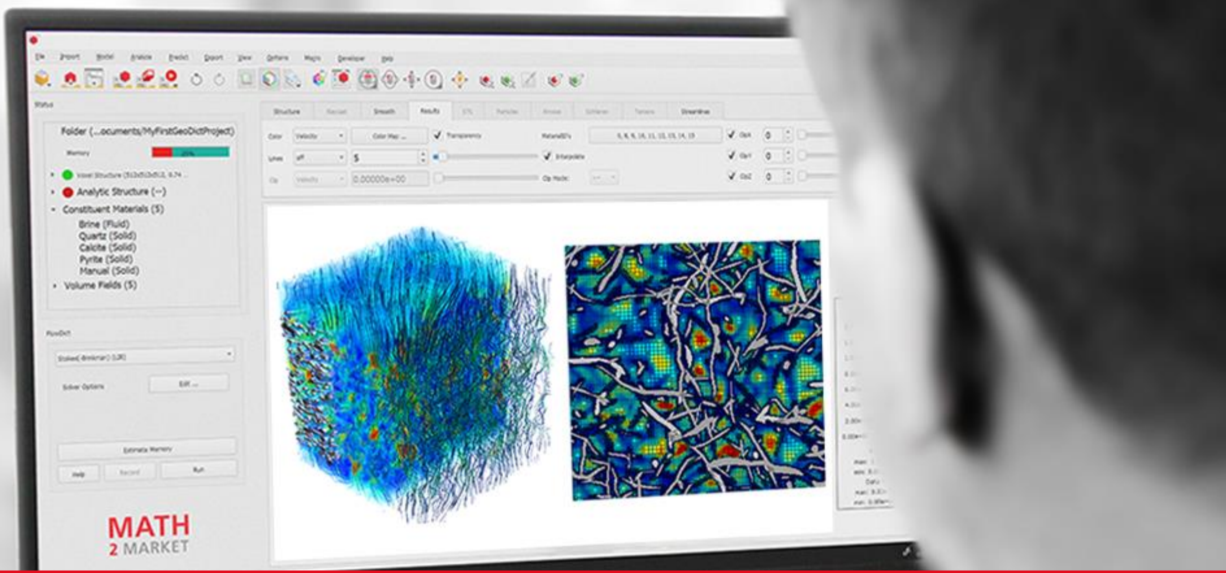
GeoDict
The Digital Material Laboratory



Specialized Methods for Direct Numerical Simulations in Porous Media

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Math2Market GmbH

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Some background information

Math2Market GmbH

- creates and markets the scientific software GeoDict®.
- was spun off in 2011 from Fraunhofer ITWM in Kaiserslautern.
- is an privately owned company based in Kaiserslautern, Germany.

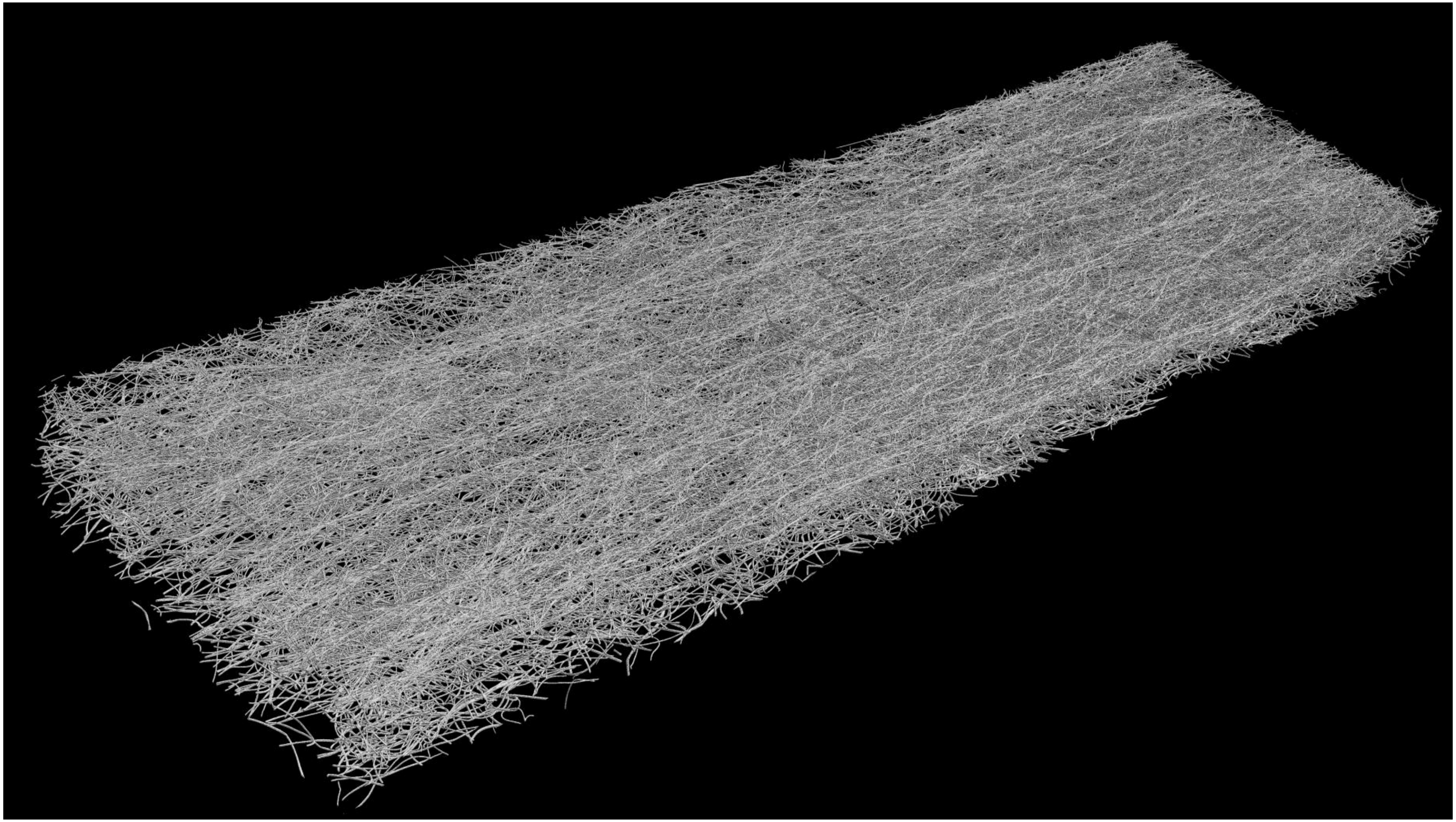
GeoDict® - The Digital Material Laboratory

