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GRAND CHALLENGE PROBLEMS IN ENVIRONMENTAL MODELING AND REMEDIATION: GROUNDWATER CONTAMINANT TRANSPORT

PARTNERSHIP IN COMPUTATIONAL SCIENCES CONSORTIUM

FINAL PROJECT REPORT 1998 FOR THE CENTER FOR SUBSURFACE MODELING

Todd Arbogast, Steve Bryant, Clint N. Dawson, and Mary F. Wheeler

Center for Subsurface Modeling
Texas Institute for Computational and Applied Mathematics
The University of Texas at Austin
Austin, Texas 78712

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1 Introduction

This report describes briefly the work of the Center for Subsurface Modeling (CSM) of The University of Texas at Austin (and Rice University prior to September 1995) on the Partnership in Computational Sciences Consortium (PICS) project entitled Grand Challenge Problems in Environmental Modeling and Remediation: Groundwater Contaminant Transport. This project was funded by the U.S. Department of Energy (DOE) under contract No. DE-AC05-96OR22464 (and earlier contracts), and administered through the Center for Computational Sciences, Bldg 4500N, MS 6203, Oak Ridge National Laboratory, Oak Ridge, TN 37831. Other participants and work was performed by Texas A&M University (Richard E. Ewing and Michael S. Pilant), Oak Ridge National Laboratory (ORNL–Kenneth Kliewer), Brookhaven National Laboratory (BNL–Ronald F. Peierls and Joseph E. Pasciak), the University of South Carolina (Robert C. Sharpley), Princeton University (Michael A. Celia), and SUNY Stony Brook (James Glimm and Brent Lindquist). The entire project is described in the full report; this report describes only the CSM contribution.

2 Deliverables

- Parssim1: The Parallel Subsurface Simulator, Single Phase. Single-phase flow, multicomponent transport, and multi-phase geochemistry, including a full complement of homogeneous and heterogeneous reactions (complexation, adsorption, ion-exchange, precipitation/dissolution, biological Monod, and radionuclide) of both equilibrium and kinetic type.
  (*http://www.ticam.utexas.edu/Groups/SubSurfMod/software.html*)
- Eye: 3D visualization tool.
  (*http://www.ticam.utexas.edu/Groups/SubSurfMod/software.html*)

3 The University of Texas

Activities at The University of Texas at Austin were centered within the Center for Subsurface Modeling (CSM) of the Texas Institute for Computational and Applied Mathematics (TICAM). The following members were involved in the project from The University of Texas at Austin and, prior to September of 1995, at Rice University. Faculty members were Mary F. Wheeler (Director of CSM), Todd Arbogast, Clint N. Dawson, and Joseph Warren. Research scientists and post doctoral researchers include Steve Bryant, Frederic d'Hennezel, Philip T. Keenan, Robert McLay, Douglas Moore, and Ivan Yotov. Graduate students include Ashokkumar Chilakapati, Lawrence C. Cowsar, Joseph Eaton, Fredrik Saaf, Carol San Soucie (Woodward), and Ivan Yotov.

These researchers, their work, the development of software connected with this project, and their publications and professional presentations were supported only in part by the U.S. Department of Energy (DOE) through the Partnership in Computational Science (PICS) Grand Challenge Program administered through the Center for Computational Sciences at the Oak Ridge National Laboratory. Support came also from other grants from the DOE, the U.S. National Science Foundation, and the State of Texas Governor's Energy Office.

3.1 The Parssim1 and GCT simulators

Parssim1 [UT–TR7] is a simulator written by CSM to develop and test algorithms and software needed for the PICS Groundwater Contaminant Transport (GCT) simulator. We first describe Parssim1, the Parallel Subsurface Simulator, Single Phase. Parssim1 is an aquifer or reservoir simulator for the incompressible, single phase flow and reactive transport of subsurface fluids through a heterogeneous porous medium of somewhat irregular geometry. It is also capable of simulating the decay of radioactive tracers or contaminants in the subsurface, linear adsorption, wells, and bioremediation [UT–O3, UT–O5, UT3, UT8, UT–O17, UT–O19].

Although the code uses very simple rectangular data structures for efficiency and accuracy, the subsurface domain can be of irregular geometry. The subsurface domain is assumed to be described by a logically rectangular grid. A mapping technique is used to map the irregular, physical domain (with its hills, valleys, internal faults and strata, etc.) to the rectangular, computational domain, without loss of accuracy or efficiency.

The code can run in serial on a single processor, or on a massively parallel, distributed memory computer or collection of computers (using MPI or PVM). The code is portable, and has been run to date on several large parallel machines (Intel Paragon, IBM SP2, and Cray T3E) and on various serial machines (Sun Sparc2, IBM RS6000, and SGI Octane). Computational results indicate that the code has very good parallel scaling properties. We use *domain decomposition* to compute in parallel. The grid is divided into subdomains, one for each parallel processor. Each subdomain is given roughly the same number of cells. Each processor is responsible for the simulation only in its subdomain. The individual processors send information to each other during the computation.

The flow, advection, diffusion/dispersion, and geochemistry subproblems are solved independently using a time splitting technique [2, 3]. Thus, the code is very modular, and consists of the four main parts: *driver*, *flow*, *transport*, and *chemistry*. The driver routines are responsible for the user interface (input and output) as well as managing the coupling between the flow and transport routines. Chemistry is called from within the transport routines.

Flow is simulated with a package called *Parcel* [UT–TR4] It allows for the simulation of incompressible, single-phase, saturated flow with wells on geometrically general domains (but logically rectangular), and it uses a locally conservative, cell-centered finite difference scheme.

The transport routine *ParTrans* allows the simulation of multiphase transport with linear sorption, radionuclide decay, simple (specialized) chemical reactions, and wells on general geometry. Transport is simulated using a locally conservative method of characteristics called the Characteristics-Mixed Finite Element Method (CMM) or a Godunov Method.

The general chemistry routine handles both equilibrium and kinetic reactions. For equilibrium reactions, it uses an interior-point algorithm for the minimization of the Gibbs free energy, and is therefore relatively robust, even when mineral phases precipitate into existence or dissolve away.

We now describe the GCT simulator. Similar to Parssim1, the GCT simulator consists of four main parts: *driver*, *flow*, *transport*, and *chemistry*. The transport and chemistry routines are essentially identical to those found in Parssim1. The driver routines are very similar and use much of the same software as found in Parssim1. Only the flow routines

are significantly different in GCT. These are the result of the Texas A&M, University of South Carolina, BNL, and Princeton efforts, as described elsewhere. Because of the time splitting approach used, the flow routines in Parssim1 can be relatively easily replaced by the PICS flow routines to form GCT, although substantial changes to the driver routine to accommodate new input and data structures are also required. It should be noted, however, that the most advanced state of development (and debugging) of the driver, transport, and chemistry routines appears only in Parssim1; earlier versions were incorporated in GCT.

3.1.1 Algorithm and Software Development for Flow

The Parcel flow package [UT–TR4] was developed at CSM primarily independently of PICS as a solver for second order elliptic partial differential equations. It uses an efficient domain decomposition solution procedure that scales nearly linearly in parallel, the Glowinski-Wheeler [5] domain decomposition procedure. This involves solving an interface problem [UT5, UT–O8]. The subdomain linear system is solved directly.

Parcel was interfaced to Parssim1 through routines that set up the physical problem of incompressible saturated flow with various types of boundary conditions and wells. This simple flow situation allowed for more rapid development of the other routines.

A locally mass conservative, logically rectangular cell-centered finite difference procedure, developed primarily through the PICS project, is used to discretize the equations. This method is based on the expanded mixed finite element method, handles tensor permeabilities accurately [UT10], and extends to non-rectangular geometry by a preprocessing of the coefficients by a mapping technique [UT13] (see also [UT–O6, UT–O9, UT–O10, UT–O13, UT–O18]). The efficiency of rectangular cell-centered finite differences is maintained. The finite difference stencil is a compact, 19-point stencil in three dimensions (the $3 \times 3 \times 3$ cube less the 6 corners). The compactness of the stencil makes the technique efficient in parallel applications. It was shown rigorously that the discrete solution to the scheme converges at the optimal rate to the true solution to the differential equations; moreover, at nodal points, there is superconvergence of the pressure and, on smooth grids, also of the mass flux. This extra accuracy in the flux between grid cells is important for subsurface flow, since the mass flux is of primary interest in transport problems. Similar results were obtained for triangular and tetrahedral meshes [UT–O4, UT13].

