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Large-Scale Three-Dimensional Geothermal Reservoir Simulation on Small Computer Systems

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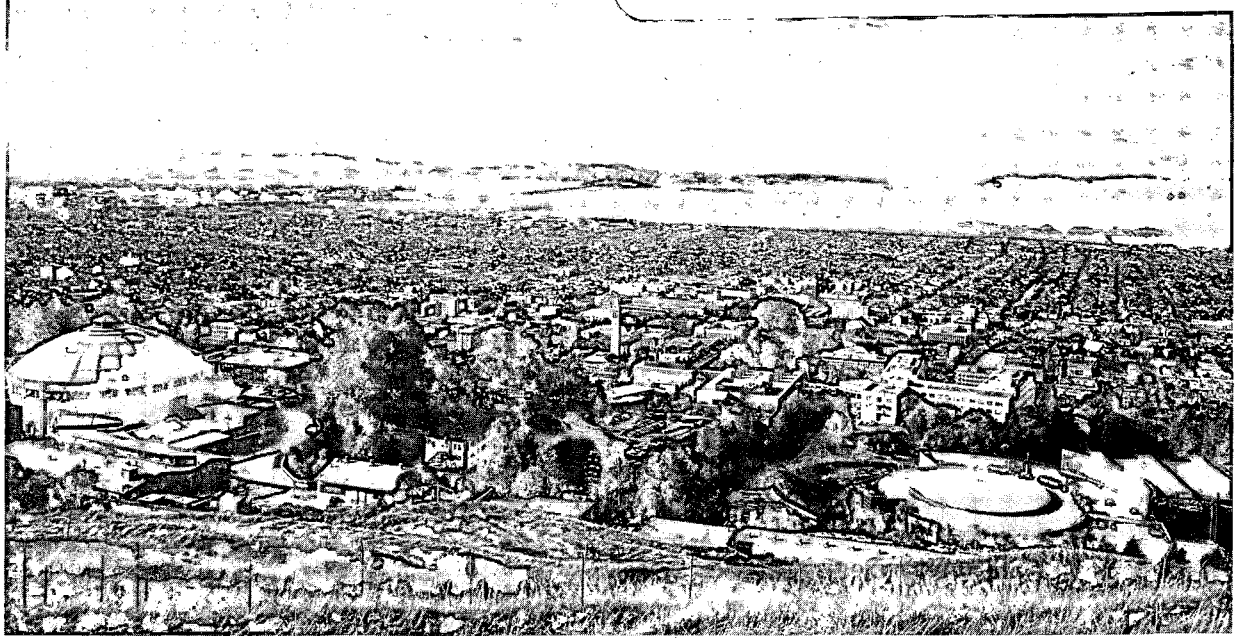

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ABSTRACT

The performance of TOUGH2, Lawrence Berkeley Laboratory's general purpose simulator for mass and heat flow and transport enhanced with the addition of a set of preconditioned conjugate gradient solvers, was tested on three PCs (486-33, 486-66, Pentium-90), a MacIntosh Quadra 800, and a workstation IBM RISC 6000.

A two-phase, single porosity, 3-D geothermal reservoir model with 1,411 irregular grid blocks, with production from and injection into the reservoir was used as the test model.

The code modifications to TOUGH2 and its setup in each machine environment are described. Computational work per time step and CPU time requirements are reported for each of the machines used.

It is concluded that the current PCs provide the best price/performance platform for running large-scale geothermal field simulations that just a few years ago could only be executed on mainframe computers and high-end workstations.

INTRODUCTION

In geothermal engineering, computers have facilitated the analysis of processes that range from the simple movement of fluids through porous media (in which mass and energy balances have to be simultaneously accounted for) to the more complex problems in which heat pipes, non-condensable gases, salinity and chemical processes have to be included in the analysis.

Considering that current personal computers (PCs) have the same or more computational power than mainframes and minicomputers of a few years ago, it is not surprising that software that was developed for mainframes and minicomputers had started migrating towards the more cost-effective PC platforms. This has been the case with Lawrence Berkeley Laboratory's general purpose reservoir simulator TOUGH2 [Pruess, 1991].

TOUGH2 is a numerical simulation program for non-isothermal flow of multicomponent, multiphase fluids in porous and fracture media. This code has been widely applied in geothermal reservoir engineering, nuclear waste disposal, environmental restoration, and unsaturated groundwater hydrology.

