A Priori Model Order Reduction for Transient Neutron Diffusion

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Outline

1. Motivation
   - Why reduced order modeling?
2. Proper generalized decomposition
3. Research Objectives
4. Results - Transient Neutron Diffusion
   - 1D
   - 2D
5. Conclusions and Future Work

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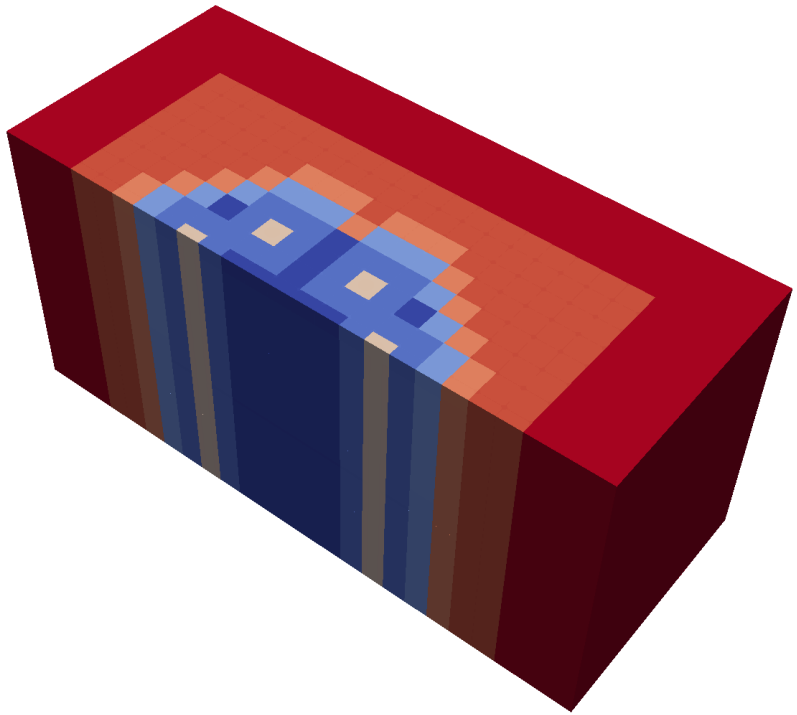
Drawbacks of high fidelity computing

- Current methods (FEM) scale exponentially with the number of dimensions and suffer from “curse of dimensionality"
- Consider a transient 3D transport simulation:
  - 2.7 million dof in space
  - 26 energy groups
  - S_8 quadrature in angle
  - 1000 points in time



Leads to $2.7E6 \times 26 \times 80 \times 1000 = 5.616E12$ dof!

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Need for reduced order models

Intractability increasingly apparent for:

a) multiscale/multiphysics problems

b) repeated evaluations (e.g. optimization and uncertainty quantification)

Development of accurate, lower order methods is needed.

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Reduced Order Modeling

Main idea - develop efficient, low order models that accurately represent high fidelity, large-scale simulations.

Parametric model reduction:

- generation of a reduced order model (ROM) that approximates the original full-order system with high fidelity over a range of parameters
- Projection methods allow for retainment of underlying physics of original full-scale model

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Projection Based Methods

Consider the following first order ODE:

$$\frac{dZ}{dt} = \mathbf{A} \cdot Z \tag{1}$$

We can define Z as the product of a *projection matrix,* $\boldsymbol{\rho}$ and the *reduced solution vector*, Z_r:

$$Z = \boldsymbol{\rho} \cdot Z_r \tag{2}$$

Plugging Equation 2 into Equation 1:

$$\frac{d}{dt}\left(\boldsymbol{\rho} Z_r\right) = \mathbf{A} \cdot \left(\boldsymbol{\rho} Z_r\right)$$

We can arrive at our reduced order system:

$$\rightarrow \frac{dZ_r}{dt} = \boldsymbol{\rho}^{-1}\mathbf{A} \cdot \boldsymbol{\rho} Z_r \tag{3}$$

Projection matrix creation

- POD basis vectors are computed *a posteriori* through the “method of snapshots"
- Assume a set of Q solutions from a series of snapshots are known and defined as:

$$\mathbf{X} = [z_i, z_{i+1}, \ldots, z_Q]$$

We can find a solution by constructing a correlation matrix and finding it’s eigenvalues and eigenvectors:

$$R = \sum_{i=1}^{Q} z_i(z_i^T) \qquad\qquad \boldsymbol{\rho} = [v_1, v_2, \ldots, v_j]$$

The eigenvectors, $v_1, v_2, \ldots, v_j$, correspond to the largest eigenvalues $\sigma_j > \sigma_1 \times \epsilon$, where $\epsilon = 10^{-8}$

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Drawbacks of POD

- Quality of ROM is *highly* sensitive to snapshot set.
  - What data/solutions are appropriate/useful? Potentially requires ad-hoc/expert knowledge of problem on hand.

- *A posteriori* methods require an online solution of the full-order system.
  - POD ROM cannot be used without a data set - either experimental or simulation. For many problems, this can be difficult or impractical.

