Use of Advanced Computing in Tomographic Surveys

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Abstract. We adopt parallel computing and adaptive mesh refinement in a class of iterative inverse solution strategies for tomographic surveys. Due to the algorithmic structure of these inverse solvers, a combination of data parallelism and task parallelism is best suited. Targeting clusters of multicore processor chips, it also justifies to use a mixture of message passing and threads. Moreover, adaptive mesh refinement is used to capture dynamic features and reduce the overall computing effort. Applications in characterizing subsurface hydraulic properties will be presented.

Key words: Tomographic surveys, parallel computing, adaptive mesh refinement, inverse problems, PDEs.

1 Introduction

Accurate modeling of groundwater resources relies on high-resolution characterization of hydraulic properties, which typically have heterogeneous spatial distributions in the subsurface. Such detailed knowledge of hydraulic properties is also important for predicting subsurface contaminant transport. A "see-through" capability into the subsurface is therefore highly desirable. This can be achieved by so-called *tomographic surveys* [5], e.g., hydraulic tomography [2, 6, 4, 1, 10], partitioning tracer tomography [9, 8], and electrical resistivity tomography [7, 3].

The common feature of different tomographic surveys is the use of a set of excitation-response tests, which are (almost) non-invasive, to indirectly characterize the subsurface hydraulic properties. Mathematically, tomographic surveys are equivalent to solving an inverse problem with the subsurface hydraulic properties as the solution objective. The underlying mathematical model for a tomographic survey consists of one or several partial differential equations (PDEs), which employ the unknown subsurface hydraulic properties as the coefficients. The excitations are incorporated as source terms or initial/boundary conditions, while the corresponding responses are measured at a number of observation locations. It is typically by an iterative process that the approximated subsurface hydraulic properties are gradually improved, together with some statistical analyses of the approximation.

Numerical solution of PDE-based inverse problems is often time-consuming, due to the large amount of computations involved. In addition, the quest for high resolution results in a large number of degrees of freedom in the solution. Therefore, efficient numerical strategies for tomographic surveys must rely on advanced computing. Two major ingredients of advanced computing are parallel computing and adaptive mesh refinement. The motivation is obvious. Use of multiple processors/cores aims at larger and/or faster computations. Use of localized fine mesh resolution in strategically chosen areas, instead of uniform resolution everywhere, may improve the overall computation efficiency. The present paper is thus concerned with applying parallel computing and adaptive mesh refinement to tomographic surveys.

2 Some Commonly Used PDEs in Tomographic Surveys

We list here a number of commonly used PDEs in tomographic surveys. These will serve as the basis for discussions in the following sections.

Let us denote by $K(\mathbf{x})$ the hydraulic conductivity and $H(\mathbf{x})$ the total hydraulic head (that is measurable at certain locations). The simplest PDE in the context of hydraulic tomography is the following steady-state flow equation:

$$\nabla \cdot [K\,\nabla H] + Q = 0, \tag{1}$$

where Q denotes a source term, e.g., the pumping rate at a specific location. It can be mentioned that the main PDE in electrical resistivity tomography has the same form as (1).

Considering time dependency, (1) can be extended as follows:

$$S_s \frac{\partial H}{\partial t} = \nabla \cdot [K \nabla H] + Q. \tag{2}$$

Here, $H(\mathbf{x}, t)$ is assumed to depend on both time and space, and $S_s(\mathbf{x})$ denotes the specific storage.

In connection with partitioning tracer tomography, the basic assumption is that there exists a steady flow field, in form of a Darcy flux,

$$\mathbf{q} = -K \nabla H,$$

where H typically arises from solving (1) for some approximation of the hydraulic conductivity field K. A pumping test of partitioning tracer tomography injects an impulse of partitioning tracers as a source term in the following transport equation:

$$\frac{\partial}{\partial t}\left(\theta_w c + K_n \theta_n c\right) = -\nabla \cdot (\mathbf{q} c) + \nabla \cdot (\theta_w \mathbf{D} \nabla c), \tag{3}$$

where c denotes the tracer concentration, θ_w denotes the volumetric water content, K_n denotes the partitioning coefficient, θ_n denotes the volumetric content of a non-aqueous phase liquid, and $\mathbf{D}$ denotes a prescribed dispersion tensor field.

3 Parallelism in Tomographic Computations

We will restrict our attention to a general class of iterative inverse solution strategies, where the solution objective (such as $K(\mathbf{x})$, $S_s(\mathbf{x})$, $\theta_w(\mathbf{x})$, $\theta_n(\mathbf{x})$) is approximated gradually. Such strategies need to repeatedly solve the main PDE, i.e., (1) or (2) for the case of hydraulic tomography, and similarly, electrical resistivity tomography. In the case of partitioning tracer tomography, (3) also needs to be repeatedly solved in addition to (1). Therefore, the speed of solving (1), (2) and (3) is essential, and thereby the need for parallel computing.

In connection with numerically solving (1), (2) and (3), parallelism can arise from a data parallel perspective, meaning that each processor or core can be assigned with a portion of the data arrays, thus a portion of the entire work load. Data partitioning via domain decomposition is explicitly needed on distributed-memory systems, whereas on shared-memory systems (such as a multicore processor chip) data partitioning can be more flexible. Collaboration between the different processors or cores is typically enabled by MPI calls or thread-based commands. On a cluster of multicore chips, a sensible choice is to use MPI for inter-chip communication and thread-based parallelism within each chip.

Another important part of computation of the iterative inverse solution strategies is solving adjoint state equations of (1) and (2). The adjoint equations have the same form of (1) and (2), and need to be solved for each measurement location (combined with each measurement time level). These adjoint state equations can be solved independently, therefore giving rise to task parallelism. In the case of a large number of available processors, in comparison with the number of measurements, some form of data parallelism must also be adopted for solving each adjoint state equation. This means that several processors or cores should work together to solve one adjoint state equation. Collaboration between these processors or cores is either message passing based or thread based.

4 Adaptive Mesh Refinement

Adaptive mesh refinement is particularly useful in connection with solving (3). This is because this PDE is often convection dominated, making it important to follow the propagation of the sharp fronts of the concentration $c(\mathbf{x}, t)$. Locally refined mesh resolution is therefore only needed in the vicinity of the sharp fronts, and the fine resolution should be able to dynamically follow the propagation of the fronts. A simple mesh refinement strategy for each time step is as follows. First, the temporally discretized form of (3) is solved on a coarse uniform mesh. Then, the intermediate c^* solution from the coarse mesh is used to indicate where the adaptive mesh refinement should be carried out. More specifically, the larger the gradient of c^*, the more need for local mesh refinement. Thereafter, the computation of c is re-done on the locally refined mesh.

5 Concluding Remarks

Parallel computing and adaptive mesh refinement have already demonstrated great success in many types of PDE-related computations. However, the use of these two ingredients of advanced computing in tomographic surveys is so far rather limited. The advantages will be shown in the upcoming full version of the present paper.

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