Method of Distributions for Quantification of Uncertainty in Multiscale Systems

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An Uncertain Journey through Uncertainty Quantification

UQ in Predictive Sciences

Natl. Res. Council report "Assessing the Reliability of Complex Models: Mathematical and Statistical Foundations of Verification, Validation, and Uncertainty Quantification", Natl. Acad. Sci., 2012*

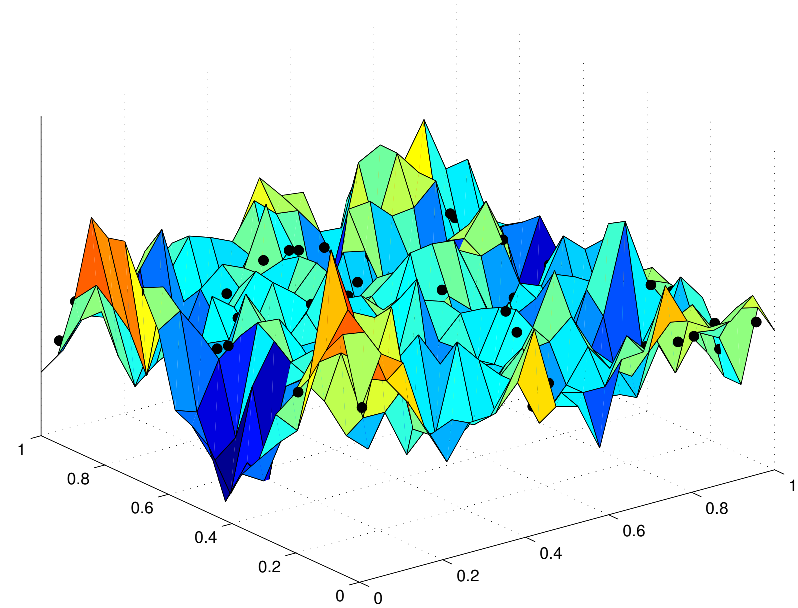
Q: Given inevitable flaws, how should computational results be viewed by those who wish to act on them?

A: The appropriate level of confidence in the results must stem from an understanding of a model's limitations and the uncertainties inherent in its predictions.

*http://www.nap.edu/catalog.php?record-id=13395

Probabilistic Framework for UQ

- Parameter,
  $p(\mathbf{x}) : \mathcal{D} \in \mathbb{R}^d \to \mathbb{R}$
- Random field,
  $P(\mathbf{x}, \omega) : \mathcal{D} \times \Omega \to \mathbb{R}$
- Governing equations become "stochastic"



parameter $p(x_1, x_2)$

$$\begin{cases} \mathcal{L}(\mathbf{x}; u) = g(\mathbf{x}), & \mathbf{x} \in \mathcal{D} \\ \mathcal{B}(\mathbf{x}; u) = b(\mathbf{x}), & \mathbf{x} \in \partial\mathcal{D} \end{cases} \Longrightarrow \begin{cases} \mathcal{L}(\mathbf{x}, \omega; U) = g(\mathbf{x}, \omega), & \mathbf{x} \in \mathcal{D} \\ \mathcal{B}(\mathbf{x}, \omega; U) = b(\mathbf{x}, \omega), & \mathbf{x} \in \partial\mathcal{D} \end{cases}$$

- Solutions are PDF $f_U(u; \mathbf{x}, t)$ or CDF $F_U(u; \mathbf{x}, t)$ or moments, e.g., $\overline{U}$ and σ_U^2

Monte Carlo Simulations

- Advantages
  - Easy to implement
  - Nonintrusive
  - Perfectly parallelizable
- Disadvantages
  - Intellectual: No physical insight into computed statistics
  - Utilitarian: Slow convergence rate, $1/\sqrt{N}$
- Search for alternatives (a historical prospective)

Moment Differential Equations (MDEs)

Given

$$\mathcal{L}(\mathbf{x},\omega;U) = g(\mathbf{x},\omega),$$

derive deterministic equations for ensemble moments of $U(\mathbf{x},\omega)$, e.g.,

$$\mathcal{L}_u(\mathbf{x};\overline{U}) = \overline{g}(\mathbf{x}), \qquad \mathcal{L}_\sigma(\mathbf{x};\sigma_U^2) = \sigma_g^2(\mathbf{x}).$$

Usually derived via perturbation expansions in parameter variance σ_P^2.

