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Modelling and Simulation in Porous Media



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Multi-scale and multi-physics modelling of flow and transport processes in porous media

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In co-operation with

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Need for Coupled Porous Media Models



Geothermal energy



Fracking fluid and salt water infiltration in groundwater?

Unconventional gas production



Fracking fluid and methane migration in groundwater?

Potential CO₂ storage site in northern Germany





- 40 km x 40 km site in northern Germany
- Injection depth: 1500m
- Injection rate:
 2.5 Mt/year
 (for 10 years)

How does the injection in structure A affect the pressure field in structure B?



Saturation and pressure distribution after 10 years









Complex Long-Term Processes: e.g. CO₂ Sequestration:

Simulation of long-term processes during CO₂ storage



(Darcis et al. 2014 WRR)



Classification of Model-Coupling Approaches





Multi-scale and multi-physics strategy



adaptive in space (multi-scale), adaptive in physics (multiphysics) + adaptive in time (multi-numerics)

Multi-scale Approaches



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Model equations: Equations for two-phase flow

- Coupled system:
 - Continuity equation:
 - Darcy's law:

$$\phi \frac{\partial S_{\alpha}}{\partial t} + \nabla \cdot \mathbf{v}_{\alpha} = q_{\alpha} \qquad \alpha \in \{\mathsf{w}, \mathsf{n}\}$$
$$\mathbf{v}_{\alpha} = -\frac{k_{\mathsf{r}_{\alpha}}\mathbf{K}}{\mu_{\alpha}} \cdot [\nabla p_{\alpha} - \varrho_{\alpha}g\nabla z]$$

$$p_{\mathsf{C}} = p_{\mathsf{n}} - p_w$$



Demands on simulators

- Simulation of huge domains
- Fine resolution of heterogeneous parameters



Demands on simulators

- Simulation of huge domains
- Fine resolution of heterogeneous parameters
- Fine resolution of fluid fronts
- Complex physics
 - Focus: e.g. Two-phase flow including **capillary pressure effects**



Some examples (Capillary pressure effects)





Fine-scale reference: Effect of capillary pressure

 Capillary pressure heterogeneities can strongly affect the fluid distribution!





Demands on simulators

- Simulation of huge domains
- Fine resolution of heterogeneous parameters
- Fine resolution of fluid fronts
- Complex physics
 - Focus: Two-phase flow including capillary pressure effects

Problems:

- Large number of grid cells/
 Large number of degrees of freedom
- - Complex non-linear models





(M. Celia)



Demands on simulators

- Simulation of huge domains
- Fine resolution of heterogeneous parameters
- Fine resolution of fluid fronts
- Complex physics
 - Focus: Two-phase flow including capillary pressure effects

Problem:

- Large number of grid cells/
 Large number of degrees of freedom
- Complex non-linear systems/models

Solution Strategies:

- Multi-scale methods
 Simplified de-coupled
 - systems
 - Multi-physics methods



Multi-scale modeling of two-phase flow: State of the art

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• Many powerfull approaches for the simplified case:

$$\nabla \cdot \left[-\lambda_{\mathsf{t}} \mathbf{K} \nabla p_{\mathsf{W}} \right] = q_{\mathsf{t}}$$

$$\phi \frac{\partial S_{\mathsf{W}}}{\partial t} + \nabla \cdot \mathbf{v}_{\mathsf{W}} = q_{\mathsf{W}}$$

- Multi-scale finite element approaches (e.g. Kippe et al., 2008, …)
- Multi-scale finite volume approaches (e.g. Lee et al., 2009, ...)
- Standard numerical upscaling/pseudo function approaches (e.g. Durlofsky,1991, Stone, 1991, Niessner etal 2009...)
- Adaptive upscaling methods (e.g. Chen and Li, 2009,...)