- is a software tool to analyze and design porous media and composites.
- works on
  - µCT and FIB-SEM 3D images or
  - random geometric material models.

Outline

Outline

Segmented CT-Scan of a Non-Woven Structure



18310 x 4816 x 1704 (>**150 billion**) voxels, 4.4 x 1.2 x 0.4 cm^3, 2.4 µm voxel length

Introduction

- 3d imaging devices (e.g. µCT) allow deep insights into the structures of porous materials
  - 2000^3 (8 billion) voxels is a standard size - imaged and reconstructed within hours
- Very fast and memory efficient methods are needed to deal with these images
- Researchers and engineers are interested in effective material properties such as
  - permeability, pressure drop and mean velocity
  - thermal and electrical conductivity, diffusivity and tortuosity,
  - stiffness, strain, stress, or elastic moduli,
  - saturation- or compression-dependent properties (e.g. relative permeability)
- Bottleneck of classical finite-element or -volume methods is the meshing step
  - Runtime of the meshing step can take more runtime than the actual solving
  - Manual adjustment of the mesh is often required
- Lattice-Boltzmann (LB) methods are advancing fast and do not require meshing
  - But they require a lot of memory due to the D3Qm lattices
- Here, we present specialized finite-volume methods designed for large 3d images

OUTLINE

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01 Introduction

02 Direct numerical methods

1. Explicit Jump
2. SIMPLE-FFT
3. LIR

Single-Phase Flow

4. Lippmann Schwinger

Mechanics

5. Pore Morphology

Two-Phase Flow

03 Application examples

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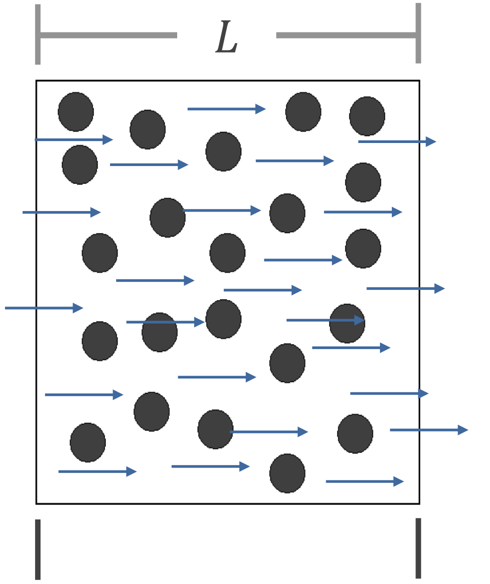
ΔP-driven Stokes

$$\mu\Delta u = \nabla p \text{ on } \Omega \quad (\text{Conservation of momentum})$$
$$\nabla \cdot u = 0 \quad \text{on } \Omega \quad (\text{Conservation of mass})$$
$$u = 0 \quad \text{on } \Gamma \quad (\text{No} - \text{slip on solid surfaces})$$
$$\Omega \subset [0, l_x] \times [0, l_y] \times [0, l_z] \quad (\text{Domain})$$

$\boldsymbol{u}$, p periodic on Ω with boundary Γ, except for pressure drop P_1-P_2 = c



As usual:

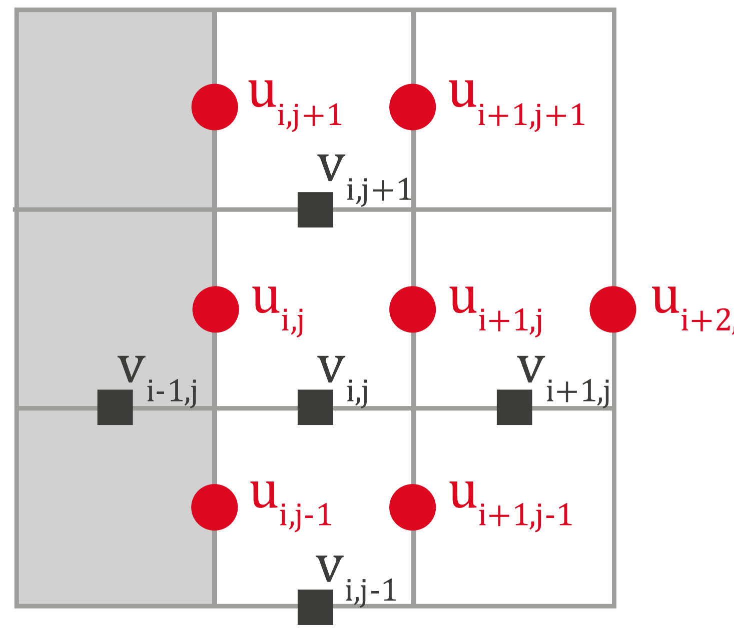
- u: velocity
- p: pressure
- μ: dynamic viscosity
- $\tilde{u}$: mean velocity

Darcy's law: $\tilde{u} = -\frac{\boldsymbol{K}}{\mu}\frac{(P_1 - P_2)}{L}$

In the linear regime, i.e. for Stokes flow, the permeability **K** is a material property, independent of viscosity, density, and velocity of the fluid.

