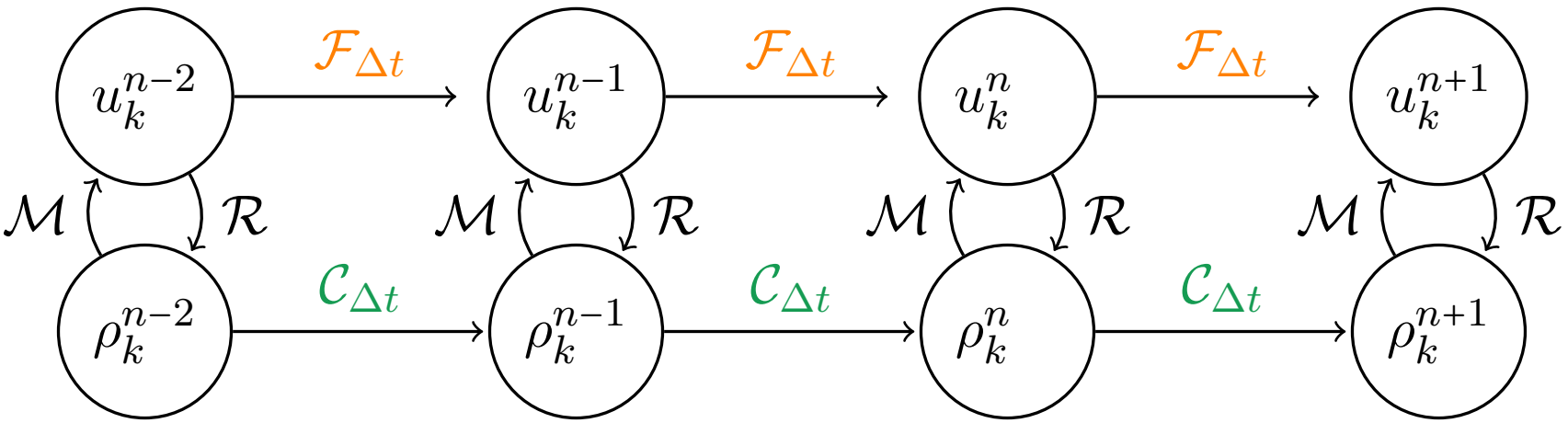
$$u_k^{n-1} \xrightarrow{\mathcal{F}_{\Delta t}} u_k^{n} \xrightarrow{\mathcal{F}_{\Delta t}} u_k^{n+1} \xrightarrow{\mathcal{F}_{\Delta t}} u_k^{n+2}$$

[2] (Lions, Maday, and Turinici 2001)

micro-Macro Parareal [3]

Original parareal $u_{k+1}^{n+1} = \mathcal{C}_{\Delta t}(u_{k+1}^{n}) + \mathcal{F}_{\Delta t}(u_k^n) - \mathcal{C}_{\Delta t}(u_k^n)$

micro-Macro Parareal



$$\rho_{k+1}^{n+1} = \mathcal{C}_{\Delta t}(\rho_{k+1}^{n}) + \mathcal{R}\mathcal{F}_{\Delta t}(u_k^n) - \mathcal{C}_{\Delta t}(\mathcal{R}u_k^n)$$
$$u_{k+1}^{n+1} = \mathcal{M}(\rho_{k+1}^{n+1}, \mathcal{F}_{\Delta t}(u_k^n))$$

[3] (Legoll, Lelièvre, and Samaey 2013), (Legoll, Lelièvre, Myerscough, and Samaey 2020)

