Solute Transport: An Application of Model Reduction

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Abstract: Being able to accurately and reliably model subsurface systems is integral to our ability to understand, monitor, and conserve groundwater, one of our most vital resources. Many analysis tools used in contaminant transport modeling, such as parameter estimation and uncertainty quantification, have an extremely high computational cost because of the high number of realizations of the forward model that are required. In previous research we have put forth the technique of reduced order modeling (ROM) via proper orthogonal decomposition (POD) as a viable means to solve diffusion-dominated linear reactive transport systems, demonstrating the method in the one-dimensional case, but did not present any data regarding the computational savings. Here we demonstrate a two-dimensional example, and the computational cost-savings of the reduced model. We will describe the processes of reactive transport, outline the method of model reduction, and demonstrate the ability of ROM to improve simulation time while maintaining accuracy. As our work continues, we turn our attention to some of the methods we are researching for treating more realistic reactive transport scenarios.

Why Study Reactive Transport?

- Water is an essential resource; access to supplies of clean fresh water is a basic necessity.
- Groundwater comprises the vast majority of Earth's available fresh water (i.e., not frozen in ice caps or glaciers). Most of the fresh water we use comes from subsurface aquifers.
- Good contaminant transport models are essential for predicting the spread of contamination and identifying sources of contamination, especially as direct subsurface observation is very difficult or impossible in general. Good predictions can help protect the public and aid in remediation efforts.

Groundwater Contamination Modeling

The fate of solute particles dissolved in groundwater is goverened by the processes of advection (particles carried along by the flow of the water), hydrodynamic dispersion (molecular diffusion and mechanical dispersion), and reactions with other chemical species present in the aquifer.

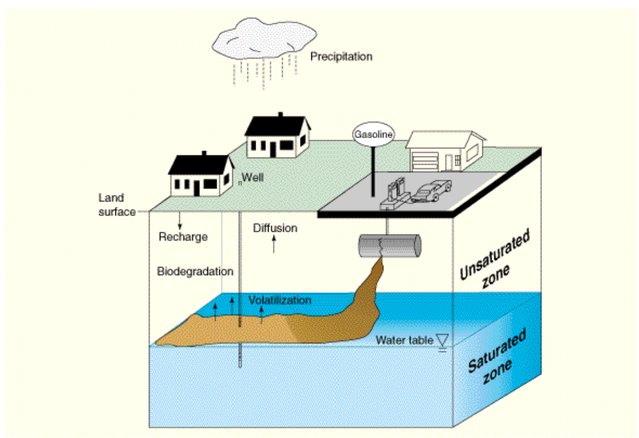

Figure 1. Conceptualization of the fate of petroleum hydrocarbons in a ground-water system.

Mathematically, we can model these processes with the *advection-dispersion-reaction equation*. Transport of solute in a long, thin aquifer with a continuous injection of contaminated water at the point $(0, 0)$ is described using the 2d advection-dispersion-reaction equation

$$\frac{\partial C}{\partial t} + \nu\frac{\partial C}{\partial x} - D_x\frac{\partial^2 C}{\partial x^2} - D_y\frac{\partial^2 C}{\partial y^2} - \sum \mathbf{R} = \frac{QC_0\delta(x,y)}{\theta} \qquad x \in [-\infty, \infty] \quad y \in [-\infty, \infty] \quad t > 0 \tag{1}$$

whe $C(x,t)$ is the concentration of the solute species at time t and location (x, y), $\mathbf{v}_x$ is the seepage velocity of the water along the length of the field, and $\mathbf{D}_x$ and $\mathbf{D}_y$ are the coefficients of hydrodynamic dispersion along the longitudinal and transverse directions, respectively. $\sum \mathbf{R}$ represents the summation of (typically nonlinear) source/sink terms resulting from chemical reactions involving the solute species.

