

Uncertainty Quantification for Complex Systems

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Outline

Discussion Points

- 1 Sources of Uncertainty
- 2 Analytic Methods
- 3 Numerical Methods
- 4 Results
- 5 Extra: Sensitivity Analysis

Introduction

Who is this guy?

Current:

- Ph.D Nuclear Engineering student, UNM
- Idaho National Laboratory (RAVEN, MOOSE)

Past:

- M.S. Nuclear Engineering, Oregon State University
- B.S. Physics, BYU-Idaho (2010)

RAVEN

...and its place in the herd.

MOOSE herd

- MARMOT: Mesoscale materials
- BISON: Engineering-scale materials
- RattleSnake: Neutronics
- RELAP-7: Thermal Hydraulics

A different kind of critter...

- RAVEN: Uncertainty Quantification

Uncertainty

Two Types

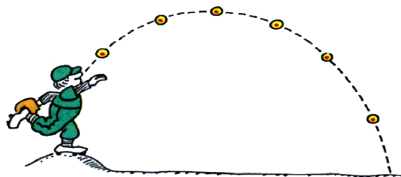
- Epistemic - Unmeasured Uncertainty
 - Tool Accuracy
 - Complicated Dependencies (arrow, double pendulum)
 - Documentation
- Aleatory - True Randomness
 - Quantum effects
 - Particle-Material interactions (gold foil)
 - Brownian Motion

Example Stochastic Problem

Projectile Motion

$$y(t) = y_i + v \sin(\theta)t - \frac{1}{2}gt^2,$$

$$x(t) = v \cos(\theta)t.$$



$$\text{Solution: } x_f = \frac{v \cos \theta}{g} \left(v \sin \theta + \sqrt{v^2 \sin^2 \theta + 2gy_i} \right)$$

Example Stochastic Problem

Solved...?

$$x_f = \frac{v \cos \theta}{g} \left(v \sin \theta + \sqrt{v^2 \sin^2 \theta + 2gy_i} \right)$$

- initial height $y_i = 2$ m
- initial velocity $v = 35$ m/s
- initial trajectory $\theta = 35^\circ$
- accel. gravity $g = 9.81$ m/s/s

Solution: $x_f \approx 120$ m

Example Stochastic Problem

...I'm not so certain anymore.

$$x_f = \frac{v \cos \theta}{g} \left(v \sin \theta + \sqrt{v^2 \sin^2 \theta + 2gy_i} \right)$$

- initial height $y_i = 1 \pm 1$ m
- initial velocity $v = 35.5 \pm 2.5$ m/s
- initial trajectory $\theta = 45 \pm 10^\circ$
- accel. gravity $g = 9.7988 \pm 0.0349$ m/s/s

Solution: $x_f = ?$

Uncertainty Quantification

Methods

Some way to quantify uncertainty:

Uncertainty Quantification

Methods

Some way to quantify uncertainty:

- Min-Max
 - Good for monotonic problems

Uncertainty Quantification

Methods

Some way to quantify uncertainty:

- Min-Max
 - Good for monotonic problems
- Sandwich Formula
 - Good for analytic solutions

Uncertainty Quantification

Methods

Some way to quantify uncertainty:

- Min-Max
 - Good for monotonic problems
- Sandwich Formula
 - Good for analytic solutions
- Perturbation
 - Valid for small uncertainty

Uncertainty Quantification

$$x_f = \frac{v \cos \theta}{g} \left(v \sin \theta + \sqrt{v^2 \sin^2 \theta + 2gy_i} \right)$$

Min-Max

$$x_{f,\min} = \frac{(33)(0.5736)}{9.8337} \left((33)(0.8192) + \sqrt{(33)^2(0.8192)^2 + 2(9.8337)(0)} \right) = 105.46 \text{ m}$$

$$x_{f,\max} = \frac{(55)(0.8192)}{9.7369} \left((55)(0.5736) + \sqrt{(55)^2(0.5736)^2 + 2(9.8337)(2)} \right) = 142.17 \text{ m}$$

Result: $x_f \approx 124 \pm 18.3 \text{ m}$

Uncertainty Quantification

$$x_f = \frac{v \cos \theta}{g} \left(v \sin \theta + \sqrt{v^2 \sin^2 \theta + 2gy_i} \right)$$

Min-Max

$$x_{f,\min} = \frac{(33)(0.5736)}{9.8337} \left((33)(0.8192) + \sqrt{(33)^2(0.8192)^2 + 2(9.8337)(0)} \right) = 105.46 \text{ m}$$

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Result: $x_f \approx 124 \pm 18.3 \text{ m}$

Flawed Reasoning

- θ not monotonic!

