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APPLICATION OF HYDROINFORMATIC METHODS AND TECHNIQUES FOR COMPLEX SYSTEMS - QUANTIFICATION OF METHANE-MIGRATION PROCESSES FROM ABANDONED COAL MINES

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This paper demonstrates the urgent necessity for a combined use of many powerful hydroinformatic methods and techniques to investigate and analyze complex processes in complex large-scale domains. This is explained for the quantification of methane-migration processes stemming from abandoned coal mines with the modeling system MUFTE-UG. The model set-up is carried out with a CAD system, a database and a mesh generator for elements of different dimensions. Uncertainties in the geology can be accounted for with geostatistical tools. Different model concepts, efficient discretization methods, fast solvers, parallel computers as well as advanced visualization are needed to understand the relevant processes and to prepare tools for future prognoses. Furthermore, optimization methods are helpful means for decision support, for example in optimizing methane-extraction measures.

INTRODUCTION

In recent years, a coupling of different hydroinformatic methods and techniques has become an urgent prerequisite for the numerical simulation and prediction of anthropogenic changes in the flow conditions as well as the water budget and quality in complex hydrosystems.

As an example application, we present the modeling of methane-migration processes stemming from abandoned coal mines through saturated and unsaturated zones in the subsurface (see Fig. 2). Methane adsorbed by coal seams is released and removed by means of ventilation as long as the mines are in operation. After a mine is closed, ventilation is stopped and the water table rises after pumping has ceased. However, closed mines continue to produce methane, which displaces the water due to the much lower density and may reach the surface of the earth via old mine workings, shafts, permeable strata, faults and mining-induced fractures. Methane-gas emission, for example close to residential areas, is dangerous because methane gas is toxic for humans, and is a fire and explosion risk; thus, the gas which accumulates in buildings can jeopardize human life. However, methane can be used to supply energy if the flow is large enough and a controlled suction is possible.

The overall aim of the work consists of setting up a three-dimensional model of an existing coal mine, calibrating the numerical model in the range of the available data and making predictions for possible remediation measures with estimations about the influences of various uncertainties. Such simulations can detect endangered areas or be used for the optimal positioning of wells which draw off the gas in a controlled way.

Hydroinformatic methods and techniques mainly comprise the interacting fields of modeling systems, decision-support, management and information systems as well as information and communication technologies. To solve the above-mentioned problems, we concentrate in this paper on the topics modeling and decision-support systems using MUFTE-UG, see Helmig [6], Bastian et al. [2] and Hinkelmann [7]. MUFTE-UG provides or has interfaces to tools for describing the geometry of complex subsurface systems, for example with a CAD system, for assigning physical parameters to the geological structures, for example using a database, for generating meshes and for accounting for uncertainties in the parameter fields, for example applying geostatistical methods; this is described in the second section. The 'heart' of MUFTE-UG consists of different model concepts for multiphase flow and transport processes in fractured subsurface systems, efficient discretization methods as well as fast solvers based on parallel adaptive multigrid methods. This is discussed for the simulation of two-phase flow processes in the subsurface together with advanced visualization in section three. Optimization methods as one means of decision support are introduced in section four and applied to a two-phase / multicomponent model concept using a special parallelization strategy. Finally, conclusions are drawn.

MODEL SET-UP

A three-dimensional model of an existing abandoned coal in the Ruhr, Germany, has been set up. It is explained in detail in Breiting et al. [4] The complex domain consists of a multilayered system of the basement and cap rock including coal seams, fault zones, fractures, shafts, transport roads etc. (see Fig. 2). We were provided with geological maps, drilling profiles and maps of coal seams, transport roads, dams and shafts. The rock matrix was discretized with 3D elements, (exhausted and non-exhausted) coal seams, fault zones and fractures with 2D elements and shafts, transport roads, dams with 1D elements. A dam closes a transport road before it ends at a shaft (see Fig. 2). As the shafts and parts of the transport roads are open tubes, they are excluded from the computational domain and treated as (inner) boundaries. The geometric data were digitized and integrated into the CAD model AutoCAD. In Figure 1, left, an isometric view of coal seams, transport roads and a shaft is given, while the surrounding basement rock is not shown. The different colors indicate different vertical levels.

