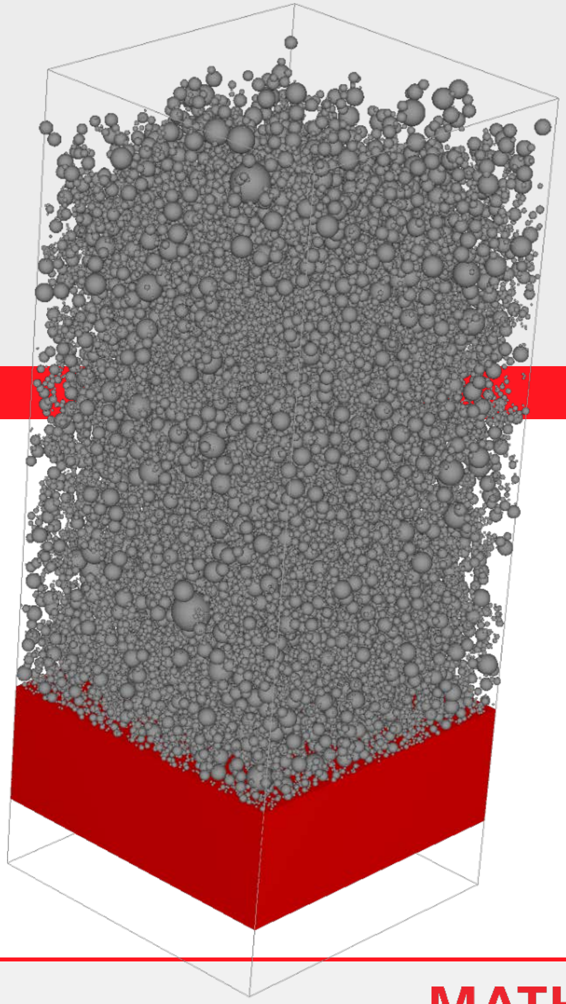
From Resolved Filtration Simulations to Effective Cake Filtration Simulation Parameters



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Liping Cheng

Sven Linden

Jürgen Becker

Cornelia Kronsbein

Andreas Wiegmann

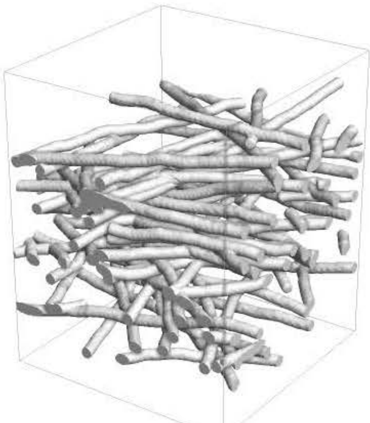
GeoDict

MATH 2 MARKET

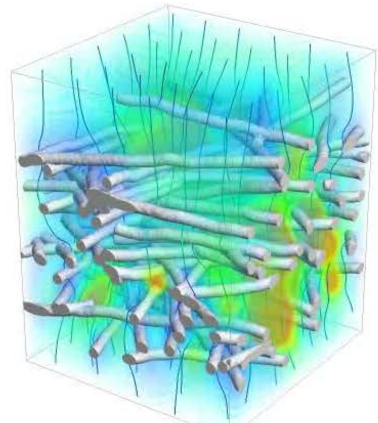
Math2Market GmbH
Some background information

- Math2Market creates and markets software for engineers and scientists that want to analyze and design porous and composite materials based on the material's geometric inhomogeneity.
- The materials can come from µCT, FIB-SEM or models and are represented as 3-dimensional images in the software.
- This software is called GeoDict, the Digital Material Laboratory.
- M2M is based in Kaiserslautern, Germany.
- M2M spun off from Fraunhofer Institute for Industrial Mathematics.
- Visit us at our booth

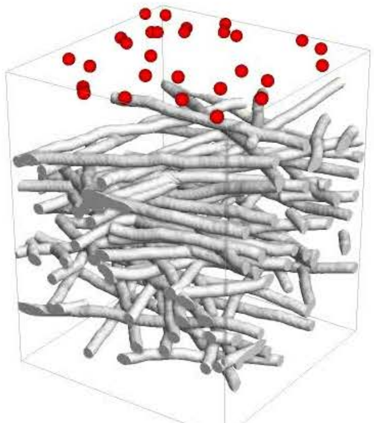
How is cake filtration simulated?