TOUGH2 with its standard direct matrix solver MA28 (Duff, 1977) and a package of three different preconditioned conjugate gradient (CG) solvers[1] (Moridis et al., 1994) were ported to a 486-66 MHz PC and extensively tested by Antúnez, et al. (1994). These memory efficient and fast CG algorithms significantly decrease the execution time and memory requirements, and thus make possible the simulation of much larger (in terms of number of equations) systems in small machines. How efficient the code is running in different machines, is the main topic of this paper.

PCs SETUP AND REQUIREMENTS

The TOUGH2 code requires 64-bit arithmetic. When using a 32-bit machine (i.e., machines with 386, 486 or higher processor and MacIntosh Quadra 800 68040 CPU), it is necessary to modify the code to declare all variables REAL*8 (or DOUBLE PRECISION), and to comply with the FORTRAN77 ANSI X-3.9-1978 standards, also all floating point constants must be converted from E##.# to D##.# format. The processing speed of the code will depend on the machine being used. The maximum size of computational grids will depend on the amount of extended memory (XMS) available on the machine[2]. A minimum configuration to run TOUGH2/PC (Antúnez et al., 1994) would be a 386 PC equipped with 4 MB of RAM, an 80 MB hard drive and an optional (but recommended) numerical coprocessor (387). This configuration will allow to perform 3-D simulations[3] with grids of approximately 1,000 elements and 3,000 connections when using the CG solvers; or approximately 500 elements and 1,500 connections using the standard version of TOUGH2/PC with the direct matrix solver (MA28). The MacIntosh (Mac) performance was disappointing as will be discussed later, but memory requirements are similar to the PC's. By the time this paper was written Apple Computers made available the Power MacIntosh with a processor that uses RISC (Reduced Instruction Set Calculations) architecture and they claim that this machine runs two to six times faster than Quadras. If these specifications are correct, the Macs will be another small machine to consider to run large-scale geothermal simulations.

Very large models of up to 10,000 grid elements were run on a 486-DX2-66 MHz PC equipped with 32 MB of RAM and a 250 MB hard drive. TOUGH2/PC was compiled and linked using Version 5.0 of the Lahey Fortran Compiler for 32-bit machines (Antúnez, et al. 1994). The study was limited to grids with a maximum of 10,000 elements; however, the previous configuration should be able to handle models with larger number of elements. Antunez, et al (1994) concluded that the Lanczos-type Bi-Conjugate Gradient Squared [Sonneveld, 1989] was the fastest of the solvers and that it is the best choice on the basis of its performance efficiency, and its slightly faster than linear growth of computation time and memory requirements with problem size. For these reasons it was selected as the solver to use for the TOUGH2/machine's performance testing.

[1] Conjugate Gradient solvers are algorithms for the iterative solution of large sets of linear equations.

[2] Extended memory (XMS) is additional memory beyond the first MByte (MB) of random access memory (RAM). The first MB of RAM is usually occupied by the Disk Operating System (DOS), the 640 KB of DOS conventional memory and the Terminate and Stay Resident applications (TSR).

[3] 3-D simulations are the most memory demanding. 1-D and 2-D problems result in arrays of smaller size.

TESTING PROCEDURE

A two-phase, single porosity reservoir model for the Cerro Prieto geothermal field with irregular gridding, and considering production and injection was used as the test model.

The testing was based on the average time it took each algorithm to complete a Newtonian iteration, which consists of:

(a) Recalculating the terms of the Jacobian matrix that results from applying the mass and energy conservation equations at each grid element,

(b) Preconditioning and solving the matrix using the Bi-Conjugate Gradient Squared solver. The matrix solution provides the changes of all primary variables, i.e., pressure, temperature for single-phase elements, and pressure, vapor saturation for elements presenting two-phases, and

(c) recalculating all the secondary variables (density, internal energy, viscosity, relative permeabilities, capillary pressure, phase saturation, mass fractions of each component) for all the elements of the grid.

Each of the CG solvers performs "internal" iterations of the algorithm[4] (CG iterations) to a maximum specified by the user (usually 10% of the number of elements times the number of equations per element). A closure criterion of 10^{-6} is generally used for the solvers.