The physical parameters of the geological and man-made subsurface structures, such as permeability or parameters of constitutive relationships, were assigned to the geometrical units. Above and below exhausted coal seams, disturbed domains were taken into account by giving higher permeability. The physical parameters are partially based on measurements and partially estimated in cooperation with geologists from the mining company DMT. They are stored in the public-domain relational database MySQL which is connected to the CAD model.

The geometric and physical information is given to the mesh generator ART which is based on a shape-optimized Delaunay triangulation, see Fuchs [5]. ART generates tetrahedra with a regular mesh structure and enables area-wise higher mesh resolutions according to user-defined density functions. It is able to include 1D and 2D subdomains which lie on the boundaries of 3D subdomains. In Figure 1, right, a mesh with about 100000 elements of the basement rock of Figure 1, left, is presented. Around the coal seams, transport roads and the shaft, the mesh resolution is much higher, which is indicated by the dark color. The different colors in the mesh show the domain decomposition into 40 subdomains; this is required for the parallel computation.

Experience has shown that the development of an appropriate geometry model is an iterative process between model set-up and simulation; if problems occurred in the first numerical simulations, changes in the CAD model and / or the mesh often led to improvements.

The geological structures and their parameter variations, whose spatial distributions are generally unknown, may significantly influence the behavior of a multiphase flow and transport system. To estimate the influences of such uncertainties, we have two possibilities. Small-scales heterogeneities, for example of a permeability field, can be determined with the geostatistical tool SIMSET, see Bárdossy [1]. Small-scale fracture networks, (see Fig. 4, left), can be generated with FRAC3D, which combines deterministical and geostatistical information, see Silberhorn-Hemminger [11]. The more geological data or reasonable estimations are available for the parameters which are required for the geostatistical methods, for example correlation length, fracture density or aperture width, the better the influence of the uncertainties can be assessed.

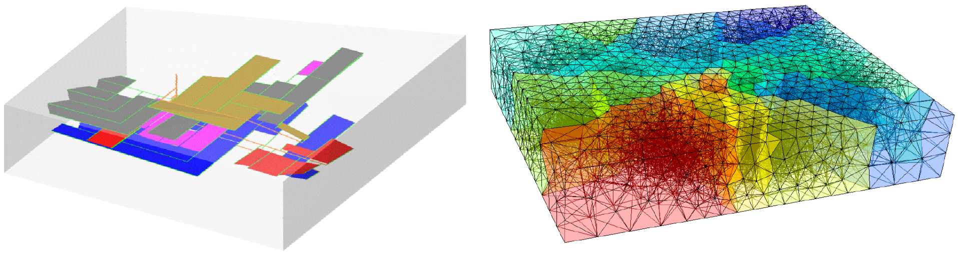

Figure 1. Basement rock with coal seams, transport roads and a shaft. Left: CAD model after Breiting et al. [4]; right: computational grid and domain decomposition.

SIMULATION

The numerical simulator MUFTE-UG is a combination of MUFTE and UG. MUFTE stands for **MU**ltiphase **F**low, **T**ransport and **E**nergy model and mainly contains the physical model concepts and discretization methods for isothermal and non-isothermal multiphase / multicomponent flow and transport processes in porous and fractured-porous media, see Helmig [6], Breiting et al. [3] and Hinkelmann [7]. UG is the abbreviation of **U**nstructured **G**rid and provides the data structures and fast solvers for the discretization of partial differential equations based on parallel, adaptive Multigrid methods, see Bastian et al. [2]. MUFTE uses UG as its fast solver.

In Figure 2, a sketch of the abandoned coal mine in the Ruhr is given. Simplified test cases are important to understand the relevant processes of the 3D methane flow through the saturated and unsaturated zones from the coal seam to the surface of the earth. The driving 'force' in our system is the methane source term which is located in the non-exhausted coal seams. The order of magnitude of the source term was estimated by colleagues from the coal-mining company DMT. Around the coal seams in the water-saturated basement rock, we assume that the relevant flow processes can be described by a two-phase flow model concept consisting of a gas and a water phase. The system properties of the gas phase are based on the assumption that the gas phase is composed of an air-methane mixture, while the water phase consists of water only. Thus, mass- and energy-transfer processes between the phases are not considered in this model concept.