At the close of the project, extensions to multi-block domains were being pursued (though not primarily by the PICS effort). These are grids formed by partitioning the domain into large "blocks," and imposing a grid independently on each block. Since the grids may not match across the interface, special care must be taken there. In one approach, a discrete "mortar" space is defined on an interface grid to impose conservation of mass and continuity of pressure [UT–O11, UT–O16, UT15, UT7]. In a second approach, these are obtained by the imposition of opposing Robin type interface boundary conditions [UT11]. Theoretical error analysis and numerical testing show that the schemes are optimally convergent.

Work was begun on an operator based upscaling technique to better handle subgrid effects, such as heterogeneities in the permeability and the exact size and location of wells. The technique is efficient and shows promise [UT–O21].

3.1.2 Algorithm and Software Development for Transport

Three options can be selected for the solution of the advection subproblem.

Characteristics-Mixed Method (CMM). An explicit characteristics method, a type of Eulerian-Lagrangian or ELLAM method, called the Characteristics-Mixed Method, was developed, numerically analyzed, and implemented [UT-01, UT4]. Mass is advected in time by a backward difference approximation. Not merely points, but entire grid cells are tracked backward along the characteristics (i.e., streamlines), and the mass from the previous time level in this region is given to the grid cell at the current time level. A postprocessing of the previous mass distribution achieves theoretically and numerically increased accuracy. The scheme has minimal numerical dispersion and is theoretically locally conservative. No CFL time step constraint is imposed (other than that related to the domain decomposition), so relatively large time-steps can be taken.

The code scales nearly linearly in parallel [UT-TR1]; however, the method suffers from numerical mass and/or volume imbalances in implementation. It is also relatively computationally expensive.

Since adsorption processes change the characteristic speed of some chemical species, when reactive transport is simulated, it may be advantageous to take relatively small time steps. This prevents inaccurate approximation of time during which species are in contact and can therefore react. Thus, we implemented the other two advection options below.

Higher Order Godunov Method (HOG). An explicit, formally second order Godunov method was added to Parssim1 for advection [1]. A postprocessing step improves the order of accuracy (except near sharp fronts or shocks). The scheme has a CFL time step constraint, so relatively small time-steps must be taken. The scheme has very little numerical dispersion, and is locally mass and volume conservative. Each time step, though small, is computationally relatively inexpensive.

A direct comparison of the two advection schemes was performed on a test case related to the Oak Ridge site. In this case flow is down a hillside toward a pit where strontium was stored. We simulated flow of a tracer for 40 days using a two-dimensional 40×40 grid and compared solutions generated by the HOG and characteristic methods in the absence of dispersion. The results were very similar. The characteristic method exhibited slightly less numerical diffusion. In this run the time step for the characteristic method was 6 times larger than a CFL constraint would allow, but the higher-order Godunov method was much faster per time-step. Thus the overall run time for the HOG method was less than that required for the characteristic method.

First Order Godunov Method (FOG). The higher order Godunov Method can be used without the postprocessing step, resulting in the first order Godunov method for advection.

Diffusion/Dispersion. This subproblem is solved by the cell-centered finite difference technique used for the flow problem, as described above. Note that Dispersion must be represented as a tensor, with (generally) greater longitudinal mixing in the direction of flow as opposed to the transverse directions. A simple Jacobi preconditioned conjugate gradient technique is sufficient to solve the resulting linear system.

Nonlinear Sorption. Studies and numerical computations on especially the long time limit profiles of nonlinear sorptive pulses was performed [UT1, UT2, UT6, UT9, UT12,

UT-O7, UT-O12]. These studies showed that the underlying algorithms for transport and nonlinear sorption were accurate, although Parssim1 uses somewhat different numerical techniques for sorption: either simple linear adsorption or sorption computed in the geochemistry routines as a phase change.

3.1.3 Algorithm and Software Development for Geochemistry

After gaining experience with bioremediation modeling [UT3, UT-O2, UT-O3, UT-O5], CSM developed and tested a geochemical reaction simulator [UT-O15, UT-TR6, UT-O20]. The local governing equations for the geochemical system are a mixture of differential and algebraic equations, including elemental mass balance equations. Discretizing the differential/algebraic system implicitly in time, which is necessary to correctly couple reactions and minimize time step restrictions, results in a system of nonlinear equations. This system can be difficult to solve numerically. One reason is that the species concentrations and rate parameters can differ by many orders of magnitude. Another is the physical requirement that species concentrations be nonnegative. The non-differentiable character of the equilibria for precipitation-dissolution reactions adds a particular complication: the possibility that a mineral can be present imposes an inequality constraint on the species concentrations, which becomes an equality only when the mineral is actually present. To handle such constraints requires iterations through different combinations of minerals. This iteration introduces a variety of problems regarding convergence, efficiency, robustness and stability.

As a first attempt at modeling geochemistry, we obtained the batch chemistry simulator KEMOD from George Yeh at Penn State University [6] and incorporated it into our transport module. In order to improve the robustness of the KEMOD routine, several enhancements were made. We incorporated a global Newton line-search procedure, and introduced variable scalings/transformations to handle the differences in magnitude between concentrations and rate parameters. We also investigated alternative strategies for selecting correct mineral assemblage, and modified the stopping criteria. These modifications have made the code more robust, but they are not sufficient for all the cases under consideration; in particular, precipitation/dissolution reactions are still problematic.

As an attempt to create a more robust and rigorous procedure, we recast the batch calculation as a free energy minimization problem and developed the new simulator. This approach is often used in calculating phase partitioning in multi-phase flow simulation. The result of this formulation is the minimization of an energy functional, subject to elemental mass balance equations and inequality constraints (concentrations are nonnegative). For solving this system we use of an interior-point algorithm, developed by Richard Tapia *et al.*, at Rice University [4, UT-O14, UT-TR5]. Calculations for simplified aqueous chemistry showed improved robustness over the modified KEMOD routine.

Work was begun on load balancing the geochemistry work in parallel. In a typical subsurface problem, reaction fronts travel through the domain. These fronts are associated with increased computational effort, and therefore require a different distribution of work than for the flow and transport, which is divided evenly by a domain decomposition that assigns an equal number of grid cells to each processor. Initial results show dramatic improvements after load balancing the reaction computations [UT-O22].

3.1.4 Documentation and User Interface Software Development

A complete, fully indexed user's manual was developed for Parssim1 [UT-TR7]. The manual describes briefly the code's capabilities and algorithms, and then provides a detailed discussion of the input and output files.

The user interface to Parssim1 allows a reasonable amount of flexibility without making the code difficult to use. It is not required that the advanced features be used to run the code. Parallelism is entirely transparent to the user.

Information is provided item-by-item in a free format style (items are separated by any number and combination of space, tab, and carriage return, as well as comma, semicolon, and colon). Comments are allowed after the pound sign. Thus, data can be set up by the user in a meaningful way. The input can be divided by the user into separate files if that is convenient, say either to separate grid information from species information from algorithm parameters, etc., or to place large data sets in separate data files. Errors in the input file(s) are identified by type of error and file and line number of occurrence, so that problem specification input errors can be reliably and rapidly corrected.

Physical units can be given inconsistently. The user interface allows for automatic units conversion and checking. Thus one gram per cc can be given in cgs units as "1" or as "1[g/cc]." The latter is one gram per cc in whatever system of units is used, and the quantity given this value must require the physical units of mass per volume (or an error will be flagged). See the manual for a complete description of capabilities.

Parssim1 was connected to the Waterways Experiment Station's GMS front-end at ORNL and used successfully. Parssim1 was also successfully connected to the pv3 package to allow interactive visualization of data in parallel.

