FINAL REPORT

Title: Grand Challenge Problems in Environmental Modeling and Remediation:
Groundwater Contaminant Transport (Partnerships In Computational Science)

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Abstract

The over-reaching goal of the Groundwater Grand Challenge component of the Partnership in Computational Science (PICS) was to develop and establish the massively parallel approach for the description of groundwater flow and transport and to address the problem of uncertainties in the data and its interpretation. This necessitated the development of innovative algorithms and the implementation of massively parallel computational tools to provide a suite of simulators for groundwater flow and transport in heterogeneous media. This report summarizes the activities and deliverables of the University of South Carolina component of the Groundwater Grand Challenge project funded through the High Performance Computing grand challenge program of the Department of Energy from 1995 through 1997.

Seven institutions were primarily involved in this project: Brookhaven National Laboratory, Oak Ridge National Laboratory, Princeton University, SUNY at Stony Brook, Texas A&M University, The University of South Carolina, and the University of Texas at Austin, with contributing efforts from the Westinghouse Savannah River Technology Center. Each institution had primary responsibility for specific research components, but strong collaboration among all institutions was essential for the success of the project and in producing the final deliverables.

PICS deliverables include source code for the suite of research simulators and auxiliary HPC tools, associated documentation, and test problems. These materials will be available as indicated from each institution's web page or from the Center for Computational Sciences Oak Ridge National Laboratory in January 1998.

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1 Introduction

The groundwater grand challenge component of the Partnership in Computational Science (PICS) High Performance Computing initiative was formed to apply the members' collective efforts towards the mathematical and scientific challenges presented by complex groundwater, soil, contaminants, and air interactions. The numerical modeling of the fate of groundwater contaminants is a critical step in the formulation of remediation policies to be used to address contaminated groundwater and soils. Such strategies as pump-and-treat and in-situ vitrification require accurate knowledge of the location and extent of the contaminant plume; furthermore, some remediation strategies themselves use complex physical and chemical processes, requiring, for example, the placement of chemical "traps" or the injection of surfactants, bacteria, or nutrients.

Remediation methods remain extremely (and potentially prohibitively) expensive and unpredictable in their success. This is due to a number of factors, including significant geologic heterogeneity, incomplete characterization of the subsurface, and the complexity of underground contaminant reactions and remediation processes.

Groundwater contamination problems typically involve organic liquids, ionic solutes, and/or radionuclides. The transfer of chemical species between the contaminant-bearing phase, the soil or aquifer, and the groundwater may involve interphase mass transfer as well as a host of intraphase chemical reactions such as dissolution, aqueous phase complexation, ion exchange, adsorption, precipitation, oxidation/reduction, and even biological degradation kinetics. The extent of mass transfer and chemical reaction is ultimately limited by thermodynamic equilibrium, but compositions far from equilibrium often arise locally because of kinetic and surface area constraints.

In addition to the basic research on coupled multi-phase flow and multi-component transport in porous media, the development of parallel algorithms for the solution of these coupled equations, and the development of computational science tools for better analysis and understanding, specific deliverables provided an overriding guide for the collaborative work among consortium members.

This report summarizes the activities and deliverables of the Groundwater Grand Challenge project funded through the High Performance Computing grand challenge program of the Department of Energy from 1995 through 1997. The goal of the project are to develop and establish the massively parallel approach for the description of groundwater flow and transport and to address the problem of uncertainties in the data and its interpretation. This required the development of innovative algorithms and the implementation of massively parallel computational tools to provide a suite of simulators for groundwater flow and transport in heterogeneous media.

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PICS deliverables include source code for the suite of research simulators and auxiliary HPC tools, associated documentation, and test problems. These materials will be available from each institution's web page or from the Center for Computational Sciences Oak Ridge National Laboratory in January 1998.

Software Deliverables:

- GCT1.2: Saturated/Unsaturated Flow and Multicomponent transport Flow based on Galerkin FEM and transport based on mixed method of characteristics and Godunov schemes.
- GCT1.3: Two-phase Flow and Multicomponent transport.

