Model Reduction for Advection-Dominated Nonlinear Reactive Transport

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Abstract: Mathematical modeling of reactive transport is critical to our understanding of the spread of contaminants in underground aquifers. In applications such as parameter estimation, the high number of degrees of freedom necessary to compute the necessary realizations of these models using standard (i.e., finite element, finite difference, finite volume) methods often cause computation to be prohibitively costly. POD-based ROM has been used in a number of application areas to reduce the cost of producing large numbers of realizations of such models. In our previous work, we have shown that POD-based ROM can be successfully applied to contaminant transport systems involving dispersion-dominated transport and linear reaction terms. We continue to explore how POD-based ROM may be applied to more general reactive transport systems.

Groundwater Contamination

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.

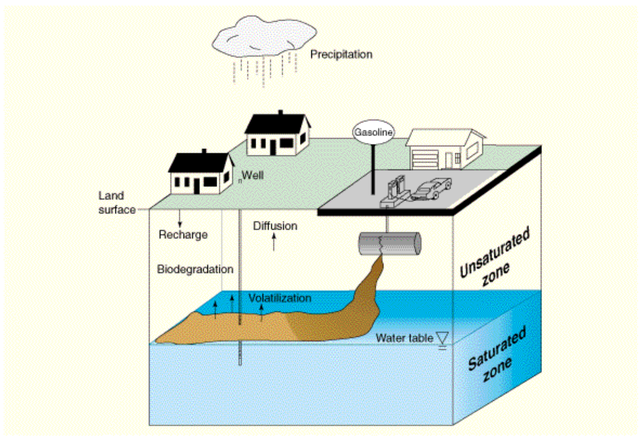


Figure 1. Conceptualization of the fate of petroleum hydrocarbons in a ground-water system.

Mathematically, we can model these processes with the *advection-dispersion-reaction equation*. Transport of solute in a column where water flows through a porous medium can be modeled using the advection-dispersion-reaction equation in one spatial dimension:

$$\frac{\partial C}{\partial t} = \mathbf{D}_x \frac{\partial^2 C}{\partial x^2} - \mathbf{v}_x \frac{\partial C}{\partial x} + \sum \mathbf{R} \qquad x \in [0, L] \quad t > 0 \tag{1}$$

whe $C(x,t)$ is the concentration of the solute species at time t and location x, $\mathbf{v}_x$ is the seepage velocity of the water along the length of the column, and $\mathbf{D}_x$ is the coefficient of hydrodynamic dispersion. $\sum \mathbf{R}$ represents the summation of (typically nonlinear) source/sink terms resulting from chemical reactions involving the solute species. In general, there may be more than one solute species in the system, and a coupled system of nonlinear partial differential equations will be needed to model the system (one governing equation for each species).

Parameter Estimation

If we know the values of $\mathbf{v}_x$, $\mathbf{D}_x$, and parameters in the reaction terms, as well as an appropriate set of boundary and initial conditions for Equation 1, then we can solve the differential equation, e.g. via finite element approximation, to find $C(x,t)$. However, this is usually not the case. Instead, we may have some knowledge of the inputs and outputs observed in a field or laboratory setting and seek values of the model parameters such that the model agrees with the observed data.

Solving this type of problem can easily carry a prohibitively high computational cost. There are a variety of methods to solve such an **inverse problem**, but they all require the computation of many realizations of the forward model. If the solution of the forward model is expensive to compute, that cost is amplified by the large number of realizations required by the parameter estimation process. This motivates us to seek ways to reduce the cost of approximating the forward model.

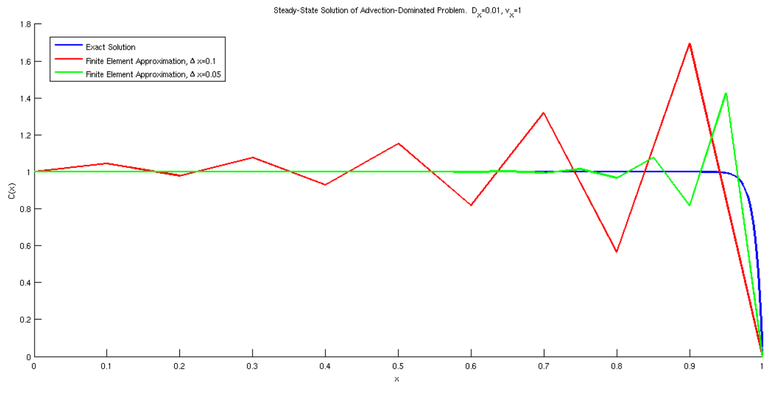
POD-based Model Reduction

In finite element approximation, the number of degrees of freedom is related to the number of nodes in the computational grid, and the resulting system is typically very large. In POD-based ROM, we choose a different set of basis functions. While these functions have global support over the domain, we seek to use a small number of them, so that the system is dense but small. Our procedure is outlined below:

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*, $S = \begin{pmatrix} s_1 & s_2 & \dots & s_m \end{pmatrix}$
3. Compress the information from the columns of S. Here, we use the Singular Value Decomposition to obtain a proper orthogonal decomposition (POD): $S = U\Sigma V^T$
4. Choose the number of basis functions, d_{ROM}, to use in the reduced model. Choose the basis functions for the reduced model to be the functions represented by the first d_{ROM} columns of U.

