Surrogate and Reduced-Order Models

Problem: Difficult to obtain sufficient number of realizations of discretized PDE models for Bayesian model calibration, design and control.

Mass
$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0$$

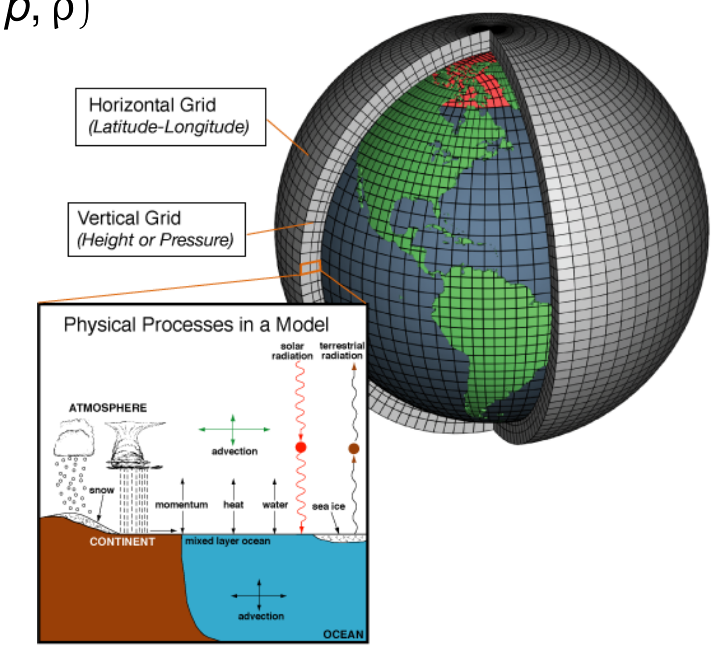
Momentum
$$\frac{\partial v}{\partial t} = -v \cdot \nabla v - \frac{1}{\rho}\nabla p - g\hat{k} - 2\Omega \times v$$

Energy
$$\rho c_V \frac{\partial T}{\partial t} + p\nabla \cdot v = -\nabla \cdot F + \nabla \cdot (k\nabla T) + \rho \dot{q}(T, p, \rho)$$

$$p = \rho R T$$

Water
$$\frac{\partial m_j}{\partial t} = -v \cdot \nabla m_j + S_{m_j}(T, m_j, \chi_j, \rho) \ , \ j = 1, 2, 3,$$

Aerosol
$$\frac{\partial \chi_j}{\partial t} = -v \cdot \nabla \chi_j + S_{\chi_j}(T, \chi_j, \rho) \ , \ j = 1, \cdots, J,$$



Solution: Construct surrogate models

- Also termed data-fit models, response surface models, emulators, meta-models
- Projection-based models often called reduced-order models (Chapter 19)

Surrogate Models: Motivation

Example: Consider the PDE

$$\frac{\partial u}{dt} = \alpha \frac{\partial^2 u}{\partial x^2} + g(t,x) \quad , \quad 0 < x < L\,, t > 0$$

$$u(t,0) = u(t,L) = 0 \quad , \quad t > 0$$

$$u(0,x) = u_0(x) \quad , \quad 0 \leqslant x \leqslant L.$$

Weak Model Formulation:

$$\int_0^L \frac{\partial u}{\partial t} \phi dx + \alpha \int_0^L \frac{\partial u}{\partial x} \frac{d\phi}{\partial x} dx + \int_0^l g\phi dx$$

for all test functions $\phi \in H_0^1(0,L) = \{\phi \in H^1(0,L) \,|\, \phi(0) = \phi(L) = 0\}$.

QOI:

$$y(t,x) = \int_\Gamma u(t,x,q)\rho(q)dq$$

Surrogate Models

Approximate Solution:

$$u_r^J(t,x) = \sum_{j=1}^{J-1} u_j(t,q^r)\phi_j(x) = \sum_{j=1}^{J-1} u_j^r(t)\phi_j(x)$$

ODE System:

$$M\dot{u}_r(t) = K(q^r)u_r(t) + g(t)$$

where

$$u_r(t) = [u_1^r(t), \ldots, u_{J-1}^r(t)]^T \quad , \quad [g(t)]_i = \int_0^L g(t,x)\phi_i(x)dx$$

$$[M]_{ij} = \int_0^L \phi_i(x)\phi_j(x)dx \quad , \quad [K(q^r)]_{ij} = \alpha^r \int_0^L \phi_i'(x)\phi_j'(x)dx$$

QOI: Monte Carlo approximation

$$y(t,x) \approx \frac{1}{R}\sum_{r=1}^{R} u_r^J(t,x) = \frac{1}{R}\sum_{r=1}^{R}\sum_{j=1}^{J-1} u_j^r(t)\phi(x)$$

