

USE OF TOUGH2 ON SMALL COMPUTERS

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ABSTRACT

TOUGH2/PC has been tested extensively on different PC platforms (486-33, 486-66, Pentium-90), with encouraging results. TOUGH2 performance has also been tested in other 32-bit computers as the MacIntosh Quadra 800, and a workstation IBM RISC 6000. Results obtained with these machines are compared with PCs' performance.

PC results for 3-D geothermal reservoir models are discussed, including: (a) a Cartesian; and (b) a geothermal reservoir model with 1,411 irregular grid blocks. Also discussed are the results of the TOUGH2-compiler performance tests conducted on small computer systems.

Code modifications required to operate on 32-bit computers and its setup in each machine environment are described.

It is concluded that in today's market PCs provide the best price/performance alternative to conduct TOUGH2 numerical simulations.

INTRODUCTION

The PC version of TOUGH2 [Pruess, 1991] was released to the Energy Sciences and Technology Software Center (ESTSC) in January 1995, for distribution. Prior to its release the code was extensively tested by LBL staff and selected Beta Testers. Because of the flexibility/price/performance of the PC environments, the applications and the demand for the TOUGH2/PC code have been steadily increasing.

The success of the PC version of the code has been mainly due to two factors: (a) the migration of applications from mainframes and workstations to PC platforms is completely transparent; and (b) to the addition of a set of three preconditioned conjugate gradient solvers¹ (CG) to TOUGH2 [Moridis *et al.*, 1995]. These solvers make a more

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

efficient use of memory and also provide matrix solutions faster than direct solvers, allowing the processing of larger simulation models in terms of number of grid elements and number of equations to solve. Models of 10,000+ grid elements have been processed successfully with TOUGH2 on PC type computers [Antúñez *et al.*, 1994, 1995]. All versions of TOUGH2 distributed by the ESTSC have been updated to include the CG solvers package to complement its standard direct solver MA28 [Duff, 1977].

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 TOUGH2 applications traditionally executed on mainframes and minicomputers had started migrating towards the more cost-effective PC platforms. The PC code is currently being used at LBL in geothermal reservoir engineering, nuclear waste disposal, environmental restoration, and unsaturated groundwater hydrology.

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 machine². A minimum configuration to run TOUGH2/PC (Antúñez *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 simulations³ 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) memory requirements are similar to the PC's.

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 (Fig. 1). TOUGH2/PC was compiled and linked using Version 5.0 of the Lahey FORTRAN Compiler for 32-bit machines (Antúñez, *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. Antúñez, *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 only slightly faster than linear growth of computation time and memory requirements with problem size. For

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.

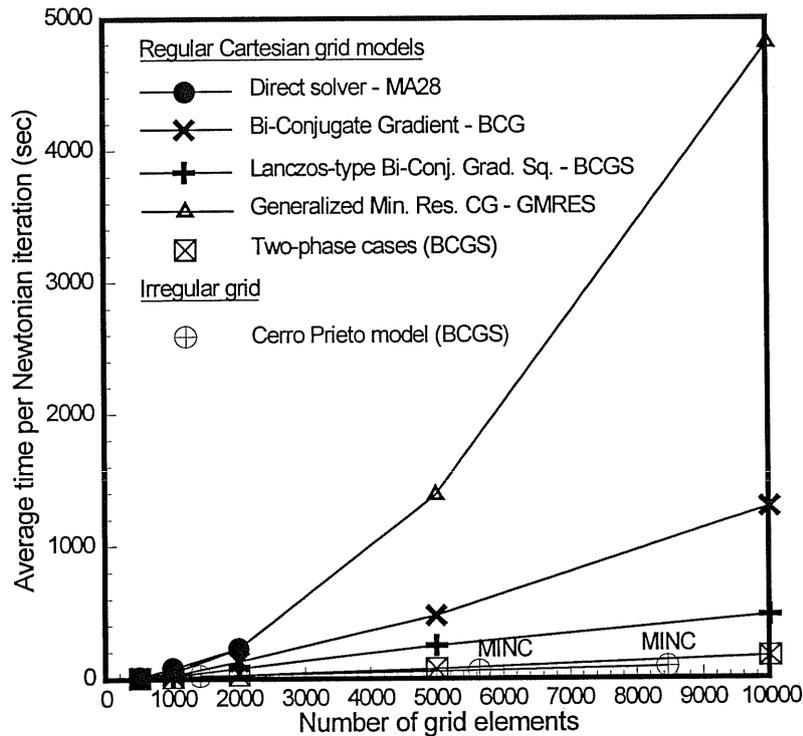


Fig. 1: Timing of Newtonian iterations for each of the analyzed matrix solvers as function of problem size [Antúnez *et al.*, 1994]

these reasons it was selected as the solver to use for the TOUGH2/machine's performance testing and became the default solver on the updated versions of TOUGH2.

DISCUSSION OF RESULTS

To compare the performance of the different solvers, the average timing of all Newtonian iterations⁴ per run was plotted by Antúnez *et al.*, (1994) against the number of elements in the grid. Timing data of the various solvers are presented in Fig. 1.