3.1.5 A Scripting Language for GCT

An input specification "scripting language" was developed to enable PICS to unify the input specification to the GCT code. This scripting language was based loosely on the "kScript" language of Phil Keenan [UT-TR3]. This new input specification allows the user to specify input data in a uniform manner, it will allow us to add features to the code without making older data sets obsolete, and it will eventually allow us to add code to perform text-based, interactive simulation. In the first phase of this project, a preprocessor was under development at BNL to translate the new input script into the old data files, so no interactivity is yet possible.

All data can be entered into GCT through data files prepared using the preprocessor by issuing commands scripted in this highly flexible, free format style scripting language. The input script can be given interactively from the keyboard, it can be prepared ahead of time and read directly from one or more input files, or it can be given in a combination of these two ways. Most data items have a default value, so generally only a small amount of data needs to be explicitly given to run the code successfully.

The input script consists of a series of commands, each describing some action to be taken. A single command may span multiple lines, and multiple commands may be on the same line. A command has a command name and optionally one or more arguments. An argument may be a subcommand name, the name of a data item (such as a variable, array,

or function), or the data itself.

The name of a data item is also the name of a command to set it to a value. The value can be specified as an arithmetical expression of numbers and/or other variable names. For example "2*cm" can be used to declare a length of 2 cm (provided that the unit "cm" has been defined appropriately). Thus, among other things, the language explicitly allows easy units conversion.

A command can be repeated with different arguments. For example, the user can prepare a script file with a different set of defaults than are provided automatically, read these defaults, and then modify them for the case at hand. The latest instance of the command overrides the effects of all former instances.

Prototypes of this system were developed; however, this work on a scripting language for GCT was not completed by the end of the PICS project.

3.2 The Eye Visualization Tool

Eye [UT-TR2] is a interactive viewer for polyhedral data. The polyhedral data is produced by tools that processes some form of scientific data and produce polygons from it. Currently available tools include iso-contour generators, cross-section generators, and steady-state flow-line generators for data arranged topologically as cubic grids. Eye is aware of these tools, and the user can invoke them from within Eye. Other tools can be built and integrated easily into Eye as needed, such as tools for producing iso-surfaces from scattered points, or tools for generating time-varying flow lines.

Eye displays three-dimensional data projected onto a flat screen; however, it actually represents data in up to five dimensions. The data that Eye receives actually consists of a collection of simplices (points, segments, triangles, tetrahedra, ...), with each vertex of the simplex a tuple of data. Conventionally, these tuples are displayed as the x-, y- and z-coordinates of a point, its time, and its value. The z-coordinate is projected away according to where the user places his "eye" with respect to the object viewed. The time coordinate is intersected away according to where the user sets a clock. The value coordinate is mapped onto a color spectrum.

The geometric data that Eye receives can be viewed as filled-in flat-shaded polygons, as a wire-frame model, or as a point cloud. The geometry can be viewed from arbitrary orientations, with lighting from several directions and with parts clipped away to reveal the most relevant parts. The figure can be moved across the screen, distorted to increase or lessen the apparent depth of the figure, or repainted to reflect a shift or stretch in the value dimension.

Eye is designed for portability; with appropriate configuration, Eye can be installed on any workstation that supports version 4 or higher of the X Window System, release 11, and provides a C++ compiler. Versions that exploit specialized graphics libraries and hardware for better performance are under development. Eye can display its images on paper as well; it can generated encapsulated Post-Script for an image in a format compatible with the Idraw program distributed with the freely available InterViews user-interface library. Thus, it produces pictures that can be rearranged manually for better presentation.

Eye presents a graphical interface with three main components: the menu-bar across the top-left, the gadgets on the right, and the viewport that dominates the application window.

The viewport is the region where the object being viewed is displayed. An optional bounding box about the object provides information on the current object position.

3.3 Model Applications

The following applications of Parssim1 have been performed to date. These applications were only partially supported by PICS, but they represent application of the codes supported by PICS.

3.3.1 Benchmark Problems

At the PNNL-hosted Workshop on Subsurface Reactive Transport (29 Oct. to 1 Nov., 1997) a set of benchmark problems were set up in order for the invited participants to compare reactive transport codes. Parssim1 functioned very well on these tests. Examples included a flow in a 2D parabolic velocity field with a conservative tracer, providing a rigorous test of the ability of a code to control numerical dispersion. The method of characteristics option in Parssim1 handled this problem very well, while the higher-order Godunov scheme exhibited larger dispersion. The test problem was particularly well suited to particle tracking transport schemes. Extensions of the test problem to simple kinetics were also handled well by Parssim1, and it should be noted that general chemical reactions of the sort incorporated in Parssim1 are difficult to implement in particle tracking schemes.

Another benchmark involved the transport of mixed waste (heavy metal cations with organic ligands) through a 1D medium. The complex chemistry included rate limited sorption and biodegradation, as well as complexation. Parssim1 replicated the benchmark results. The extension to very fast kinetic reactions introduced some minor numerical difficulties; converting the fast kinetics to equilibrium reactions gave essentially the same concentration profiles without the numerical problems.

A particularly instructive benchmark involved the speciation of a redox-sensitive solution with pyrite. This proved to be an extremely rigorous test of the mass balance of any code. As a matter of fact we were able to demonstrate discrepancies in the reported solutions to the problem.

Another benchmark involved the migration of a square concentration wave in a 2D domain. The flow field was transverse to the coordinate axes, again giving a severe test of a code's capability to avoid numerical dispersion. The method of characteristics scheme preserved the square wave well, though it was costly to compute. The higher-order Godunov scheme exhibited some dispersion but did run more rapidly.

3.3.2 Site Characterization

Partitioning tracers are a novel technology for locating NAPLs in the subsurface and assessing their saturations. This approach offers significant cost advantages over other characterization technologies, but it requires very powerful forward simulation models in order for the inversion problem to be feasible. The general chemistry capabilities in Parssim1 make this forward modeling straightforward. We have carried out several test cases with multiple wells, heterogeneous rock properties and heterogeneous distributions of NAPL phase. These

clearly demonstrate the different velocities of conservative and partitioning tracers in the presence of the NAPL phase.

3.3.3 Radionuclide migration

One of the most intriguing applications of Parssim1 has been the investigation of radionuclide migration on the Oak Ridge Reservation [UT14]. Waste pits and trenches on the Reservation were filled with low-level radioactive waste during the Manhattan Project. The pH of the waste was increased in order to promote precipitation of radioactive cations as hydroxyl salts. Simulation of transport of this high pH waste showed remarkable behavior in form of a pulse of radionuclide moving at approximately tracer velocity. This result is completely unexpected from classical chromatography theory, but it has been verified independently by numerical means. More importantly, the prediction explains the field observation of rapid radionuclide movement. An investigation of the underlying mathematics of this mode of propagation continues, as well as further simulation of the field situation.

3.3.4 Pump-and-treat Remediation Simulation

The mixed-waste (heavy metal plus organics) benchmark problem described above was extended to provide an example of a pump-and-treat remediation strategy. A waste source was imposed for 500 days in a small region of the recharge zone of an aquifer, in which an east-to-west flow field prevailed. The aquifer was highly heterogeneous in permeability, but its sorption properties were assumed constant with position. Three wells were turned on in a region downstream of the contaminant plume after 1250 days of simulated time. This 3D simulation showed the importance of correctly scaling up laboratory derived conditions. The naturally occurring microbe population decreased very rapidly in this simulation, indicating that the microbe death rate kinetics used in the lab scale benchmark problem would give a much more optimistic prediction of natural attenuation in the lab than would be obtained in the field.

3.3.5 Well Stimulation

The stimulation of wells with acid is an important application of reactive flow. Such treatments are carried out in thousands of oil and gas wells annually, as well as in many injection wells operated by waste disposal companies. When concentrated hydrofluoric and hydrochloric acids contact sedimentary rocks, a large suite of dissolution reactions occurs at a wide range of rates. High concentrations of mineral ions are generated, making many precipitation reactions possible, along with several important secondary dissolution reactions. Overlaying this chemical complexity is the near-wellbore flow field. Previous studies of acid stimulation usually assume a radial flow field, but this assumption can greatly oversimplify local variations due to the geometry of perforations and the distribution of permeability. The competition between advection and reaction is critical for determining local extents of reaction, and so variations at this scale can be important. The rock itself is mineralogically heterogeneous, further complicating the problem. Thus the question of what is the optimum design for well stimulation remains open.

