micro-Macro parareal: exploratory analysis of the effect of reduced models in parallel-in-time PDE simulation

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In a Nutshell

Motivation Parallel-in-time (PinT) methods have the potential to speed up PDE simulations on massively parallel computers. We analyse convergence of mM-parareal as a candidate for multiscale PinT simulation

Goal Exploratory (numerical) analysis of the effect of reduced models in parallel-in-time PDE simulation

Model 1D/2D slow-fast Ornstein-Uhlenbeck process

Method Numerical experiments: Julia implementation

mM-parareal method

- Iterative method to accelerate timestepping simulation
- **Classical parareal** [LMT01]

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

where n is timestep index, k is iteration index, $\mathcal{C}_{\Delta t}$ is a coarse (cheap) propagator, $\mathcal{F}_{\Delta t}$ is a fine propagator

- **micro-Macro parareal** [LLS13]

$$\rho_{k+1}^{n+1} = \mathcal{J}(\mathcal{C}_{\Delta t}(\rho_{k+1}^{n}),\ \mathcal{R}\mathcal{F}_{\Delta t}(\mathcal{X}_k^n),\ \mathcal{C}_{\Delta t}(\mathcal{R}\mathcal{X}_k^n))$$
$$\mathcal{X}_{k+1}^{n+1} = \mathcal{M}(\mathcal{X}_{k+1}^{n+1}, \rho_{k+1}^{n+1})$$

- ρ_k^n macroscopic state, $\mathcal{X}_k^n$ microscopic state
- $\mathcal{R}(\mathcal{X})$: **restriction operator** transfers the micro state $\mathcal{X}$ to the macro level
- $\mathcal{M}(\mathcal{X}, \rho)$: **matching operator** modifies micro state $\mathcal{X}$ in order to be compatible with a given macro state ρ
- $\mathcal{J}(\rho_1, \mathcal{X}, \rho_2)$: **iteration operator** defines updating formula. In classical parareal: $\mathcal{J}(\rho_1, \mathcal{X}, \rho_2) = \rho_1 + \mathcal{X} - \rho_2$

Slow-fast Systems

- **Slow-fast SDEs** (time scale separation parameter ϵ)

$$\frac{dx}{dt} = f(x,y) + \alpha(x,y)\frac{dU}{dt}$$
$$\frac{dy}{dt} = \frac{1}{\epsilon}g(x,y) + \frac{1}{\sqrt{\epsilon}}\beta(x,y)\frac{dV}{dt}$$

- Corresponding slow-fast PDE (Fokker-Planck equation): $\mu(x,y)$ is the joint probability density

$$\frac{\partial \mu}{\partial t} = \left[\frac{\partial f\mu}{\partial x} + \frac{\partial^2 \alpha\mu}{\partial x^2}\right] + \frac{1}{\epsilon}\left[\frac{\partial g\mu}{\partial y} + \frac{\partial^2 \beta\mu}{\partial y^2}\right]$$

Reduced models: averaging

- Assumption: the fast dynamics y possess an invariant distribution $\rho^\infty(y;x)$
- **Reduced SDE** [PS08]

$$dx = \bar{F}(x)dt + \sqrt{2\bar{D}(x)}dW$$

- PDE equivalent

$$\frac{\partial \rho}{\partial t} = \left[\frac{\partial \bar{F}(x)\rho}{\partial x} + \frac{\partial^2 \bar{D}(x)\rho}{\partial x^2}\right]$$

→ $F(x) = \int_{\mathcal{Y}} f(x,y)\rho^\infty(y,x)dy$

→ $A(X)A(X)^T = \int_{\mathcal{Y}} \alpha(x,y)\alpha(x,y)^T\rho^\infty(y,x)dy$

Ornstein-Uhlenbeck (OU) process

- Definition of n-dimensional OU process

$$dX = -\lambda X dt + \sigma dW$$

where $\lambda, \sigma \in \mathbb{R}^{n\times n}$ and $X, dW \in \mathbb{R}^n$

- **Analytical solution: 0D *moment models***
  * Gaussian distributions remain Gaussian
    → simple evolution law for mean and (co)variance
  * Mean: $\mu(t) = e^{-\lambda t}X_0$
  * (Co)variance:

$$\Sigma(t) = e^{-\lambda t}\Sigma(0)e^{-\lambda^T t} + \int_0^t e^{\lambda(s-t)}\sigma\sigma^T e^{\lambda^T(s-t)}ds$$

micro-Macro parareal: example

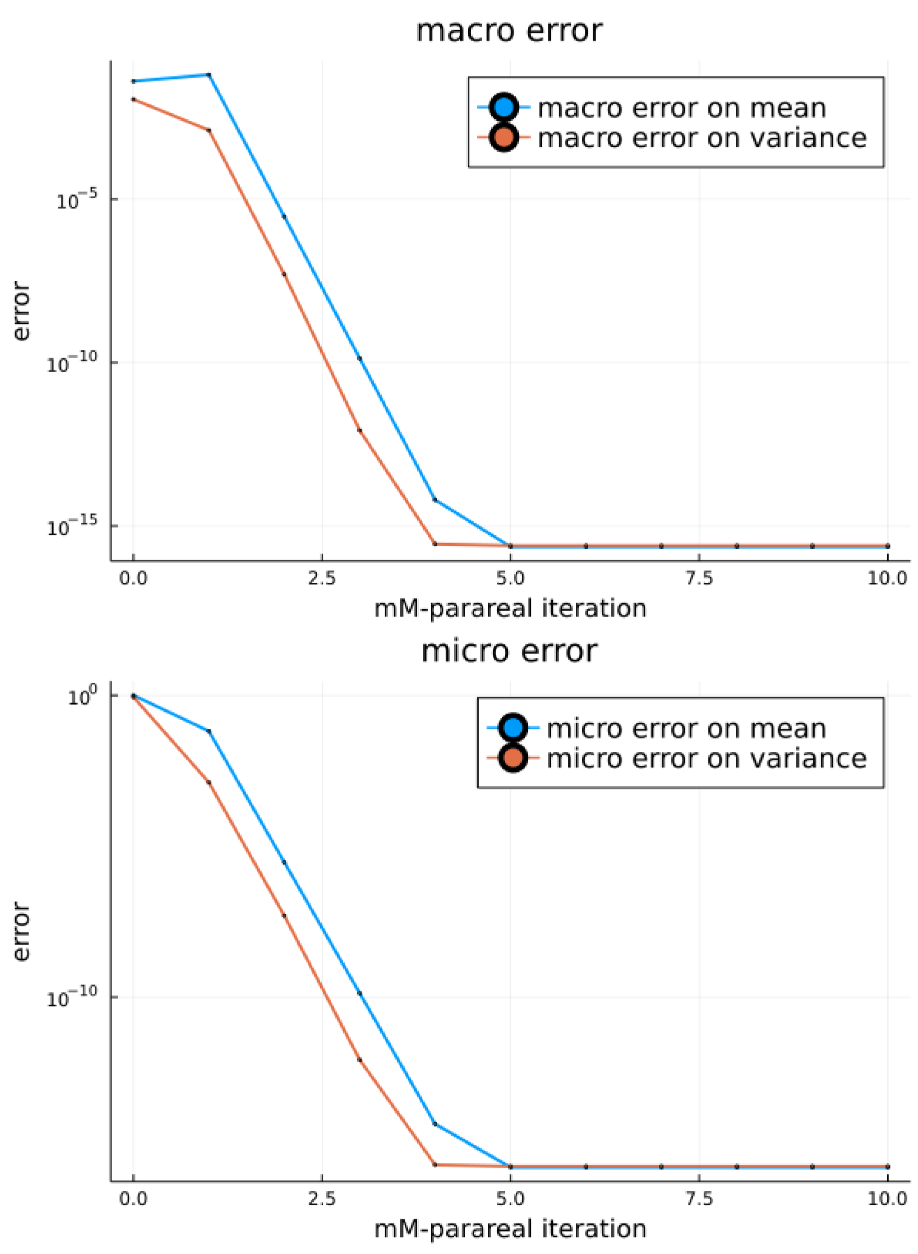
Model parameters

$$\lambda = \begin{pmatrix}1 & 0\\ 0 & 1/\epsilon\end{pmatrix}, \quad \sigma = \begin{pmatrix}1 & 0\\ 0 & 1/\sqrt{\epsilon}\end{pmatrix}$$