- G3D: Graphical pre- and post-processing software.
(<http://www.math.sc.edu/~sharp/leym/G3D/colormannual.ps>)
- Steer: Steering and Tracking Library.
(<http://www.math.sc.edu/~sharp/leym/Steer.html>)
- Parsimm: Single-phase flow, radionuclide decay, and biogeochemistry.
- EDONIO/DOLIB: Scalable I/O library and Parallel distributed object library.
- PERM: Parameter estimation.
- US3D-MP: Saturated/Unsaturated Flow and Single component transport Based on Galerkin FEM
- 2D Front tracking code from SUNY-SB.

2 University of South Carolina Component

The University of South Carolina contributed primarily in five areas to the PICS project: (i) ELLAM algorithm development for advection-diffusion-reaction equations, (ii) development and testing of data compression algorithms to enable interactive simulations over standard bandwidth networks, (iii) development of graphical user interfaces for preprocessing input data, model development, and post-processing simulations for analysis, (iv) development of an general purpose library for remote interactive tracking and steering of simulations on massively parallel machines, and (v) collaboration with the Savannah River Site in providing realistic field site data as test cases for the PICS simulators. More details on the University of South Carolina's PICS contributions and activities are available at "<http://www.math.sc.edu/~sharp/leym/pics.html>".

2.1 Numerical Algorithms for Advection-Diffusion-Reaction Equations - ELLAM

The sensitive numerics of advection-diffusion equations, appearing both in the saturation equation of the flow code and in the transport equations, require careful treatment in order to efficiently achieve the accuracy required for these coupled model equations. South Carolina continued its collaboration with Princeton and Texas A&M on Eulerian-Lagrangian Localized Adjoint Methods (ELLAM) for the numerical solution of advection-dominated partial differential equations. Significant results have been obtained on the convergence analysis of ELLAM schemes [10, 11], development of algorithms for advection-diffusion-reaction equations [9, 10, 11, 12, 13], domain decomposition and space-time local refinements [11, 13], and the numerical simulation of compositional models [9].

Many numerical methods for the solution of one- and two-dimensional advection-diffusion-reaction partial differential equations, including ELLAM schemes, Galerkin finite element methods, quadratic Petrov-Galerkin methods, cubic Petrov-Galerkin methods, streamline diffusion methods, Flux Corrected Transport, and Godunov schemes, have been systematically compared under a variety of initial and boundary conditions. The result of these comparisons have demonstrated the strong potential of ELLAM schemes to address the model transport equations.

2.2 Input Modules for GCT 1.3

South Carolina, in collaboration with Princeton, Savannah River, and Texas A&M provided boundary condition specifications. The primary input modules were developed by Mohamed Al-Lawatia and have been delivered to satisfy the corresponding part of the milestones. Complete documentation and examples were included. The modules were merged into the official GCT 1.3 code and

conform to the new input standards. This effort was coordinated with Pasciak (BNL), Vassilev (TAMU), Celia (Princeton), and the G3D development team. Thorough testing has been completed for each of the primary WEB modules (grid, initial conditions, boundary conditions, and material properties). Special data structures were designed and implemented for the efficient building, handling and storage of time-dependent boundary condition data sets.

2.3 Graphical User Interfaces for Model Development and Analysis

A comprehensive suite of graphical pre- and post-processors has been developed to assist practitioners with model formulation and development. These GUI's allow for easy input of all necessary parameters and system properties, and for meaningful graphical display of output from the numerical simulations. The current version of these interfaces, referred to as G3D([6]),

["http://www.math.sc.edu/~sharpely/PICS/USC_PICS_4b.html"](http://www.math.sc.edu/~sharpely/PICS/USC_PICS_4b.html),

has been developed through funding from DOE with matching funds from the University of South Carolina. G3D currently provides a fully functional pre- and post-processing graphical interface that allows the user to easily generate and modify the numerical grid, to input and modify soil and rock properties, and to impose appropriate initial and boundary conditions. It provides a data synthesis capability which facilitates detection of user input errors as well as providing an efficient methodology for refinement of the modeling process. G3D provides animated graphical display of evolving contaminant plumes in three-dimensions, with options to plot iso-concentration surfaces or color shadings with varying degrees of opacity.

