# Uncertainty quantification for nonlinear hyperbolic PDEs

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### Lituya Bay, Alaska



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- ► Took place on July 9, 1958.
- Magnitude 7.8 Earthquake along Fairweather fault (Alaska).
- Triggered massive Rock slide of  $3 \times 10^7 m^3$  volume.
- Wave run-up to shore of 525 m !!!
- ▶ Maximum Wave height of 50 80 m !!!
- Most powerful tsunami ever recorded.

# Lituya Bay Post-Tsunami



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Two-layer Savage-Hutter (Shallow water) model.

$$\begin{cases} \frac{\partial h_1}{\partial t} + \frac{\partial q_1}{\partial x} = 0\\ \frac{\partial q_1}{\partial t} + \frac{\partial}{\partial x} \left(\frac{q_1^2}{h_1} + \frac{g}{2}h_1^2\right) + gh_1\frac{\partial h_2}{\partial x} = gh_1\frac{dH}{dx} + S_f + S_{b_1}\\ \frac{\partial h_2}{\partial t} + \frac{\partial q_2}{\partial x} = 0\\ \frac{\partial q_2}{\partial t} + \frac{\partial}{\partial x} \left(\frac{q_2^2}{h_2} + \frac{g}{2}h_2^2\right) + rgh_2\frac{\partial h_1}{\partial x} = gh_2\frac{dH}{dx} - rS_f + S_{b_2} + \tau \end{cases}$$
(1)

With

- Coulomb friction:  $\tau = -g(1-r)h_2\frac{q_2}{|q_2|}\tan(\delta_0)$ ,
- Interlayer friction:  $S_f = \frac{c_f h_1 h_2}{h_2 + r h_1} (u_2 u_1) |u_2 u_1|$

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 Savage-Hutter equations are Non-conservative hyperbolic system

 $\mathbf{U}_t + \mathbf{A}(\mathbf{U})\mathbf{U}_x = 0.$ 

- Specially designed Path conservative finite volume scheme
- Need to discretize Non-conservative product carefully.
- Optimized GPU implementation.

- Initial data.
- Boundary conditions.
- Model parameters:
  - Acceleration due to gravity g.
  - Interlayer density ratio r
  - Bottom friction parameters  $S_{b_{1,2}}$
  - Coulomb friction angle  $\delta_0$
  - Interlayer friction parameter c<sub>f</sub>

# Run-up at T = 39s



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#### Sources of Errors

- Modeling error
  - Savage-Hutter is a good model (checked in the lab).
- Numerical (discretization) error.
  - Good numerical scheme (Discretization error can be made as small as possible).
- Measurement (Data) errors:
  - Rather low for initial data and boundary conditions.
  - Unacceptably high for  $r, c_f, \delta_0$  (even in the lab !!!)
  - Standard deviation is more than 50 percent of mean !!!
- High measurement error  $\Rightarrow$  low trust in simulation ?

#### Generic situation in Science and Engineering

- Mathematical modeling of any physical/chemical/biological phenomena:
- Model inputs: are obtained by Measurements:
  - Initial conditions.
  - Boundary data.
  - Coefficients.
  - Parameters.
- Measurements are Uncertain.
- ► Uncertain Inputs ⇒ Uncertain Solutions (Outputs).
- + Many models based on Uncertain Dynamics (high Model + Numerical error).

- Uncertainty quantification includes:
  - Modeling of uncertain inputs and dynamics.
  - Efficient Computation of the resulting output uncertainty.
  - Interpretation of the uncertain output.

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#### Run-up Mean at T = 39s



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#### Run-up Variance at T = 39s



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#### Run-up Mean at T = 120s



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#### Run-up Variance at T = 120s



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$$\begin{aligned} \mathbf{U}_t + \operatorname{div}(\mathbf{F}(k(x, t), \mathbf{U})) &= S(x, t, \mathbf{U}), \\ \mathbf{U}(x, 0) &= \mathbf{U}_0(x), \\ \mathbf{U}|_{\partial D} &= \mathbf{U}_b(x, t). \end{aligned}$$

Uncertainty in determining:

- Flux Coefficients (Equations of state, Material properties of porous media)
- Initial data (Initial wave displacement in tsunamis)
- Source terms (Bottom topography in shallow water waves)
- Boundary data (Plasma circuit breakers)
- ► UQ: Given uncertainty in inputs ⇒ Compute uncertainty in the solution.

