Automated Generation of Spatially Varying Stochastic Expansions for Embedded Uncertainty Quantification

LABORATORY DIRECTED RESEARCH & DEVELOPMENT

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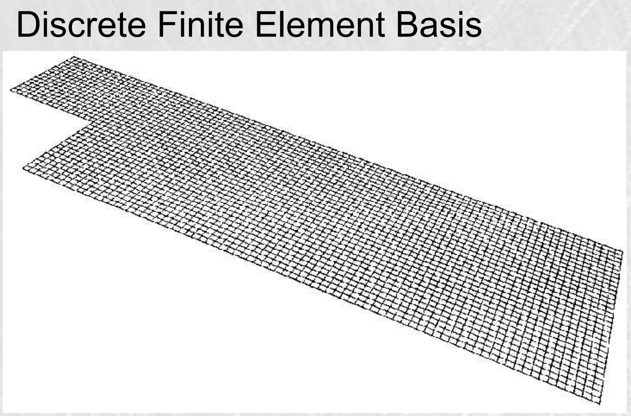
Early Career R&D Program

Problem

- UQ allows computation of PDE solution over uncertain parameter space
- Two techniques using **Tensor Product** discretization: black box and embedded
  - Black-box: Samples PDE code over parameter space
  - Embedded: Requires modification of PDE code
- Size of discrete solution: (PDE unknowns)*(Size stochastic expansion)
  - Black-box: Rapid growth of PDE solves
  - Embedded: Rapid growth of unknown counts
  - High cost for full simulation
- GOAL: Reduce computational cost by exploiting higher granularity of embedded methods

Tensor-Product discretization

Discrete Finite Element Basis



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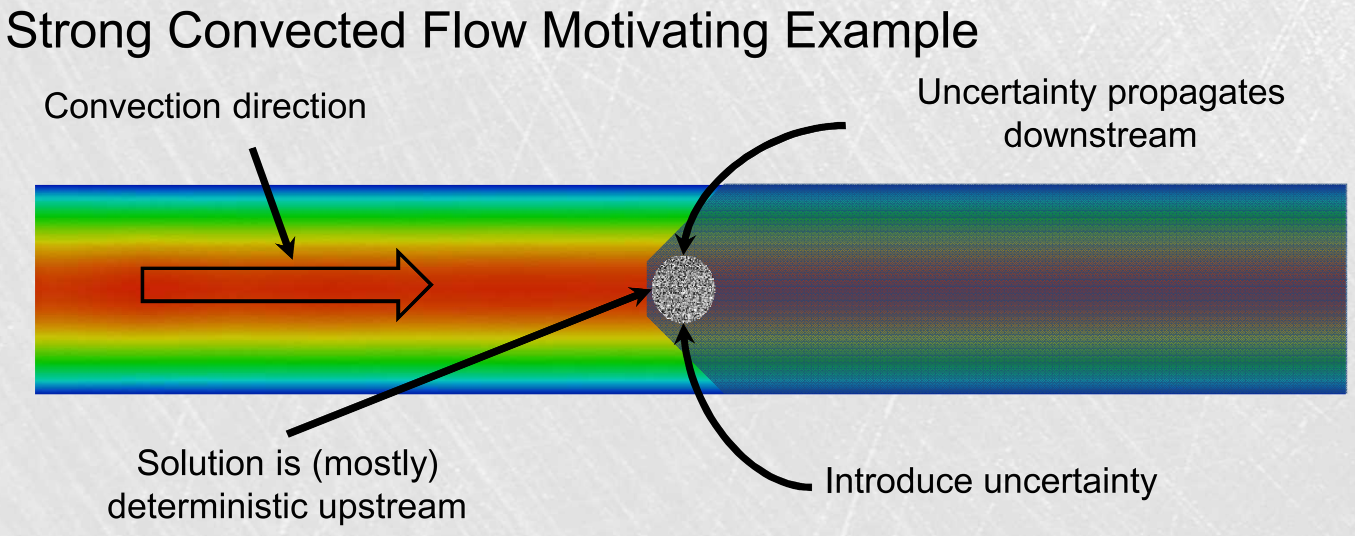
Polynomial Chaos Basis

$$\psi_0(\xi) = 1$$
$$\psi_1(\xi) = 2\xi$$
$$\psi_2(\xi) = 4\xi^2 - 2$$
$$\psi_3(\xi) = 8\xi^3 - 12\xi$$
$$\psi_4(\xi) = 16\xi^4 - 48\xi^2 + 12$$