Does increasing θ make a longer or shorter range?

Uncertainty Quantification

Sandwich Formula (simplified):

$$\sigma_{x_f} = \sqrt{\left(\frac{\partial x_f}{\partial y_i}\right)^2 \sigma_{y_i}^2 + \left(\frac{\partial x_f}{\partial v}\right)^2 \sigma_v^2 + \left(\frac{\partial x_f}{\partial g}\right)^2 \sigma_g^2 + \left(\frac{\partial x_f}{\partial \theta}\right)^2 \sigma_\theta^2}$$

Works well for simple functions

- Simple derivatives
- Analytic solution
- Assumes mean is reference value

Uncertainty Quantification

$$x_f = \frac{v \cos \theta}{g} \left(v \sin \theta + \sqrt{v^2 \sin^2 \theta + 2gy_i} \right)$$

Sandwich Formula:

$$\sigma_{x_f} = \sqrt{\left(\frac{\partial x_f}{\partial y_i}\right)^2 \sigma_{y_i}^2 + \left(\frac{\partial x_f}{\partial v}\right)^2 \sigma_v^2 + \left(\frac{\partial x_f}{\partial g}\right)^2 \sigma_g^2 + \left(\frac{\partial x_f}{\partial \theta}\right)^2 \sigma_\theta^2}$$

Result: $x_f = 120 \pm 62.44$ m

A More Difficult Problem

Air Resistance

With Air Resistance:

$$y(t) = \frac{v_T}{g}(v \sin \theta + v_T) \left(1 - e^{-gt/v_T}\right) - v_T t,$$

$$x(t) = \frac{vv_T \cos \theta}{g} \left(1 - e^{-gt/v_T}\right).$$

$$v_T = \frac{mg}{D}, \quad D = \frac{\rho CA}{2}, \quad A = \pi r^2$$

Solve numerically to get x_f (Forward Euler).

A More Difficult Problem

Aside: Forward Euler

Take small Δ_t time steps while $y^t > 0$: $t = t + \Delta_t$,

$$a_x^{(t+\Delta_t)} = \frac{-D}{m} v_x^{(t)}, \quad a_y^{(t+\Delta_t)} = -g - \frac{D}{m} v_y^{(t)},$$

$$v_x^{(t+\Delta_t)} = v_x^{(t)} + a_x^{(t+\Delta_t)} \Delta_t, \quad v_y^{(t+\Delta_t)} = v_y^{(t)} + a_y^{(t+\Delta_t)} \Delta_t,$$

$$x^{(t+\Delta_t)} = x^{(t)} + v_x^{(t+\Delta_t)} \Delta_t + \frac{1}{2} a_x^{(t+\Delta_t)} \Delta_t^2,$$

$$y^{(t+\Delta_t)} = y^{(t)} + v_y^{(t+\Delta_t)} \Delta_t + \frac{1}{2} a_y^{(t+\Delta_t)} \Delta_t^2.$$

(video)

Uncertainty Summary

$$\rho_{\text{air}} = 1.2 \pm 0.1 \text{ kg/m}^3.$$

► Sensitivity Study



A More Difficult Problem

Equation Summary

$$y(t) = \frac{v_T}{g}(v \sin \theta + v_T) \left(1 - e^{-gt/v_T}\right) - v_T t,$$

$$x(t) = \frac{vv_T \cos \theta}{g} \left(1 - e^{-gt/v_T}\right).$$

$$v_T = \frac{mg}{D}, \quad D = \frac{\rho CA}{2}, \quad A = \pi r^2$$

Uncertainty Quantification

Complicated Problems

How do we quantify uncertainty for problems without simple analytic solutions?

