Numerical Methods and UQ Analysis for Phase Field Equations

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Outline

1. Diffuse Interface / Phase Field Model
2. Uncertainty Quantification (UQ)
3. UQ and stability
   - Stochastic Galerkin methods
4. Sample-based methods and stability
5. Conclusions and references

Phase field model

- A very simple/popular tool

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- Long history, extensive literature

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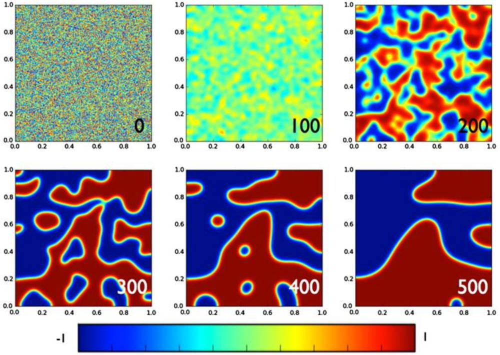
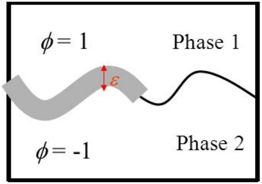
- Long history, extensive literature
- An approximation to the sharp interface

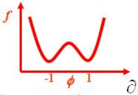


Phase-Field Models

- **Approach to moving boundary problems**
  - Phases associated with value of ϕ
    - Interface implies $\phi = 0$
  - Diffuse interface
    - Original problem obtained when $\varepsilon \to 0$

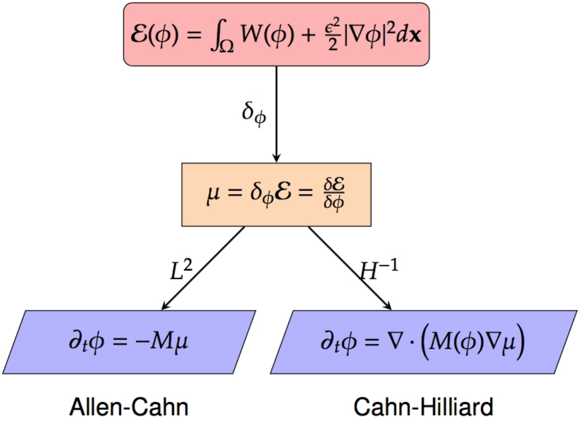


- **Dynamics of ϕ**
  - Can be derived from a free energy $F[\phi, \varepsilon]$



  - Non-conserved order parameter: Allen-Cahn equation $\dfrac{\partial \phi}{\partial t} = -\dfrac{\delta F}{\delta \phi}$
  - Conserved order parameter: Cahn-Hilliard equation $\dfrac{\partial \phi}{\partial t} = \nabla^2 \dfrac{\delta F}{\delta \phi}$

Allen-Cahn and Cahn-Hilliard Equation



ϕ : concentration or temperature
W : double-well function
μ : chemical potential
M : diffusion mobility

Allen-Can/ Cahn-Hilliard Eqns

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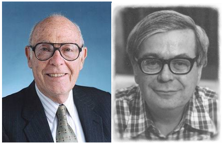

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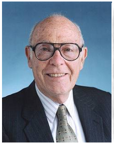


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$$u_t = -\delta \Delta^2 u + \nabla \cdot f(\nabla u),$$

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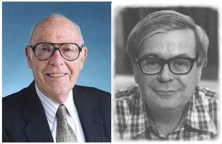

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$$u_t = -\delta\Delta^2 u + \nabla \cdot f(\nabla u),$$

- Typical f: $f(\phi) = \phi|\phi|^2 - \phi$. An important feature is that they can be viewed as the gradient flow of the following energy functionals:

$$E_{MBE}(u) = \int_\Omega \left[\frac{\delta}{2}|\Delta u|^2 + \frac{1}{4}(|\nabla u|^2 - 1)^2\right] dx$$

$$E_{CH}(u) = \int_\Omega \left[\frac{\delta}{2}|\nabla u|^2 + \frac{1}{4}(|u|^2 - 1)^2\right] dx$$