- Coupled system:
 - Continuity equation:
 - Darcy's law:

$$\phi \frac{\partial S_{\alpha}}{\partial t} + \nabla \cdot \mathbf{v}_{\alpha} = q_{\alpha} \qquad \alpha \in \{\mathsf{w}, \mathsf{n}\}$$
$$\mathbf{v}_{\alpha} = -\frac{k_{\mathsf{r}_{\alpha}}\mathbf{K}}{\mu_{\alpha}} \cdot [\nabla p_{\alpha} - \varrho_{\alpha}g\nabla z]$$

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- Reformulation → Decoupled equations:
 - Pressure equation:

$$\nabla \cdot [-\lambda_{t} \mathbf{K} \nabla p_{\mathsf{W}} - \lambda_{\mathsf{n}} \mathbf{K} \nabla p_{\mathsf{C}} - (\lambda_{\mathsf{W}} \rho_{\mathsf{W}} + \lambda_{\mathsf{n}} \rho_{\mathsf{n}}) \mathbf{K} g \nabla z] = q_{\mathsf{t}}$$
$$p_{\mathsf{C}} = p_{\mathsf{n}} - p_{w}$$

Transport equation:

$$\phi \frac{\partial S_{\mathsf{W}}}{\partial t} + \nabla \cdot \mathbf{v}_{\mathsf{W}} = q_{\mathsf{W}}$$



Multi-scale modeling modeling of two-phase flow

→ including capillary pressure

 $\nabla \cdot \left[-\lambda_{\mathsf{t}} \mathbf{K} \nabla p_{\mathsf{W}} \right] = q_{\mathsf{t}}$

$\nabla \cdot [-\lambda_{t} \mathbf{K} \nabla p_{\mathsf{W}} - \lambda_{\mathsf{n}} \mathbf{K} \nabla p_{\mathsf{C}} - (\lambda_{\mathsf{W}} \rho_{\mathsf{W}} + \lambda_{\mathsf{n}} \rho_{\mathsf{n}}) \mathbf{K} g \nabla z] = q_{\mathsf{t}}$ Outline part I

- Numerical upscaling
- Adaptive grid refinement
- Multi-scale modeling



Numerical Upscaling

- **Coarse scale equations:** \bullet $\phi^* - \partial S_{\alpha}$
 - Mass balance:

Darcy's law:

$$\frac{\partial S_{\alpha}}{\partial t} + \nabla \cdot \mathbf{v}_{\alpha} = q_{\alpha} \qquad \qquad \alpha \in \{\mathsf{w}, \mathsf{n}\}$$

 $\rho_{\alpha}g\nabla z$]

$$\mathbf{v}_{\alpha} = -\underbrace{\mathbf{K}_{\mathsf{tot}_{\alpha}}^{*}}_{\mu_{\alpha}} \cdot [\nabla p_{\alpha} -$$

- Choose representative subscale problems (problem setups)
- Calculate coarse scale quantities from (local) fine-scale \bullet simulations



Numerical Upscaling

- Coarse scale equations:
 - Mass balance:
 - Darcy's law:

$$\phi^* \frac{\partial S_{\alpha}}{\partial t} + \nabla \cdot \mathbf{v}_{\alpha} = q_{\alpha} \qquad \alpha \in \{\mathsf{w}, \mathsf{n}\}$$
$$\mathbf{v}_{\alpha} = \underbrace{\mathbf{K}_{\mathsf{r}_{\alpha}}^* \mathbf{K}^*}_{\mu_{\alpha}} \cdot [\nabla p_{\alpha} - \varrho_{\alpha} g \nabla z]$$

- Reformulation:
 - Pressure equation:

Transport equation:

$$\nabla \cdot \left[\begin{array}{c} \mathbf{\Lambda}_{t}^{*} \mathbf{K}^{*} \nabla \Phi_{\mathsf{W}} - \begin{array}{c} \mathbf{F}_{\mathsf{n}}^{*} \mathbf{\Lambda}_{t}^{*} \mathbf{K}^{*} \nabla \Phi_{\mathsf{c}}^{*} \right] = q_{\mathsf{t}} \\ \Phi_{\alpha} = p_{\alpha} + \varrho_{\alpha} gz \qquad \Phi_{\mathsf{c}} = \Phi_{\mathsf{n}} - \Phi_{w} \\ \phi^{*} \frac{\partial S_{\mathsf{W}}}{\partial t} + \nabla \cdot \mathbf{v}_{\mathsf{W}} = q_{\mathsf{W}} \end{array}$$

