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DUMUX: A MULTI-SCALE MULTI-PHYSICS TOOLBOX FOR FLOW AND TRANSPORT PROCESSES IN POROUS MEDIA

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Abstract. *Flow and transport processes in porous media occur on different spatial and temporal scales and may also exhibit different physical behavior in different parts of the model domain. Additionally, the structure of the porous medium itself generally shows a high dependence on the spatial scale. Employing a complex fine scale model throughout the whole domain is in general very expensive and often limited by the available computational resources. Moreover, in many cases, it is not needed to use the full model everywhere, and one can choose a simpler one and/or consider one on a coarser scale in large parts of the domain.*

Our goal is to develop a multi-scale multi-physics toolbox DuMu^x for nonisothermal compositional multiphase flow and transport processes in porous media which makes use of the locally different behavior. In particular, we aim to use in each part of the domain the model which is the less expensive but still accurate enough to describe the physics correctly. Furthermore, we want to be able to choose the best discretization in space and time for each model. We use modern programming techniques within the framework of DUNE, the Distributed and Unified Numerics Environment which has been developed recently. It allows to implement the necessary numerical algorithms independent of the ultimately used data structures. This paper presents the current possibilities of our toolbox.

1 INTRODUCTION

Flow and transport processes in porous media occur on different spatial and temporal scales and may also exhibit different physical behavior in different parts of the model domain. Additionally, the structure of the porous medium itself generally shows a high dependence on the spatial scale. As an example, the contamination of the unsaturated zone with a light non-aqueous phase liquid (NAPL) is studied, corresponding to a domain with randomly distributed heterogeneities where complex three-phase three-component processes are relevant only in a small (local) subdomain. This subdomain needs fine resolution as the complex processes are governed by small-scale effects. For a comprehensive fine-scale model taking into account three-phase three-component processes as well as heterogeneities in the whole (global) model domain, data collection is expensive and computational time is long.

Therefore, we developed a multi-scale model where on the one hand, the global flow field influences the local three-phase three-component processes on the fine-scale. On the other hand, a coarse-scale saturation equation is solved where the effects of the fine-scale multi-phase multi-component processes in the subdomain are captured by source/sink terms and the effects of fine-scale heterogeneities by a macrodispersion term. The new multi-scale algorithm represents a flexible and extendable tool for incorporating processes of different complexity occuring at different locations in one model domain, while reducing the amount of required data. For the implementation, we started to develop the general toolbox **DuMu^{x}**, "**DU**NE for **Mu**lti-{phase, component, scale, physics, ...} Flow and Transport in Porous Media," based on the recently released DUNE framework, [1].

The rest of the paper is organized as follows. Section 2 describes the nonisothermal compositional multiphase flow model we are interested in. This is followed by a presentation of the current state of the DuMu^{x} toolbox in Section 3. We finally give an outlook in Section 4. Since the development of DuMu^{x} just started recently, we postpone the presentation of numerical results to the talk given at the conference and to subsequent publications.

2 NON-ISOTHERMAL MULTI-PHASE/MULTI-COMPONENT SYSTEMS

Modeling nonisothermal compositional multiphase flow and transport processes in porous media requires the consideration of the transfer of mass and energy between the phases in addition to the flow processes such as advection and diffusion. Such processes occur in several fields of environmental engineering and reservoir engineering in the subsurface. While first applications appeared in the oil industry in the 1970s [2], these concepts have subsequently been transfered, adapted and extended to issues of groundwater protection and remediation [3, 4], as well as to the storage of CO_2 in deep geological formations [5, 6], or to biomedical applications. Recently, multiphase multicomponent models have also been developed for technical applications on a much smaller scale for the simulation of the water management in the cathode diffusion layer of fuel cells [7].

Characteristic of compositional multiphase models is that the phases are not only matter of a single chemical substance. Instead, their composition in general includes several species, and for the mass transfer, the component behavior is quite different from the phase behavior. In the following, we give some basic definitions and assumptions that are required for the formulation of the model concept below. As an example, we take a three-phase three-component system water-NAPL-gas [3]. The modification for other multicomponent systems is straightforward and can be found, e. g., in [5, 7].

2.1 Basic Definitions and Assumptions for the Compositional Model Concept

Components: The term *component* stands for constituents of the phases which can be associated with a unique chemical species, or, more generally, with a group of species exploiting similar physical behavior. In this work, we assume a water-gas-NAPL system composed of the phases water (subscript w), gas (g), and NAPL (n). These phases are composed of the components water (superscript w), air (a), and the organic contaminant (c) (see Fig. 1).