Additional G3D tools include 3-D mouse view control, multiple views, VCR record and playback, overlay and stereo imaging, grid and model editing, including full boundary condition GUI editing for time-dependent boundary conditions of all types. Multiple scalar and vector data are simultaneously processed, as well as the simultaneous rendering of soil and fluid features. Additional images, model animations, and source codes are available from the WEB site printed above, and the URL *["http://www.math.sc.edu/~sharpely/PICS/USC_PICS_4a.html#movie"](http://www.math.sc.edu/~sharpely/PICS/USC_PICS_4a.html#movie)*.

In order to provide for efficient and effective use of both the GUI's and the parallel simulators on remote massively parallel machines, we have also developed a general purpose Controller Library which is described in more detail in the next subsection.

2.4 Tracking/Steering Library

An Interactive Tracking/Steering Library with the parallel machine (e.g., Paragon) as server and UNIX workstations (e.g. Silicon Graphics) as clients has been developed and may be obtained from the ORNL repository or from South Carolina's ftp site. This is a general purpose library which was developed for interactive remote tracking and steering of simulations and which conforms to specifications as set by GCT code developer J. Pasciak (BNL). The library has been tested on the satellite PICS Paragons, as well as the main production machines at ORNL, to ensure compatibility of the remote procedure calls with security at each site. Components delivered include: (i) client and server libraries, (ii) Steering/Tracking instrumented versions of GCT1.2 and US3D ([5]) for interactive remote use with the G3D graphical interface, (iii) four additional working example codes in increasing order of complexity, (iv) TeX user documentation, (v) FAQ (Frequently asked questions), 'Man' pages for on-line help. Additional information and a user manual is available online at the URL

<http://www.math.sc.edu/~sharpely/Steer.html>

The library permits remote tracking and steering of simulations on supercomputers from local workstations with user-determined levels of interruption to maintain load-balance, synchronization, and integrity of data to be transferred. This library has been ported to the MPI message passing language, has been coupled with G3D, specialized data compression modules, and three of the PICS groundwater contaminant codes [5, 8] to provide interactive groundwater simulations on remote Paragons.

2.5 Data Compression

Extensive testing and usage of network connections to PICS machines at ORNL and member institutions, provided convincing evidence that the use of compatible data compression tools will be necessary for hydrologists and field engineers to perform interactive Grand Challenge simulations from their local workstations.

South Carolina has developed algorithms ([4]) for both client and server compression modules to address this problem and are tuning them for groundwater applications. During this grant period, we have developed and implemented 3D algorithms (both single and multiple processor versions on the server machine, i.e. Paragon) designed to be coupled with the user interface codes and compress data as it is generated by GCT applications in a non-interruptive manner. The algorithms and research codes use nonlinear approximation and specialized entropy encoders, which have proven to be extremely successful for wavelet compression of 2D images applied to hyperbolic wavelet bases. We have developed 3D variants of Shapiro's method for comparison and have tested these implementations with our Steering library coupling US3D with our *G3D* graphical user interface.

These compression algorithms applied to the both smooth (e.g., pressures) and to rough fields (transport solutions generated by the highly heterogeneous Old Burial Ground data at SRS) have achieved impressive rates of compression without discernible loss of visual information, and provides up to 1,200 times compression with excellent visual retention of qualitative features

"http://www.math.sc.edu/~sharpley/PICS/USC_PICS_4b.html#4b3".

2.6 Field Application Simulations

Data was provided in several forms by our collaborators in the Environmental Sciences Division of the Savannah River Technology Center

"http://www.math.sc.edu/~sharpley/PICS/USC_PICS_4c.html".

