A Full Multiscale Computational Approach for Groundwater Management Modeling

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Abstract

This paper presents the computational framework of a full multiscale method for solving groundwater management modeling. The management model used in this paper, which was developed in previous work, uses an optimal control algorithm called successive approximation linear quadratic regulator (SALQR) to identify optimal well locations and pumping rates for in-situ bioremediation design. The multiscale method integrates a one-way spatial multiscale approach, a V-cycle multiscale derivative calculation and a local effect derivative calculation. Application of this method starts from a coarsest mesh and solves for the optimal solution at that level, then uses the obtained solution as the initial guess for the finer mesh. While at the finer mesh, the method switches back to the coarser mesh to solve for the derivatives and uses those derivatives to interpolate back to the finer mesh. Only the peak area of the derivatives is solved at the finer mesh, with the flat area of the derivatives obtained by the interpolation. Full results combining these methods will be given at the conference, but initial results presented in this paper indicate great potential for computational savings. The reduction of computing time is about 79% for a case with over 1600 state variables. Much more savings can be expected for larger size problems.

Introduction

Groundwater management modeling can be very computationally challenging. For example, when using Minsker and Shoemaker's SALQR optimal control model (Minsker and Shoemaker, 1998b) to identify an optimal groundwater in-situ bioremediation design, prohibitive computational efforts would be required to model realistic sites with thousands of numerical mesh nodes. Their model defines control variables as pumping rates and state variables as hydraulic heads and concentrations of substrate, oxygen and biomass. The model identifies optimal well locations and pumping rates to minimize pumping costs. As presented by Minsker and Shoemaker (1998a), a substantially finer mesh is required for in situ bioremediation than for traditional pump-and-treat design, due to the nonlinearity and dynamic properties of this remediation strategy. Thus, overcoming this computational bottleneck while still preserving the accuracy of the modeling is a key issue for applying this model to large-scale field sites.

In this paper, a full multiscale computational approach is presented to explore the potential for reducing the computational burden associated with solving this model. By integrating the local effect principle of the derivatives information with the one-way spatial

multiscale methodology developed by Liu et al. (2001, in press) and the numerical derivatives and multiscale derivatives V-cycle calculation methods by Liu and Minsker (2000, submitted), this method is expected to significantly improve the computational efficiency. The full multiscale method starts from the coarsest mesh and proceeds to finer meshes progressively until sufficient accurate solutions are identified. While it is on a finer mesh, it switches back to a coarser mesh to calculate the numerical derivatives, which are then interpolated back to the finer mesh to approximate the derivatives on the finer mesh. A locally finer mesh is used to solve the peak area of the derivatives in order to maintain a satisfied accuracy and reduce the computational effort.

This paper is organized as follows. A brief description of the optimal control model of in-situ bioremediation is presented in the next section. In section three, the full multiscale computational methodology is presented. The results are presented in section four, which discusses the significant improvement by the individual components of this full multiscale computational approach and the potential to further reduce the computing time once it is completely implemented. A brief summary and conclusion is presented in the last section.

Description of the Optimal Control Model

The discrete-time optimal control model of in-situ bioremediation of groundwater can be described as follows (Minsker and Shoemaker, 1998b):

$$\underset{U_1 \ldots U_2}{Min}\ J(U) = \sum_{k=1}^{K} G(X_k, U_k, k) \qquad (1)$$

subject to

$$X_{k+1} = Y(X_k, U_k, k),\ k = 1,\ldots,K \qquad (2)$$

$$L(X_k, U_k, k) \le 0,\ k = 1,\ldots,K \qquad (3)$$

where *J(U)* = the objective function, i.e. the sum of cost functions *G* in each management period k; *K* = the total number of management periods; *U* = the control vector, i.e. the pumping rate; and *X* = the state vector, which includes hydraulic heads and concentrations of the contaminant, oxygen and biomass. Equation 2 is a transition equation, which describes the change in state vector *X* from one management period to the next under the current control policy U. The transition equation is a two-dimensional finite-element contaminant fate and transport simulation model called Bio2D. Equation 3 is a set of constraints that stipulate the water quality standard to be met at the end of the clean-up, the upper and lower bound of the hydraulic heads at each well location, and any other possible conditions required for either state or control variables. When this model is solved using SALQR, these constraints are incorporated into the objective function using a penalty function (see the penalty function description in Minsker and Shoemaker (1998b)).

SALQR is a variant of differential dynamic programming (Yakowitz and Rutherford, 1984) in which the second derivative of the transition equation is assumed to be zero. SALQR consists of two iterative steps: a forward sweep and a backward sweep. An initial guess of the control policy is needed to start the algorithm. The forward sweep runs the simulation model to evaluate the effects of the current pumping rates, and the backward sweep computes derivatives of the objective function and transition equation to find an improved strategy. The algorithm

stops when it converges to the optimal pumping policy. More details on SALQR can be found in the literature (e.g., Culver and Shoemaker, 1992).

Ignoring sparsity considerations, the computational work for solving a SALQR model is proportional to $O(N^3)$ (Liao and Shoemaker, 1991), where N is the total number of state variables. The state variables are defined at the nodes of the finite element mesh within the simulation model, so significant increases in computational effort can be expected when using a fine mesh rather than a coarse mesh.