- Advantages
  - Physical insight: equations for $\overline{U}$ are nonlocal, etc.
  - Can be more efficient than MCS
- Disadvantages
  - Not practical for higher moments of $U(\mathbf{x},\omega)$
  - (*Formally*) valid for $\sigma_P^2 \leq 1$

Frish; Papanicolaou; Van Kampen; etc

Direct Numerical Solutions of SPDEs

⋆ Polynomial chaos expansions

⋆ Stochastic collocation on sparse grids

⋆ Stochastic finite elements

- Disadvantages
  - Curse of dimensionality (small correlation lengths)
  - The same (lack of) insight as MCS
- Advantages
  - Claim: Non-perturbative alternatives to MDEs (arbitrary σ_P^2)

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	Ref [5]	Ref [6]	Ref [7]	Ref [12]	Ref [17]	Ref [19]
σ_P^2	0.5	0.1	0.1	0.04	0.02	0.01

Effect of Parameter Variance σ_P^2 (1/5)

Approximation of an input parameter $P(x,\omega)$ via, e.g., K-L expansion

$$P = \bar{P} + \sigma_P \sum_{n=0}^{\infty} \sqrt{\lambda_n}\gamma_n(x)\xi_n(\omega), \quad P_N = \bar{P} + \sigma_P \sum_{n=0}^{N} \sqrt{\lambda_n}\gamma_n(x)\xi_n(\omega)$$

A global truncation error,

$$\mathcal{E}_P^g \equiv \int_D \|P - P_N\|_{L^2}^2 \mathrm{d}\mathbf{x} = \sigma_P^2 \sum_{n=N+1}^{\infty} \lambda_n$$

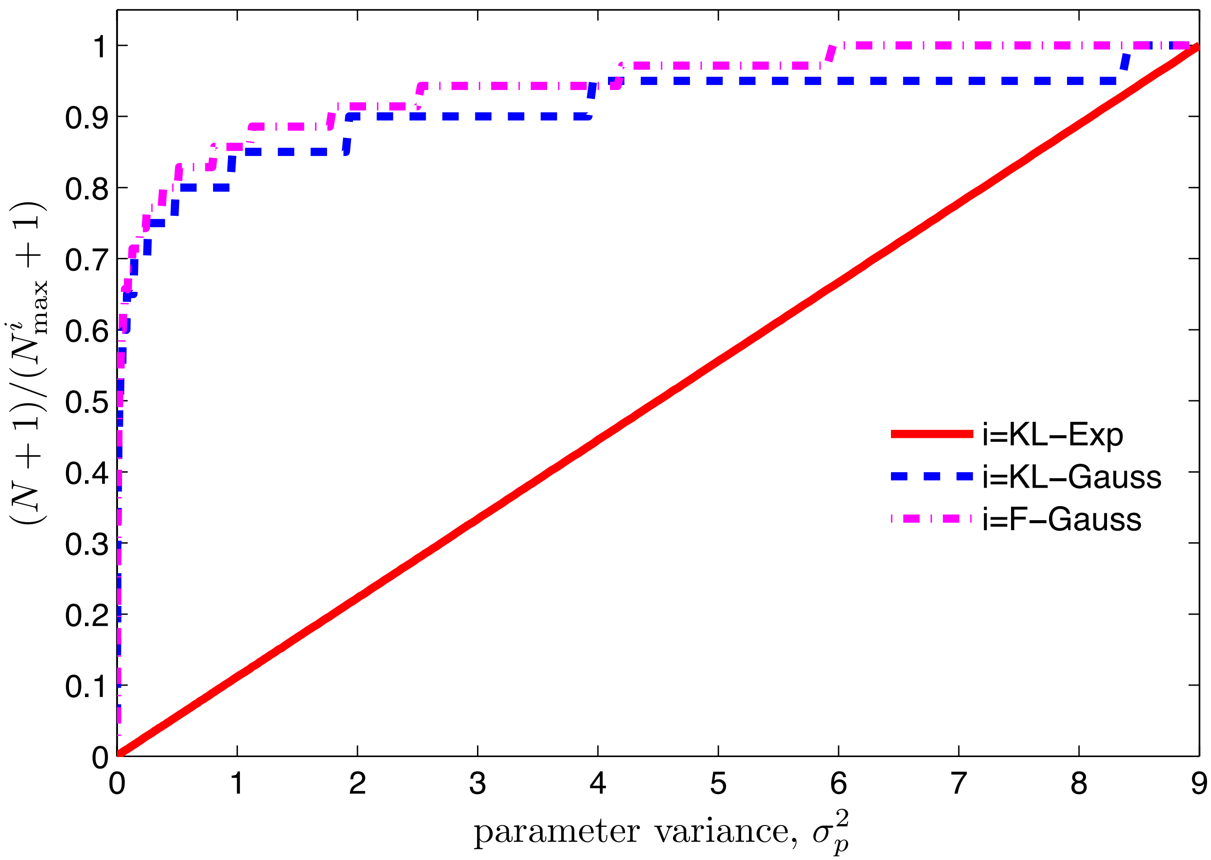
Convergence of the series depends on the choice of correlation function

⋆ Exponential function: $\rho_p = \exp(-r/\ell_p)$

⋆ Gaussian function $\rho_p = \exp(-r^2/\ell_p^2)$

Effect of Parameter Variance σ_P^2 (2/5)

For exponential ρ_p, it takes $N = \begin{cases} 20 & \sigma_P^2 = 0.1 \\ 203 & \sigma_P^2 = 1.0 \end{cases}$ to achieve $\mathcal{E}_P^g \leq 10^{-3}$.



