### Additional Results

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University of New Mexico

Dissertation Defense, November 3, 2016

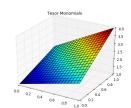
Funded by a Laboratory Directed Research effort at Idaho National Laboratory



**Tensor Monomials** 

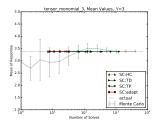
#### **Tensor Monomials**

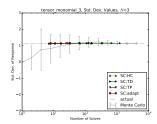
$$u(Y) = \prod_{n=1}^{N} (y_n + 1)$$

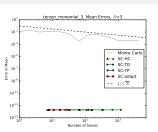


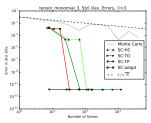
- ► Linear response
- All polynomial combinations

#### Tensor Monomials, N=3







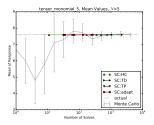


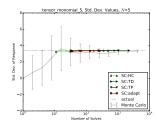


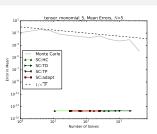


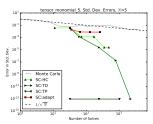


#### Tensor Monomials, N = 5







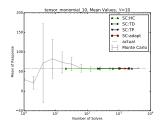


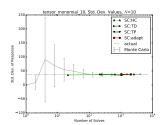


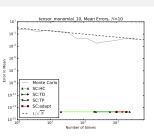


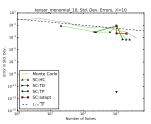


#### Tensor Monomials, N = 10











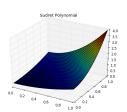




Sudret Polynomials

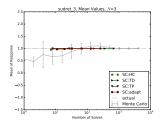
### Sudret Polynomials

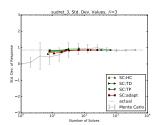
$$u(Y) = \frac{1}{2^N} \prod_{n=1}^N (3y_n^2 + 1)$$

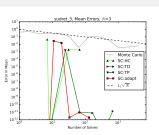


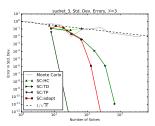
- Exclusively second-order interactions
- ▶ All second-order polynomial combinations

### Sudret Polynomials, N=3





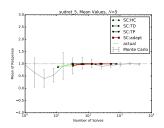


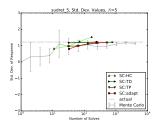


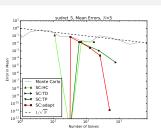


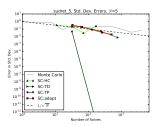


### Sudret Polynomials, N=5











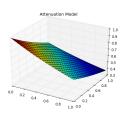




Attenuation

#### Attenuation

$$u(Y) = \prod_{n=1}^{N} \exp(-y_n/N)$$

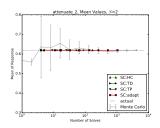


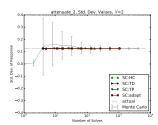
- ► Tensor of decreasing-importance polynomials
- ► Combination terms over single-variable

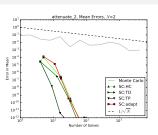
Attenuation, Taylor Expansion

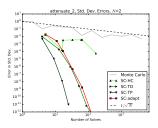
$$e^{-ay} = 1 - ay + \frac{(ay)^2}{2} - \frac{(ay)^3}{6} + \frac{(ay)^4}{24} - \frac{(ay)^5}{120} + \mathcal{O}(y^6)$$

		Polynomial Order $(y_1)$						
		0	1	2	3	4		
	0	1	а	$a^{2}/2$	$a^{3}/6$	$a^4/24$		
Polynomial	1	а	$a^2$	$a^{3}/2$	$a^{4}/6$	$a^{5}/24$		
Order	2	$a^{2}/2$	$a^{3}/2$	$a^{4}/4$	$a^5/12$	a <sup>6</sup> /48		
$(y_2)$	3	$a^{3}/6$	$a^4/6$	$a^5/12$	$a^{6}/36$	$a^{7}/144$		
	4	$a^4/24$	$a^{5}/24$	$a^{6}/48$	$a^{7}/144$	$a^{8}/576$		