Energy decay (the key for numerical stability)

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$$E(u(t) \leq E(u(s)), \quad \forall t \geq s.$$

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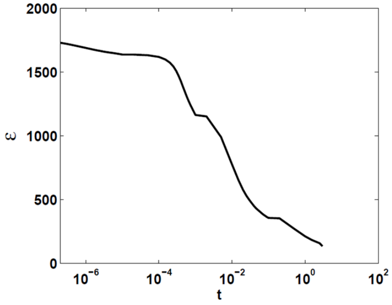
- Example: Cahn-Hilliard impainting

$$u_t = \Delta\left(-\delta\Delta u - \frac{1}{\delta}F'(u)\right) + \lambda(f - u)$$

[Bertozzi etc. IEEE Tran. Imag. Proc. 2007, Commun. Math. Sci, 2011]



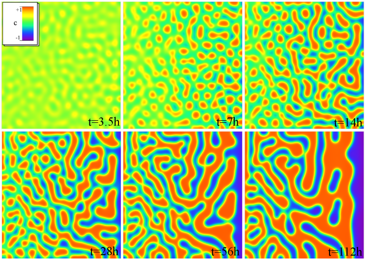
Numerical Challenge for Phase Field Computations

- Difficulties:

  Catch dynamics (small Δt) & steady state (large Δt)

  Higher order methods vs. efficiency

  Long-Time Integration



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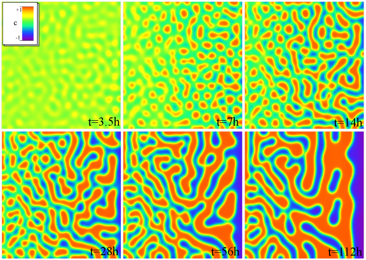

- Different Approaches:
  Energy decay methods (numerous efforts)

  Adaptivity in time/space; Moving mesh spectral method etc

start from Allen-Cahn eqn

- To demonstrate the main idea, we consider

$$
\begin{aligned}
&u_t = u_{xx} + u(1-u^2), \quad x \in (-1,1), \\
&u(\pm 1, t) = 0, \\
&u(x,0) = f(x).
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- Define the energy function in L^2- space

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E(u) = \int_\Omega (\frac{1}{2}|\nabla u|^2 + F(u))dx
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where $F(u) = \frac{1}{4}(1 - u^2)^2$.

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- Multiplying u_t on both sides of the AC eqn, and then use integration by parts gives

$$\frac{d}{dt}E(u) \leq 0, \quad \forall t > 0.$$

Implicit scheme: Crank-Nicholson

- The CN scheme

$$\frac{u_j^{n+1}-u_j^n}{\Delta t}=\frac{1}{2\Delta x^2}\left(\delta_-\delta_+u_j^{n+1}+\delta_-\delta_+u_j^n\right)+\frac{u_j^{n+1}+u_j^n}{2}\left(1-\frac{(u_j^{n+1})^2+(u_j^n)^2}{2}\right).$$

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$$\delta_+u_j=u_{j+1}-u_j,\quad \delta_-u_j=u_j-u_{j-1}.$$

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where

$$\delta_+ u_j = u_{j+1} - u_j, \quad \delta_- u_j = u_j - u_{j-1}.$$

- For the CN scheme, the following gradient flow property is satisfied

$$\hat{E}(u^{n+1}) \leq \hat{E}(u^n),$$

where

$$\hat{E}(u^{n+1}) := \sum_j \left(\frac{u_{j+1}^{n+1} - u_j^n}{\Delta x}\right)^2 \Delta x + \sum_j \frac{1}{4}\left(1 - (u_j^{n+1})^2\right)^2$$

simple proof

- Multiplying $u_j^{n+1} - u_j^n$ on both sides of the CN scheme gives

$$\left(u_j^{n+1} - u_j^n\right)^2 = \frac{\lambda}{2}\left(u_j^{n+1} - u_j^n\right)\left(\delta_-\delta_+ u_j^{n+1} + \delta_-\delta_+ u_j^n\right) + \frac{\Delta t}{2}\left((u_j^{n+1})^2 - (u_j^n)^2\right)\left(1 - \frac{(u_j^{n+1})^2 + (u_j^n)^2}{2}\right),$$