Approach

Strong Convected Flow Motivating Example



- Resolution of uncertainty needed only downstream
- Tensor product basis resolves uncertainty uniformly
- Computational effort could be reduced

My Approach: Vary Stochastic Expansion Spatially:

Tensor Product

$$u(x,\xi) \approx \sum_{i=1}^{N}\sum_{j=1}^{M} u_{ij}\phi_i(x)\psi_j(\xi)$$

➡

Spatially Varying

$$u(x,\xi) \approx \sum_{i=1}^{N}\sum_{j=1}^{M_i} u_{ij}\phi_i(x)\psi_j^i(\xi)$$

How to construct spatially varying discretization? Construct discretization adaptively

Adaptive refinement shopping list:

1. Error Indicator
2. Marking strategy

Error Indicator

Let $g(\xi)$ be PC expansion of a DOF

$$g(\xi) = \sum_{j=1}^{M} g_j\psi_j(\xi)$$

Error indicator for $g(\xi)$ is

$$\eta_g = \frac{g_M}{\mathrm{Var}[g]}$$

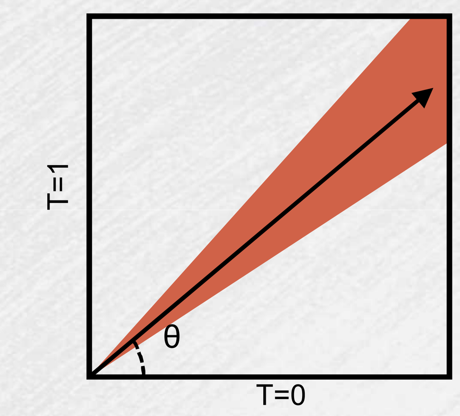
Marking Strategy

```
Order = markingA(DOFs,ErrorInd)
  Order <- [0,0,…,#DOFs]
  for each dof in DOFs
    err <- ErrorInd[dof]
    if err >= lower
      Order[dof] += lower_bump
    if err >= higher
      Order[dof] += higher_bump
```

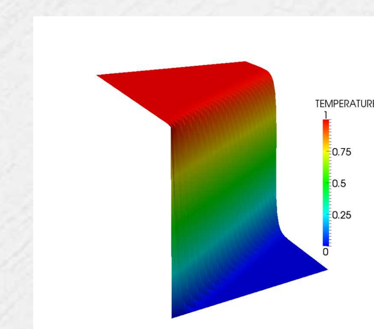
Results

Problem setup

- Convection-Diffusion on unit square
- Strong Convection: Peclet Number=10^7
- Angle varies stochastically: $\mathcal{N}(40,4)$
- Using SUPG stabilization