A Priori Model Reduction

Ideally, one would want to be able to:

1. Create a ROM *a priori*
   - i.e. without having to rely on previous simulation/experimental data or any previous knowledge of the problem
2. Assess the accuracy of the ROM on-the-fly and improve accuracy if need be.

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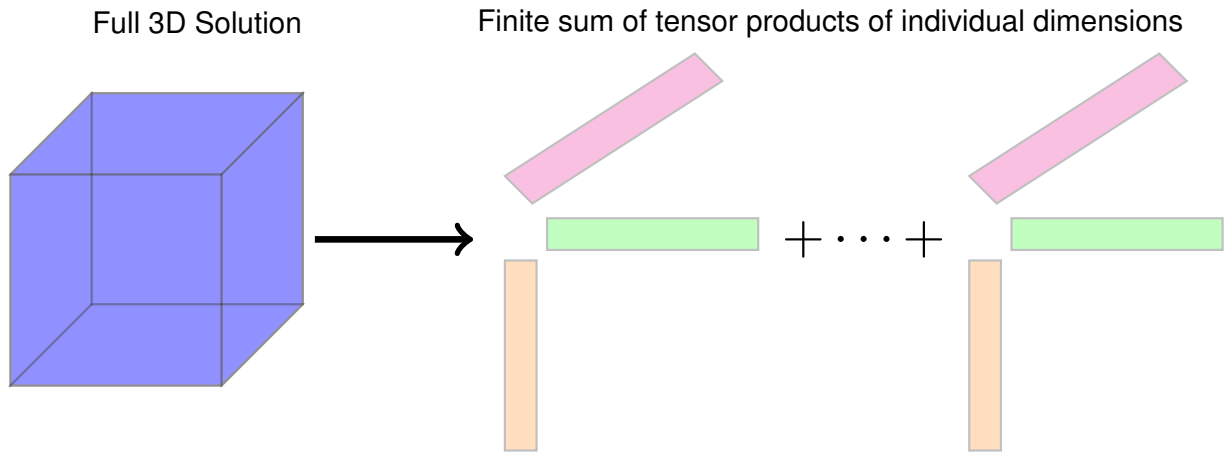
Proper Generalized Decomposition (PGD)

PGD seeks a solution that is a series expansion whose components are products of separable functions in each dimension of interest:



$$u(x_1, x_2, \ldots, x_D) = \sum_{i=1}^{n} \prod_{k=1}^{D} X_{i,k}(x_k)$$

“Curse of dimensionality" is overcome by linear relationship!

F. Chinesta, et al. *The Proper Generalized Decomposition for Advanced Numerical Simulations: A Primer.* Springer 2014.

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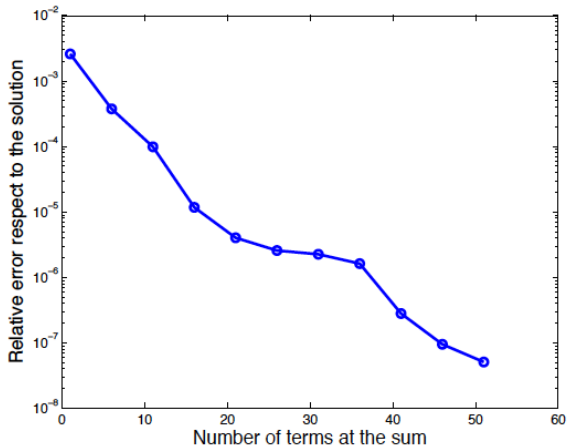
Select Applications of PGD

1. A. Ammar et. al. applied PGD to multi-bead-spring molecular models of polymer solutions in complex fluids
   - Order reduction from 2.56E6 dof (standard) to 3200 dof (PGD)

2. González-Pintor et. al. applied PGD to calculate the dominant mode eigenvalue of a nuclear reactor



3. In nearly all works to date, only a few terms have been required in PGD expansions.

1. A. Ammar, et. al. A new family of solvers for some classes of multidimensional partial differential equations encountered in kinetic theory modeling of complex fluids. Journal of Non-Newtonian Fluid Mechanics, 139:153-176, 2006.
2. S. González-Pintor, et. al.. Using proper generalized decomposition to compute the dominant mode of a nuclear reactor. Mathematical and Computer Modelling 57:1807-1815, 2013.

Potential of PGD in Radiation Transport

Revisiting our 3D transport problem, we can separate the solution into a series of products of 7 1D basis functions:

$$\psi(\mathbf{r}, \mathbf{\Omega}, E, t) = \sum_{i=1}^{n} R(x, y, z)\xi(\theta, \varphi)E(\epsilon)T(t)$$

where:

$$R(x, y, z) = X(x)Y(y)Z(z), \text{ and } \quad \xi(\omega) = A(\theta)P(\varphi)$$

“Curse of dimensionality" overcome by linear relationship!

$$n(140 + 140 + 140 + 26 + 80 + 1000) << 5.616\text{E}12$$

Research Objectives

Using the diffusion approximation:

1. Assess the relationship between model reduction and accuracy of an a priori ROM for two-dimensional, energy dependent transient flux calculations.
   - Theoretically possible to include energy as a “dimension" in the PGD approximation and obtain a continuous energy flux distribution.