THE CERRO PRIETO MODEL

The Cerro Prieto geothermal field developed by the Comisión Federal de Electricidad (CFE), is located approximately 35 km south of Mexicali, Baja California, México. Since the beginning of the exploitation of Cerro Prieto in 1973, one of the most important operational problems that CFE has had to face was the handling of the waste brine [Hiriart and Gutiérrez Puente, 1992]. Up to date most of the brine is sent to evaporation ponds that presently cover an area of 18.6 km^2 (Figure 1). An infiltration area west of the ponds is used during the winter, when the evaporation rate is significantly lower.
During 1992 and 1993, CFE started a series of cold (approximately at 20°C) brine injection tests, using brine from the evaporation ponds. The objective of these tests was to monitor the reservoir's response to the injection and to test the injectivity of different areas of CP1 in the western part of the field. CFE's final goal is to inject all the separated brine back into the system, to eliminate its surface disposal and, at the same time, provide pressure maintenance to the reservoir.

Under the DOE/CFE cooperative agreement on geothermal energy, a numerical model for CP1 was developed, using data provided by CFE. The computational grid representing an area of 89 km^2, was defined based on the geological model of the field and the location and completion of the production and injection wells (Fig. 1).

In the vertical direction the model extends from the surface to 5,000 m depth, and is divided into six layers. All the layers have the same discretization and have 235 grid elements (Fig. 1), except for layer 5 that has 47 additional blocks in the NE simulating the volume of the CP2, CP3 and CP4 areas. An additional block was used at the top of the model to simulate the atmospheric conditions. The model used for this paper does not include the 47 elements in layer 5. Therefore, it has a total of 1411 elements and was developed as a single porosity model [Antúnez and Lippmann, 1992]. The model was calibrated against production and piezometric data, and was used to test several injection strategies.

The timing of the Newtonian iterations was conducted using the following scenario: Inject 3,500 t/h of 20°C water evenly distributed between injection wells M-48, 101, 104, E-6, O-473 and M-6. Production wells were assumed to produce at a rate equal to that measured at the end of 1991 (for that year, the average field production was 5,459 t/h of steam and 6,394 t/h of separated brine).

[4] Not to be confused with the Newtonian iterations which are external to the CG algorithm.

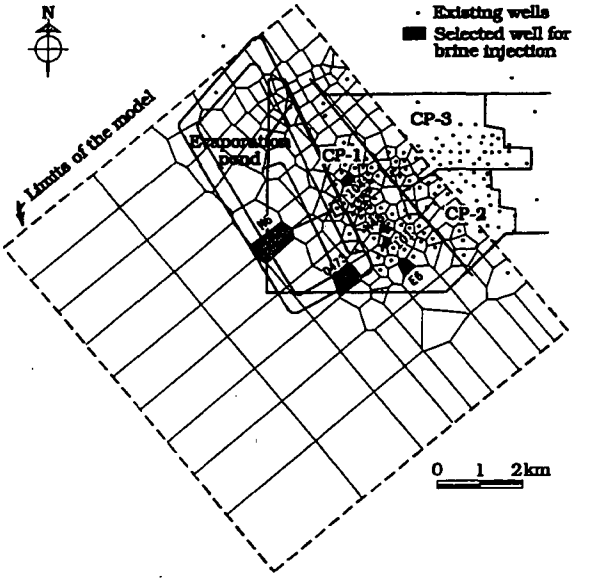

Fig. 1: Cerro Prieto model. Characteristics of the irregular computational grid.

Injection well locations are shown in Figure 1. The reservoir parameters used on the Cerro Prieto model are given in Table 1.

DISCUSSION OF RESULTS

All machines were allowed to run the Cerro Prieto model for 25 time steps. An average of 3 to 4 Newtonian iterations were required to reach convergence in each time step (see Fig. 2). Each Newtonian iteration for a given time step is identified in Fig. 2 with a number on the upper left quadrant of the symbol. The straight line corresponds to the arithmetic average of all iterations. To compare the performance of TOUGH2 on different machines, the average timing of all Newtonian iterations per run was plotted against the machine type; results are presented in Figure 3. Using the 486-33 timing as the basis for comparison, Figure 4 shows the relative performance for each machine.

Table 2 presents a summary of the test results using the different machines. The reported total number of iterations are the sum of: a) the Newtonian iterations (external iterations); b) the repeated external iterations in cases with convergence failure (after nine Newtonian iterations without reaching convergence, the incremental time used in the current time step is divided by five and the iteration procedure for that time step is repeated); and c) one "convergence" iteration per time step (iteration that does not need to call the solver since convergence has been attained). The average timing per Newtonian iteration only includes the completed Newtonian iterations; convergence iterations are not considered in this column. The CPU time corresponds to execution time for all iterations Newtonian and non-Newtonian, plus the time to write the output files.