- How to model uncertainty in inputs ??
- Mathematical framework for uncertain solutions.
- Efficient numerical methods for UQ.

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- ► Use the Probabilistic framework a la Kolmogorov.
- Complete Probability space:
  - Ω (Set of Outcomes)
  - $\Sigma$  ( $\sigma$ -algebra (field) of Events)
  - $\mathbb{P}: \Omega \mapsto [0,1]$  with  $\mathbb{P}(\Omega) = 1$  (Probability measure).

#### Random fields

- Use Random fields to model Uncertain:
  - Initial data.
  - Boundary conditions.
  - Fluxes.
  - Sources.
- $(\Omega, \Sigma, \mathbb{P})$  is a complete probability space.
- ► Random field  $\mathbf{U}$  :  $(\Omega, \Sigma) \mapsto (\mathcal{F}, \mathcal{B}(\mathcal{F}))$  measurable
- *F* is a function space (separable Banach space) with Borel
   *σ*-algebra *B*(*F*)
- For  $\omega \in \Omega$ ,  $\mathbf{U}(\omega) \in \mathcal{F}$ .
- Example: Random initial data (scalar conservation laws):

$$egin{aligned} &u_0:(\Omega,\Sigma)\mapsto (L^1(\mathbb{R}^d),\mathcal{B}(L^1(\mathbb{R}^d)))\ &u_0(.,\omega)\in L^\infty(\mathbb{R}^d)\cap BV(\mathbb{R}^d),\mathbb{P}-a.s. \end{aligned}$$

# Representation of Random fields I: Parametric representation

- Random field represented by a finite number of parameters (Random Variables).
- Example I: Euler equations Sod Shock tube Uncertain initial location + amplitude:

$$\mathbf{U}_{0}(x,\omega) = \begin{cases} \mathbf{U}_{l} + \alpha(\omega) & \text{if } x \leq \beta(\omega), \\ \mathbf{U}_{r} & \text{if } x > \beta(\omega), \end{cases}$$
$$\alpha \sim 0.05\mathcal{U}[-1,1] \\ \beta \sim 0.2\mathcal{U}[-1,1] \end{cases}$$

2 Uniformly distributed random parameters.

# Euler equations – Sod Shock tube – Uncertain initial location + amplitude

 $\bullet$  Mean  $\pm$  Standard deviation.



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#### Ex II: Euler equations - Cloud shock interaction

• Deterministic Initial data:



#### Ex II: Euler equations - Cloud shock interaction

• Uncertain initial data in terms of 11 uniformly distributed parameters:



• Uncertainty in Shock location, amplitude, Bubble location, amplitude and geometry.

### Ex III: Shallow water equations- bottom topography

- Real data bottom topography given by Digital Terrain Models.
- Typical representation:



Interpolation using hierarchical hat basis (SM, Schwab, Sukys, 2013)

#### Bottom topography: one sample (realization)

Hierarchical hat basis representation

• 962 Random parameters !!!



#### Bottom topography: mean and standard deviation

Hierarchical hat basis representation

• 962 Random parameters !!!



#### Random fields II: Karhunen-Loeve expansions

- Bi-orthogonal decomposition ( a la Fourier Series).
- General form of KL expansion:

$$f=\overline{f}+\sum\sqrt{\lambda_k}Z_kf_k.$$

- $Z_k$ 's are Uncorrelated random variables as  $\mathbb{E}(Z_i Z_j) := \lambda_j \delta_{ij}$ .
- ▶  $\lambda_k, f_k$  are eigenvalues (vectors) of the Covariance operator:  $K_C : L^2(D) \mapsto L^2(D)$ :

$$\mathcal{K}_{C_f}[g](x) = \int_D C_f(x, y)g(y)dy, C_f(x, y) := \mathbb{E}(f(x, \omega)f(y, \omega)).$$

#### Ex I: Perturbed Burgers' flux

Has the KL expansion:

$$f(\omega; u) = f(\mathbf{y}; \mathbf{u})\Big|_{\mathbf{y}=\mathbf{Y}(\omega)} = \frac{\mathbf{u}^2}{2} + \delta\Big(\sum_{\mathbf{j}\geq\mathbf{1}} \mathbf{y}_{\mathbf{j}}\sqrt{\lambda_{\mathbf{j}}}\mathbf{\Phi}_{\mathbf{j}}(\mathbf{u})\Big),$$