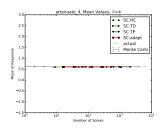


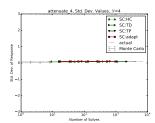


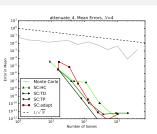


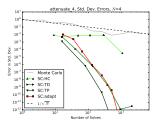






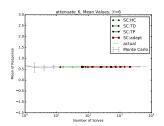


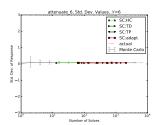


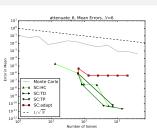


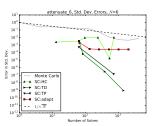












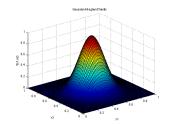




Gauss Peak

### Gauss Peak

$$u(Y) = \prod_{n=1}^{N} \exp(-3^{2}(y_{n} - 0.5)^{2})$$



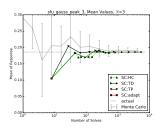
- ► Tensor of polynomials
- Slow, inconsistent decay

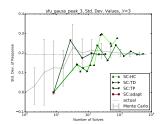
Gauss Peak, Taylor Expansion

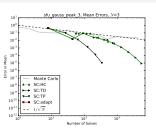
$$e^{-a^2y^2} = 1 - a^2y^2 + \frac{a^4}{2}y^4 - \frac{a^6}{6}y^6 + \frac{a^8}{24}y^8 + \mathcal{O}(y^{10})$$

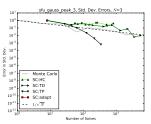
		Polynomial Order $(y_1)$				
		0	1	2	3	4
	0	1	0	$a^2$	0	$a^4/2$
Polynomial	1	0	0	0	0	0
Order	2	$a^2$	0	$a^4$	0	$a^{6}/2$
$(y_2)$	3	0	0	0	0	0
	4	$a^4/2$	0	$a^{6}/2$	0	$a^{8}/4$

#### Gauss Peak, N = 3







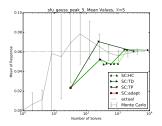


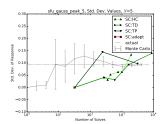


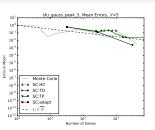


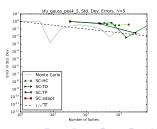


### Gauss Peak, N = 5









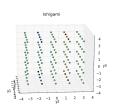




Ishigami Function

#### Ishigami Function

$$u(Y) = \sin y_1 + a \sin^2 y_2 + b y_3^4 \sin y_1$$



- ► Not a tensor combination
- ▶ Strange interplay between  $y_1, y_3$

Ishigami Function, Taylor Expansion

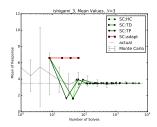
### Ishigami Function

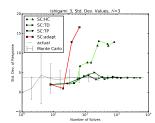
$$u(Y) = \sin y_1 + a \sin^2 y_2 + b y_3^4 \sin y_1$$

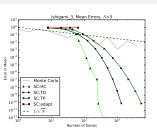
$$\sin y = x - \frac{x^3}{6} + \frac{x^5}{120} + \mathcal{O}(x^7)$$

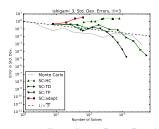
$$\sin^2 y = x^2 - \frac{x^4}{3} + \frac{2x^6}{45} + \mathcal{O}(x^8)$$

### Ishigami Function, N=3









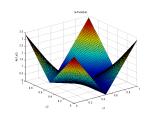




Sobol G-Function

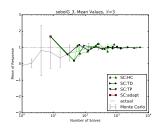
### Sobol G-Function

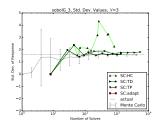
$$u(Y) = \prod_{n=1}^{N} \frac{|4y_n - 2| - a_n}{1 + a_n}, \quad a_n = \frac{n-2}{2}$$

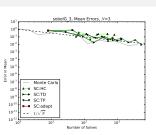


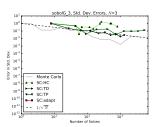
- ▶ Tensor combination of terms
- Only zeroth-order continuity

#### Sobol G-Function, N = 3

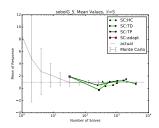


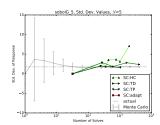


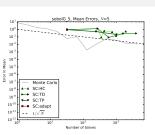


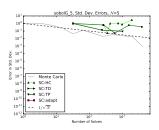


#### Sobol G-Function, N = 5













#### Conclusions

### Regarding static SCgPC:

- Great in low input space dimensionality
- Better with regular responses
- ► Total Degree often great choice

