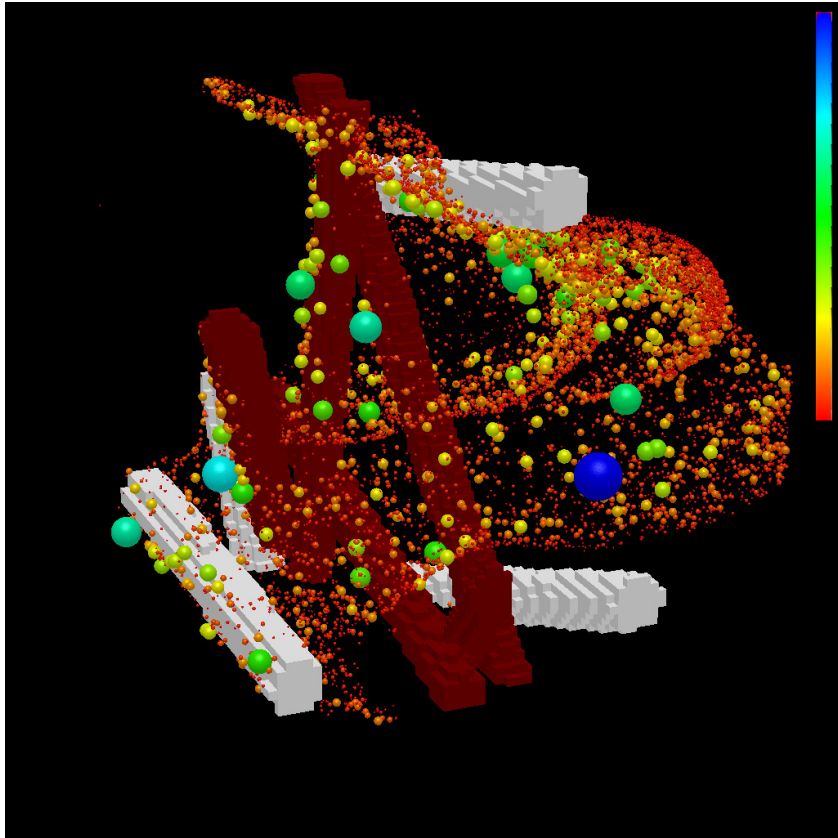

Explicit jump solvers for virtual material design



- I. Electric field from singular charges on fiber surfaces (filtration)
- II. Heat equation for piecewise constant coefficients (insulation)
- III. Stokes solver (effective permeability; filtration)

Andreas Wiegmann

Work on the electrostatics and heat equations
is joint with

Aivars Zemitis

Ventspils University College,
Ventspils, Latvia

What is the relation of the explicit jump solvers with Virtual Material Design (VMD) and Multiscale modelling?

The VMD design cycle:

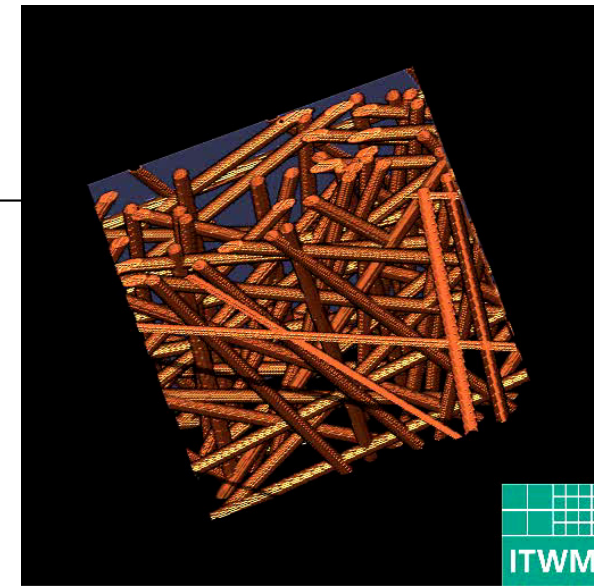
- A. Have a 3d geometry model
- B. Do fast solve for many variable problem**
- C. Evaluate quality criteria
- D. Apply rule for geometry improvement

(e.g. P. Toint)

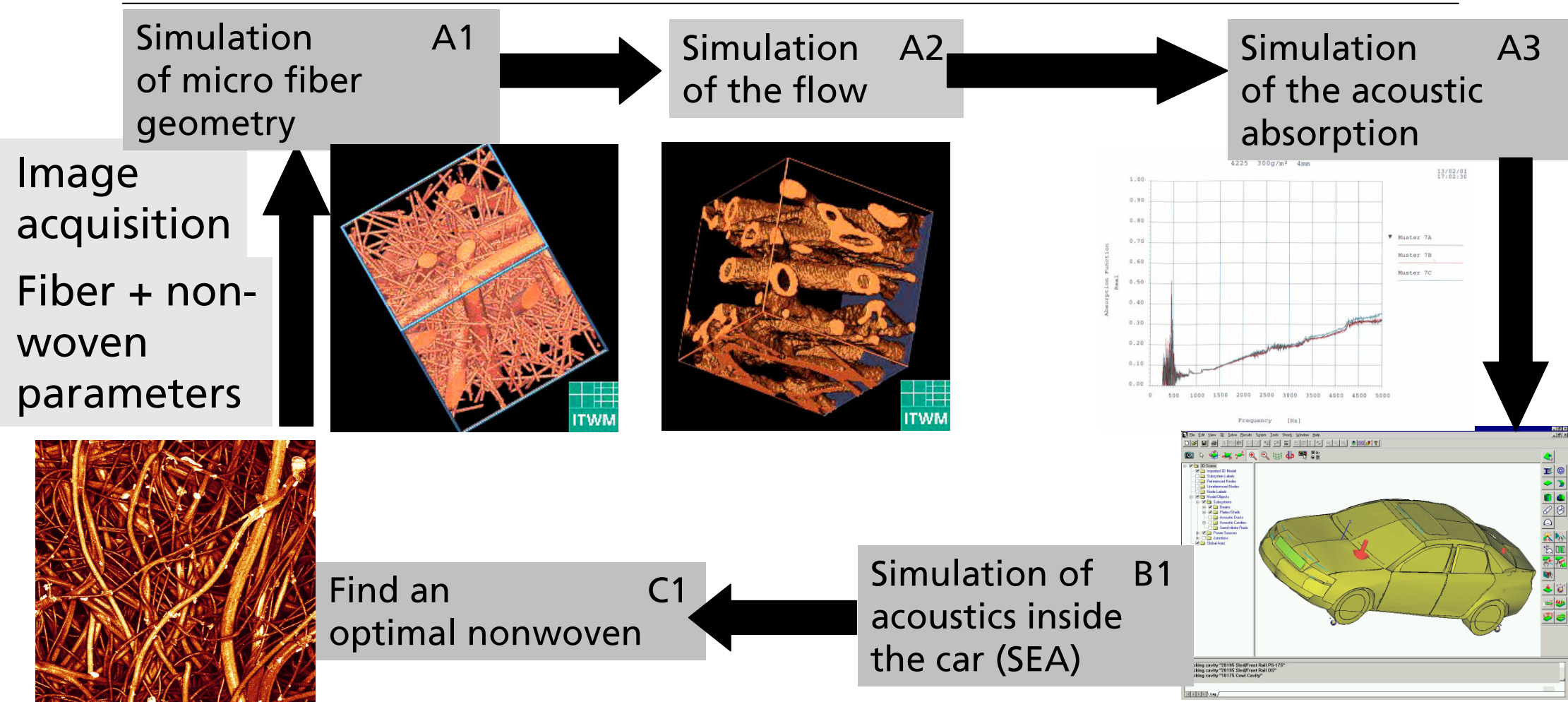
Multiscale modelling:

- A. Nano scale
- B. Micro scale**
- C. Mini scale
- D. Macro scale (product)

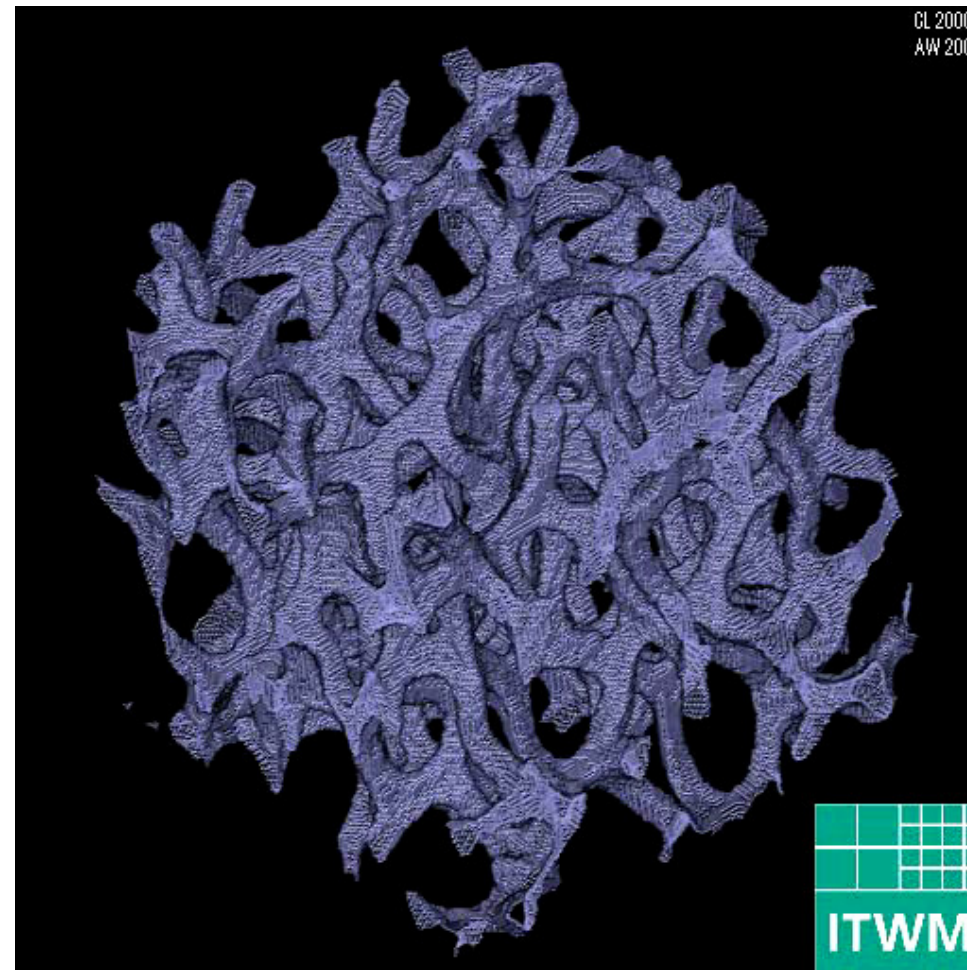
(e.g. W. E)



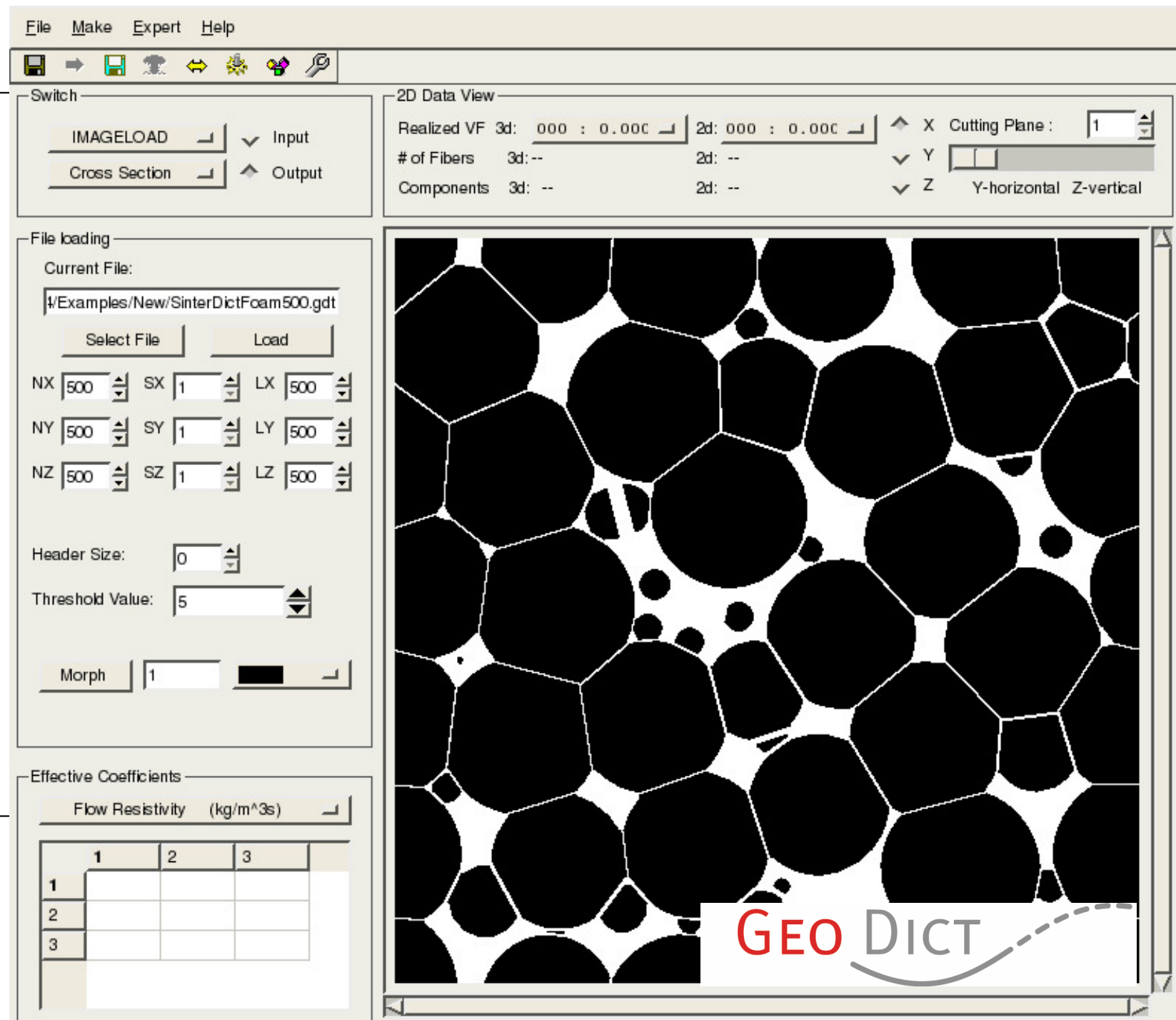
Example of virtual material design and product design cycle



Tomographed foam: open pores



Generated
foam:
closed pores



Why elliptic BVP on voxelized geometries?