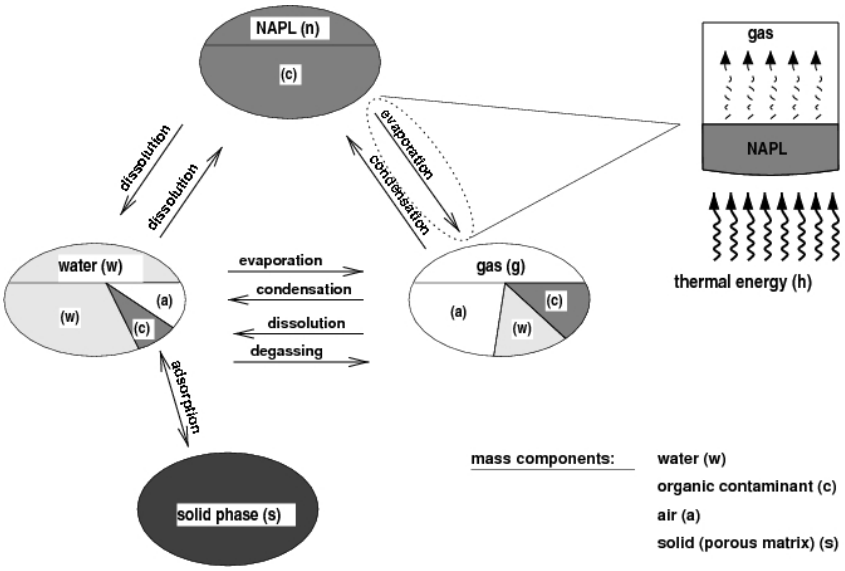

Figure 1: Mass and energy transfer between the phases

Equilibrium: For the nonisothermal multiphase processes in porous media under consideration, we state that the assumption of local thermal equilibrium is valid since flow velocities are small. We neglect chemical reactions and biological decomposition and assume chemical equilibrium. Mechanical equilibrium is not valid in a porous medium, since discontinuities in pressure can occur across a fluid-fluid interface due to capillary effects.

Notation: The index $\alpha \in \{\mathrm{w}, \mathrm{n}, \mathrm{g}\}$ refers to the phase, while the index $\kappa \in \{\mathrm{w}, \mathrm{a}, \mathrm{c}\}$ refers to the component.

p_α	phase pressure	ϕ	porosity
T	temperature	K	absolute permeability tensor
S_α	phase saturation	τ	tortuosity
x_α^κ	mole fraction of component κ in phase α	$\boldsymbol{g}$	gravitational acceleration
X_α^κ	mass fraction of component κ in phase α	q^κ	volume source term
$\varrho_{\mathrm{mol},\alpha}$	molar density of phase α	u_α	specific internal energy
$\varrho_{\mathrm{mass},\alpha}$	mass density of phase α	h_α	specific enthalpy
$k_{\mathrm{r}\alpha}$	relative permeability	c_s	specific heat enthalpy
μ_α	phase viscosity	λ_pm	heat conductivity
D_α^κ	diffusivity of component κ in phase α	q^h	heat source term

2.2 Balance Equations

For the balance equations for multicomponent systems, it is in many cases convenient to use a molar formulation of the continuity equation. Considering the mass conservation for each component allows us to drop source/sink terms for describing the mass transfer between phases.

Then, the molar mass balance can be written as:

$$\phi\frac{\partial(\sum_\alpha \varrho_{\text{mol},\alpha}x_\alpha^\kappa S_\alpha)}{\partial t} - \sum_\alpha \operatorname{div}\left(\frac{k_{\text{r}\alpha}}{\mu_\alpha}\varrho_{\text{mol},\alpha}x_\alpha^\kappa K(\operatorname{grad} p_\alpha - \varrho_{\text{mass},\alpha}\boldsymbol{g})\right)$$

$$-\sum_\alpha \operatorname{div}\left(\tau\phi S_\alpha D_\alpha^\kappa \varrho_{\text{mol},\alpha}\operatorname{grad} x_\alpha^\kappa\right) - q^\kappa = 0, \qquad \kappa \in \{\text{w,a,c}\}.$$

In the case of non-isothermal systems, we further have to balance the thermal energy. We assume fully reversible processes, such that entropy is not needed as a model parameter. Furthermore, we neglect dissipative effects and the heat transport due to molecular diffusion. The heat balance can then be formulated as:

$$\phi\frac{\partial\left(\sum_\alpha \varrho_{\text{mass},\alpha}u_\alpha S_\alpha\right)}{\partial t} + (1-\phi)\,\frac{\partial \varrho_{\text{s}}c_{\text{s}}T}{\partial t} - \operatorname{div}\left(\lambda_{\text{pm}}\operatorname{grad} T\right)$$

$$-\sum_\alpha \operatorname{div}\left(\frac{k_{\text{r}\alpha}}{\mu_\alpha}\varrho_{\text{mass},\alpha}h_\alpha K\left(\operatorname{grad} p_\alpha - \varrho_{\text{mass},\alpha}\boldsymbol{g}\right)\right) - q^h \;=\; 0.$$

In order to close the system, supplementary constraints for capillary pressure, saturations and mole fractions are needed, [8]. According to the Gibbsian phase rule, the number of degrees of freedom in a non-isothermal multiphase multicomponent system is equal to the number of components plus one. This means we need as many independent unknowns in the system description. The available primary variables are, e. g., saturations, mole/mass fractions, temperature, pressures, etc.