### Regarding adaptive SCgPC:

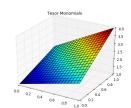
- Optimal for small input dimensionality
- Monotonically-decreasing variance moments
- Very poor if oscillating moments



**Tensor Monomials** 

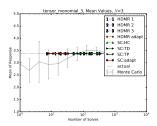
#### **Tensor Monomials**

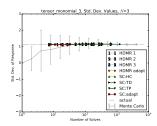
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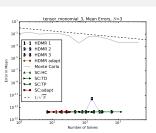


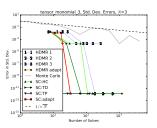
- ► Linear response
- All polynomial combinations

#### Tensor Monomials, N=3





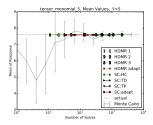


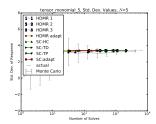


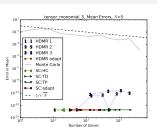


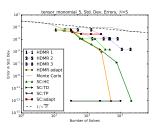


#### Tensor Monomials, N = 5

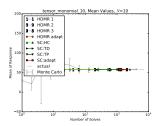


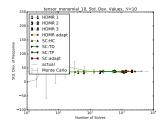


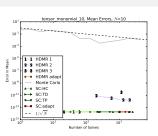


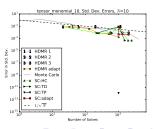


#### Tensor Monomials, N=10









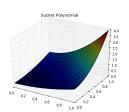




**Sudret Polynomials** 

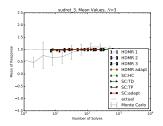
### Sudret Polynomials

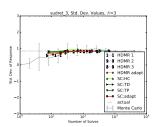
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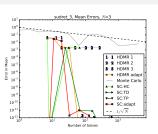


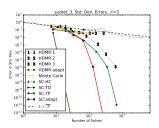
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### Sudret Polynomials, N=3





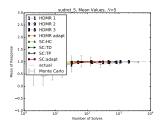


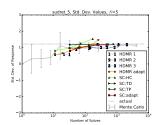


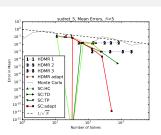


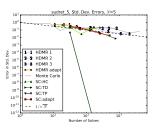


### Sudret Polynomials, N=5









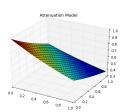




#### Attenuation

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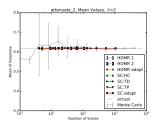


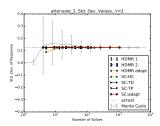
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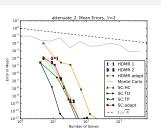
Attenuation, Taylor Expansion

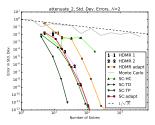
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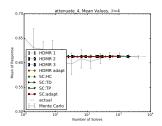


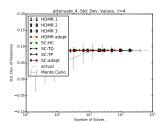


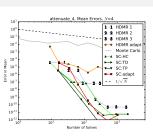


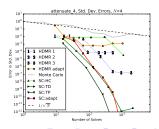






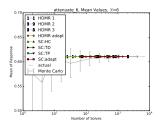


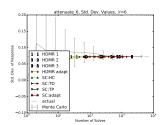


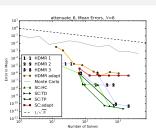


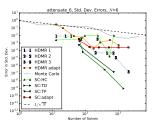












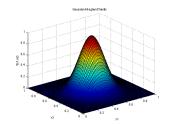




#### Gauss Peak

### Gauss Peak

$$u(Y) = \prod_{n=1}^{N} \exp(-3^{2}(y_{n} - 0.5)^{2})$$



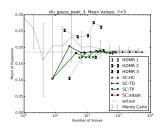
- ► Tensor of polynomials
- Slow, inconsistent decay

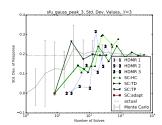
Gauss Peak, Taylor Expansion

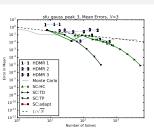
$$e^{-a^2y^2} = 1 - a^2y^2 + \frac{a^4}{2}y^4 - \frac{a^6}{6}y^6 + \frac{a^8}{24}y^8 + \mathcal{O}(y^{10})$$

