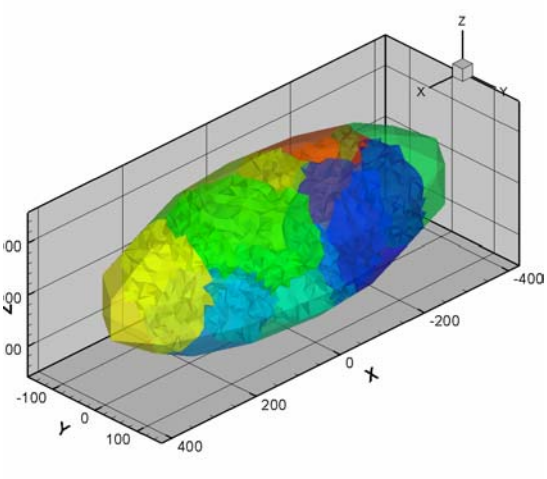
University of Tübingen
Center for Applied Geosciences
GeoSystemsResearch

LANDESSTIFTUNG
Baden-Württemberg

Ideenwettbewerb

Modellierung und Simulation auf Höchstleistungscomputern



Höchstleistungsrechnen in den Angewandten Geowissenschaften

Abschlußbericht

O Kolditz, P Adamidis, S Bauer, Y Du, M Hess, D Kemmler,
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High Performance Computing in Applied Geosciences

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1 Project summary

This report presents development, implementation and use of High Performance Computing (HPC) methods in order to solve modelling problems in applied geoscience. These applications are mostly not academic problems but have arisen from field work at several 'real' investigation sites. 'Real world problems' are still very difficult to simulate, because available conventional computing power is still too low for detailed structure models for geosystems. Especially the problems that we are dealing with in this project are influenced by a lot of complicating aspects like multi-field (e.g. thermo-hydro-mechanical-chemical (THMC) coupled) and multi-scale problems. Numerical results are given which provide the complete thermal, two-phase-flow, inelastic deformation court (TH^2M problems).

For the computing part we develop the open source, scientific software platform GeoSys/RockFlow (GS/RF) which is based on numerical domain schemes (finite elements and finite volumes). GS/RF is relying on object-oriented methods and the parallelization concept as well.

Four applications from different disciplines in applied geosciences are presented. The analysis of the geotechnical FEBEX and DECOVALEX experiments, which require fully coupled TH^2M (two-phase flow) simulations. Further applications presented in this paper are models for water resources management purposes in the Jordan Valley area and geothermal reservoir analysis of the Bad Urach hot-dry-rock site in South Germany. Finally, an application of a parallel regional soil model for the Reuze-Beerzel drainage basin is presented. These numerical models are very demanding in terms of computation time and memory requirements which exceeds the capabilities of single processor architecture. The introduction of HPC methods in geoscience was very important for more realistic models capturing the complex structure of geosystems as well as all related processes.

2 Conducted research work

2.1 Introduction

With increasing computing power it is becoming feasible to tackle real world problems with High Performance Computing (HPC). In the area of geoscience employing HPC can reduce the amount of field work done, it can save money by reducing the monitoring facilities. Unfortunately nature is not very kind to modelers, so the models have to be complex to cover even the most relevant aspects of geoscience problems, in order to produce good results that really can substitute costly field work. Another strong point for employing HPC in geoscience are long term forecasts. Because of the limited human life-span, forecasts can only be done with the help of modelling. But because of the long times involved in these forecasts, many time steps are required to obtain even qualitatively correct results.

2.2 Model features

The finite element simulator GeoSys/RockFlow (GS/RF) [1] covers a wide range of physical and biogeochemical processes relevant to geo- and hydrosystems. The processes can be grouped in four different categories as summarized below:

- **Hydromechanical processes:**
  - Groundwater flow in confined and unconfined aquifers
  - Multi phase flow, gas flow
  - Fracture flow, dual continua
  - Density dependent flow (thermal, salinity)
  - River flow (based on averaged 1-D Saint-Venant equations)
  - Overland flow (based on averaged 2-D Saint-Venant equations)
- **Thermal processes:**
  - Heat transport with density and viscosity changes
  - Non isothermal multiphase flow with phase changes
- **Chemical processes:**
  - Multi-component transport with density changes
  - Reactive Transport
  - Sorption models
  - Equilibrium and kinetic chemical and biogeochemical reactions
- **Mechanical processes:**
  - Poro-elasticity
  - Thermo-elasticity
  - Visco-elasticity (creep)
  - Elasto-plasticity (hardening)
  - Dynamic deformation

GS/RF finds 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.