A Full Multiscale Computational Approach

This section presents the methodology of the full multiscale computational approach. As can be seen from Figure 1, this method starts from the coarsest mesh (Level 1) and solves the model to convergence. Then the converged results are interpolated up to the finer mesh (Level 2), at which the model runs using the converged results from Level 1 as the starting point. At Level 2, when the derivatives are needed at the backward sweep, instead of calculating them directly at the current level, it switches back to the coarser level (Level 1) and obtains the coarse grid derivatives first, and then interpolates back to the current level using a standard bilinear interpolator. An efficient one-sided divided difference method (Liu and Minsker, submitted, 2000) is used to calculate the numerical derivatives so that those derivatives that cannot be interpolated can be calculated separately on the Level 2. However, the derivatives on Level 2 are only calculated within a peak local area, while the smooth area can be approximated using the coarse grid derivatives information. When examining the spatial structure of the first derivatives of the transition equation with respect to the state variables, we found two distinct regions: a peak region and a smooth region. Figure 2 shows an example spatial structure of such derivative information. We call this the "local-effect" of the derivative information, which means that a small perturbation of the value of one state variable can only have significant impact in its surrounding area but will have little effect in remote areas. Note that in order to solve the derivatives at the current level (Level 2) only at the peak area, the boundary conditions must be obtained from the coarse grid derivatives calculation. Once the model converges at Level 2, we can continue to interpolate up to the finer mesh (Level 3) and perform a similar procedure as at Level 2. This process continues until the model reaches the finest level (in Figure 1, the finest level is Level 3) and converges.

An algorithmic description of this method is presented as follows:

(1) For a given problem, set up a hierarchy of meshes where the mesh sizes $h_1 > h_2 > \ldots > h_{L-1} > h_L$, L being the finest level with the desired level of accuracy and 1 being the coarsest level.

(2) Starting from the coarsest level (Level 1), solve the model (both forward and backward sweep) to convergence.

(3) For Level 2 to L
   a. Interpolate the results from Level –1 to Level using a bilinear interpolator
   b. Start with this value to perform a two-level cycle of the V-cycle multiscale derivatives calculation. Solve the peak area of the derivatives at the current Level and interpolate the smooth are from the previous level (i.e., Level –1).

(4) Stop after the convergence at the finest level.

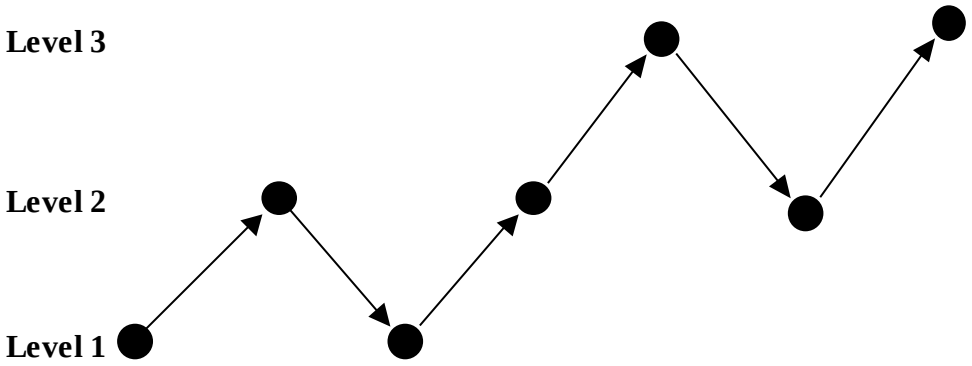

Figure 1. The structure of the full multiscale computational approach for SALQR model