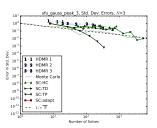
		Polynomial Order $(y_1)$				
		0	1	2	3	4
	0	1	0	$a^2$	0	$a^4/2$
Polynomial	1	0	0	0	0	0
Order	2	$a^2$	0	$a^4$	0	$a^{6}/2$
$(y_2)$	3	0	0	0	0	0
	4	$a^4/2$	0	$a^{6}/2$	0	$a^{8}/4$

#### Gauss Peak, N = 3





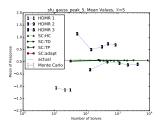


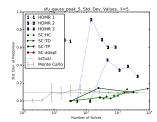


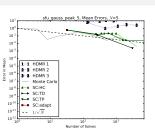


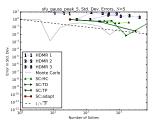


#### Gauss Peak, N = 5









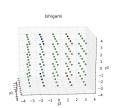




Ishigami Function

### Ishigami Function

$$u(Y) = \sin y_1 + a \sin^2 y_2 + b y_3^4 \sin y_1$$



- ► Not a tensor combination
- ▶ Strange interplay between  $y_1, y_3$

Ishigami Function, Taylor Expansion

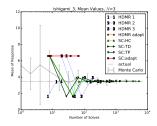
### Ishigami Function

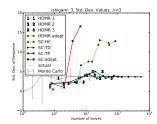
$$u(Y) = \sin y_1 + a \sin^2 y_2 + b y_3^4 \sin y_1$$

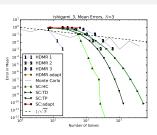
$$\sin y = x - \frac{x^3}{6} + \frac{x^5}{120} + \mathcal{O}(x^7)$$

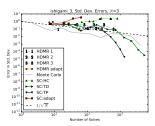
$$\sin^2 y = x^2 - \frac{x^4}{3} + \frac{2x^6}{45} + \mathcal{O}(x^8)$$

#### Ishigami Function, N=3









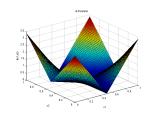




Sobol G-Function

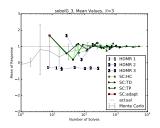
### Sobol G-Function

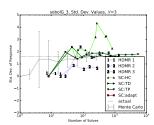
$$u(Y) = \prod_{n=1}^{N} \frac{|4y_n - 2| - a_n}{1 + a_n}, \quad a_n = \frac{n-2}{2}$$

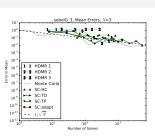


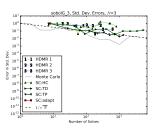
- Tensor combination of terms
- Only zeroth-order continuity

#### Sobol G-Function, N=3





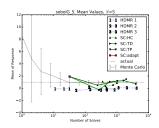


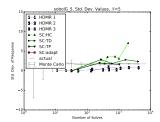


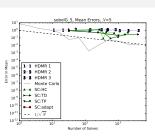


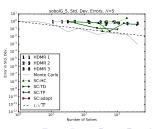


#### Sobol G-Function, N = 5











#### Conclusions

#### Regarding static HDMR:

- Never outperforms associated SCgPC
- Does produce results with less evaluations

### Regarding adaptive HDMR:

- Sometimes outperforms adaptive SCgPC
- Yields results with fewer evaluations

HDMR is most useful when very few evaluations possible

## Outline

- 1 Results
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#### Introduction

More complicated than an analytic case

$$\begin{split} -D_{g}(\mathbf{r})\nabla^{2}\phi_{g}(\mathbf{r}) + \Sigma_{a,g}(\mathbf{r}) &= \sum_{g'=1}^{G} \Sigma_{g' \to g} \phi_{g'}(\mathbf{r}) \\ &+ \frac{\chi_{p,g}}{k} \sum_{g'=1}^{G} \nu \Sigma_{f,g'}(\mathbf{r}) \phi_{g'}(\mathbf{r}) \end{split}$$

Quantities of interest

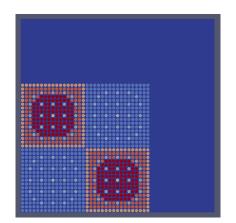
- $\phi_g(\mathbf{r})$ : Group neutron flux
- ▶ k eigenvalue: Neutron multiplication factor