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.

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 (project start) 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/RockFlow consisting of three object-libraries GEOLib, MSHLib, PCSLib as well as the creation and encapsulation of process-oriented objects (PCS) [2], [3]. These changes provide a solid basis for further program development within a growing research team.

Within this project the original serial software of GS/RF was transformed into a object-oriented performing, parallel system (section 2.3).

2.3 HPC Methods

In this section we will describe briefly the methods employed from the field of High Performance Computing (HPC). We used different approaches to HPC: parallelization, domain decomposition and vectorization which have been incorporated into GS/RF in order to be flexible in the variety of applications.

From the top 500 list of Supercomputers [4] it is clear that nearly all HPC architectures are based on distributed memory and a lot of them are cluster-like or clusters themselves. At the same time modern PC-CPUs get more computing cores which share memory and caches and increasingly vector operation sets, e.g. SSE3, are used in these processors. One of our target platforms is a NEC SX-8, a cluster of vector SMP nodes. Hence we also contemplate vector optimizations and consider shared memory cluster nodes.

Parallelization There are two obvious strategies for the parallelization of GS/RF.

1. Due to the many processes that have to be calculated, one can execute loosely coupled processes in parallel and synchronize them every once in a little while. This parallelization strategy requires careful analysis of the coupling strength of the different processes to prevent communication bottlenecks.

This parallelization concept has been successfully applied for the simulation of regional flow processes in watersheds (section 2.4).

2. As GS/RF is based on finite elements we use well established methods for the parallelization in the first place. There are basically two steps when using finite elements. Firstly, one has to assemble an equation system from the node values of the elements and then this equation system must be solved. If the target architecture is a distributed memory system, domain decomposition techniques are used (see section 2.3) to partition the calculation domain into smaller pieces which in turn are processed by different computing nodes. Every computing node assembles a local equation system and prepares the data in such a way that the resulting global equation system can be solved. Depending on the solver preconditioning should also be done concurrently. The PetSC library [5] provides exactly these features. In future we aim to implement more sophisticated methods, based on the work of Nakajima [6], which promises a huge performance gain, especially for the SX-8.

Domain Decomposition Each parallelization has to deal with the determination of subdomains and their assignment to processors. Therefore, the original FE grid is transformed into an adjacency graph, Fig. 1, which serves as a better foundation for the following decomposition process. The partitioning process tries to find a good distribution of the input data of equally sized chunks as there are numbers of processors. This is essential in regard to load balancing and communication aspects.

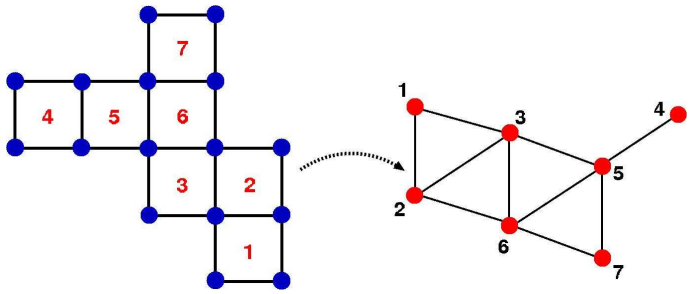


Fig. 1. Transformation of FE grid into an adjacency graph

Load balancing refers to the practice of distributing work among processing nodes so that all computing units are kept busy all the time. It can be considered a minimization of task idle time. Load balancing is also important to parallel programs for performance reasons. If, for example, all tasks are subject to a barrier synchronization point, the slowest task will determine the overall performance which can be seen in Fig. 2.