The two-phase flow equations are discretized with the so-called Box method, which comprises a node-centered Finite-Volume method in space with fully upwinding for the advective terms and a fully implicit Euler method in time. The non-linear systems of equations are solved with the Newton-Raphson method as the outer solver and the BiCGSTAB method with Multigrid preconditioning as the inner solver. The parallelization in UG is carried out in the algebraic operations, such as scalar or matrix-vector products. The parallel-programming model which is specially suitable for graph-based data structures enables portability to nearly all common High-Performance Computational architectures; however, the use of vector computers is not reasonable. Static (see Fig. 1, right) and dynamic load-balancing techniques are available. Compared to a sequential code, only a few lines must be added for the parallel version.

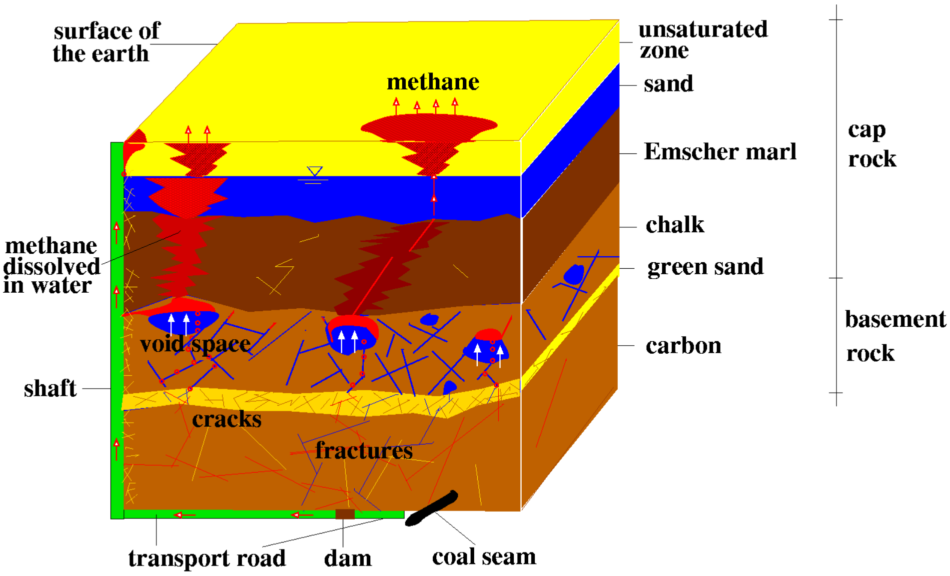

Figure 2. Sketch of the abandoned coal mine in the Ruhr, after Sheta et al. [10].

In Figure 3, left, a simplified subsystem of Figure 1, left, is shown with just a few coal seams and transport roads. It is closed along all boundary surfaces and, initially, fully saturated with water. The exhausted coal seams have a much higher permeability than the rock matrix. The methane source is then activated in the lower (non-exhausted) coal seams. In Figure 3, right, the isoareas of the gas saturation are visualized. Up to the considered time step, the methane only migrated into the exhausted coal seams, not into the rock matrix. In Figure 4, the influence of a small-scale fracture network, whose existence is known from field data, on the methane-migration behavior is investigated. Figure 4, left, shows the same system as in Figure 3, left; however, it is extended by a geostatistically generated fracture network. In figure 4, right, the isoareas of the gas-saturation are given for the same time as in Figure 3, right. The fracture network causes a much faster upward migration of the methane through the fractures and a migration of methane into the rock matrix, see Sheta et al. [10]. This comparison demonstrates that the geological structures have an important influence on the flow processes, the amount of methane escaping to the atmosphere as well as its locations at the surface of the earth.

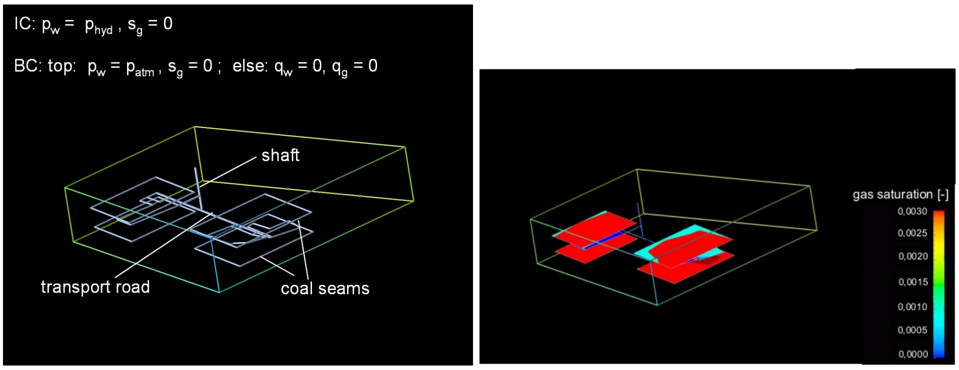

Figure 3. System, initial and boundary conditions, left; gas-saturation, right.