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- Summing over j and using integration by parts give

$$\begin{aligned}
&\sum_j \left(u_j^{n+1} - u_j^n\right)^2 \Delta x \\
= \quad & -\frac{\lambda}{2}\sum_j \delta_+\left(u_j^{n+1} - u_j^n\right)\left(\delta_+ u_j^{n+1} + \delta_+ u_j^n\right)\Delta x \\
& + \frac{\Delta t}{2}\sum_j \left[(u_j^{n+1})^2 - (u_j^n)^2 - \frac{1}{2}\left((u_j^{n+1})^4 - (u_j^n)^4\right)\right]\Delta x \\
= \quad & -\frac{\lambda}{2}\sum_j \left[\left(\delta_+ u_j^{n+1}\right)^2 - \left(\delta_+ u_j^n\right)^2\right]\Delta x - \frac{\Delta t}{4}\sum_j \left[\left(1 - (u_j^{n+1})^2\right)^2 - \left(1 - (u_j^n)^2\right)^2\right]\Delta x.
\end{aligned} \tag{1}$$

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- As the left-hand side of (1) is non-negative, we obtain

$$\frac{1}{2}\sum_j \left[\left(\frac{\delta_+ u_j^{n+1}}{\Delta x}\right)^2 - \left(\frac{\delta_+ u_j^n}{\Delta x}\right)^2\right]\Delta x + \frac{1}{4}\sum_j \left[\left(1 - (u_j^{n+1})^2\right)^2 - \left(1 - (u_j^n)^2\right)^2\right]\Delta x \le 0.$$

Linear approximation

- Note that CN scheme is nonlinear. Consider *linear* scheme:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{1}{\Delta x^2}\delta_-\delta_+ u_j^{n+1} + u_j^{n+1}\Big(1 - (u_j^n)^2\Big), \quad 1 \le j \le J - 1$$

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Linear scheme satisfying gradient flow property

- consider

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- If $\Delta t < 1$ and

$$\Delta t \|u_0\|_\infty e^{cT} < 1,$$

then the following gradient flow property is satisfied

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Convex splitting for Cahn-Hillard eqn

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$$E(u) = E_c(u) - E_e(u)$$

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where $E_c, E_e \in C^2$ and are strictly convex.
- The semi-implicit discretization is given by

$$\frac{U^{n+1} - U^n}{\Delta t} = -\Big(\nabla E_c(U^{n+1}) - \nabla E_e(U^n)\Big).$$

Various Eyre’s type or various extension

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- Using the splitting form for CHE

$$E_c(u) = \int_\Omega \left(\frac{\delta}{2}|\nabla u|^2 + \frac{\beta}{2}u^2\right)dx, \quad E_e(u) = \int_\Omega \left(\frac{\beta}{2}u^2 - F(u)\right)dx,$$

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- we have

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- If the constant β is sufficiently large, then

$$E(u^{n+1}) \leq E(u^n), \quad n = 0, 1, \cdots .$$

Lower order with p-adaptivity

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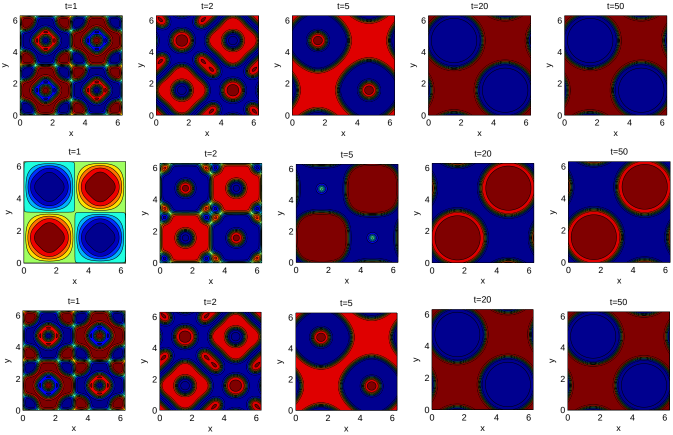
- (a)

