Semi-intrusive Uncertainty Quantification for Multiscale models

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Abstract

- Sub-models on micro scales usually represent the most computationally intensive part of multiscale models.
- Our goal is to reduce the computation time spent on uncertainty quantification of multi-scale models.
- We exploit the multiscale nature of the model and limit the inspection of the multiscale model up to the level of the subscale systems.

Multiscale modeling

Consider a PDE of the form

$$\frac{\partial u(x,t,\xi)}{\partial t} = \mathcal{L}(u(x,t,\xi),\xi),$$

where $\mathcal{L}$ is an operator acting in the space variable, and ξ denotes n-dimensional space of uncertain input. The analytical solution of this PDE satisfies

$$u(x,t+\Delta t,\xi) = e^{\Delta t \mathcal{L}} u(x,t,\xi).$$

Let us assume for $\mathcal{L}$ a two-term splitting:

$$\mathcal{L} = \mathcal{L}^{\mu} + \mathcal{L}^{M},$$

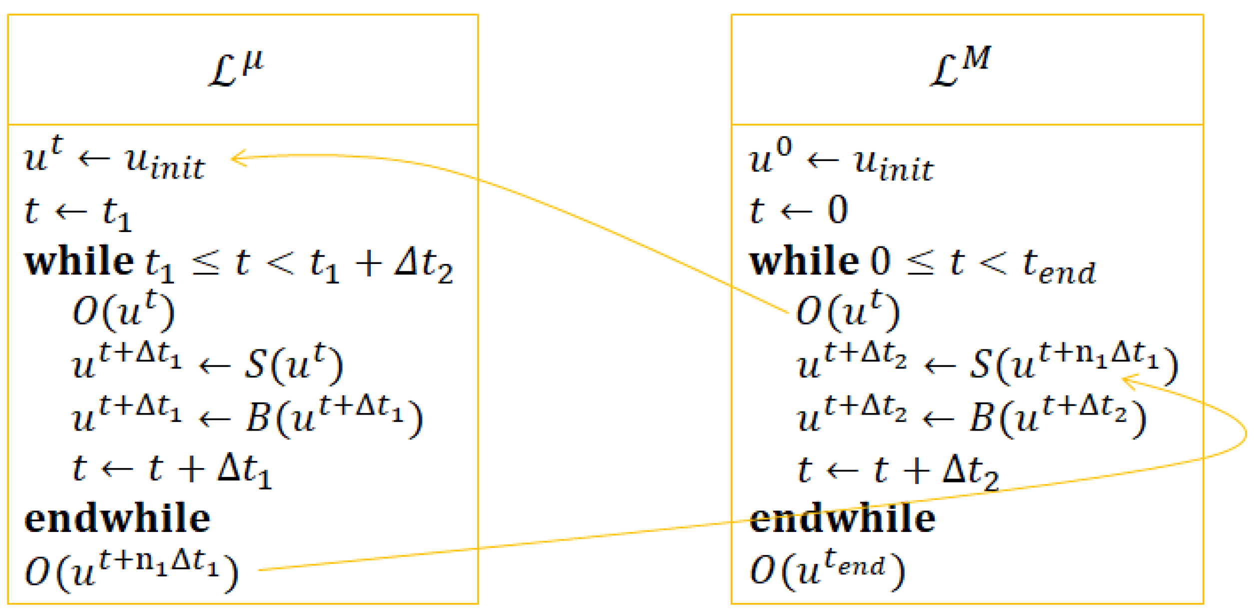
where $\mathcal{L}^{\mu}$ and $\mathcal{L}^{M}$ are subscale models with micro and macro time scale, respectively. Thus, the equation can be rewritten

$$u(x,t+\Delta t,\xi) \approx e^{\Delta t \mathcal{L}^{M}} e^{\Delta t \mathcal{L}^{\mu}} u(x,t,\xi)$$

The original PDE can be approximated as a sequence of the following two sub-systems

$$\frac{\partial u^{*}(x,t,\xi)}{\partial t} = \mathcal{L}^{\mu} u^{*}(x,t,\xi), \text{ for } t_n < t < t_{n+1},$$
$$\text{with } u^{*}(x,t_n,\xi) \approx u(x,t_n,\xi)$$
$$\frac{\partial u^{**}(x,t,\xi)}{\partial t} = \mathcal{L}^{\mathcal{M}} u^{**}(x,t,\xi), \text{ for } t_n < t < t_{n+1},$$
$$\text{with } u^{**}(x,t_n,\xi) = u^{*}(x,t_{n+1},\xi)$$

In general, a model with two or more different time scales can be illustrated by a *Submodel Execution Loop* [1, 2].



u_{init} are some initial conditions for a sub-scale model, O is the observation of the current state, S is the solver, and B is the application of boundary conditions.