(Wolff et al. Treatment of tensorial relative permeabilities with multipoint flux approximation. *International journal of numerical analysis & modeling*, 2012)



Definition of the phase permeability tensor

$$\mathbf{K}_{\mathsf{tot}_{\alpha}}^* = \mathbf{K}^* \mathbf{K}_{\mathsf{r}_{\alpha}}^*$$

- Total and absolute permeability:
 - Second order tensors
- <u>Relative permeability:</u>
 - <u>Second order tensor</u> (e.g. *Nordbotten et al.* On the definition of macroscale pressure for multiphase flow in porous media, 2008)



Local numerical upscaling



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Local steady state upscaling

- Calculate full absolute permeability tensor from local 1-p problems
 - e.g. Wen et al. 2003, ...



Local steady state upscaling

- Calculate full absolute permeability tensor from local 1-p problems
 - e.g. Wen et al. 2003, ...
- Calculate capillary pressure using a macroscale percolation approach
 - e.g. Braun et al 2005,



Local steady state upscaling:



(Braun et al. JCH 2005, Nuske et al WRR, 2010)



Local steady state upscaling

- Calculate full absolute permeability tensor from local 1-p problems
 - e.g. Wen et al. 2003, ...
- Calculate capillary pressure using a macroscale percolation approach
 - e.g. Braun et al 2005,
- Calculate full relative permeability tensor from local 2-p problems
 - Extention of Wen et al. 2003 for relative permeabilities



Local steady state upscaling:



Relative permeability upscaling

$$\begin{pmatrix} \Psi_{\alpha,x}^{x} & \Psi_{\alpha,y}^{x} & 0 & 0\\ 0 & 0 & \Psi_{\alpha,x}^{x} & \Psi_{\alpha,y}^{x}\\ \Psi_{\alpha,x}^{y} & \Psi_{\alpha,y}^{y} & 0 & 0\\ 0 & 0 & \Psi_{\alpha,x}^{y} & \Psi_{\alpha,y}^{y}\\ 0 & 1 & -1 & 0 \end{pmatrix} \begin{pmatrix} K_{\text{tot}_{xx\alpha}}^{*}\\ K_{\text{tot}_{yx\alpha}}^{*}\\ K_{\text{tot}_{yy\alpha}}^{*} \end{pmatrix} = - \begin{pmatrix} \langle v_{\alpha_{x}} \rangle_{\alpha}^{x}\\ \langle v_{\alpha_{y}} \rangle_{\alpha}^{x}\\ \langle v_{\alpha_{x}} \rangle_{\alpha}^{y}\\ \langle v_{\alpha_{y}} \rangle_{\alpha}^{y}\\ 0 \end{pmatrix}$$

$$\Psi_{\alpha,x}^{x} = \frac{1}{\mu_{\alpha}} \frac{\partial}{\partial x} \langle \Phi_{\alpha} \rangle_{\alpha}^{x} \qquad \qquad \Psi_{\alpha,y}^{x} = \frac{1}{\mu_{\alpha}} \frac{\partial}{\partial y} \langle \Phi_{\alpha} \rangle_{\alpha}^{x}$$

$$\Psi^{y}_{\alpha,x} = \frac{1}{\mu_{\alpha}} \frac{\partial}{\partial x} \langle \Phi_{\alpha} \rangle^{y}_{\alpha} \qquad \qquad \Psi^{y}_{\alpha,y} = \frac{1}{\mu_{\alpha}} \frac{\partial}{\partial y} \langle \Phi_{\alpha} \rangle^{y}_{\alpha}$$

$$\mathbf{K}_r^* = \mathbf{K}_{\mathsf{tot}}^* \mathbf{K}^{*^{-1}}$$

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Local steady state upscaling

- Calculate full absolute permeability tensor from local 1-p problems (e.g. Wen et al. 2003, ...)
- Calculate capillary pressure using a macroscale percolation approach (e.g. Braun et al 2005,)
- Calculate full relative permeability tensor from local 2-p problems (Extention of Wen et al. 2003 for relative permeabilities)
- Use effective flux boundary conditions to account for the global distribution of the heterogeneous parameters
- Permeability tensors are forced to be symmetric and positive definit (Avoid unphysical flow!)
- Continuous relative permeability curves are interpolated using monotone splines



Upscaled constitutive relations





Multi-scale = Upscaling + Downscaling

• Upscaling:

- From detailed information to less detailed information
- Information is thrown away
- Unique!

