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

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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 Maclntosh 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 piper, non-condensable gases, salinity and chemical processes have to he 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 rhe 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) There memory efficient and fast CG algorithms significantly decrease the execution time and memory requirements, and **thus** make possihle 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 Maclntosh Quadra 800 68040 CPU), it is necessary to modify the code to declare **all** vanables REAL*8 (or DOUBLE PRECISION), and to comply with the FORTRAN77 ANSI X-3.9-1978 standards. also all floating paint constants must be converted from E##.# to D##.# formal. The processing speed of the *code* will depend on the machine king 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 TOUGHUPC (Antúnez et ill., 1994) would be **a** ***386*** PC equipped with 4 MB of RAM. an 80 MB hard dive and an optional (but recommended) numerical coprocessor (387). This configuration will allow to perform **3-D** simulations] with gnds 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 TOUGHUPC with the direct matrix **solver** (MA28). The Maclntosh (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 Maclntosh 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 an 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 f a 32-hit 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 **an** 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 hy** 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 **problem** result in arrays of smaller size

TESTING PROCEDURE

A two-phasr. 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' (CG iterations) to a maximum specified hy 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 CERKO 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 CPI 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 DOFJCFE cooperative agreement on geothermal energy. a numerical model for CPI was developed. using data provided by CFE. The computational grid representing an area of 89 km^2, war 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. l). 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

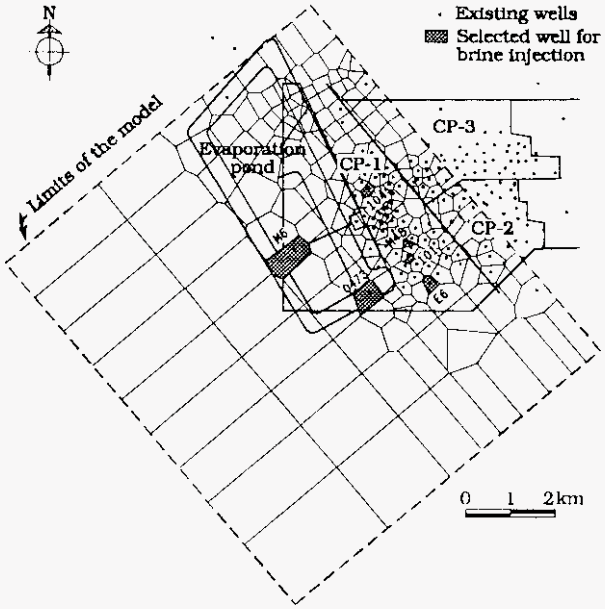

Fig. 1: Cerro Prieto model. Characteristics of the irregular computational grid.

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

DISCUSSION OF RESULTS

All machines were allowed to run the Cerro Prieto model fur 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 liming as the basis for comparison, Figure 4 shows the relative performance for rach machine.

Tahle 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 limed 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 hy tightening the closure criteria for the conjugate gradient (from $1x10^{-6}$ to $1x10^{-8}$)

Table I: Reservoir **parameters far 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	

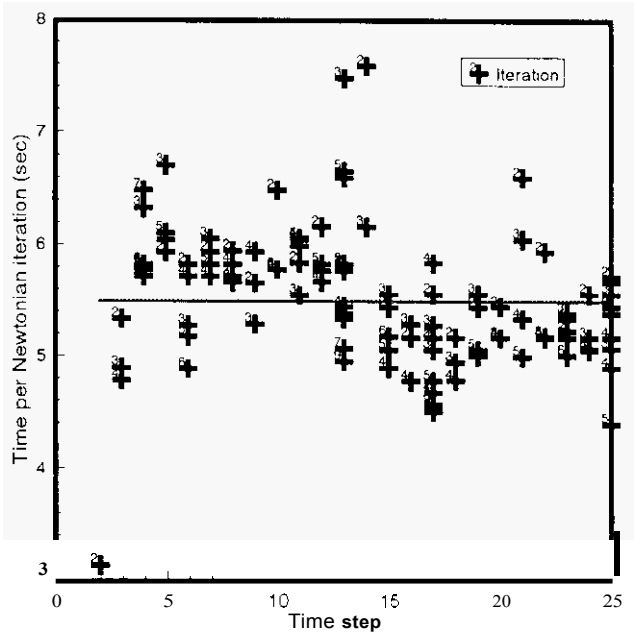

Fig. **2:** Timing **of Newtonian** iterations **far a 1411 element irregular grid for Cerro** Prieto using the Lanczos-type Bi-**Conjugate** Gradient Squared solver on **a** PC **with** Pentium **90MHz CPU.**

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 I 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 hut 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 thr 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

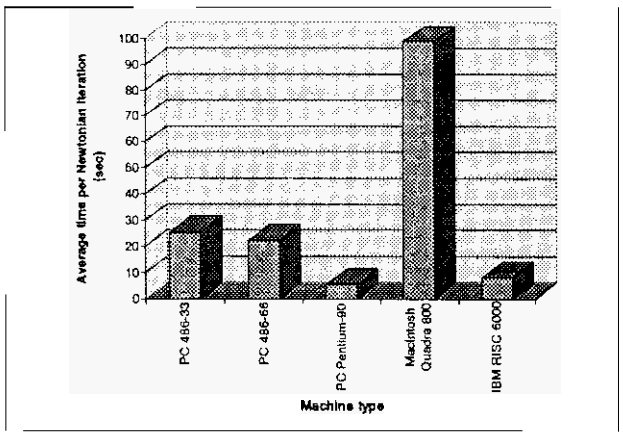

Fig. *3:* **Timing of Newtonian** iterations **for different** machines using **the** Cerro Prieto **model,** the simulation code **TOUGH2 and a Lanczos** type **biconjugate** Gradient **Squared solver**

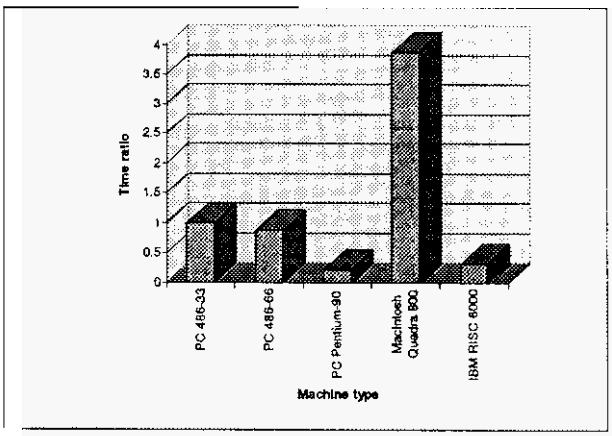

Fig. 4: Comparative performance ratio, taking the timing of Newtonian iterations of a PC 486-33 machine as the basis for the comparison.

and memory requirements with problem size

- A two-phase. single porosity reservoir model far the Cero 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 tu 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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Table 2: Timing of the test runs for TOUGH2 with different machines

Newtonian iteration tolerance = $1x10^{-5}$
Closure in CG solvers = $1x10^{-6}$

	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.