(b)

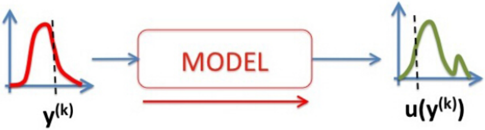
(c)



Uncertainty Quantification (UQ)

Uncertainty propagation: non-intrusive

- Non-intrusive methods: only require (multiple) solutions of the original (deterministic) model



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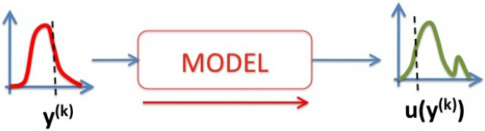

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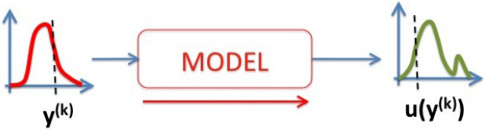

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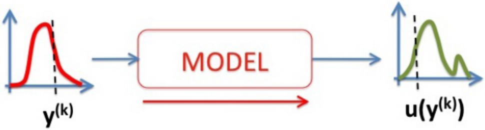

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- Monte Carlo (low order), stochastic collocation (High order), ect.

Non-intrusive approach: Monte Carlo

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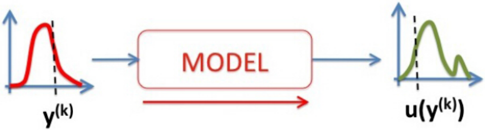

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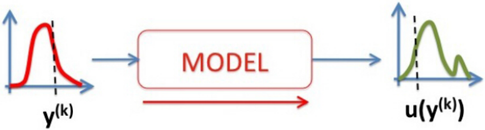
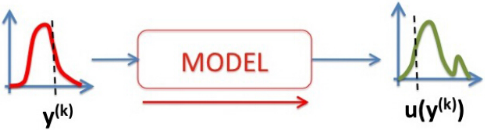


- Approximation of statistic moments

$$\mathbb{E}[u] \approx \frac{1}{M}\sum_{k=1}^{M} u\left(\mathbf{y}^{(\mathbf{k})}\right).$$

Non-intrusive approach: Monte Carlo

- If you know how to sample $\left\{\mathbf{y}^{(\mathbf{k})}\right\}_{k=1}^{M}$ ... it's done



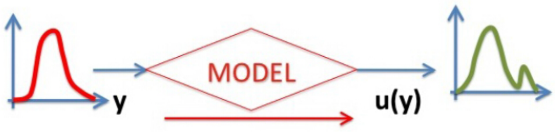
- Approximation of statistic moments

$$\mathbb{E}[u] \approx \frac{1}{M} \sum_{k=1}^{M} u\left(\mathbf{y}^{(\mathbf{k})}\right).$$

- Slow convergence rate $M^{-\frac{1}{2}}$, but independent of the dimension d.

Uncertainty propagation: intrusive

- Intrusive methods: require the formulation and solution of a stochastic version of the original model



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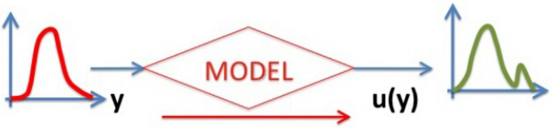

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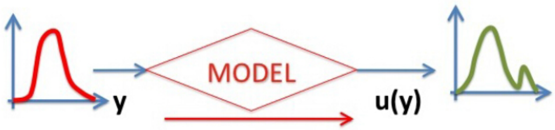

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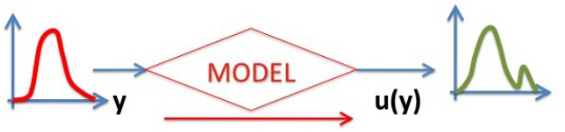