The second important aspect of load balancing and therefore the need of domain decomposition is the ratio between computation and communication. In

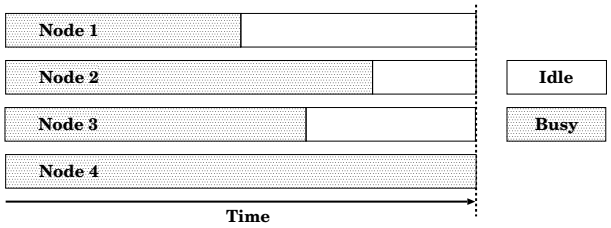


Fig. 2. Load balancing: slowest node determines the overall performance

parallel computing, granularity is a qualitative measure of this ratio. Periods of computation are typically separated from periods of communication by synchronization events. There is no general receipt of the most efficient granularity. The best granularity depends on the algorithm and the hardware environment in which a program runs. In most cases the overhead associated with communication between the processing nodes and their synchronization is high relative to execution speed so it is advantageous to have a coarse granularity. A fine-grain parallelism can help reduce overheads due to load imbalances. I/O operations are generally regarded as inhibitors to parallelism.

With an effective domain decomposition the number of edges crossing partition boundaries can be minimized and thus communication is reduced to the smallest possible extent. The related mapping problem to the domain decomposition is NP-complete and there exist almost no efficient sequential or parallel heuristics which solve this problem sufficiently. There are a couple of well known domain decomposition tools available like Jostle [7] or Metis [8], Fig. 3.

Inputfile:	Heat Flow, 2D
Number of Nodes:	1002001
Number of Elements:	2000000
Type of Elements:	triangle
Number of Partitions:	50

Jostle		Metis
1.0300	Balance Factor	1.0284
88527	Number of Cut Edges	98585
41196	Size of Biggest Partition	41136
29776	Size of Smallest Partition	38834
82575.5	Processing Time of Tool (ms)	16800.1

Fig. 3. Results from Jostle and Metis of a 2D FE grid with 2 mio. elements

Vectorization In order to be able to exploit a vector processor it is necessary that the code can be vectorized by the compiler. This means that special data structures have to be implemented, which support vectorization.

One major part of a finite element program is the solution of the resulting linear system of equations. One of the solvers used in GS/RF is the BiCGSTAB

method. The most CPU-time consuming operation is the matrix-vector multiplication where the matrix is sparse. The best known data structure for this type of operation for vector computers is the *Jagged Diagonal Format* (JDF).

Applying the original non-optimized code with the *Modified Sparse Row* (MSR) on a problem consisting of 1002501 nodes on the NEC SX-8 took 15043.83 sec of total CPU time. The time spent in the matrix-vector multiplication was 13981.15 sec (92.9CPU-time). With the JDF the time needed for the matrix-vector multiplication drops down to 193.20 seconds and the total CPU time is now 1286.18 sec.

2.4 HPC Applications in Geoscience

Today's modern (single) processor machines and desktop computers are improving in terms of speed, performance and storage capacity. However, they are far from being powerful enough to process large scale numerical models necessary for the realistic simulation of highly complex geosystems. Through the combination of geoscience and high performance computation, supported by effective mathematical algorithms developed in computer science, a new level in environmental modelling can be attained. To reach the aim of computing numerical models with several million grid nodes, parallel computation methods have to be used. Computational work as well as the required data have to be distributed to the individual processors of a parallel computer by domain decomposition techniques or process parallelization. Utilization of these techniques for geosystem analysis will allow for a much needed move towards realistic integrated modelling.

Computational analysis of geosystems offers challenges to high performance computation in many ways. In the first sense this is related to the inherent complexity of physico-chemical-biological (THMC) processes as well as the geometric complexity (3-D, multi-scales) of real-world applications. We present results of HPC application in following areas:

- Geotechnics (section 2.4)
- Water resources (section 2.4)
- Geothermics (section 2.4)
- Watershed hydrology (section 2.4)

THM Processes in Geotechnical Applications Numerical analysis of thermo-hydro-mechanical (THM) coupled problems leads to an extremely high computational expense. Several geotechnical applications, in particular for waste management problems, have been successfully conducted, such as simulations of the FEBEX experiment [3] and the DECOVALEX test cases which represent full scale engineering barriers experiments in crystalline rock (Fig. 4) for high level radioactive waste (HLW) repositories.