- Monte Carlo sampling
- Stochastic Collocation

Uncertainty Quantification

Monte Carlo

- Let $u(Y)$ be any system, like $x_f(y_i, v, \theta, g, m, r, C, \rho)$
- Randomly sample input parameters, record outputs
- Repeat M times
- Calculate moments (mean, variance, skew, kurtosis)

$$\text{Mean: } \bar{u} \approx \frac{1}{M} \sum u(Y^{(m)})$$

(video)

Uncertainty Quantification

Stochastic Collocation

- Let $u(Y)$ be any system, like $x_f(y_i, v, \theta, g, m, r, C, \rho)$
- Represent original model with polynomials
- Calculate moments (mean, variance, skew, kurtosis)

$$u(Y) \approx S[u(Y)] \equiv \sum_{k \in \Lambda} c_k \Phi_k(Y),$$

$$\Phi_k(Y) = \phi_{k_1}(Y_1) \cdot \phi_{k_2}(Y_2) \cdot \dots \cdot \phi_{k_N}(Y_N)$$

Uncertainty Quantification

Stochastic Collocation

Our case:

$$\begin{aligned} x_f(y_i, v, \theta, g, m, r, C, \rho) &\approx S[x_f(y_i, v, \theta, g, m, r, C, \rho)], \\ &\approx \sum_{k \in \Lambda} c_k \Phi_k(y_i, v, \theta, g, m, r, C, \rho), \end{aligned}$$

$$\Phi_k(y_i, v, \theta, g, m, r, C, \rho) = \phi_{y_i}(y_i) \cdot \phi_v(v) \cdot \dots \cdot \phi_\rho(\rho).$$

$$c_k = \frac{\int \int \int \int \int \int \int \int x_f \Phi \, d(y_i, v, \theta, g, m, r, C, \rho)}{\int \int \int \int \int \int \int \int \Phi^2 \, d(y_i, v, \theta, g, m, r, C, \rho)}.$$

Uncertainty Quantification

Combining polynomials?

For example, let ϕ be monomials $(1, x, x^2, x^3, x^4, \dots)$.

$$\Lambda = \left\{ \begin{array}{l} (0, 0, 0, 0, 0, 0, 0, 0), \\ (1, 0, 0, 0, 0, 0, 0, 0), \\ (0, 1, 0, 0, 0, 0, 0, 0), \\ \vdots \\ (1, 2, 3, 4, 5, 6, 7, 8), \\ \vdots \end{array} \right\}$$

k	polynomial Φ
$(0, 0, 0, 0, 0, 0, 0, 0)$	$y_i^0 \cdot v^0 \cdot \theta^0 \cdot g^0 \cdot m^0 \cdot r^0 \cdot C^0 \cdot \rho^0 = 1$
$(1, 2, 3, 4, 5, 6, 7, 8)$	$y_i^1 \cdot v^2 \cdot \theta^3 \cdot g^4 \cdot m^5 \cdot r^6 \cdot C^7 \cdot \rho^8$
$(1, 1, 1, 1, 1, 1, 1, 1)$	$y_i \cdot v \cdot \theta \cdot g \cdot m \cdot r \cdot C \cdot \rho$

Uncertainty Quantification

Stochastic Collocation

Comparison

Monte Carlo	Stochastic Collocation
Dimension-independent	Calculations grow with dimension*
Slow converging	Very fast convergence*
	Can replace original model

Uncertainty Quantification

Results: pdf

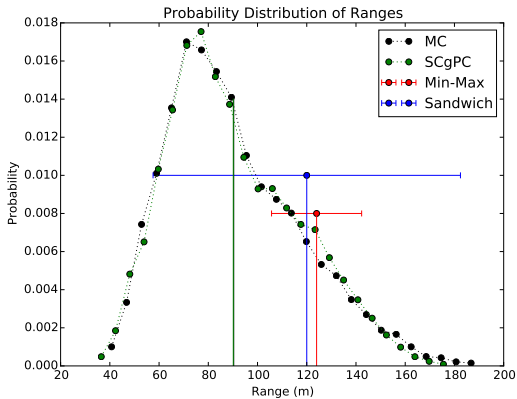
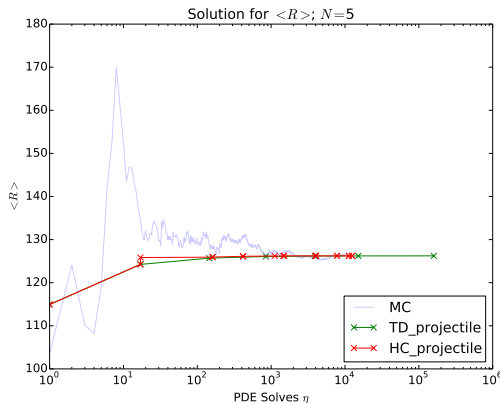


