Reduced Order Modeling of Reactive Transport in a Column

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Background

It is estimated that approximately 93% of the earth's available fresh water supply is stored underground. The fate of solutes that contaminate this source of fresh water are a matter of serious concern.

Computational modeling aids understanding of solute fate in the subsurface environment, where direct observation is difficult or impossible. This modeling of reactive contaminant transport systems can be a computationally demanding task, requiring the computation of many thousands of unknown coefficients at every time step using standard methods (i.e.,finite difference, finite element). This is compounded in settings such as parameter estimation, when a simulation must be repeated many times with parameters that vary in a given range.

We create a reduced order model to approximate the solution of a system of reactive transport equations with a decreased number of unknown coefficients. We show that the reduced model is able to approximate the high-order finite element model.

Problem

Transport of four reactive species through a column 150cm long:

$$\frac{\partial C_1}{\partial t} = \epsilon\frac{\partial^2 C_1}{\partial x^2} - \nu\frac{\partial C_1}{\partial x} - k_1 C_1$$
$$\frac{\partial C_2}{\partial t} = \epsilon\frac{\partial^2 C_2}{\partial x^2} - \nu\frac{\partial C_2}{\partial x} - k_2 C_2 + \alpha_{2,1} C_1$$
$$\frac{\partial C_3}{\partial t} = \epsilon\frac{\partial^2 C_3}{\partial x^2} - \nu\frac{\partial C_3}{\partial x} + \alpha_{3,1} C_1 + \alpha_{3,2} C_2$$
$$\frac{\partial C_4}{\partial t} = \epsilon\frac{\partial^2 C_4}{\partial x^2} - \nu\frac{\partial C_4}{\partial x} + \alpha_{4,1} C_1 + \alpha_{4,2} C_2$$

on the domain

$$0 < x < 150, \qquad t > 0$$

where all boundary and initial conditions are zero with the exception of

$$C_1(0,t) = e^{-5t}$$

Discretization

We use uniform discretization in both the time and space domains, with Δx=0.1cm, Δt=0.01min.

We use a first-order backward difference scheme to discretize the time derivative in the governing equation ($O(\Delta t)$).

For the finite element approximation, we use piecewise-linear polynomials for approximation in space ($O((\Delta x)^2)$ in the L_2 norm).

Parameters

We assign a range for each parameter in the governing system..

Parameter	Meaning	Median Value	Uncertainty	Range
ν	Seepage Velocity	5 cm/min	± 10%	(4.5, 5.5)
ϵ	Dispersion Coefficient	5 cm^2/min	± 99%	(5.0×10^{-2}, 10)
		–Reaction Rates–		
k_1	S_1 Decay	5×10^{-3} min^{-1}	± 50%	(2.5×10^{-3}, 7.5×10^{-3})
k_2	S_2 Decay	4×10^{-3} min^{-1}	± 50%	(2.0×10^{-3}, 6.0×10^{-3})
$\alpha_{2,1}$	$S_1 \rightarrow S_2$	6×10^{-4} min^{-1}	± 50%	(3.0×10^{-4}, 9.0×10^{-4})
$\alpha_{3,1}$	$S_1 \rightarrow S_3$	4×10^{-4} min^{-1}	± 50%	(2.0×10^{-4}, 6.0×10^{-4})
$\alpha_{4,1}$	$S_1 \rightarrow S_4$	3×10^{-4} min^{-1}	± 50%	(1.5×10^{-4}, 4.5×10^{-4})
$\alpha_{3,2}$	$S_2 \rightarrow S_3$	5×10^{-4} min^{-1}	± 50%	(2.5×10^{-4}, 7.5×10^{-4})
$\alpha_{4,2}$	$S_2 \rightarrow S_4$	6×10^{-4} min^{-1}	± 50%	(3.0×10^{-4}, 9.0×10^{-4})

We assume that the parameter values will be uniformly distributed in these ranges.

