

Semi-intrusive Uncertainty Quantification for Multiscale models

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Multiscale models

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

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

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Multiscale models

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

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

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

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

Multiscale models

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

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

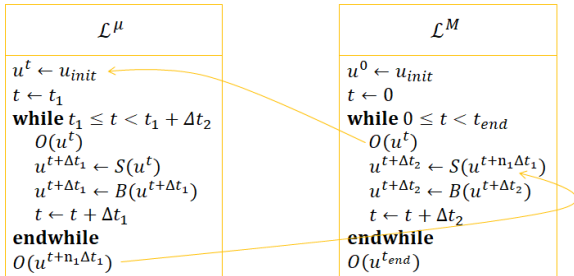
$$\text{with } u^*(x, t_n, \xi) \approx u(x, t_n, \xi)$$

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

$$\text{with } u^{**}(x, t_n, \xi) = u^*(x, t_{n+1}, \xi)$$

Submodel Execution Loop

In general, a model with two or more different time scales can be illustrated by a *Submodel Execution Loop* [BFL⁺13, CFHB11].

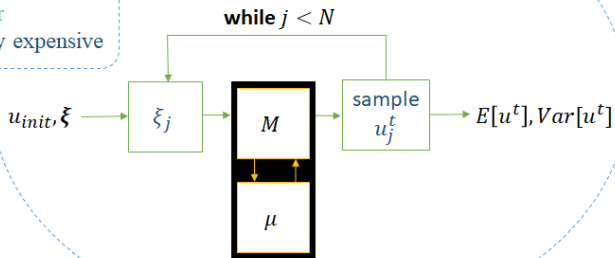


u_{init} are some initial conditions for a sub-scale model, O is the observation of the current state, S is the solver, and B is the application of boundary conditions.

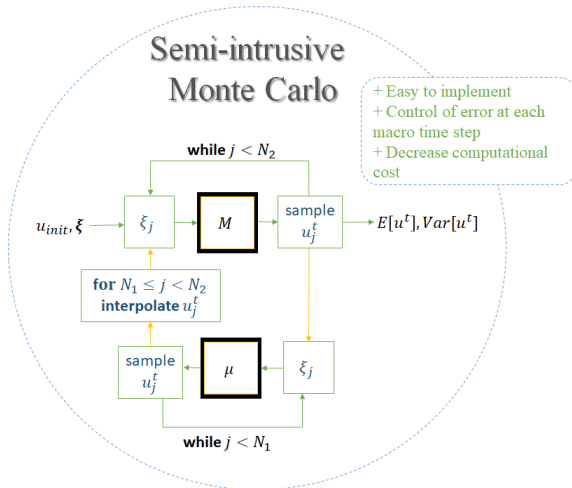
Black Box Monte Carlo

Crude Monte Carlo

- + Easy to implement
- + Control of error
- Computationally expensive



Semi-intrusive Monte Carlo



The Gray-Scott reaction diffusion model

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

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

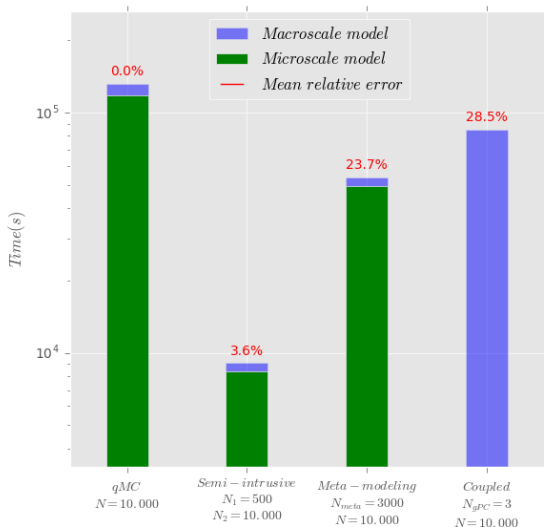
where the model reaction and diffusion coefficients contain 10% uncertainty with mean values

$$\mathbb{E}(D_u(\xi_1)) = 2 \cdot 10^{-5}, \quad \mathbb{E}(F(\xi_2)) = 0.025,$$




$$\mathbb{E}(D_v(\xi_3)) = 1 \cdot 10^{-5}, \quad \mathbb{E}(K(\xi_4)) = 0.053.$$

The model reproduces a complex pattern formation with a transition map studied in [HsQHS16].

Comparisomn of the performance of the UQ methods



References I

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-  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 reaction–diffusion model*, Journal of Statistical Mechanics: Theory and Experiment (2016), 43301.