3 THE DUMUX TOOLBOX

3.1 The DUNE framework

DUNE, the Distributed and Unified Numerics Environment is a modular toolbox for solving partial differential equations with grid-based methods, [1]. The main intention is to create slim interfaces allowing an efficient use of legacy and new libraries. Using C++ techniques, DUNE allows to use different implementations of the same concept (i.e. grids, solvers, ...) using a common interface with a very low overhead. DUNE is based on three main principles. The first one is the separation of data structures and algorithms by abstract interfaces, providing more functionality with less code and also ensuring maintainability and extendability of the framework. The second one is efficient implementation of these interfaces using generic programming techniques, [9], where static polymorphism allows the compiler to do more optimizations. The third principle is reuse of existing finite element packages with a large body of functionality.

The framework consists of a number of modules which are downloadable as separate packages. The current stable core modules are `dune-common` containing basic classes used by all modules (debugging, exceptions, ...), `dune-grid` for nonconforming, hierarchically nested, multi-element-type, parallel grids in arbitrary space dimensions, and `dune-istl`, the Iterative Solver Template Library (Krylov methods, ILU, algebraic and geometric multigrid, ...). Furthermore, there exist two modules `dune-disc` and `dune-fem`, which provide discretization algorithms, shapefunctions, and frameworks for defining operators between vector spaces.

3.2 DuMu$^{\text{x}}$

DuMu$^{\text{x}}$ comes in form of an additional module `dune-mux`. It inherits functionality from all available DUNE modules. Its main intention is to provide a framework for easy and efficient

implementation of models from porous media flow problems, ranging from problem formulation, the selection of spatial and temporal discretization schemes, as well as nonlinear solvers, up to general concepts for model coupling. Moreover, DuMu$^{\text{x}}$ includes ready to use numerical models and example applications.

Currently, the following models are available in DuMu$^{\text{x}}$:

- **diffusion:** Solves the stationary diffusion equation

$$-\operatorname{div}(K \operatorname{grad} u) = q.$$

  The permeability field K can be generated by Simset, [10]. Available spatial discretization methods: finite elements, cell centered finite volumes, mimetic finite differences. The diffusion term may be enhanced to account for the coupling with the transport equation within the context of the fractional flow formulation.

- **transport:** Solves

$$\phi \partial_t S - \operatorname{div}(f(S)\boldsymbol{v} + D(S, \operatorname{grad} S)) = 0.$$

  The diffusion term D may be arbitrarily specified to account for, e.g., capillary pressure or dispersion due to upscaling. Available spatial discretization method: cell centered finite volumes. Available time integration: explicit Runge-Kutta schemes.

- **decoupled fractional flow:** Solve

$$\begin{aligned} -\operatorname{div}(\lambda_{\text{t}}(S) K \text{grad} p) &= 0, \\ \phi \partial_t S - \operatorname{div}(f(S)\boldsymbol{v}_{\text{t}}(S,p)) &= 0. \end{aligned}$$

  Combination of diffusion and transport model. Available constitutive relations: linear, Brooks-Corey, van Genuchten. The pressure and the saturation equation may be discretized on different levels and with different spatial discretizations. Thus, we are flexible to perform upscaling for only one of the two equations or for both. However, currently, only an upscaling of the transport equation based on [11] is implemented. Available algorithm for decoupling: IMPES scheme.

- **fully coupled twophase flow:** Solves the $p_{\text{w}} - S_{\text{n}}$ formulation

$$\begin{aligned} -\phi \partial_t S_{\text{n}} - \operatorname{div}(\lambda_{\text{w}} K (\text{grad} p_{\text{w}} - \rho_{\text{w}} \boldsymbol{g})) - q_{\text{w}} &= 0, \\ \phi \partial_t S_{\text{n}} - \operatorname{div}(\lambda_{\text{n}} K (\text{grad}(p_{\text{w}} + p_{\text{c}}) - \rho_{\text{n}} \boldsymbol{g})) - q_{\text{n}} &= 0. \end{aligned}$$

  Discretization scheme: box method. Nonlinear solver: Newton's method. Time integration: implicit Euler.

A key issue is to reduce the time needed for the implementation of new models. First steps have been done in this direction. Based on the discretization module `dune-disc`, we started developing a general framework for nonlinear evolution equations of first order in time, discretized by either the box method or piecewise linear finite elements. Apart from eventually having to specify a new problem type, i.e., the kind of boundary and initial conditions, and from implementing new material properties and constitutive relations, the task is basically reduced to provide a routine for calculating the local defect on each element/cell. The Jacobian needed for the Newton method is then approximated by finite differences. Alternatively, a problem-specific routine for the element-wise Jacobian can be given by the user.

4 OUTLOOK

Concerning the DuMu^x toolbox, the immediate next steps are to generalize and optimize the box method, the mimetic finite difference method, and the Newton solver, as well as to implement an interface with external grid generators used in our research groups. In the long run, two key issues are to be resolved. The first one is the development of a general strategy for coupling different numerical models in various ways: horizontally, i.e., from different subdomains, vertically, i.e., on different spatial scales, temporally, i.e., different time step sizes / discretizations, and, finally, different problem dimensions. The second major issue is the implementation on parallel architectures, for which the DUNE framework provides an excellent starting point.

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