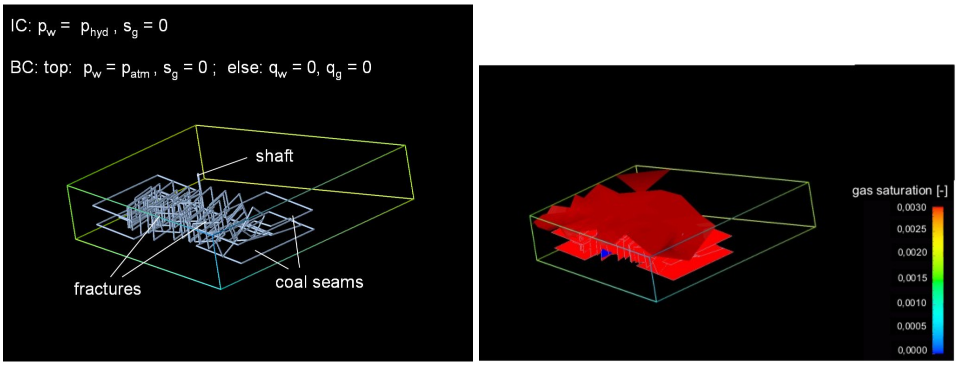

Figure 4. System with fractures, initial and boundary conditions, left,;gas-saturation, right, after Sheta et al. [10].

Two further aspects are briefly addressed. In Figure 5, left, the parallel speed-up obtained on a Linux cluster at our institute is shown. The parallel speed-up, which is the ratio of the run time on 1 processor to the run time on p processors, indicates a reasonable parallel run-time behavior up to 32 processors. However, the problem size is too small for more than 32 processors because the inclination of the parallel speed-up decreases.

The results in Figures 3 and 4 were visualized with the public-domain Data Explorer, which is an advanced visualization tool. To get even better insight into the complex processes in the complex domain, the results were also visualized in the CAVE of the computer center of Stuttgart University, see Figure 5, right. The CAVE is a special Virtual Reality room with an all-round projection where a user can immerge into the representation of the results and can interact with the simulation model. In the CAVE, physical effects which had not been seen before have been discovered.

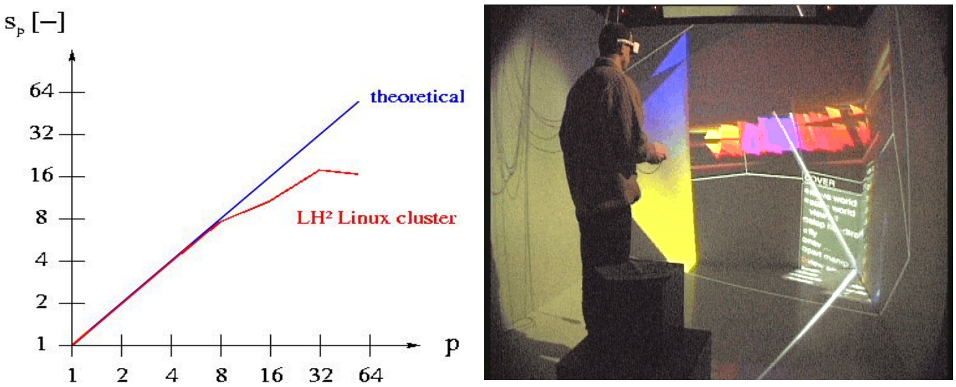

Figure 5. Parallel speed-up on a Linux cluster, left; visualization in a CAVE, right.

OPTIMIZATION

Optimization methods are one means of decision support. In the context of the methane-migration problem, such methods are required to determine, for example, optimal locations and / or numbers of gas-extraction wells in order to keep buildings free of methane. Optimization methods should compute optima of a so-called objective function which depends on the simulation results and possibly also on other parameters, for example costs. As the objective function can have (many) local optima, the major problem of optimization methods consists of determining the global optimum among the local ones. Generally, derivative-type and heuristic optimization methods can be distinguished.

