Stabilized Reduced-Order Modeling of Reactive Transport

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Abstract: In this work, we consider the use of model order reduction in solving the advection-dispersion-reaction equation. Equations of this form appear in a wide range of application areas, but we focus on the study of reactive transport in groundwater systems. In cases where transport is dominated by advective forces, numerical models often suffer from instability which may pose a serious computational challenge by producing non-physical oscillations in the approximations. We aim to reduce the burden of the computational challenges in this setting through model order reduction, employing the method of snapshots and the singular value decomposition to construct a reduced basis via proper orthogonal decomposition (POD). We study the incorporation of Streamline Upwind Petrov-Galerkin (SUPG) methods to lend stability to full- and reduced-order transport models in 2d, considering advection-dominated transport and nonlinear reactive transport.

Groundwater Contamination Modeling

Fresh water is a vital resource, yet most of the fresh water available for human consumption is actually stored in underground aquifers. Responsible management of this resource is critical, but direct observation of these subsurface systems is often expensive, impractical, or even impossible. Because of this, computational modeling and simulation are essential to our understanding and conservation practices in this field.

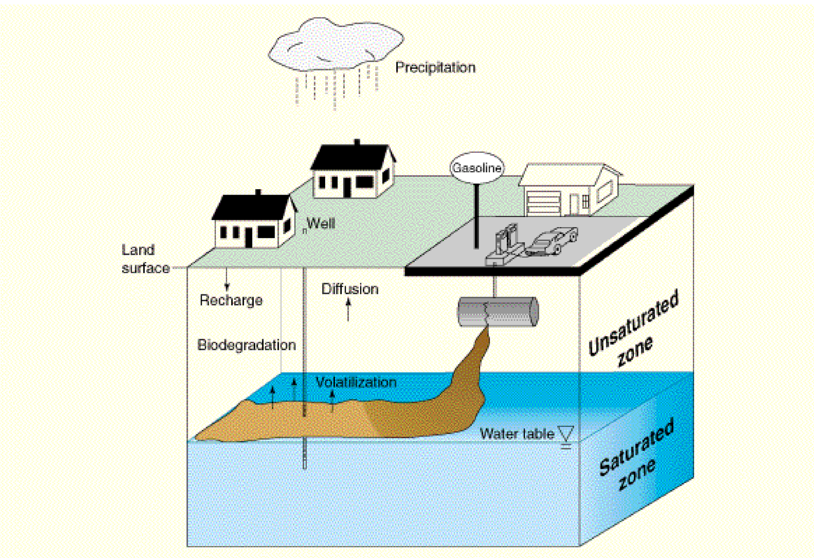


Figure 1. Conceptualization of the fate of petroleum hydrocarbons in a ground-water system.

The fate of solute particles dissolved in groundwater is goverened by the processes of advection, hydrodynamic dispersion, and chemical reactions. Mathematically, we model the effect of these processes on solute concentration as a system of *advection-dispersion-reaction equations*.

$$\frac{\partial C}{\partial t} = \nabla \cdot (\mathbf{D}\nabla C) - \nabla \cdot (\mathbf{a}C) + \sum \mathbf{R}(C) \tag{1}$$

for $t > 0$ on a domain Ω, with suitable initial conditions at $t = 0$ and boundary conditions on $\partial\Omega$. The reaction terms in $\sum \mathbf{R}(C)$ are often nonlinear and may produce coupled systems for multispecies models.

POD-based Model Reduction

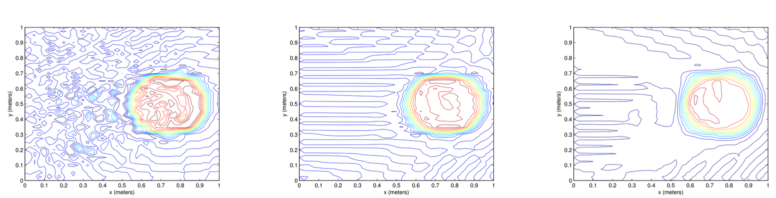
For many problems of interest in hydrology, we have to generate many realizations of the advection-dispersion-reaction model to address issues such as **parameter estimation/model identification** and **uncertainty quantification**. If the computational model is expensive, however, such a procedure becomes prohibitively costly. **POD-based model reduction gives us a way to use the information from a small number of expensive realizations to compute additional realizations with significant cost-savings.**

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 ($d << n$). In this work, we use the Singular Value Decomposition to compress the snapshot data:
$$\mathbf{S} = \mathbf{U}\Sigma\mathbf{V}^T \tag{2}$$
where we choose basis functions that are represented by the first d columns of $\mathbf{U}$.
4. Use this new basis to compute realizations for different parameter values in the same parameter space (via Galerkin projection).