 \rightarrow A certain distribution has exact one average (unless the average operator is changed)

• Downscaling:

- From less detailed information to detailed information
- Information has to be generated!
- Non-unique!
 - \rightarrow What is the distribution to a certain average?



Downscaling of two-phase flow

- Small scale phase pressures and saturations have to be reconstructed from coarse scale information
- Problem 1: Phase pressure and saturation are coupled by capillary pressure
- Problem 2: Information about extreme values is lost/averaged at the coarse scale
- Local downscaling is not possible if capillary effects are important!?
- Global downscaling is not efficient!
- An adaptive grid is "a natural and efficient global downscaling strategy"!



Adaptive grid refinement

Numerical method:

- Cell centered finite volumes with multi-point flux approximation (MPFA L-method, e. g. Aavatsmark et al., 2008.)
 - Development of a MPFA L-method for two-phase flow including capillarity and gravity based on the decoupled formulation
 - ✓ Non-conforming refinement with hanging nodes (Faigle et al. CompGeo 2013)
 - ✓ Unstructured grids
 - Heterogeneities (e.g. Helmig and Huber, AWR 1999)
 - ✓Permeability, Porosity
 - ✓Capillary pressure (interface conditions)



The MPFA L-method

- 2d-quadrilaterals: Aavatsmark et al., Numer Meth Part D E, 2008
- Works on **unstructured** and **non-K-orthogonal** grids
- Correct treatment of grid block heterogeneities and material interfaces
- Maximum flux stencil: 9-point stencil (2-d), 18-point stencil (3d)





Adaptation examples: 1) Nine-spot water flood





0.6

0.4



Adaptation examples: 2) Low permeable lenses





Adaptation examples: 3) Anisotropic permeability





Adaptive grid refinement: Example (DNAPL infiltration)

- Two-phase flow with capillary pressure and gravity
- Homogeneous domain, anisotrop absolute and relative permeability



(Wolff et al. sub. DeGrutyer 2013)



Multi-Scale Modeling

Demands on simulators:

- Simulation of huge domains
- Fine resolution of heterogeneous parameters
- Fine resolution of fluid fronts
- Complex physics



Focus: Two-phase flow including capillary pressure effects





Multi-scale approach

- Combination of numerical upscaling and grid adaptive discretization schemes (Wolff et al. WRR 2013)
 - If a grid cell is on the finest level and fine-scale parameters/functions are available use these
 - Else use upscaled parameters/functions
- Control of the multi-scale behavior by choice of the adaption criterion!
 - Error control by **standard criteria**
 - e.g. saturation gradients, flux integrals, etc.
 - Error control by **multi-scale criteria**
 - Check if assumptions of the upscaling method are sufficiently satisfied (e.g. capillary equilibrium assumption → capillary number, etc.)



(Criteria)

- Standard mark element for $\begin{cases} \text{coarsening} &, \Delta S_{\text{local}} < \epsilon_{\text{coarsen}} \Delta S_{\text{max}} \\ \text{refinement} &, \Delta S_{\text{local}} > \epsilon_{\text{refine}} \Delta S_{\text{max}} \\ \text{nothing} &, \text{else} \end{cases}$
- Standard + ds/dt \rightarrow flux integral!
 - additional coarsening criterion

mark element for $\left\{ \text{coarsening} \quad , \left(\frac{\Delta S}{\Delta t} \right)_{\text{local}} < \epsilon_{\text{coarsen}} \right\}$

- Standard + multi-scale (only with capillary pressure):
 - Check if capillary equilibrium assumption for coarse scale parameters is valid

mark element for $\begin{cases} coarsening &, Ca_{local} < \epsilon_{coarsen} \\ refinement &, Ca_{local} > \epsilon_{refine} \end{cases}$