- Simplest 3d material model: a voxel is a cube with constant properties
- Can use 3d images directly (e.g. from synchrotron tomography)
- Can discretize easily from parameterized models
- Homogenize to find effective permeability
- Homogenize to find effective diffusivity
- Need stationary flow field or electrostatic field for simulation of filtration processes

On a voxelized geometry, a first order method is sufficient!

What are **desired fields or material properties**?

Poisson eq: **Electric field E**

$$-\Delta u = f, \text{ singular } f \text{ lives on } \partial G$$

- Potential u

$$u(x + il_x, y + jl_y, z) = u(x, y, z) \text{ for } i, j \in \mathbb{Z}, -d_z < z < d_z$$

$$u(x, y, -d_z) = u(x, y, d_z) = 0$$

Heat eq:

$$\mathbf{E} = -\nabla u$$

effective conductivity β^*

- Temperature u
- piecewise constant β
- Direction of interest $\mathbf{f}$

$$\nabla (\beta(\nabla u + \mathbf{f})) = 0 \in \Omega,$$

$$u(x + il_x, y + jl_y, z + kl_z) = u(x, y, z) \text{ for } i, j, k \in \mathbb{Z}$$

Stokes eq:

$$\mu \Delta \mathbf{u} + \mathbf{f} = \nabla p \text{ in } \Omega \setminus G,$$

$$\nabla \cdot \mathbf{u} = 0 \text{ in } \Omega \setminus G,$$

- **Velocities $\mathbf{u}$**

$$\mathbf{u}(x + il_x, y + jl_y, z + kl_z) = \mathbf{u}(x, y, z) \text{ for } i, j, k \in \mathbb{Z}$$

- **Pressure p**

$$p(x + il_x, y + jl_y, z + kl_z) = p(x, y, z) \text{ for } i, j, k \in \mathbb{Z}$$

- Direction of interest $\mathbf{f}$

$$\mathbf{u} = 0 \text{ on } \partial G$$

$$\mathbf{f} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \text{ or } \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

Why and how use FFT(W)?

- $\Delta u = f \Leftrightarrow (\xi_1^2 + \xi_2^2 + \xi_3^2)\hat{u} = \hat{f}$

- for periodic 7-point central differences:

Later we will denote
a subspace inverse
applied by FFT by $\Delta_h^\dagger$.

$$\hat{U}_{k,m,p} = \frac{h^2 \hat{F}_{k,m,p}}{\left\{ 2 \cos\left(\frac{2k\pi}{N_1}\right) + 2 \cos\left(\frac{2m\pi}{N_2}\right) + 2 \cos\left(\frac{2p\pi}{N_3}\right) - 6 \right\}}$$

$$k = 0, 1, \dots, n_1, \quad m = 0, 1, \dots, n_2,$$

$$p = 0, 1, \dots, n_3 \text{ and } k + m + p > 0.$$

$$\text{Require } \hat{F}_{0,0,0} = 0 \text{ and set } \hat{U}_{0,0,0} = 0.$$

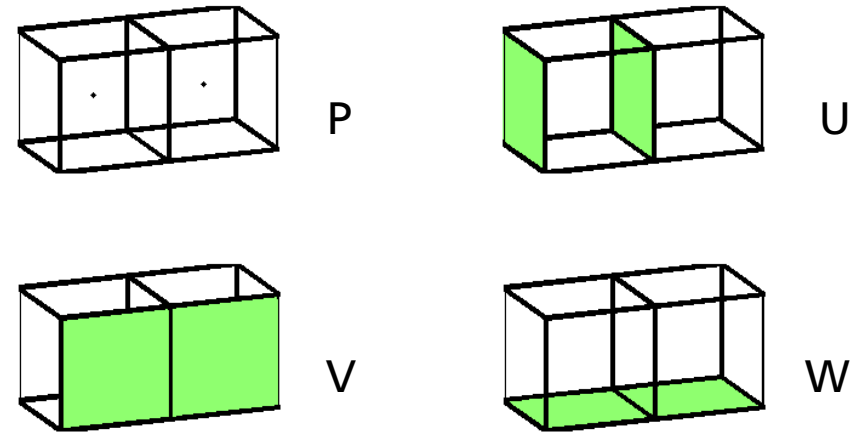
Direct Poisson solvers were
invented and popular in the
1970s, see Swarztrauber.

- Solve periodic Poisson equation in $O(n \log n)$
(**FFTW** is extremely well implemented)
Use inverse Laplacian as preconditioner!



The MAC grid: variable position

- In electrostatics, forces lie on U, V and W grids
- In homogenized heat, jumps occur on one of U, V or W grids
- In Stokes flow, boundary conditions are given on U, V and W grids, but are extended also into the obstacles!



$P_{i,j,k}$ is pressure at

$U_{i,j,k}$ is x-component of velocity at

$V_{i,j,k}$ is y-component of velocity at

$W_{i,j,k}$ is z-component of velocity at

$((i + 0.5)h, (j + 0.5)h, (k + 0.5)h),$

$((i + 1)h, (j + 0.5)h, (k + 0.5)h),$

$((i + 0.5)h, (j + 1)h, (k + 0.5)h),$

$((i + 0.5)h, (j + 0.5)h, (k + 1)h).$



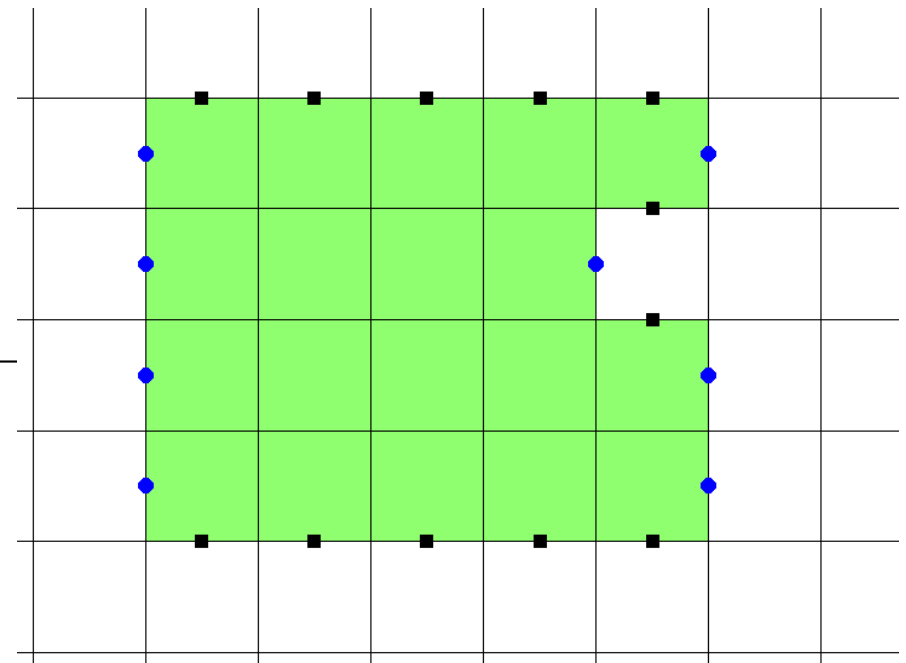
How does the singular source enter in the electrostatic problem?