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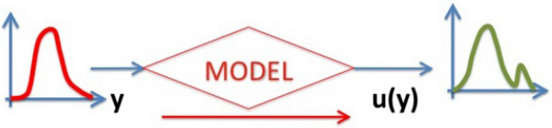

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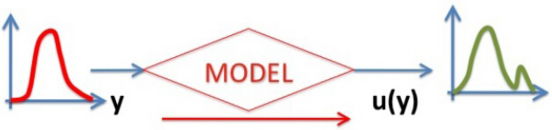

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- Computational cost can be high for large-scale problems.

Numerical Study for Uncertainties

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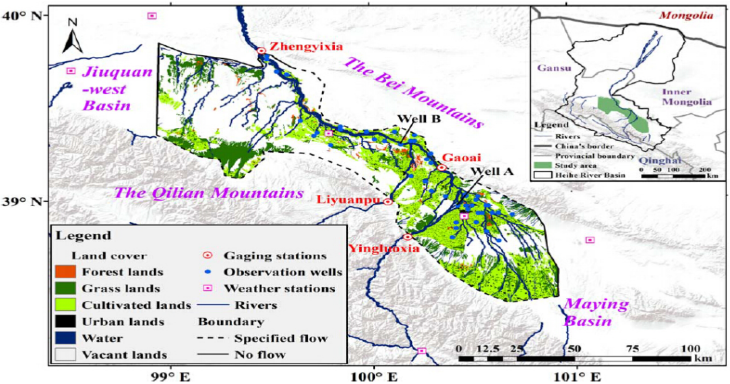
Subsurface flow in random media (Dagan '89, Zhang '02)



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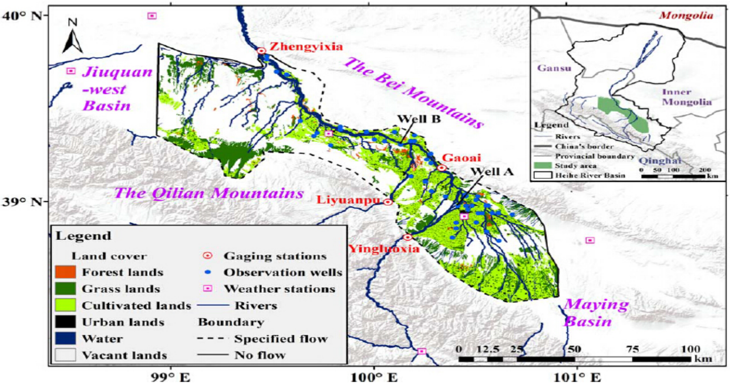
$$\begin{cases} \nabla \cdot (K(x,\omega)\nabla h(x)) + g(x) = 0, & x \in \Gamma, \\ h(x) = H(x), & x \in \Gamma_D, \\ K(x,\omega)\nabla h(x) \cdot \mathbf{n}(x) = -Q(x), & x \in \Gamma_n. \end{cases}$$



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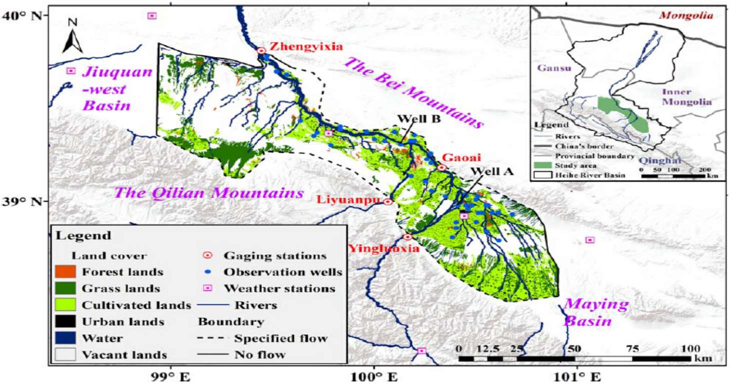
Log-normal conductivity:

$Y(x,\omega) = \ln K(x,\omega)$,

$Y(x,\omega) \sim$ Gaussian random field



The elliptic model problem

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  - Babuska-Nobile et al '07, Cohen-DeVore-Schwab '10

Generalized Polynomial Chaos (Xiu & Karniadakis '03)

- Multivariate polynomial expansions:

$$u(x, \mathbf{y}) \approx \sum_{\alpha \in \mathcal{I}} \widehat{c}_\alpha(x) \phi_\alpha(\mathbf{y}), \quad \text{with} \quad \int \rho(\mathbf{y}) \phi_\alpha(\mathbf{y}) \phi_\beta(\mathbf{y}) d\mathbf{y} = \delta_{\alpha\beta}.$$

Input	Polynomial	Density	Support
Normal	Hermite $He_n(x)$	$e^{-\frac{x^2}{2}}$	$[-\infty, +\infty]$
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- Total degree polynomial spaces with degree q:

$$\mathcal{I} := \{\alpha : \|\alpha\|_1 \le q\} \quad \Rightarrow \quad N = \binom{q+d}{d} = \frac{(q+d)!}{q!d!}.$$

Advantages of gPC

- Computation of statistic moments:

$$\mathbb{E}[u] \approx \mathbb{E}[u_N] = \widehat{c}_1(x), \quad \mathbb{V}ar[u] \approx \mathbb{V}ar[u_N] = \sum_{n=2}^{N} \widehat{c}_n^2(x)$$

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- High order rate of convergence for smooth problems
- The goal: efficient recover the unknown coefficients $\{\widehat{c}_n(x)\}$

Intrusive Approach: Stochastic Galerkin

$$\left\langle \phi_n(\mathbf{y}), -\nabla \cdot (\kappa(x, \mathbf{y})\nabla u) \right\rangle_{\rho(\mathbf{y})} = \left\langle \phi_n(\mathbf{y}), f(x, \mathbf{y}) \right\rangle_{\rho(\mathbf{y})}, \quad n = 1, ..., N.$$

$$\Downarrow$$

$$-\nabla \cdot [\mathbf{A}(x)\nabla \mathbf{c}] = \mathbf{f} \quad \text{Deterministic system}$$

- $\mathbf{c} = (\widehat{c}_1(x), ..., \widehat{c}_N(x))^\top, \ \mathbf{f} = (\widehat{f}_1(x), ..., \widehat{f}_N(x))^\top, \ \mathbf{A}(x) = [\mathbf{A}_{n,m}(x)]$

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- Drawbacks: coupled system, hard to solve in general.

Non-intrusive Approach: Stochastic Collocation

- Sampling the parametric space:

$$\left\{\mathbf{y}^{(\mathbf{m})}\right\}_{m=1}^{M} \xrightarrow[\text{PDE Solver}]{} \left\{u\left(x, \mathbf{y}^{(\mathbf{m})}\right)\right\}_{m=1}^{M}$$

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- The approximation "$\approx$" will be explained later.

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  - Various sampling methods can be adopted, again, stability & efficiency are important

Stability results for unbounded domain (Tang-Zhou, 'SISC14)

- Stable with high probability:

$$\Pr\left\{ |||\hat{\mathbf{A}} - \mathbf{I}||| \geq \frac{5}{8} \right\} \leq M^{-\gamma} \text{ provided that } \frac{M}{\log M} > \gamma N,\ L > 5\sqrt{N}.$$

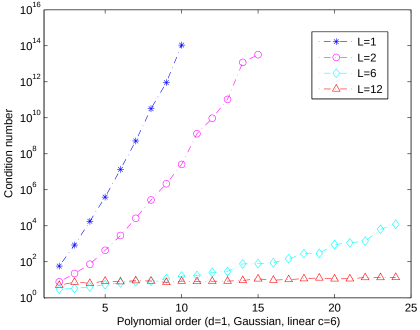

Figure: Condition number against polynomial order in 1D (Gaussian)

Allen-Cahn Eqn

Consider a simple stochastic ACE:

$$u_t(x,t,\mathbf{z}) = \delta(\mathbf{z})u_{xx} + u(1-u^2), \quad x \in (-1,1),$$
$$u(\pm 1, t, \mathbf{z}) = 0, \quad u(x,0) = u_0(x,\mathbf{z}).$$

- ... the input random vector $\mathbf{z} = (z_1, \cdots, z_d) \in \mathbb{R}^d$, where $\{\mathbf{z}_k\}_{k=1}^d$ are independent random parameters.