Multi-scale: Random permeability field



fine-scale reference



adaptive, multiscale, conservative refinement



adaptive, multiscale, intermediate refinement

wetting saturation



adaptive, multiscale, lax refinement









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SPE 10 Model 2 (Christie and Blunt, 2001)





Combination of all indicators

- One indicator which accounts for errors in the saturation transport (local sat gradient)
- One indicator which accounts for errors in the flow field (total velocity)
- Multi-scale: Permeability upscaling + adaptive grid



Solutions averaged to the coarse scale grid



Multi-scale: SPE 10

- Layer from bottom formation
- With capillary pressure





Refined for max. accuracy









scale solution



SPE 10 Model 2





Adaptive time discretization







Transport equations

Two-Phase Flow equations:

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Fractional Flow Formulation:

$$\phi \frac{\partial S_w}{\partial t} + \nabla \cdot v_w = q_w \qquad \nabla \cdot \left[-\lambda_t \mathbf{K} (\nabla \Phi_w + f_n \nabla \Phi_c) \right] = q_w + q_n$$
$$\phi \frac{\partial S_n}{\partial t} + \nabla \cdot v_n = q_n \qquad \qquad \phi \frac{\partial S_w}{\partial t} + \nabla \cdot v_w = q_w$$

Phase and Capillary Potential:

$$\Phi_{\alpha} = p_{\alpha} + \rho_{\alpha}gz, \ \alpha = w, n, \ \Phi_c = p_c + (\rho_n - \rho_w)gz$$

elliptic + parabolic equation



Fully Implicit Methods



Discretization of Fractional Flow Equation

IMPES

$$\mathbf{A}_{\Phi}(\mathbf{S}_w^n)\mathbf{\Phi}_w^{n+1} + \mathbf{A}_c(\mathbf{S}_w^n)\mathbf{\Phi}_c(\mathbf{S}_w^n) = \mathbf{Q}_{\Phi}^{n+1}$$

$$\mathbf{M}\frac{\mathbf{S}_{w}^{n+1} - \mathbf{S}_{w}^{n}}{\Delta t^{n}} + \mathbf{A}_{w}(\mathbf{S}_{w}^{n})\mathbf{\Phi}_{w}^{n+1} = \mathbf{Q}_{w}^{n+1}$$

FL

$$\mathbf{A}_{\Phi}(\mathbf{S}_{w}^{n+1})\mathbf{\Phi}_{w}^{n+1} + \mathbf{A}_{c}(\mathbf{S}_{w}^{n+1})\mathbf{\Phi}_{c}(\mathbf{S}_{w}^{n+1}) = \mathbf{Q}_{\Phi}^{n+1}$$

$$\mathbf{M}\frac{\mathbf{S}_{w}^{n+1} - \mathbf{S}_{w}^{n}}{\Delta t^{n}} + \mathbf{A}_{w}(\mathbf{S}_{w}^{n+1})\mathbf{\Phi}_{w}^{n+1} = \mathbf{Q}_{w}^{n+1}$$

Assumptions: no

Problems: convergence of solver

IMPSAT

IMPCAP

$$\mathbf{A}_{\Phi}(\mathbf{S}_{w}^{n})\mathbf{\Phi}_{w}^{n+1} + \mathbf{A}_{c}(\mathbf{S}_{w}^{n})\mathbf{\Phi}_{c}(\mathbf{S}_{w}^{n}) = \mathbf{Q}_{\Phi}^{n+1} \quad \mathbf{A}_{\Phi}(\mathbf{S}_{w}^{n})\mathbf{\Phi}_{w}^{n+1} + \mathbf{A}_{c}(\mathbf{S}_{w}^{n})\mathbf{\Phi}_{c}^{\operatorname{approx}}(\mathbf{S}_{w}^{n+1}) = \mathbf{Q}_{\Phi}^{n+1}$$
$$\mathbf{M}\frac{\mathbf{S}_{w}^{n+1} - \mathbf{S}_{w}^{n}}{\Delta t^{n}} + \mathbf{A}_{w}(\mathbf{S}_{w}^{n})\mathbf{\Phi}_{w}^{n+1} = \mathbf{Q}_{w}^{n+1} \qquad \mathbf{M}\frac{\mathbf{S}_{w}^{n+1} - \mathbf{S}_{w}^{n}}{\Delta t^{n}} + \mathbf{A}_{w}(\mathbf{S}_{w}^{n})\mathbf{\Phi}_{w}^{n+1} = \mathbf{Q}_{w}^{n+1}$$