Finite Element Example

If we consider transport as described in Equation 1 with a conservative solute species ($\sum \mathbf{R} = 0$), then an analytical solution to the problem is available from Wilson and Miller, 1978. We use problem parameters:

- $\nu = \frac{1}{3}\,\mathrm{m/d}$
- $D_y = 1\,\mathrm{m}^2/\mathrm{d}$
- $Q = 0.1\mathrm{m}^2/\mathrm{d}$
- $D_x = \frac{10}{3}\,\mathrm{m}^2/\mathrm{d}$
- $\theta = 0.3$
- $C_0 = 1\,\mathrm{g/m}^3$

The Dirac delta function, $\delta(x, y)$, has units of m^{-2}, and we shift the source location to $(150, 150)$.

We partition the domain into a uniform triangular mesh and discretize the governing equation using piecewise-quadratic basis functions in space and a second-order backward difference approximation in time. We simulate the system from $t = 0$ to $t = 365$ using $\Delta t = 0.5\,\mathrm{d}$, $\Delta x = \Delta y = 10\,\mathrm{m}$.

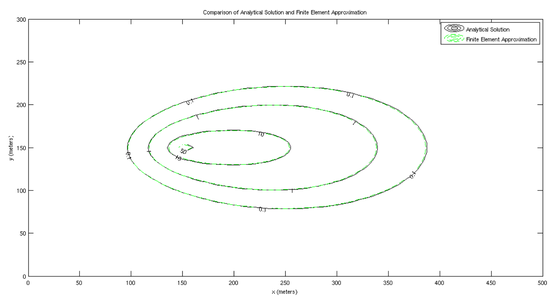

Figure 2: Comparison of analytical solution and finite element approximation

POD-based Model Reduction

In finite element approximation, we choose the basis functions functions, $\{\phi_i\}_{i=1}^n$, to be piecewise-continuous nodal polynomials, so that the resulting linear system is sparse and banded. However, this system is generally large (n depends on the number of grid nodes).
In POD-based ROM, we seek a small set of global basis functions that can reproduce the solution. This produces a small, dense linear system.

1. Obtain a sampled set of parameter values in the parameter space and time instants in the time domain.
2. Compute approximations to the PDE solution corresponding to the sampled values. Store vectors representing these particular approximations, $\{s_k\}_{k=1}^m$, as columns in the **snapshot set**, S.
3. Compress the information from the columns of S to obtain d vectors defining the functions in the reduced basis ($d << n$).
4. Use this reduced basis to solve the PDE for other parameters in the prescribed space.

In this work, we use the Singular Value Decomposition to compress the snapshot data. The SVD compression is advantageous because the resulting vectors are linearly independent and the singular values can be used to assess data loss due to truncation.

Why Use Model Reduction?

In many applications we are driven to find ways to reduce the associated computational cost, such as

- Parameter Estimation/Model Identification
- Uncertainty Quantification (UQ)
- Stochastics
- Real-Time Calculations

Because of the pre-processing cost associated with constructing the basis functions for the reduced model, it is not an attractive option if we only want to solve a particular PDE one time. However, **ROM is a very attractive option if we want to solve the PDE many times, or if we need to be able to solve it in real time**.

ROM Example

Using the method described to obtain a reduced basis, we repeat the approximation of our 2d example problem in hopes of reproducing the finite element data with a small number of basis functions. Results for approximations using 2, 4, 8, and 16 basis functions are displayed.