2. Extend the energy dependent transient flux ROM to include coupled sets of ODEs
   - E.g. reactor kinetics and/or depletion
   - Purpose is to investigate the applicability of a priori ROMs for a select multiscale problem in reactor physics.

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Results so far...

1. 1D Transient Heat Transfer (FDM) ✓

2. 1D Transient Neutron Diffusion ✓
    a) Assume constant cross sections, discretize each independent variable with FDM.
    b) Expand into spatially dependent cross sections, discretize with FEM.
        i. Dirichlet BC's, MMS.
        ii. Reflecting BCs, "real" problem with heterogeneity, reference CFEM solver with backward euler in time.

3. 2D Transient Neutron Diffusion
    - Dirichlet BC's, MMS 1/2

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Mechanics of PGD - Preliminaries

Consider 1D transient neutron diffusion:

$$\frac{1}{v}\frac{\partial \phi}{\partial t} - \frac{\partial}{\partial x} \cdot D\frac{\partial}{\partial x}\phi + \Sigma_a(x)\phi(x,t) = S \tag{4}$$

Assume a solution in space and time:

$$\phi(x,t) \approx \sum_{j=1}^{n} X_j(x)\,T_j(t) \tag{5}$$

where the:

a) number of enrichment steps, n and

b) basis functions, $X_j(x)$ and $T_j(t)$ are unknown a-priori.

Mechanics of PGD - Enriching the Solution

Separated representation is built progressively by “enriching".

- At enrichment step $n+1$, assume we know the previous n terms.

$$\begin{aligned}\phi_{n+1}(x,t) &= \phi_n(x,t) + X_{n+1}(x)T_{n+1}(t) \\ &= \sum_{j=1}^{n} X_j(x)T_j(t) + \mathcal{X}(x)\mathcal{T}(t) \end{aligned} \tag{6}$$

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Mechanics of PGD - Alternating Direction Algorithm

1. Solve for $\mathcal{X}(x)$ assuming $\mathcal{T}(t)$
2. Solve for $\mathcal{T}(t)$ with obtained $\mathcal{X}(x)$
3. Check convergence of $\mathcal{X}(x)\mathcal{T}(t)$
4. Check convergence of ROM

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Alternating Direction Algorithm - Step 1

Starting with weighted residual form of the 1D transient neutron diffusion equation

$$\int_{\Omega_x \times \Omega_t} \phi^* \left(\frac{1}{v} \frac{\partial \phi}{\partial t} - \nabla \cdot D \nabla \phi + \Sigma_a(x) \phi(x,t) - S \right) dx dt = 0 \qquad (7)$$

where the test function, ϕ^*, defined as:

$$\phi^*(x,t) = u(x)\mathcal{T}(t) \qquad (8)$$

- $\mathcal{T}(t)$ is assumed known

Plugging our test function into the weighted residual form, we can obtain a BVP that is solved via CFEM

$$\int_{\Omega_x} u(x)\left[\left(\frac{1}{v}t_2 + t_1\Sigma_a(x)\right)\mathcal{X}(x) - t_1\frac{d}{dx}\cdot D(x)\frac{d\mathcal{X}(x)}{dx}\right]dx$$

$$= -\sum_{j=1}^{n}\int_{\Omega_x} u(x)\left[\left(\frac{1}{v}t_{4,i} + t_{3,i}\Sigma_a(x)\right)X_i(x)dx - t_{3,i}\frac{d}{dx}\cdot D(x)\frac{dX_i(x)}{dx}dx\right]$$

$$+ \int_{\Omega_x}\int_{\Omega_t} u(x)S(x,t) \tag{9}$$

Alternating Direction Algorithm - Step 2

Revisiting our weighted residual form:

$$\int_{\Omega_x \times \Omega_t} \phi^* \cdot \left(\frac{1}{v} \frac{\partial \phi}{\partial t} - \nabla \cdot D \nabla \phi + \Sigma_a(x) \phi(x,t) - S \right) dx dt = 0 \qquad (10)$$

This time, with a new test function, ϕ^*, defined as:

$$\phi^*(x,t) = \mathcal{X}(x) w(t) \qquad (11)$$

- $\mathcal{X}(x)$ is known from previous step

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- Plugging our test function into the weighted residual form, we can obtain an IVP that is solved via DFEM

$$\frac{1}{v}x_1\left(w(t)\mathcal{T}(t)\big|_{surf} - \int_{\Omega_t}\mathcal{T}(t)\frac{dw}{dt}dt\right) + (x_2 - x_3)\int_{\Omega_t} w(t)\mathcal{T}(t)dt$$

$$= -\sum_{i=1}^{n}\left[\frac{1}{v}x_{4,i}\left(w(t)T_i(t)\big|_{surf} - T_i\frac{dw}{dt}dt\right) + (x_{6,i} - x_{5,i})\int_{\Omega_t} w(t)T_i(t)dt\right]$$

$$+ \int_{\Omega_t}\int_{\Omega_x} w(t)S(x,t) \tag{12}$$

- Closure obtained by upwinding on surface terms.
- Initial condition in all tests $= 0.0$.