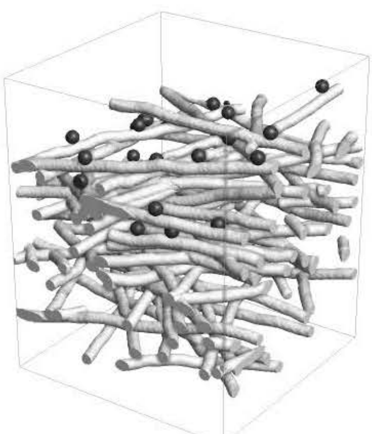
1. Filter Model



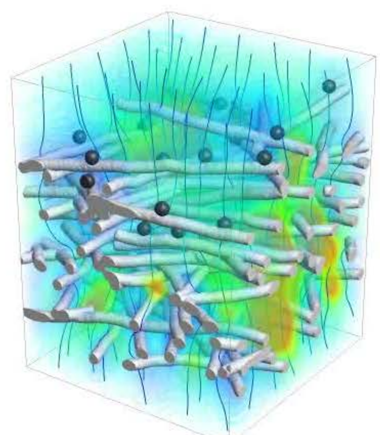
2. Flow Field



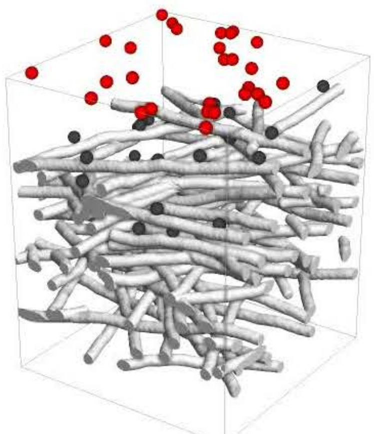
3. Track Particles



4. Deposit Particles



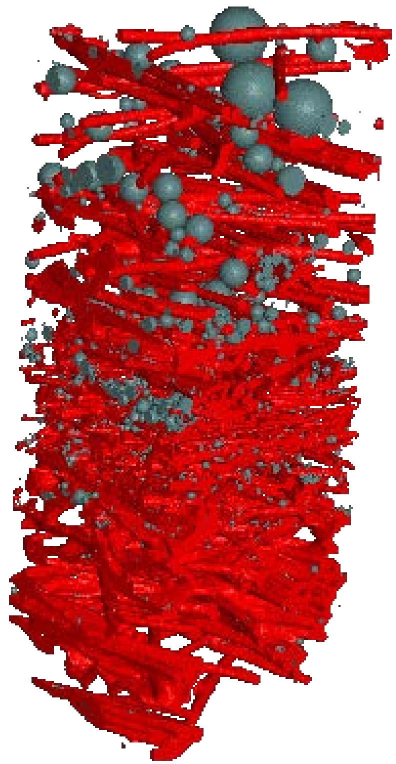
5. Flow Field



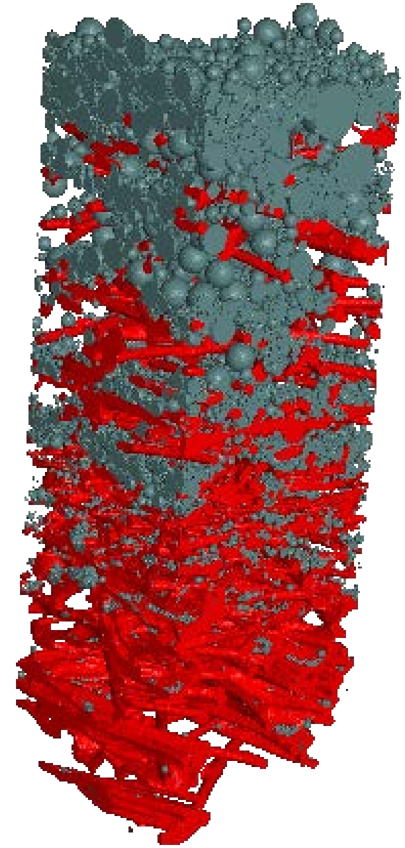
6. Repeat …

Depth filtration vs. cake filtration

Clean filter medium

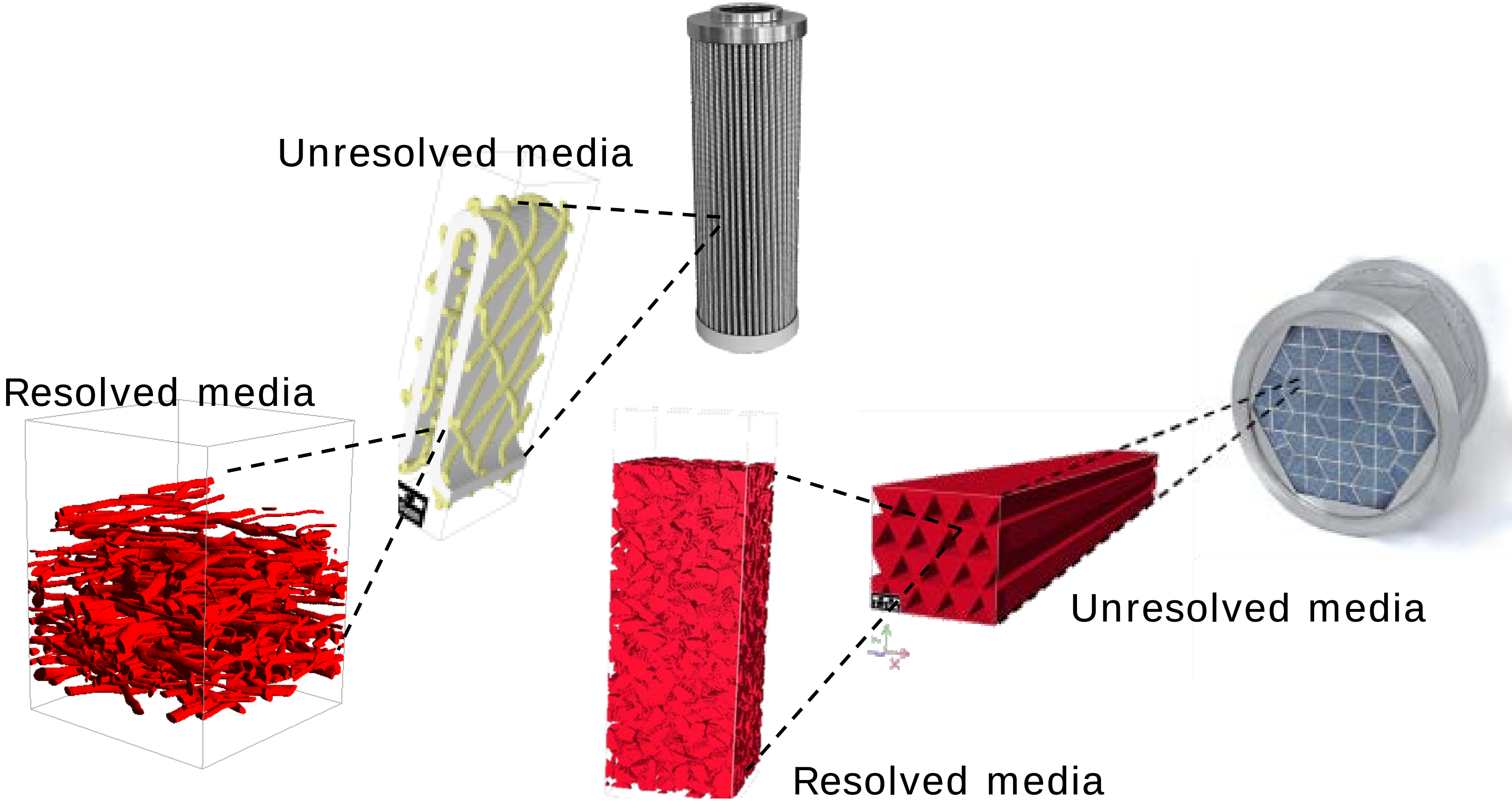


Depth filtration

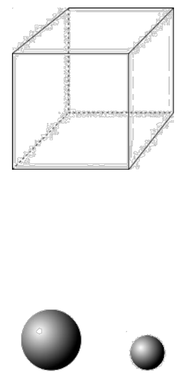
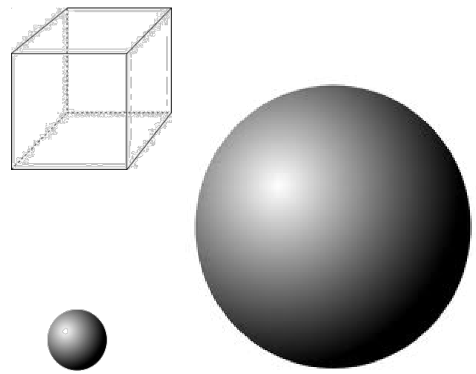
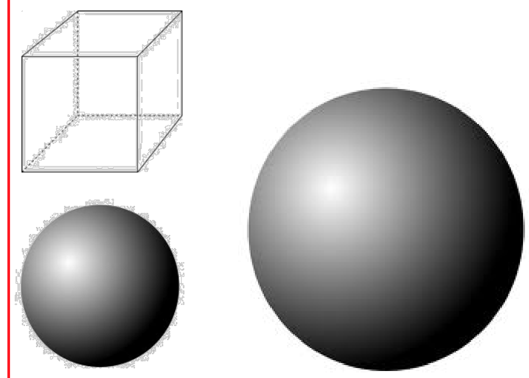
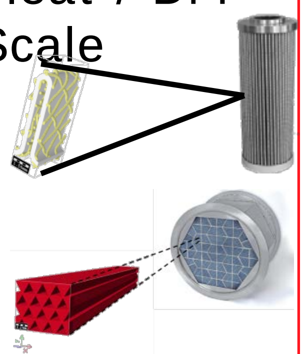
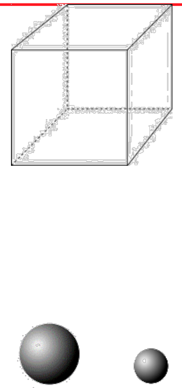
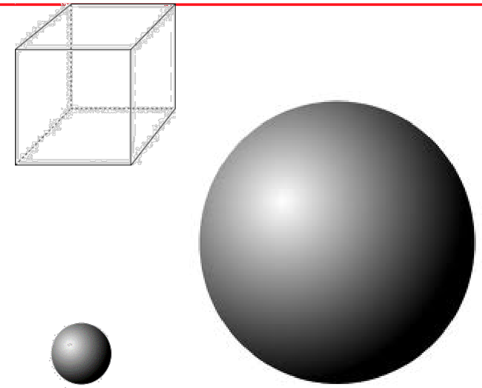
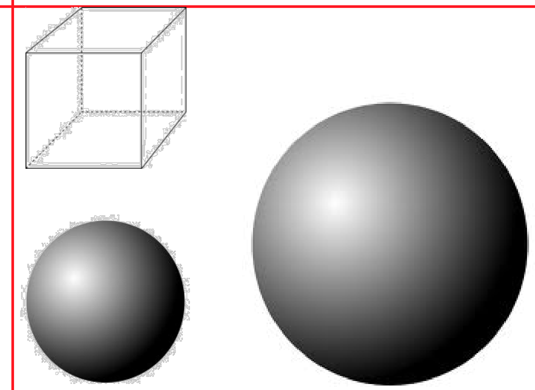


Cake filtration

Resolution: filter media



Resolution: particles

Particles Domain	Unresolved	Mixed	Resolved
Media Scale 			
Pleat / DPF Scale 			

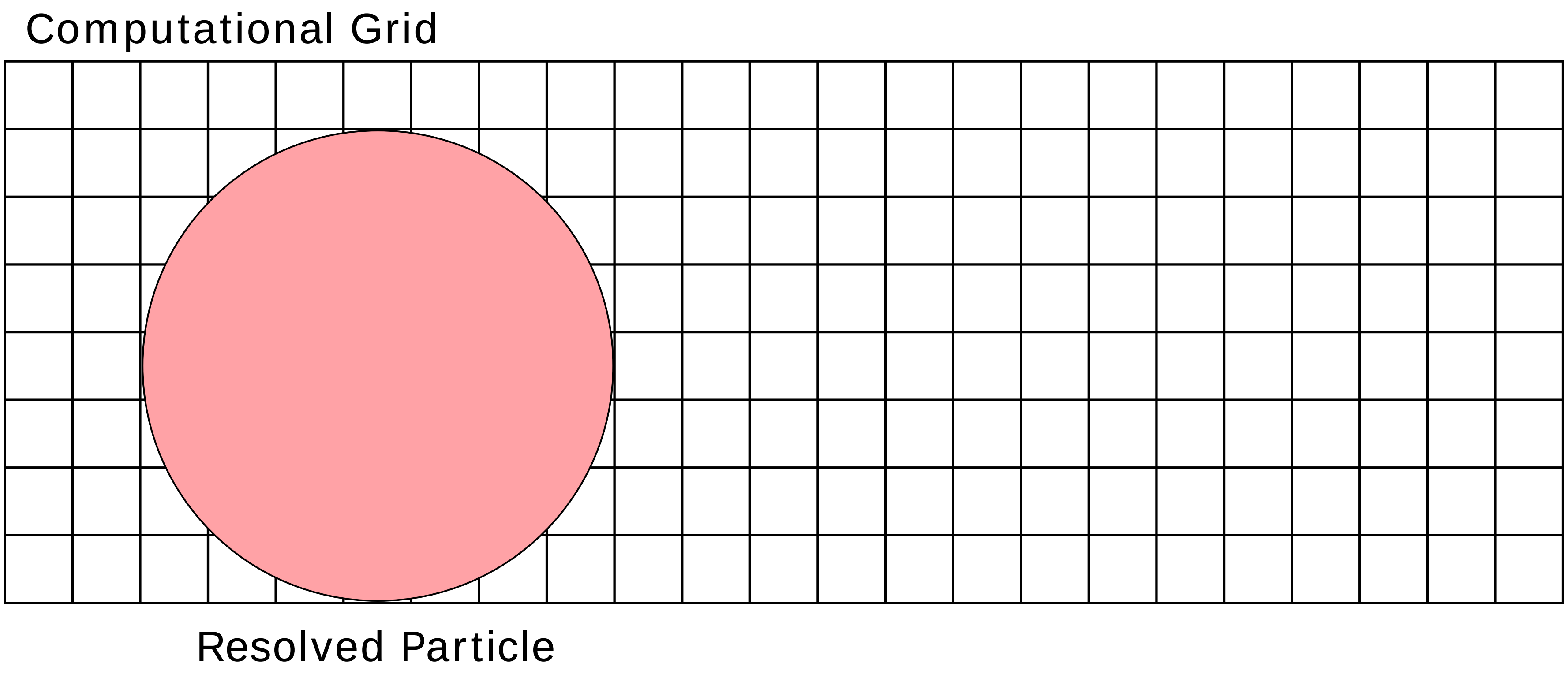
Scale Issue of Cake Filtration Simulation on Uniform 3d Grids

- When all particles are much larger than the grid size, then solid and empty cells suffice to represent them.
- When all particles are much smaller than the computational grid size, then an homogeneous porous media approach works.

- Resolved and unresolved particles are both present in the poly-disperse particles.
- When the particle size distribution includes larger particles and smaller particles than the grid size, then sub-grid resolution and parameters for inhomogeneous porous media are required.

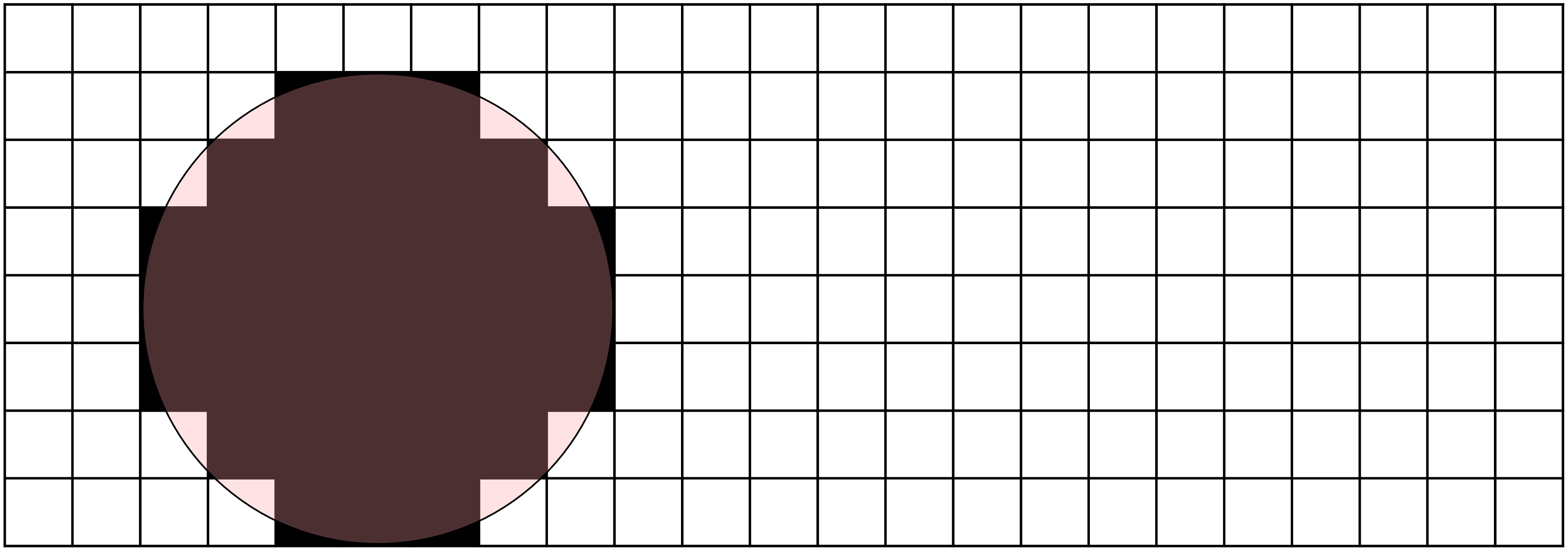
- We describe two approaches to find these parameters.