We have simulated a variety of scenarios, the first goal being to evaluate whether crossflow in the vertical direction will compromise the effectiveness of a stimulation treatment. Thus far it appears that simple layered formations behave just as predicted from simpler models. Work is still underway to determine how this conclusion changes when flow is radial rather than linear, with a consequent variation of Damkohler number (ratio of characteristic reaction time to characteristic advection time) along the flow field. We are also investigating the effect of heterogeneities, both mineralogical and hydraulic, in the near-wellbore region.

3.3.6 Diagenesis

As brines percolate through buried sediments over geologic time, mineral precipitation and dissolution can occur. These reactions can alter porosity substantially and can change permeability by orders of magnitude. Thus an ability to predict how and where such reactions occur can greatly improve the understanding of flow fields in aquifers and reservoirs. Researchers in the Department of Geological Sciences at UT-Austin have produced a detailed description of a carbonate rock (the Lower Ismay in Utah) both in outcrop and at depth. We are using this data, along with constraints on possible fluid compositions derived from laboratory measurements, as input to Parssim1 for simulation of reactive flow through the sediment. Because the field and lab data so thoroughly characterize the rock, this will provide an excellent test of the model, providing insight into what chemical and physical mechanisms must have been at work.

3.3.7 Biotic/Abiotic Competition

Biodegradation reactions rarely occur in isolation; there is commonly competition between multiple microorganisms and multiple pathways for reaction. For example, inorganic reactions may consume or produce species involved in biodegradation. Biodegradation of toluene using a multi-component model illustrates how competition between components can affect the degradation rate. Parssim1 allows the user to select chemical and biological components for reactive transport modeling including kinetics and accounts for coupling between biotic and abiotic species. The model quantified the inhibition of toluene degradation when either benzene or pyrite competes with toluene for electron acceptors. Simplified uncoupled models will not account for this behavior, so it is important to collect site-specific data to determine whether chemically heterogeneous conditions exist before deciding whether to use simplified or multi-component models.

3.3.8 Bioremediation

Parssim1 has been used to quantify the migration of contaminants in complex flow geometries with a variety of chemical interactions. In order to compare the effects of different reaction pathways, we considered the case of a residual NAPL phase dissolving into a flowing groundwater, with subsequent biodegradation of the dissolved NAPL. The simulations involved from three to 27 species and two phases (flowing water, immobile NAPL). The flow of approximately 10 pore volumes of groundwater was simulated through a unit cube of porous medium which contains several regions of residual non-aqueous phase liquid (NAPL). A constant velocity is imposed at the x-faces of the cube; the y and z faces are no-flow boundaries.

A 32 × 32 × 32 grid was used to discretize the porous medium, and isotropic permeabilities were assigned to the grid blocks from a Gaussian distribution spanning 3 orders of magnitude. The spatial distribution of permeability causes a very heterogeneous flow field, despite the simple boundary conditions.

The residual NAPL phase dissolves into the flowing groundwater. The rate of dissolution depends on the difference between the local aqueous NAPL concentration and the maximum possible concentration (i.e. the concentration in equilibrium with the residual phase, which is 0.1 mol/l in this example). In the base case, in which there are no naturally occurring processes to degrade the NAPL, the contamination plume expands downstream of the NAPL sources. The groundwater contains dissolved oxygen at typical background levels. Thus when a uniform distribution of microbes is placed in the porous medium, the microbes utilize the oxygen to degrade the dissolved NAPL. Consequently the contamination plume is much smaller than in the base case.

In natural environments, the dissolved oxygen may participate in many other reactions. For example, reducing minerals such as pyrite will consume dissolved oxygen until the porous medium reaches Eh equilibrium. Such redox reactions will delay the propagation of the injected oxygen concentration through the porous medium. In this example case, all the incoming oxygen was consumed by inorganic redox reactions (assumed to proceed to thermodynamic equilibrium instantaneously) during the first year. This leaves no oxygen for biodegradation. Consequently the contamination plume is as severe as if no microbes were present. This illustrates the importance of considering all the chemical interactions in a system, both biotic and inorganic.

If the redox reactions occur at a finite rate, rather than going to thermodynamic equilibrium, more oxygen is available for biodegradation. The amount available depends on the rate of redox reaction. In this case study, the redox consumption during the first year of flow was so fast that little biodegradation occurred. In this case the contamination plume is only slightly smaller than in the case of equilibrium redox reactions.

After three years of simulated flow, the base case contamination plume is still quite large. In the case of biodegradation only, the natural attenuation process has greatly reduced the extent of the plume; the contamination is limited to the immediate vicinity of the residual NAPL phase. However, if substantial pyrite is present, the equilibrium redox front will have propagated only a small distance even after three years, consuming nearly all the incoming oxygen. If the redox reactions are rate-limited, enough oxygen is getting into the porous medium after three years to substantially reduce the contamination plume.

Ultimately the incoming oxygen changes the Eh of the porous medium, so that eventually oxygen becomes available for biodegradation, even if large amounts of pyrite are present. All the situations in which microbes are present exhibit smaller contamination plumes than the worst case.

3.4 Prospective Model Applications

The following applications of Parssim1 are being investigated in the CSM.

3.4.1 Heavy Metal Transport

We have available a data set from a small chemical plant, the soil of which is contaminated with heavy metals including arsenic and chromium. The data includes the flow field and extensive chemical analysis of samples from monitoring wells. A pump-and-treat remediation scheme has started on site, and siting of additional wells is currently being studied. The sorption, cation exchange and precipitation of heavy metals have a dramatic effect on their migration in the subsurface, and a modeling study of the site would provide important insight as alternative remediation schemes are considered. Parssim1's ability to handle general inorganic chemistry and detailed flow fields, including wells, would be very useful in this case.

3.4.2 Coal Ash Leaching

We have an extensive data set from experiments conducted on the leaching of coal ash. Processes have been developed which improve the combustion of coal so that many pollutants which otherwise enter the flue gas instead remain in the ash. While these processes hold the promise of greatly reducing air pollution from coal-fired power plants, the question arises as to whether the pollution problem is merely being transferred from the atmosphere to the groundwater. Coal ash from these advanced combustion processes is particularly reactive, and the percolation of rainwater through an ash pile can result in highly alkaline effluent with significant metal loading. It would be of considerable practical interest to model both the leaching process and the migration of the leachate through the subsurface with Parssim1. The experimental data would provide a useful validation of available kinetic and thermodynamic parameters for heavy metals.

3.5 Refereed Publications

[UT1] C. Dawson, C., J. van Duijn and M. F. Wheeler, Characteristic-Galerkin methods for contaminant transport with non-equilibrium adsorption kinetics, *SIAM J. Numer. Anal.*, 31 (1994), 982–999.

[UT2] R. E. Grundy, C., J. van Duijn and C. Dawson, Asymptotic profiles with finite mass in one-dimensional contaminant transport through porous media: the fast reaction case, *Quarterly Journal of Mechanics and Applied Math.*, 47 (1994), 69–106.

[UT3] T. Arbogast, C. N. Dawson and M. F. Wheeler, A parallel algorithm for two phase multicomponent contaminant transport, *Applications of Math.*, 40 (1995), 163–174.

[UT4] T. Arbogast and M. F. Wheeler, A characteristics-mixed finite element method for advection dominated transport problems, *SIAM J. Numer. Anal.*, 32 (1995), 404–424.

[UT5] C.L. Cowsar, J. Mandel, and M.F. Wheeler, Balancing domain decomposition for mixed finite element methods, *Math. of Comp.* 64 (1995), 989–1015.

[UT6] C.N. Dawson, High-resolution upwind-mixed finite element methods for advection-diffusion equations with variable time stepping, *Numerical Methods for Partial Differential Equations*, 11 (1995), 525–538.