Stochastic Spectral Methods

Representation:

$$u^K(t,x,q) = \sum_{k=0}^{K} u_k(t,x)\Psi_k(q)$$

Mean and Variance:

$$\mathbb{E}\left[u^K(t,x,q)\right] = u_0(t,x)$$

$$\mathrm{var}[u^K(t,x,q)] = \sum_{k=1}^{K} u_k^2(t,x)\gamma_k$$

Strategy: Employ Galerkin, discrete projection, collocation to determine coefficients $u_k(t,x)$

Evolutionary PDE

Evolutionary PDE:

$$\frac{\partial u}{dt} = q\frac{\partial^2 u}{\partial x^2} + g(t,x) \quad , \quad 0 < x < L\,, t > 0$$

$$u(t,0) = u(t,L) = 0 \quad , \quad t > 0$$

$$u(0,x) = u_0(x) \quad , \quad 0 \leqslant x \leqslant L.$$

Deterministic Weak Formulation: Holds for all $v \in V$

$$\int_0^L \frac{\partial u}{\partial t}\phi dx + q\int_0^L \frac{\partial u}{\partial x}\frac{d\phi}{\partial x}dx + \int_0^l g\phi dx$$

QOI:

$$y(t,x) = \int_\Gamma u(t,x,q)\rho(q)dq$$

Evolutionary PDE

Deterministic Weak Formulation: Holds for all $v \in V$

$$\int_0^L \frac{\partial u}{\partial t} \phi dx + q \int_0^L \frac{\partial u}{\partial x} \frac{d\phi}{\partial x} dx + \int_0^l g\phi dx$$

Approximate Solutions:

$$u^K(t,x,q) = \sum_{k=0}^{K} u_k(t,x)\Psi_k(q) = \sum_{k=0}^{K} \sum_{j=1}^{J-1} u_{jk}(t)\phi_j(x)\Psi_k(q)$$

Discrete Projection: Let

$$u_r^J(t,x) = \sum_{j=1}^{J-1} u_j^r(t)\phi_j(x)$$

solve weak formulation for sampled q^j; i.e.,

$$\int_0^L \frac{\partial u_r^J}{\partial t} \phi dx + q^r \int_0^L \frac{\partial u_r^J}{\partial x} \frac{d\phi}{\partial x} dx + \int_0^l g\phi dx$$

Coefficients:

$$u_k(t,x) \approx \frac{1}{\gamma_k} \sum_{r=1}^{R} u_r^J(t,x)\Psi_k(q^r)\rho(q^r)w^r$$

Evolutionary PDE

Example:

$$\frac{\partial u}{dt} = q\frac{\partial^2 u}{\partial x^2} + g(t,x) \quad , \quad 0 < x < L\,, t > 0$$

$$u(t,0) = u(t,L) = 0 \quad , \quad t > 0$$

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Deterministic Weak Formulation: Holds for all $v \in V$

$$\int_0^L \frac{\partial u}{\partial t}\phi dx + q\int_0^L \frac{\partial u}{\partial x}\frac{d\phi}{\partial x}dx + \int_0^l g\phi dx$$

Note: Take $g(t,x) = x(2-x)^4 \sin(3\pi t), u_0(x) = \sin(\frac{3\pi x}{2})$ and $L = 2$

Parameter: $q = \alpha \sim \mathcal{U}(a,b)$, with $a > 0$

Approximate Solution:

$$u^K(t,x,q) = \sum_{k=0}^{K} u_k(t,x)\Psi_k(q) = \sum_{k=0}^{K}\sum_{j=1}^{J-1} u_{jk}(t)\phi_j(x)\Psi_k(q)$$

Evolutionary PDE

Approximate Solution:

$$u^K(t,x,q) = \sum_{k=0}^{K} u_k(t,x)\Psi_k(q) = \sum_{k=0}^{K}\sum_{j=1}^{J-1} u_{jk}(t)\phi_j(x)\Psi_k(q)$$

Discrete Projection: Take $q = \alpha = \frac{a+b}{2} + \frac{b-a}{2}\xi$ where $\xi \sim \mathcal{U}(-1,1)$

Coefficients:

$$u_k(t,x) = \frac{1}{\gamma_k}\sum_{r=1}^{R} u_r^J(t,x)\psi_i(\xi^r)\rho(\xi^r)w^r$$

where

$$u_r^J(t,x) = \sum_{j=1}^{J-1} u_j^r(t)\phi_j(x)$$

is obtained by numerically integrating

$$M\dot{u}_r(t) = K(\xi^r)u_r(t) + g(t)$$

where

$$[K(\xi^r)]_{ij} = \left(\frac{a+b}{2} + \frac{b-a}{2}\xi^r\right)\int_0^L \phi_i'(x)\phi_j'(x)dx$$

Evolutionary PDE

Results: Mean and variance with $q = \alpha \sim \mathcal{U}(1,2)$

Note:

- Discrete projection: R = 10
- Collocation: R = 15
- Monte Carlo: R = 5000