▶ Represented as a Gaussian process with exponential covariance: C<sub>Y</sub>(u<sub>1</sub>, u<sub>2</sub>) = σ<sup>2</sup><sub>Y</sub>e<sup>-|u<sub>1</sub>-u<sub>2</sub>|/η</sup>

#### Ex II: Rock permeability for seismic imaging

Seismic Acoustic pulses modeled by Wave equation:

$$p_{tt} + div(\mathbf{c}\nabla p) = 0.$$

- Rewritten as a linear system of conservation laws.
- **c** is the rock permeability coefficient
- Highly uncertain modeled by a log normal Gaussian random field:

$$\log(\mathbf{c}(x,\omega)) := \log(\overline{c}(x)) + \sum_{k=1}^{\infty} \sqrt{\lambda_k} Z_k(\omega) g_k(x).$$

- Many different Covariance functions.
- Need Spectral FFT + Upscaling for efficient generation.

### Ex II: 2-D log normal layered permeability field (sample)

•  $\approx$  1000 uncertain parameters !!!



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### Ex II: 2-D log normal layered permeability field (statistics)

•  $\approx$  1000 uncertain parameters !!!



### Ex II: 3-D log normal layered permeability field (sample)

•  $\approx 10^6$  uncertain parameters !!!

DB: c at time 1



Random scalar conservation laws:

$$u_t(x, t, \omega) + \operatorname{div}(f(\omega; u(x, t, \omega))) = 0.$$
  
$$u(x, 0, \omega) = u_0(x, \omega).$$

with initial data and flux:

$$u_0: (\Omega, \Sigma) \mapsto (L^1(\mathbb{R}^d), \mathcal{B}(L^1(\mathbb{R}^d)))$$
$$f: (\Omega, \Sigma) \mapsto (C^1(\mathbb{R}^1; \mathbb{R}^d); \mathcal{B}(C^1(\mathbb{R}; \mathbb{R}^d)))$$

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#### Random entropy solution

- Solution is a random field that satisfies,
  - Measurability:  $u : \Omega \in \omega \mapsto u(x, t; \omega)$  is measurable from  $(\Omega, \Sigma)$  to  $C((0, T); L^1(\mathbb{R}^d))$ .
  - Weak solution: *u* satisfies the integral identity:

$$\begin{split} \int_{\mathbb{R}^{d}\times\mathbb{R}_{+}} (u(x,t,\omega)\varphi_{t}(x,t) + \langle f(\omega;u(x,t,\omega),\nabla\varphi(x,t)\rangle) dx dt \\ &+ \int_{\mathbb{R}^{d}} u(x,0,\omega)\varphi(x,0) dx = 0. \end{split}$$

for  $\mathbb{P}$ -a.e  $\omega \in \Omega$ .

Entropy conditions: satisfied for all entropy-entropy flux pairs and for P-a.e ω ∈ Ω.

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# Well-posedness theorem: SM, Schwab, 2010, SM et al 2012.

► For sufficiently regular *u*<sub>0</sub>,:

Existence: There exists a unique random entropy solution

$$u: \Omega \ni \omega \mapsto C_b(0, T; L^1(\mathbb{R}^d))$$

Construction:

$$u(\cdot, t; \omega) = S(t)u_0(\cdot, \omega), \quad t > 0, \ \omega \in \Omega$$

• Stability:  $\mathbb{P}$ -a.s  $\omega \in \Omega$ ,

$$\begin{aligned} \|u\|_{L^{k}(\Omega;C(0,T;L^{1}(\mathbb{R}^{d})))} &\leq \|u_{0}\|_{L^{k}(\Omega;L^{1}(\mathbb{R}^{d}))}, \\ \|S(t) u_{0}(\cdot,\omega)\|_{(L^{1}\cap L^{\infty})(\mathbb{R}^{d})} &\leq \|u_{0}(\cdot,\omega)\|_{(L^{1}\cap L^{\infty})(\mathbb{R}^{d})} \\ TV(S(t)u_{0}(\cdot,\omega)) &\leq TV(u_{0}(\cdot,\omega)) \end{aligned}$$