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- Mean value and variance function:

$$\mathbb{E}[u](x,t) = \int_\Gamma \rho(\mathbf{z})u(x,t,\mathbf{z})d\mathbf{z}, \quad \mathbb{V}\text{ar}[u](x,t) = \int_\Gamma \rho(\mathbf{z})(u-\mathbb{E}[u])^2 d\mathbf{z}.$$

Free energy for ACE

- Consider a new free energy in the expectation sense, i.e.

$$\widehat{E}(u) := \mathbb{E}\left[\int_\Omega \left(\frac{\delta}{2}|\nabla u|^2 + F(u)\right) dx\right] = \int_\Gamma \int_\Omega \rho(\mathbf{z}) \left(\frac{\delta}{2}|\nabla u|^2 + F(u)\right) dx d\mathbf{z}.$$

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$$\widehat{E}(u) := \mathbb{E}\left[\int_{\Omega}\left(\frac{\delta}{2}|\nabla u|^2 + F(u)\right)dx\right] = \int_{\Gamma}\int_{\Omega}\rho(\mathbf{z})\left(\frac{\delta}{2}|\nabla u|^2 + F(u)\right)dxd\mathbf{z}.$$

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- Another interesting problem is to investigate the following free energy:

$$\overline{E}(u) := \int_\Omega \left(\frac{\delta}{2}|\nabla \bar{u}|^2 + F(\bar{u})\right) \mathrm{d}x \quad \text{with} \quad \bar{u} = \mathbb{E}[u].$$

i.e.,consider the free energy with respect to the mean

Stochastic Galerkin methods

- Expand the solution in the parametric space by polynomials

$$u(x,t,\mathbf{z}) \approx u_M = \sum_{k=1}^{M} v_k(x,t)\phi_k(\mathbf{z}), \quad \int_\Gamma \rho(\mathbf{z})\phi_k(\mathbf{z})\Phi_j(\mathbf{z})d\mathbf{z} = \delta_{kj}.$$

... $\mathbf{v} = \{v_1, \ldots, v_M\}$ are the expansion coefficients to be determined, and $\{\phi_k\}_{k=1}^M$ are orthogonal polynomials in Γ.

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$$\|u_M\|_{L^2(\Gamma\otimes D)} \leq \mathrm{e}^{2t}\|u_{0,M}\|_{L^2(\Gamma\otimes D)},$$

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  $$\mathbf{v}_t = \mathbf{A}\Delta\mathbf{v} - \mathbf{f}(\mathbf{v}),$$

  where

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- IC and BC are given by

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The energy law for the Galerkin system

- Consider the Galerkin system

$$\mathbf{v}_t = \mathbf{A}\mathbf{v}_{xx} - \mathbf{f}(\mathbf{v}). \tag{2}$$

We define the associated free energy as

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- Multiplying both sides of (2) by $-\mathbf{v}_t^\top$ to obtain $-\mathbf{v}_t^\top \mathbf{A}\mathbf{v}_{xx} + \mathbf{v}_t^\top \mathbf{f}(\mathbf{v}) \le 0$. Then