Sources occur at $(x_{i-1/2}, y_j, z_k)$ on u -grid (blue),
or similarly on v (black) or w grids, strength ρ .

$$\frac{u_{i-1,j,k} + u_{i,j-1,k} + u_{i,j,k-1} - 6u_{i,j,k} + u_{i+1,j,k} + u_{i,j+1,k} + u_{i,j,k+1}}{h^2} = -\frac{\rho}{2h}$$

$$\frac{u_{i-2,j,k} + u_{i-1,j-1,k} + u_{i-1,j,k-1} - 6u_{i-1,j,k} + u_{i,j,k} + u_{i-1,j+1,k} + u_{i-1,j,k+1}}{h^2} = -\frac{\rho}{2h}$$

In simplest version, material (green) has same
electrical conductivity as void.



How to compute the electric field?

Use periodic problem to solve Dirichlet boundary problem in z-direction via reflection:

$$\frac{\dots + u_{i-1,j,k} - 6u_{i,j,k} + u_{i+1,j,k} + \dots}{h^2} = \tilde{f}_{ijk}$$

where

$$\tilde{f}_{ijk} = \begin{cases} 0, & k = 0 \\ f_{ijk}, & 0 < k < n_3 \\ 0, & k = n_3 \\ -f_{ij(2n_3-k)}, & n_3 < k < 2n_3. \end{cases}$$

Periodically identify

$i = 0$ with $i = n_1$,

$j = 0$ with $j = n_2$ and

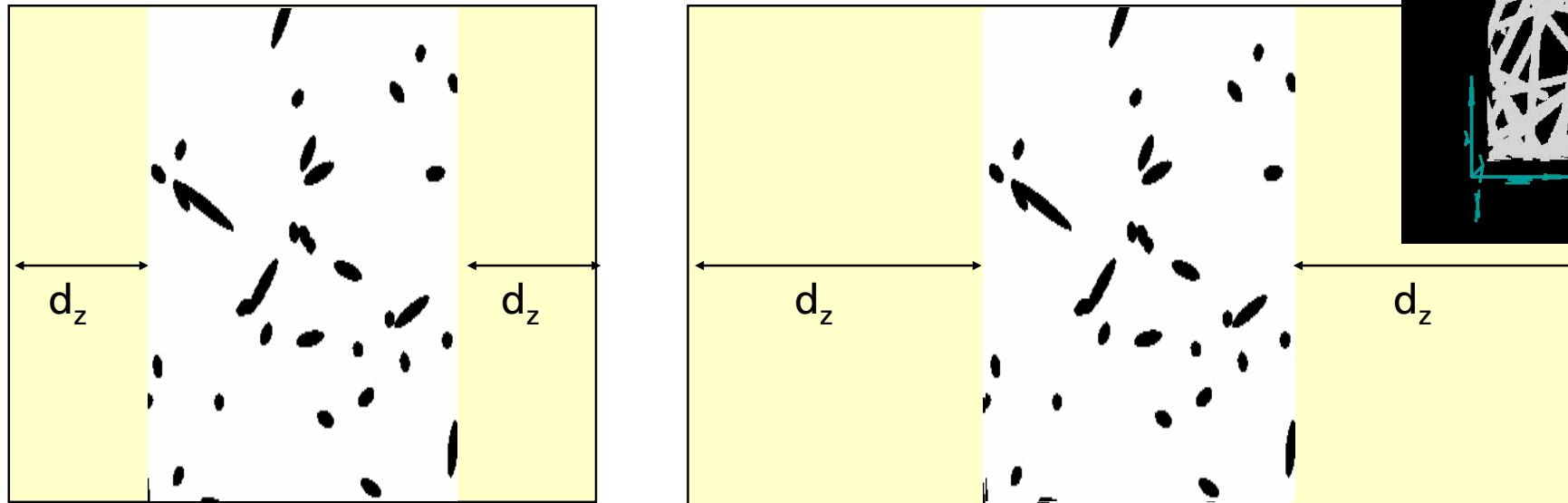
$k = 0$ with $k = 2n_3$.

Remark:

Could use discrete sine transform, would want equally good implementation as for FFT!



Where to place the Dirichlet condition?



Want $E = \nabla u$ inside the media (**white**), how far away impose the Dirichlet condition?

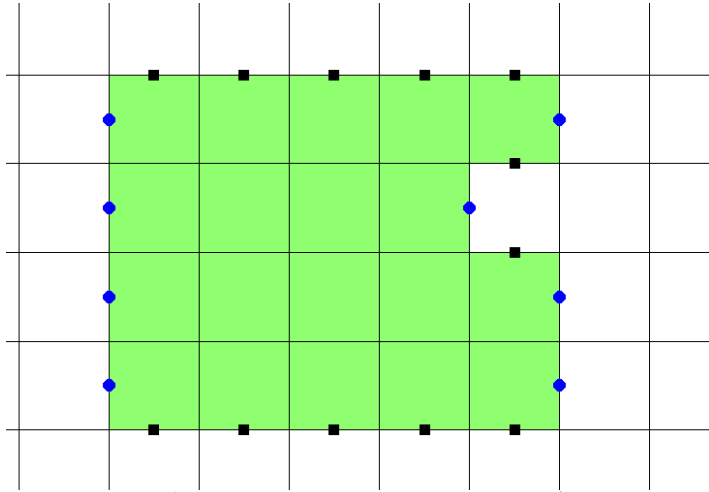
u is not independent of the position of the Dirichlet boundary condition, d_z !

Fortunately, E is almost independent for $d_z > C$.

FFT solves electrostatic with periodic / Dirichlet boundary conditions in a single solve.



Jumps for the heat equation and discretization



$$\nabla \cdot (\beta \nabla u) = -\nabla \cdot (\beta (1, 0, 0)') \Rightarrow$$

$$[\partial_x u]_{i+\frac{1}{2}} = -\left(\frac{u_{i+1} - u_i}{h} + 1\right) \frac{2(\beta_{i+1} - \beta_i)}{\beta_{i+1} + \beta_i}$$

$$[\partial_y u]_{j+\frac{1}{2}} = -\left(\frac{u_{j+1} - u_j}{h} + 0\right) \frac{2(\beta_{j+1} - \beta_j)}{\beta_{j+1} + \beta_j}$$

$$[\partial_z u]_{k+\frac{1}{2}} = -\left(\frac{u_{k+1} - u_k}{h} + 0\right) \frac{2(\beta_{k+1} - \beta_k)}{\beta_{k+1} + \beta_k}$$

$$\frac{\beta_i}{h} \left(\frac{\left(u_{i+1} - \frac{h}{2} [\partial_x u]_{i+\frac{1}{2}}\right) - u_i}{h} - \frac{u_i - \left(u_{i-1} - \frac{h}{2} [\partial_x u]_{i-\frac{1}{2}}\right)}{h} \right) = 0$$

$$\frac{1}{h} \left(\left(\frac{1}{2\beta_{i+1}} + \frac{1}{2\beta_i} \right)^{-1} \frac{u_{i+1} - u_i}{h} - \left(\frac{1}{2\beta_i} + \frac{1}{2\beta_{i-1}} \right)^{-1} \frac{u_i - u_{i-1}}{h} \right) = -\frac{\beta_i(\beta_{i+1} - \beta_i)}{h(\beta_{i+1} + \beta_i)} - \frac{\beta_i(\beta_i - \beta_{i-1})}{h(\beta_i + \beta_{i-1})}$$

$$\frac{1}{h} \left(\left(\frac{1}{2\beta_{j+1}} + \frac{1}{2\beta_j} \right)^{-1} \frac{u_{j+1} - u_j}{h} - \left(\frac{1}{2\beta_j} + \frac{1}{2\beta_{j-1}} \right)^{-1} \frac{u_j - u_{j-1}}{h} \right) = 0$$



This is simply harmonic
averaging on voxels!