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Conservation law with uncertain initial data:

$$u_t(x, t, \omega) + \operatorname{div}(f(u(x, t, \omega))) = 0.$$
$$u(x, 0, \omega) = u_0(x, \omega).$$

- Discretization of Physical space-time.
- Standard Finite volume method
### Finite volume Grid



Of the form:

$$u_j^{n+1} - u_j^n + \frac{\Delta t}{\Delta x}(F_{j+1/2} - F_{j-1/2}) = 0$$

Have the following convergence rate:

$$\|u(.,t)-u_{\tau}(.,t)\|_{L^1(\mathbb{R}^d)}\leq C\Delta x^s.$$

Work estimate:

$$\operatorname{Work}_{\tau} = \mathcal{O}(\Delta x^{-(d+1)}).$$

Accuracy vs. Work:

$$\|u(.,t)-u_{\tau}(.,t)\|_{L^1(\mathbb{R}^d)} \leq C(\operatorname{Work}_{\tau})^{-rac{s}{d+1}}.$$

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Random conservation law:

$$u_t(x, t, \omega) + \operatorname{div}(f(\omega; u(x, t, \omega))) = 0.$$
$$u(x, 0, \omega) = u_0(x, \omega).$$

- Need to discretize the probability space.
- Statistical sampling methods: Monte Carlo (MC) method.

#### The MC algorithm:

- Draw *M* i.i.d samples for the initial data and flux:  $\{u_0^i, f^i\}_{1 \le i \le M}$ .
- For each sample: Solve conservation law by FVM to obtain  $u_{\tau}^{i}$ .
- Sample statistics:

$$\mathcal{M}^1 u(\cdot, t) pprox E_M[u_{ au}(\cdot, t)] := rac{1}{M} \sum_{i=1}^M u^i_{ au}(\cdot, t).$$
  
 $\mathcal{M}^k u(t_1, \dots, t_k) := rac{1}{M} \sum_{i=1}^M \underbrace{(u^i_{ au}(\cdot, t_1) \otimes \dots \otimes u^i_{ au}(\cdot, t_k))}_{k- ext{times}}.$ 

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#### Convergence:

$$\|\mathbb{E}[u(\cdot,t)] - E_{\mathcal{M}}[u_{\tau}(\cdot,t;\omega)]\|_{L^{2}(\Omega;L^{1}(\mathbb{R}^{d}))} \leq C_{\mathrm{stat}}M^{-\frac{1}{2}} + C_{\mathrm{st}}\Delta x^{s}.$$

• Number of samples: 
$$M = \mathcal{O}(\Delta x)^{-2s}$$
.

► Accuracy vs. Work:

$$\|\mathbb{E}[u(\cdot,t)] - E_M[u_{\tau}(\cdot,t;\omega)]\|_{L^2(\Omega;L^1(\mathbb{R}^d))} \leq C(\operatorname{Work}_{\tau})^{-\frac{s}{d+1+2s}}.$$

► Slow convergence ⇒ very high computational cost.

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- ▶ Heinrich 1995: Quadrature.
- Giles 2002: Stochastic ODEs.
- Barth, Schwab, Zollinger 2010: Elliptic PDEs.

#### MLMCFVM algorithm:

- Different nested levels of resolution: *I*.
- Draw  $M_i$  i.i.d samples for the initial data:  $\{u_{i,0}^i\}_{1 \le i \le M_i}$ .
- For each draw: Solve conservation law by FVM to obtain  $u_{l,\tau}^i$ .
- Sample statistics: with  $u_{\tau,-1} = 0$ ,

$$\mathcal{M}^1 u(\cdot, t) \approx E^L[u(\cdot, t)] = \sum_{\ell=0}^L E_{M_\ell}[u_{\tau,\ell}(\cdot, t) - u_{\tau,\ell-1}(\cdot, t)]$$
$$\mathcal{M}^k u(t_1, \dots, t_k) := \sum_{\ell=0}^L E_{M_\ell}[u_{\tau,\ell}^{(k)}(\cdot, t) - u_{\tau,\ell-1}^{(k)}(\cdot, t)]$$