1 Intro

2 mM-Parareal

3 Model error

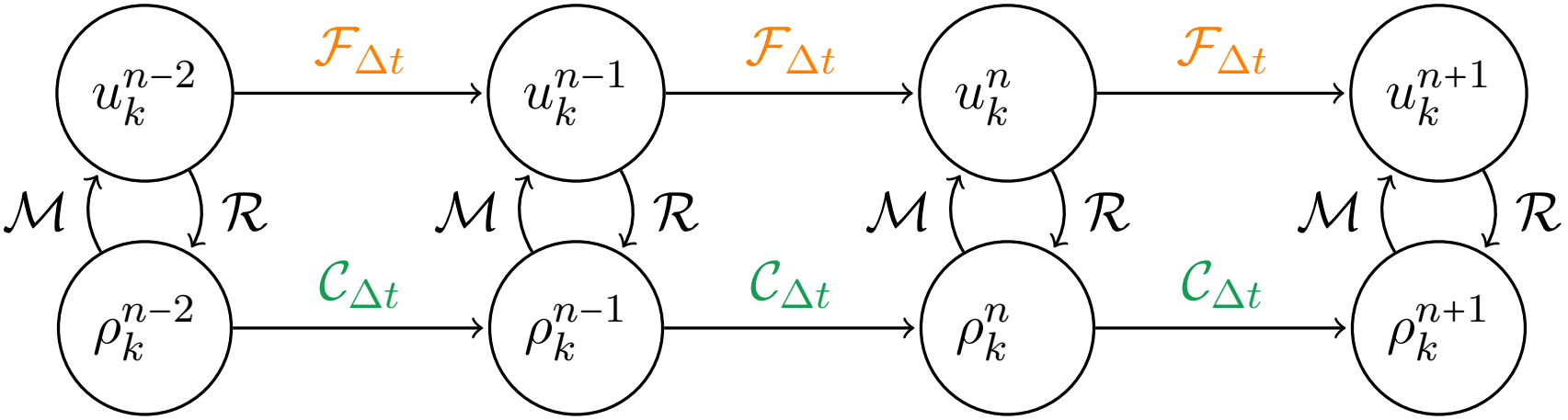
4 Linear ODE

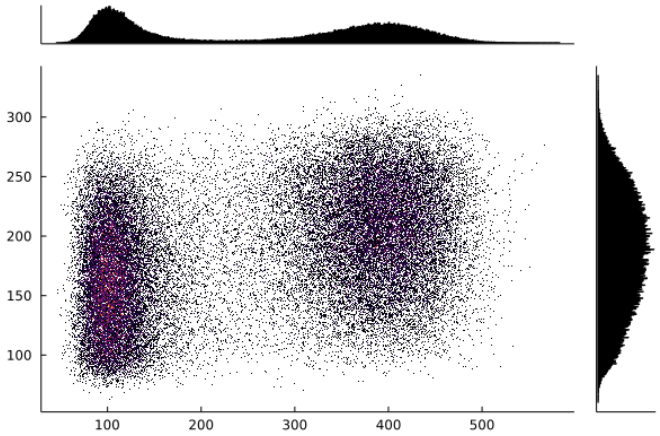
5 Linear SDE

6 Nonlinear SDE

7 Conclusion and outlook

Brief recap





- $\mathcal{F}_{\Delta t}(\cdot)$: highD model, MC simulation
- $\mathcal{C}_{\Delta t}(\cdot)$: reduced model
- Sources of error:
  - Timestep Δt vs. δt
  - Statistical error
  - **Model error**

