Multiscale Modeling of Flow and Transport

and the simulation toolbox DuMu\textsuperscript{X}

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Outline

Multiscale / multiphysics modeling
- Motivation
- Concept
- Outlook

DuMu$^X$
- What is Dune? What is DuMu$^X$?
- 1p1c / 2p2c multiphysics example
LNAPL contamination in the unsaturated zone

- LNAPL in residual saturation
- Unsaturated zone
- Saturated zone
- Soil vapor extraction
- Drinking water well
- Groundwater flow

(Niessner)
LNAPL – spatial dependence of processes

(Niessner)
Motivation—General Idea

Modeling of complex physical processes in larger domains:

- available computer power + data → coarse-scale models
- processes dependent on phase & material interfaces → fine-scale modeling

coarse-scale models accounting for fine-scale processes!

multi-scale modeling

(Niessner)
Definition of Scales

- MICRO SCALE
  - REV effective parameters ($\phi$, $S$)
  - constitutive relationships
  - equations of state

- LOCAL SCALE
  - material interphase oriented processes
  - continuity in intensive state variables
  - discontinuities in primary unknowns

- MOLECULAR SCALE
  - phase interphase oriented processes
  - mass transfer
  - reaction
  - capillarity

- MACRO SCALE
  - larger scale heterogeneities
  - lack of detailed knowledge of smaller scales

(Niessner)
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Concept

- Modeling of complex processes on fine scale only where needed
  -> Multiphysics
- Modeling of ‘simple’ processes on macro scale with account to local scale heterogeneities
  -> Multiscale

Concept for 2p2c / 3p3c developed by J. Niessner
[Niessner & Helmig 2007]
- No gravity, capillarity, compressibility
- Isothermal conditions
- Mass transfer only in Subdomain, one phase immobile
- Fractional Flow Formulation
2p2c concept
2P / 2P2C Flow Equations

Pressure equation

$$\nabla \cdot \mathbf{v} = 0, \quad \mathbf{v} = -\lambda(S_w)K\nabla p$$

Saturation equation (upscaled)

$$\frac{C_{\bar{V}_z}}{C_w} \cdot \mathbf{u} f + \mathbf{i}_z \mathbf{y} . \mathbf{G}, @ 3$$

Concentration equations

$$\frac{C_{\bar{F}^\text{in}}}{C_w} \cdot \mathbf{u} f + \mathbf{i} \mathbf{F}^\text{in} \mathbf{y}, @ 3$$

with

$$C_{\kappa} = \rho_\alpha X_{\kappa}$$

and

$$C_{\kappa} = \sum_{\alpha} \left( C_{\kappa} S_\alpha \right)$$
Solution Strategy

1. Flow Field
2. Concentration
3. Saturation
4. Saturation
3p3c concept

residual NAPL

3p3c

2p3c
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Enhanced Remediation

- LNAPL in residual saturation
- Unsaturated zone
- Saturated zone
- Soil vapor extraction
- Groundwater flow
- Drinking water well
- Thermal energy
- 200°C
- 10°C
- Several km
- 100 m
# Processes and Models

<table>
<thead>
<tr>
<th>Processes</th>
<th>Model in T</th>
<th>Model in U</th>
</tr>
</thead>
<tbody>
<tr>
<td>Immobile spill of contaminant in saturated zone, isothermal</td>
<td>1P1C upscaled</td>
<td>2P2C</td>
</tr>
<tr>
<td>Immobile spill of contaminant in unsaturated zone, isothermal</td>
<td>2P1C upscaled</td>
<td>3P3C</td>
</tr>
<tr>
<td>As above, non-isothermal</td>
<td>(as above), T</td>
<td>(as above), T</td>
</tr>
<tr>
<td>Locally advection dominated, non-isothermal</td>
<td>(as above), T conductive</td>
<td>(as above) T conv + cond</td>
</tr>
<tr>
<td>Locally fast -&gt; no thermal equilibrium</td>
<td>(as above), T</td>
<td>(as above), T for each phase</td>
</tr>
</tbody>
</table>
Goals

Jennifer Niessner

Multiscale Multiphysics Approach

Gravity and Capillary Effects

Bernd Flemisch

Discretizations, Mathematical Multiscale Approaches

Jochen Fritz

Compressibility, non-iso-thermal Processes

Implementation in DUNE

Multiscale Toolbox

Physical Processes

- Phases/Components
- Capillary Forces
- Non-isothermal Effects

Discretizations

- Spatial Scales (adapt.)
- Implicit/Explicit Time
- Element shapes

Math. Modeling

- Finite Volume
- Finite Element
- Multiscale FV/FE
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DuMu$^X$

Dune for Multi-{phase, component, scale, physics, …}\nFlow in Porous Media

Current development by:
• Bernd Flemisch
• Jochen Fritz
• Onur Dogan
• Melanie Darcis
• Klaus Mosthaf
What is Dune?

- Modular toolbox for solving PDEs with grid-based methods.
- Allows different implementations of the same concept (grids, solvers, ...) using a common interface with low overhead.
- Developed by groups in Stuttgart (AG Bastian), Freiburg (AG Kröner), Berlin (AG Kornhuber), Münster (AG Ohlberger).
- Free software licensed under GPL: [www.dune-project.org](http://www.dune-project.org)
- Modules: dune-common, dune-grid, dune-istl, dune-disc, dune-fem
- Main principles:
  - Separation of data structures and algorithms by abstract interfaces.
  - Efficient implementation using generic programming techniques.
  - Reuse of existing packages with a large body of functionality.
Available Dune modules

Core, stable

- **dune-common**: basic classes used by all modules (debugging, exceptions, …).
- **dune-grid**: nonconforming, hierarchically nested, multi-element-type, parallel grids in arbitrary space dimensions.
- **dune-istl**: Iterative Solver Template Library (Krylov methods, ILU, algebraic and geometric multigrid, …).

External, unstable

- **dune-disc**: discretizations, shapefunctions, operators (AG Bastian).
- **dune-fem**: discretization algorithms, function spaces, operators (AG Kröner).
What is DuMu^x? 

- Additional module **dune-mux**. 
- Inherits functionality from all available Dune modules. 
- Provides a framework for easy and efficient implementation of models from porous media flow problems:
  - problem formulation. 
  - spatial and temporal discretization schemes. 
  - nonlinear solvers. 
  - concepts for model coupling. 
- Includes ready to use numerical models and example applications.
Sample DuMu$^X$ Functionality

• Diffusion model
  - Generation of K by SIMSET (Bardossy)
  - Spatial discretizations: FEM, FVM, Mimetic FDM

\[
\nabla \cdot ( f(S) \mathbf{v} + D(S, \nabla S) ) = 0
\]

• Transport model
  - Arbitrary diffusion term (capillarity, upscaling)
  - Spatial discretisation: FVM
  - Temporal discretization explicit Runge-Kutta

\[
\frac{CV}{C_w} \nabla \cdot ( f_i + V,y ) . \ G + V > u \ V , , @ 3
\]
Sample DuMuX Functionality

• Transport model
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  - Spatial discretisation: FVM
  - Temporal discretization explicit Runge-Kutta

\[
\phi \frac{\partial C}{\partial t} - \nabla \cdot \left( \sum_{\alpha} C_{\alpha} f(S) v \right) = 0
\]

• Fractional Flow
  - Combines diffusion and transport model
  - Time discretisation: IMPES
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Example Simulation

Initial Condition

Permeability Field
Example Simulation
Example Simulation
Example Simulation