Description of the master's thesis

In numerous applications, multi-phase flow takes place on a huge spatial domain and occurs over large time scales. In most cases, however, complex flow regimes occur only in small regions of the domain. For example, if CO$_2$ is injected into brine-bearing formations, saline groundwater might propagate along a pressure gradient induced by the injection, thereby putting freshwater resources at risk. In addition it is of interest whether the CO$_2$ could leak back into the atmosphere, and which kind of pathways allow for such rising up from the deep underground. A risk evaluation requires simulations on a large domain, including local features such as fault zones and a representation of the transient saline front. In these areas, the numerical solution benefits from a fine grid resolution. However, it is computationally very expensive or even impossible with standard hardware resources to simulate fluid flow on such a fine grid in the entire domain during the whole simulation time. Local grid adaptation can decrease the computational cost of simulations. It is one way to reduce the number of global degrees of freedom and thus the size of the system of equations that has to be solved.

The simulator DuMux (Flemisch et al., 2011) that is built on top of DUNE (Distributed and Unified Numerics Environment) offers several models which allow using nonconforming adapted grids. So far, the grid adaptation is performed based on various heuristic indicators such as the gradients of the unknowns. The aim of this work is to improve the available grid adaptation strategies by including rigorous and theory-based a posteriori error estimators. A posteriori error estimators can balance the global error of the discrete solution on the whole domain through the global upper bound (Ohlberger, 2009):

$$\|u - u_h\| \leq \eta(u_h),$$

with the exact solution $u$ and the approximated solution $u_h$. Local lower bounds guarantee that the required tolerance is achieved with a minimal amount of work by selecting local areas with large errors for refinement. This results in an equal distribution of the error throughout the domain, leading to an efficiently refined grid. The a posteriori error chosen in this work was developed by Kröner and Ohlberger (2000) in the L1-norm for upwind finite volume schemes. By applying this error estimator we neglect errors caused by the boundary conditions that need to be fixed. It can be written as:

$$\int_K |u - u_h| \leq T[a_0 \int_{|x-x_0|<R+1} |u_0(x) - u_h(x,0)| dx + aQ + 2\sqrt{bcQ}]$$

(14)
where

\[
Q : = \sum_{n \in I_0} \sum_{j \in M(n)} |u_{n+1}^j - u_n^j| \Delta t^n h_N^j
+ \sum_j \sum_{n \in I_0} \sum_{m \in M(n)} \Delta t^n (\Delta t^n + h_{jl}) \max_{u_j^m \leq \xi \leq u_j^n} (g_{jl}^n(d, c) - g_{jl}^n(d, d)) \delta_{jl}^n
+ \sum_j \sum_{n \in I_0} \sum_{m \in M(n)} \Delta t^n (\Delta t^n + h_{jl}) \max_{u_j^m \leq \xi \leq u_j^n} (g_{jl}^n(d, c) - g_{jl}^n(c, c)) \delta_{jl}^n
+ 2M_1 \sum_{n \in I_0} \sum_{j \in J} \Delta t^n h_{jl}^{N-1} (\Delta t^n + h_{jl})^2 \delta_{jl}^n,
\]

with the simulation time \( T \), constants \( a_0, a, b, c \) and the numerical flux \( g_{jl} \). The a posteriori error estimator was implemented in this form and in a reduced form for the Buckley-Leverett equation. Results showed that the estimators were not able to estimate the global error with a satisfying accuracy. Neither the simplified Buckley-Leverett error estimator nor the general estimator can be seen as reliable. It was shown that the influence of time-related effects on the global error proved a difficulty for the error estimators. Especially for hyperbolic problems (like the Buckley-Leverett problem), the influence of such errors is difficult to estimate because of the inherent characteristic of the problem. However, the error estimators showed a good convergence rate behavior and good applicability in grid adaptation.

For more complex problems, the a posteriori error estimator showed stability problems during grid refinement because of a direct dependence on the number of grid cells. This dependence was relaxed and a new grid adaptation indicator based on error estimation was developed. This heuristic estimator showed an improved applicability in an adaptive process compared to the already existing heuristic grid adaptation indicators. The benefit of the error estimators in particular is a good regulation of the adaptation process by the user-specified error tolerances. These can be varied independently for errors due to finite time or space discretization. This possibility offers opportunities to select the grid adaption strategy specific to the individual problem simulated. Most importantly, the error estimators guarantee an equal distribution of the local error and thus a most efficiently adapted grid. For more complex problems, the new heuristic estimator is e.g. able to track the moving fingers of DNAPL for low tolerance (efficient grid), whereas the original grid adaptation indicator loses them. This results in a more accurate saturation distribution for the heuristic estimator while reducing the simulation time by 70%.

References