Alternating Direction Algorithm - Steps 3 & 4

- Solving for $\mathcal{X}(x)$ and $\mathcal{T}(t)$ involves a nonlinear iteration.
- Convergence criteria, $\nu = 1 \times 10^{-6}$

$$\nu = \sqrt{(\| \mathcal{X}^p \| \| \mathcal{T}^p \| - \| \mathcal{X}^{p-1} \| \| \mathcal{T}^{p-1} \|)^2}$$

note, $\| \cdot \| = \| \cdot \|_{L_2}^2$

- ROM convergence criteria, $\epsilon = 1 \times 10^{-6}$

$$\begin{aligned} \epsilon &= \|\phi_{n+1} - \phi_n\| \\ &= \| \left(\sum_{i=1}^{n} X_i T_i + X_{n+1} T_{n+1} \right) - \sum_{i=1}^{n} X_i T_i \| \\ &\leq \|X_{n+1}\| \|T_{n+1}\| \end{aligned}$$

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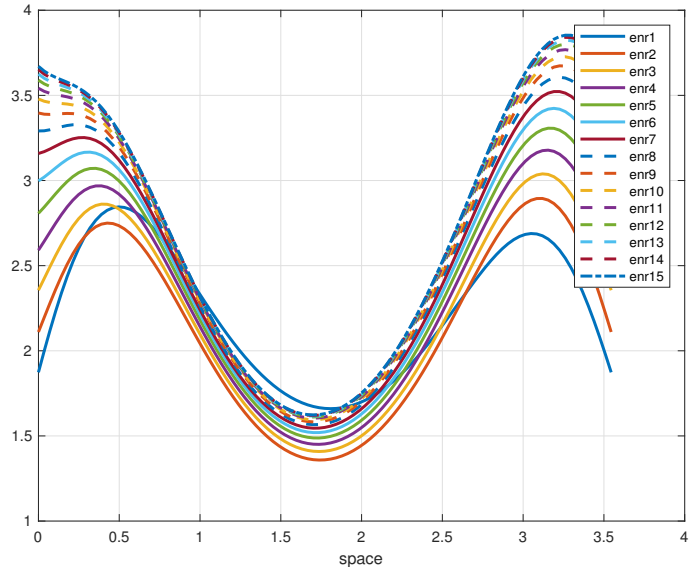
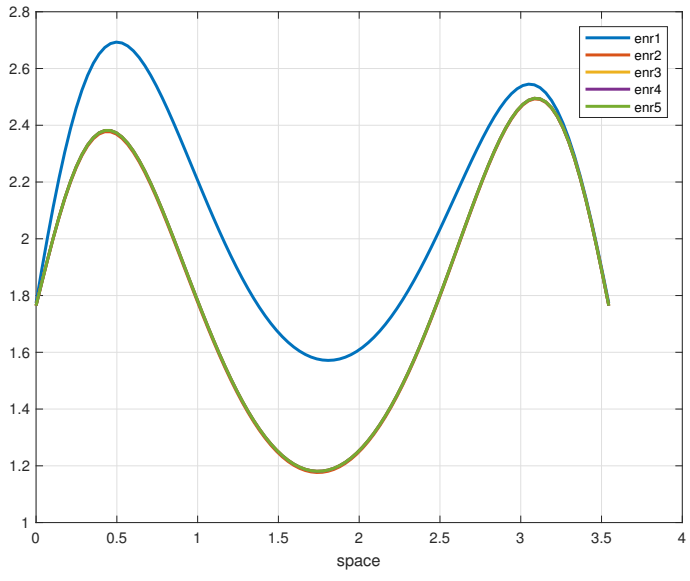
Alternating Direction Algorithm - Review