In ROM, we solve a small, dense system of equations rather than the large, sparse system from the high-order method.

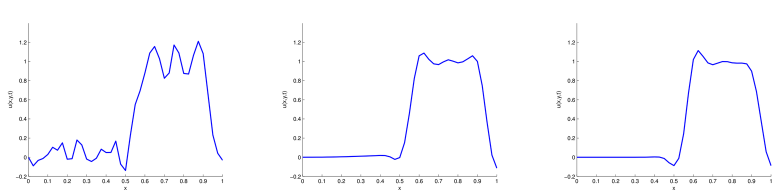
Instability in Convection-Dominated Problems

Instabilities arise when transport is advection-dominated and the computational grid is too coarse, but we want to eliminate the non-physical artifacts without making the grid arbitrarily fine. Here we use a **S**treamline-**U**pwind **P**etrov-**G**alerkin (SUPG) method (Bochev, 2004) to stabilize the finite element model by adding diffusion only along the solution streamline. Some oscillations near steep gradients in directions orthogonal to the streamline remain, which may be improved by adding some small artificial diffusion in this direction to form a **S**purious **O**scillations at **L**ayers **D**iminishing (SOLD) method (John/Knobloch, 2007).



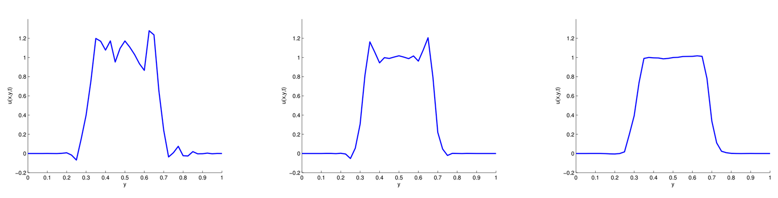
(a) FE (b) FE-SUPG (c) FE-SOLD

Figure 2: Finite Element Approximations for Cylinder Advection



(a) FE (b) FE-SUPG (c) FE-SOLD

Figure 3: Streamline cross-section view of transported cylinder



(a) FE (b) FE-SUPG (c) FE-SOLD

Figure 4: Cross-section view of transported cylinder perpendicular to streamline

Stabilization in ROM

Using stabilized methods for snapshot generation alone is not sufficient to stabilize the reduced-order approximation. Since the SUPG and SOLD methods are enforced on the weak form of the problem by the inclusion of weighted residual terms, they can be readily applied within the ROM framework.

As an example, consider a nonlinear advection-dispersion-reaction system with second-order decay:

$$\frac{\partial u}{\partial t} = \mathbf{D}_x\frac{\partial^2 u}{\partial x^2} + \mathbf{D}_y\frac{\partial^2 u}{\partial y^2} - \mathbf{a}_x\frac{\partial u}{\partial x} - \mathbf{k}u^2 \tag{3}$$

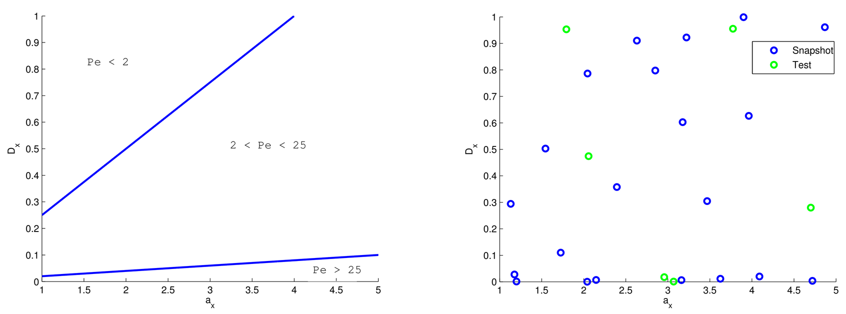
on the domain $x, y \in [0, 10]$, $t > 0$, subject to $u(x, y, 0) = 0$ with

$$\frac{\partial u(x,0,t)}{\partial y} = \frac{\partial u(x,10,t)}{\partial y} = \frac{\partial u(10,y,t)}{\partial x} = 0 \qquad u(0,y,t) = \begin{cases} 1 \text{ for } 0.4 \le y \le 0.6 \\ 0 \text{ otherwise} \end{cases} \tag{4}$$

We wish to construct a reduced model that can compute realizations for parameter choices within the specified parameter space. Figure 5 shows the randomly selected parameter points for snapshot generation and model testing. We produce distinct snapshot sets and ROM bases for each stabilization type. As an example, we show plots for the first test problem, which occurs in the more highly advection-dominated region of the parameter space. Table 1 contains results for all of the tests for the ROM-SUPG method.