In this section we briefly present the methodology for the reduction of the computational expense for THM coupled multi-field problems by parallel computing methods [9] and some illustrative results. To this purpose, parallelization is applied to the most time consuming portions of finite element simulations, i.e.

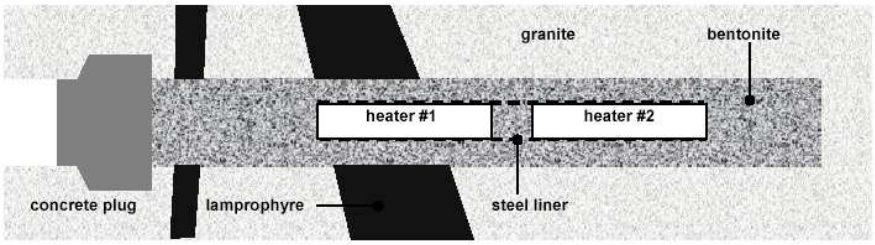
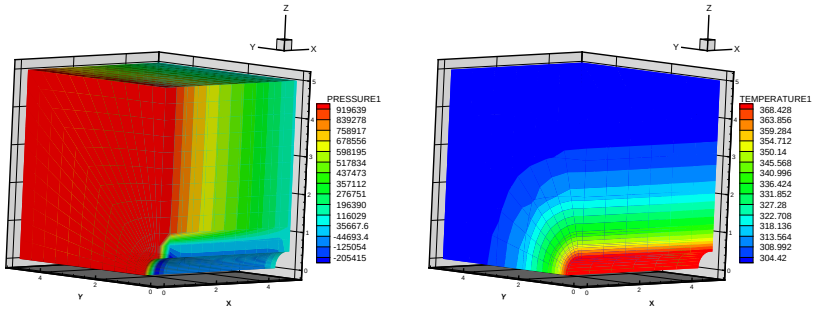


Fig. 4. Layout of the FEBEX experiment

assembly of linear equation systems (LES) and solving them. Since an iterative solver is adopted in the present study, the sub-structuring technique of domain decomposition plays an important role in both assembly and solving of LES. Three principles of the parallelization procedure are: (1) all processes of a coupled problem share a unique finite element mesh; (2) this mesh is discretized into sub-domains, each of them are established with mesh topology for both linear and quadratic interpolation, the assembly of linear equation systems is performed in sub-domains and is distributed to the involved processors (CPU-nodes); (3) matrix-vector multiplications, which are the basic computational operations in an iterative solver, are split to sub-domain level and are also performed by the involved processors concurrently. The parallel FEM is applied successfully to the solution of a THM coupled problem in partially saturated bentonite which are used as buffer material in geotechnical sealings [10,9].

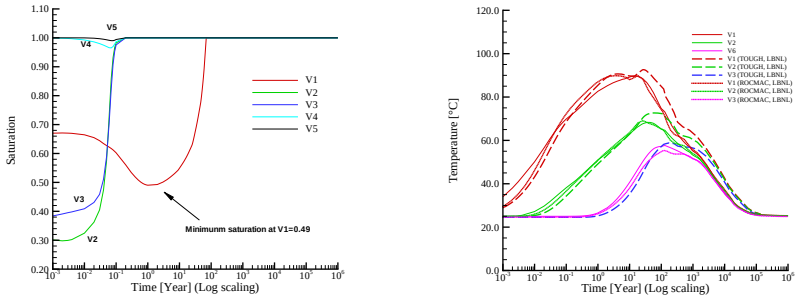


Gas pressure p^g Temperature T

Fig. 5. TH^{2}M FEBEX simulations

The FEBEX as well as DECOVALEX simulations require the solution of fully coupled TH^{2}M problems in which the complete thermal, two-phase-flow, inelastic deformation court is provided by one unique code. TH^{2}M simulations

are very sensitive to time and space scale discretizations and such simulations are very expensive with respect to computation time. As demonstrative examples we present some results of the TH^{2}M simulation for the FEBEX (Fig. 5) as well as DECOVALEX studies [11] (Fig. 6).