Effect of Parameter Variance σ_P^2 (3/5)

$\star$ Other errors: $|\langle u \rangle - \hat{u}_N| \leq |\langle u \rangle - \langle u_N \rangle| + |\langle u_N \rangle - \hat{u}_N| = \epsilon_{\text{KL}} + \epsilon_{\text{est}}$

$\star$ Richards equation

$$\frac{\partial \theta(\mathbf{x}, \psi)}{\partial t} = \nabla \cdot [K(\mathbf{x}, \psi) \nabla \psi] - \frac{\partial K(\mathbf{x}, \psi)}{\partial x_3}$$

with constitutive laws $\theta = \theta[\Lambda_\theta(\mathbf{x}), \psi]$ and $K = K[\Lambda_K(\mathbf{x}), \psi]$

$\star$ Uncertain parameters

$$\Lambda_\theta(\mathbf{x}),\ \Lambda_K(\mathbf{x}) \Rightarrow \Lambda_\theta(\mathbf{x}, \omega),\ \Lambda_K(\mathbf{x}, \omega)$$

This SPDE was studied extensively with moment equations (e.g., WRR 2002; JFM 2003; JH 2003)

Effect of Parameter Variance σ_P^2 (4/5)

⋆ Stochastic Collocation on Sparse Grids

1. Karhunen-Loève expansions of n parameters, e.g., $Y_i = \ln \Lambda_\theta(\mathbf{x})$

$$Y_i(\mathbf{x}, \omega) = \mathbb{E}[Y_i] + \sum_{j=1}^{P} \sqrt{\lambda_{ij}} \gamma_{ij}(\mathbf{x}) \xi_{ij}(\omega), \qquad i = 1, \ldots, n$$

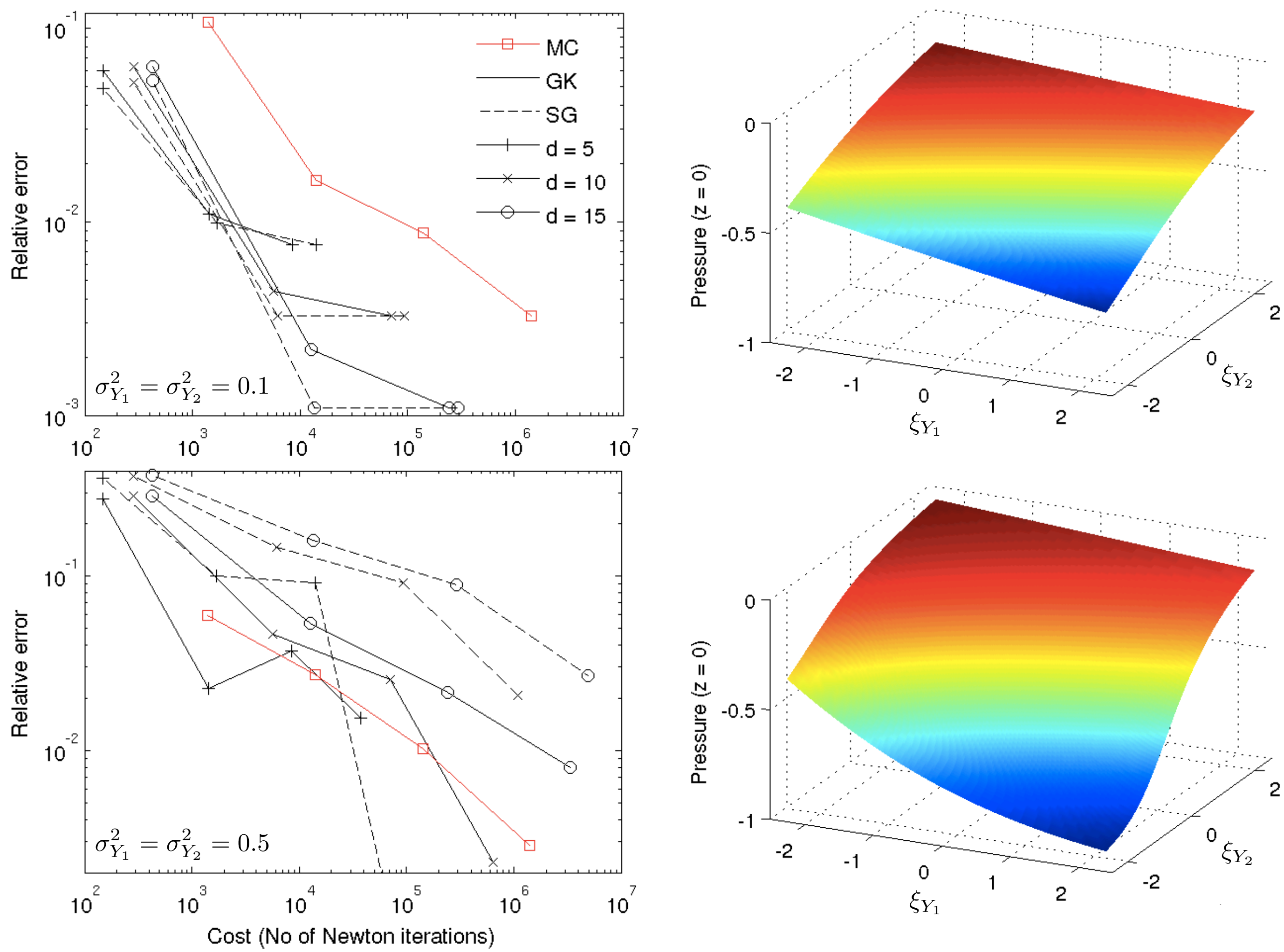
2. N-dimensional ($N = nP$) outcome space characterized by a *multi-Gaussian* random vector $\boldsymbol{\xi} = (\xi_{11}, \ldots, \xi_{1P}, \xi_{n1}, \ldots, \xi_{nP})^\top$
3. Statistics of quantities of interest, e.g. ψ, are computed as