Case study

We studied the Gray-Scott reaction diffusion model with uncertain coefficients:

$$\frac{\partial u(t,x,y,\xi)}{\partial t} = \underbrace{D_u(\xi_1)\nabla^2 u - uv^2}_{\text{Macro scale model}} + \underbrace{F(\xi_2)(1-u)}_{\text{Micro scale model}}$$
$$\frac{\partial v(t,x,y,\xi)}{\partial t} = \overbrace{D_v(\xi_3)\nabla^2 v + uv^2} - \overbrace{(F(\xi_2)+K(\xi_4))v}$$

where the model reaction and diffusion coefficients contain 10% uncertainty with mean values

$$\mathbb{E}(D_u(\xi_1)) = 2\cdot 10^{-5},\ \mathbb{E}(F(\xi_2)) = 0.025,$$
$$\mathbb{E}(D_v(\xi_3)) = 1\cdot 10^{-5},\ \mathbb{E}(K(\xi_4)) = 0.053.$$

The model reproduces a compex pattern formation with a transition map studied in [3].

Conclusions

- Our semi-intrusive method can result in a significant decrease in computational time while maintaining the quality of UQ estimates.
- The method allows to choose the number of samples N_1 at each time scale according to errors estimated by the cross-validation approach.

Acknowledgements

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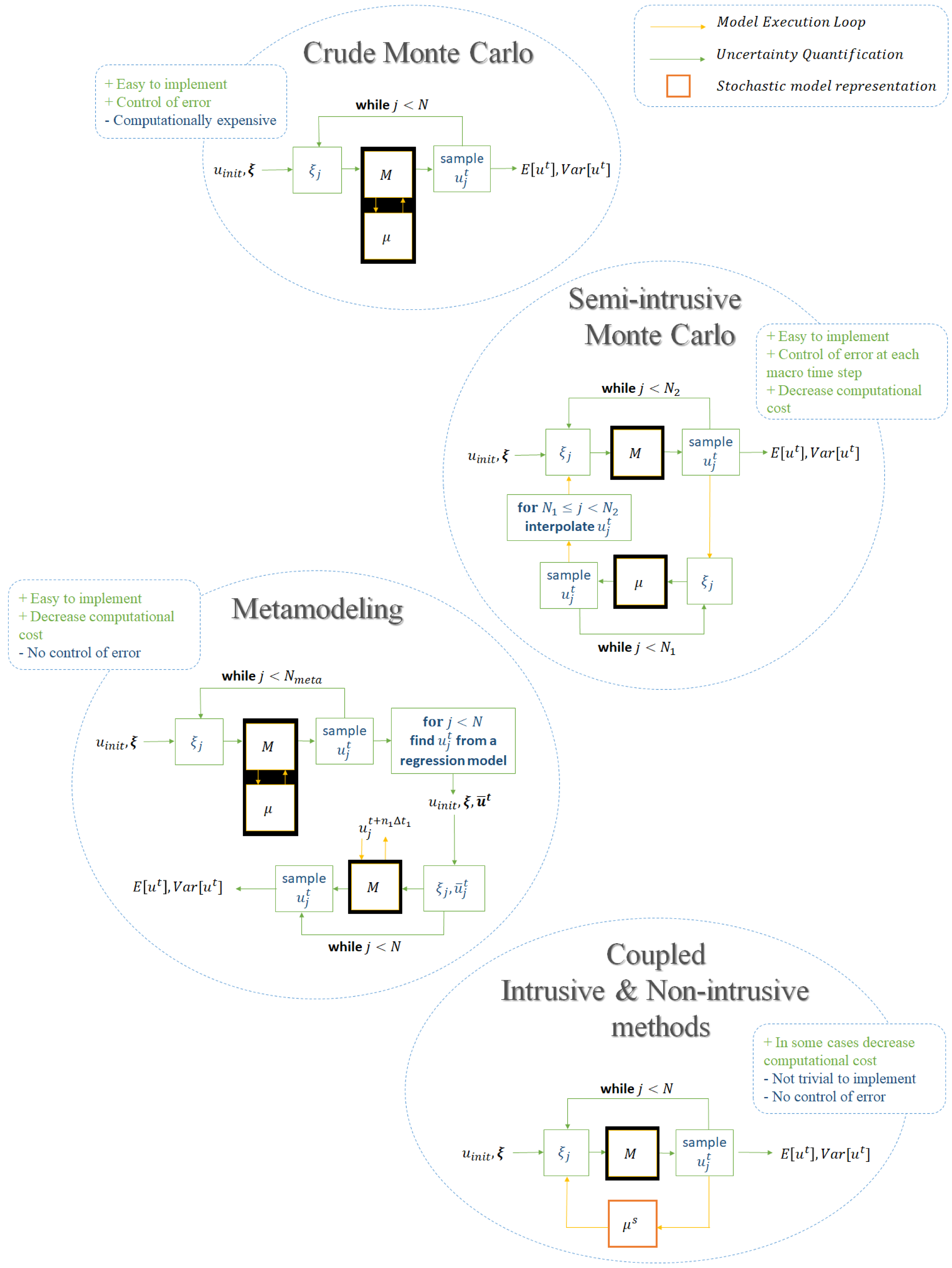
Uncertainty Quantification methods