Liquid saturation S^l Temperature T

Fig. 6. TH^{2}M DECOVALEX simulations

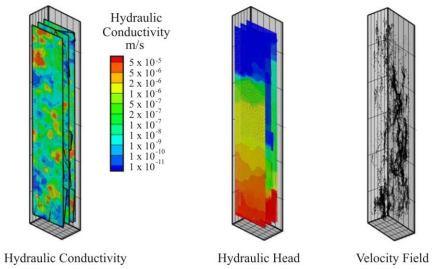
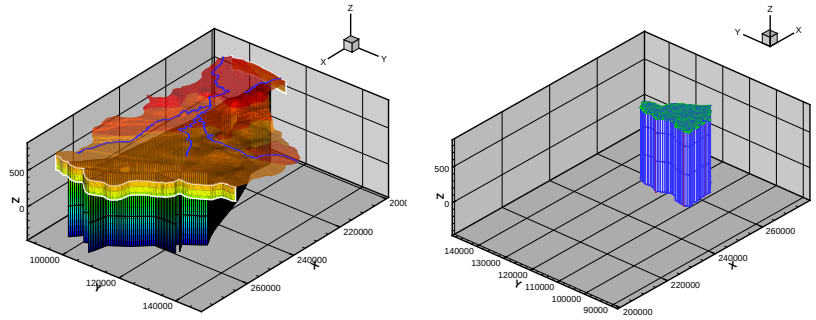


Fig. 7. Fracture network simulation

Recently, the paralleled GS/RF version could be successfully applied also to hydro-chemical (HC) fracture network simulations (Fig. 7). Due to the statistical description of fracture network systems, a large number of realizations has to be considered [12]. Thiss work was conducted in close cooperation with the Paul-Scherrer-Institute in Switzerland.

TH Processes in Hydrosystems An example which shows the necessity of high performance computing in environmental science results of a water resources management model for the Jordan Valley area [13] are presented in this section. Fig. 8 (left) depicts the structural model of the investigation area which consists of 84 geometric entities (volumes) based on geological considerations. Geometric complexity is one of the features of those environmental systems. This requires spatial high-resolution discretisations in the order of several million grid points and, in particular, domain decomposition for hybrid finite element methods consisting different geometric element types (Fig. 8, right).



Structure model Hybrid domain decomposition

Fig. 8. Hydrosystem model in the Jordan Valley

The hydraulic system is controlled by recharge and discharge conditions to or from the model area as well as by discharges from several springs. Geothermal basic processes are illustrated in Fig. 9. There is a permanent heat flow from the base to the system. Through the North colder groundwater is entering the upper aquifer and through the East of the lower aquifer.

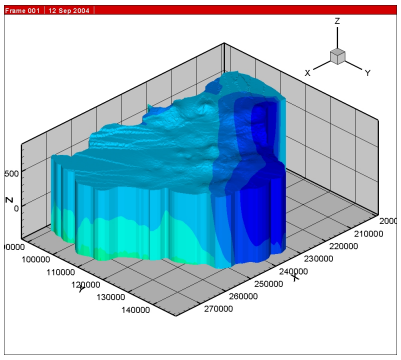
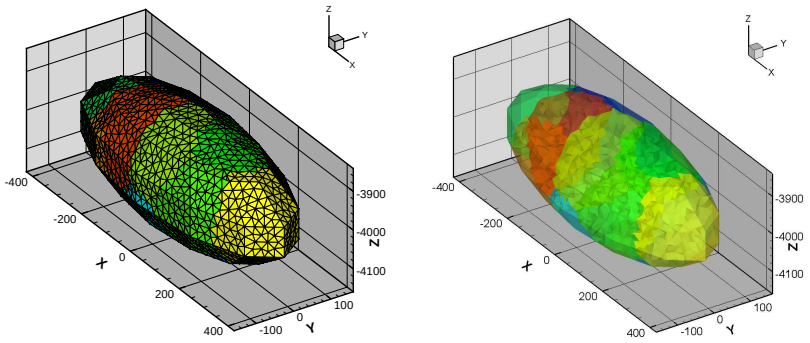