As a first step, we decided on a simple method and chose Simulated Annealing as one of the heuristic methods which is implemented as an iteration process in the form of an outer loop around MUFTE-UG. As we were looking for optimal well locations, a new mesh had to be generated with ART in each iteration step (see Fig. 6). A special coarse-grain parallelization strategy was developed because a huge amount of CPU time had to be expected. The domain is subdivided into subdomains (see Fig. 6, right) and the optimization method just searches the optimum within its assigned subdomain. Finally, the global optimum is determined by global communication among all processors. The details are described in Kobayashi et al. [8] and Kobayashi [9].

A system in the unsaturated zone is investigated where methane flows from the coal seams to the transport roads which are partially filled with rock material and which have a high permeability. As a further first step, we just considered the transport roads in a horizontal plane and the methane inflow is prescribed by conditions, see Figure 6. For the processes under investigation, for example including rainfall, a two-phase / three-component model concept (phases: water, gas; components: water (vapor), (dissolved) methane, (dissolved) air) was required and had to be adapted to the methane-migration problem. This model concept takes mass-transfer processes into account, for example the dissolution of methane in water or the evaporation of water. The objective function describes the maximum methane flux for a given time period and underpressure and depends on the coordinates in the horizontal plane. In Figure 7, left, the optima found in subdomains 1 to 23 are given. The global optimum is found in segment number 23. Figure 7, right, shows the pressure field for the optimal solution in segment 23 which is located at the cross-section of two roads. The area influenced by the prescribed underpressure at the extraction well is very small.

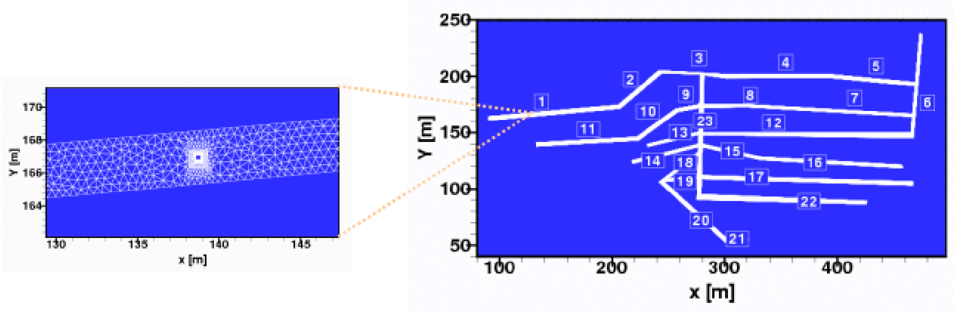

Figure 6. System for optimization. Left: zoom in subdomain 1 with location of the extraction well; right: domain and domain decomposition, after Kobayashi [9].

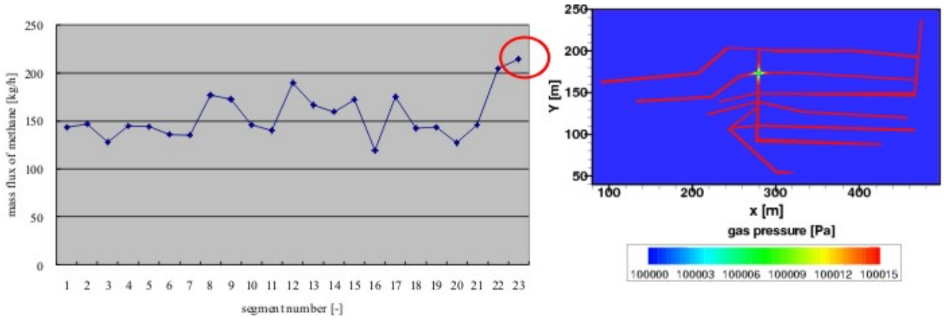

Figure 7. Methane mass fluxes in the subdomains, left; gas pressure field in subdomain 23, after Kobayashi [9].

CONCLUSIONS

A combined application of many powerful hydroinformatic methods and techniques is urgently required to understand complex processes in large-scale complex domains. It is a prerequisite to prepare tools for prediction as well as for optimization purposes. For the quantification of the methane-migration processes, the next major step is an adjustment of the magnitude of the methane source in such a way that measured methane fluxes at the shaft will be reproduced. Additionally, the influences of different uncertainties must be estimated to determine the bandwidths and the reliability of the results.

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