#### Convergence:

$$\begin{split} \|\mathbb{E}[u(\cdot,t)] - E^{L}[u_{\tau}(\cdot,t,\omega)]\|_{L^{2}(\Omega;L^{1}(\mathbb{R}^{d}))} &\leq C_{1}\Delta x_{L}^{s} + C_{3}M_{0}^{-\frac{1}{2}} \\ &+ C_{2}\Big\{\sum_{\ell=0}^{L}M_{\ell}^{-\frac{1}{2}}\Delta x_{\ell}^{\frac{s}{2}}\Big\} \end{split}$$

- Level dependent number of samples:  $M_l = \mathcal{O}\left(\frac{\Delta x_l^s}{\Delta x_c^{2s}}\right)$
- Accuracy vs. Work: If  $0 \le s < (d+1)$ ,

$$\|\mathbb{E}[u(\cdot,t)] - E^{L}[u_{\tau}(\cdot,t;\omega)]\|_{L^{2}(\Omega;L^{1}(\mathbb{R}^{d}))} \leq C(\mathrm{Work})^{-\frac{s}{d+1+s}}$$

- Significantly more efficient than MCFVM !!!
- Sparse tensor higher moments computation with same efficiency.

### 1-D Burgers' with uncertain initial phase

• 1 random parameter.



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### Mean $\pm$ Standard deviation



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# Mean: MC vs MLMC



# Variance: MC vs MLMC



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# log(resolution) vs. log(relative error)



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# log(runtime) vs. log(relative error)



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### Buckley Leverette with uncertain relative permeabilities

#### • 2 random parameters.



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Random linear symmetrizable systems of conservation laws:

$$\mathbf{U}_t(x, t, \omega) + \sum_{r=1}^d \frac{\partial}{\partial \mathbf{x}_r} \left( \mathbf{A}_r(\mathbf{x}, \omega) \mathbf{U} \right) = 0.$$
$$\mathbf{U}(x, 0, \omega) = \mathbf{U}_0(x, \omega).$$

with uncertain initial data an flux:

$$\begin{split} \mathbf{U}_0 &: (\Omega, \Sigma) \mapsto (L^2(\mathbf{D}), \mathcal{B}(L^2(\mathbf{D})) \\ \mathbf{A}_r &: (\Omega, \Sigma) \mapsto (C^1(\mathbf{D})^{m \times m}; \mathcal{B}(C^1(\mathbf{D})^{m \times m})) \end{split}$$

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### Random Weak solution

- Solution is a random field that satisfies,
  - Measurability:  $\mathbf{U} : \Omega \in \omega \mapsto \mathbf{U}(x, t; \omega)$  is measurable from  $(\Omega, \Sigma)$  to  $C((0, T); L^2(\mathbf{D}))$ .
  - Weak solution: U satisfies the integral identity:

$$\int_{\mathbb{R}^{d} \times \mathbb{R}_{+}} \left( \mathbf{U} \cdot \boldsymbol{\varphi}_{t} + \sum_{r=1}^{d} \mathbf{A}_{r} \mathbf{U} \cdot \frac{\partial}{\partial \mathbf{x}_{r}} \boldsymbol{\varphi} \right) d\mathbf{x} dt + \int_{\mathbb{R}^{d}} \mathbf{U}_{0} \cdot \boldsymbol{\varphi}(t=0) \ d\mathbf{x} = 0.$$

for  $\mathbb{P}$ -a.e  $\omega \in \Omega$ .

 THM (SM, Schwab, Sukys 2014): Random weak solutions exist and are unique.

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### Schemes for Linear systems I: FVM





Under suitable assumptions on initial data + coefficients A<sub>r</sub>, FVM Convergence rate:

$$\|\mathbf{U}-\mathbf{U}^{\Delta x}\|_{L^2}\leq C\Delta x^s$$

#### The MC algorithm:

- Draw *M* i.i.d samples for the initial data and flux:  $\{\mathbf{U}_0^i, \mathbf{A}_r^i\}_{1 \le i \le M}$ .
- For each sample: Solve linear system by FVM to obtain  $\mathbf{U}_{\tau}^{i}$ .
- Sample statistics:

$$\mathbb{E}(\mathbf{U}(\cdot,t)) pprox E_M[\mathbf{U}_{ au}(\cdot,t)] := rac{1}{M}\sum_{i=1}^M \mathbf{U}^i_{ au}(\cdot,t).$$

Convergence (SM,Schwab,Sukys,2014):

 $\|\mathbb{E}[\mathbf{U}(\cdot,t)] - E_{\mathcal{M}}[\mathbf{U}_{\tau}(\cdot,t;\omega)]\|_{L^{2}(\Omega;L^{2}(\mathbf{D}))} \leq C_{\mathrm{stat}}M^{-\frac{1}{2}} + C_{\mathrm{st}}\Delta x^{s}.$ 

► Slow convergence ⇒ very high computational cost.