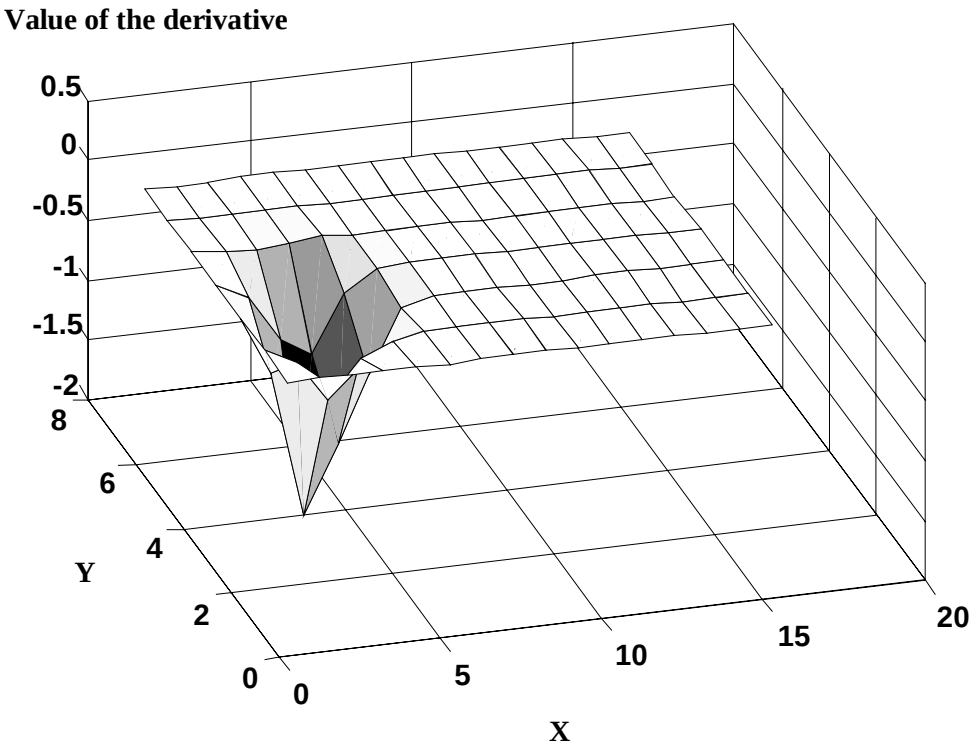

Figure 2. Local spatial structure of an example derivative, showing the first derivative of oxygen concentration at the beginning of management period 2 relative to the biomass concentration at the beginning of management period 1.

The V-cycle multiscale derivatives calculation was presented in Liu and Minsker (2000, submitted) and is part of the full multiscale method. For example, if the model is currently at Level 3, to calculate the derivatives, it has to first switch back to Level 2 and obtain the coarse grid derivatives, and then interpolate the derivatives to Level 3. Incorporating the local-effect of the derivatives information to solve the fine mesh derivatives, however, was introduced in the full multiscale method, which was not used in Liu and Minsker (2000, submitted).

A Comparison Results Analysis

This section presents a comparison of CPU time for the different components of the full multiscale method for a three-level case study presented in Liu and Minsker (2000, submitted). The CPU time was obtained on an SGI/Cray Origin 2000 supercomputer using only one 195MHz processor. Level 3 is the finest level consisting of 1651 state variables, Level 2 is the intermediate one consisting of 441 state variables and Level 1 is the coarsest one with only 124 state variables.

As can be seen from Figure 3, computational efficiency has been improved by using components of the full multiscale method. The CPU time shown is for obtaining converged optimal results at Level 3. A single run on the Level 3 mesh starting from a random initial guess using the original analytical derivatives needs about 117 hours, while a single run on Level 3 with the numerical derivatives method required only 37.8 hours. Using our one-way spatial multiscale approach with analytical derivatives, however, about 54.5 hours are needed to get satisfactory results at Level 3. When applying the one-way spatial multiscale approach with numerical derivatives method, only about 24 hours are needed. The total computing time for using V-cycle multiscale numerical derivatives is about 27 hours. The V-cycle multiscale method is not applicable to the analytical derivatives method because, in the analytical derivatives method, all the derivatives are coupled and solved simultaneously (see discussion in Liu and Minsker (2000, submitted)). We are expecting more computing time reduction once the full multiscale method is implemented and these methods are combined.

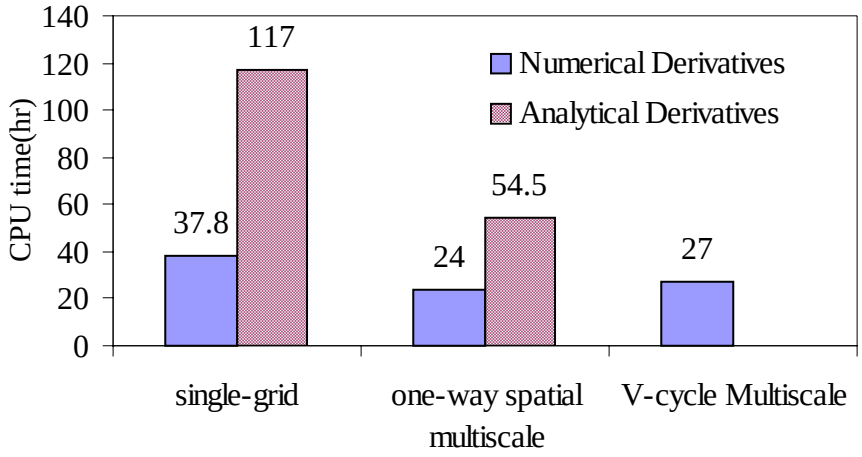

Figure 3. Comparison of CPU time used for obtaining optimal results at Level 3 using different methods

Conclusion

We described a full multiscale method for an optimal control model of groundwater in-situ bioremediation. This method integrates the one-way spatial multiscale method, V-cycle multiscale numerical derivatives calculation and the local-effect principle of the derivative information. Initial results indicate substantial promise for reducing computational effort, with over 79% reduction in CPU time from combining two of the components of the full multiscale method (i.e., using the one-way spatial multiscale method with numerical derivatives), comparing to the original single-grid analytical derivatives method. Higher percentage reduction in computing time should be expected when the number of state variables increases because the computing time was reduced by almost an order of magnitude with respect to the number of state variables, as shown in Liu and Minsker (submitted, 2000). Research is ongoing to complete implementation of the method and results will be present at the conference.

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