Computational Grid, Resolved



Discretization of Resolved Particles

Computational Grid

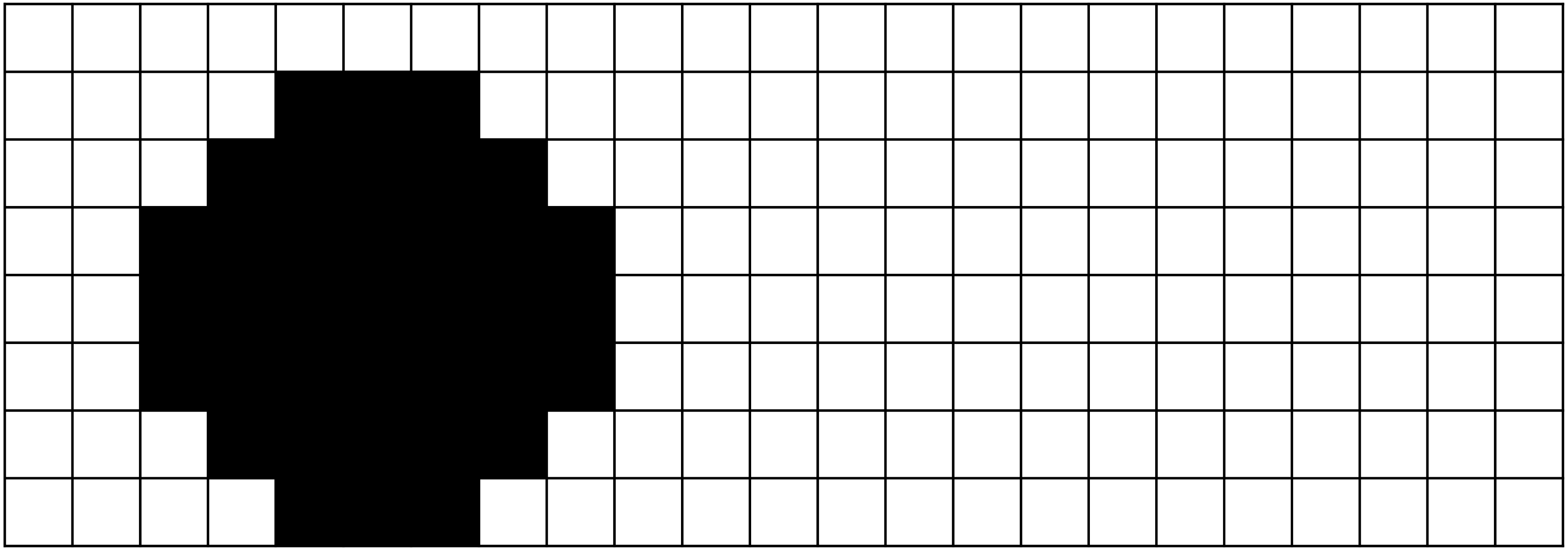


Resolved Particle

Empty/Solid Cells

Discretization of Resolved Particles

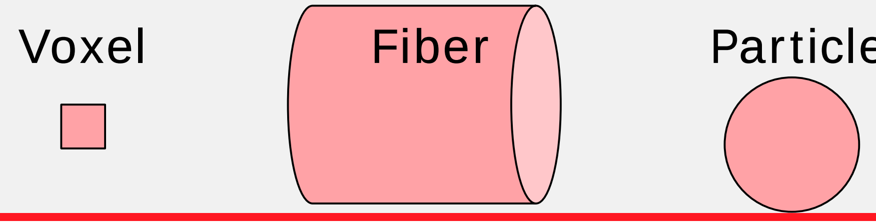
Computational Grid



Resolved Particle

Empty/Solid Cells

Resolved Particles



- Voxels are solid or empty

- Stationary incompressible Navier-Stokes equation

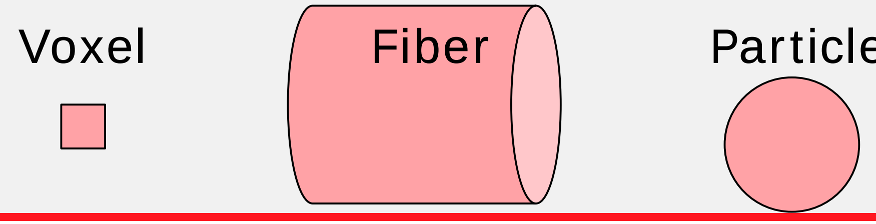
$$-\mu\Delta\vec{u} + \rho(\vec{u}\cdot\nabla)\vec{u} + \nabla p = 0, \qquad \nabla\cdot\vec{u} = 0$$

μ	viscosity
ρ	density
u	velocity
p	pressure

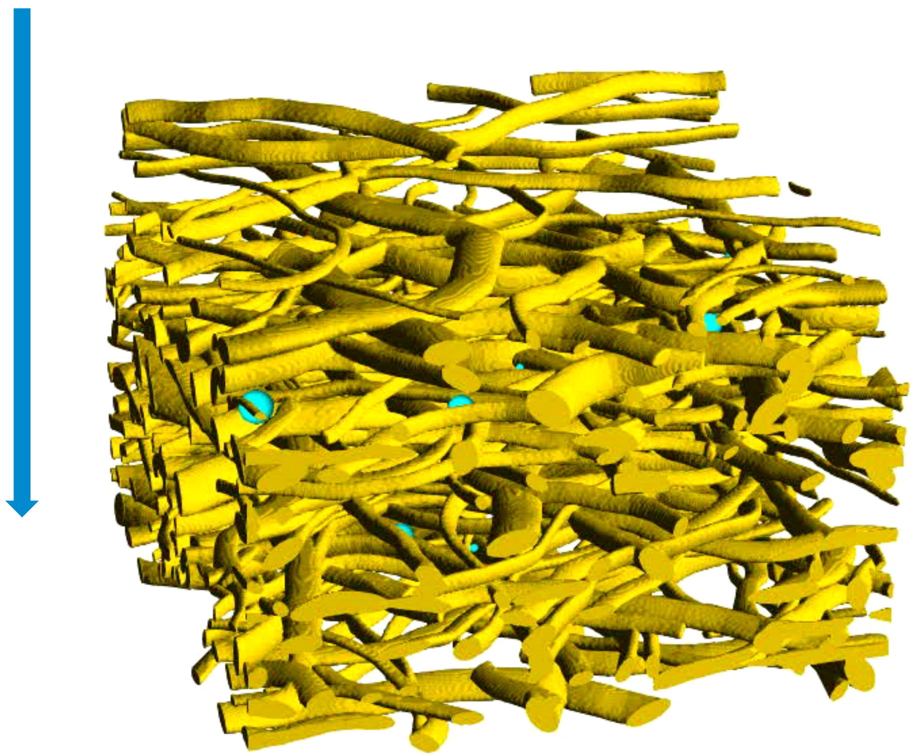
- Particles are discretized into solid/empty grid cells

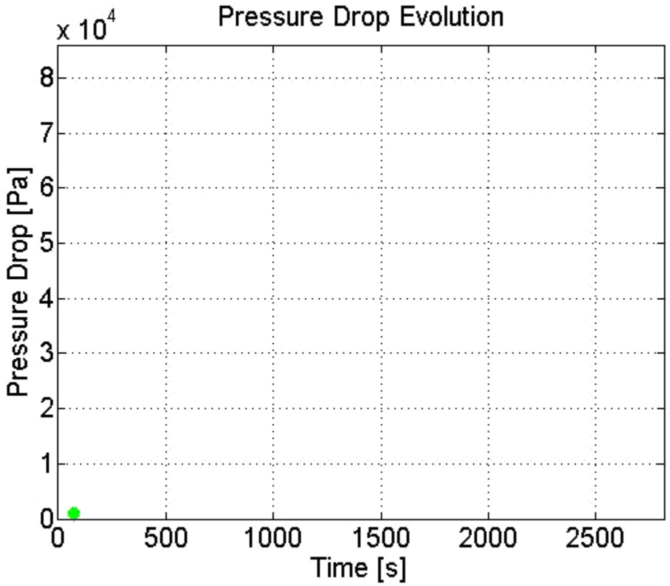
Output parameters: f_{max} (maximal solid volume fraction)
and σ_{max} (maximal flow resistivity)