Assumptions: weakly coupled Problems: time step restrictions Assumptions: weakly coupled Problems: CFL, expensive assembling



Comparison of Efficiency and Accuracy

SPE 10, Layer 15





Problem Setting $p_{w,min}$ $p_{w,min} = 20 \text{ MPa}$ $S_{w,init} = 0.0$ $p_{w,max} = 40 \text{ MPa}$ $p_{w,max} S_w = 1.0$

• similar results

• FI and IMPSAT: more numerical diffusion



Comparison of Efficiency and Accuracy

- IMPES fastest up to ~ 10^4 cells, lowest order
- IMPSAT faster than FI
- FI highest efficiency order



- All methods converge
- FI higher accuracy than IMPSAT
- Jocobian reassembling has no effect on accuracy



Problem with capillary pressure





Problem with capillary pressure



IMPSAT:

- Wrong front movement
- Assumption of weakly coupled equations is not fullfilled

IMPES:

- CFL Coats criteria produces small time step sizes
- Equations are only for small steps weakly coupled

IMPSAT + IMPCAP:

- Correct solution
- Bigger time step sizes are possible
- Loss of sparsity pattern for matrices



Motivation Adaptive Implicit Method (AIM)

For each numerical method you can design a poblem where it performs bad





Regions are changing per time, they move with the physical processes

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Two-phase flow with gravity and capillary pressure



 \mathcal{X}



More complex example

including gravity + capillary pressure



no optimal AIM example





Next Steps / Outlook

- Implementation of MPFA for AIM
- Further investigation of AIM approach
- Increase convergence of solver / better preconditioner:

$$\mathbf{R_1} = \mathbf{A}_{\Phi}(\mathbf{S}_w^{n+1})\mathbf{\Phi}_w^{n+1} + \mathbf{A}_c(\mathbf{S}_w^{n+1})\mathbf{\Phi}_c(\mathbf{S}_w^{n+1}) - \mathbf{Q}_{\Phi}^{n+1} \quad \text{elliptic}$$

$$\mathbf{R_2} = \mathbf{M} rac{\mathbf{S}_w^{n+1} - \mathbf{S}_w^n}{\Delta t^n} + \mathbf{A}_w(\mathbf{S}_w^{n+1}) \mathbf{\Phi}_w^{n+1} - \mathbf{Q}_w^{n+1}$$
 parabolic

$$\mathbf{X} = (\mathbf{P}_{\mathbf{w}}, \mathbf{S}_{\mathbf{w}}) \qquad \mathbf{J}_{\mathbf{R}} = \frac{\partial \mathbf{R}}{\partial \mathbf{X}} = \begin{pmatrix} \mathbf{A}_{\mathbf{1}, \mathbf{P}_{\mathbf{w}}} & \mathbf{A}_{\mathbf{1}, \mathbf{S}_{\mathbf{w}}} \\ \mathbf{A}_{\mathbf{2}, \mathbf{P}_{\mathbf{w}}} & \mathbf{A}_{\mathbf{2}, \mathbf{S}_{\mathbf{w}}} \end{pmatrix}$$

- use different preconditioner for elliptic and parabolic equation
- → CPR-AMG preconditioner



0.2505 0.24

0.2

0.1626

Johansen Formation





Summary – State of current work

- Adaptive grid refinement: Hanging nodes, MPFA Lmethod (3D)
- Numerical upscaling of phase permeabilities: tensorial relative permeabilities
- Treatment of tensorial relative permeabilities using MPFA
- **Multi-scale**: Combination of numerical upscaling and adaptive grid refinement

Future work:

- Adaptive time discretization (IMPES, sequential and fully implicit)
- Large scale simulation
- Include **multi-physics** concept (e.g. 3-phase 2-phase flow)

The End







References

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http://dune-project.org/