Solving Coupled Geoscience Problems on High Performance Computing Platforms

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Abstract. This paper describes a finite element geo-process modeling software, which is able to solve multiphysics problems in the area of geo science. It is one of the first applications providing complete thermal, two-phase-flow, inelastic deformation court within one framework. As a real-life example the FEBEX TH^2M coupling problems are described. These kind of problems are very demanding in terms of CPU time and memory space which cannot be provided by single processor architecture. Therefore the exploitation of high performance architectures is required. Here we present the results of the vectorization of the existing serial code as a first step towards parallelization.

1 Introduction

Modeling complex coupled transient and dynamic processes found in geo-systems requires increasingly high resolution models for a more precise and qualified validation and evaluation. The more exactly the investigation of the given problem can be accomplished, the better the utilization, management and planning of the given geo-resources can be undertaken.

1.1 GeoSys/RockFlow

GeoSys/RockFlow (GS/RF) [1] is a finite element geo-process modeling software tool finding increased application in modeling and simulation in fields such as water resource management, geotechnics, design of geo-engineered barriers, exploitation of geothermal energy, soil and groundwater contaminant transport and remediation strategies. Its current design is based upon a sequential approach.

Here we present a new project which started in fall 2004 and is funded by the German Research Foundation (DFG) and the State of Baden-Wuerttemberg (BW). Its goal is to bundle the knowledge of the experts at the High Performance Computing Center (HLRS) in Stuttgart and the scientists and researchers working at the Center for Applied Geology, (ZAG) at the University of Tuebingen. This project is truly interdisciplinary and multinational as specialists in mathematics, computer science, hydrology, geo science, chemistry, just to name a few,

are continuing to develop the already existing serial software and to finally transform it into a GRID application deploying massive-parallel systems in Stuttgart and Tuebingen.

2 GeoSys/RockFlow Model Features

The finite element simulator GS/RF covers a wide range of physical and chemical processes relevant to environmental hydrosystems. The processes can be grouped in 4 different categories as summarized below:

1. **Hydrological Processes:**
  - Groundwater flow in confined and unconfined aquifers
  - Multi phase flow
  - Fracture flow, dual porosity
  - Density dependent flow (thermal, tracer)
  - River flow (based on averaged 1-D Saint-Venant equations)
2. **Thermal Processes:**
  - Heat transport with density changes
  - Non isothermal multiphase flow with phase changes
3. **Chemical Processes:**
  - Multi-component transport with density changes
  - Sorption models
  - Reactive Transport (i.e. Freundlich Isotherm)
  - Chemical reactions via coupling to PHREEQC2
4. **Mechanical Processes:**
  - Poro elasticity
  - Thermo elasticity
  - Elasto plasticity (hardening)

Models can be created and run using a graphical user interface (Windows application). Built-in mesh generators are: gmsh, PrisGen and TetMesh. Meshing of complex structures can be done using gOcad or the pre-processor GINA developed by the Federal Institute for Geosciences and Natural Resources (BGR). Hybrid meshing is possible. ArcGIS shape files can be read and converted to polylines which are then used to create meshes or assign boundary or initial conditions etc. An interface to Gstat allows for the generation of three dimensional heterogeneous conductivity fields. Two dimensional contour plots and time-value graphs are displayed during the simulation in the GUI or Tecplot output files are written directly or created with the post-processor RF2TP also developed by the BGR.

Despite its long history dating back to 1985 the code is programmed according to recent programming principles. The software was constantly improved. In 2003/2004 the code underwent a major re-organization to benefit even more from object-orientation and to allow an easier switching between process couplings. Most recent changes are: use of C++, organization of RockFlow into GeoSys: GEOLib, MSHLib, FEMLib and the creation and encapsulation of process-oriented objects (PCS). These changes provide a solid basis for further program development within a growing research team.

3 The FEBEX Experiment

As an example of the necessity of high performance computing in environmental science we present results of different simulations of the FEBEX experiment [2] which is a full scale engineering barriers experiment in crystalline rock (Fig. 1) for high level radioactive waste (HLW) repository.

Fig. 1. Layout of the FEBEX experiment

In the experiment, the heaters experienced a temperature of 100°C . Bentonite was used as filling material (geotechnical barrier) around the heater. The heaters and geotechnical barrier were in a tunnel (2.4 m in diameter) surrounded by granite. The bentonite swells as a result of the intrusion of ground water from fractures. The swelling effect changed the microstructure of bentonite, i.e. porosity and in particular permeability of the bentonite. On the other hand it increased the swelling pressure and accordingly the effective tension in the bentonite. The expanded bentonite in turn exerted pressure on the surrounding granite and affected the stress conditions and possibly the water path in it. Gas was produced by the high temperature of the heaters from the water, which moved outward. The experiment was conducted in order to understand the thermo-hydro-mechanically (THM) coupled phenomena in the bentonite and surrounding granite and furthermore provide a valid reference for long term HLW repository.

3.1 Simulation Results

One part of the simulation was the analysis of the TH^2M coupling problems (always with the same boundary conditions and with the same material parameters) using a fine mesh of 3276 nodes and 2640 hexahedra. The geometry and mesh are depicted in Fig. 2, in which a cross section close to the front of the present saturation propagation is selected to portray the inside domain and z direction points downward in order to permit a close look around the canister surface.

In the following figures (Fig. 3) the primary variables of the TH^2M simulations after 10 ($t = 10^5$ sec) time steps are depicted.

The FEBEX simulations are to our knowledge the first all-in-one 3D fully coupled TH^2MC^n simulations in which the complete thermal, two-phase-flow,

Fig. 2. Mesh and slice section

inelastic deformation court is provided by one unique code. TH^2MC^n simulations are very sensitive to time and space scale discretizations and such simulations are very expensive with respect to computation time.