Results

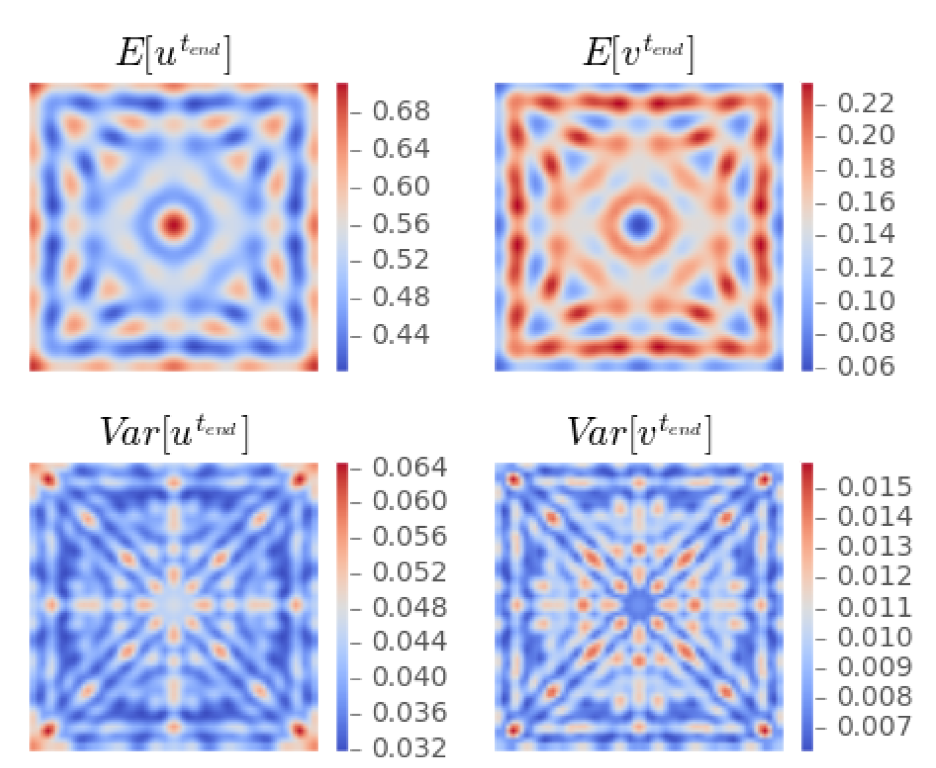


Fig. 3: Mean and variance of the concentration u and v at the final time step

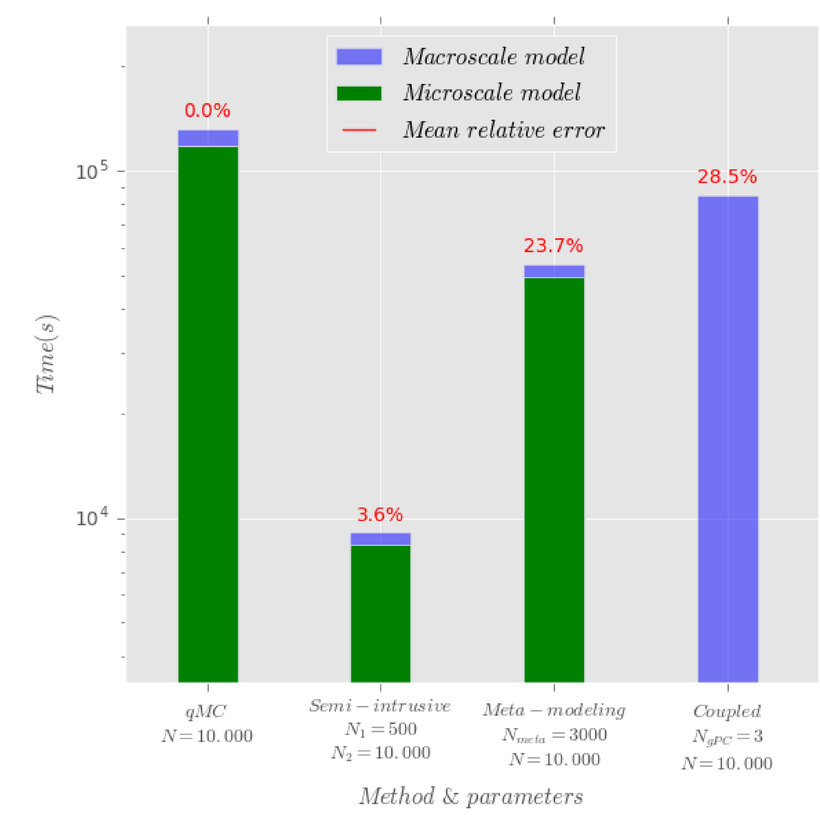


Fig. 4: Comparison of the performance of the different Uncertainty Quantification methods

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[3] Omri Har-shemesh, Rick Quax, Alfons G Hoekstra, and Peter M A Sloot. Information geometric analysis of phase transitions in complex patterns: the case of the Gray-Scott reactionâĂŞdiffusion model. *Journal of Statistical Mechanics: Theory and Experiment*, page 43301, 2016.