Resolved Particles

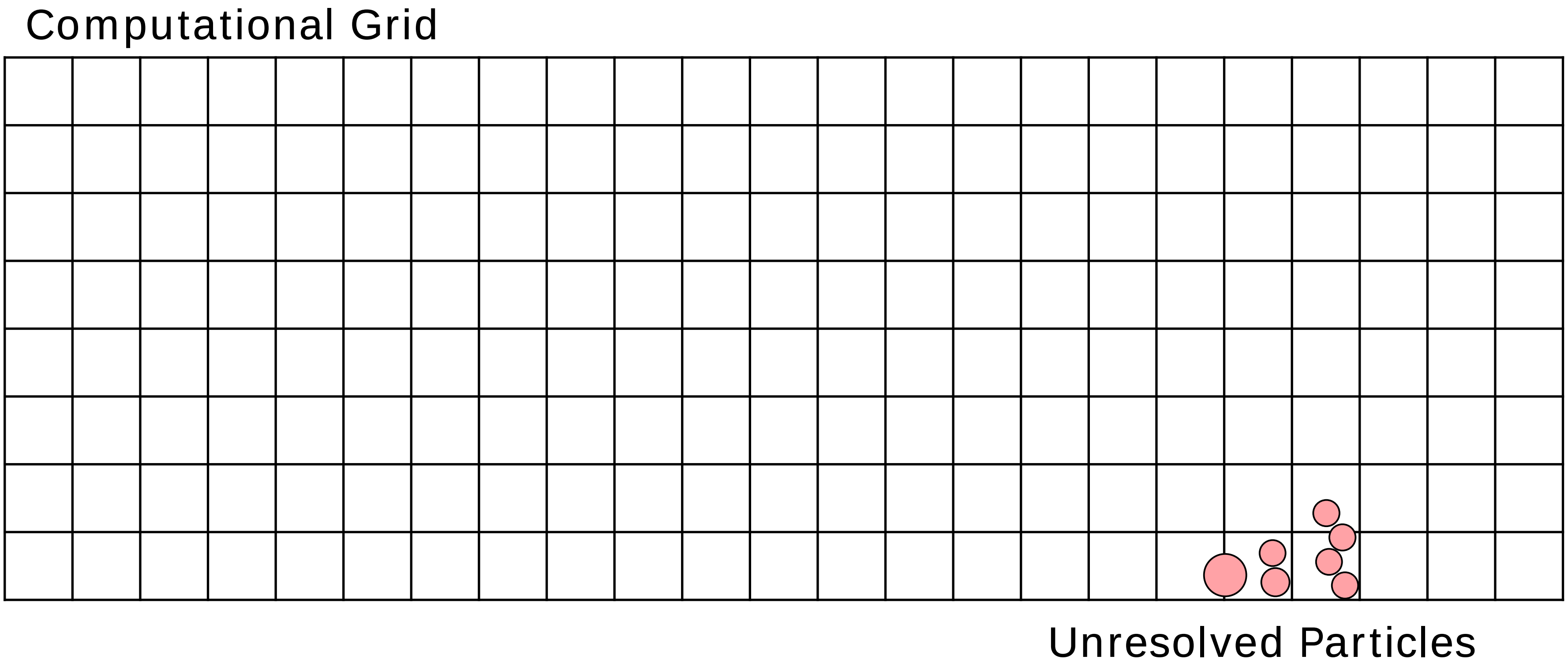


Example: Oil filtration – Multi Pass test; sieving model



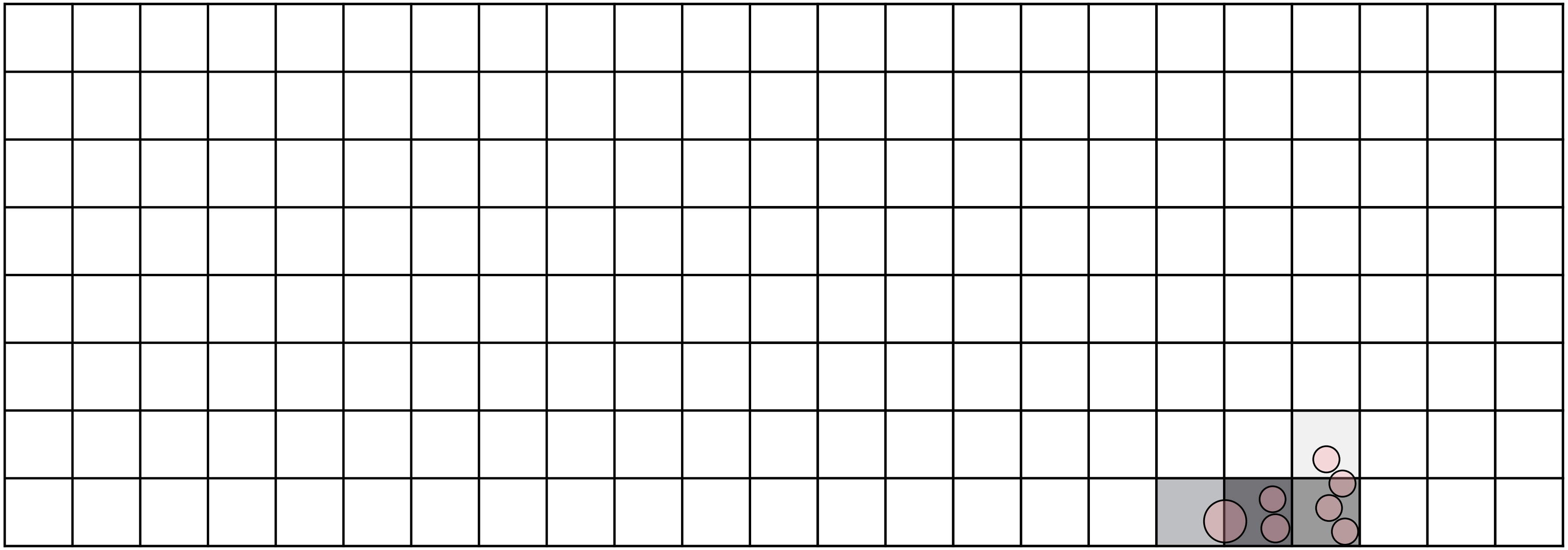


Computational Unresolved Particles



Discretization of Resolved and Unresolved Particles

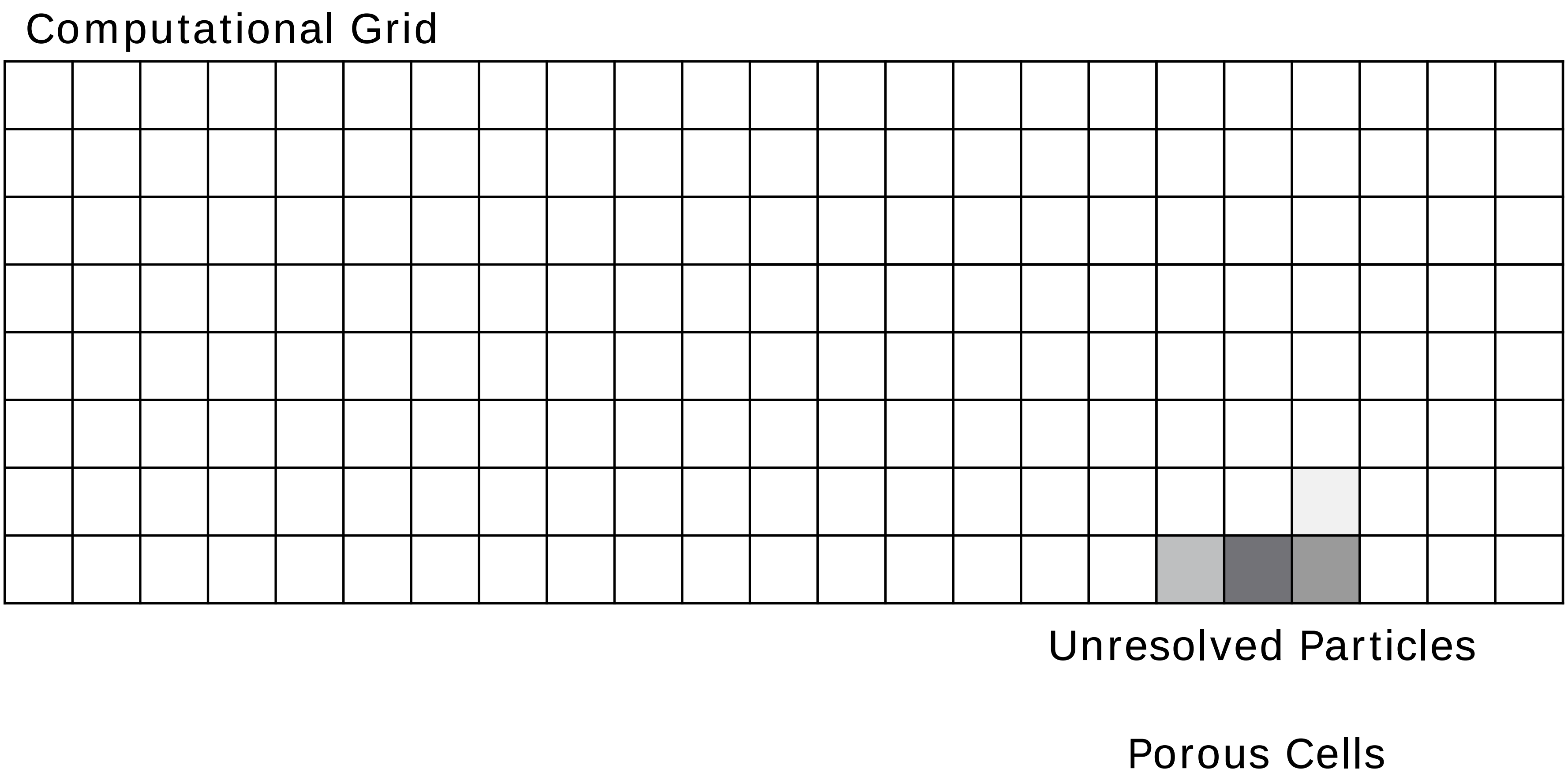
Computational Grid



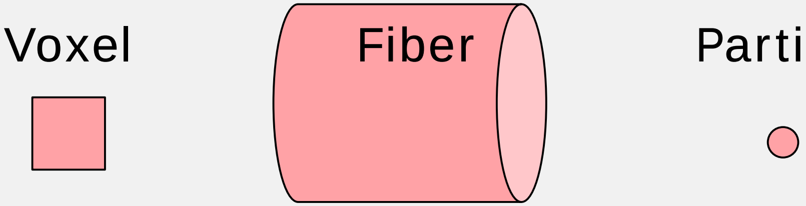
Unresolved Particles

Porous Cells

Discretization of Resolved and Unresolved Particles



Unresolved Particles



- Voxels are solid, empty or porous
- Stationary incompressible Navier-Stokes-Brinkman equation

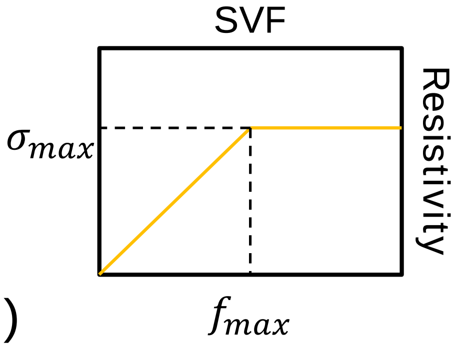
$$-\mu\Delta\vec{u} + \rho(\vec{u}\cdot\nabla)\vec{u} + \sigma\vec{u} + \nabla p = 0, \qquad \nabla\cdot\vec{u} = 0$$

σ: resistivity

In porous voxels:

- Local solidity f changes when a particle is added.
- When f_{max} is reached, no more particles can be added.
- Local flow resistivity:

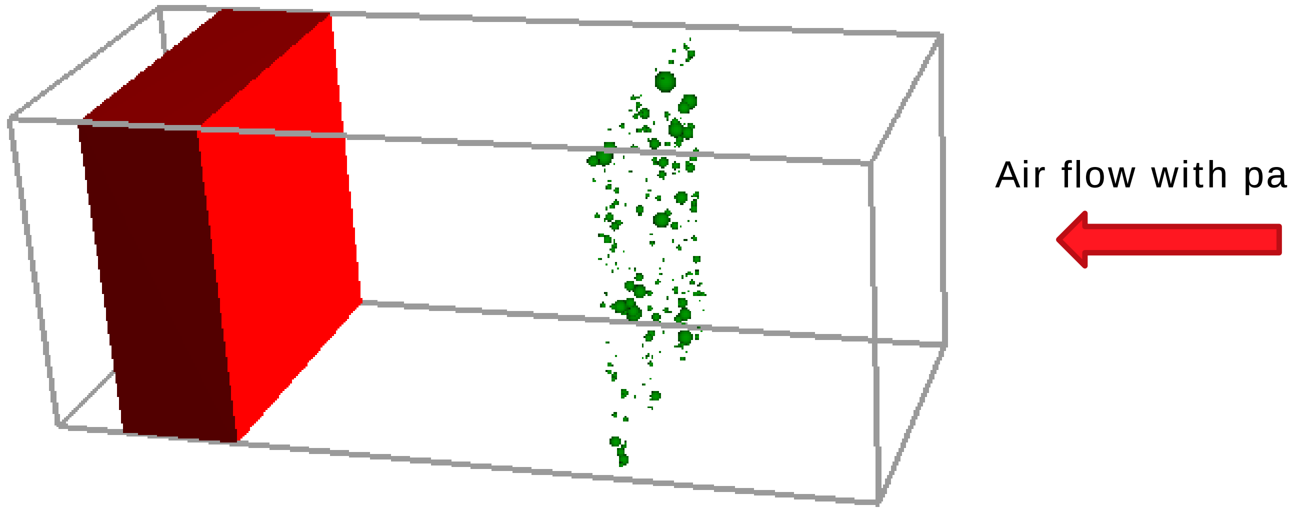
$$\sigma = \begin{cases} \frac{f}{f_{max}}\sigma_{max} & \text{for } 0 < f < f_{max} \\ \sigma_{max} & \text{for } f_{max} \le f \le 1 \end{cases}$$



Input parameters: f_{max} (maximal solid volume fraction)

and σ_{max} (maximal flow resistivity)

Simulation Setup



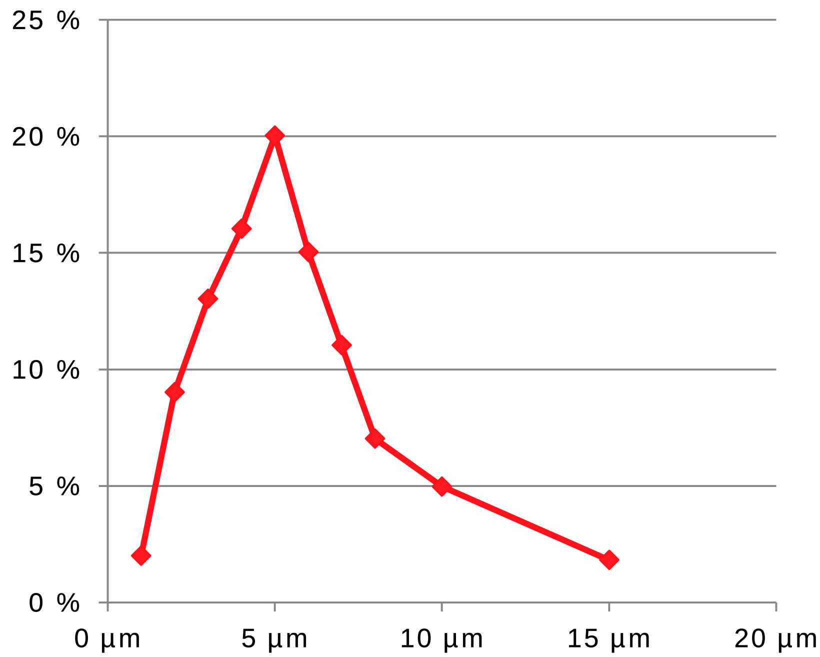
Air flow with particles

- No depth filtration, only cake filtration
- Unresolved filter media: 48 µm thick, fixed permeability
- Particles are *caught on first touch*
- Particle diameter range between 1µm and 15µm

1. Vary resolution between 0.5 µm per voxel and 24 µm per voxel
2. Determine flow resistivity and cake solidity

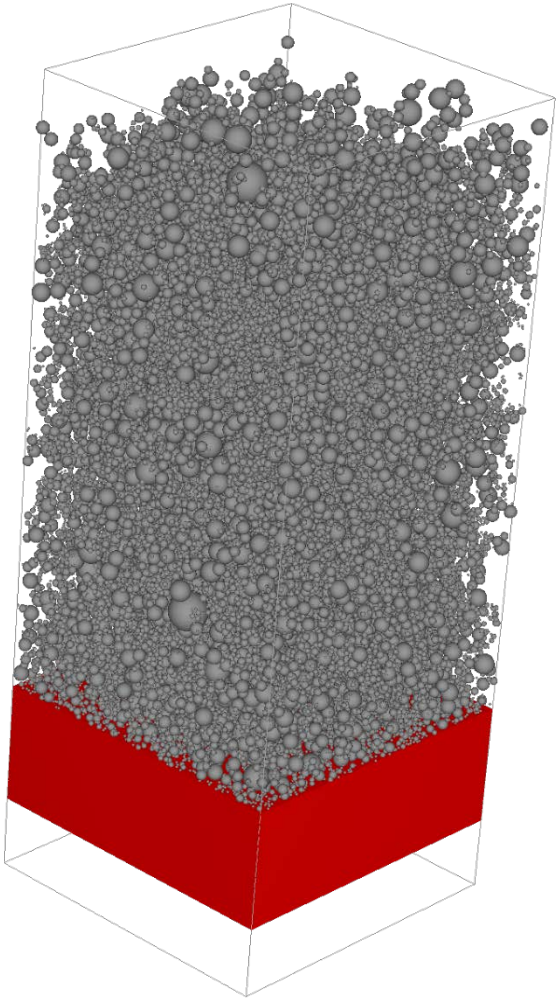
Particle Size Distribution

Particle Diameter	Mass %	Count %
1 µm	2.00	48.340
2 µm	9.01	27.190
3 µm	13.03	11.640
4 µm	16.04	6.040
5 µm	20.04	3.870
6 µm	15.03	1.680
7 µm	11.03	0.780
8 µm	7.03	0.330
10 µm	4.97	0.120
15 µm	1.82	0.013