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# Schemes for Linear systems III: MLMCFVM-SM,Schwab,Sukys 2014



#### Convergence:

$$\begin{split} \|\mathbb{E}[\mathbf{U}(\cdot,t)] - E^{L}[\mathbf{U}_{\tau}(\cdot,t,\omega)]\|_{L^{2}(\Omega;L^{2}(\mathbb{R}^{d}))} &\leq C_{1}\Delta x_{L}^{s} + C_{3}M_{0}^{-\frac{1}{2}} \\ &+ C_{2}\Big\{\sum_{\ell=0}^{L}M_{\ell}^{-\frac{1}{2}}\Delta x_{\ell}^{s}\Big\} \end{split}$$

- Level dependent number of samples:  $M_l = O\left(\frac{\Delta x_l^{2s}}{\Delta x_r^{2s}}\right)$
- Same complexity as deterministic FVM !!!

Seismic Acoustic pulses modeled by Wave equation:

$$p_{tt} + div(\mathbf{c} \nabla p) = 0.$$

- Rewritten as a linear system of conservation laws.
- **c** is the rock permeability coefficient
- Highly uncertain modeled by a log normal Gaussian random field:

$$\log(\mathbf{c}(x,\omega)) := \log(\overline{c}(x)) + \sum_{k=1}^{\infty} \sqrt{\lambda_k} Z_k(\omega) g_k(x).$$

- Many different Covariance functions.
- Need Spectral FFT + Upscaling for efficient generation.

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# Ex : 2-D log normal layered permeability field (sample)

•  $\approx$  1000 uncertain parameters !!!



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## Ex : 2-D log normal layered permeability field T = 0.4

#### $\bullet \approx 1000$ uncertain parameters !!!



## Ex : 2-D log normal layered permeability field T = 0.6

#### $\bullet \approx 1000$ uncertain parameters !!!



# Ex : 2-D log normal layered permeability field T = 1.0

#### $\bullet \approx 1000$ uncertain parameters !!!



### Convergence of mean

•  $\approx$  1000 uncertain parameters !!!



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# Convergence of variance

•  $\approx$  1000 uncertain parameters !!!



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# Ex II: 3-D log normal layered permeability field (sample)

•  $\approx 10^6$  uncertain parameters !!!

DB: c at time 1



## Ex II: Mean at T = 0.4

 $\bullet \approx 10^6$  uncertain parameters !!!

DB: mean of p at time 0.4



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## Ex II: Mean at T = 0.6

 $\bullet \approx 10^6$  uncertain parameters !!!

DB: mean of p at time 0.6



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## Ex II: Mean at T = 1.0

 $\bullet \approx 10^6$  uncertain parameters !!!

DB: mean of p at time 1



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#### Ex II: Variance at T = 0.4

 $\bullet \approx 10^6$  uncertain parameters !!!

DB: variance of p at time 0.4



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#### Ex II: Variance at T = 0.6

 $\bullet \approx 10^6$  uncertain parameters !!!

DB: variance of p at time 0.6



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## Ex II: Variance at T = 1.0

 $\bullet \approx 10^6$  uncertain parameters !!!

DB: variance of p at time 1



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# Euler equations with uncertain shock location and amplitude



Siddhartha Mishra UQ for hyperbolic PDEs

#### Mean $\pm$ Standard deviation



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#### Mean: MC vs MLMC





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## log(resolution) vs. log(relative error in mean)



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## log(runtime) vs. log(relative error in mean)



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# Uncertain Orszag-Tang vortex for MHD (2 Sources of uncertainty)



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# Uncertain Orszag-Tang vortex for MHD (Convergence of mean)



# Uncertain Orszag-Tang vortex for MHD (Convergence of variance)



### Flow past aerofoils: Left: NACA0012, Right:RAE2826



Siddhartha Mishra UQ for hyperbolic PDEs

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## Mean $\pm$ STD for $C_p$ : Left: NACA0012, Right: RAE2826



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#### Variance decay: Left: NACA0012, Right:RAE2826



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