Reduced Order Modeling for use in Contaminant Transport Modeling

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Background

Groundwater contamination affects the lives of people across the globe. Contaminant transport modeling is an important way to gain knowledge that helps to mitigate and control contamination of groundwater.

Contaminant transport is described mathematically by the advection-dispersion equation, a partial differential equation that can be solved with numerical techniques such as the Finite-Element Method.

Unfortunately, computing a solution using a high-resolution finite-element scheme requires the solution of a large, sparse linear system. For transient problems, this linear system must be solved at every time step.

In this work, we show that Reduced-Order Modeling is a viable way to reduce the computational complexity of solving the advection-dispersion quation.

Problem

In this demonstration, we use the heat equation in one spatial dimension, which could also be considered a special case of the advection-dispersion equation (where flow velocity is zero). We have:

$$u_t - u_{xx} = f(x,t)$$

$$0 \le x \le 2 \qquad 0 \le t \le 1$$

$$f(x,t) = \sin(\pi x) + t\,\pi^2 \sin(\pi x)$$

$$u(x,0) = 0$$

$$u(0,t) = u(2,t) = 0$$

with the exact solution to this problem given by:

$$u(x,t) = t\sin(\pi x)$$

Reduced-Order Approach

- Use high-resolution finite-element code to generate solutions to the problem for a sampling of parameter values at different time steps, collecting these "snapshots" as the columns of the matrix Φ.
- Compute the singular value decomposition of Φ:

$$\Phi = U\Sigma V^*$$

- Define the POD (proper orthogonal decomposition) basis of cardinality n as the set of the first n left singular vectors.
- Use Galerkin approximation to approximate the solution as a linear combination of n POD basis vectors.

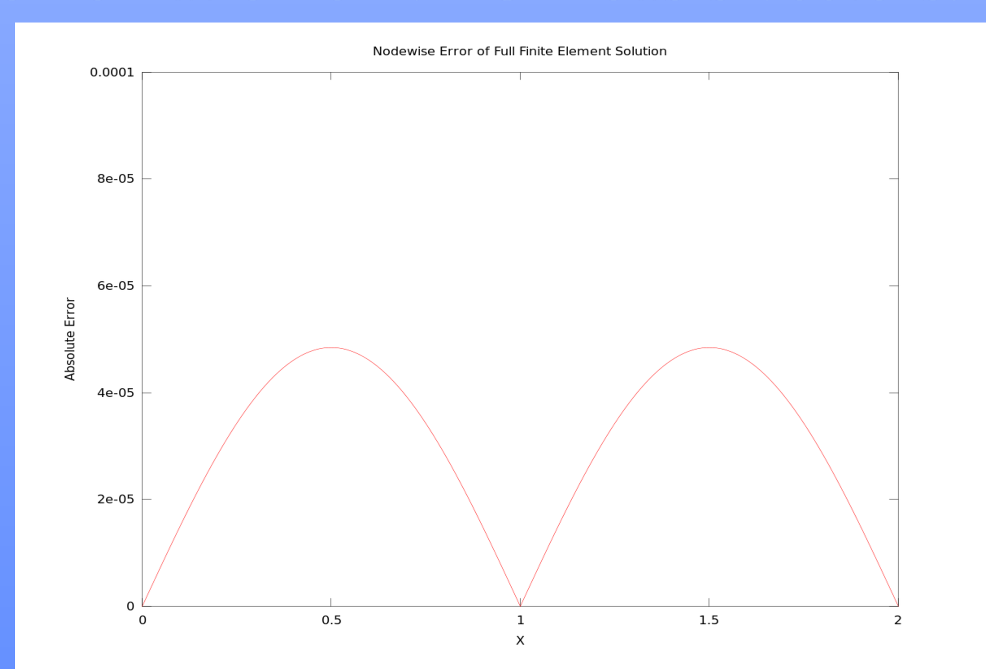

Figure 1: Node-wise absolute error of full finite element solution with Δx=0.0025, Δt=0.00005

Full Solution

We solve the equation first using the standard finite element method with piecewise linear "hat" basis functions and using a first-order backward difference scheme to advance in time. At the final time, we calculate the error (Figure 1).

Collecting snapshots at various time steps, the snapshot set is assembled. The basis vectors are generated using the singular value decomposition (Figure 2).