Fig. 9. Thermal hydrosystem model

Fig. 9 shows a long-term simulation (30.000 years) of the thermal system based on the hydraulic model presented above. The simulation shows a permanent increase of temperatures. The groundwater entering the system is not equilibrating the base heat flux. This indicates to possible defects in the current model. First, the outside groundwater recharge to the domain is underestimated. Second, the base heat flux is overestimated. This means, involving thermal data to the simulation, the hydraulic model can be improved.

THM Processes in Geothermal Systems Without any doubt geothermal energy forms a massive under exploited renewable and environmentally friendly energy resource, less than 5 km beneath the ground surface. The problem is getting at this energy in an economical and environmentally coherent approach. During in situ heat energy extraction several coupled processes are operating at a wide variety of scales in a complex three dimensional geological media. Experience shows that the complex interaction of several Geothermal related THMC processes (thermal, hydraulic, mechanical, as well as geochemical and biological) forms a major undefined related risk to the effective utilization of the geothermal energy resources.



Tetrahedra meshing Domain decomposition

Fig. 10. Geothermal reservoir simulation

Numerical coupling of the THMC processes can be addressed in a number of different ways. Principally the processes can be all solved simultaneously, leading to an enormous computing effort, and at the current standard only small areas, at the most of a meter scale can be addressed. Alternatively the processes can be solved one after the other in a monolithic approach, allowing larger areas to be addressed, but leading to potential cumulative computational errors.

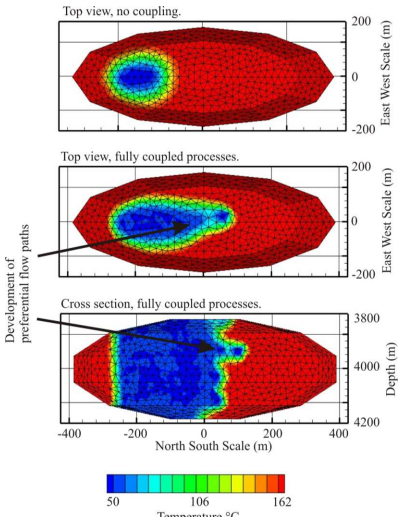
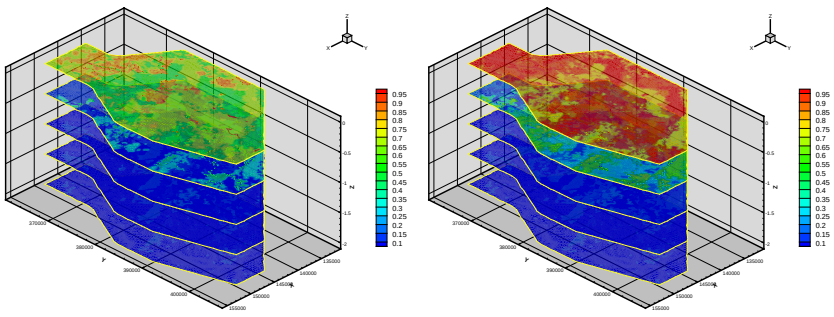


Fig. 11. Preferential flow in reservoirs

[14] presented a method of using scale dependent functional approximations to investigate HM coupling at the Urach site, which was further expanded to investigate HT(MC) coupling, where the mechanical and fluid response was considered a functional response to the temperature and pressure conditions. The challenges to HPC in geothermal reservoir simulation are manyfold. First, deep geothermal sites have multifaceted geologic structures including complex 3-D fracture systems. This leads to enormous spatial discretization efforts. Second, the fully coupling of THMC processes has to be considered. The German geothermal research site for the exploration of deep hot-dry-rock reservoirs is located near Bad Urach in the South-West. Fig. 11 shows results of THM simulations for the Urach site.