SAE Ultrafine Dust (ISO 12103-1)

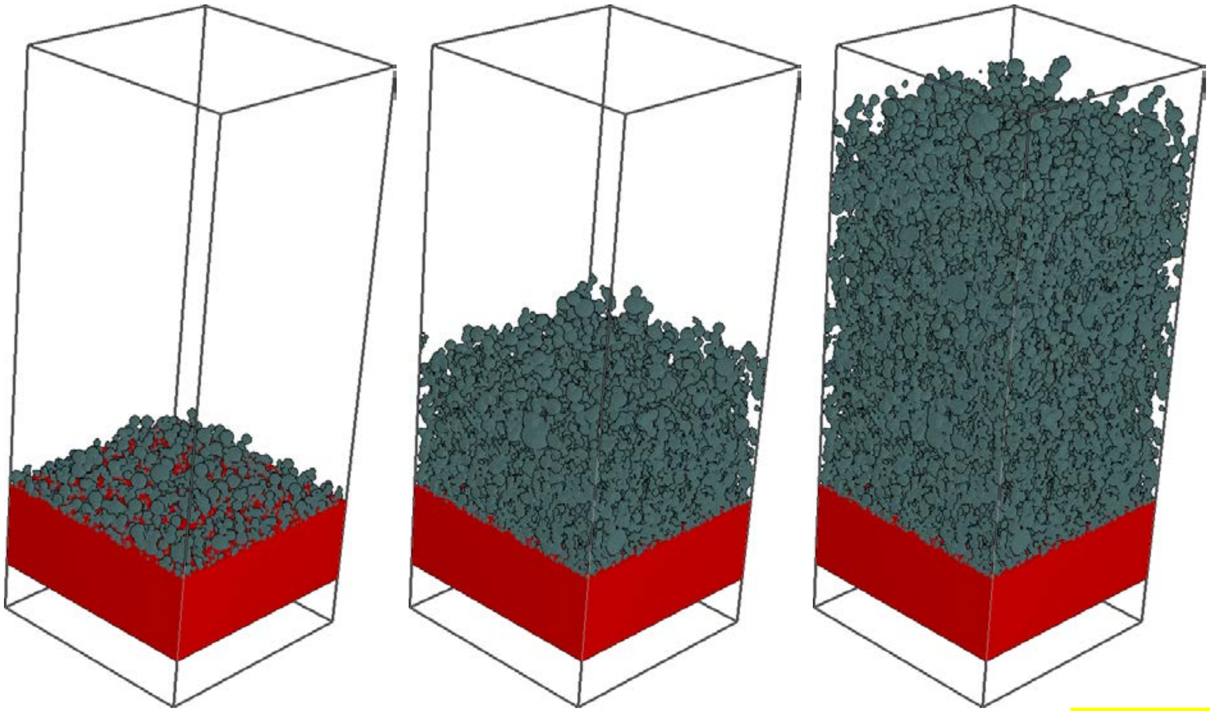
Resolved Particles

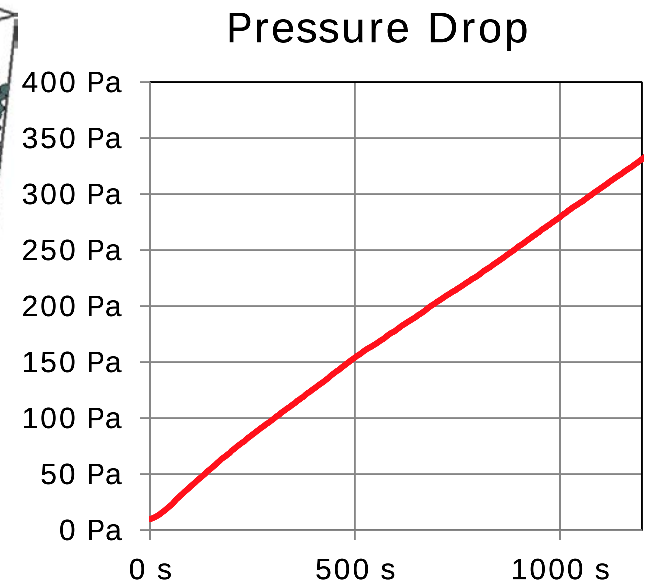


- Simulation with all resolved particle works by entering them as solid / empty and computing Stokes flow in the pores.
- The solid volume fraction f_{max} and the resistivity σ_{max} agrees to the experimental cake valules f_{real} and σ_{real}.

Resolved Particles
Caught On First Touch

Resolution 0.5µm

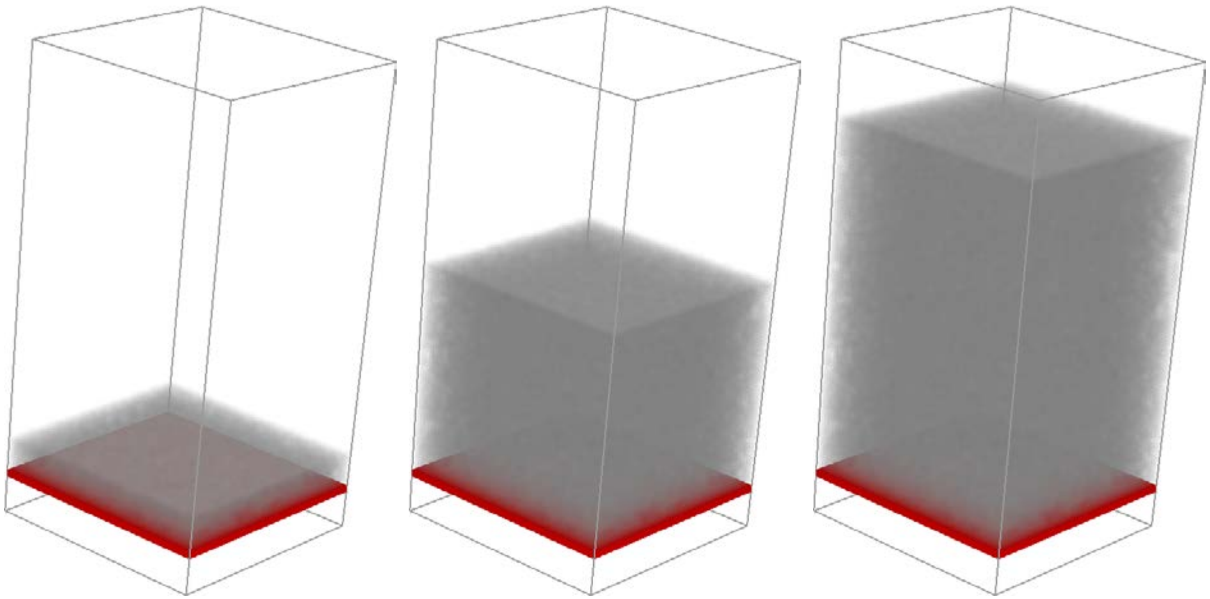


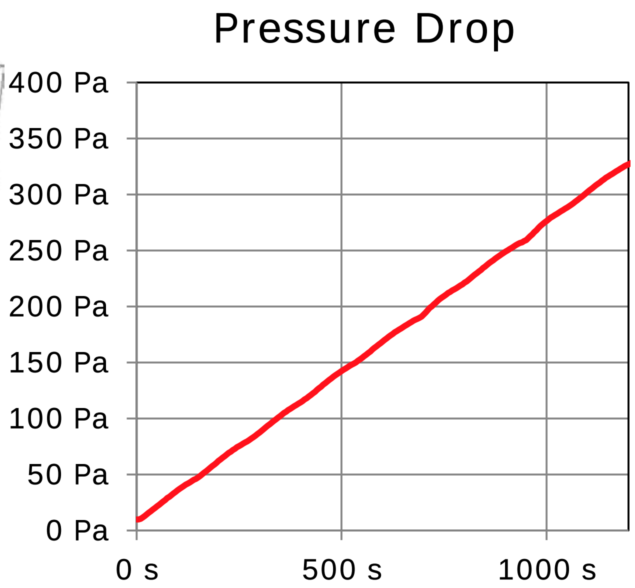


Result:
- Flow resistivity 14.4 e+6 kg/m³s
- Cake solidity 0.1953

Fully Unresolved Particles Caught On First Touch

Resolution 24µm





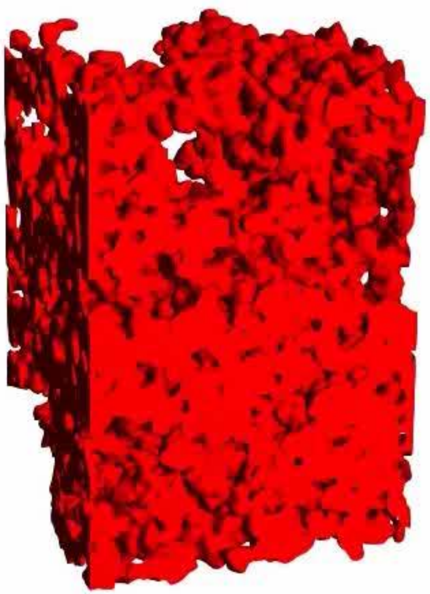
Input (porous voxels):
σ_{max} = 14.4 e+6 kg/m³s
f_{max} = 0.1953

