CALCULATING TRANSIENT NEUTRON FLUX USING THE PROPER GENERALIZED DECOMPOSITION

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Summary

High fidelity simulations in nuclear engineering inherently lie in high-parameter spaces and commonly suffer from the "curse of dimensionality". Current methods used to overcome this computational expense include low-order moments-based angular treatments, few-group energy discretizations, and spatial homogenization/upscaling [2]. However, the the effect of errors and uncertainties associated with these approaches increases when they are coupled to other physical systems (i.e. fluid dynamics, structural mechanics, material models, etc) [7]. The combination of high parametric space and increasing need for high-fidelity calculations has led to a developing interest in applications of contemporary reduced order modeling methods [1, 8].

Introduction

A relevant example is the solution of a nuclear reactor dynamics problem with deterministic treatments of each of the phase space variables. A high fidelity solution to this problem includes solving an integro-differential Boltzmann transport equation (BTE) describing the neutron population as a function of time coupled to a set of ordinary differential equations (ODE) that govern the dynamics of various nuclear reactions (up to 10^3 additional equations). The dimensionality of this problem is driven by the solution to the BTE in which there are seven degrees of freedom; three in space (x, y, z), two in direction of flight (θ, ϕ), one in energy (E), and one in time (t). In order to capture detailed physics involved in radiation transport, fine mesh discretizations are often required.

A few common (and reasonable) approximations to alleviate the computational cost associated with the above example are as follows: 1) disregard the ODEs governing nuclear reaction dynamics; 2) in the BTE, assume that the angular dependence of the neutron flux can be adequately represented through a linearly anisotropic angular dependence [6]; and 3) assume that the neutron population can be characterized by a single energy group. Applying these approximations yields the monoenergetic neutron diffusion equation:

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

Proper Generalized Decomposition (PGD)

Proper generalized decomposition is a modern *a priori* decomposition-based method where functions can be represented through a finite sum decomposition [4]. Consider the three dimensional solution to Equation 1 in space, x, time, t, and diffusivity, D:

$$\phi(x,t,D) = \sum_{j=1}^{n} X_j(x) \cdot T_j(t) \cdot P_j(D) \tag{2}$$

where n is the total number of "enrichment steps" in the solution and $X_j(x)$, $T_j(t)$, and $P_j(D)$ are the basis functions defining the spatial, time, and diffusivity dependence at enrichment step, j, respectively.

Additional enrichment steps can be computed in the following manner:

$$\phi(x,t,D) = \sum_{j=1}^{n} X_j(x)\cdot T_j(t)\cdot P_j(D) + X_{n+1}(x)\cdot T_{n+1}(t)\cdot P_{n+1}(D) \tag{3}$$

For notational simplicity, we will define $X_{n+1}(x)$, $T_{n+1}(t)$, and $P_{n+1}(D)$ as $\mathcal{X}(x)$, $\mathcal{T}(t)$, and $\mathcal{P}(D)$, respectively.

Consider the weighted residual form of Equation 1 with u^* defined as a suitable test function:

$$\int_\Omega u^* \cdot \left(\frac{1}{v}\frac{\partial \phi}{\partial t} - D\nabla^2\phi + \Sigma_a\phi - S \right) dx \cdot dt \cdot dD = 0 \tag{4}$$

Using Equation 3 as the definition for ϕ, Equation 4 yields a non-linear problem for the unknown functions $\mathcal{X}(x)$, $\mathcal{T}(t)$, and $\mathcal{P}(D)$. Using an alternating direction implicit (ADI) scheme, this problem can be treated as three successive subproblems: first, assume a solution for $\mathcal{T}(t)$ and $\mathcal{P}(D)$ and solve the resulting BVP for $\mathcal{X}(x)$; then, using the updated $\mathcal{X}(x)$ and the guess for $\mathcal{P}(D)$, solve the resulting IVP for $\mathcal{T}(t)$; and finally, using the updated $\mathcal{T}(t)$ and $\mathcal{X}(x)$ solve the resulting analytic expression for $\mathcal{P}(D)$.

The strong form of each of these subproblems is shown below (detailed derivations of each can be found in [3]).