Staggered Grid

- We present three different single-phase stationary Stokes flow solver methods
  - Each has its own advantages and disadvantages
  - Common denominator is the staggered grid discretization on voxel grids
- Staggered grid discretization [Harlow & Welch, 1965]
  - Pressure lives at the center of the voxel
  - Velocity components live at the center of the different voxel faces
    - X-Velocity lives at the vertical X-faces
    - Y-Velocity lives at the horizontal Y-faces
    - Z-Velocity lives at the Z-faces



Staggered grid for velocity variables

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Explicit Jump Methods

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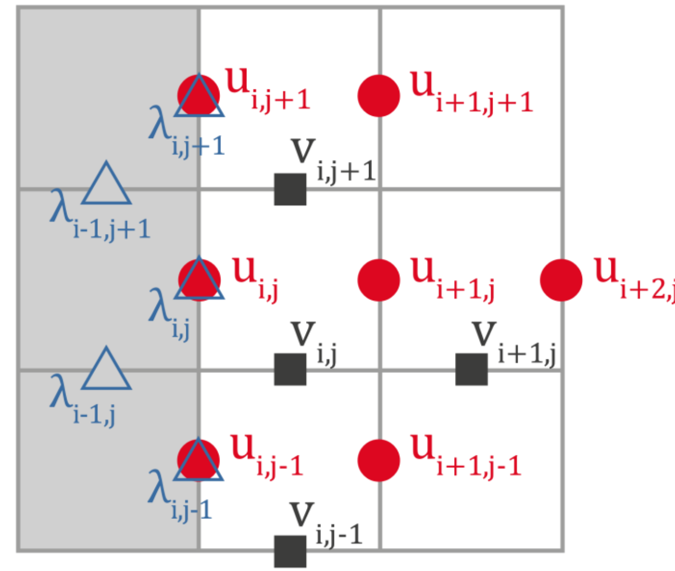
- Basic idea: introduce *jump* variables λ in the momentum equation for no-slip conditions
$$\mu\Delta u - \nabla p + \Psi\lambda = f \qquad (1)$$
- Then we apply the divergence operator $\nabla\cdot$ to the momentum equation
$$\mu\Delta(\nabla\cdot u) - \Delta p + \nabla\cdot\Psi\lambda = \nabla\cdot f$$
$$\Delta p - \nabla\cdot\Psi\lambda = \nabla\cdot f \qquad (2)$$
- The no-slip boundary condition is discretized by
$$\Upsilon u = 0 \qquad (3)$$
- The final system of equations is given by
$$\begin{pmatrix} \mu\Delta & -\nabla & \Psi \\ 0 & \Delta & -\nabla\cdot\Psi \\ \Upsilon & 0 & 0 \end{pmatrix}\begin{pmatrix} u \\ p \\ \lambda \end{pmatrix} = \begin{pmatrix} f \\ \nabla\cdot f \\ 0 \end{pmatrix}$$
- A Schur-complement eliminates velocity and pressure and the remainder $M\lambda = b$ is solved by Krylov subspace methods and FFTs [Wiegmann, 2007]



Staggered grid for velocity variables with jumps for no-slip conditions

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Explicit Jump Methods

- The location of the jump variables depends on the specific no-slip discretization
- The natural domain boundary conditions are periodic
  - Symmetric boundary conditions can be achieved by mirroring of the structure or using cosine transforms
- The convergence depends on the number of jump variables
  - Converges very fast for highly porous structures
- Requires much less memory compared to LB methods
- Not (yet) extended to Navier-Stokes-Brinkman equations
- The Explicit Jump methods can also be used to solve poisson equations
  - Convergence speed is independent of the phase contrast!

SIMPLE-FFT Method

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- SIMPLE (Semi-Implicit Method for Pressure Linked Equations) algorithms are widely used to solve Navier-Stokes-Brinkman equations [Patankar, 1980]
- The SIMPLE algorithm works as follow (start with u^n and p^n)
  1. Solve the momentum equation with Gauß-Seidel and get u^*
  2. Solve pressure correction equation $\Delta p' = \mu\Delta(\nabla \cdot u^*)$ which is simplified to $\Delta p' = -\mu \operatorname{diag}[\Delta](\nabla \cdot u^*)$ with Gauß-Seidel and get p'
  3. Update pressure with $p^{n+1} = p^n + p'$
  4. Correct velocity with $u^{n+1} = u^* + \operatorname{diag}[\Delta](\nabla p')$
- The SIMPLE methods converge very slowly for low porosity structures due to the ineffective pressure correction step
- Basic idea: Exact pressure correction by FFT instead of approximate solve in step 2.
- Convergence speed dramatically higher than SIMPLE (up to 10 times)!
  - Very fast for low porosity structures
  - Runtime per iteration is higher due to the FFT

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LIR Method – 1: Mesh Coarsening