Diffusion-Dominated Transport

In our previous work, we found that POD-based ROM worked well for advection-dispersion-reaction systems where the chemical reaction terms are linear and transport is dominated by diffusion. In general, however, we must be able to handle a number of nonlinear reaction terms, and cannot guarantee that the system we wish to solve will always be diffusion-dominated. In cases where diffusion is small relative to advection, numerical approximations can become unstable. To illustrate this, consider using the finite element method to solve the steady-state ($\frac{\partial C}{\partial t} = 0$) problem corresponding to Equation 1 with $\mathbf{D}_x = 0.01$, $\mathbf{v}_x = 1.0$, $\sum \mathbf{R} = 0$, $C(0) = 1$, $C(1) = 0$.



Operator Splitting

We may use the technique of *operator splitting*, as described by Ropp and Shadid, 2009, to separate the processes represented in Equation 1.

$$\frac{\partial C^*}{\partial t} = -\mathbf{v}_x \frac{\partial C}{\partial x}, \quad t \in [t^n, t^{n+1}], \quad C^*(t^n) = C^n \tag{2}$$

$$\frac{\partial C^{**}}{\partial t} = \mathbf{D}_x \frac{\partial^2 C}{\partial x^2}, \quad t \in [t^n, t^{n+1}], \quad C^{**}(t^n) = C^*(t^{n+1}) \tag{3}$$

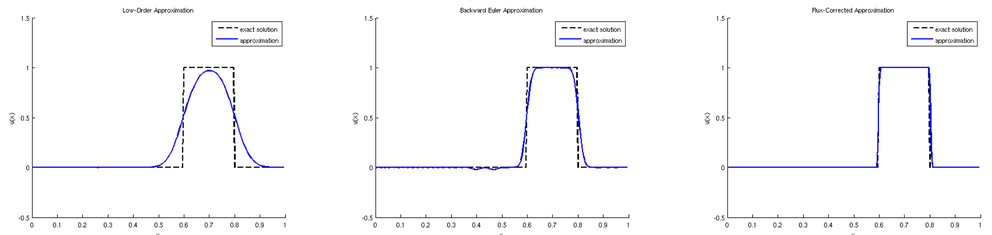
$$\frac{\partial C^{***}}{\partial t} = \sum \mathbf{R}, \quad t \in [t^n, t^{n+1}], \quad C^{***}(t^n) = C^{**}(t^{n+1}) \tag{4}$$

$$C^{n+1} = C^{***}(t^{n+1}) \tag{5}$$

Using this approach allows for each phase of the transport process to be computed using an appropriately selected method. Additionally, we are free to change the order in which the phases are computed. The reaction phase, while nonlinear, can be treated as an initial value problem at each grid node. We are also free to choose a method for the advection phase that maintains a more physically realistic solution.

Flux-Corrected Transport

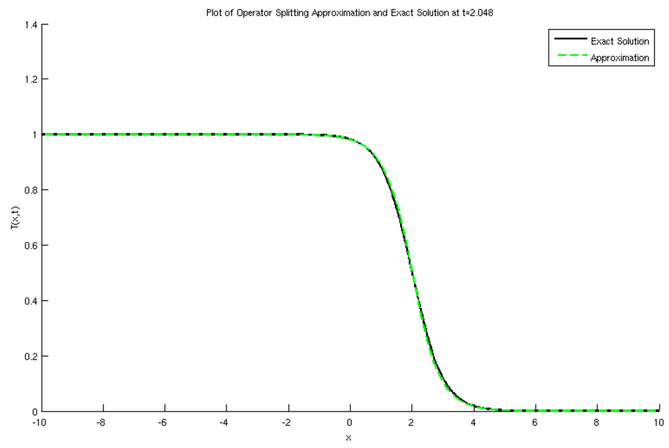
Kuzmin and Turek, 2002, describe application of the Flux Corrected Transport (FCT) method within the context of finite element approximation. FEM-FCT is a method for improving the accuracy of finite element approximations to advective problems. The idea of the method is to consider both a "low-order" approximation, which maintains positivity in the approximation but admits significant diffusion, and a "high-order" approximation, which maintains sharper fronts but may contain oscillations.



The FEM-FCT approximation is obtained by updating the low-order approximation at each node with an anti-diffusive corrective term computed from the high-order approximation and scaled by a flux-limiter chosen at each node.

Example

Let us consider a test problem where $\mathbf{v}_x = \mathbf{D}_x = 1$, $\sum \mathbf{R} = 8C^2(1-C)$, with boundary conditions $C(-\infty, t) = 1$, $C(\infty, t) = 0$. We compare the exact solution with the results of applying operator splitting to separate the phases of the problem, using finite element approximation to solve the diffusion phase and FEM-FCT to solve the advective phase.



Research Goals

Our goal is to ease the computational burden of the parameter estimation process by using ROM to solve more general reactive transport problems.

- Use FEM-FCT and operator splitting to improve the accuracy of snapshots used to construct the reduced model.
- Test the viability of a straightforward application of ROM given these improved snapshots.
- Determine how best to use snapshots and reduced basis in conjunction with operator splitting and FCT, so that we may better handle advection-dominated problems.
- Explore whether the data contained in the reduced basis can be used to ease computation of the reactive phase.

References

- Kuzmin, D., and S. Turek. "Flux correction tools for finite elements." *Journal of Computational Physics* 175.2 (2002): 525-558.
- Ropp, David L., and John N. Shadid. "Stability of operator splitting methods for systems with indefinite operators: advectiondiffusionreaction systems." *Journal of Computational Physics* 228.9 (2009): 3508-3516.
- Figure 1 provided by US Geological Survey.