Reduced Order Model

We begin by computing particular solutions to the problem using the finite element model for several sets of parameters. We call these particular solutions "snapshots," and construct a *snapshot set*, S. S is a matrix where each column is one of these snapshots.

- 10 parameter sets generated by performing a Latin hypercube sampling of the parameter space.

-For each parameter set, the FE model is used to solve the system from t=0 to t=50, and 366 snapshots are written at different values of t.

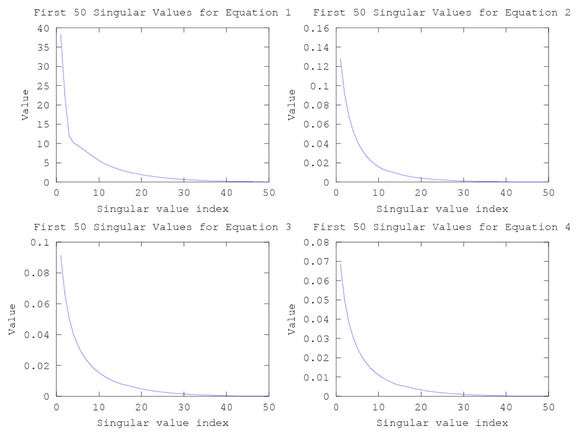
-3660 Total snapshots collected into the snapshot set, S.

We compute the Singular Value Decomposition of S,

$$S = U\Sigma V^T$$

The columns of U form a basis for the columnspace of S in order of decreasing dominance. To construct a reduced model of order *n*, we choose the first *n* columns of U as basis functions in the reduced model. Since these functions have global support, *n* must be small.

Choosing *n*

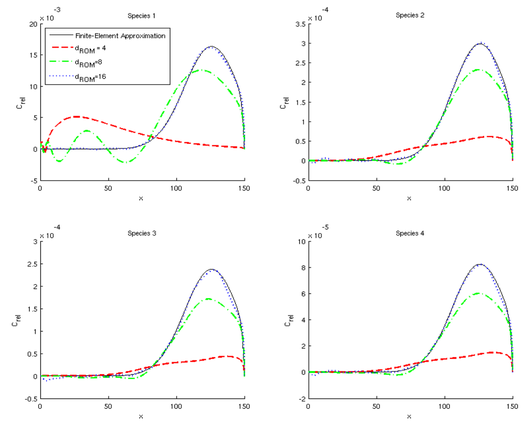


For accuracy, choose *n* after the "elbow" in the singular value curve.

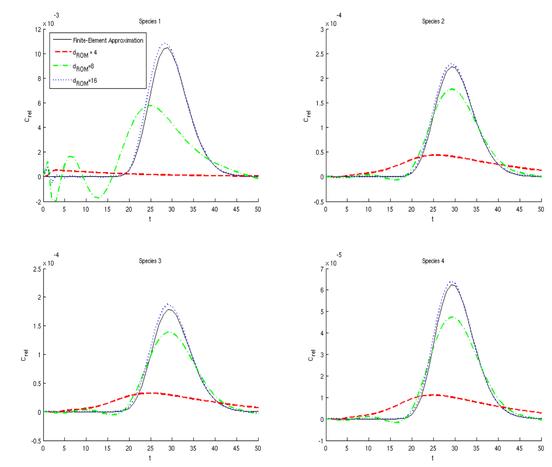
Test Problem

Here we show test results using a randomly selected set of parameters within the specified ranges. Results of the reduced order model with 4,8, and 16 basis vectors with the finite element solution.

Concentration Profile at *t*=20min



Breakthrough Curve (*x*=148cm)



Relative Error in Breakthrough Curve Using 16 Basis Vectors

Equation 1	Equation 2	Equation 3	Equation 4
8.07%	4.08%	6.50%	4.65%

Current and Future Work

-Use higher-order approximating functions.

-Validate results against third-party software.

-Revise problem to include more complex reaction system.

References

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