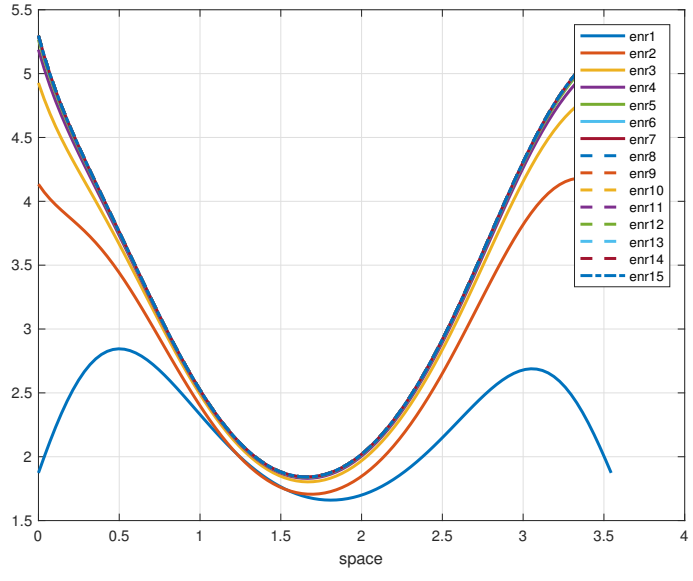
for $m = 1$ to m_{max}
define $X^{(0)}, T^{(0)}$ (initialization)
  for $k = 1$ to k_{max}
  compute $X^{(k)} = F_m\left(T^{(k-1)}\right)$
  compute $T^{(k)} = G_m\left(X^{(k)}\right)$
  normalize, s.t. $\|T^{(k)}\|_{L2}^2 = 1$
  check convergence, $\nu < X^{(k)} T^{(k)}$
  end
normalize $X^{(k)}$ and $T^{(k)}$
set $X^{(k)} = X_m$ and $T^{(k)} = T_m$
check convergence, $\epsilon < \|X_m\| \|T_m\|$
end

Importance of Normalizing in Non-linear Iterations

- Not commonly observed in literature
- Crucial to quality and convergence behavior of enrichment steps
- Normalization of time domain enhances convergence behavior and improves solution quality.







Test Problem 1

Using MMS with assumed solution of $\phi_{ref}(x,t) = t\sin(x)$:

Assume $v = 1.5$, $D = \Sigma_a = x + 1$

$\Omega_x = [0, \pi]$; CFEM; 250 elements

$\Omega_t = [0, 1$; DFEM; 60 elements

Both are discretized via 1st order linear polynomials

dof $= n(251 + 120)$

Error quantification is defined by the following:

$$\text{error}_i = \sqrt{\int_{\Omega_t}\int_{\Omega_x}\left(\phi_{ref}(x,t) - \sum_{j=1}^{i}\phi_{pgd,j}(x,t)\right)^2 dxdt}$$

where, i, is the enrichment step of interest

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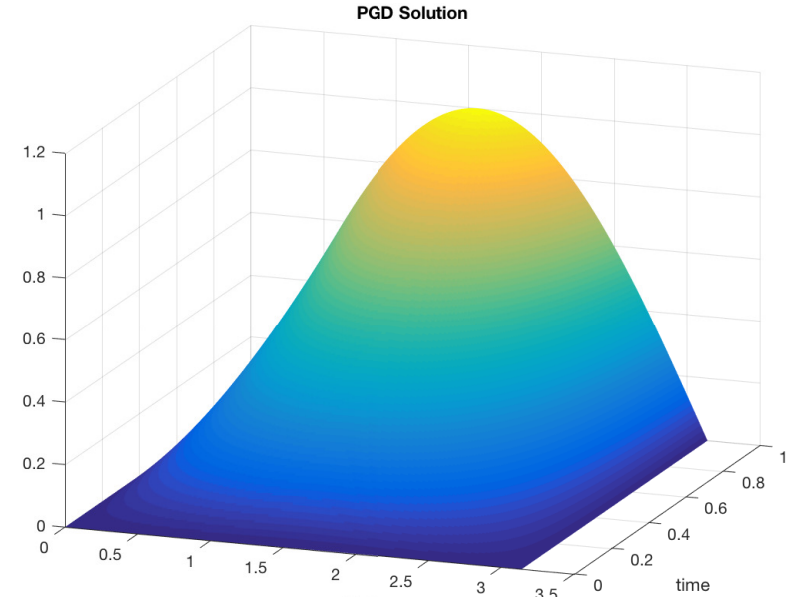
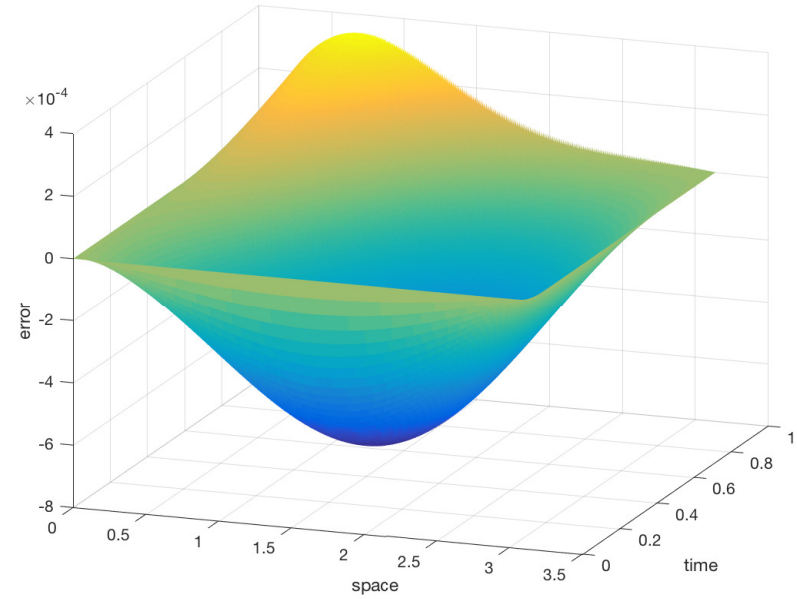
Test Problem 1 - Results

- PGD solution captures reference solution within first enrichment step.
- Higher enrichment steps have negligible effects.