EJIM system for the heat equation

$$\frac{\beta_i}{h} \left(\frac{\left(u_{i+1} - \frac{h}{2} [\partial_x u]_{i+\frac{1}{2}} \right) - u_i}{h} - \frac{u_i - \left(u_{i-1} - \frac{h}{2} [\partial_x u]_{i-\frac{1}{2}} \right)}{h} \right) = 0$$

divide by β_i and get

$$\begin{aligned} \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} - \frac{[\partial_x u]_{i+\frac{1}{2}} + [\partial_x u]_{i-\frac{1}{2}}}{2h} &= 0 \\ \frac{u_{i+1} - u_i}{h} + [\partial_x u]_{i+\frac{1}{2}} &= -\frac{2(\beta_{i+1} - \beta_i)}{\beta_{i+1} + \beta_i} \\ \frac{u_i - u_{i-1}}{h} + [\partial_x u]_{i-\frac{1}{2}} &= -\frac{2(\beta_i - \beta_{i-1})}{\beta_i + \beta_{i-1}} \end{aligned}$$

This is an explicit jump (immersed interface method) system or EJIM system:

$$\begin{bmatrix} A & \Psi \\ D' & I \end{bmatrix} \begin{bmatrix} U \\ J \end{bmatrix} = \begin{bmatrix} 0 \\ F_2 \end{bmatrix}$$



Solution of the EJIM system for the heat equation by BiCGStab

$$\begin{bmatrix} \Delta_h & \Psi \\ D' & I \end{bmatrix} \begin{bmatrix} U \\ J \end{bmatrix} = \begin{bmatrix} 0 \\ F_2 \end{bmatrix}$$

Δ_h is the 7-point Laplacian with periodic boundary conditions, i.e. singular! The magic is:

$\sum D'U = 0$ for all $U \in \mathbb{R}^n$, also $\sum F_2 = 0$.
Thus $\sum J = 0 \Rightarrow \sum \Psi J = 0 \Rightarrow \Delta_h^\dagger$, the FFT-based "inverse" on $\mathbb{R}^n \setminus \{\mathbf{x} \in \mathbb{R}^n : \sum \mathbf{x} = 0\}$ can be used.

$$\Rightarrow (I + D' \Delta_h^\dagger \Psi) J = F_2$$

is a nonsymmetric regular linear system of equations on $\mathbb{R}^n \setminus \{\mathbf{x} \in \mathbb{R}^n : \sum \mathbf{x} = 0\}$.

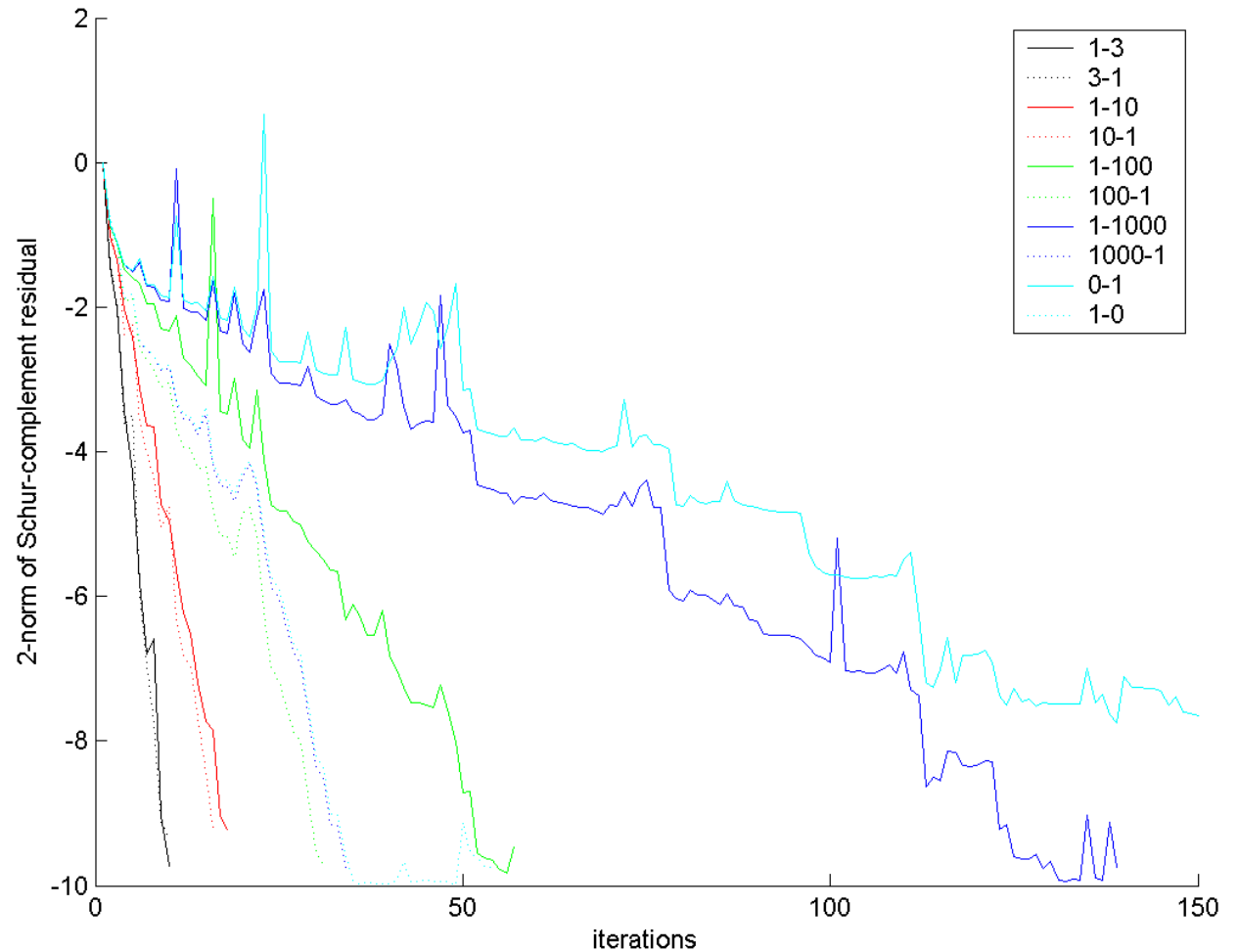
Solve by BiCGStab. Matrix-vector multiplication is performed by applying operators, the "singular Schur-complement" is not formed.