Problem

# Neutronics Example

Geometry

Quarter-symmetric 4-assembly reactor core



### **Energy Groups**

7 energy groups, 7 materials, 32 mesh elements per pin

Group	Upper Energy Bound				
7	0.02 eV				
6	0.1 eV				
5	0.625 eV				
4	3 eV				
3	500 keV				
2	1 MeV				
1	20 MeV				

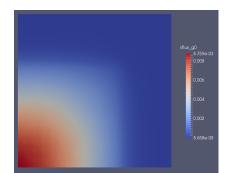
Solved using RATTLESNAKE's linear CFEM

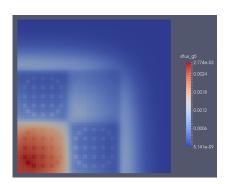


Problem

# Neutronics Example

Flux Profiles





## Outline

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#### Uncertainty

### Specific Responses

- k-eigenvalue
- Group 1 flux at reactor center
- Group 5 flux at reactor center

### 168 correlated uncertain inputs

- Material macroscopic cross sections
- Assigned 10% correlation
  - ▶ Same material and reaction, different energies
  - Same material and energy, different reaction
- ▶ Relative variance of 5% for all inputs



**Uncertainty Correlations** 

Need to de-correlate input space

RAVEN has two-step reduction

- Karhunen-Loeve expansion (PCA)
- Sensitivity reduction
- Combined yields importance rank

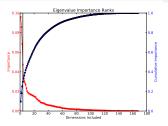
#### **Uncertainty Correlations**

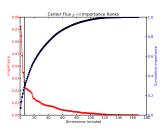
	k-eigenvalue		Center F	ux, g = 1	Center Flux, $g = 5$	
Rank	Dimension	Importance	Dimension	Importance	Dimension	Importance
1	24	0.09606	24	0.07231	24	0.07032
2	9	0.08555	9	0.06472	9	0.06648
3	0	0.06861	0	0.04856	100	0.06474
4	17	0.04737	116	0.03472	13	0.03396
5	23	0.03415	17	0.03470	0	0.03092
6	158	0.03047	10	0.02726	17	0.02716
7	164	0.02852	8	0.02468	10	0.02651
8	50	0.02695	164	0.02174	118	0.02600
9	6	0.02315	20	0.02157	117	0.02420

Retained latent dimensions 24, 9, 0, 17, 10, 116, 100, 13

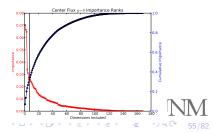


#### **Uncertainty Correlations**





- ► Truncated after gradients
- ► Some importance lost
- Mean preserved well
- ► Std dev partially preserved

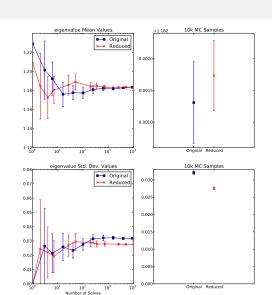


Uncertainty

# Neutronics Example

#### **Uncertainty Correlations**

k-Eigenvalue



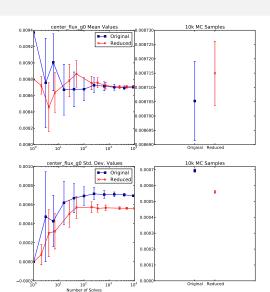


Uncertainty

# Neutronics Example

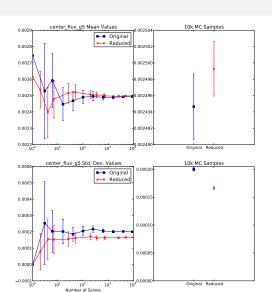
#### **Uncertainty Correlations**

Center Flux, g = 1



#### **Uncertainty Correlations**

Center Flux, g = 5





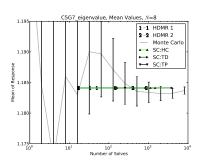
## Outline

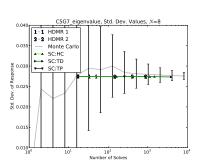
- 1 Results
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Results