Toy problem: perturbed Dahlquist equation

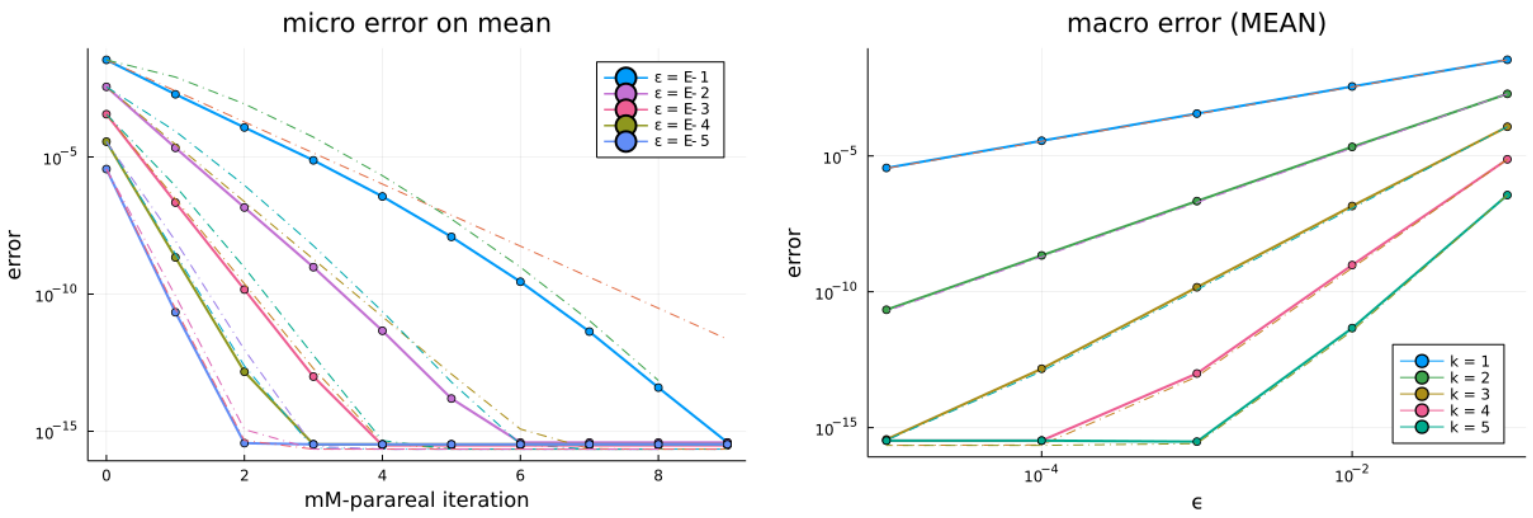
Dahlquist equation

$$\dot{u}(x,t) = \alpha u$$
$$u(t_0) = u_0$$

- $\mathcal{F}_{\Delta t}(u) = \exp(\alpha \Delta t) u$
- $\mathcal{C}_{\Delta t}(u) = \exp((\alpha + \epsilon)\Delta t) u$
- Error: ∞-norm over time

Toy problem: perturbed Dahlquist equation

- $\mathcal{F}_{\Delta t}(u) = \exp(\alpha \Delta t) u$
- $\mathcal{C}_{\Delta t}(u) = \exp((\alpha + \epsilon)\Delta t) u$



- Theoretical results on convergence behavior[4]
- Effect of *coupling operators* $\mathcal{M}$, $\mathcal{R}$ not considered

[4] Similar to convergence results in (Gander and Vandewalle 2007) and (Legoll, Lelièvre, and Samaey 2013)

Results: 2D SDE (moments) - 1D SDE (moments)

Linear Multiscale SDE

- $\mathcal{F}_{\Delta t}(\cdot)$: slow-fast Ornstein-Uhlenbeck

$$\begin{bmatrix} dx \\ dy \end{bmatrix} = \begin{bmatrix} \alpha & \beta \\ \gamma/\epsilon & \zeta/\epsilon \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} dt + \begin{bmatrix} \sigma_x & \sigma_{xy} \\ \sigma_{yx}/\sqrt{\epsilon} & \sigma_y/\sqrt{\epsilon} \end{bmatrix} dW$$

- $\mathcal{C}_{\Delta t}(\cdot)$: reduced model $dX = \left(\alpha - \frac{\beta\gamma}{\zeta}\right) X dt + \sigma_x dW$
- Instead of simulating SDE (Monte Carlo method), moment model for mean and variance[5]

[5] (Arnold 1974)

2D SDE (moments) - 1D SDE (moments) - linear

$\mathcal{F}_{\Delta t}$: multiscale system:

$$\begin{bmatrix} dx \\ dy \end{bmatrix} = \begin{bmatrix} \alpha & \beta \\ \gamma/\epsilon & \zeta/\epsilon \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} dt + \begin{bmatrix} \sigma_x & \sigma_{xy} \\ \sigma_{yx}/\sqrt{\epsilon} & \sigma_y/\sqrt{\epsilon} \end{bmatrix} dW$$