* Model error (mean/covariance of the 2D model vs. mean/variance of 1D reduced model) behaves as $\mathcal{O}(\epsilon)$ as $\epsilon \to 0$
* Chosen time scale separation parameter $\epsilon = 0.1$

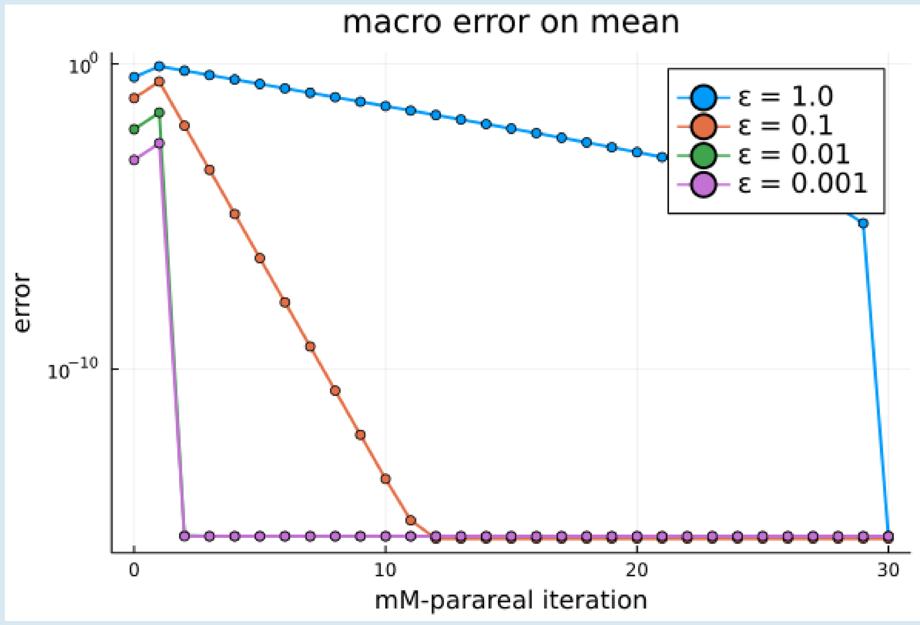
mM-parareal parameters

* **Fine propagator** $\mathcal{F}_{\Delta t}$: 0D *moment model* for mean μ and covariance Σ of the full 2D model
* **Coarse propagator** $\mathcal{C}_{\Delta t}$: 0D *moment model* for mean μ_{macro} and variance Σ_{macro} of the reduced 1D model
* $\mathcal{R}$: restriction operator selects marginal mean $\mu_{\text{macro}} = \mu[1]$ and marginal variance $\Sigma_{\text{macro}} = \Sigma[1,1]$
* $\mathcal{M}$: matching operator leaves the fast mean/variance untouched, while replacing $\mu[1] \leftarrow \mu_{\text{macro}}$ and $\Sigma[1,1] \leftarrow \Sigma_{\text{macro}}$
* $\mathcal{J}$: classical parareal iteration operator, applied to μ_{macro} and Σ_{macro}
* Number of coarse timesteps $N = 10$



Effect of time scale separation

Experiment parameters: $N = 30$, other parameters identical to example



- Models with large time scale separation converge faster
- The convergence above is a best scenario indication for convergence of mM-parareal on the OU process

Conclusions

Summary * mM-parareal convergence depends on the scale-separation parameter ϵ

* mM-parareal might be effective in the parallel-in-time simulation of multiscale PDEs, especially for models with big time-scale separation

Future work * Numerical experiments with non-Gaussian initial condition and other (more general) driving processes (the 0D *moment models* are only exact with Gaussian initial condition)

* Study effect of using more informative reduced models (e.g. modeling the full probability density) on convergence of mM-parareal
* Apply Monte Carlo simulation for the fine model
  → study additional effect of stochastic error on mM-parareal convergence

Thank you for taking a look at this poster!

References

[LLS13] Frédéric Legoll, Tony Lelièvre, and Giovanni Samaey. "A micro-macro parareal algorithm: application to singularly perturbed ordinary differential equations". In: *SIAM journal on scientific computing* 35.4 (2013), A1951–A1986.

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