## Neutronics Example

Results: k-eigenvalue

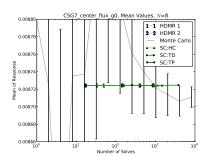


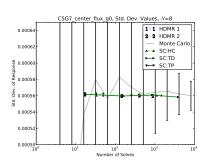


Results

## Neutronics Example

Results: Center Flux, g = 1

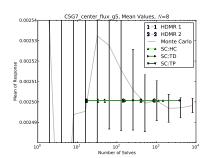


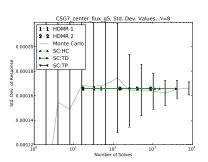


Results

## Neutronics Example

Results: Center Flux, g = 5





## Outline

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└ Problem

# Multiphysics Example

Introduction

### Coupled multiphysics problem

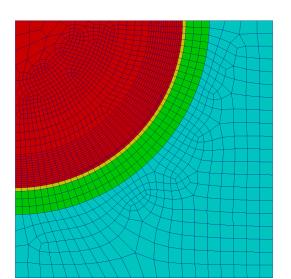
- Neutronics
  - neutron transport and interaction
  - Provides flux/power shapes to fuels performance
- Fuels Performance
  - ▶ temperature, depletion, fuel oxidation,
  - fission product swelling, densification, fuel fracture,
  - ▶ interstitial heat transfer, mechanical contact,
  - cladding creep, thermal expansion, plasticity
  - Provides temperature fields to neutronics



Problem

# Multiphysics Example

Geometry





## Outline

- 1 Results
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## Multiphysics Example

#### Geometry and Uncertainty

#### Dimensions

- ▶ Domain is 6.3 mm square
- Reflective boundaries
- ► Fuel pin radius is 4.09575 mm with clad

### Response is k-eigenvalue

### Uncertain inputs

- ▶ 671 correlated interaction cross sections
- ► Fuel thermal expansion coefficient
- Clad thermal conductivity
- ► Fuel thermal conductivity

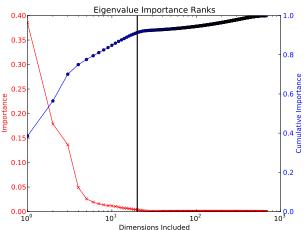




Uncertainty

# Multiphysics Example

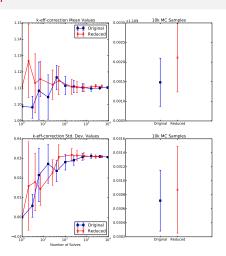
#### **Uncertainty Correlation**



Uncertainty

# Multiphysics Example

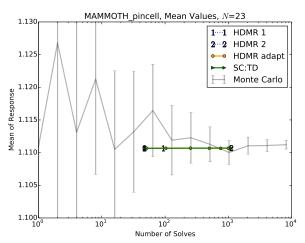
#### **Uncertainty Correlation**



## Outline

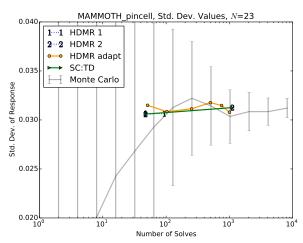
- 1 Results
- 2 Results
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# Multiphysics Example





# Multiphysics Example





# Multiphysics Example

Run Times

Method	Degree	Runs
Total Degree	1	47
Total Degree	2	1105
Total Degree*	3	17389
HDMR (1)	1	47
HDMR (1)	2	47
HDMR (1)	3	93
HDMR (1)	4	93
HDMR (1)	5	139
HDMR (2)	1	47
HDMR (2)	2	1105
HDMR $(2)^{\dagger}$	3	3221
HDMR $(2)^{\dagger}$	4	7361
HDMR (2)*	5	13571



Introduction

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  - Uncertainty
  - Results

Introduction

## Time-Dependent Analysis

Introduction

#### Transient Problems

- ► Response is time-dependent
- ► Response may evolve in time
- Physics may change in time

"Time" could be any monotonically-increasing parameter

# Time-Dependent Analysis

Approach

#### RAVEN approach

- ► Divide time into snapshots
- ► Evaluate ROM on each snapshot
- ► Interpolate between snapshots

We extended SCgPC and HDMR to do this as well

Limitation: Adaptive methods



└ Problem

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  - Results

## Time-Dependent Example

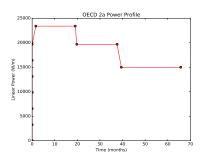
#### Introduction

#### Fuels Performance problem

- OECD Benchmark
- PWR Fuel Rod
- "Steady-State"
- ▶ Power Changes

#### Responses

- max clad temp
- % fission gas released
- clad elongation
- clad creep strain



└─ Problem

## Time-Dependent Example

Introduction

#### Geometry

- Fuel and Cladding
- 2D Axisymmetric R-Z
- ▶ 4 m by 0.55 cm
- ▶ 4290 QUAD8 Elements