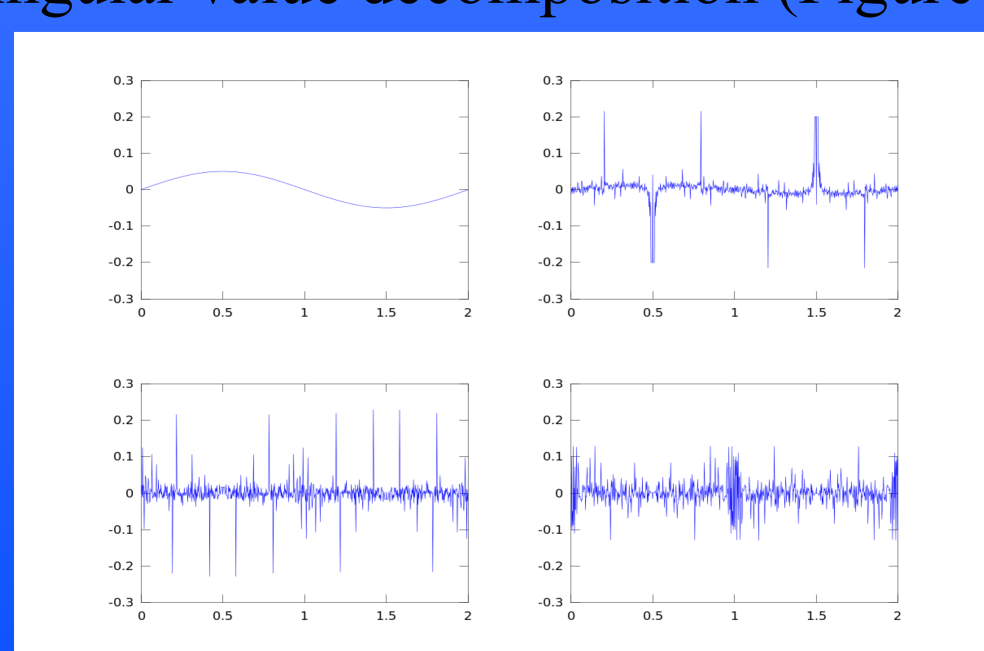

Figure 2: First 4 basis "solution" vectors from SVD of snapshot set

ROM Solution

Performing Galerkin approximation using an increasing number of basis vectors gives an increasingly accurate solution. However, for this particular problem, the added improvement from additional basis vectors declines sharply. It is possible to compare the error from the reduced-basis solution (using 4 basis vectors) to that of the full finite-element solution (Figure 3).

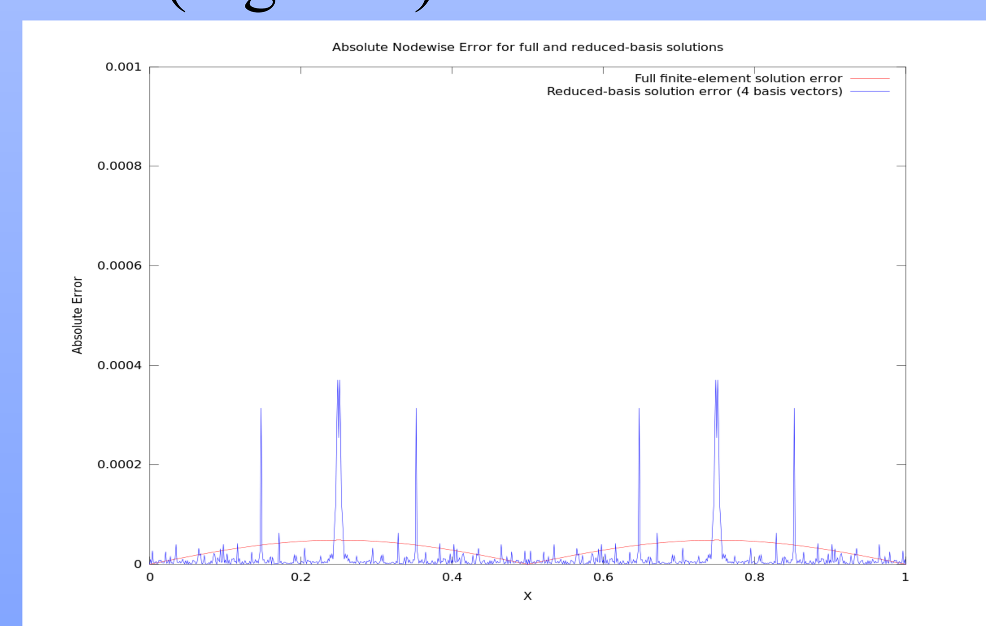

Figure 3: Absolute node-wise error for the standard (full) finite element solution and the reduced basis (4 basis vectors) solution.

Analysis

- The error is larger for the reduced-basis solution, but still controlled (error decreases when more basis vectors are used).
- The reduced-basis solution has a much smaller linear system (n=4 in this case) that must be solved compared to the full solution (n=799).
- We may continue using this approach to reduce the complexity of modeling contaminant transport.

REFERENCES

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