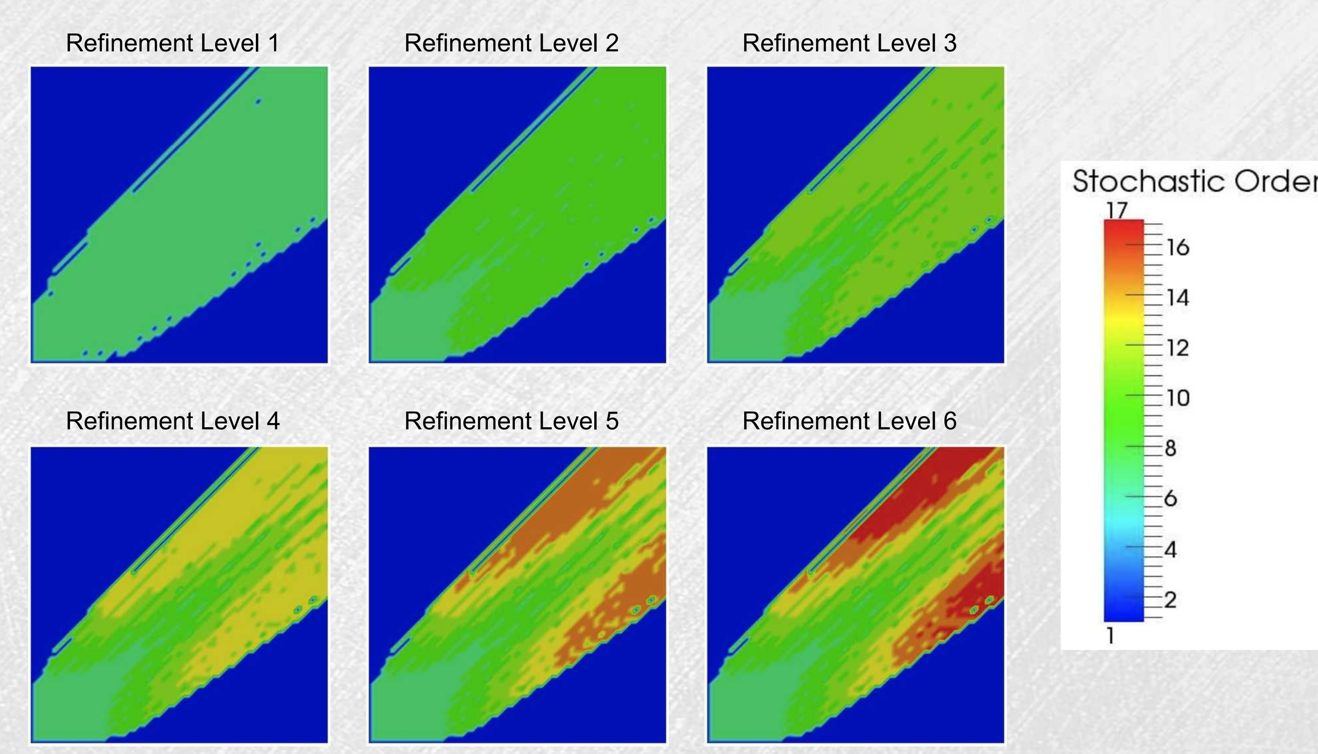


Deterministic Solution: θ=40

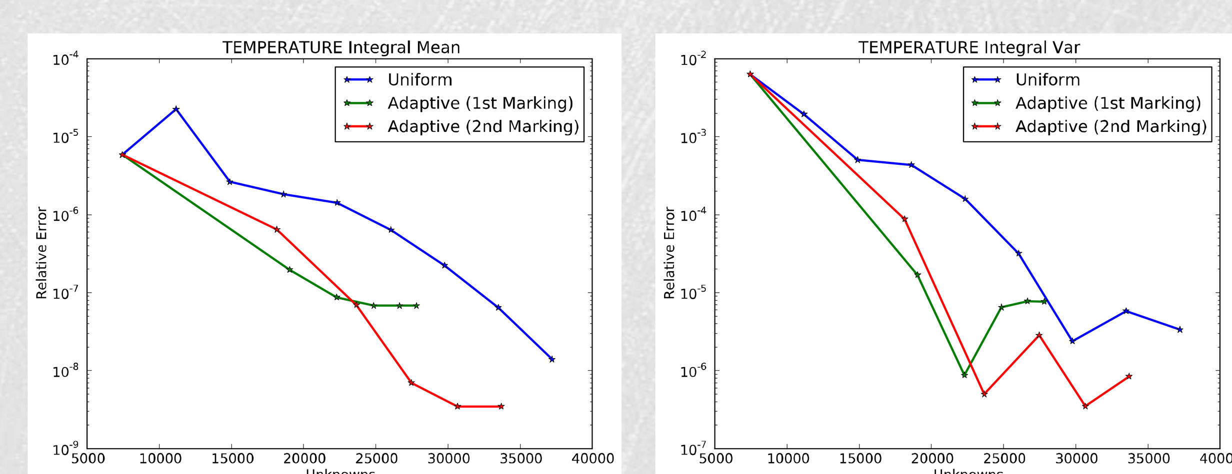


Compare uniform to adaptive refinement

- Reference is 20th order uniform stochastic galerkin
- Start from 2 term stochastic expansion
- Response quantities: Spatial average



Take Home: Refinement focuses high order where needed



- Horizontal Axis: Number of unknowns
- Vertical Axis: Relative error in response values

Take Home: Refinement yields less work for same accuracy

Significance

Spatially varying discretization yields same accuracy with less work

- Enables higher fidelity simulations with UQ
- Provides greater understanding of propagation of uncertainty (not always spatially uniform!)

Work is "proof of principle" for spatially varying discretizations

- Multi dimensional parameter space
- On going effort in multiphysics
- CFD and Semi-conductor modeling are next targets

Follow on work needed

- Improvement error indicators
- Marking rules
- Efficient parallel implementation
- Preconditioners for adapted solution

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