$$\mathbb{E}[\psi] = \int_{\mathbb{R}^N} \psi(\mathbf{x}, t, \boldsymbol{\xi}) \rho(\boldsymbol{\xi}) \mathrm{d}\boldsymbol{\xi} \approx \sum_{i=1}^{M} \psi(\mathbf{x}, t, \boldsymbol{\xi}_i) w_i$$

4. Locally adaptive sparse grids
   - Smolyak algorithm
   - Gauss-Kronrod extensions of Gauss-Hermite quadratures

Effect of Parameter Variance σ_p^2 (5/5)

Pressure Estimate $\mathbb{E}[\psi]$



Alternative Strategies

- Stochastic finite elements
- Accelerated Monte Carlo methods
  - Quasi Monte Carlo (e.g., Latin hypercube or stratified sampling)
  - Multi-level Monte Carlo
- Reduced complexity models
  - Data & cost-accuracy tradeoff in model selection (JUQ 2015)
- Method of distributions: PDF and CDF methods (SERRA '03, WRR '09, JCP '12...)

Multi-Level Monte Carlo

$\star$ Given: PDE with random coefficients, $\mathcal{N}(\psi) = 0$, e.g., Richards equation

$\star$ Goal: Compute statistics of system states, e.g., $\mathbb{E}[\psi(\mathbf{x}, t)]$

$\star$ MLMC approach: Solve a sequence $\mathcal{N}_M(\psi) = 0$ and compute statistics of their solutions $\psi_M(\mathbf{x}, t)$, such that (hypothesis)

$$\mathbb{E}[\psi_M - \psi] = \mathcal{O}(M^{-\alpha}) \text{ as } M \to \infty,$$