Project personnel James Brannan of Clemson University worked closely with Luther Hamm and Gregory Flach of SRS to assist in developing the theory, algorithms and software tools for processing raw data into input files for both HPC codes. The goal is to create software which incorporates scale-up techniques, data fusion methods, and permits input of soft or subjective geological knowledge. These issues will be critical for providing practicing hydrologists access to HPC simulators developed through the PICS project.

The SRS raw data was assimilated and used for flow and transport simulations on $128 \times 128 \times 64$ model runs, as well as several smaller model versions. Qualitative feedback of the model runs by SRS collaborators has resulted in a detailed flow field of the site. The model data were also critical in debugging several components of the GCT codes and illustrated the need for distributed I/O for model data in this application field. QuickTime and MPEG animations of the simulations were produced by applying *G3D* to the output of these models for both flow

"http://www.math.sc.edu/~sharp/leym/PICS/USC_PICS_4a.html#movie2".

and transport

"http://www.math.sc.edu/~sharp/leym/PICS/USC_PICS_4a.html#movie".

The original flow runs were performed on the XPS150 at ORNL by South Carolina personnel and the results were demonstrated at the ORNL booth during *SuperComputing '95*.

3 Publications Resulting from DOE Grant DE-FG05-95ER25266

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2. K. J. Bene, E. K. Paleologos, M. M. Meadows, Geostatistical Analyses of Laboratory and In-situ Measurements of Saturated Hydraulic Conductivity, *Abstracts of the 46th Annual Southeastern Section of the Geological Society of America* 29(3)(March 1997), p. 4.
3. K. J. Bene, R. P. Ray, M.M. Meadows, E. K. Paleologos, Application of Geostatistics to Site Characterization, *Annales Geophysicae*, European Geophysical Society (1997), p. C266.
4. Z. Gao, A. Andreev and R.C. Sharpley, *Elementary Encoding of Wavelet Coefficients*, IMI Report 97:02, Department of Mathematics, University of South Carolina, Columbia, SC (Jan. 97).
5. L.S. Johnson, A. Kaulgud, R.C. Sharpley, R.E. Ewing, Z. Leyk, J. Pasciak, M. Celia, and J.R. Brannan, *Integration of Contaminant Transport Simulators on Parallel Machines with a Graphical User Interface for Remote Interactive Modeling*, in “Proceedings of the 1997 Simulation Multiconference,” Atlanta, April 1997, Soc. for Computer Simulation International, San Diego.
6. L.S. Johnson, A. Kaulgud and R.C. Sharpley, *G3D: A 3D User Environment for Partial Differential Equations*, IMI Report 97:01, Department of Mathematics, University of South Carolina, Columbia, SC (Jan. 97).
7. A. Kaulgud and R.C. Sharpley. *An Interactive Tracking/Steering Library*, IMI Report 95:10, Department of Mathematics, University of South Carolina, Columbia, SC (Aug. 1995, rev. July 1997).
8. G. Mahinthakumar, R.C. Sharpley, A. Kaulgud, and L.S. Johnson, *Groundwater remediation experiments using interactive computational steering on the Intel Paragon*, Intel Supercomputer Users Group Annual Conference (ISUG97), Albuquerque, NM, June 11-13, 1997.
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10. H. Wang, M. Al-Lawatia, and S.A. Telyakovskiy, A Runge-Kutta characteristic method for first-order linear hyperbolic equations, *Numerical Methods for PDEs*, 13, (1997), 617–661.
11. H. Wang, M. Al-Lawatia, and R.C.Sharpley, A characteristic domain decomposition and space-time local refinement method for first-order linear hyperbolic equations with interfaces, submitted.
12. H. Wang, H.K. Dahle, R.E. Ewing, M.S. Espedal, R.C. Sharpley, and S. Man, An Eulerian-Lagrangian localized adjoint method for advection-dispersion equations in two dimensions and its comparison to other schemes, accepted for publication in *SIAM J. Scientific Computing*.
13. H. Wang and B-G Ersland, A characteristic domain decomposition technique for two-phase flows with interfaces, accepted for publication in *Proceedings of the Ninth International Conference on Domain Decomposition Methods*, Ullensvang, Norway, June, 1996.