[UT7] Y.A. Kuznetsov and M.F. Wheeler, Optimal order substructuring preconditioners for mixed finite element methods on nonmatching grids, *East-West J. Numer. Math.* (1995), 127–143.

[UT8] T. Arbogast, S. Bryant, C. Dawson, F. Saaf, Chong Wang and M. Wheeler, Computational methods for multiphase flow and reactive transport problems arising in subsurface contaminant remediation, *J. Computational Appl. Math.*, 74 (1996), 19-32.

[UT9] C. Dawson, C., J. van Duijn and R. E. Grundy, Large-time asymptotics in contaminant transport in porous media, *SIAM J. Appl. Math.*, 56 (1996), 965–993.

[UT10] T. Arbogast, M. F. Wheeler and I. Yotov, Mixed finite elements for elliptic problems with tensor coefficients as cell-centered finite differences, *SIAM J. Numer. Anal.*, 34 (1997), 828–852.

[UT11] T. Arbogast and I. Yotov, A non-mortar mixed finite element method for elliptic problems on non-matching multiblock grids, *Comp. Meth. in Appl. Mech. and Engng.*, 149 (1997), 225–265.

[UT12] C. J. van Duijn, R. E. Grundy and C. Dawson, Limiting profiles in reactive solute transport, *Transport in Porous Media*, 27 (1997), 57–84.

[UT13] T. Arbogast, C. N. Dawson, P. T. Keenan, M. F. Wheeler and I. Yotov, Enhanced cell-centered finite differences for elliptic equations on general geometry, *SIAM J. Sci. Comput.*, 19 (1998), 404-425.

[UT14] L. Toran, S. Bryant, J. Saunders, and M.F. Wheeler, Sr mobility under variable pH: application of a coupled geochemistry and transport model, to appear in *Groundwater*.

[UT15] T. Arbogast, L. C. Cowsar, M. F. Wheeler and I. Yotov, Mixed finite element methods on non-matching multiblock grids, *SIAM J. Numer. Anal.*, Submitted.

3.6 Other Publications

[UT–O1] T. Arbogast, A. Chilakapati and M. F. Wheeler, A characteristic-mixed method for contaminant transport and miscible displacement, in *Computational Methods in Water Resources* IX, Vol. 1: *Numerical Methods in Water Resources*, T. F. Russell et al., eds., Computational Mechanics Publications, Southampton, U.K. (1992), 77–84.

[UT–O2] A. Chilakapati, K.R. Robertson, and M.F. Wheeler, Three-Dimensional Bioremediation Modeling in Heterogeneous Porous Media, *Computational Methods in Water Resources* IX, Vol. 1: *Numerical Methods in Water Resources*, T.F. Russell et al., eds., Computational Mechanics Publications, Southampton, U.K. (1992), 299–316.

[UT–O3] T. Arbogast and M. F. Wheeler, A parallel numerical model for subsurface contaminant transport with biodegradation kinetics, in *The Mathematics of Finite Elements and Applications* VIII (MAFELAP 1993), J. R. Whiteman, ed., Wiley, New York (1994), 199-213.

[UT–O4] T. Arbogast, C. N. Dawson and P. T. Keenan, Efficient mixed methods for groundwater flow on triangular or tetrahedral meshes, in *Computational Methods in Water Resources* X, Vol. 1, A. Peters, et al., eds., Kluwer Academic Publishers, Dordrecht, The Netherlands (1994), 3–10.

[UT–O5] T. Arbogast, C. N. Dawson and M. F. Wheeler, A parallel multiphase numerical model for subsurface contaminant transport with biodegradation kinetics, in *Computa-*

tional Methods in Water Resources X, Vol. 2, A. Peters et al., eds., Kluwer Academic Publishers, Dordrecht, The Netherlands (1994), 1499–1506.

[UT–06] T. Arbogast, M. F. Wheeler and I. Yotov, Logically rectangular mixed methods for groundwater flow and transport on general geometry, in *Computational Methods in Water Resources* X, Vol. 1, A. Peters et al., eds., Kluwer Academic Publishers, Dordrecht, The Netherlands (1994), 149–156.

[UT–07] C. Dawson, Modeling of nonlinear adsorption in contaminant transport, *Computational Methods in Water Resources* X, A. Peters et al., eds., Kluwer, Dordrecht, pp. 233–240, 1994.

[UT–08] L. C. Cowsar, Some domain decomposition and multigrid preconditioners for hybrid mixed finite elements, *Ph.D. thesis*, Department of Computational and Applied Mathematics, Rice University, April, 1994.

[UT–09] T. Arbogast, P. T. Keenan, M. F. Wheeler and I. Yotov, Logically rectangular mixed methods for Darcy flow on general geometry, note SPE 29099, in *Proceedings of the 13th SPE Symposium on Reservoir Simulation*, held in San Antonio, Texas, Society of Petroleum Engineers (February 12–15, 1995), 51–59.

[UT–010] T. Arbogast, Mixed Methods for Flow and Transport Problems on General Geometry, in *Finite Element Modeling of Environmental Problems*, G. F. Carey, ed., Wiley, Cichester, England, (1995), 275–286.

[UT–011] M. F. Wheeler and I. Yotov, Mixed finite element methods for modeling flow and transport in porous media, in *International Conference on Mathematical Modeling of Flow through Porous Media*, Saint Etienne, France, A. P. Bourgeat et al.,eds., World Scientific (1995), 337–357.

[UT–012] C. Dawson, Contaminant transport with nonlinear, nonequilibrium adsorption kinetics, *Finite Element Modeling of Environmental Problems*, G. F. Carey, ed., Wiley, New York, pp. 265–274, 1995.

[UT–013] T. Arbogast, M. F. Wheeler and I. Yotov, Logically rectangular mixed methods for flow in irregular, heterogeneous domains, in *Computational Methods in Water Resources* XI, vol. 1, Á. A. Aldama et al., eds, Computational Mechanics Publications, Southampton, (1996), 621–628.

[UT–014] S. Bryant, F. Saaf, R. Tapia, and M.F. Wheeler, Computing General Chemical Equilibria with an Interior-point Method, *Computational Methods in Water Resources* XI, Vol. 2, A.A. Aldama et al., eds, Computational Mechanics Publications Southampton, U.K., (1996), 201–209.

[UT–015] F. Saaf, A study of reactive transport phenomena in porous media, *Ph. D. thesis*, Rice University, Houston, Texas, 1996.

[UT–016] I. Yotov, Mixed finite element methods for flow in porous media, *Ph. D. Thesis*, Rice University, Houston, Texas, May 1996. TR96-09, Dept. Comp. Appl. Math., Rice University and TICAM report 96-23, University of Texas at Austin.

[UT–017] M. F. Wheeler, T. Arbogast, S. Bryant, C. N. Dawson, F. Saaf and Chong Wang, New computational approaches for chemically reactive transport in porous media, in *Next Generation Environmental Models and Computational Methods* (NGEMCOM), Proceedings of the U.S. Environmental Protection Agency Workshop (NGEMCOM), G. Delic and M.F. Wheeler, eds., SIAM, Philadelphia (1997), 217–226.

[UT–018] T. Arbogast, C. N. Dawson, P. T. Keenan, M. F. Wheeler and I. Yotov, The

application of mixed methods to subsurface simulation, in *Modeling and Computation in Environmental Sciences*, Proceedings of the ICA seminar on Modelling and Computation in Environmental Sciences, Univ. of Stuttgart, R. Helmig et al., eds., Notes on Numerical Fluid Mechanics, 59, Vieweg Publ., Braunschweig, (1997), 1–13.

[UT–O19] J. Eaton, C.N. Dawson, and M.F. Wheeler, Transport of Multispecies Components with Biological and Chemical Kinetics, *Modeling and Computation for Applications in Mathematics, Science, and Engineering*, J. Jerome, ed., Oxford University Press, Oxford, England, 1997.

[UT–O20] M.F. Wheeler, Transport of Multispecies Contaminants in Porous Media, in *Nonlinear Applications*, INRIA (1997), 1–70.

