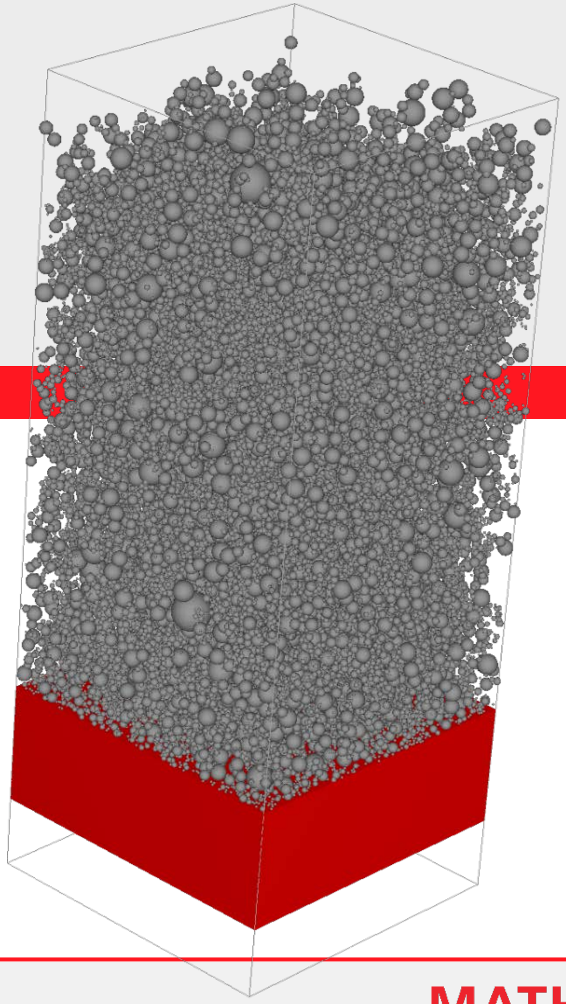
Estimation of Effective Cake Filtration Simulation Parameters from Resolved Filtration Simulations



Interpore 2016

Cincinnati, Ohio

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Liping Cheng

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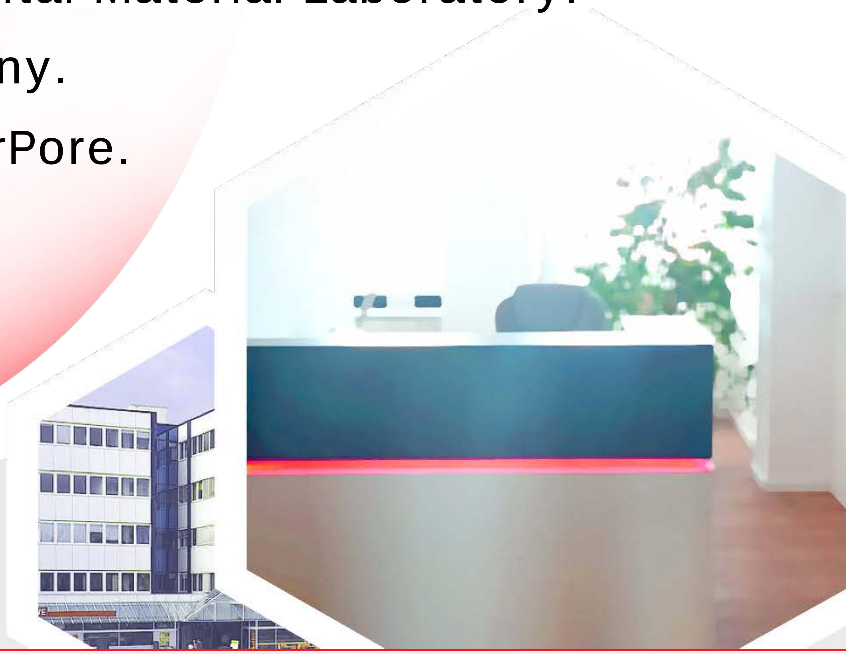
GeoDict

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 is an institutional member of InterPore.
- M2M spun off from Fraunhofer Institute for Industrial Mathematics, a founding institute of InterPore.