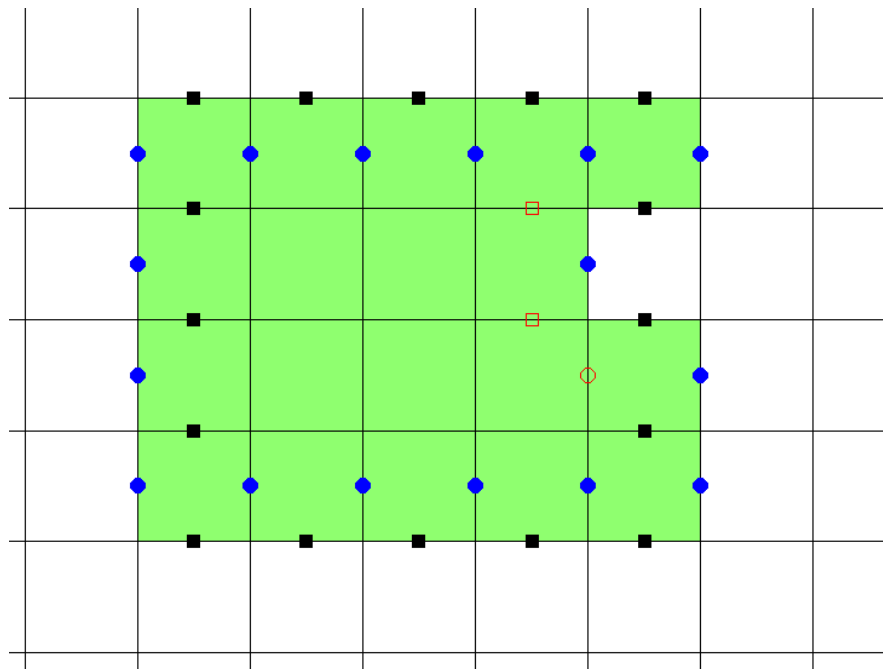
Results: Heat solver

128³, 95% type 0, 5% type 1,
fibrous media,
required about 170MB RAM,
10 seconds / iteration

type	value	its
0.3̄ : 1	0.35	10
0.1 : 1	0.12	18
0.01 : 1	0.0185	57
0.001 : 1	0.0033	139
0 : 1	0.0	(*)150
1 : 0.3̄	0.95	10
1 : 0.1	0.93	16
1 : 0.01	0.912	31
1 : 0.001	0.910	34
1 : 0	0.910	54



Surface variables for the Stokes equations



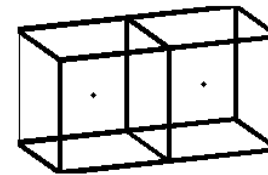
$P_{i,j,k}$ is pressure at

$U_{i,j,k}$ is x-component of velocity at

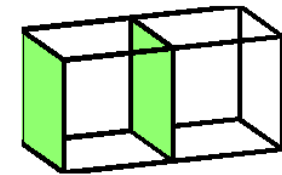
$V_{i,j,k}$ is y-component of velocity at

$W_{i,j,k}$ is z-component of velocity at

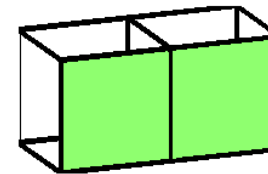
No need for pressure boundary condition!



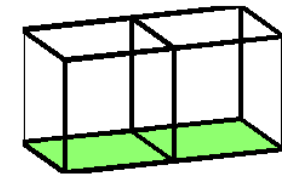
P



U



V



W

$((i + 0.5)h, (j + 0.5)h, (k + 0.5)h),$
 $((i + 1)h, (j + 0.5)h, (k + 0.5)h),$
 $((i + 0.5)h, (j + 1)h, (k + 0.5)h),$
 $((i + 0.5)h, (j + 0.5)h, (k + 1)h).$



Stokes via

4 Poisson problems

$$\mu \Delta \mathbf{u} + \mathbf{f} = \nabla p \text{ in } \Omega \setminus G,$$

$$\nabla \cdot \mathbf{u} = 0 \text{ in } \Omega \setminus G,$$

$$\mathbf{u}(x + il_x, y + jl_y, z + kl_z) = \mathbf{u}(x, y, z) \text{ for } i, j, k \in \mathbb{Z}$$

$$p(x + il_x, y + jl_y, z + kl_z) = p(x, y, z) \text{ for } i, j, k \in \mathbb{Z}$$

$$\mathbf{u} = 0 \text{ on } \partial G$$

$$\begin{aligned} \operatorname{div} \operatorname{grad} p = \Delta p &= \operatorname{div}(\mu \Delta \mathbf{u}) + \operatorname{div} \mathbf{f} = \\ &\mu \Delta(\operatorname{div} \mathbf{u}) + \operatorname{div} \mathbf{f} = \operatorname{div} \mathbf{f} \end{aligned}$$

$$\Delta p = \operatorname{div} \mathbf{f} \text{ in } \Omega \setminus G,$$

$$\mu \Delta u = \frac{\partial p}{\partial x} - f_x \text{ in } \Omega \setminus G,$$

$$\mu \Delta v = \frac{\partial p}{\partial y} - f_y \text{ in } \Omega \setminus G,$$

$$\mu \Delta w = \frac{\partial p}{\partial z} - f_z \text{ in } \Omega \setminus G,$$

$$\mathbf{u} = 0 \text{ on } \partial G.$$



Discretized Stokes

$$\begin{aligned}\mu \tilde{\Delta}_h \tilde{U} + \tilde{F}^x &= D_x^- \tilde{P} \text{ in } \Omega \setminus G, \\ \mu \tilde{\Delta}_h \tilde{V} + \tilde{F}^y &= D_y^- \tilde{P} \text{ in } \Omega \setminus G, \\ \mu \tilde{\Delta}_h \tilde{W} + \tilde{F}^z &= D_z^- \tilde{P} \text{ in } \Omega \setminus G, \\ \tilde{D}_x^+ \tilde{U} + \tilde{D}_y^+ \tilde{V} + \tilde{D}_z^+ \tilde{W} &= 0 \text{ in } \Omega \setminus G, \\ \tilde{U} &= U^0 \text{ on } \partial G, \\ \tilde{V} &= V^0 \text{ on } \partial G, \\ \tilde{W} &= W^0 \text{ on } \partial G.\end{aligned}$$

$\tilde{\cdot}$: valid only in the pores

Embedded Stokes

$$\Sigma_l = (1, 1, \dots, 1) \in \mathbb{R} \text{ "find sum of a vector"}$$

$$S_l = \mathbb{R}^l \setminus \{\Sigma_l\} \text{ "space of vectors summing to zero"}$$

$$M_l = \frac{1}{l} \Sigma_l' \Sigma_l \in \mathbb{R}^{l \times l} \text{ "write average of a vector to a vector,"}$$

$$P_l = (I_l - M_l) \text{ "orthogonal projector" } \mathbb{R}^l \rightarrow S_l$$

$$\Psi_x = E_x P_{m_x} \in \mathbb{R}^{n \times m_x} \text{ "embeds the projection" to } S_{m_x}$$

$$\Psi_y = E_y P_{m_y} \in \mathbb{R}^{n \times m_y} \text{ "embeds the projection" to } S_{m_y}$$

$$\Psi_z = E_z P_{m_z} \in \mathbb{R}^{n \times m_z} \text{ "embeds the projection" to } S_{m_z}$$

Artificial forces
on solid
surfaces

$$\Delta_h U - D_x^- P + \Psi_x \overset{\text{red}}{F_x} = -\bar{F}_x,$$

$$\Delta_h V - D_y^- P + \Psi_y F_y = -\bar{F}_y,$$

$$\Delta_h W - D_z^- P + \Psi_z F_z = -\bar{F}_z,$$

$$D_x^+ U + D_y^+ V + D_z^+ W = 0,$$

$$\Psi_x' U = P_{m_x} U^0,$$

$$\Psi_y' V = P_{m_y} V^0,$$

$$\Psi_z' W = P_{m_z} W^0.$$

$$\Delta_h P = D_x^+ \Psi_x F_x + D_y^+ \Psi_y F_y + D_z^+ \Psi_z F_z + D_x^+ \bar{F}_x + D_y^+ \bar{F}_y + D_z^+ \bar{F}_z.$$