Time comparisons for the different machines presented in Figures 3 and 4 and Table 2 indicates that the three PCs showed performances very similar to the high-end workstation IBM RISC 6000 and one of them, the PC Pentium 90, gave 50% faster performance than the workstation. At the current prices a well equipped Pentium 90 costs two to three times less than a comparably equipped RISC 6000. The MacIntosh developed some roundup errors that did not allow the simulation to advance in time. The problem was solved by tightening the closure criteria for the conjugate gradient (from $1x10^{-6}$ to $1x10^{-8}$).

Table 1: Reservoir parameters for the Cerro Prieto model

	Single-Porosity	Double-Porosity
Matrix properties		
density	2000-2800 kg/m^3	2000-2800 kg/m^3
porosity	5-20 %	15 %
saturated thermal conductivity	0.5-1.3 W/m °C	0.5-1.3 W/m °C
specific heat	600-2200 J/kg °C	600-2200 J/kg °C
permeability	0.1-100 md	0.001-1 md
initial steam saturation	spatially variable	spatially variable
Fracture domain properties		
rock grain density		2000-2800 kg/m^3
porosity		1 %
rock specific heat		600-2200 J/kg °C
fracture spacing		50 m
permeability		0.1-6,000 md
initial steam saturation		spatially variable

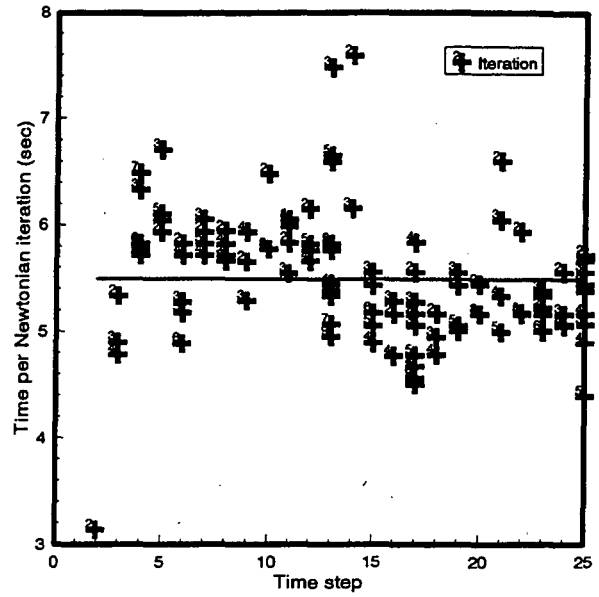

Fig. 2: Timing of Newtonian iterations for a 1411 element irregular grid for Cerro Prieto using the Lanczos-type Bi-Conjugate Gradient Squared solver on a PC with Pentium 90MHz CPU.

This way the roundup errors did not continue increasing and the Mac was able to attain the same total simulation time as the other machines.

The overall simulation took a higher number of Newtonian iterations to converge. The results for the MacIntosh presented in Figures 3, 4 and Table 1 correspond to the run conducted with the same closure criteria for the CG solver ($1x10^{-6}$) as for the other machines to keep a comparative basis.

It is worth noticing that the results presented in Figures 3, 4 and Table 2 reflect not only the performance of the machine but also the efficiency of the executable code produced by their respective Fortran compiler. Each of the compilers listed in Table 2 were used on their respective machine set to full optimization.

SUMMARY AND CONCLUSIONS

- Lawrence Berkeley Laboratory's general purpose simulator TOUGH2 together with a set of three preconditioned conjugate gradient solvers was ported to three PCs, a MacIntosh, and their performance were compared to a high end IBM workstation.
- The testing of the different machines was conducted using TOUGH2 and a Lanczos-type Bi-Conjugate Gradient Squared solver that was chosen based on its performance efficiency, and because of its slightly faster than linear growth of computation time

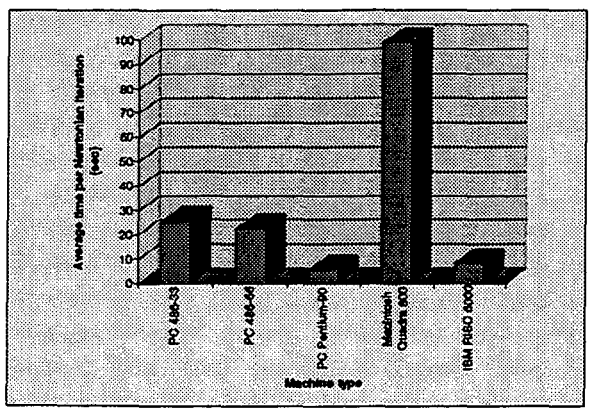

Fig. 3: Timing of Newtonian iterations for different machines using the Cerro Prieto model, the simulation code TOUGH2 and a Lanczos type biconjugate Gradient Squared solver