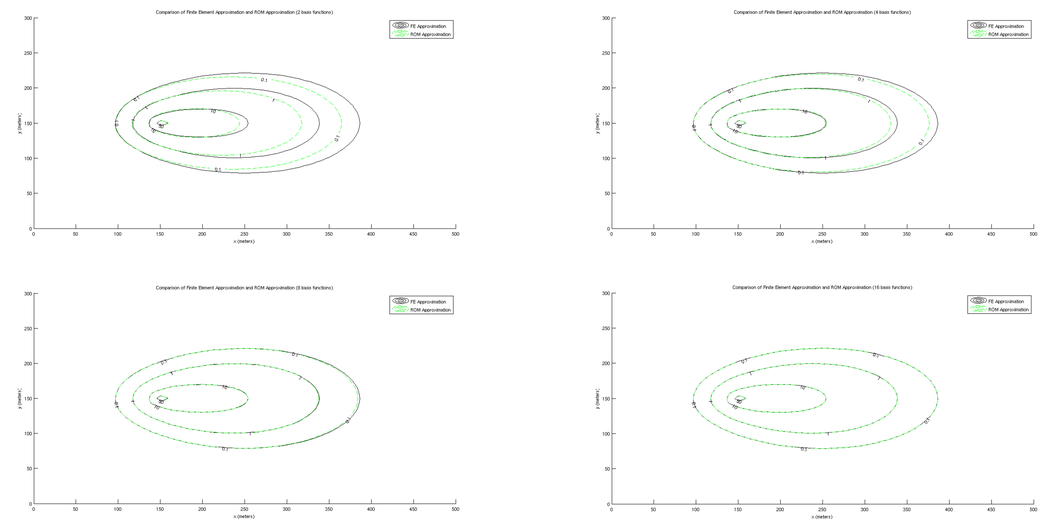

Table 1: Error of Reduced Order Model Compared to Finite Element Approximation

Basis Functions	L_2 Error	H_1 Error	Relataive L_2 Error	Relative H_1 Error	SVD-based Error Estimate	Computational Time(s)
2	1.8151×10^{3}	1.8561×10^{3}	2.2173×10^{-1}	2.2655×10^{-1}	1.1053×10^{-1}	68.4
4	5.1865×10^{2}	6.4909×10^{2}	6.3358×10^{-2}	7.9225×10^{-2}	2.3662×10^{-2}	88.9
8	5.3572×10^{1}	3.9505×10^{2}	6.5443×10^{-3}	4.8219×10^{-2}	1.2365×10^{-3}	130.9
16	2.4096×10^{-1}	3.9131×10^{2}	2.9436×10^{-5}	4.7763×10^{-2}	1.6198×10^{-6}	213.9
32	2.2027×10^{-3}	3.9131×10^{2}	2.6908×10^{-7}	4.7763×10^{-2}	1.8407×10^{-13}	380.7

We can see the trade-off between accuracy and computational time in the reduced model in Table 1 and Figure 3.

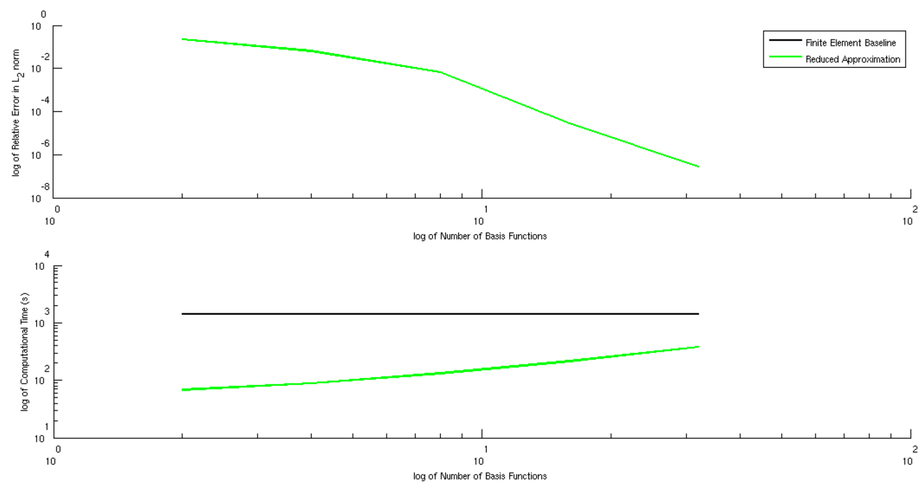

Figure 3: Behavior of Error and Computational Cost of the Reduced Model

Work in Progress

- Incorporate realistic chemical reactions into the model.
- Determine how best to account for chemical reactions in the reduced model setting.
- Test how well ROM performs in the UQ framework.
- Consider ways to make ROM more robust for advection-dominated problems.

References

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4. Figure 1 provided by US Geological Survey (*http://pubs.usgs.gov/fs/FS-019-98*).