Figure: Probability Distributions

Uncertainty Quantification

Results: Expected Value, Values



Uncertainty Quantification

Results: Expected Value, Errors

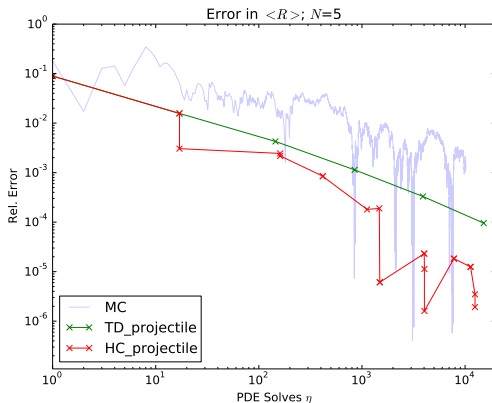


Figure: Error in $\mathbb{E}[x_f]$

So...what?

- Understand range of possible solutions
- Worse-case scenarios
- Sensitivity Analysis
 - Who is contributing the most to our spread?
 - Which measurements should I focus on improving?
 - Which design specification should I tighten down on?



Sensitivity Analysis

Polynomial Expansion Revisited

Recall: $u(Y) \approx S[u(Y)] = \sum_{k \in \Lambda} c_k \Phi_k(Y)$,
 so for $x_f(y_i, v, \theta, g, m, r, C, \rho)$:

$$\begin{aligned}
 x_f &\approx S[x_f] = c_{(0,0,0,0,0,0,0,0)} \\
 &+ c_{(1,0,0,0,0,0,0,0)} y_i + c_{(0,1,0,0,0,0,0,0)} v + c_{(0,0,1,0,0,0,0,0)} \theta + \dots \\
 &+ c_{(2,0,0,0,0,0,0,0)} y_i^2 + c_{(1,1,0,0,0,0,0,0)} y_i \cdot v + c_{(1,0,1,0,0,0,0,0)} y_i \cdot \theta + \dots \\
 &+ c_{(3,0,0,0,0,0,0,0)} y_i^3 + c_{(1,1,1,0,0,0,0,0)} y_i \cdot v \cdot \theta + \dots \\
 &\dots
 \end{aligned}$$

Sensitivity Analysis

Polynomial Expansion Revisited

Rearrange:

$$\begin{aligned}
 x_f \approx S[x_f] &= c_{(0,0,0,0,0,0,0,0)} \\
 &+ c_{(1,0,0,0,0,0,0,0)} y_i + c_{(2,0,0,0,0,0,0,0)} y_i^2 + c_{(3,0,0,0,0,0,0,0)} y_i^3 + \dots \\
 &+ c_{(0,1,0,0,0,0,0,0)} v + c_{(0,2,0,0,0,0,0,0)} v^2 + c_{(0,3,0,0,0,0,0,0)} v^3 + \dots \\
 &\dots \\
 &+ c_{(1,1,0,0,0,0,0,0)} y_i \cdot v + c_{(1,2,0,0,0,0,0,0)} y_i \cdot v^2 + \dots \\
 &\dots
 \end{aligned}$$

Sensitivity Analysis

“It is simple to show...”