$$\begin{aligned}
&\int_\Omega \left(-\mathbf{v}_t^\top \mathbf{A}\mathbf{v}_{xx} + \mathbf{v}_t^\top \mathbf{f}(\mathbf{v})\right) dx \\
&= \int_\Omega \left(\mathbf{v}_{tx}^\top \mathbf{A}\mathbf{v}_x + \sum_j \frac{\partial v_j}{\partial t} \int_\Gamma \rho(\mathbf{z}) f(u_M)\phi_j(\mathbf{z}) d\mathbf{z}\right) dx \\
&= \int_\Omega \left(\mathbf{v}_{tx}^\top \mathbf{A}\mathbf{v}_x + \sum_j \frac{\partial v_j}{\partial t} \int_\Gamma \rho(\mathbf{z}) f(u_M)\phi_j(\mathbf{z}) d\mathbf{z}\right) dx \\
&= \int_\Omega \left(\mathbf{v}_{tx}^\top \mathbf{A}\mathbf{v}_x + \int_\Gamma \rho(\mathbf{z}) f(u_M)\frac{\partial u_M}{\partial t} d\mathbf{z}\right) dx \\
&= \frac{d}{dt}\int_\Omega \left(\mathbf{v}_x^\top \mathbf{A}\mathbf{v}_x + \int_\Gamma \rho(\mathbf{z}) F(u_M) d\mathbf{z}\right) dx.
\end{aligned}$$

Monte Carlo method

- First generates randomly a sample set $\{\mathbf{z}_l\}_{l=1}^{L}$ according to $\rho(\mathbf{z})$, and then solve the random ACE for each $\mathbf{z}_l$ to obtain $u_l = u(x, t, \mathbf{z}_l)$.

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- Good: the energy law is preserved

$$\frac{d}{dt}\widehat{E}_L(u) =: \frac{1}{L}\sum_{l=1}^{L}\frac{d}{dt}E(u_l) \leq 0,$$

Bad: the associated convergence rate is only one half :$1/\sqrt{L}$.

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- For example, if uniform density is considered, then one choose the Legendre Gaussian points as samples; while if normal distribution is considered, the Hermite Gaussian points will be used as samples.
- Suppose the $\{\mathbf{z}_k\}_{k=1}^K$ are those samples (i.e., the tensor product of Gaussian-type points), we solve the random ACE for each point $\mathbf{z}_k$

$$
\begin{aligned}
&u_t(x,t,\mathbf{z}_k) = \delta(\mathbf{z}_k)u_{xx} + u(1-u^2), \quad x \in (-1,1), \\
&u(\pm 1, t, \mathbf{z}_k) = 0, \quad u(x,0) = u_0(x,\mathbf{z}_k).
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$$u_K(x,t,\mathbf{z}) = \sum_{k=1}^{K} u_k(x,t,\mathbf{z}_k)\mathbf{T}_k(\mathbf{z}).$$

Notice that the Lagrange bases $\{\mathbf{T}_k\}_{k=1}^{K}$ are of tensor-product type. the Lagrange interpolation is constructed by tensorize the one-dimensional interpolation.

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- We have

$$\frac{d}{dt}\widehat{E}_K(u(x,t,\mathbf{z})) =: \sum_{k=1}^{K} \mathbf{w}_k \frac{d}{dt} E(u(x,t,\mathbf{z}_k)) \le 0.$$

Here $\{\mathbf{w}_k\}$ are the quadrature weights associated with the Gaussian-type points

$$\mathbf{w}_k = \int_\Gamma \rho(\mathbf{z})\mathbf{T}_k(\mathbf{z})d\mathbf{z} \ge 0, \quad k = 1, ..., K.$$

Some remarks

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- This number is huge when d is large (known as the curse of dimensionality).
- To overcome this, one may resort to the so called sparse grid rule. However, in sparse grid approach, the positivity of the weights are no longer guaranteed, and the energy stability may not hold.

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- UQ introduces new analysis, e.g., probabilistic based analysis
- UQ can be very interdisciplinary, and often involves subjects such as scientific computing, approximation theory, probability, random matrix, compressed sensing ect

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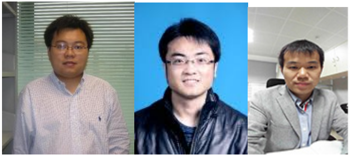

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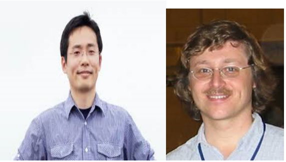

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