$Enr.Step$	$\|\|Ref - PGD\|\|_{L2}$
1	3.516E-3
2	4.325E-3
3	3.686E-3
4	3.679E-3
5	3.715E-3





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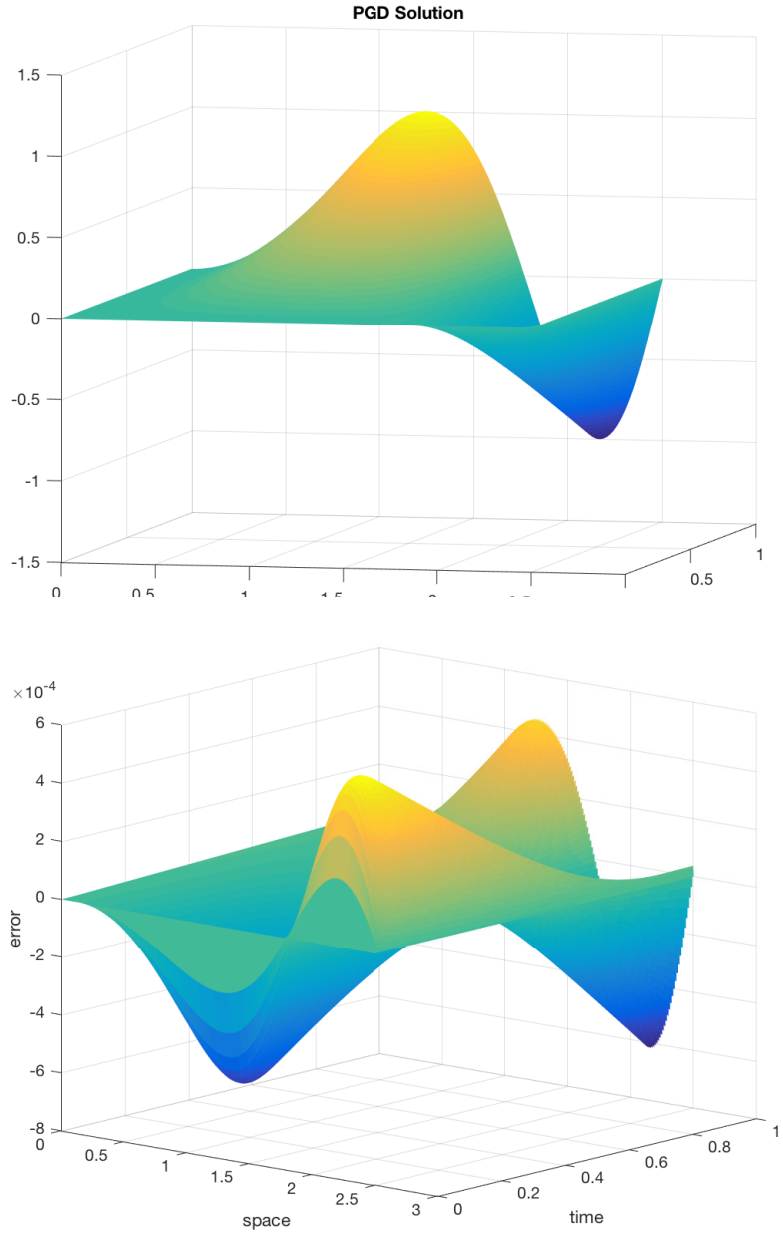
Test Problem 2

- $\phi_{ref} = t\sin(x^2)$
- $\Omega_x \in [0,\ \sqrt{2}\sqrt{\pi}]$; CFEM; 250 elements.
- $\Omega_t = [0, 1]$; DFEM; 60 elements
- Both are discretized via 1st order linear polynomials
- dofs = n(201+120)
- Again, PGD solution captures reference solution within first enrichment step.