Moments:

$$\begin{aligned}
\frac{dm_x}{dt} &= \alpha m_x + \beta m_y \\
\frac{dm_y}{dt} &= \frac{\gamma}{\epsilon} m_x + \frac{\zeta}{\epsilon} m_y \\
\frac{d\Sigma_x}{dt} &= 2\left(\alpha \Sigma_x + \beta \Sigma_{xy}\right) + \sigma^2 \\
\frac{d\Sigma_y}{dt} &= 2\left(\frac{\zeta}{\epsilon}\Sigma_y + \frac{\gamma}{\epsilon}\Sigma_{xy}\right) + \frac{\sigma^2}{\epsilon} \\
\frac{d\Sigma_{xy}}{dt} &= \beta \Sigma_y + \frac{\gamma}{\epsilon}\Sigma_x + \left(\alpha + \frac{\zeta}{\epsilon}\right)\Sigma_{xy}
\end{aligned}$$

2D SDE (moments) - 1D SDE (moments) - linear

$\mathcal{C}_{\Delta t}$: reduced system:

$$dX = \left(\alpha - \frac{\beta\gamma}{\zeta}\right) X\,dt + \sigma_x dW$$

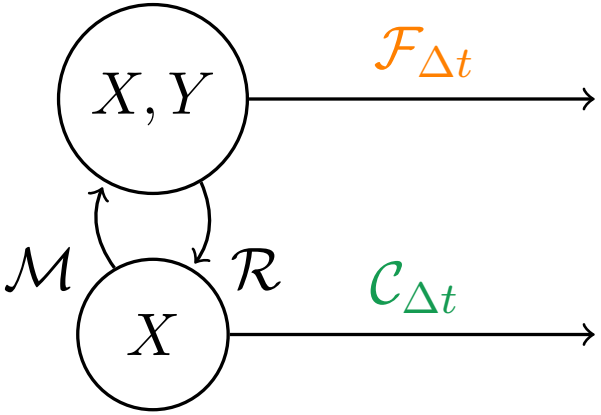
Moments:

$$\frac{dm_X}{dt} = \left(\alpha - \frac{\beta\gamma}{\zeta}\right) m_X$$

$$\frac{d\Sigma_X}{dt} = 2\left(\alpha - \frac{\beta\gamma}{\zeta}\right) \Sigma_X + \sigma_x^2$$

These moment models are exact for all initial conditions.

Results: 2D SDE (moments) - 1D SDE (moments)



- Restriction operator

$$\mathcal{R}\left(\begin{bmatrix} m_x & m_y & \Sigma_x & \Sigma_x & \Sigma_y & \Sigma_{xy} \end{bmatrix}\right) = \begin{bmatrix} m_x & \Sigma_x \end{bmatrix}$$