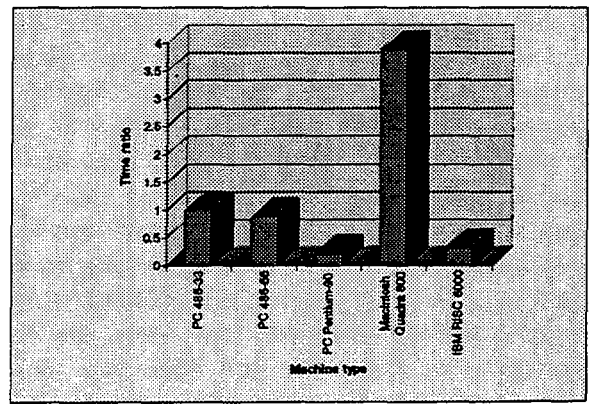

Fig. 4: Comparative performance ratio, taking the timing of Newtonian iterations of a PC 486-33 machine as the basis for the comparison.

and memory requirements with problem size.

- A two-phase, single porosity reservoir model for the Cerro Prieto geothermal field with irregular gridding, and considering production and injection into a model was used as the test model.
- This study demonstrates that the current PCs (386 and higher) are an economical and efficient platform to conduct large-scale three-dimensional geothermal reservoir simulations, and that they compare or surpass the performance of some of the most popular high-end workstations.

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REFERENCES

Antúnez, E., and Lippmann, M. (1993) Numerical Study of the Effects of Brine Injection on the CP1 Production Area of Cerro Prieto. Earth Sciences Division Annual Report 1992, Lawrence Berkeley Laboratory report LBID-33000, pp. 97-99

Antúnez, E., Moridis, G., and Pruess, K. (1994) Large-Scale Three-Dimensional Geothermal Reservoir Simulation on PCs. Proceedings of the Nineteenth Workshop on Geothermal Reservoir Engineering, Stanford, CA, pp 99-106.

Duff, I. S. (1977) MA28 - A set of Fortran Subroutines for Sparse Unsymmetric Linear Equations, AERE Harwell Report R 8730.

Hiriart, G.L. and Gutiérrez Puente, H. (1992) An Update of Cerro Prieto Geothermal Field, Twenty Years of Commercial Power. Geothermal Resources Council Bull. Sept/Oct, pp. 289-294.

Moridis et al., (1994) LBL Report on the implementation of the Conjugate Solvers to the TOUGH2 code, in preparation.

Pruess, K. (1991) *TOUGH2* - A General-Purpose Numerical Simulator for Multiphase Fluid and Heat Flow, Lawrence Berkeley Laboratory report LBL-29400.

Sonneveld, P. (1989) CGS, A fast Lanczos-type solver for nonsymmetric linear systems. SIAM J. Sci. Stat. Comput., Vol. 10, No. 1, pp. 36-52.

Table 2: Timing of the test runs for TOUGH2 with different machines

Newtonian iteration tolerance = 1×10^{-5}
Closure in CG solvers = 1×10^{-6}

	Number of iterations			Time (sec)						
Case	Total[5]	Newtonian	Repeated due to convergence failure	per Newtonian iteration	Input	CPU	Total execution	Simulated	Machine	Fortran Compiler
1	145	117	3	25.38	40.48	3130.70	3171.18	4.8061E8	486-33	Lahey F77L-EM/32 V. 5.2
2	145	117	3	22.26	29.22	2722.93	2752.15	4.8061E8	486-66	Lahey F77L-EM/32 V. 5.2
3	145	117	3	5.49	11.92	675.86	687.78	4.8061E8	Pentium-90	Lahey F77L-EM/32 V. 5.2
4	198	160	13	98.68	377.47	17151.87	17529.33	4.1951E8	Mac Quadra 800	Language Systems V. 3.0
5	145	117	3	8.10	28.98	1009.50	1038.93	4.8061E8	IBM RISC 6000	6000 V.2.3

[5] The total number of iterations column includes one additional convergence iteration per prescribed time step, 25 in total. At each iteration convergence is checked and if satisfied a new time step is started.

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