Rewritten for Schur-complement

$$\left[\begin{array}{ccc|ccc} \Delta_h & \mathcal{O} & \mathcal{O} & -D_x^- & \psi_x & \mathcal{O} & \mathcal{O} \\ \mathcal{O} & \Delta_h & \mathcal{O} & -D_y^- & \mathcal{O} & \psi_y & \mathcal{O} \\ \mathcal{O} & \mathcal{O} & \Delta_h & -D_z^- & \mathcal{O} & \mathcal{O} & \psi_z \\ \hline \mathcal{O} & \mathcal{O} & \mathcal{O} & \Delta_h & -D_x^+ \psi_x & -D_y^+ \psi_y & -D_z^+ \psi_z \\ \hline \psi'_x & \mathcal{O} & \mathcal{O} & \mathcal{O} & \mathcal{O} & \mathcal{O} & \mathcal{O} \\ \mathcal{O} & \psi'_y & \mathcal{O} & \mathcal{O} & \mathcal{O} & \mathcal{O} & \mathcal{O} \\ \mathcal{O} & \mathcal{O} & \psi'_z & \mathcal{O} & \mathcal{O} & \mathcal{O} & \mathcal{O} \end{array} \right] \begin{bmatrix} U \\ V \\ W \\ P \\ F_x \\ F_y \\ F_z \end{bmatrix} = \begin{bmatrix} -\bar{F}_x \\ -\bar{F}_y \\ -\bar{F}_z \\ \operatorname{div} \bar{F} \\ P_{m_x} U^0 \\ P_{m_y} V^0 \\ P_{m_z} W^0 \end{bmatrix}$$

The Schur-complement

Solve

$$M \begin{bmatrix} F_x \\ F_y \\ F_z \end{bmatrix} = \begin{bmatrix} \Psi'_x U^2 - P_{m_x} U^0 \\ \Psi'_y V^2 - P_{m_y} V^0 \\ \Psi'_z W^2 - P_{m_z} W^0 \end{bmatrix}$$

with

$$M = \begin{bmatrix} \Psi'_x \Delta_h^\dagger \left(-I + D_x^- \Delta_h^\dagger D_x^+ \right) \Psi_x & \Psi'_x \Delta_h^\dagger D_x^- \Delta_h^\dagger D_y^+ \Psi_y & \Psi'_x \Delta_h^\dagger D_x^- \Delta_h^\dagger D_z^+ \Psi_z \\ \Psi'_y \Delta_h^\dagger D_y^- \Delta_h^\dagger D_x^+ \Psi_x & \Psi'_y \Delta_h^\dagger \left(-I + D_y^- \Delta_h^\dagger D_y^+ \right) \Psi_y & \Psi'_y \Delta_h^\dagger D_y^- \Delta_h^\dagger D_z^+ \Psi_z \\ \Psi'_z \Delta_h^\dagger D_z^- \Delta_h^\dagger D_x^+ \Psi_x & \Psi'_z \Delta_h^\dagger D_z^- \Delta_h^\dagger D_y^+ \Psi_y & \Psi'_z \Delta_h^\dagger \left(-I + D_z^- \Delta_h^\dagger D_z^+ \right) \Psi_z \end{bmatrix}$$

M is symmetric since $\Delta_h^\dagger$ is symmetric,

$D_x^+ = -D_x^-$, $D_y^+ = -D_y^-$, $D_z^+ = -D_z^-$ and

because the one-sided differences D_x^- , D_y^- , D_z^- , D_x^+ , D_y^+ and D_z^+ commute with $\Delta_h^\dagger$.



Fast multiplication for use in CG

$$\tilde{F}_x = \Psi_x F_x, \tilde{F}_y = \Psi_y F_y, \tilde{F}_z = \Psi_z F_z.$$

$$P^1 = \Delta_h^\dagger (D_x^+ \tilde{F}_x + D_y^+ \tilde{F}_y + D_z^+ \tilde{F}_z),$$

$$U^1 = \Delta_h^\dagger (D_x^- P^1 - \tilde{F}_x),$$

$$V^1 = \Delta_h^\dagger (D_y^- P^1 - \tilde{F}_y),$$

$$W^1 = \Delta_h^\dagger (D_z^- P^1 - \tilde{F}_z),$$

$$M \begin{bmatrix} F_x \\ F_y \\ F_z \end{bmatrix} = - \begin{bmatrix} \Psi'_x U^1 \\ \Psi'_y V^1 \\ \Psi'_z W^1 \end{bmatrix}.$$

Argument is in

$$\mathbb{R}^n \setminus \{\mathbf{x} \in \mathbb{R}^n : \sum \mathbf{x} = 0\}$$

for each of the

4 direct Poisson solves
that are needed per
CG iteration

Final answer:

$$U = U^1 + U^2,$$

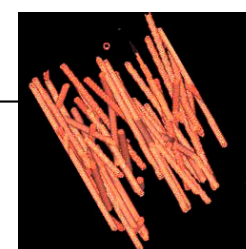
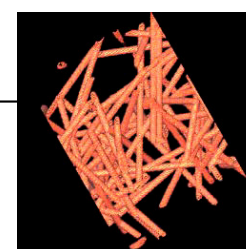
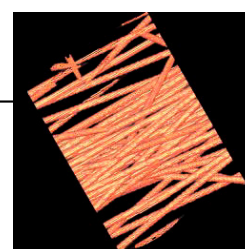
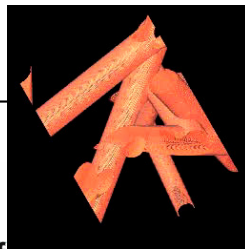
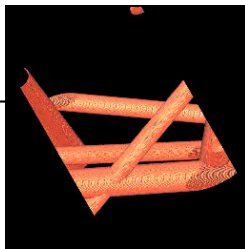
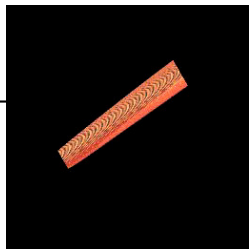
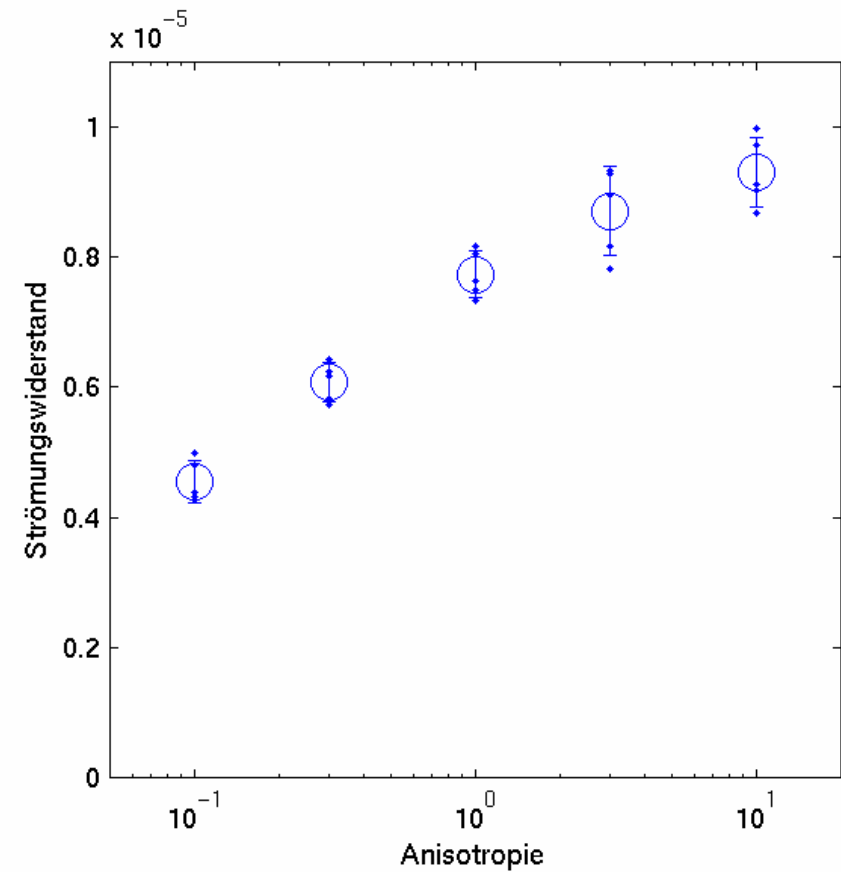
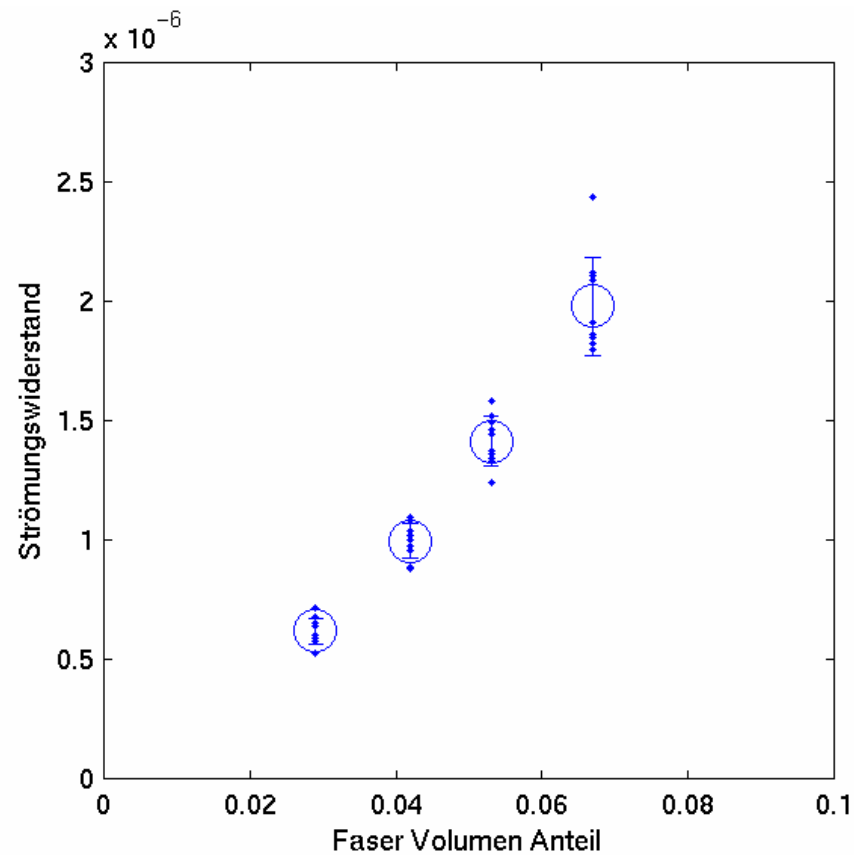
$$V = V^1 + V^2,$$

$$W = W^1 + W^2,$$

$$P = \mu (P^1 + P^2).$$



Influence of porosity and fiber directions on flow resistivity?



Effect of prime factorization on solution efficiency?

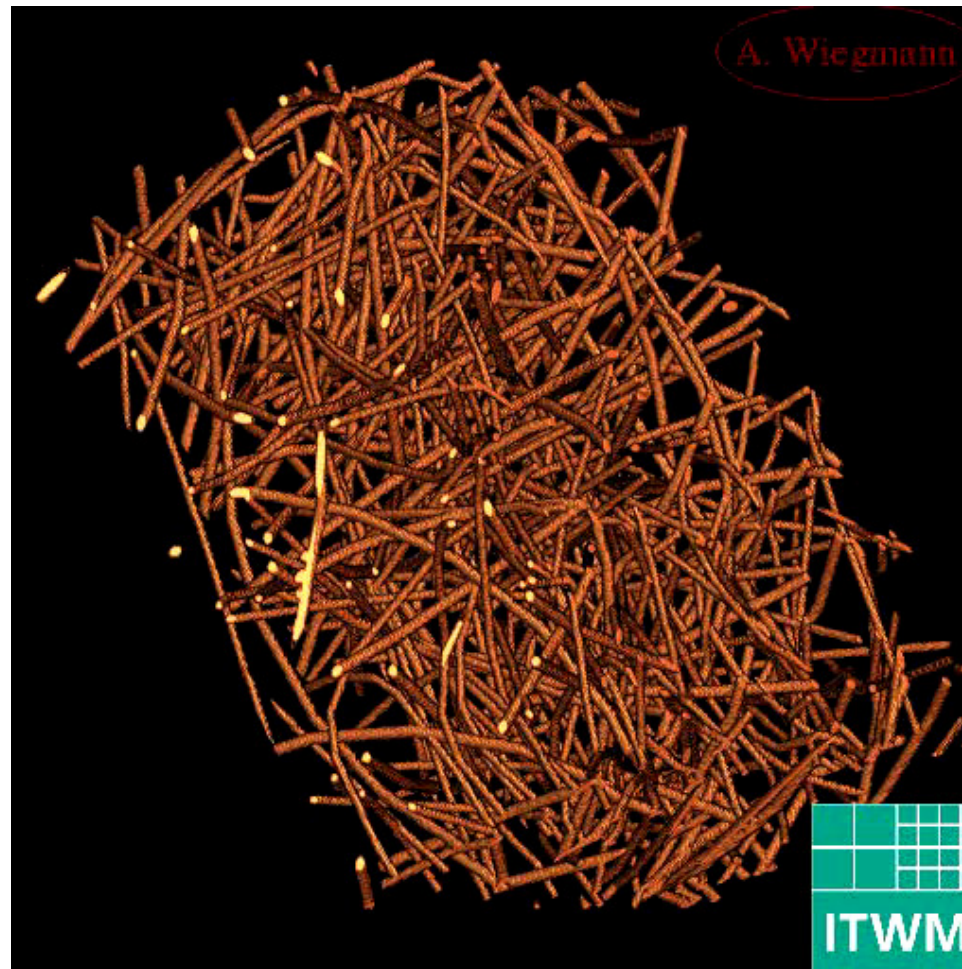
Stokes solver was run to 1 digit accuracy merely to get the time / iteration, required approximately 400MB RAM.

n	$n_x = n_y = n_z$	iterations	run time (s)	time / iteration (s)
2,048,383	127	4	156	39
2,097,152	$2^7 = 128$	6	131	22
2,146,689	$3 * 43 = 129$	6	167	28

Clearly powers of 2 work better than other prime factorizations, but as long as all directions remain fairly short (or have “good” prime factorization), FFTW is very fast!



Compression of fibrous media



Summary

- FFT(W) based explicit jump solvers solve electrostatics, diffusive heat transfer & Stokes
 - Direct Poisson solvers can be a viable alternative to multigrid
 - Fundamental idea: „discretize first, then do Schur-complement“, not „do integral equation, then discretize“
 - FFT replaces the kernel (fundamental solution) of the integral equation
 - Even on laptops, REVs can be achieved
 - If anyone is interested, we can meet for an online demo later
 - Thank you for your attention
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