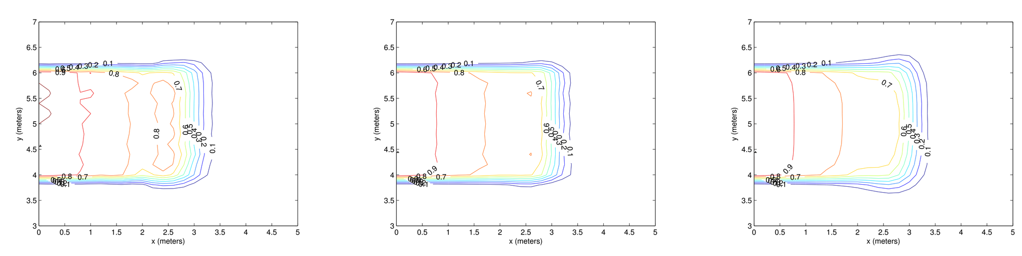
Parameter Space:

$$\mathbf{a}_x \in [1, 5] \tag{5}$$
$$\mathbf{D}_x \in [0, 1] \tag{6}$$
$$\mathbf{k} \in [5.0 \times 10^{-2}, 5.0 \times 10^{-1}] \tag{7}$$
$$\mathbf{D}_y = 0.10(\mathbf{D}_x) \tag{8}$$



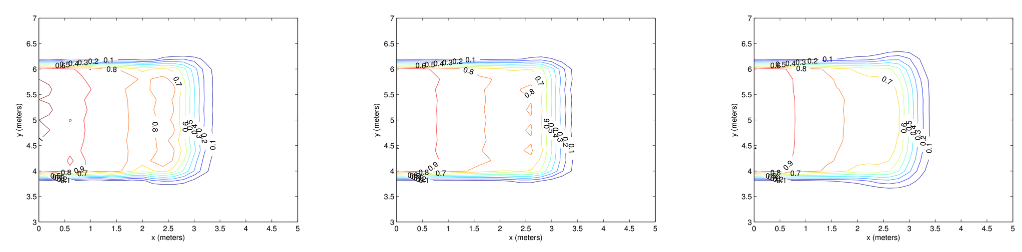
(a) Problem variation (b) Sampled parameter sets

Figure 5: Cross-section view of parameter space



(a) FE (b) FE-SUPG (c) FE-SOLD

Figure 6: Full-order approximations for test case 1



(a) ROM (b) ROM-SUPG (c) ROM-SOLD

Figure 7: ROM approximations for test case 1 (16 basis functions)

Our results demonstrate that we can reproduce the qualitative features of FE, FE-SUPG, or FE-SOLD in a reduced-order approximation in a nonlinear reactive transport setting. Increasing the number of basis functions in the model increases both the accuracy of ROM and the computational cost. ROM offers considerable savings in computational time if the number of basis functions in the model can be kept small.

Table 1: Relative L_2 error of ROM-SUPG, as compared to FE-SUPG

Basis Size	Rel. CPU Time	Test 1	Test 2	Test 3	Test 4	Test 5	Test 6
8	13.9%	0.0799	0.0677	0.0199	0.0871	0.0653	0.1196
16	40.9%	0.0171	0.0129	0.0156	0.1054	0.0602	0.0256
32	146.1%	0.0090	0.0031	0.0079	0.0521	0.0109	0.0118

Continuing Work

- Apply stabilized ROM to a more realistic reactive transport application (bioremediation)
- Explore the use of operator splitting with ROM and SUPG to separate phases and de-couple multispecies problems.

References

1. Bochev, Pavel B., Max D. Gunzburger, and John N. Shadid. "Stability of the SUPG finite element method for transient advection-diffusion problems." *Computer Methods in Applied Mechanics and Engineering* 193.23 (2004): 2301-2323.
2. Gunzburger, Max D., Janet S. Peterson, and John N. Shadid. "Reduced-order modeling of time-dependent PDEs with multiple parameters in the boundary data." *Computer Methods in Applied Mechanics and Engineering* 196.4 (2007): 1030-1047.
3. John, Volker, and Petr Knobloch. "On spurious oscillations at layers diminishing (SOLD) methods for convection-diffusion equations: Part I-A review." *Computer Methods in Applied Mechanics and Engineering* 196.17 (2007): 2197-2215.
4. Figure 1 courtesy of US Geological Survey (*http://pubs.usgs.gov/fs/FS-019-98*).