Hydraulic processes in regional soil systems The parallelized regional soil model (RSM) is developed based on the Richards equations and finite element method by [15]. The responses and water budget of alterations in timing and distribution of precipitation on the unsaturated zone are focused on by deterministic physically-based RSM, which is flexible and adaptable to extent one dimensional vertical column to three dimensional spatial area according to the heterogenous characteristics of climatological conditions, soil properties, geographic elevation and so on. Aiming for the numerical simulation of a wide range catchment which combines enormous information, parallel computation is obligatory as an effective tool to break the restriction of computation abilities, reduce calculation time and provides an approach to deal with realistic application. The parallelized RSM is running on Linux supported symmetric multi-processing computers with MPI (Message Passing Interface) environment, and it is the key technology to realized the high performance computation of regional scale hydrosystem models. The Beerze-Reuzel drainage basin is used as a study area, the high solution of saturation distribution and wet front movements in this area are presented by using the parallel computation of RSM [16]. It takes about 5 mins for each time step in the whole region (12210 soil columns) with 3GHz processor and about one Gigabyte memory consumption without parallel comparing to 0.1 min 6 CPU nodes with parallel.

The regional evolution of the soil water distribution is presented in Fig. 12 for day 25, 50 of the year 2000. It can be seen that the infiltration process into the soil compartment is very heterogeneous. As the meteorological precipitation-evaporation conditions are rather homogeneously distributed in the region, the pronounced differential moisture propagation in the region is caused by the local variation of hydraulic soil properties. The regional groundwater recharge distribution is calculated from the soil water Darcy velocities multiplied by the corresponding influence area of each soil profile.



30 days 60 days

Fig. 12. Evolution of regional water saturation distribution

3 Use of high performance computers

The following HPC platforms have been used for this project:

Strider (HLRS)

- 125+2+1 Dual-Opteron Knoten (256 Opteron CPUs)
- 1.024 TFlop/s nominell
- 516 GB RAM
- PGI 6.1.3 and GNU Compiler tested
- Myrinet Netzwerk

Cacau (HLRS)

- 200+1 Dual-Xeon EM64T (mittlerweile 20 Knoten weniger) insgesamt 401 EM64T
- 2.5 TFlop/s nominell
- 160 GB + 80 GB RAM (160 Knoten mit 1 GB, 40 mit 2 GB)
- Intel Compiler 9.0
- Infiniband Netzwerk
- Voltaire MPI

SX6 (HLRS)

- 4 nodes * 8 CPU's * 9.2 GFlops
- 294,4 GFlop/s nominell
- 512 GB RAM (8 nodes * 64 GB RAM)
- NEC SX Compiler
- Node-node interconnect: IXS 8GB/s

SX8 (HLRS)

- 72 nodes * 8 CPUs
- 12 TFlop/s nominell
- 9.2 TB RAM
- NEC SX Compiler
- Node-node interconnect: IXS 6 GB/s per node

Merlin 3 (Paul-Scherrer-Institute, Switzerland)

- 14 new compute nodes, dual core AMD Opteron 2.4 GHz CPUs
- 14x8 GB RAM, 12 TByte of disk storage
- Scientific Linux 4 (PSI cluster customization, 64-bit), 64-bit PGI compilers

ZAG-Cluster (ZAG)

A small Linux cluster was provided for this project for development purposes.

- 4 Dual-Nodes (8 CPU)
- 35.2 GFlop/s
- 16 GB RAM

Additionally tests have been made on test nodes of the IBM BlueGene/L (FZJ) and Cray XT3 (PSI, Switzerland).

Benchmarking

In order to test consecutive parallel versions on different platforms, a benchmarking procedure was developed. Different types of T-HM- problems have to be tested on different platforms for each new release (Fig. 13). The version management is conducted using WebSVN through the internet.