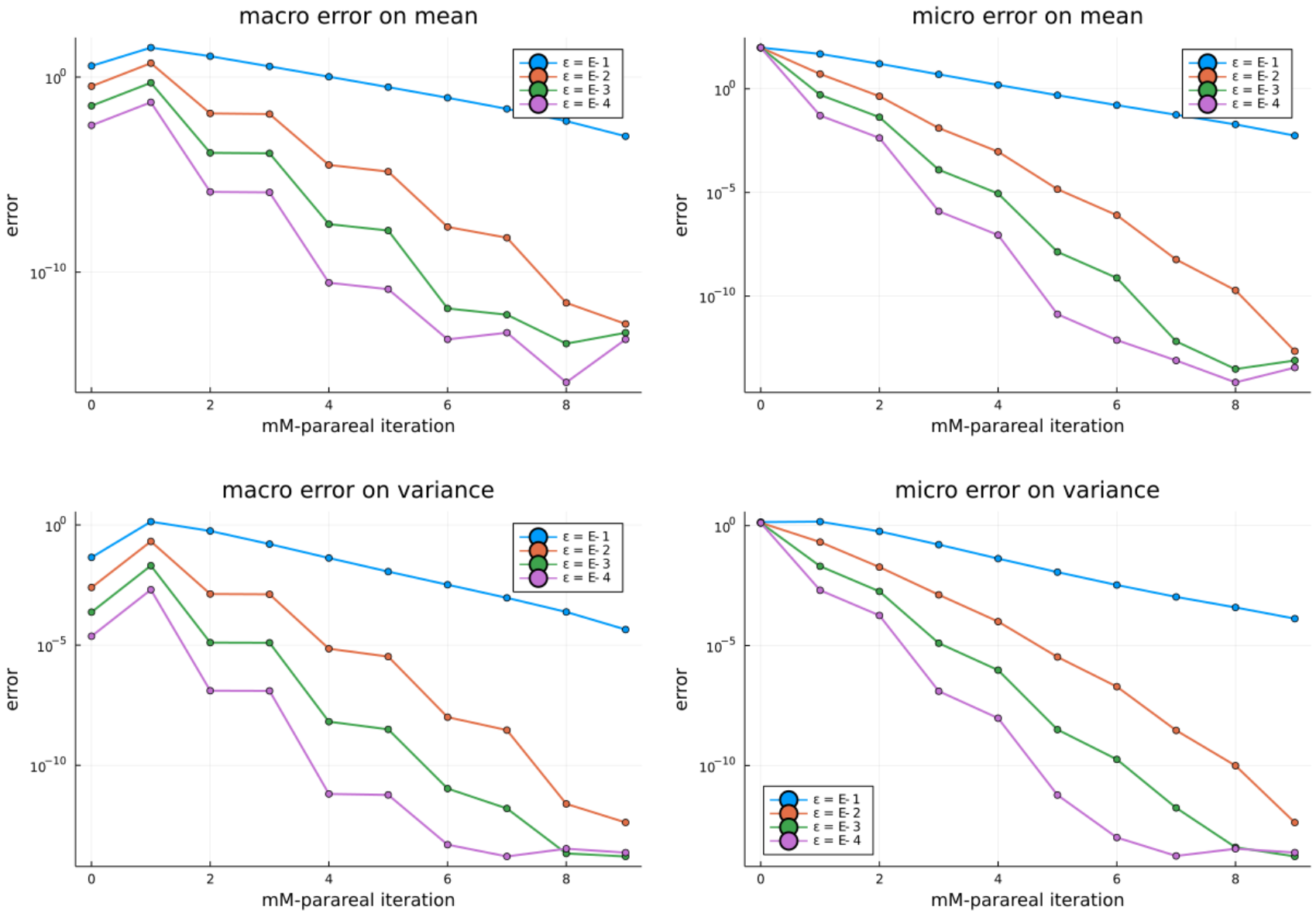
- Matching operator:

$$\mathcal{M}\left(\begin{bmatrix} M_X \\ S_X \end{bmatrix}, \begin{bmatrix} m_x \\ m_y \\ \Sigma_x \\ \Sigma_y \\ \Sigma_{xy} \end{bmatrix}\right) = \begin{bmatrix} M_X \\ m_y \\ S_X \\ \Sigma_y \\ \Sigma_{xy} \end{bmatrix}$$