[UT–O21] T. Arbogast, S. E. Minkoff and P. T. Keenan, An operator-based approach to upscaling the pressure equation, in *Computational Methods in Water Resources* XII, (1998), to appear.

[UT–O22] M. F. Wheeler, T. Arbogast, S. Bryant and J. Eaton, Efficient parallel computation of spatially heterogeneous geochemical reactive transport, in *Computational Methods in Water Resources* XII, (1998), to appear.

3.7 Technical Reports

[UT–TR1] T. Arbogast, C. N. Dawson, D. Moore, F. Saaf, C. San Soucie, M. F. Wheeler and I. Yotov, Validation of the PICS transport code, Department of Computational and Applied Mathematics, Rice University, Houston, Texas, (1993).

[UT–TR2] P. Cheng, M. Wells, D. Moore, Eye: 3D Graphics Visualizer User's Guide, Rice UNiversity (1994).

[UT–TR3] P.T. Keenan, kScript User Manual, Version 2, TICAM Tech. Report, The University of Texas at Austin, December 1995.

[UT–TR4] L. C. Cowsar, C. A. San Soucie, and I. Yotov, Parcel v1.01 user guide, Tech. Rep. TICAM 96–28, Texas Institute for Computational and Applied Mathematics, The University of Texas at Austin, June 1996.

[UT–TR5] F. Saaf, A user's manual for nipsf: Nonlinear interior-point solver, fortran, Tech. Rep., TR96–24, Department of Computational and Applied Mathematics, Rice University, Houston, Texas, 1996.

[UT–TR6] F. Saaf and S. Bryant, A user's manual for the geochemistry module in parsim1 reactive flow and transport code, tech. rep., Center for Subsurface Modeling, Texas Institute for Computational and Applied Mathematics, The University of Texas at Austin, Austin, Texas, Jan. 1997.

[UT–TR7] T. Arbogast, User's Guide to Parssim1: The Parallel Subsurface Simulator, Single Phase, The Center for Subsurface Modeling, Texas Institute for Computational and Applied Mathematics, The University of Texas at Austin, Austin, Texas, (1998).

3.8 Presentations

1. M.F. Wheeler, T. Arbogast, S. Bryant, C. Celentano, C.N. Dawson, P.T. Keenan, H. Klie, F. Saaf, C. San Soucie, and I. Yotov. All work was discussed at the Center

for Subsurface Modeling Industrial Affiliates Annual Meetings from 1992–1997. This program has attracted the support of several major petroleum companies and a few computer companies.

2. M.F. Wheeler, T. Arbogast, C.N. Dawson, D. Moore, and J. Warren, video presentation on, "A demonstration of the Rice transport code," *Supercomputing '92*, Minneapolis, Minnesota, November, 1992.
3. T. Arbogast, "A characteristics-mixed method for advection dominated transport problems," at the Institute for Mathematics and its Applications, University of Minnesota, summer program on *Environmental studies: mathematical, computational, and statistical analysis*, organized by M. F. Wheeler, J. Chang, M. Chil, D. McTigue, J. Seinfeld, and P. Switzer, July 6–31, 1992.
4. T. Arbogast, "A characteristics-mixed method for advection-dominated transport," at the *Texas Finite Element Circus*, the Texas Institute for Computational Mechanics (TICOM), University of Texas, Austin, Texas, April, 1992.
5. C. N. Dawson, "Godunov Mixed Methods for Nonlinear Contaminant Transport," Texas Finite Element Circus, University of Texas, March 1992.
6. C. Dawson, "Mixed Finite Element Methods on General Geometry for Flow Through Porous Media," Dept. of Mathematics and Infomatics, Delft University of Technology, Netherlands, May 1992.
7. C. N. Dawson, "Large Time Behavior of Solutions for Contaminant Transport Problems in One Space Dimension," Mathematical Problems in Flow in Porous Media, Oberwolfach, Germany, June 1992.
8. C. Dawson, "Error Estimates for Godunov Mixed Methods Applied to Nonlinear Contaminant Transport," Department of Mathematics, University of Houston, October 1992.
9. M. Wheeler, "A Mixed-Characteristic Method for Contaminant Transport," Institute for Mathematics and Its Applications (IMA) and Mathematics Department, the University of Minnesota, Minneapolis, Minnesota, February 28, 1992.
10. M.F. Wheeler, "Three-Dimensional Bioremediation Modeling in Heterogeneous Porous Media," "Scientific Computation on Massively Parallel Machines" and "Mixed Characteristic Methods for Linear Advection Problems," Distinguished Visitor Series on Challenges for Computational Mathmetics in the 1990's, Mathematical Sciences Department, Clemson University, Clemson, South Carolina, March 9 -12, 1992.
11. M. Wheeler, "A Mixed-Characteristic Method for Contaminant Transport" Plenary Address, International Conference on Differential Equations and Mathematical Physics, Georgia Tech, Atlanta Georgia, March 22, 28, 1992.
12. M. Wheeler, "Parallel Algorithms for Energy and Environmental Problems," Texaco Research and Development, Houston, Texas, April 9, 1992.
13. M.F. Wheeler, "Characteristic Finite Element Methods for Modeling Transport Phenomena in Porous Media," the 28*th* Dutch Mathematics Congress, Delft University, Netherlands, April 22, 1992.
14. M.F. Wheeler, "Modeling Contaminant Transport of Toxic Waste Sites in Porous Media," University of Houston, Environment and Immunolgy Conference, Invited Speaker, May 1992.

15. M.F. Wheeler, "Three-Dimensional Bioremediation Modeling in Heterogeneous Porous Media," Water Resources IX, International Conference, invited speaker, Denver, June 1992.
16. M. Wheeler, "Modeling of Biodegradation of Contaminants in Groundwater," Institute for Mathematics and its Applications, University of Minnesota, Workshop on Environmental Problems, July 1992.
17. M. Wheeler, "Modeling Flow in Porous Media," International Congress on Nonlinear Analysis, Tallahasse, Florida, Invited Speaker, August 1992.
18. M.F. Wheeler, "High Performance Computing in Modeling Flow in Porous Media," Cray Technology Symposium, Houston, Texas, invited speaker, October, 1992.
19. M.F. Wheeler, "Characteristic Methods for Modeling Transport Dominated Flow Problems," Batalle Pacific Northwest Laboratory, invited speaker, August, 1992.
20. M.F. Wheeler, "Parallel Domain Decomposition Algorithms for Mixed Finite Element Methods," University of Kentucky Center for Computational Science, invited speaker, December 1992.
21. M.F. Wheeler, "Three Dimensional Bioremediation Model for Porous Media," AGU National Meeting, San Francisco, California, December 9, 1992, with Kyle Robinson, Batalle Pacific Northwest Laboratory.
22. M.F. Wheeler, "Mathematical Modeling in Porous Media," Mathematics Association of America, State of Texas Meeting, Houston, Texas, April 11, 1992.
23. M.F. Wheeler, "Parallel Algorithms for Modeling Flow in Porous Media," Supercomputer '92, invited speaker, Minneapolis, Nov. 1992.
24. M.F. Wheeler, "Rice Flow in Porous Media," Industrial Meeting with the Shell Research Group, Rice University, December 8, 1992.
25. T. Arbogast, "Computational justification of a dual-porosity model for two-phase flow in fractured media," Second SIAM Conference on Mathematical and Computational Issues in the Geosciences, Houston, Texas, April, 1993.
26. T. Arbogast, "A characteristics-mixed method for contaminant transport and miscible displacement," SIAM Conference on Mathematical and Computational Issues in the Geosciences, Houston, Texas, April, 1993.
27. T. Arbogast, "Equations with dual-porosity microstructure for modeling flow in fractured porous media," Differential Equations Conference, Ohio University, Athens, OH, August, 1993.
28. T. Arbogast, "Characteristic and mixed methods for approximating advection-diffusion equations," Georgia Tech, Atlanta, Georgia, November, 1993.
29. T. Arbogast, "Mixed methods for flow and transport problems on general geometry", Workshop on *Finite Element Modeling of Environmental Problems*, University of Texas, Austin, Texas, March 4–5, 1994.
30. C. Dawson, "Numerical Simulation of Flow Through Porous Media," Dept. of Mathematics and Infomatics, Delft University of Technology, Delft, Netherlands, May 1993.
31. C. Dawson, "Modeling of Multiphase Flow in Porous Media," Dept. of Environmental Engineering, Rice University, November 1993.
32. M.F. Wheeler, "Parallel Algorithms for Modeling Flow in Porous Media," AMS/MAA Invited Speaker, the American Mathematical Society National Meeting, San Antonio, January 1993.