1D BVP, $\mathcal{X}(\mathbf{x})$:

$$
\begin{aligned}
&- \nabla^2 \mathcal{X}(x)\,(t_2\,p_3) + \mathcal{X}(x)\left(t_3\,\frac{1}{v}\,p_2 + t_2\,\Sigma_a\,p_2\right) \\
&= \sum_{i=1}^{n-1}\left[\nabla^2 X_i(x)\,(t_4\,p_5) - X_i(x)\left(t_5\,\frac{1}{v}\,p_4 + t_4 \Sigma_a\,p_4\right)\right] \\
&\quad + S_x t_1 p_1 \\
&\phi(0,t) = \phi(L,t) = 0.0
\end{aligned} \tag{5}
$$

1D IVP, $\mathcal{T}(\mathbf{t})$:

$$
\begin{aligned}
&\frac{d\mathcal{T}(t)}{dt}\left(x_2\,\frac{1}{v}\,p_2\right) - \mathcal{T}(t)\,(x_3\,p_3 - x_2\,\Sigma_a\,p_2) \\
&= \sum_{i=1}^{n-1}\left[-\frac{dT_i}{dt}\left(x_4\,\frac{1}{v}\,p_4\right) + T_i(t)\,(x_5\,p_5 - x_4\,\Sigma_a\,p_4)\right] \\
&\quad + S_t\,x_1\,p_1 \\
&\phi(x,0) = 0.0
\end{aligned} \tag{6}
$$

Analytical, $\mathcal{P}(\mathbf{D})$:

$$
\mathcal{P}(D) = \frac{\mathcal{C}_1 + S_D\,x_1\,t_1}{\left[\frac{1}{v}\,(x_2\,t_3) - D\,(x_3\,t_2) + \Sigma_a\,(x_2\,t_2)\right]} \tag{7}
$$

where:

$$
\mathcal{C}_1 = \sum_{i=1}^{n-1}\left[P_i(D)\left(-\frac{1}{v}\,(x_4\,t_5) + D\,(x_5\,t_4) - \Sigma_a\,(x_4\,t_5)\right)\right]
$$

Results

The solution procedure described above (Equations 5, 6, 7) was tested with finite differencing for $v = 1.25$, $\Sigma_a = 0.025$, and $S(x,t) = t \cdot \sin(x)$. The spatial domain is discretized via central differencing with 400 nodes over the interval $(0,\pi)$; the time domain consists of 525 nodes over the interval $(0,1)$ with central differencing over the interior nodes and a 3-point first derivative approximation for the boundary element (to maintain $\mathcal{O}(\Delta t^2)$ accuracy); and the diffusivity domain consists of 25 nodes over the domain $(1,4)$. A Crank-Nicholson finite difference solution was used as the reference solution.

Error quantification was defined by arbitrarily choosing a time, t, and a diffusivity, D, and taking the square of the difference of the reference and PGD approximated solutions:

$$
\epsilon_i = \left(\int_{\Omega_x} \phi_{ref}(x,t,D)\,dx - \int_{\Omega_x}\sum_{j=1}^{i}\phi_{pgd,j}(x,t,D)\,dx\right)^2 \tag{8}
$$

where i is the enrichment step of interest

Figure 1 shows that as the PGD approximation is enriched, the approximated solution converges to an absolute difference of about 4.5×10^{-5}.

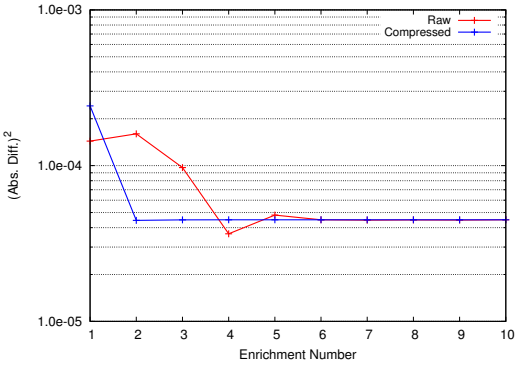

Figure 1: Absolute difference of PGD approximation as a function of enrichment step for $t = 0.5$ and $D = 2.25$.

It has been shown that PGD approximations of parabolic equations can be non-optimal [5]. The "Compressed" data series of Figure 1 shows the effects of applying an a posteriori data compression and smoothing algorithm that attempts to recover some optimality [5, 3].

The compressed PGD also allows for significant gains in data storage. To cover the entire problem domain, $\Omega_x \times \Omega_t \times \Omega_D$, the converged reference solution requires 6MB while the "raw" and "compressed" PGD solutions require 76 KB (10 enrichment steps) and 15 KB (2 enrichment steps), respectively. This represents a savings of two orders of magnitude for the PGD solutions.

Future Work

In its current state, the quality of the PGD approximation is sensitive to selections of v and Σ_a. For practical applications, this sensitivity will need to be addressed.

Increasing the complexity of the problem to include energy dependence in the solution as well as coupling the ODE's that govern the dynamics of nuclear reactions is also of interest.

Conclusions

Many problems in nuclear engineering lie in high-parameter spaces and suffer from the "curse of dimensionality". Developing *a priori* reduced order models for nuclear applications is a developing field. This work shows that by using PGD on a transient monoenergetic neutron diffusion problem, reasonable accuracy and significant data storage gains are achievable. Future work will lie in further stabilizing the nonlinear iteration scheme and improving the optimality of the approximation.

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