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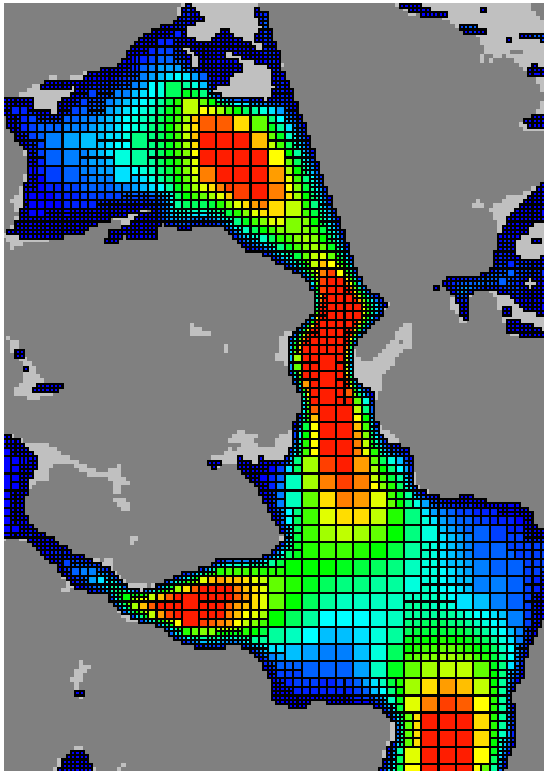
- Adaptive grid: LIR-Tree [Linden et al., 2014]
  - Combination of Octree and KD-tree
  - Very low memory overhead
  - Efficient neighborhood retrieval
  - Grid adapts to geometry, 2:1 size ratios, velocity and pressure fields
- Minimize the number of tree traversals per iteration by a special block pde formulation
- This formalism allows to solve Navier-Stokes-Brinkman and Poisson equations with full anisotropy
- Convergence speed depends on the number of cells and the porosity of the structure
  - Extremly fast for highly porous structures
- Very low memory requirements



Adaptive grid inside the pore space of a Berea sandstone

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LIR Method – 2: block PDE formulation

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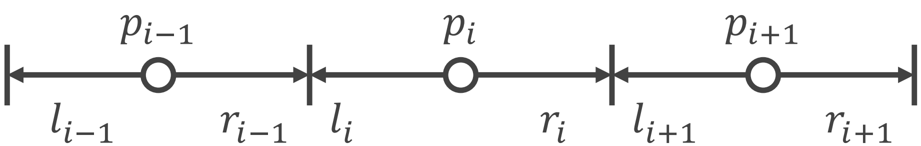
- Basic idea: split velocity variable u into a left sided l and right sided r variable



  - The momentum equation is discretized in two ways

$$\frac{\partial^2 u}{\partial x^2} - \frac{\partial p}{\partial x} \rightarrow \frac{1}{h^2}\left((r_i - l_i) - (l_i - l_{i-1})\right) - \frac{1}{h}(p_i - p_{i-1})$$

$$\rightarrow \frac{1}{h^2}\left((r_i - r_{i-1}) - (r_{i-1} - l_{i-1})\right) - \frac{1}{h}(p_i - p_{i-1})$$

  - The mass conservation is discretized with

$$\frac{\partial u}{\partial x} \rightarrow \frac{1}{h}(r_i - l_i)$$

- The Stokes equations are discretized as linear block system of equations per cell and can be solved by block Gauß-Seidel / SOR methods combined with Multigrid [Linden et al., 2015]

$$\begin{pmatrix} -2 & 1 & -1 \\ 1 & -2 & 1 \\ -1 & 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} l_i^{n+1} \\ r_i^{n+1} \\ p_i^{n+1} \end{pmatrix} = \begin{pmatrix} -l_{i-1}^{n+1} - p_{i-1}^{n+1} \\ -r_{i+1}^{n} + p_{i+1}^{n} \\ 0 \end{pmatrix}$$

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Lippmann Schwinger Methods

- Boundary value problem of linear elasticity:

$$\nabla \cdot \sigma = 0 \qquad \text{Equilibrium of stresses}$$
$$\sigma = C : \epsilon \qquad \text{Hooke's law}$$
$$2\epsilon = 2E + \nabla u^* + (\nabla u^*)^T$$

where u^* is periodic and $\sigma \cdot n$ is anti-periodic

- We introduce a reference material C^0 and define a polarization field τ

$$\tau = (\mathbb{C} - C^0) : \epsilon$$

- Hooke's law can then be transformed to

$$\sigma = C^0 : \epsilon + \tau$$

- Equilibrium of stresses can be solved by using the elastic Green operator Γ^0

$$\epsilon = E - (\Gamma^0 * \tau)$$

- Substitution of polarization yields the Lippmann Schwinger equation [Moulinec,Suquet 1994,1998]

$$\epsilon + \Gamma^0 * \left((C - C^0) : \epsilon\right) = (I + B_\epsilon)\epsilon = E$$

Lippmann Schwinger Methods

- The Lippmann Schwinger equations can be solved by using Neumann series or Krylov subspace methods using FFT and is implemented in the FeelMath solver
  - Basis scheme with Neumann series [Kabel et al., 2014]

$$\tau = (C - C^0) : \epsilon^n$$
$$\hat{\tau} = FFT(\tau)$$
$$\hat{\eta} = -\Gamma^0 : \hat{\tau}, \qquad \hat{\eta}(0) = E$$
$$\epsilon^{n+1} = FFT^{-1}(\hat{\eta})$$