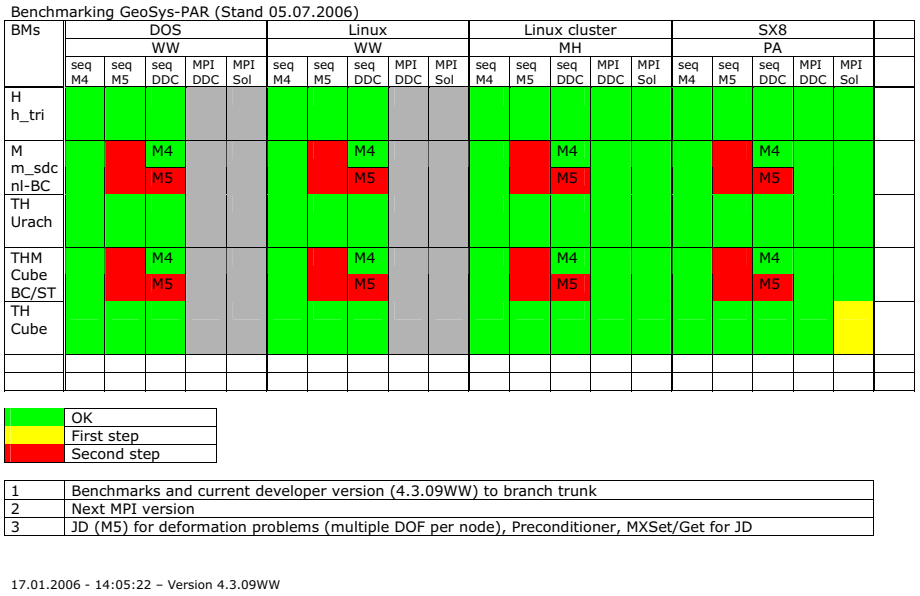


Fig. 13. Benchmarking procedure of the parallel version

4 Conclusions and outlook

The major result of this project is the parallelization of GS/RF. The basic methods for improving the computational efficiency are process parallelization, domain decomposition, solver parallelization, improved matrix storage and vectorization techniques. The parallel features of GS/RF are available since official version 4.3. GS/RF have been tested on several platforms (Linux clusters and parallel-vector-computers (NEC-SX family)). GS/RF is already being applied by external users (PSI, Switzerland).

Thanks to the object-oriented software concept, even for the parallelization, a large variety of thermo-hydro-mechanical-chemical problems can be solved now for practical needs in applied geoscience. Examples from geotechnics, water resources management, geothermics and watershed hydrology have been presented and demonstrate the applicability of the paralleled version of GS/RF.

Nonetheless further improvements are necessary concerning the speed-up of the parallelization. A hybrid concept for reactive multi-componential mass transport processes should be developed, i.e. process parallelization of mass transport, domain decomposition of the model domain and, in particular, parallelization of reaction processes which are usually the most time consuming computations.

5 Project publications

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6 Recent developments

6.1 Recent developments

The latest new developments after the evaluation in January 2006 are:

- Process parallelization for regional soil models,
- Parallelization of coupled THM problems, where the degree of freedom is different for the thermal, hydraulical sub-problems (linear elements) and the mechanical sub-problem (quadratic elements),
- Parallel solver:
  - Implementation of a MPI parallel BiCGSTAB solver,
  - Pre-conditioner,
  - Memory optimization (local topology for subdomains)
- Modifications for Linux clusters,
- Completion of Jagged Diagonal (JAD) storage scheme for vectorization
- Test of several platforms, benchmarking.

6.2 Milestones

All milestones have been achieved in time except of the following deviations from the project proposals.

6.3 Deviations from milestones

- The application case "Testfeld Süd" was not conducted. Instead another application study was accomplished for the "Brand/Niedergörsdorf" site which has similar contamination characteristics (mineral oil contamination from a former military site) [17]. For this case study an excellent data base is available.
- In addition to the work plan, Linux clusters have been included to the HPC platforms. An extra Linux cluster was installed at the ZAG, available to the research team every time, in order to facilitate the software development.

6.4 Deviations from financial planing

The project was conducted according to the financial planing.

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