MUFTE-UG: Structure, Applications and Numerical Methods.

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Structure and Tools

MUFTE-UG is a combination of MUFTE and UG. MUFTE stands for **Mu**ltiphase **F**low, **T**ransport and **E**nergy model. This software package 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 (HELMIG (1997), HELMIG et al. (1998)). It is possible to make a discrete description of the fractured porous media (Dietrich et al. (2005)). UG is the abbreviation for **U**nstructured **G**rid. This toolbox provides the data structures and fast solvers for the discretization of partial differential equations based on parallel, adaptive Multigrid Methods (UG, BASTIAN (1996), BASTIAN et al. (1997)). Figure 1 presents an overview of the modeling system with its pre- and postprocessors.

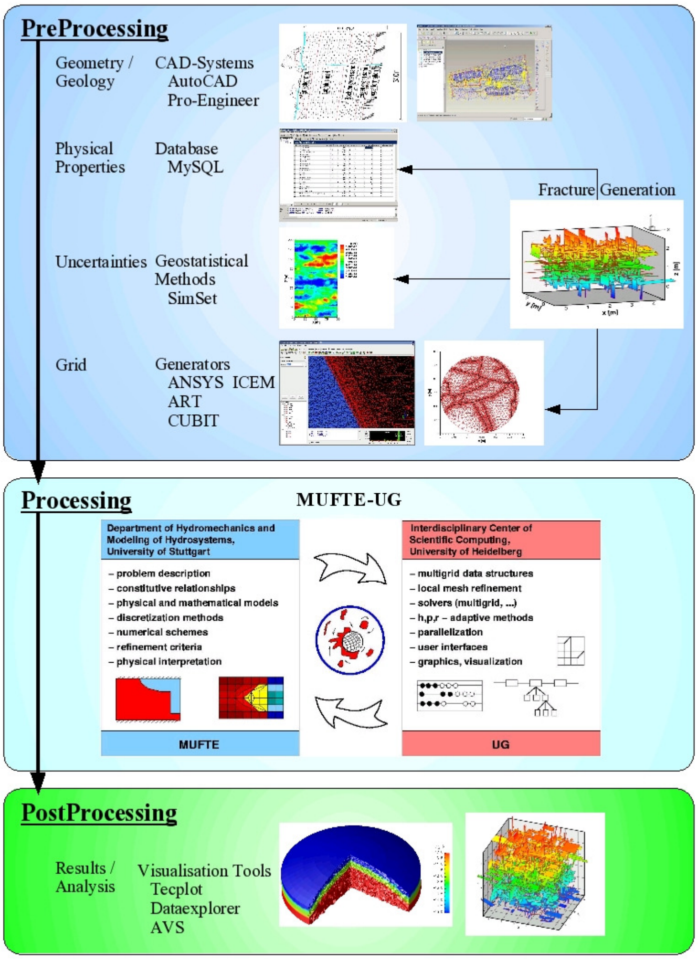

Figure 1: Modeling System *MUFTE-UG*.

MUFTE-UG has a modular structure and provides therefore an easy adaptation to various problem specific requirements.

Applications

Due to its modular composition, *MUFTE-UG* allows for many different environmental and technical applications. For example in the field of **environmental applications**, *MUFTE-UG* is capable of simulating

- NAPL (Non Aqueous Phase Liquid) infiltration into saturated and unsaturated soils. The optimization of enhanced remediation techniques is an extensive field of research and development within MUFTE.
- CO_2 sequestration in the subsurface. CO_2 is injected at high pressures and temperatures into geological formations several hundred meters below the surface. Point of interest is the plume evolution in the heterogeneous aquifer (advective and diffusive transport), along with temperature effects (due to expansion / compression) and mutual solution of the components (brine and CO_2).
- Enhanced coalbed methane recovery. During coalmining, an enhanced release of methane (CH_4) from the coal surface is observed due to the pressure drop in the close vicinity of the coal seams. By applying a negative pressure, gas with a high fraction of methane can be collected and used for energy production. The modeling task is to simulate the desorption process along with the gas flow in fractured porous media to optimize the location of the extraction wells.
- Salt water intrusion. This is a good example for very sensitive density driven flow. Dispersion mainly determines the shape as well as the position of the saltwater / freshwater transition zone.

Examples of **technical applications** include:

- Flow in the cathode of PEM fuel cells. The cathode of the H_2-PEM is the performance-limiting component in the assembly due to the slower kinetics of the oxygen reduction reaction and a sophisticated water management within the fuel cell. The membrane always has to be humidified, but water accumulation has to be prevented. The task is to give qualitative information on the effects of various operating conditions and on material properties.
- Leaking of contaminant gas from atomic waste containers in deep rock depositories.

Numerical Methods

Discretization techniques include a Fully Upwind Box Method, which is a Finite-Volume formulation with piecewise linear shape functions including fully upwinding of upstream mobilities, and a Control-Volume Finite-Element Method (CVFEM), which is a mass-conservative formulation on a discrete patch including a first order upwinding scheme. Time integration employs the Finite Difference method, and the temporal discretization is carried out fully implicitly.

Multigrid Methods are used as very fast solvers for large-scale problems with many unknowns. The procedure of this method is to decompose the error between the iterative and the exact solution into a “high-frequency” and a “low-frequency” part. It can be shown that the error-parts can be solved faster on different grids, whereas the “high-frequency” part is diminished on a fine grid, the “low-frequency” part on a coarse one. Fine grid solvers are often Jacobi, Gauss-Seidel and ILU algorithms. Coarse grid solvers (cgs) are typically direct solvers (e.g. Cholesky, Gauss).

MUFTE-UG’s special advantages also include the data-structures for unstructured grids, functional parallelization, especially designed for MIMD parallel computers and an adaptive local grid refinement.

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