- Staggered grid for discretization of displacement, strain, and stress [Schneider et al., 2016]
- Convergence speed is independent of grid size but depends on phase contrast ρ
  - $\mathcal{O}(\rho)$ for Neumann series
  - $\mathcal{O}(\sqrt{\rho})$ for Krylov subspace methods
- Supports isotropic and anisotropic constituent materials
- Works for linear and non-linear constitutive equations of stresses
- LS methods can also be used to solve conduction or flow equations

Two-Phase Flows and Saturation-dependent Properties

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- The Explicit-Jump, SIMPLE-FFT, and LIR methods solve the single-phase stationary (Navier-)Stokes(-Brinkman) equations
  - But in many application areas, researchers are interested in saturation-dependent properties (e.g. relative permeability)
- For relative permeability, we must solve two-phase flow equations instead of single-phase flow equations
- We assume flow regimes where capillary forces caused by surface tension and capillary pressure are dominating (i.e. low capillary number)
- Solving two-phase flow equations is very challenging and runtimes are very high
- Here, we present an alternative approach ...

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Pore Morphology Methods

… predict the distribution of the two phases inside porous media and the capillary pressure curve

Basic Idea

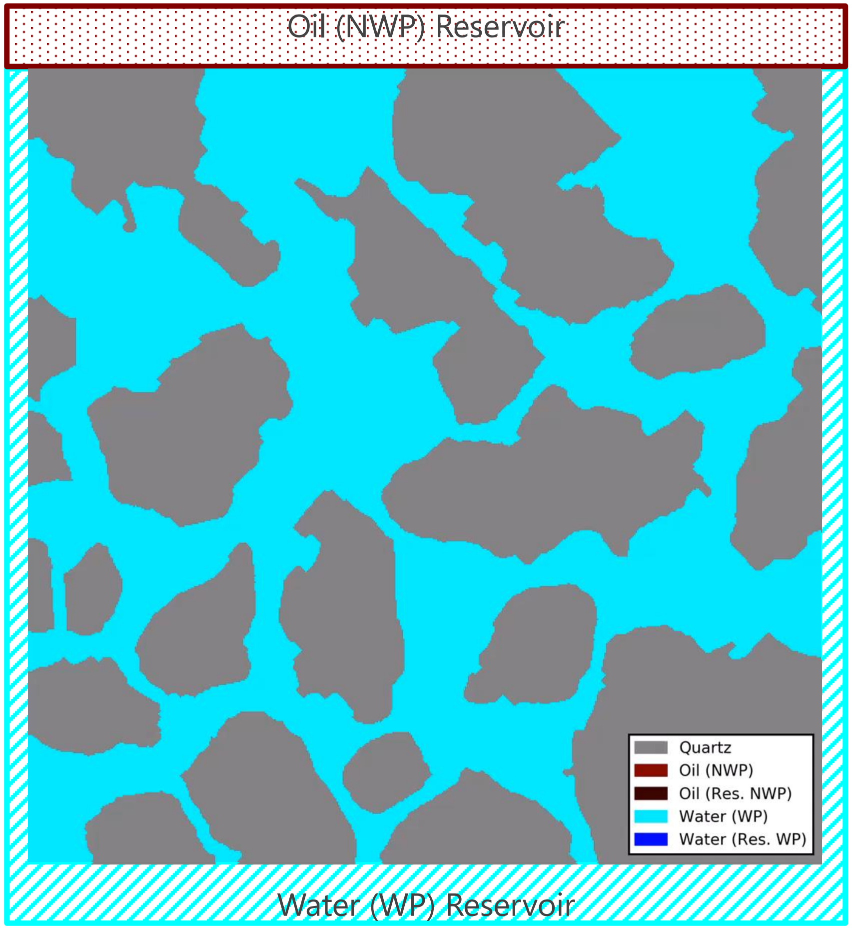
- "Push" spheres into/outside the structure & reduce/increase sphere radii [Hilpert and Miller, 2001]
- Superposition of spheres represent the non-wetting phase
- Perform connectivity checks to consider trapped/residual phases [Ahrenholz et al., 2008]
- Use sphere radii & Young-Laplace $p_c = 2\frac{\gamma}{r}\cos\alpha$ to predict the capillary pressure
- Inscribe different contact angles by sphere radii $\frac{r}{\cos\alpha}$ [Schulz et. al., 2015]

Advantage

- No partial differential equations are solved
- Very low runtime & memory requirements

Assumption

- Quasi-stationary phase distribution
- Low capillary number



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Filtration Simulation at different scales