This is the same as

$$\begin{aligned}
 X_f &\approx X_{f,\text{ref}} \\
 &+ S[x_f(y_i)] + S[x_f(v)] + \dots + S[x_f(g)] \\
 &+ S[x_f(y_i, v)] + S[x_f(y_i, \theta)] + \dots + S[x_f(C, \rho)] \\
 &+ \dots \\
 &+ S[x_f(y_i, v, \theta, g, m, r, C, \rho)].
 \end{aligned}$$

ANOVA - [AN]alysis [O]f [VA]riance:

$$\text{Sensitivity}(v) \equiv \frac{\text{var}(S[x_f(v)])}{\text{var}(x_f)}$$

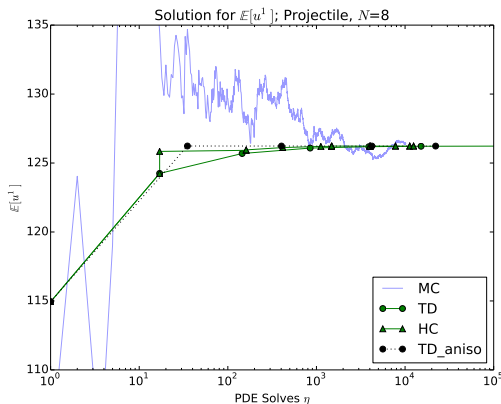
ANOVA

How much does each input contribute to the variance?

Input	Δ Variance	% Variance	Weight
C	0.523	0.6657	1
θ	0.236	0.3006	1/2
r	0.00868	0.0111	1/5
m	0.00862	0.0110	1/5
y_i	0.00671	0.0085	1/5
ρ	0.00209	0.0027	1/6
v	0.000348	0.0004	1/7
g	2.83×10^{-6}	3.601×10^{-6}	1/12

Sensitivity Analysis

Results: Expected Value, Values



Uncertainty Quantification

Results: Expected Value, Errors

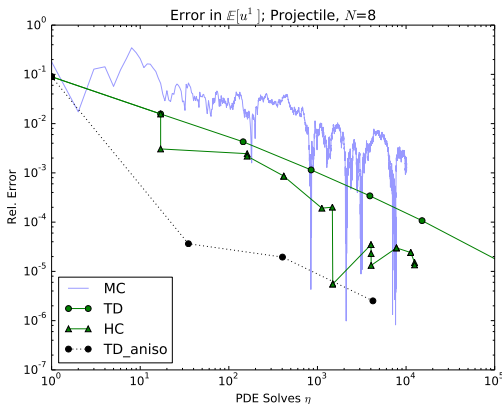
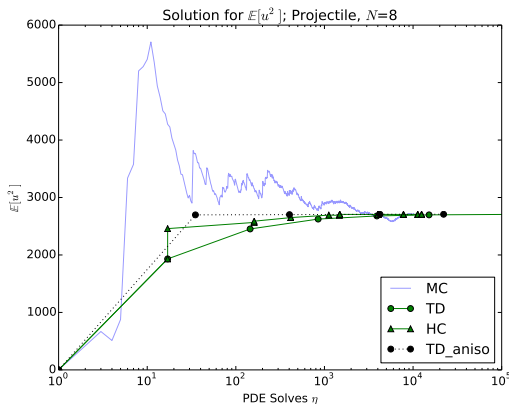


Figure: Error in $\mathbb{E}[x_f]$

Uncertainty Quantification

Results: Second Moment, Values



Uncertainty Quantification

Results: Second Moment, Errors

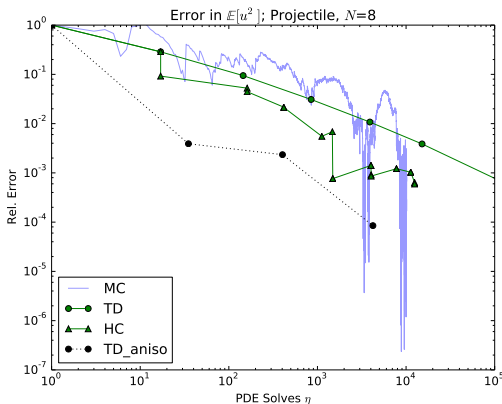


Figure: Error in $\mathbb{E}[x_f^2]$

Conclusions

- Uncertainty Quantification methods
 - Analytic methods: good, but possible deceiving
 - Numerical methods: expensive, but robust
- Sensitivity Analysis
 - Reveals importance of parameters
 - Tighten uncertainty in experiment/model
- Areas of study
 - Adaptive sampling
 - Sparse quadrature integration
 - Improved Monte Carlo methods
 - Efficient statistics algorithms

The End (\pm a few slide-minutes).