33. M.F. Wheeler, "Characteristic Mixed Finite Element Methods for Modeling Transport Dominated Flow Problems," DOE, Sandia National Lab, invited speaker, February 1993.
34. M.F. Wheeler, "Computational Science Programs" & "Parallel Algorithms for PDE's" Department of Mathematics, Trinity University, February 1993.
35. M. F. Wheeler, "Parallel Algorithms for Reservoir Engineering and Groundwater Modeling," SIAM, Norfolk Parallel Computation Meeting, Invited Minisymposium Speaker, Norfolk Virginia, March 1993.
36. M. Wheeler, "Advanced Numerical Algorithms for Groundwater Modeling," Lawrence Livermore Laboratory, invited speaker, March 1993.
37. M.F. Wheeler, "Domain Decomposition for Mixed Finite Element Methods for Elliptic Equations," VI International Domain Decomposition Meeting, Cuomo, Italy, June 1993.
38. M.F. Wheeler, "Parallel Algorithms for Modeling Flow in Porous Media," Rice Mechanical Engineering Department, Colloqium Speaker, April 1993.
39. M.F. Wheeler, "A Parallel Numerical Model for Subsurface Contaminant Transport with Biodegradation Kinetics," MAFELAP Conference, Brunel University, invited speaker, April 26–29, 1993.
40. M.F. Wheeler, "Grand Challenge Problems in Porous Media," High Performance CompuPCC Meeting, Pittsburgh, PA, May 3–6, 1993.
41. M.F. Wheeler, "A Parallel Multicomponent Two-phase Simulation with Biological and Chemical Kinetics," AGU National Meeting, Baltimore, MD, May 24–27, 1993.
42. M.F. Wheeler, "Parallel Algorithms for Modeling Multiphase Flow and Transport," Congress of the American Physical Society, Albuquerque, June 1–4, 1993.
43. M.F. Wheeler, "Domain Decomposition Algorithms for Partial Differential Equations," Computer Science Department Colloqium Presentation, University of Illinois, Urbana, IL, September 1993.
44. M.F. Wheeler, "Mixed Characteristic Method Fluids," Domain Decomposition Methods for Porous Media Meeting, Pennsylvania State University, University Park, Pennsylvania, October 1993.
45. M.F. Wheeler, "Modeling Adsorption and Bioremediation in Porous Media," Department of Mathematics, University of Arizona, Tucson, Arizona, November 1993.
46. T. Arbogast, "Logically rectangular mixed methods for groundwater flow and transport on general geometry," the Tenth International Conference on Computational Methods in Water Resources, Heidelberg, Germany, July, 1994.
47. T. Arbogast, "Mathematical simulation of flow in porous media," Joint American Mathematical Society & Mathematical Association of America Invited Address, Mathfest, Minneapolis, Minnesota, August, 1994.
48. T. Arbogast, "Mixed finite element methods as finite difference methods on general geometry," Sociedade Brasileira de Matemática Aplicada e computacional (SBMAC), XVII Congresso Nacional de Matemática Aplicada e Computacional CNMAC 94, Vitória, ES, Brasil, August–September, 1994.
49. T. Arbogast, "Superconvergent cell-centered finite difference mixed methods for flow through geometrically heterogeneous porous media," Society of Engineering Science 31*st* Annual Technical Meeting, Texas A&M University, College Station, Texas, Octo-

ber, 1994.

50. C. Dawson, "Modeling Nonlinear Adsorption in Contaminant Transport," Workshop on Finite Elements in Environmental Problems, University of Texas at Austin, March 1994.
51. C. Dawson, "Simulation of Groundwater Remediation," RCI Ltd. Symposium on High Performance Computing in Energy and the Environment, Houston, March 1994.
52. C. Dawson, "Domain Decomposition Methods for Elliptic and Parabolic Equations," Numerical Analysis Colloquium, University of Chicago, May 1994.
53. C. Dawson, "Asymptotic Behavior of Solutions to Nonlinear Contaminant Transport Problems," Computational Methods in Water Resources '94, Heidelberg, Germany, July 1994.
54. M.F. Wheeler, "Parallel Domain Decomposition Methods for Porous Media Problems" and "HPCC Grand Challenge Problems in Reservoir Engineering and Groundwater," Center for Research on Parallel Computation Annual Meeting, California Institute of Technology, Pasadena, California, January 1994.
55. M.F. Wheeler, "Parallel Algorithms for Modeling Flow in Porous Media," Louisiana State University Terraflop Mardi Gras Conference, Baton Rouge, Louisiana, February 1994.
56. M.F. Wheeler, "Mathematical Modeling in Flow in Porous Media," BAM Conference, University of Sheffield, Sheffield, England, April 1994.
57. M.F. Wheeler, "Mathematical Models for Porous Media," Barkley Rosser Lecture, University of Wisconsin, Madison, Wisconsin, May 1994.
58. M.F. Wheeler, "Mathematical Flow in Porous Media Models," IBM, T.J. Watson Center, Physics Division, May 19, 1994.
59. M.F. Wheeler, "A Nonlinear Mixed Finite Element Method for a Degenerate Parabolic Equation Arising in Flow in Porous Media," Transport in Porous Media Symposium, International Conference on Nonlinear Dynamics and Pattern Formation in the Natural Environment, ICPF'94 Leeuwenhorst Congress Center, Noordwijkerhout, the Netherlands, July 4–7, 1994.
60. M.F. Wheeler, "Transport, Bioremediation, Radionuclide Decay and Geochemistry," DOE Review, Washington, DC, July 13, 1994.
61. M.F. Wheeler, "A Parallel Multiphase Numerical Model for Subsurface Contaminant Transport with Biodegradation Kinetics," X International Conference on Computational Methods in Water Resources, Heidelberg, Germany, July 19-22, 1994.
62. M.F. Wheeler, "Logically Rectangular Mixed Methods for Groundwater Flow and Transport on General Geometry," X International Conference on Computational Methods in Water Resources, Heidelberg, Germany, July 19–22, 1994.
63. M. F. Wheeler, "A parallel multiphase numerical model for subsurface contaminant transport with biodegradation kinetics," at the Computational Methods in Geosciences Porous Medium Symposium, SIAM Annual Meeting, San Diego, July 26, 1994.
64. M.F. Wheeler, "Role of Computations in Energy and Environment," Mathematical and Computational Sciences Awareness Workshop, Rice University, July 27, 1994.
65. M.F. Wheeler, "Modeling Flow in Porous Media on Distributive Memory Machines," Plenary Lecture, Numerical Modeling in Continuum Mechanics, Theory, Algorithms, Applications, Prague, Czech Republic, Charles University, August 22–25, 1994.