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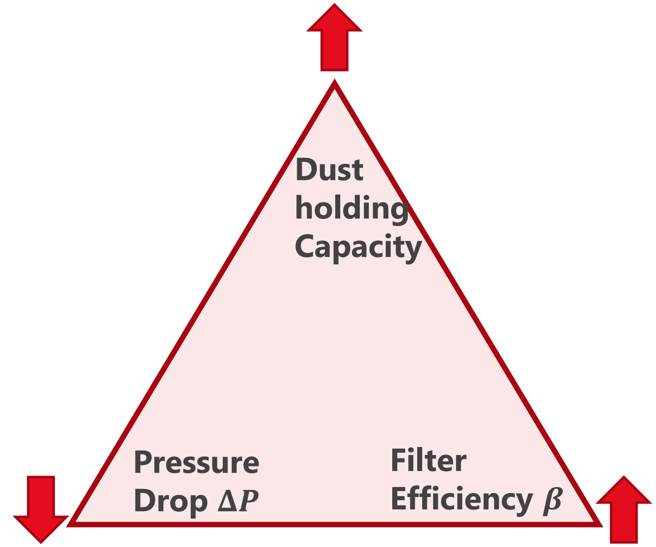
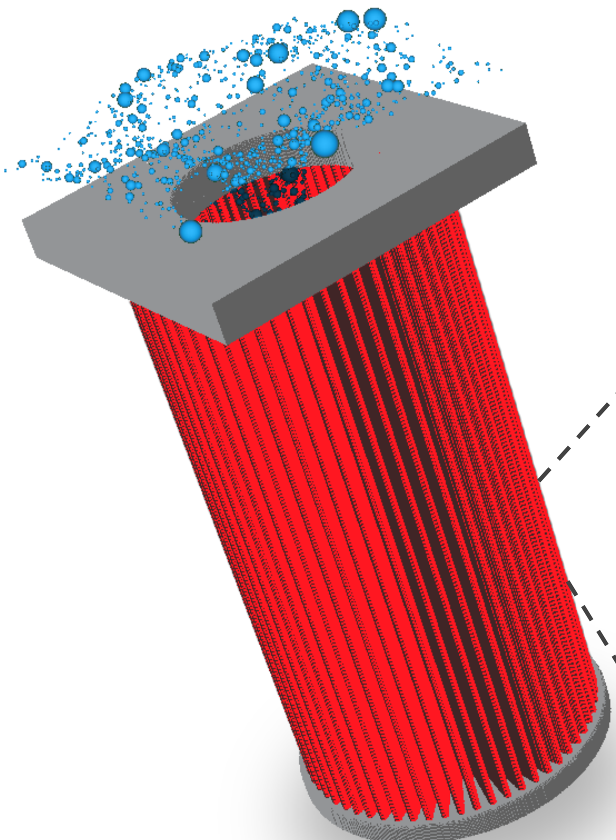
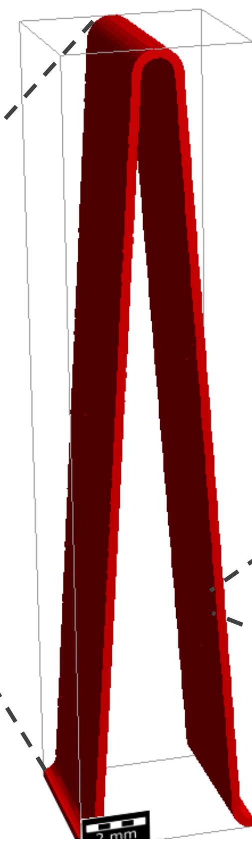
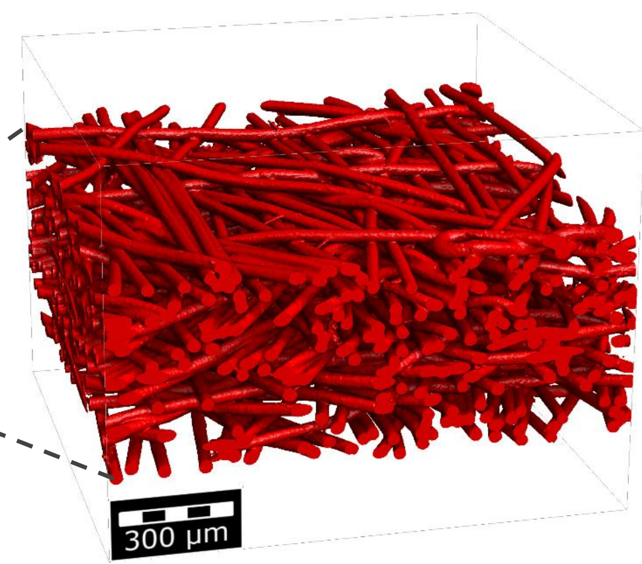




Filter element
(macro scale)



Single pleat
(macro/meso scale)



Filter media
(micro scale)

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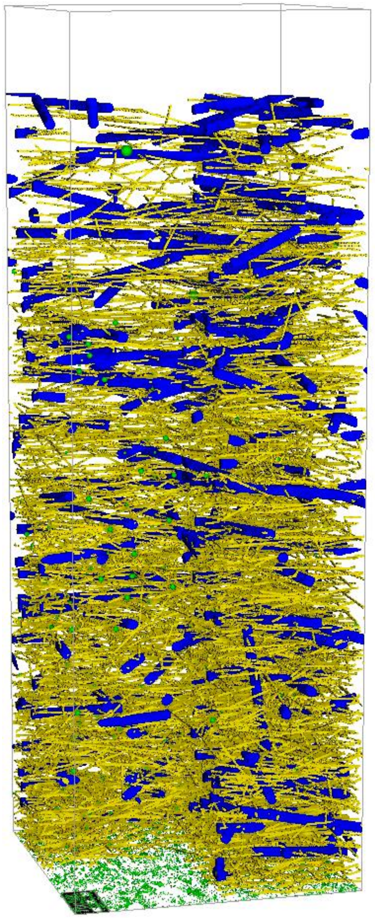
Filtration Simulation