More questions? talbotpne@gmail.com

Polynomial Index Sets

Choosing what polynomial degrees to use

■ Tensor Product:

$$\Lambda_{\text{TP}}(L) = \left\{ \bar{p} = [p_1, \dots, p_N] : \max_{1 \leq n \leq N} p_n \leq L \right\}, \eta = (L+1)^N$$

■ Total Degree:

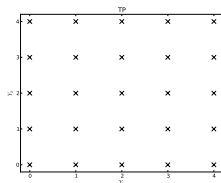
$$\Lambda_{\text{TD}}(L) = \left\{ \bar{p} = [p_1, \dots, p_N] : \sum_{n=1}^N p_n \leq L \right\}, \eta = \binom{L+N}{N}$$

■ Hyperbolic Cross:

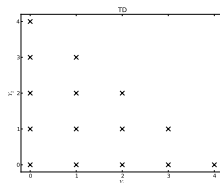
$$\Lambda_{\text{HC}}(L) = \left\{ \bar{p} = [p_1, \dots, p_N] : \prod_{n=1}^N p_n + 1 \leq L + 1 \right\}, \eta \leq (L+1)(1 + \log(L+1))^{N-1}$$

Polynomial Index Sets

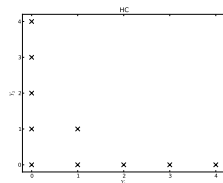
2D Example



(a) Tensor Product



(b) Total Degree



(c) Hyperbolic Cross

Figure: Index Set Examples: $N = 2, L = 4$

Calculating c_k

Where the algorithmic rubber hits the mathematical road.

$$u(Y) \approx \mathcal{S}_{N,\Lambda(L)}[u](Y) = \sum_{i \in \Lambda(L)} c(i) \bigotimes_{n=1}^N \mathcal{U}_{n,p(i_n)}[u](Y),$$

$$c(i) = \sum_{\substack{j=\{0,1\}^N, \\ i+j \in \Lambda(L)}} (-1)^{|j|_1},$$

$$\begin{aligned} \bigotimes_{n=1}^N \mathcal{U}_{n,p(i_n)}[u](Y) &\equiv \sum_{k_1=0}^{p(i_1)} \cdots \sum_{k_N=0}^{p(i_N)} u_h(Y^{(k_1)}, \dots, Y^{(k_N)}) \prod_{n=1}^N \mathcal{L}_{k_n}(Y_n), \\ &= \sum_k^{p(\vec{i})} u_h(Y^{(k)}) \mathcal{L}_k(Y), \end{aligned}$$

Calculating c_k

2D Examples

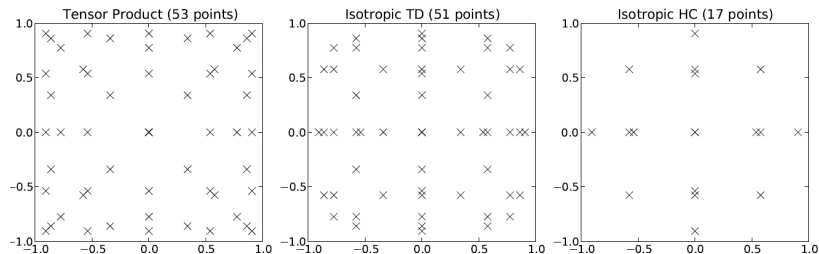


Figure: Sparse Grids, $N = 2$, $L = 4$, $p(i) = i$, Legendre points

Calculating c_k

Some Numbers

N	L	TP	TD		HC	
		$ \Lambda(L) $	$ \Lambda(L) $	η	$ \Lambda(L) $	η
3	4	125	35	165	16	31
	8	729	165	2,097	44	153
	16	4,913	969	41,857	113	513
	32	35,737	6,545	1,089,713	309	2,181
5	2	293	21	61	11	11
	4	3,125	126	781	31	71
	8	59,049	1,287	28,553	111	481

Table: Index Set and Collocation Size Comparison