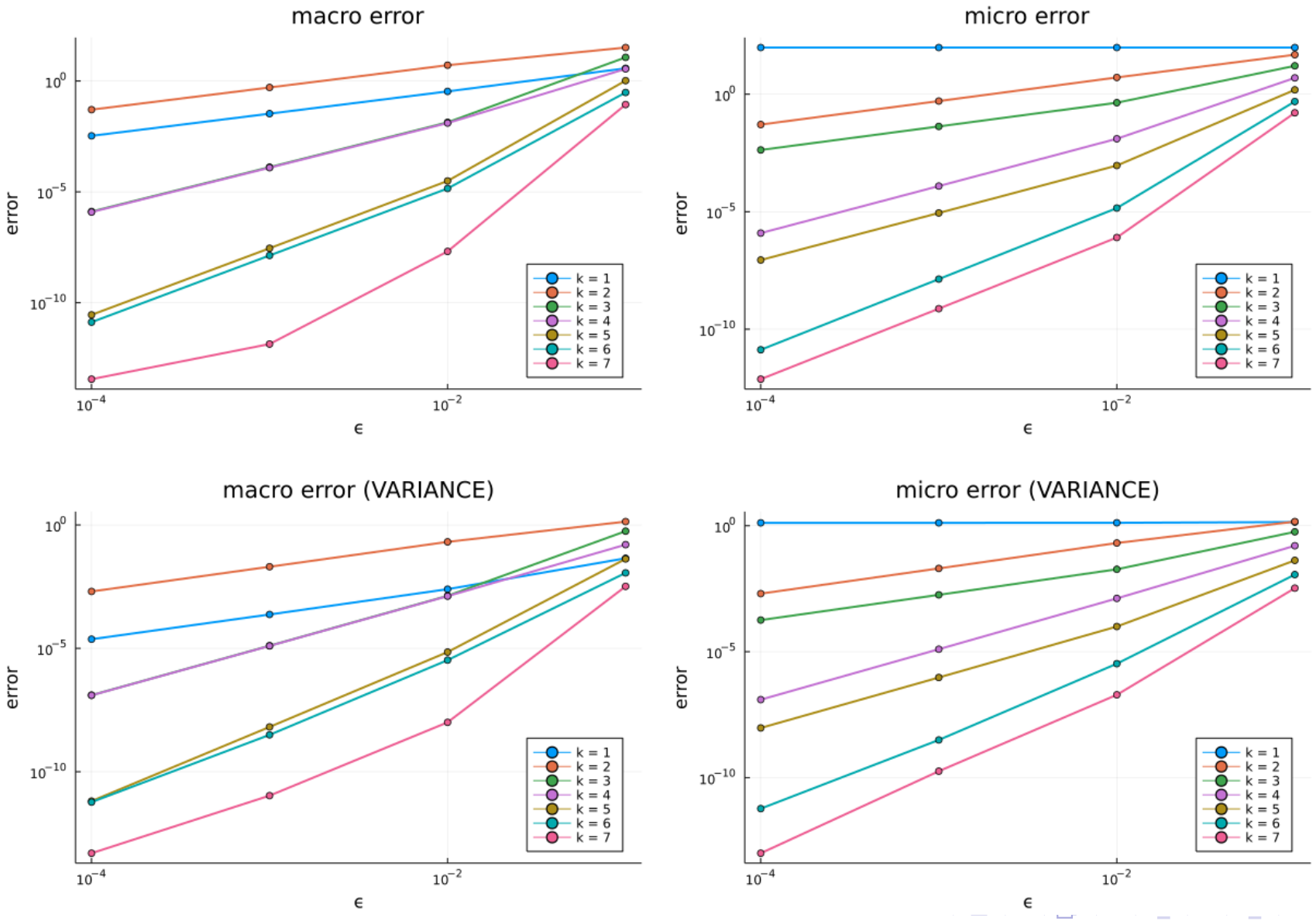
Results: 2D SDE (moments) - 1D SDE (moments)

- Error: ∞-norm over time
- Micro-error: error on full state variable $\begin{bmatrix} m_x & m_y & \Sigma_x & \Sigma_x & \Sigma_y & \Sigma_{xy} \end{bmatrix}$
- Macro error: error on macro variables $\begin{bmatrix} m_x & \Sigma_x \end{bmatrix}$

Results: 2D SDE (moments) - 1D SDE (moments)



Results: 2D SDE (moments) - 1D SDE (moments)



Results: 2D SDE - 1D SDE (nonlinear)