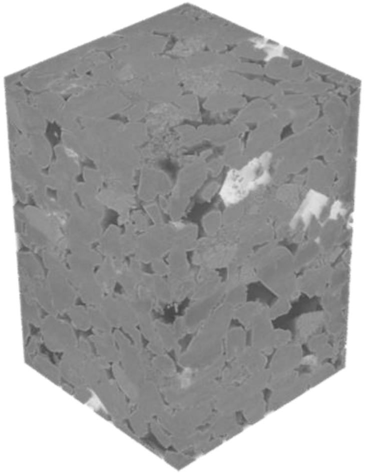
- EJ, SIMPLE-FFT, or LIR compute permeability, flow resistivity, or pressure drop, even frequency dependent acoustic absorption [Schladitz, 2015]
- Filtration process is simulated by a Lagrangian formulation of particle transport (repeat steps 1.-3.) [Latz, 2003]
  1. A flow field is computed
  2. Particles start from the inlet and move due to their own mass, friction with the fluid and Brownian motion
  3. Particles may be captured on fibers or deposited particles
- Electrostatic forces can be considered using the gradient of a potential field [Rief, 2006]
- Computed filter properties agree with measurements [Becker, 2013]
- Particle diameters usually span multiple length scales and are modelled by an empty-solid model or porous media approaches [Becker, 2016]



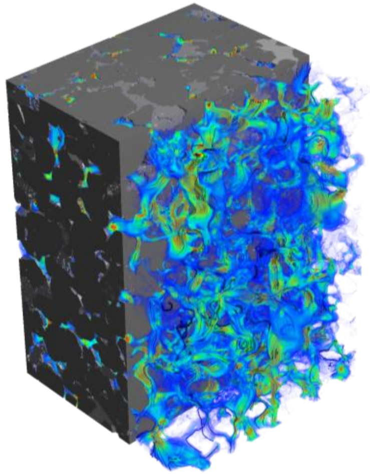
Filtration simulation on a gradient fiber media [Azimian, 2018]

Digital Rock Physics

- Digital rock physics (DRP) is the determination of physical rock properties by numerical simulations and
  - complements or replaces laboratory measurements
  - reduce time and cost compared to measurements
- Researchers and petroleum engineers are interested in
  - Porosity, pore-body and pore-throat size distributions
  - Tortuosity, electrical conductivity
  - Absolute and relative permeability
  - Capillary pressure curves
  - Stiffness and compression-dependent properties
- Porosity is often below 20% and pore networks are very complex
- EJ, SIMPLE-FFT, and LIR showed very good performance in a benchmark study with six other methods [Saxena, 2017]



CT-scan of a Berea sandstone



Stokes flow through a segmented Berea sandstone

Battery Electrode Design Workflow

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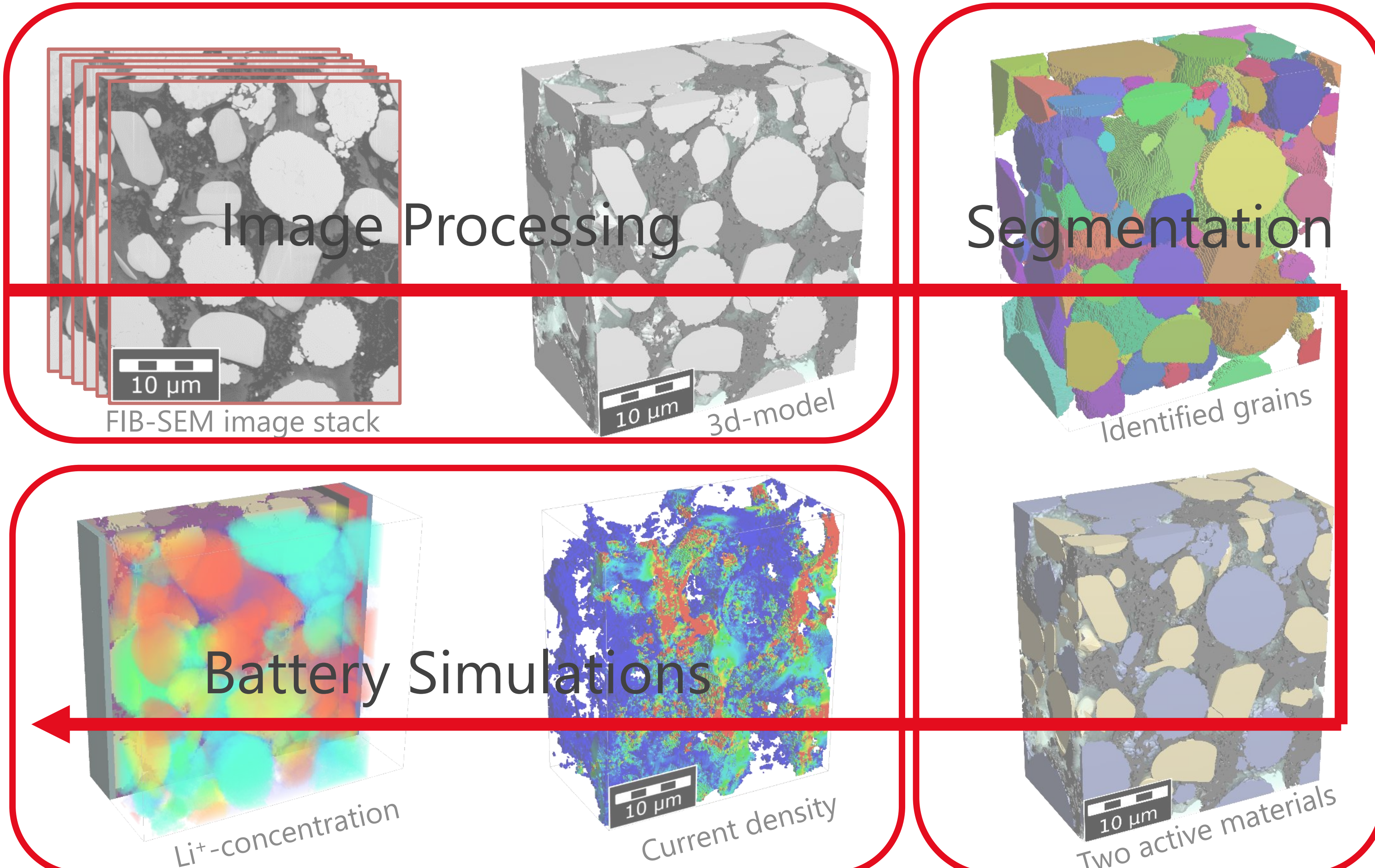