Enr.Step	$\|\|Ref - PGD\|\|_{L2}$
1	2.5661E-3
2	2.5693E-3
3	2.5694E-3

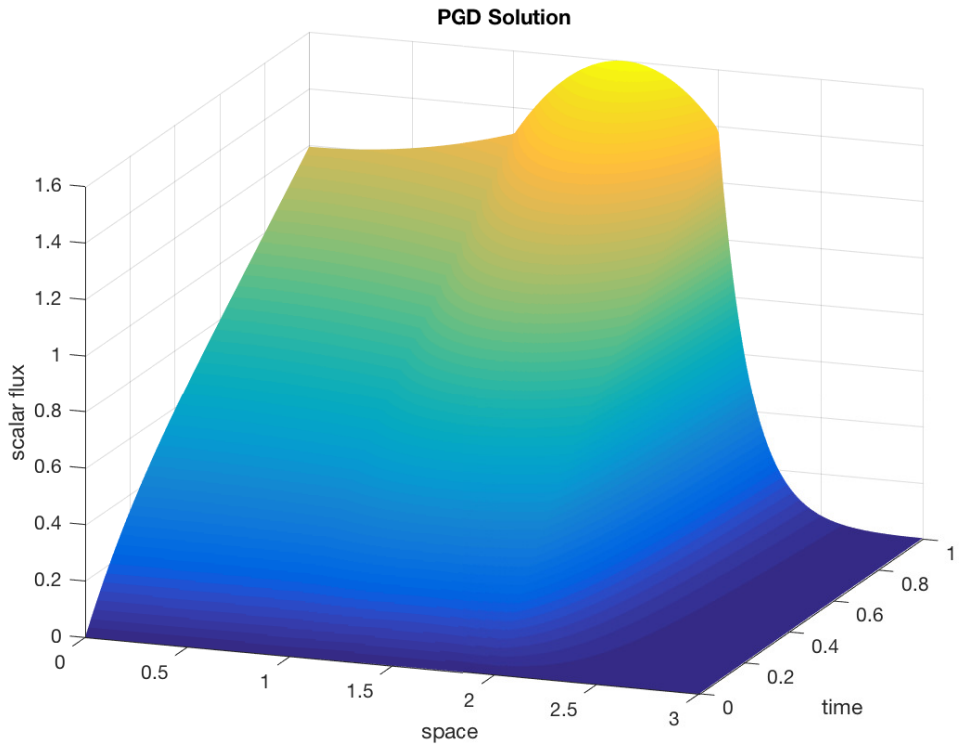


Test Problem 3 - A “real" problem

- Define 3 region heterogeneous problem (v$=$ 1.5):

Region	D	Σ_a	Source
1	5.0	0.001	0.0
2	1.0	0.5	3.0
3	0.1	3.5	0.0

- $\Omega_x = [0, 3]$; CFEM; 300 elements
- $\Omega_t = [0, 1]$; DFEM; 100 elements
- 1st order linear polynomials.
- dofs $= n(301 + 200)$



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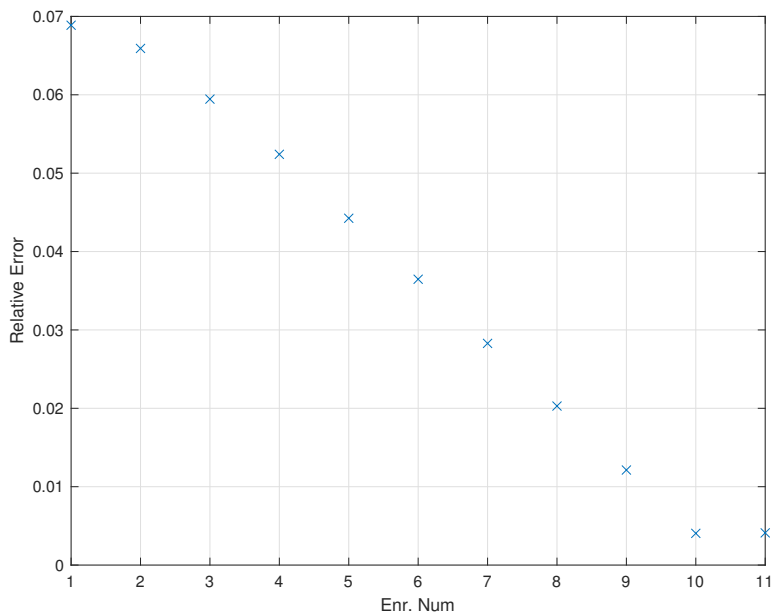
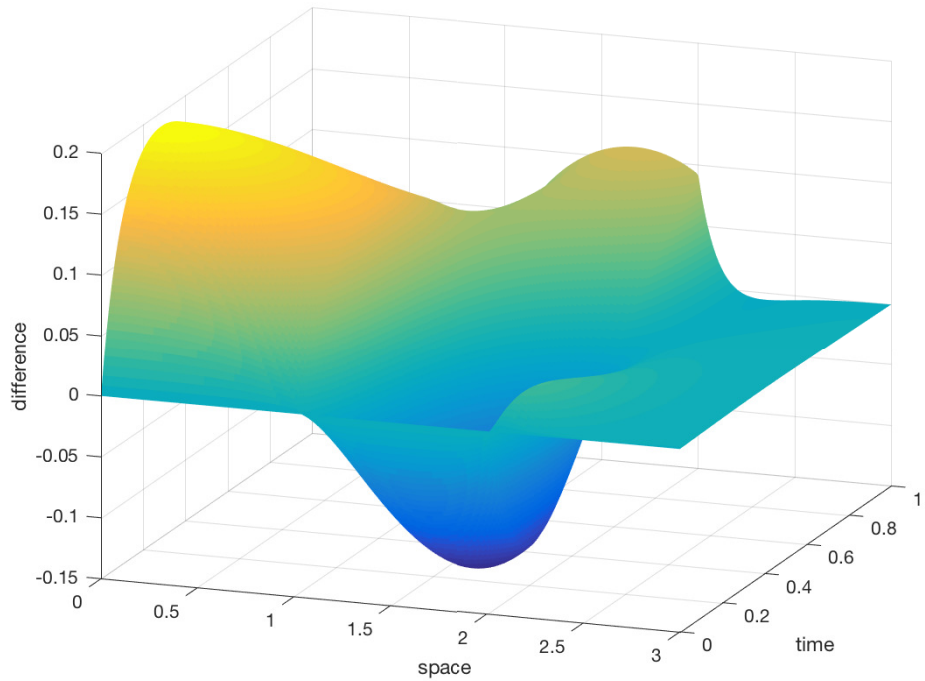
Test Problem 3 - Error Analysis