Result:
- Flow resistivity 14.3 e+6 kg/m³s
- Cake solidity 0.2027

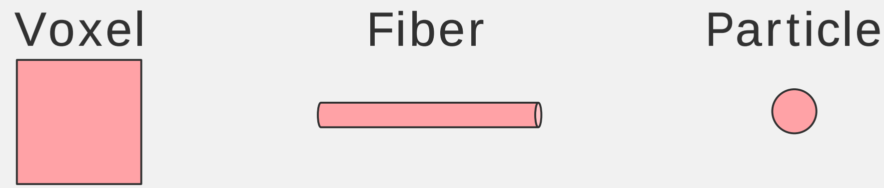
Unresolved Particles resolved media

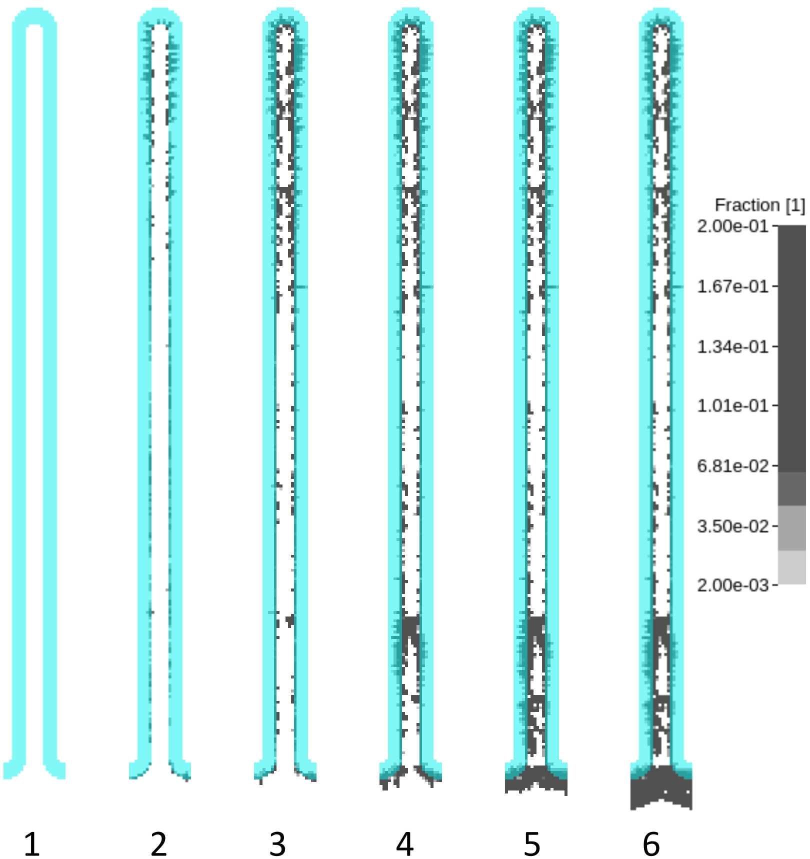
Voxel Fiber Particle

Example: Soot filtration – ceramic filter; caught on first touch model



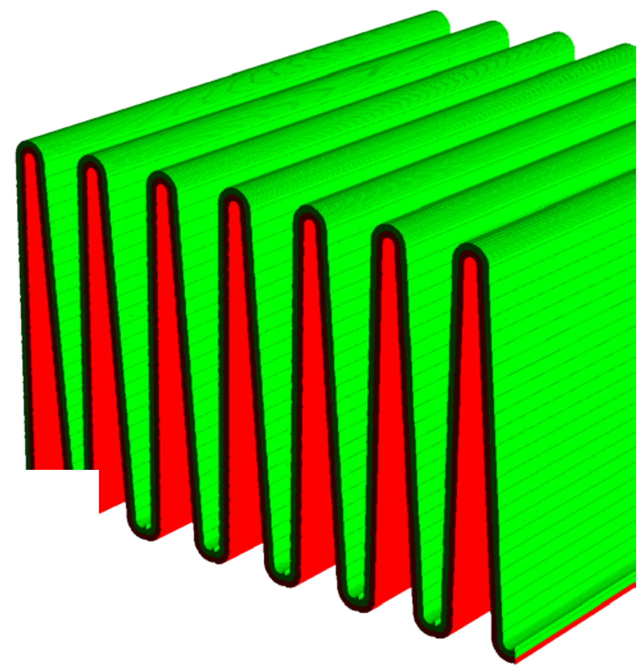
Unresolved Particles unresolved media



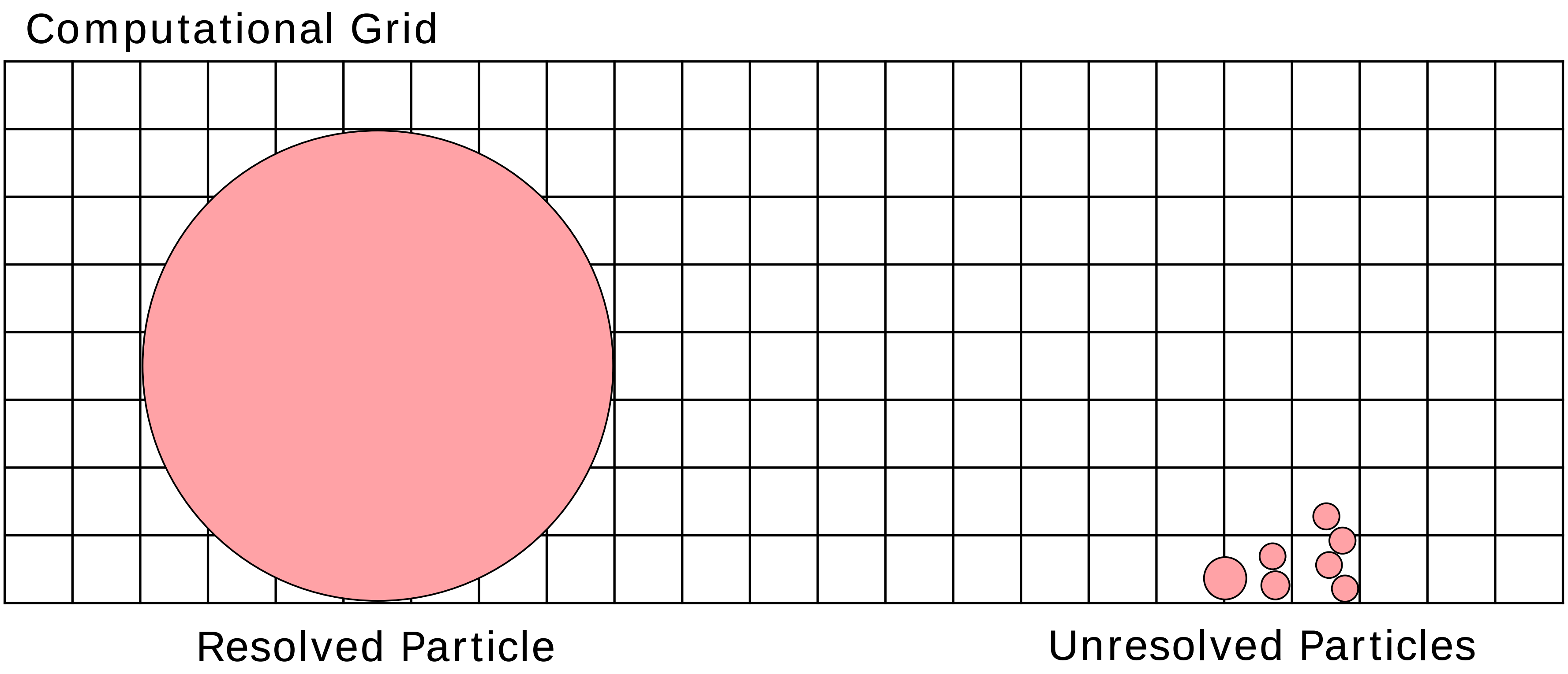


Filter material described by

- porosity
- permeability
- capturing probability model

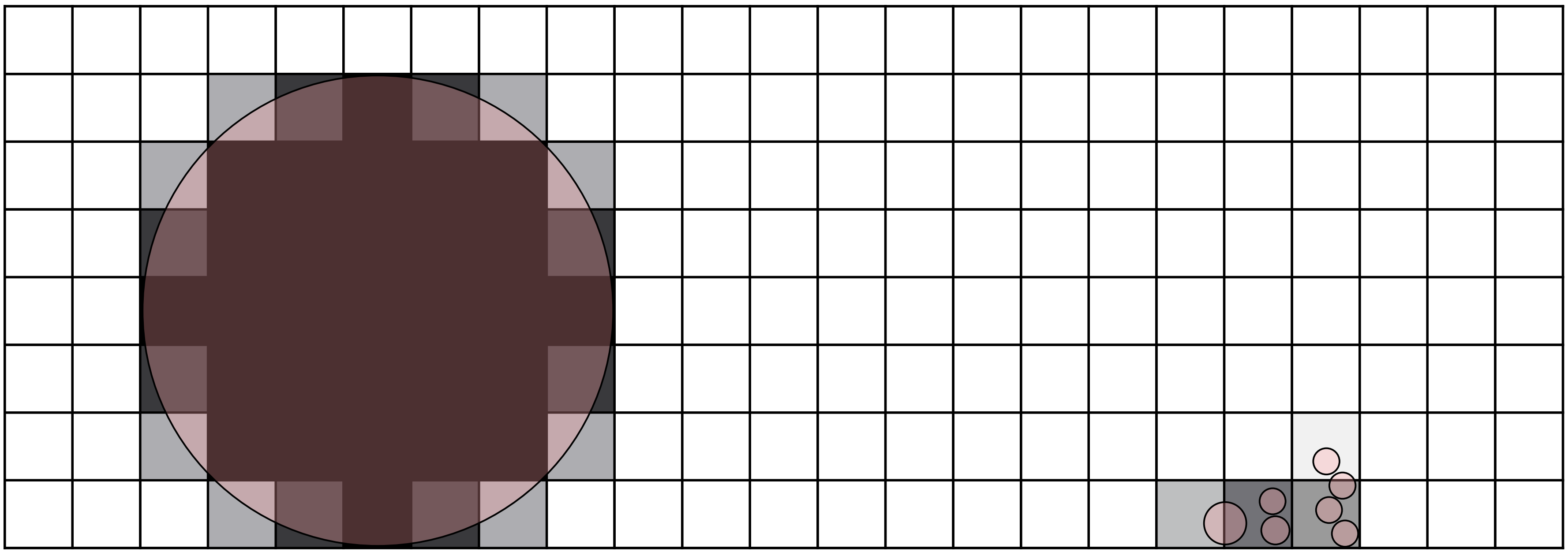


Computational Grid, Resolved & Unresolved Particles



Discretization of Resolved and Unresolved Particles

Computational Grid



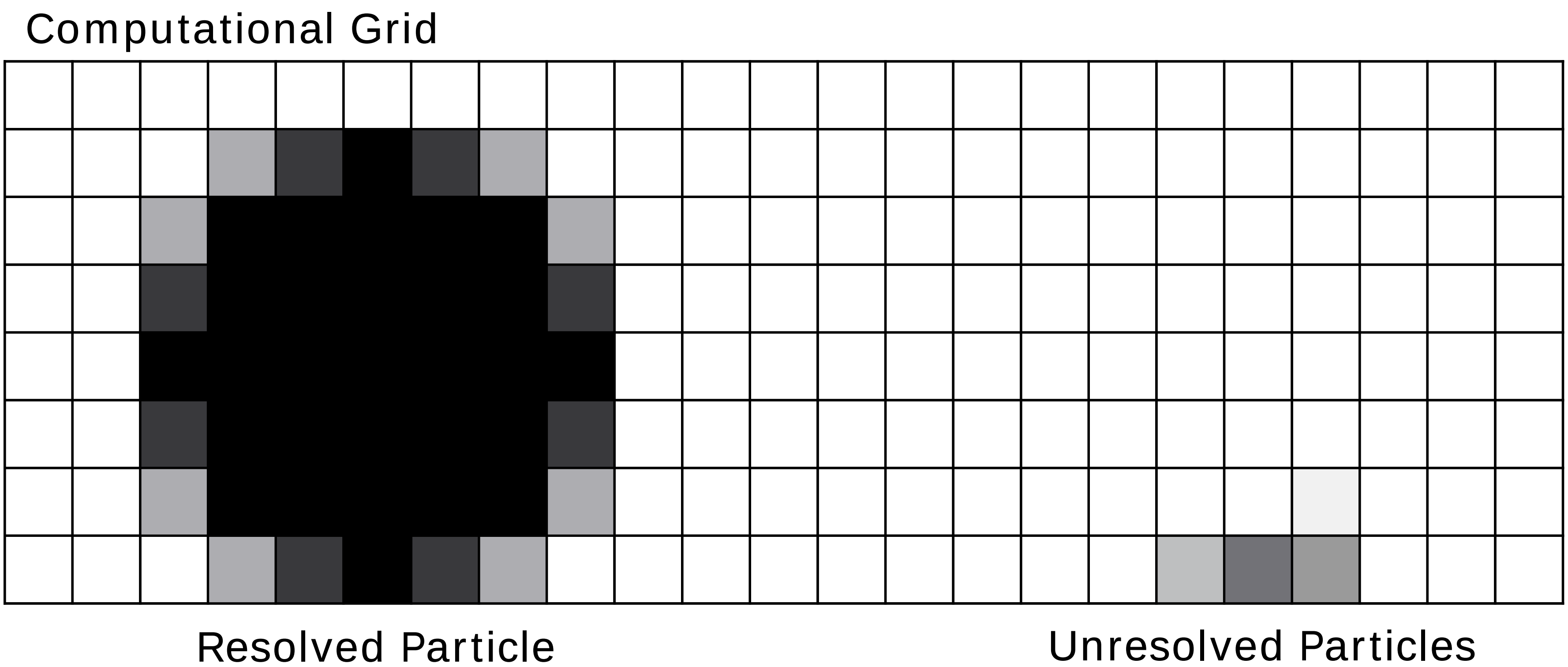
Resolved Particle

Unresolved Particles

Empty/Solid/porous Cells

Porous Cells

Discretization of Resolved and Unresolved Particles



Empty/Solid/porous Cells

Porous Cells

Resolved and Unresolved Particles

- Particles turn voxels into solid or porous.
- Stationary incompressible Navier-Stokes-Brinkman equation

In porous voxels:

- Local flow resistivity:

$$\sigma = \begin{cases} \frac{f}{f_{max}} \sigma_{max} & \text{for } 0 < f < f_{max} \\ \sigma_{max} & \text{for } f_{max} \leq f \leq 1 \\ \infty & \text{for } f = 1 \end{cases}$$