⁴ 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 (except for the direct solver MA28) and solving the matrix using one of the CG solvers. The matrix solution provides the changes of all primary variables (pressure, temperature) for single-phase elements or (pressure, vapor saturation) for elements in 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. For each Newtonian iteration, the CG solvers perform "internal" iterations of the CG algorithm (CG iterations) up to a hardcoded maximum (usually 10% of the number of elements times the number of equations per element). A closure (convergence) criterion of 10^{-6} was used in all three CG solvers.

Cartesian models and an irregular grid model developed for the Cerro Prieto geothermal field [Antúñez and Lippmann, 1993] were used to test the matrix solvers. The Cerro Prieto model was used for testing with: (a) a single porosity and (b) double-porosity formulations. The MINC method [Pruess, 1991] was used for the double-porosity calculations. From this study it was concluded that:

- Time comparisons for the different tested cases indicate that of the three CG tested, the BCGS solver showed the best performance, followed by BCG, MA28 and GMRES.
- The tested conjugate gradient solvers significantly reduced the execution time and storage requirements, making possible the execution of considerably larger problems (10,000+ grid blocks) on PCs.
- Memory requirements for TOUGH2/PC with the conjugate gradient solvers are approximately linear
- The Antúñez *et al.*, (1994) study demonstrates that the combination of the analyzed preconditioned conjugate gradient solvers and the current PCs (386 and higher) are a feasible, economical and efficient combination to conduct large-scale three-dimensional simulations that just a few years ago could only be executed on mainframe computers and high-end workstations.

It is important to emphasize that iterative methods are problem specific. A solver that showed good performance for a given problem is not guaranteed to work for all problems. Testing of the solvers with a specific problem is strongly recommended to determine which is the best for the task.

A comparison of the performance of TOUGH2 on different machines was conducted by Antúñez *et al.* (1995). The average timings of all Newtonian iterations per run were plotted against the machine type and are presented in Figure 2. Time comparisons for the different machines presented in this figure indicate that the three PCs showed performances very similar to the high-end workstation IBM RISC 6000 (model 320H-7012) and one of them, the PC Pentium 90, gave 50% faster performance than the workstation. At the current prices a well-equipped Pentium 90 - based PC costs three to five 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 1×10^{-6} to 1×10^{-8}). 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.

By the time this extended abstract 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.

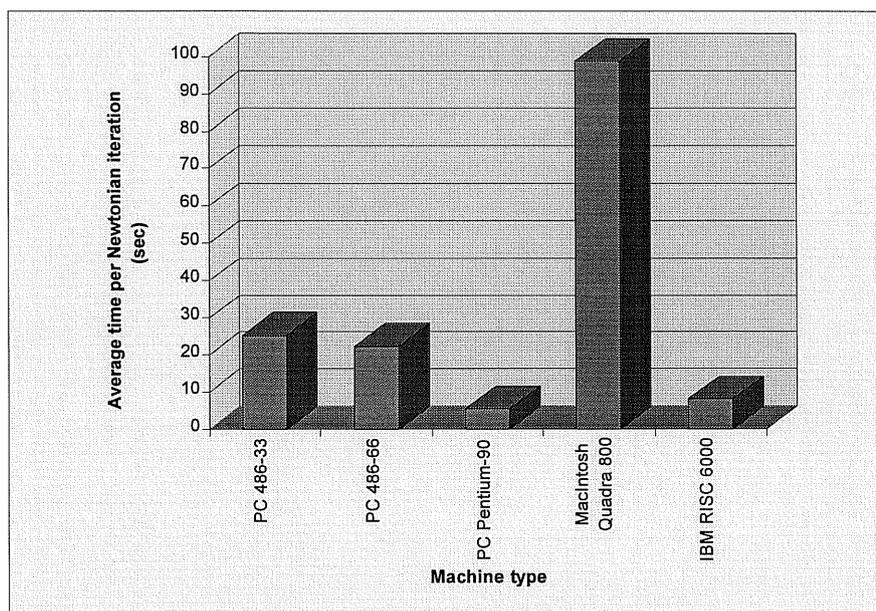


Fig. 2: Timing of Newtonian iterations for different machines using the Cerro Prieto model, the simulation code TOUGH2 and a Lanczos type biconjugate Gradient Squared solver [Antúnez *et al.*, 1995].

It is worth noticing that the results presented in Fig. 2 reflect not only the performance of the machine but also the efficiency of the executable code produced by its respective FORTRAN compiler. The details of the compilers used on each machine are given by Antúnez *et al.*, (1995). Each FORTRAN compiler was used on its respective computer system set to full optimization.

The discussed studies by Antúnez *et al.*, (1994 and 1995) demonstrate that the current PCs (386 and higher) are an economical and efficient platform to conduct large-scale three-dimensional simulations, and that they compare or surpass the performance of some of the most popular high-end workstations.

DISCLAIMER

Mention of specific products and/or manufacturers in this document implies neither endorsement of preference nor disapproval by the U.S. Government, any of its agencies, the University of California, or LBL of its use for any purpose.

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