for a certain constant α independent of M

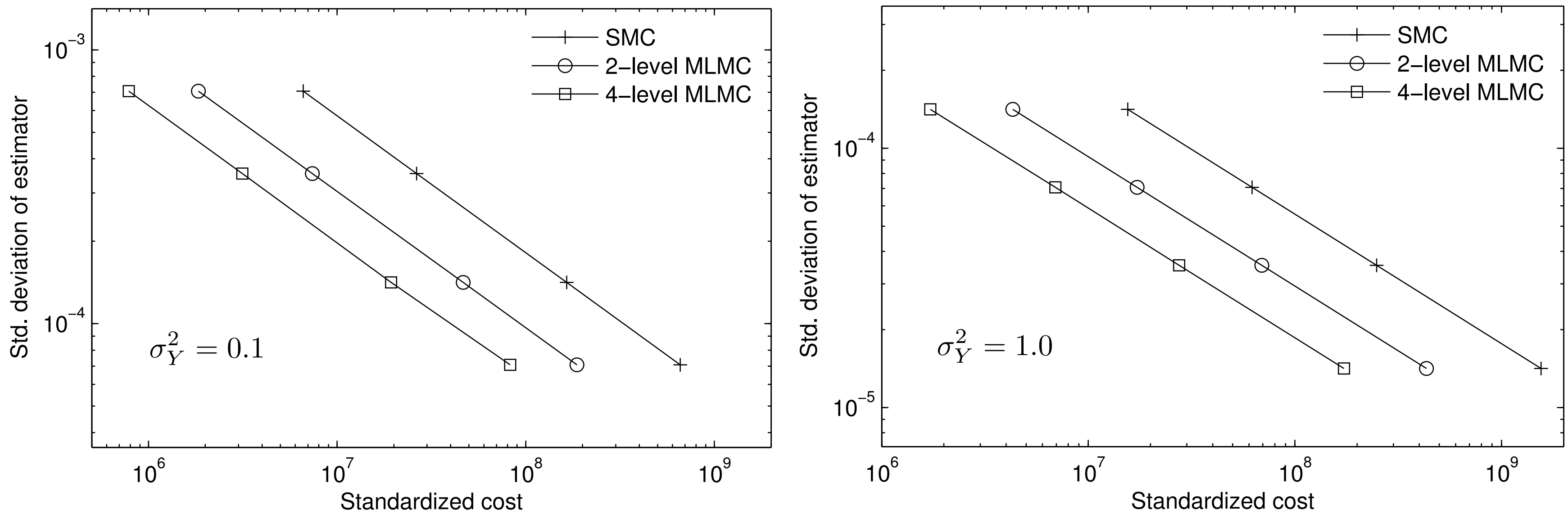
$\star$ MLMC implementation (R. Scheichl, U of Bath). Let $\{M_l\}_{l=0}^{L}$ be a sequence in $\mathbb{N}$, such that $M_L = M$ and $M_l = sM_{l-1}$ for $1 \leq l < L$ and an $s \in \mathbb{N}\backslash\{1\}$. Then

$$\mathbb{E}[\psi_M] = \sum_{l=1}^{L} \mathbb{E}[\psi_{M_l} - \psi_{M_{l-1}}] + \mathbb{E}[\psi_{M_0}] \equiv \sum_{l=0}^{L} \mathbb{E}[Y_l], \qquad \mathbb{E}[Y_l] \approx \frac{1}{N_l} \sum_{k=1}^{N_l} (\psi_{M_l}^{(k)} - \psi_{M_{l-1}}^{(k)})$$

such that N_l decreases with l.

Relative Performance of MLMC

$\sigma_\psi(x = 0)$:



$$\frac{\mathrm{d}}{\mathrm{d}z}\left[K\frac{\mathrm{d}(\psi - z)}{\mathrm{d}z}\right] = 0, \qquad K\frac{\mathrm{d}\psi}{\mathrm{d}z}(z = 0, \omega) = -Q, \qquad \psi(z = 1, \omega) = 0$$

$$K(z, \psi, \omega) = \begin{cases} K_s(z, \omega)\,\mathrm{e}^{\alpha(z,\omega)\psi(z,\omega)}, & \psi \le 0 \\ K_s(z, \omega), & \psi > 0 \end{cases}$$

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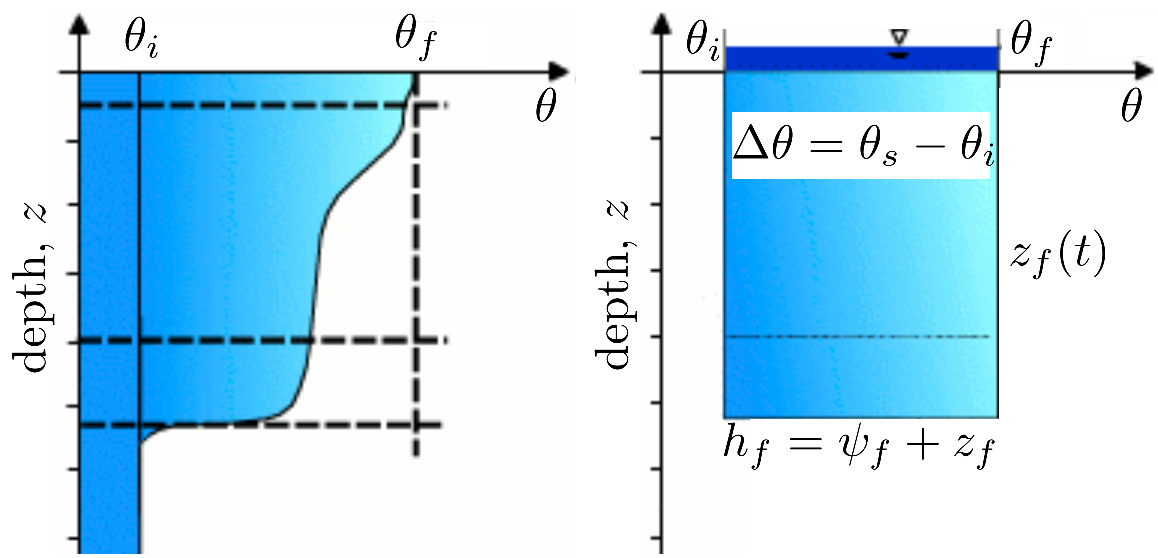
Reduced Complexity Model