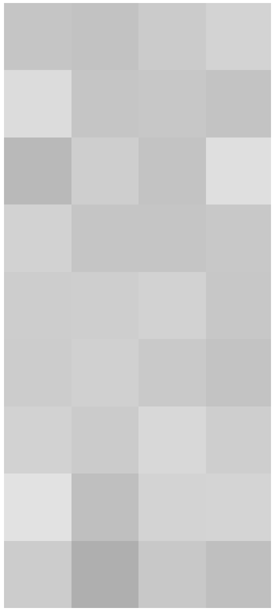
Input parameters: f_{max} (maximal solid volume fraction)

and σ_{max} (maximal flow resistivity)

Fully Resolved vs. Fully Unresolved particles

0.5 µm

Resolved Particles

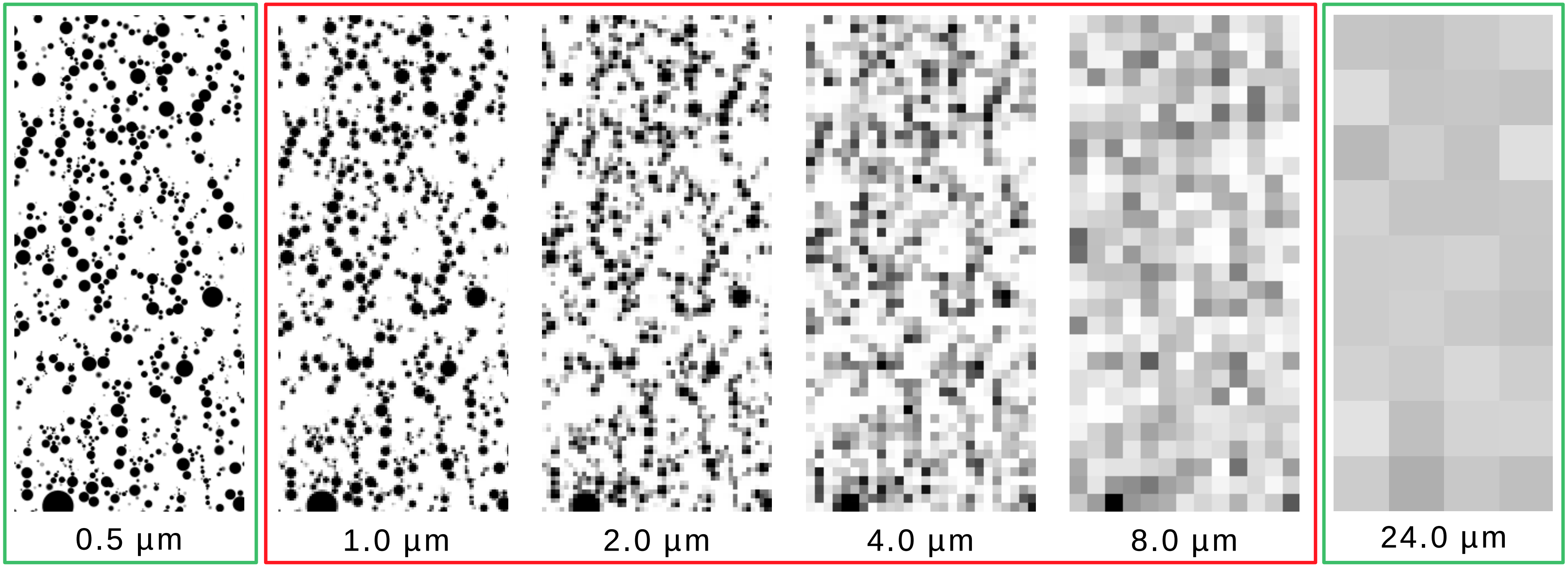


24.0 µm

Unresolved Particles

□	SVF=0	(empty)
■ (grey)	0<SVF<1	(porous)
■	SVF=1	(solid)

Mixed Resolved & Unresolved particles for varying resolutions



Resolved particles

Resolved and Unresolved particles

Unresolved particles

□	SVF=0	(empty)
▩	0<SVF<1	(porous)
■	SVF=1	(solid)

Results for Partially Resolved particles with parameters for Unresolved particles

Resolution	Input parameters		Resulting cake	
	f_{max}	σ_{max} [10^6 kg/m³s]	Solidity	Flow resistivity [10^6 kg/m³s]
24 µm	0.1953	14.4	0.2027	14.30
0.5 µm	solid/empty	solid/empty	0.1953	14.40

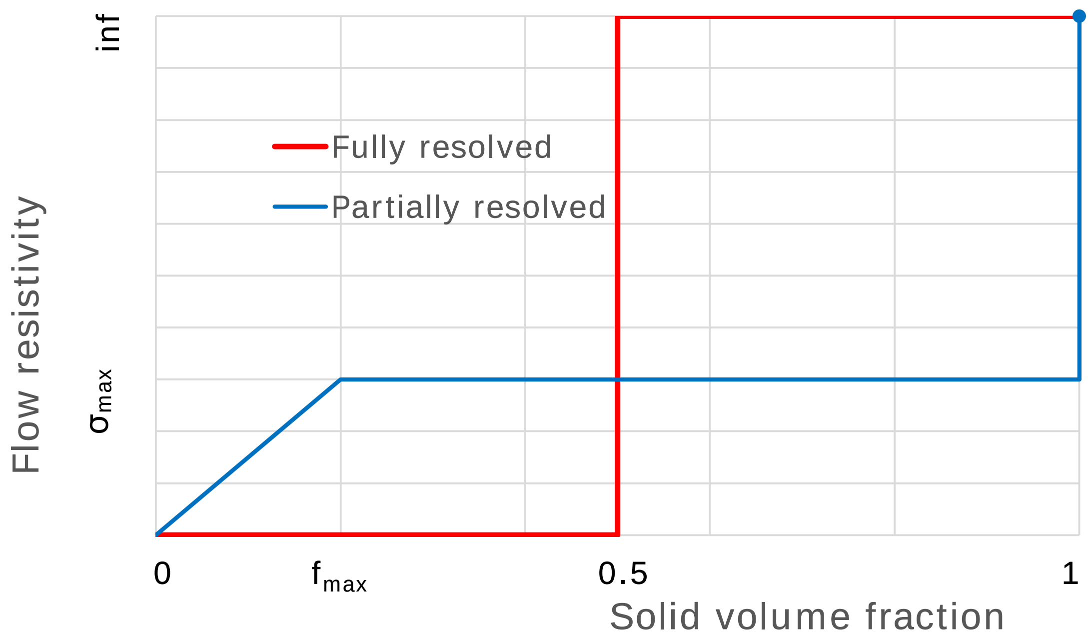
Results for Partially Resolved particles with parameters for Unresolved particles

Resolution	Input parameters		Resulting cake	
	f_{max}	σ_{max} [10^6 kg / m³s]	Solidity	Flow resistivity [10^6 kg / m³s]
24 µm	0.1953	14.4	0.2027	14.30
8 µm	0.1953	14.4	0.1953	10.17
4 µm	0.1953	14.4	0.1422	4.02
2 µm	0.1953	14.4	0.1346	3.09
1 µm	0.1953	14.4	0.1535	4.41
0.5 µm	solid/empty	solid/empty	0.1953	14.40

Solidity too low
Need higher f_{max}

Resistivity too low
Need higher σ_{max}

Results for Partially Resolved particles with parameters for Unresolved particles



Quick parameter fitting

Resolution 4 µm

1. Use result of resolved model
2. Use other values

Input parameters		Resulting cake	
f_{max}	σ_{max} [10^6 kg / m³s]	Solidity	Flow resistivity [10^6 kg / m³s]
0.1953	14.40	0.1422	4.02
0.4000	200.00	0.2505	50.00

Quick parameter fitting

Resolution 4 µm

1. Use result of resolved model
3. Assume linear dependency
   - solidity from f_{max}
   - resistivity from σ_{max}
2. Use other values

Input parameters		Resulting cake	
f_{max}	σ_{max} [10^6 kg / m³s]	Solidity	Flow resistivity [10^6 kg / m³s]
0.1953	14.40	0.1422	4.02
0.2956	56.34	0.1904	13.50
0.4000	200.00	0.2505	50.00

Results for mixed resolutions with fitted parameters

Resolution	Input parameters		Resulting cake	
	f_{max}	σ_{max} [10^6 kg/m³s]	Solidity	Flow resistivity [10^6 kg/m³s]
24 µm	0.1953	14.4	0.2027	14.3
8 µm	0.1953	20.19	0.1967	14.4
4 µm	0.2956	56.34	0.1904	13.5
2 µm	0.4600	170.00	0.1949	13.8
1 µm	0.5000	441.50	0.1928	15.2
0.5 µm	solid/empty	solid/empty	0.1953	14.4

Summary of previous work

- Solidity and flow resistivity of a filter cake can be modeled by
  - Simulating one cake filtration with fully resolved particles
  - Simulating two cake filtrations with partly resolved particles
  - Parameter fitting

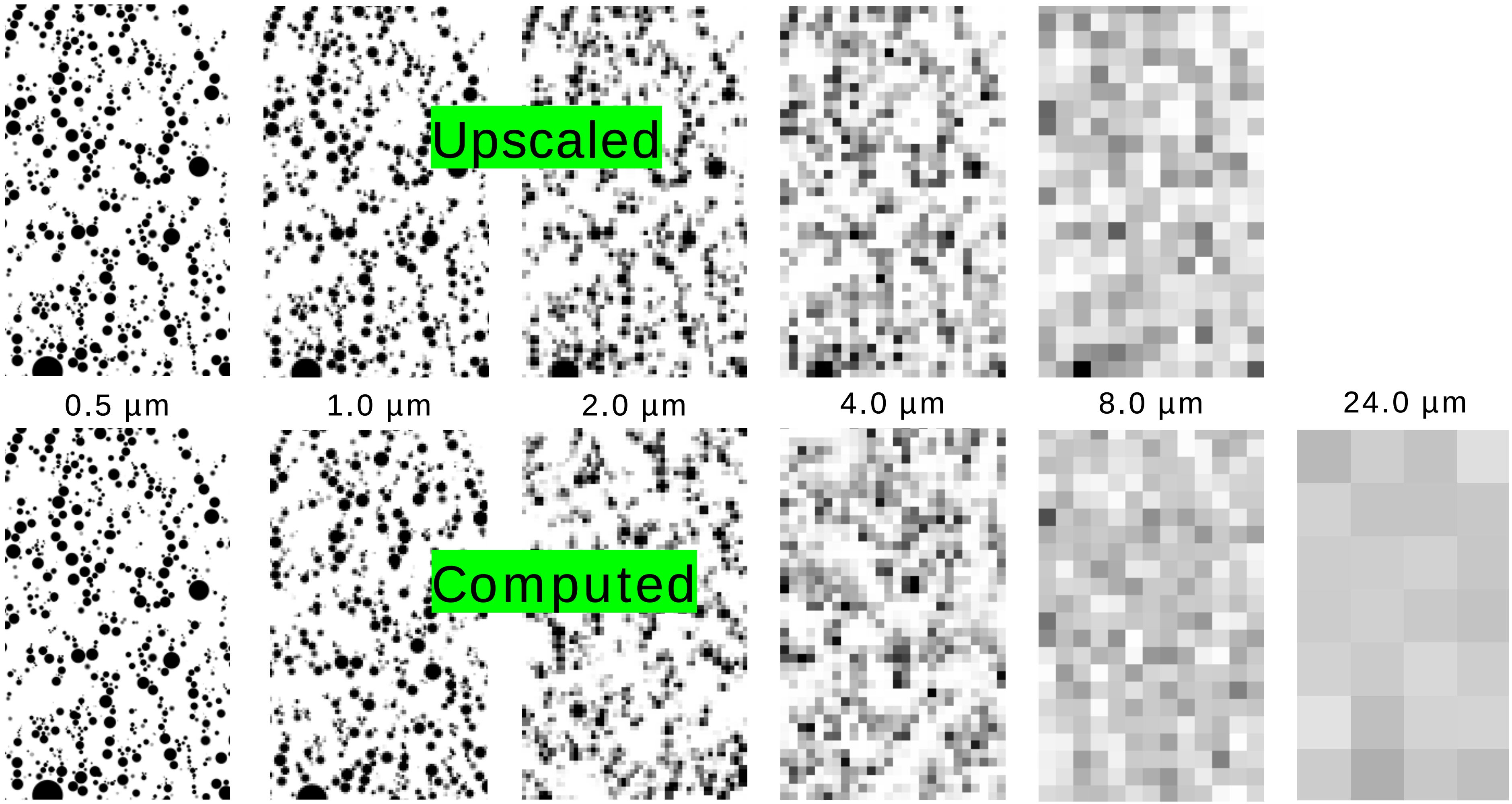
Questions:

- Do *local solidity* and *local flow resistivity* distributions match for resolved and mixed resolution computations?