3.2 FEBEX Performance

The results obtained from this analysis show strong TH^2M coupling phenomena in the present FEBEX type problem. The change of displacements and stresses is large in the buffer. This change is partially due to the material properties of the buffer but mainly it is induced by stiff boundary condition around the buffer. Therefore, the safety assessment must be focused on this domain. This computation required much more CPU time due to the necessity of solving four algebraic equations within coupling iterations, nonlinear iterations for different processes. For example, a converged Newton step for plasticity deformation took an average of 2.5 hours using a machine with an Intel III 2.0GHz CPU. To compute 100 time steps of FEBEX on 4 processors the serial version of GS/RF runs nonstop for one week. To improve computation efficiency high performance computing on powerful parallel machines has to be deployed.

4 Parallelization Strategy

Today's modern single processor machines are not powerful enough to process large scale models necessary for the realistic simulation of in situ highly complex geoscience systems.

Through the combination of the wide field of geoscience and high performance computation supported through effective algorithms found in computer science a complete new level in simulation and modeling can be attained. The final goal is to compute models consisting of more than ten million of elements with a higher grade of specialization.

Fig. 3. Primary variables of TH²M simulations for $t = 10^5$ sec

4.1 Computing Platform

The target parallel platform for the work presented in this paper is a GRID consisting of three parallel computing platforms, located at the computing center of

the University of Tuebingen, the HLRS in Stuttgart and a institute-own Linux cluster. As the most powerful environment within the GRID can be found in Stuttgart we have ported a first version of GS/RF on a NEC SX6 at the HLRS. The SX6, in summer being replaced by a SX8, implements a parallel architecture with distributed memory, in particular a cluster of symmetric multi-processors (SMPs). Each of its SMP nodes consists of 8 vector processors. To take advantage of the features of such an architecture the code has to be vectorised and parallelized.

In order to run an application on such a computational environment the work and the data have to be distributed among the processors. The decision that has to be made is what work will be done on which data. In case each process is performing a different task on different data we are talking about a MPMD (Multiple Program Multiple Data) programming model. If on the other hand the same program is running on every processor but with different data, this corresponds to a SPMD (Single Program Multiple Data) programming model. In this project we decided to use the SPMD paradigm.

Domain decomposition and load balancing techniques are a very suitable way of decomposing data and work in numerical analysis. Using load balancing tools like those of *Jostle*[3], *Metis* [4] or *ParMetis* the original computational domain can be divided into a number of subdomains, equal to the number of available computing units, and these subdomains can be distributed to the processors. In this way the resulting linear systems become smaller compared to the global one. Generally, the two CPU time-consuming parts of a finite element program are the calculation of the entries in the system matrices (element loop) and the solving of the resulting linear systems.

In particular, the calculation of the system matrices is done element-wise without any dependency on the computation between different elements. Therefore, the contributions of different elements can be calculated on different processors. When solving the linear system of equations additional care has to be taken for the unknowns residing on the artificial boundaries.

5 GS/RF Performance

We tested GS/RF on the SX6 with an artificial 2D test model consisting of 10620 elements.

The fastest solver used to solve the linear system of equations is the BiCGSTAB method. Applying the original non-optimized code took 3412.62 seconds and achieved 21.2 MFlops on one NEC SX6 processor. A more detailed analysis of the relevant GS/RF code showed that the most CPU time-consuming part of the BiCGSTAB algorithm is the matrix-vector multiplication. 99.7 % of the CPU time (3403.294 sec) is spent in computing the matrix-vector product.

The available NEC compilers offer directives which support code vectorization. Employing some of these directives the same test case terminates after only 74.04 secs, thus achieving a performance of 1015.1 MFlops. The overall

Table 1. Comparison of non-vectorized and vectorized code versions

	non-vectorized version		vectorized version	
	total	matrix-vector	total	matrix-vector
Computation time [secs]	3412.62	3403.29	74.04	63.46
Performance [MFlops]	21.2	21.2	1015.1	1182.6

time spent in the matrix-vector multiplication of the vectorized code is only 63.46 seconds at a rate of 1182.6 MFlops. Table 1 summarizes these performance measurements.

Fig. 4 depicts the resulting pressure distribution between the top right and bottom left corner of the computational domain calculated on the SX6.

Fig. 4. Pressure distribution between top right and bottom left

Not all codes are suitable for vectorization. Our results presented above show that the GS/RF code is suitable for vectorization.

Our real-world target models consist of hundreds of millions of elements. Thus, in order to take advantage of the architecture of the NEC SX6 and the SX8 respectively and to achieve higher performance, it is necessary to parallelize the code. The next step of our project is therefore to implement a parallel version of the BiCGSTAB algorithm based on domain decomposition and load balancing techniques. In a later stage GS/RF should be imbedded either in the *Globus* [5] or *UNICORE* [6] environment. For parameter studies the usage of *Condor* [7] seems to be very interesting.

6 Conclusion

In this work we have presented a geo-process software system, modeling complex coupled processes found in geo-systems. The results of the simulation of the FEBEX problem, a full scale engineering barriers experiment in crystalline rock for high level radioactive waste (HLW) repository show that the use of conventional hardware impose limitations on reliable modeling and simulation due to computation time.

A GRID environment can provide and enable the exploitation of the necessary resources to overcome the above mentioned limitations. As shown in this paper, vectorization of the serial GS/RF code leads to performance gains which is the first step in porting the code to high performance computing architectures. Further work on the GS/RF code will be done on parallelizing the solver algorithm alongside the coupling of shallow water and groundwater flow, as well as including kinetic biogeochemical reactions as well as improving the multi-view and three-dimensional graphics for the GUI.

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