Development of the porous media simulator DuMu\textsuperscript{x}

Project number: GA13
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Motivation
The quality of any type of computational modelling crucially depends on the quality of the employed software framework. Research codes very often fail to be developed and maintained in a continuous manner. On the contrary, software development at academic institutions usually is highly fragmented and driven by individual short-term needs. There is an urgent need for the sustainable and consistent development and maintenance of our in-house porous media simulator.

Objectives
The simulator DuMu\textsuperscript{x} (Flemisch et al. 2007) is (going to be) a multi-scale multi-physics toolbox for the simulation of flow and transport processes in porous media. Its development started in January 2007. It is based on Dune, the Distributed and Unified Numerics Environment (Bastian et al. 2007). The main intention is to provide a sustainable and consistent framework for easy and efficient implementation of models from porous media flow problems, ranging from problem formulation, the selection of spatial and temporal discretisation schemes, as well as nonlinear solvers, up to general concepts for model coupling. Moreover, DuMu\textsuperscript{x} should include ready to use numerical models and example applications.

Achievements
The main achievements are made by the researchers themselves within their individual projects, see the list below. In summary, DuMu\textsuperscript{x} meanwhile is capable of simulating two-phase two-component non-isothermal flow and transport processes in porous media. It is possible to choose between fully coupled implicit formulations and decoupled IMPES-like schemes. For the fully coupled part, a flexible general box discretisation framework has been created, admitting an easy extension of existing models and implementation of new ones. Within the decoupled part, several model-specific discretisations have been developed, and first successful steps for the integration of multi-physics and multi-scale approaches could be done. The most crucial milestone for a sustainable code development was the release of DuMu\textsuperscript{x} under the GNU general public license on July 1\textsuperscript{st} 2009, paving the way for a fruitful exchange with a large scientific community.

Current and Future work
The simulator is constantly being enhanced and improved. Exemplarily, current and future work is done on the extension to three phases and more than two components, enhancing the capabilities of the decoupled formulations, improving the multiscale framework, incorporating mechanical and chemical processes, and the coupling to free flow domains. See the individual project reports for details.

Link to other projects
The simulator DuMu\textsuperscript{x} is developed and used in the following projects, see the corresponding individual reports:
NUPUS doctoral researchers:

- Yufei Cao: Robust numerical algorithms based on corrected operator splitting for two-phase flow in porous media.
- Benjamin Faigle: Multi-physics modelling of two (three) phase flow with capillary pressure.

Andreas Lauser: Multiphase-, multicomponent processes within gas diffusion layers in fuel cells and their interactions with channel flow.

Associated doctoral researchers:

- Melanie Darcis: Coupling models of different complexity for the simulation of CO2 storage in saline aquifers.
- Philipp Nuske: Modelling mass transfer processes for multi-phase flow in porous media including interfacial areas.

NUPUS qualifying fellows:

- Katherina Baber: Modelling the transfer of therapeutic agents from the vascular space to the tissue compartment (a continuum approach).
- Benjamin Faigle: Two-phase flow modelling in porous media with kinetic inter-phase mass transfer processes in fractures.
- Karen-Helene Støverud: Modelling convection-enhanced delivery into brain tissue using information from magnetic resonance imaging.
- Markus Wolff: Comparison of mathematical and numerical models for twophase flow in porous media.

References