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Gas Diffusion Layers

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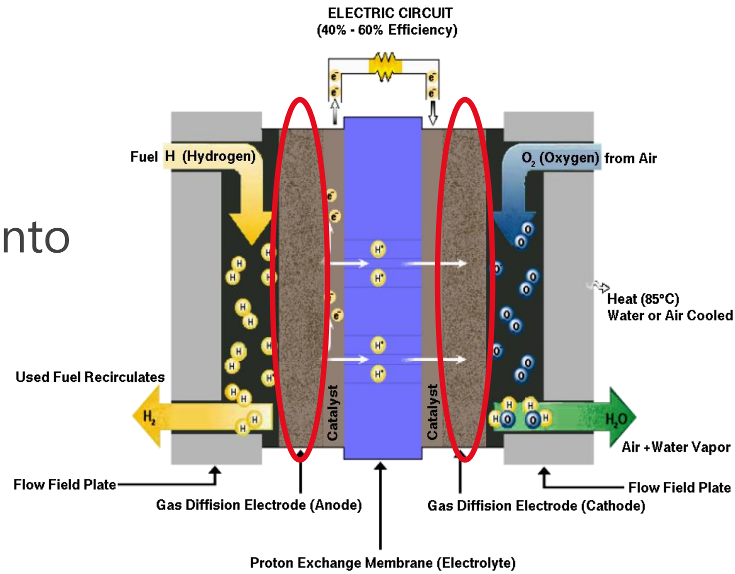
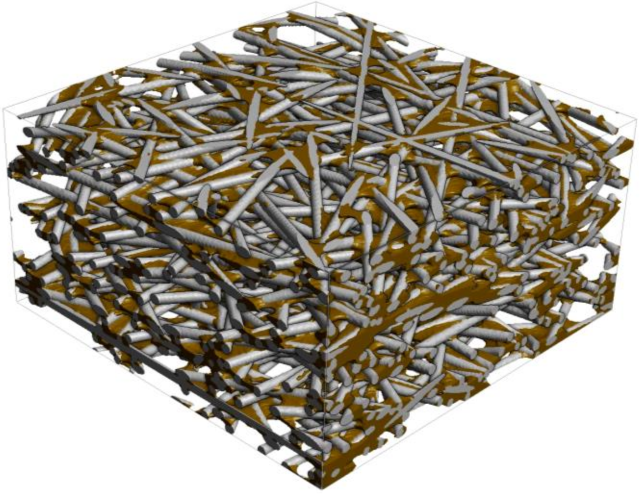
- Fuels are another promising technology used in automotive industry to convert chemical energy into electricity
  - The structure has similarities to a battery: anode, separator, and cathode
- Gas diffusion layers (GDL) are nonwoven porous structures made of carbon fibers
  - Plays an important role for the transport of reactants and products
- Important properties of GDLs that can be simulated
  - Distribution of fluids and gas, capillary pressure [Schulz, 2007]
  - Absolute and relative permeability [Becker, 2009]
  - Gas diffusivity, electrical and thermal conductivity [Zamel, 2010]
  - Compression dependent behavior





Water invades a GDL and displaces Air

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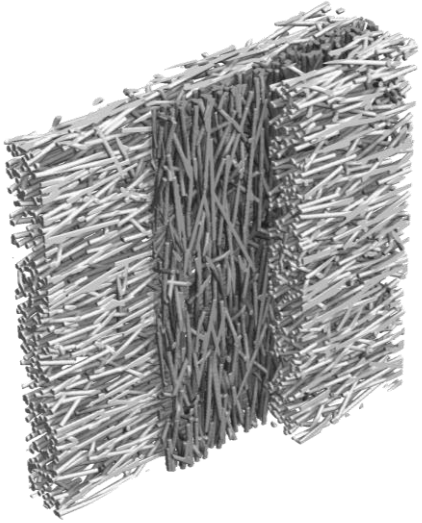
COMPOSITES

- Composite materials and digital material engineering of composites are essential in current component development
  - Creation of realistic microstructure models and
  - Determination of their physical properties helps in product development
- Applications: e.g. carbon or glass fiber-reinforced plastics
- Lippmann-Schwinger methods are especially suited for simulation of mechanical properties and they agree with measurements [Sliseris, 2014]
- Engineers are interested in
  - Full mechanical stiffness tensor, elastic moduli
  - Evolution of deformation and damage [Fliegener, 2016]
  - Permeability



Short/Long fiber composite

Woven structure

Summary & Conclusions

- We presented three different single-phase flow solver methods designed for porous media
  - Each has its own advantages and disadvantages
  - One can choose the best solver for a given application
  - Development of new features is easier in the presence of different solver methods
  - Alternative to LBM methods
- The flow solvers can be combined with mechanics or two-phase flow methods
- Solvers are successfully used in different application areas
- A standard workstation is enough for simulation on large 3d images

Thank you for your Attention!

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