- Can we estimate f_{max} and σ_{max} from just a single resolved cake filtration simulation?
  - Reduce estimation effort from three to one simulation
  - Develop a theory or provide a data base with effective parameters depending on particle size distribution and grid resolutions

- A methodology to measure *local solidity* and *local flow resistivity* on square blocks of 1×1×1, 2×2×2, 4×4×4 cells with the finest resolution results (0.5µm)
  - 1×1×1 -> 0.5µm
  - 2×2×2 -> 1.0µm
  - 4×4×4 -> 2.0µm
  - …

Comparison: Computations with Resolved particles vs. Partially Resolved particles and up to Unresolved particles



Top: SVF from computations with resolved particles upscaled by post-processing

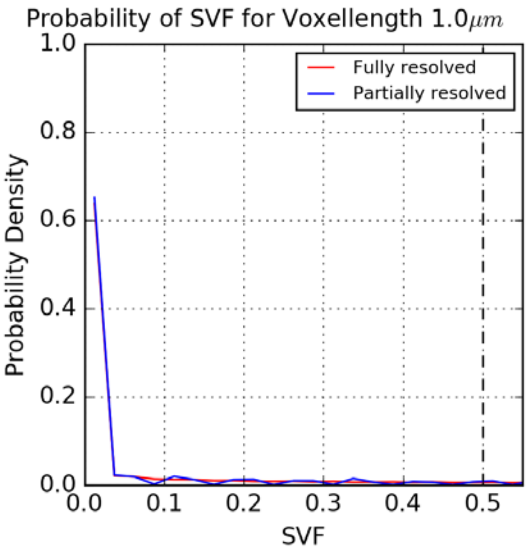
Bottom: SVF from computations with fit-parameters on partially resolved and unresolved particles

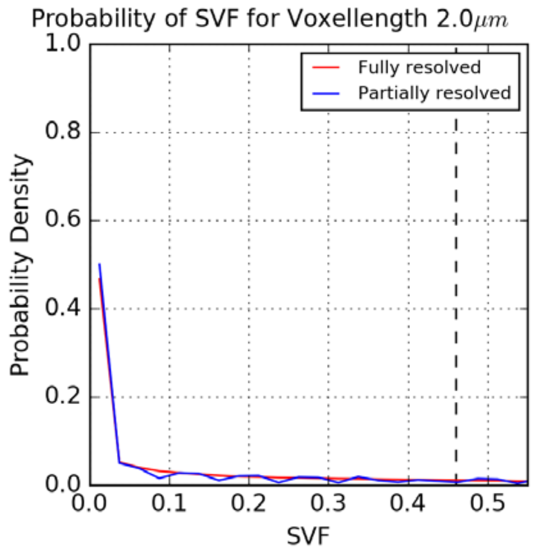
SVF=0 (empty)

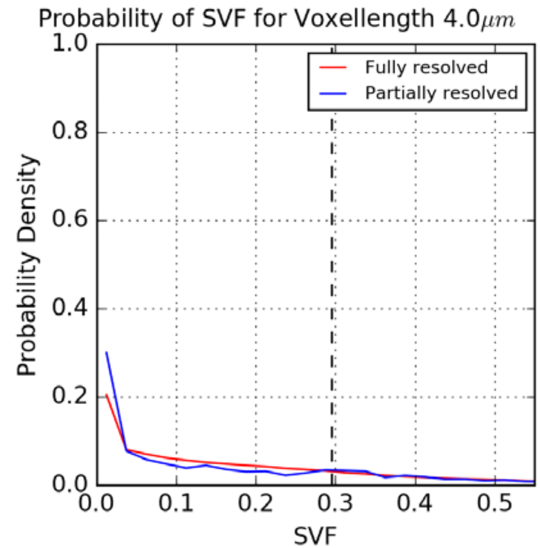
0<SVF<1 (porous)

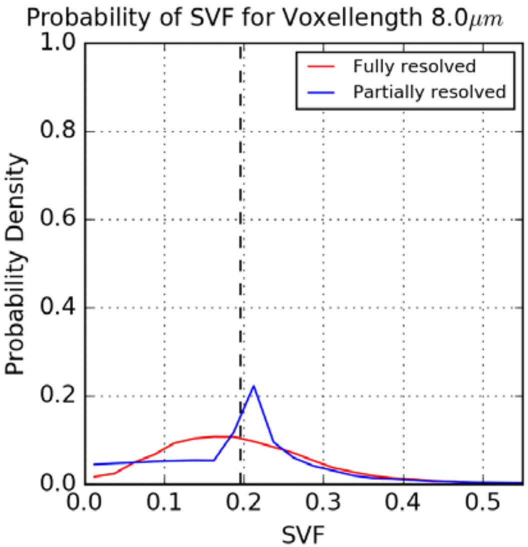
SVF=1 (solid)

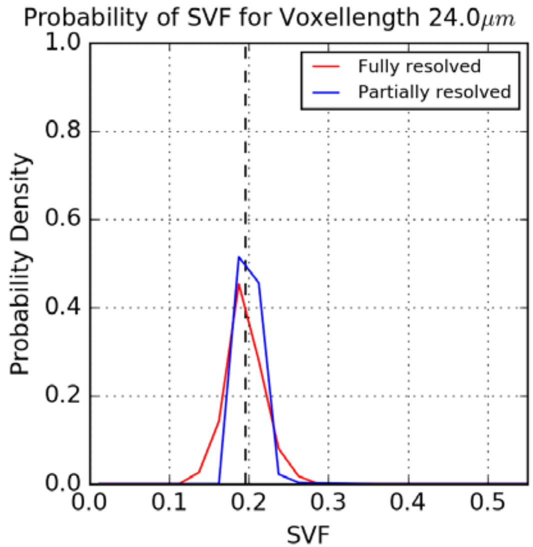
Comparison of SVF probability density





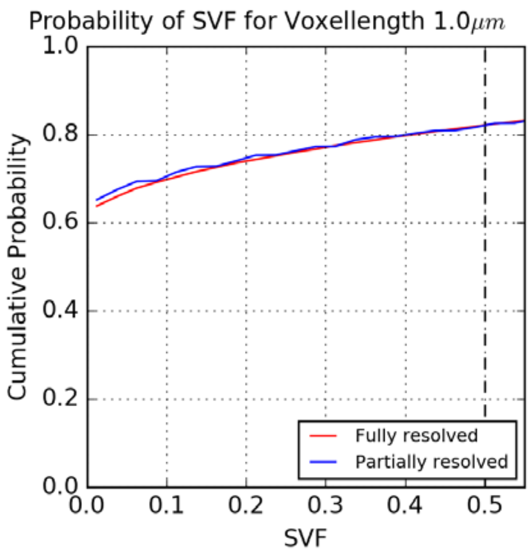


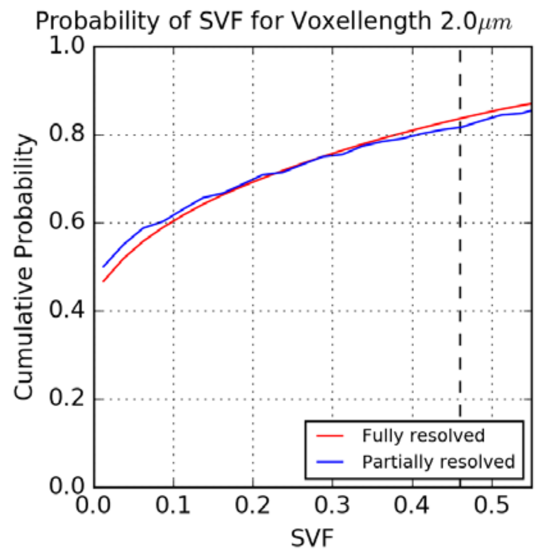


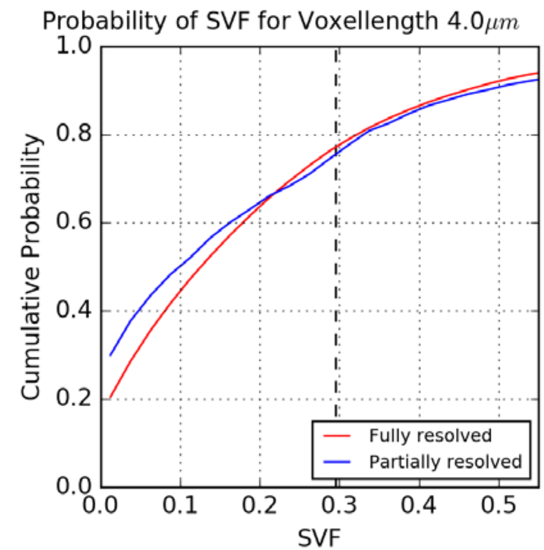


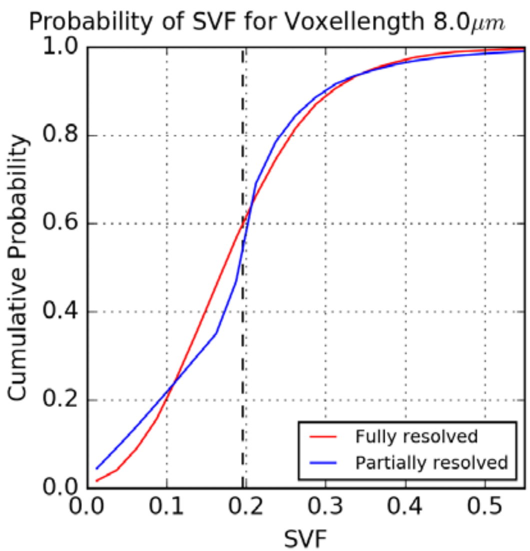
- SVF probability of fully and partially resolved particles match

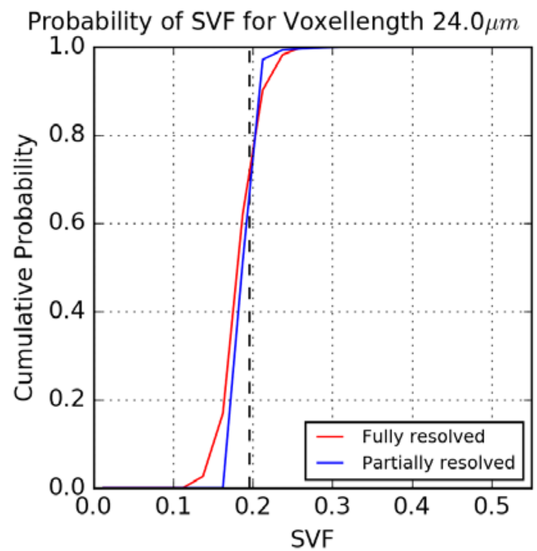
Comparison of SVF cumulative probability











- SVF probability of Fully and Partially Resolved particles match
- Cumulative probability between 60% and 80% at f_{max}

Conclusions and outlook

- Cake formation can be modeled at different resolutions
- Parameters f_{max} and σ_{max} can be estimated by linear fitting
- Local solidity and flow resistivity of Fully Resolved and Partially Resolved computations match

- The σ function for different resolutions can be estimated from Fully Resolved computations

- Open questions:
  - How to estimate f_{max} from one Fully Resolved cake filtration?
  - Can the f_{max}, σ_{max} model be replaced?

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info@math2market.de
www.geodict.com

Software Design:
Dr. Jürgen Becker, Liping Cheng, PhD,
Dr. Erik Glatt, Dr. Sven Linden,
Dr. Christian Wagner, Dr. Rolf Westerteiger,
Nicolas Harttig, Andreas Grießer,
and Andreas Wiegmann, PhD

Art Design:
Steffen Schwichow

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