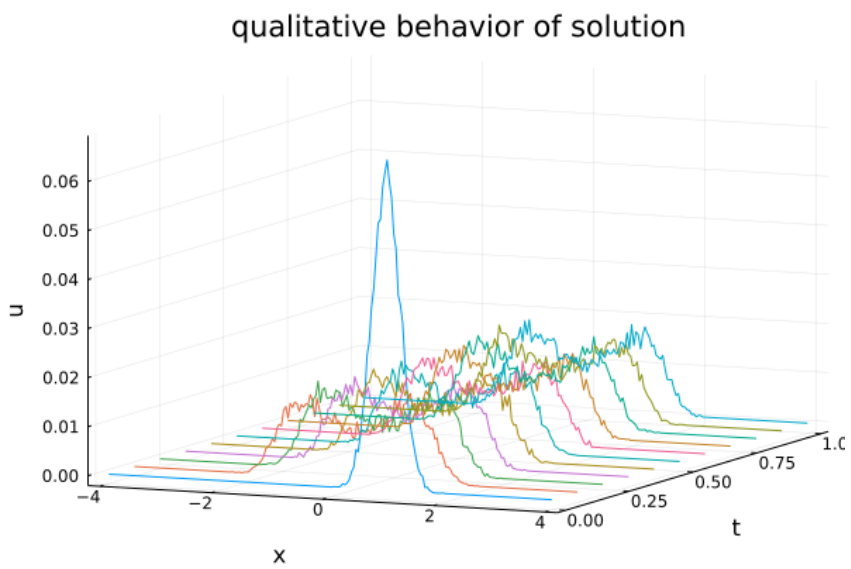
Nonlinear Equation Multiscale model

$$dx = (-2x + y)dt + 0.1dW$$

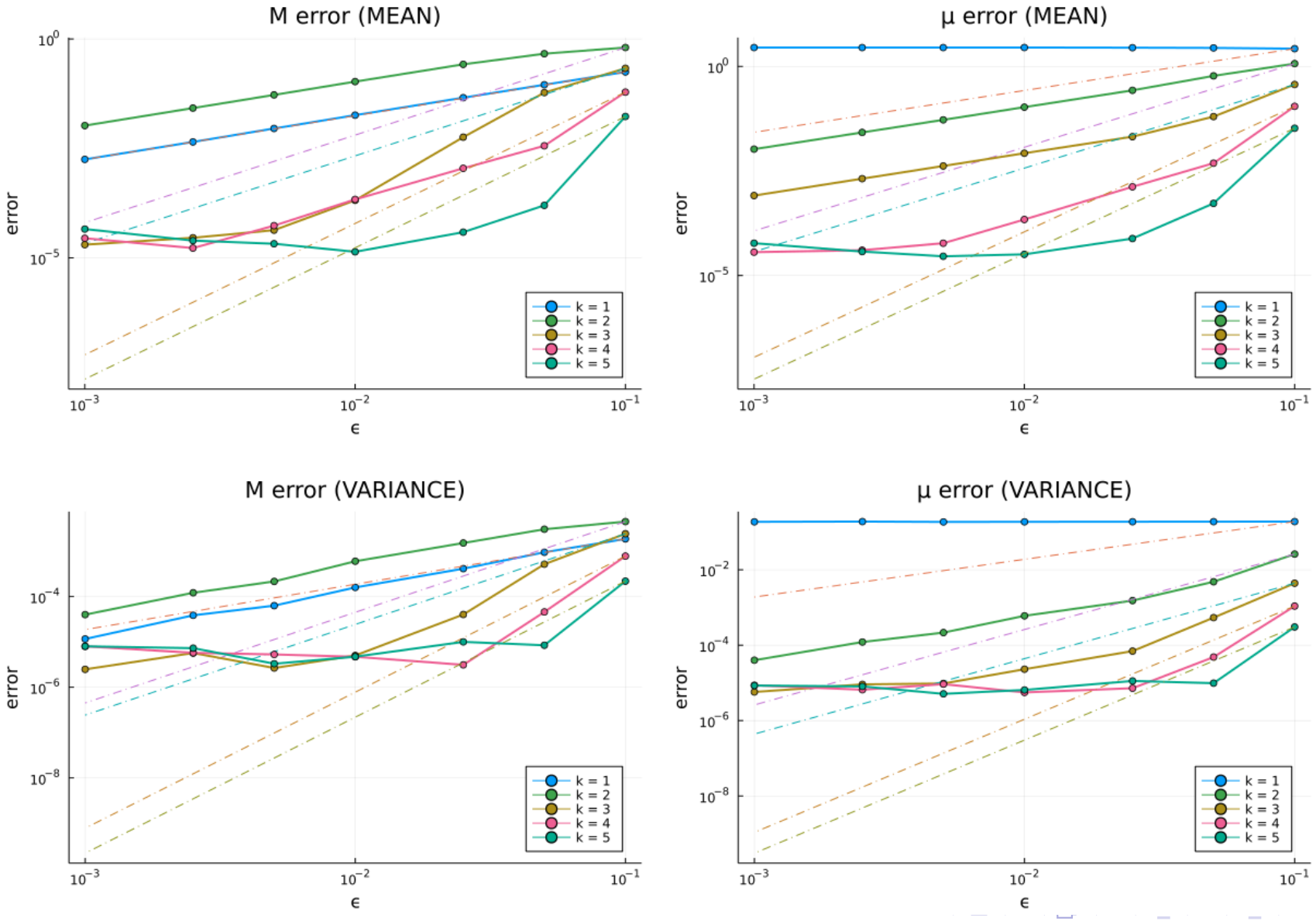
$$dy = \frac{y - y^3}{\epsilon}dt + \frac{1.0}{\sqrt{\epsilon}}dW_y$$