⋆ Richards equation

$$\frac{\partial \theta(\mathbf{x}, \psi)}{\partial t} = \nabla \cdot [K(\mathbf{x}, \psi) \nabla \psi] - \frac{\partial K(\mathbf{x}, \psi)}{\partial z}$$

⋆ Green-Ampt model (analogous to Buckley-Leverett equation)

$$\frac{\mathrm{d}z_{\mathrm{f}}}{\mathrm{d}t} = -K_s \frac{\psi_{\mathrm{f}} - z_{\mathrm{f}} - \psi_0}{z_{\mathrm{f}}}, \qquad \psi_{\mathrm{f}} = -\int_{\psi_{\mathrm{dry}}}^{0} K_r(\psi)\,\mathrm{d}\psi$$



IJUQ, 2011; AWR, 2011

Cost-Accuracy Tradeoff in Multifidelity Models

Q: Given parametric uncertainty, is the use of a high-fidelity model warranted?

A1: It depends: $\mathcal{E}_{\text{total}} = \mathcal{E}_{\text{representation}} + \mathcal{E}_{\text{sampling}}$

A2: System state measurements impact the model selection problem

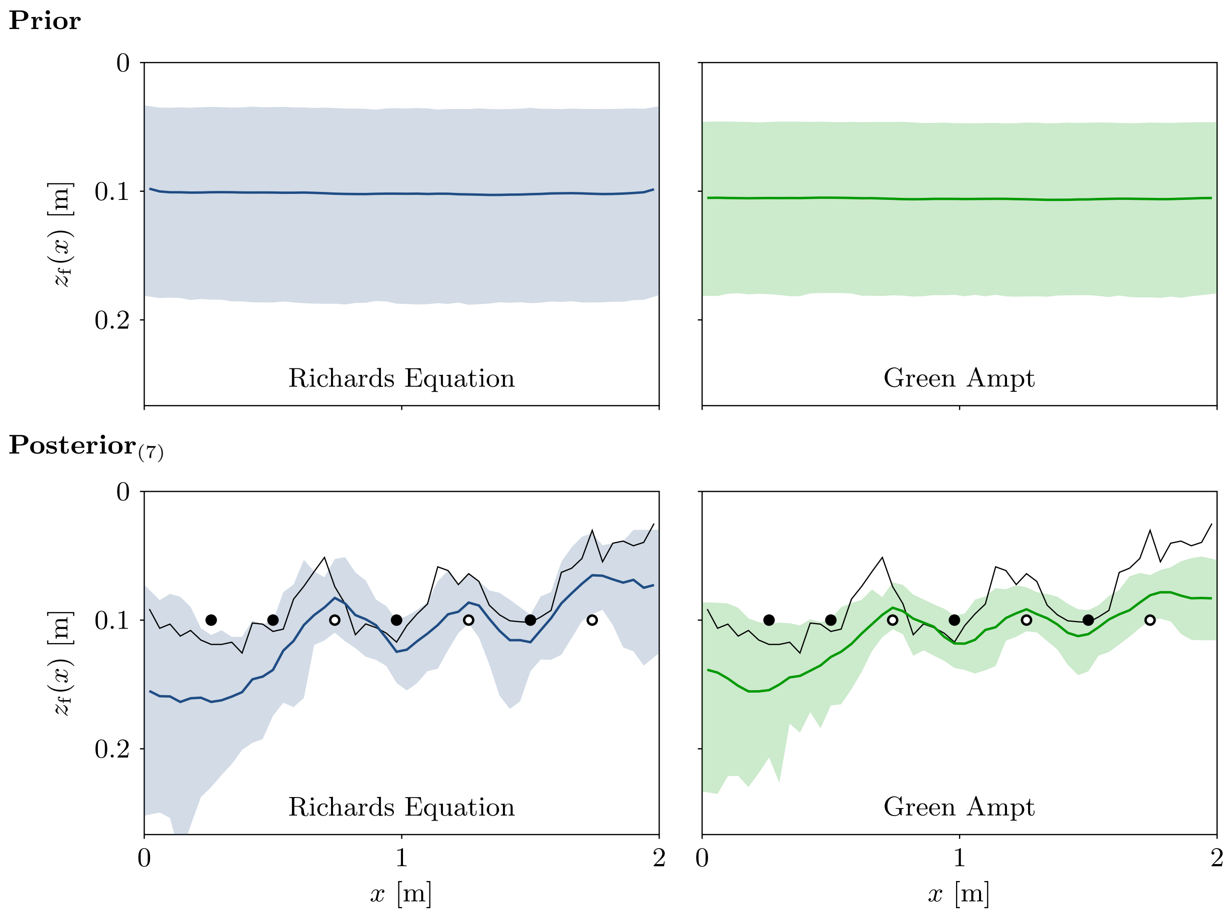
Bayesian framework:

1. Solutions of high- and low-fidelity models are *prior* PDFs

2. Assimilation of system state data yields *posterior* PDFs

Statistics of Infiltration Depth $z_\mathrm{f}(x, t = 30)$

No sampling error



Thick lines: ensemble mean. Light colored areas: pointwise 0.1 and 0.9 percentiles.

Black thin line: virtual truth. Circles: moisture sensors, wet - black, dry - white.

UCSD

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PDF and CDF Methods

⋆ Goal: Derive deterministic equations for PDF, $f_C(c; \mathbf{x}, t)$, or CDF, $F_C(c; \mathbf{x}, t)$, of a random system state $C(\mathbf{x}, t, \omega)$

⋆ Motivation:

- Avoid approximations of random system parameters, e.g.,

$$P(x, \omega) \approx \overline{P}(x) + \sigma_P \sum_{m=1}^{N} \sqrt{\lambda_m} \gamma_m(x) \xi_m(\omega)$$

- Be applicable to both SPDEs and PDEs with random coefficients
- Gain insight into the evolution of uncertainty, i.e., $f_C(c; \mathbf{x}, t)$, or $F_C(c; \mathbf{x}, t)$

⋆ Tools: physics- and/or perturbation-based closure approximations

CDF/PDF Methods for First-Order SDEs

A system of $N_{\mathbf{eq}}$ SDEs for $\mathbf{C}(\mathbf{x}, t, \omega) = (C_1, \ldots, C_{N_{\mathbf{eq}}})$,

$$\frac{\partial C_i}{\partial t} + \nabla_{\mathbf{x}} \cdot \mathbf{f}_i(\mathbf{x}, t, \mathbf{C}) = r_i(\mathbf{x}, t, \mathbf{C}), \qquad \mathbf{x} \in D \subset \mathbb{R}^d, \qquad t \in \mathbb{R}^+$$

Sources of uncertainty:

- M_i parameters $\{p_m(\mathbf{x}, t)\}_{m=1}^{M_i}$ in $\mathbf{f}_i$ and r_i
- Initial conditions $C_i(\mathbf{x}, 0) = C_{\text{in}_i}(\mathbf{x})$

CDF Methods for First-Order SDEs

Let $\Pi(c, C; \mathbf{x}, t) \equiv \mathcal{H}[c - C(\mathbf{x}, t, \omega)]$. Then

$$\langle \Pi \rangle_C = \int \Pi(c, s; \mathbf{x}, t) f_C(s; \mathbf{x}, t) \mathrm{d}s = \int^c f_C(s; \mathbf{x}, t) \mathrm{d}s = F_C(c; \mathbf{x}, t)$$

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CDF Approach to UQ:

$$\frac{\partial C}{\partial t} + \nabla_{\mathbf{x}} \cdot \mathbf{f}(\mathbf{x}, t, C) = r(\mathbf{x}, t, C), \qquad \mathbf{x} \in D \subset \mathbb{R}^d, \qquad t \in \mathbb{R}^+$$

Step 1: $\mathcal{L}(\Pi) = 0$

Step 2: $\langle \mathcal{L}(\Pi) \rangle_{\{p_1, \ldots, p_M\}} = 0 \qquad \Rightarrow \qquad \mathcal{L}_1(F_C) = 0$

Examples of SPDEs

⋆ Hyperbolic balance laws

$$\boxed{\frac{\partial C_i}{\partial t} + \nabla \cdot \mathbf{f}_i(\mathbf{x}, t, \mathbf{C}) = r_i(\mathbf{x}, t, \mathbf{C})}, \qquad i = 1, \dots, N_{\mathrm{eq}}$$

- Saint-Venant (kinematic wave) equation / smooth solutions

$$\frac{\partial C}{\partial t} + \frac{\partial Q(C)}{\partial x} = r(x, t; \omega) \quad \text{with } Q = \alpha(x; \omega) C^{1/\beta}$$

⋆ Other problems

- Advection-reaction equations (JCP 2012, PRSA 2014...)
- Buckley-Leverett (two-phase flow) equation / shocks (MMS 2013)
- Systems of Langevin equations with colored noise (PRL 2013)
- Systems of 1st-order hyperbolic balance laws (UQ Handbook 2016)