66. M.F. Wheeler, "Flow in Porous Media Parallel Computation Project," Arctic Region Supercomputing Center and the University of Alaska at Fairbanks, October 1994.
67. M.F. Wheeler, "Parallel Algorithms for Modeling Flow in Porous Media," The University of Texas Computational and Applied Mathematics Speaker, October 1994.
68. M.F. Wheeler, T. Arbogast, C.N. Dawson, and P.T. Keenan, Exhibitor for the Center for Research on Parallel Computation and the Center for Subsurface Modeling at the *Society of Petroleum Engineers Petroleum Computer Conference*, Houston, Texas, June, 1995.
69. T. Arbogast, "A nonlinear mixed finite element method for a degenerate parabolic equation arising in flow in porous media," Third SIAM Conference on Mathematical and Computational Issues in the Geosciences, San Antonio, Texas, February, 1995.
70. T. Arbogast, "Mathematical simulation of flow in porous media," Texas Institute for Computational and Applied Mathematics (TICAM), University of Texas, Austin, Texas, March, 1995.
71. T. Arbogast, "The application of mixed finite element methods to subsurface simulation," First GAMM Seminar on Modelling and Computation in Environmental Sciences, University of Stuttgart, Stuttgart, Germany, October, 1995.
72. C. Dawson, "Numerical Simulation of Large Time Behavior of Solutions for Nonlinear Adsorption in Contaminant Transport," Third SIAM Conference on Geosciences, San Antonio, February 1995.
73. C. Dawson, "Numerical Methods for Flow Through Porous Media," TICAM Seminar, University of Texas at Austin, March 1995.
74. C. Dawson, "Modeling of Groundwater Cleanup," Dept. of Aerospace Engineering and Engineering Mechanics, University of Texas at Austin, April 1995.
75. C. Dawson, "Upwind Mixed Methods for Advective Transport with Variable Time Stepping," Conference on Advances and Trends in Computational and Applied Mathematics, University of Texas at Austin, April 1995.
76. C. Dawson, "Problems in Remediation of Contaminated Porous Media," Program in Environmental Fluid Dynamics Colloquium, Arizona State University, Sept. 1995.
77. M.F. Wheeler, "Logically Rectangular Mixed Methods for Darcy Flow on General Geometry," 13th Symposium on Reservoir Simulation, San Antonio, Texas, February 1995.
78. M.F. Wheeler, "A Parallel Multiphase Model for Subsurface Transport with Biological and Chemical Kinetics," University of Vermont, March 1995.
79. M.F. Wheeler, "Computational Methods for Multiphase Flow and Reactive Transport Problems Arising in Subsurface Contaminant Remediation," TICAM Symposium on Advances and Trends in Computational and Applied Mathematics, April 1995.
80. M.F. Wheeler, "Parallel Algorithms for Modeling Multiphase Flow and Transport in Porous Media," Glimm '95 Conference, Stony Brook, New York, April 1995.
81. M.F. Wheeler, "Mixed Finite Element Methods for Modeling Flow and Transport in Porous Media," Mathematical Modeling of Flow through Porous Media Conference, St. Etienne, France, May 1995.
82. M.F. Wheeler, "New Computational Approaches for Chemically Reactive Transport in Porous Media," New Generation Environmental Models Computational Methods, U.S. EPA Sponsors, Bay City Michigan, August 8, 1995.

83. M.F. Wheeler, "Advanced Numerical Models for Treating Porous Media Geology," Michigan Institute of Technology, Hoboken, Michigan, August 10, 1995.
84. M.F. Wheeler, "New Generation Simulators for Modeling Subsurface and Surface Flows; Mixed Finite Element Methods for Partial Differential Equations," "Parallel Algorithms for Permeable Media," and "Frontiers in Science," Texas A&M University, College Station, Texas, November 1995.
85. Ivan Yotov, "Mixed finite elements for elliptic problems with tensor coefficients as cell-centered finite differences", Texas Finite Element Circus, Texas A&M University, Mar. 1995.
86. T. Arbogast, "Mixed finite element methods on multi-block domains," at the Mathematisches Forschungsinstitut Oberwalfach meeting on *Porous Media*, organized by J. Douglas, Jr., U. Hornung, and P. Knabner, Oberwalfach, Germany, February–March, 1996.
87. T. Arbogast, "Finite difference or volume methods for subsurface simulation arising from mixed finite elements," Pacific Northwest National Laboratory, Richland, Washington, September, 1996.
88. C. Dawson, "A Summary of Results on Asymptotic Behavior of Solutions to Nonlinear Contaminant Transport Problems," Workshop on Mathematical Problems in Flow Through Porous Media, Oberwolfach, Germany, February 1996.
89. M.F. Wheeler, "Emerging New Algorithms for Parallel Computation in Subsurface and Surface Flows," Institute for Geophysics, The University of Texas at Austin, Jan. 19, 1996.
90. M.F. Wheeler, "Parallel Algorithms for Modeling Multiphase Flow and Transport in Porous Media," Geology Seminar, The University of Texas, January 30, 1996.
91. M.F. Wheeler, "Modeling Activities at the Center for Subsurface Modeling," Bureau of Economic Geology, Austin, Texas, January 31, 1996.
92. M.F. Wheeler, "Modeling Multiphase Flow and Transport with Biological and Chemical Kinetics," German Mathematical Institute, Oberwolfach, Germany, February 26 - March 2, 1996.
93. M.F. Wheeler, "Impact of Computation on Modeling in Porous Media," NSF CISE Site Visit, Computer Science Department, March 4, 1996.
94. M.F. Wheeler, "Impact of Computation on Science and Engineering," AAAS Meeting, The University of Texas at Austin, Austin, March 6, 1996.
95. M.F. Wheeler, "Numerical Algorithms for Grand Challenge Problems," NSF Workshop on Grand Challenge Problems, NSF, Arlington, Virginia, March 21, 1996.
96. M. Wheeler, "Mathematical Modeling of Subsurface and Surface Flow," University of Maryland Computational Science and Engineering Meeting, College Park, Maryland, March 23, 1996.
97. M.F. Wheeler, "Emerging Parallel Computational Methodologies," University of Central Florida, Orlando Florida, April 1, 1996.
98. M.F. Wheeler, "Algorithms for Modeling Subsurface and Surface Flows," University of Central Florida, Orlando, Florida, April 2, 1996.
99. M.F. Wheeler, "Parallel Algorithms for Subsurface Flow," Computer Science Workshop, The University of Texas at Austin, April 22, 1996.

100. M.F. Wheeler, "Mathematical Modeling of Multiphase Flow in Porous Media," Modeling and Computation for Applications in Science and Engineering, Northwestern University, Evanston, Illinois, May 3-4, 1996.
101. M.F. Wheeler, "Subsurface and Surface Modeling at the Center for Subsurface Modeling at The University of Texas," NSF Center for Research in Parallel Computation Annual Meeting, Argonne National Laboratory, Chicago, Illinois, May 16, 1996.
102. M.F. Wheeler, "Subsurface and Surface Flow Simulation," 12th Candian Symposium of Fluid Dynamics, Winnipeg, Manitoba, Canada, May 29–31, 1996.
103. M. Wheeler, "Modeling Multicomponent, Multispecies, Multiphase Flow and Transport in Porous Media," 10th Conference on Mathematics of Finite Elements and Applications, Brunel University, Uxbridge, Middlesex, UK, June 25-28, 1996.
104. M.F. Wheeler, "Mixed Finite Element Methods with Nonmatching Grids for Partial Differential Equations," SIAM Annual Meeting, Kansas City, Missouri, July 23, 1996.
105. M.F. Wheeler, "Modeling Activities at The Center for Subsurface Modeling at The University of Texas at Austin," Center for Research on Parallel Computation Interim Site Visit, Rice University, August 1996.
106. Ivan Yotov, "Logically rectangular mixed methods for flow in irregular, heterogeneous domains", Eleventh International Conference on Computational Methods in Water Resources, Cancún, México, July 1996.
107. T. Arbogast, "A non-mortar mixed finite element method for elliptic problems on non-matching multiblock grids," Interdisciplinary Symposium on Advances in Computational Mechanics, The University of Texas at Austin, Austin, Texas, January, 1997.
108. T. Arbogast, "A non-mortar mixed finite element method for elliptic problems on non-matching multiblock grids," at the *Finite Element Rodeo*, The University of Texas at Austin, Austin, Texas, February–March, 1997.
109. T. Arbogast, "Mixed Finite Element Methods on Non-Matching Multiblock Grids," Spring Southeastern Sectional Meeting of the American Mathematical Society, Memphis, Tennessee, March, 1997.
110. T. Arbogast, "Mixed finite elements on multiblock grids for subsurface flow," Third IMACS International Symposium on Iterative Methods in Scientific Computation, Jackson Hole, Wyoming, July 1997.
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