Reduced model

$$dX = -2Xdt + 0.1dW$$



Results: 2D SDE - 1D SDE (nonlinear)



Conclusion and outlook

Conclusion:

- Interest in high-dimensional sytems: MC simulation.
- Cheap coarse integrators → hope to improve efficiency.
- Convergence of mM-parareal for SDEs is not fully understood. Studying the **effect of model error** looks interesting.

Current work:

- Effect of model errors on convergence: theoretical analysis
- Experiments with nonlinear drift/diffusion coeffcients

Outlook:

- Put everything together in **3-level method**
  - → Slow-fast system - Reduced system - Moment model
- Other challenges: theory on convergence, adaptivity

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[9] Roger Rodriguez and Henry C. Tuckwell. 'Statistical properties of stochastic nonlinear dynamical models of single spiking neurons and neural networks'. en. In: Physical Review E 54.5 (Nov. 1996), pp. 5585–5590. ISSN: 1063-651X, 1095-3787. DOI: 10.1103/PhysRevE.54.5585.

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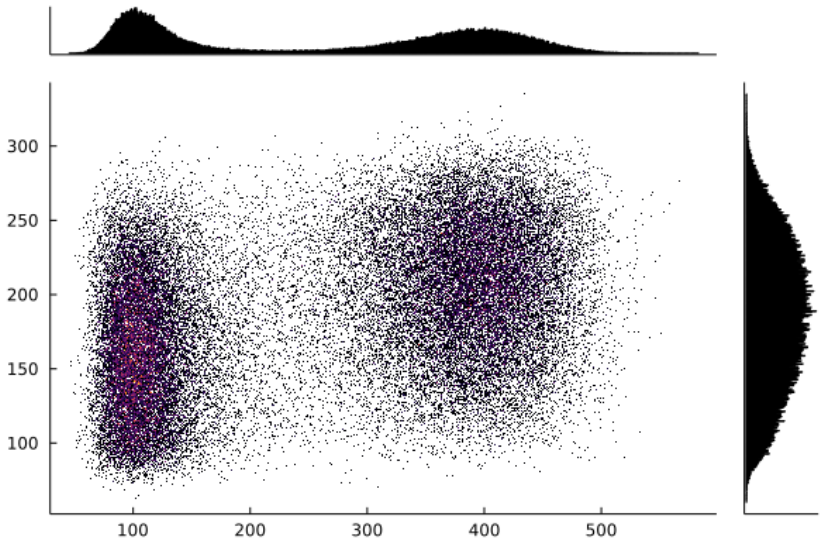

Thank you for attending!

You may overload me now with questions and suggestions/comments.
Always happy to discuss ☺.

`ignace.bossuyt1@kuleuven.be`