Saint-Venant (Kinematic Wave) Equation

$$\frac{\partial C}{\partial t} + \frac{\partial Q}{\partial x} = r(x,t;\omega), \qquad Q = \alpha(x;\omega) C^{1/\beta}$$

Cumulative density function (CDF):

$$\Pi(q,Q;x,t) = \mathcal{H}[q - Q(x,t,\omega)], \qquad \langle \Pi \rangle = F_Q(q;x,t)$$

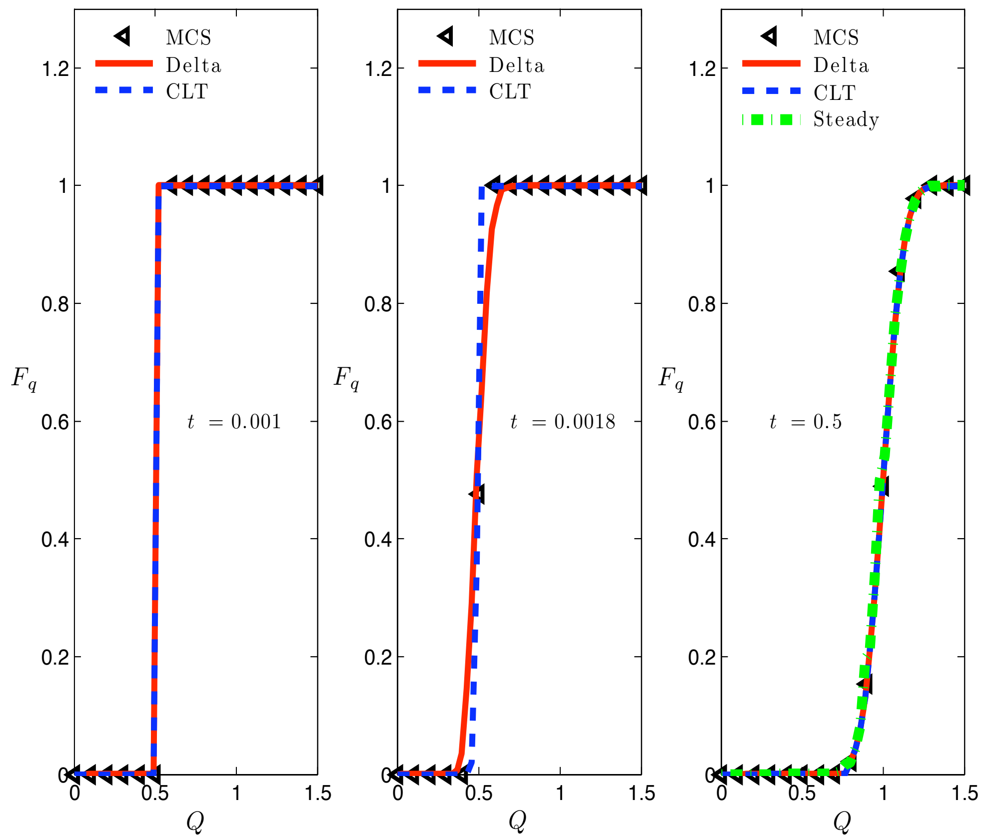
Step 1:

$$\frac{\partial \Pi}{\partial t} + \tilde{\mathbf{U}} \cdot \tilde{\nabla} \Pi = 0, \quad \tilde{\mathbf{x}} = (x,q)^\top, \quad \tilde{\mathbf{U}} = \frac{q^{1-\beta}}{\beta} \alpha \, (1,r)^\top$$

Step 2:

$$\frac{\partial F_Q}{\partial t} + \tilde{\mathbf{v}}_{\mathrm{eff}} \cdot \tilde{\nabla} F_Q = \tilde{\nabla} \cdot (\tilde{\mathbf{D}} \tilde{\nabla} F_Q), \qquad \tilde{\mathbf{x}} \in \tilde{D} \subset \mathbb{R}^{d+1}$$

CDF Solution



Flow rate CDF computed with MCS, the white noise α approximation (Delta), and the CLT-based approximation (CLT).

Conclusions

- Stochastic homogenization applied to the method of distributions, is a promising UQ technique
- Monte Carlo simulations (MCS) are simple to use and often outperform their “computationally efficient alternatives” in *realistic settings*
- Multi-level Monte Carlo provides a further boost in terms of computational efficiency, without sacrificing the MCS robustness
- Given ubiquitous parametric uncertainty, reduced complexity models might provide the most adequate predictions
- “Simplicity is often the sign of truth and a criterion of beauty.”

  (Mahlon Hoagland, Toward the Habit of Truth)