#### **Physics**

- Displacement/Creep
- Thermal expansion
- Heat conduction
- Heat convection
- Contact stress



Uncertainty

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  - Results

Uncertainty

## Time-Dependent Example

#### Uncertainty

Uncertain Parameter	Mean	Std. Dev.
Clad Thermal Conductivity	16.0	2.5
Cladding Thickness	6.7e-4	8.3e-6
Cladding Roughness	5.0e-7	1.0e-7
Clad Creep Rate	1.0	0.15
Fuel Thermal Conductivity	1.0	0.05
Fuel Density	10299.24	51.4962
Fuel Thermal Expansion	1.0e-5	7.5e-7
Fuel Pellet Radius	4.7e-3	3.335e-6
Fuel Pellet Roughness	2.0e-6	1.6667e-7
Solid Fuel Swelling	5.58e-5	5.77e-6
Gas Conductivity	1.0	0.025
Gap Thickness	9.0e-5	8.33e-6
Mass Flux	3460	57.67
Rod Fill Pressure	1.2e6	40000.0
System Pressure	1.551e7	51648.3
System Power	1.0	0.016667
Uncertain Parameter	Lower Bound	Upper Bound
Inlet Temperature	558.0	564.0

Uncertainty

## Time-Dependent Example

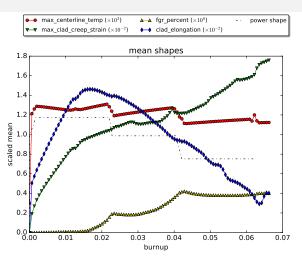
Uncertainty

#### Dependent Parameters

Dependent Parameter	Calculation
Clad inner radius	2*(fuel_rad + gap_width)
Outer Diameter (Hot)	2*(fuel_rad + gap_width + clad_thick)
Outer Diameter (Cool)	2*(fuel_rad + gap_width + clad_thick)
System Pressure (Cool)	sys_press
Thermal Porosity	1 - fuel_dens/10980
Fuel Diameter	2*fuel_rad
Gap Diameter	2*gap_thick
SIFGR Porosity	1 - fuel_dens/10980

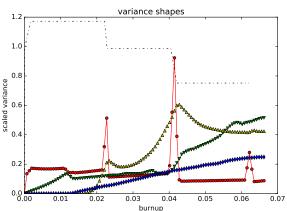
- 1 Results
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  - Uncertainty
  - Results

# Time-Dependent Example



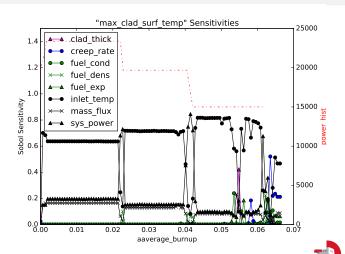
## Time-Dependent Example







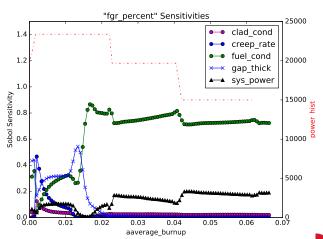
## Time-Dependent Example



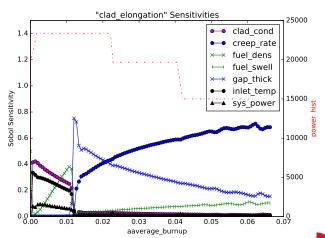
Time-Dependent Example

Results

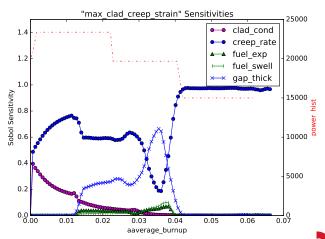
## Time-Dependent Example



## Time-Dependent Example



# Time-Dependent Example



## Time-Dependent Example

Conclusions

#### Time-Dependent Analysis with SCgPC and HDMR

- Same benefits as with static analysis
- ▶ No additional solves for time-dependent
- Increased understanding of physics
- Informed decision making