- Reference solution generated from solver with CFEM in space and Backward Euler in time
- Reference solution has $256 \times 256 = 65,536$ dof.
- PGD with 10 enrichment steps has $10(301 + 200) = 5,010$ dof.





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Test Problem 4 - 2D Transient

- $\phi_{ref} = t \sin(x) \sin(y)$

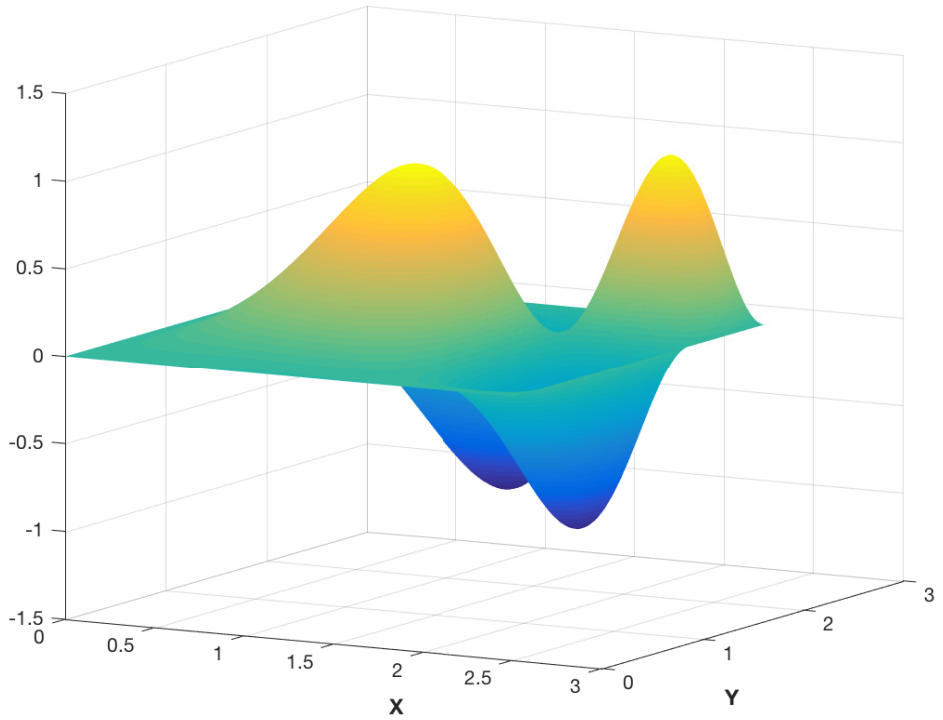
  $\Omega_x = \Omega_y \in [0, \sqrt{2}\sqrt{\pi}]$; CFEM; 100 elements.

  $\Omega_t = [0, 1]$; DFEM; 100 elements.

  $D = (xy) + 1.0$

  $\Sigma_t = ((x_r - x)(y_r - y)) + 1.0$

$Enr.Step$	$\|\|Ref - PGD\|\|_{L2} / \|\|Ref\|\|$
1	0.0287
2	0.0221
3	0.3395
4	0.2772
5	0.3184



- 1st order linear polynomials.
- dofs = n(100+100+100)

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Conclusions

- “Curse of dimensionality" is apparent in reactor physics calculations
- More well developed, data driven methods are potentially impractical
- Proper generalized decomposition provides an avenue for a priori model reduction
- 1D Transient results show promise that PGD is a potentially viable solution to dimensionality issues

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Moving Forward

1. 1D Transient problem
   - Mesh refinement studies.
2. 2D Transient problem
   - Improve understanding of normalization process in enrichment process.
   - Non-separable problems.
3. Expand to energy dependence
   - 1D transient formulation under construction now
   - Include energy as PGD dimension - *continuous* in energy
4. Couple energy dependent PGD ROM to ODEs
   - Reactor kinetics; precursor equations and delayed neutrons

Along the way...

- Spatial discontinuities
- Increasingly real problems (fission source, etc)

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Questions?

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