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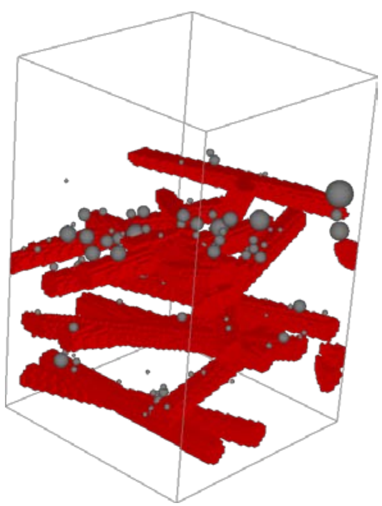
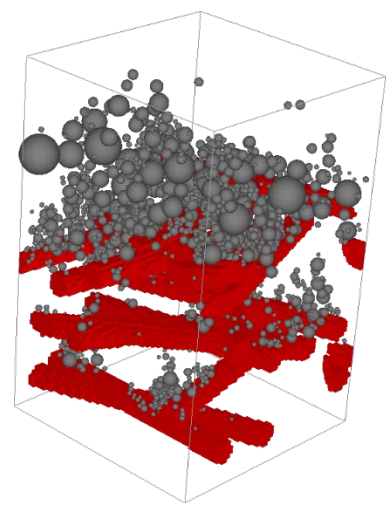
The Regimes of Fluid-Solid Filtration

In fluid-solid filtration processes, solid particles are carried by a fluid (liquid or gas) and trapped inside a filter media or on top of a filter media.

- Trapping *inside* the filter media is called *depth filtration*
- Trapping *on top* of the filter media is called *cake filtration*
  - In cake filtration, the filtration is achieved primarily by previously deposited particles, not so much by the filter media.



Depth Filtration



Cake Filtration

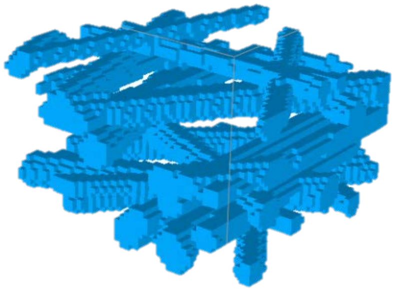
Scale Issue of Cake Filtration Simulation on Uniform 3d Grids

- While the inhomogeneity of the filter media may be on a single scale, poly-disperse particles usually span multiple scales.

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

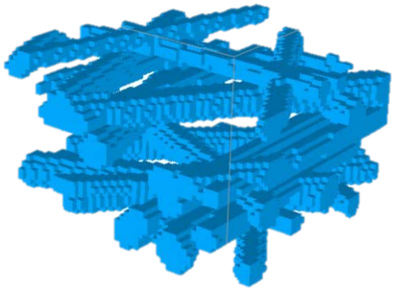
- We describe two procedures by which these parameters can be found.

How Cake Filtration is Simulated



1. Filter Model

How Cake Filtration is Simulated



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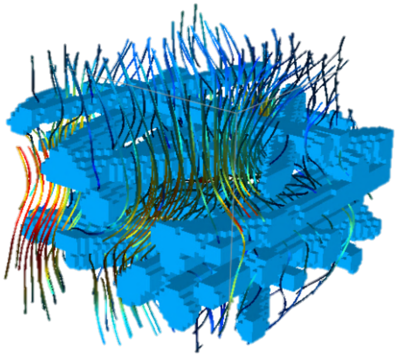
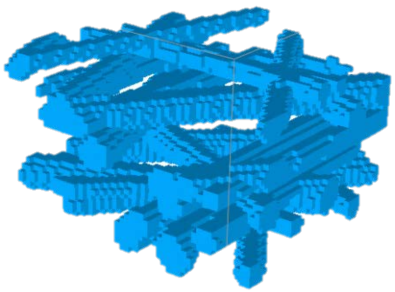


2. Flow Field

How Cake Filtration is Simulated



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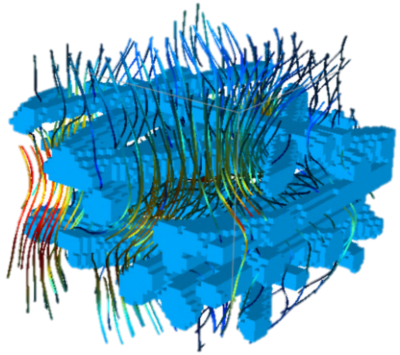

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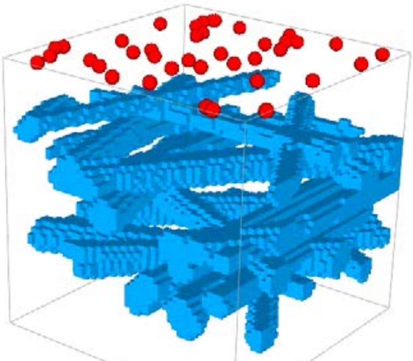
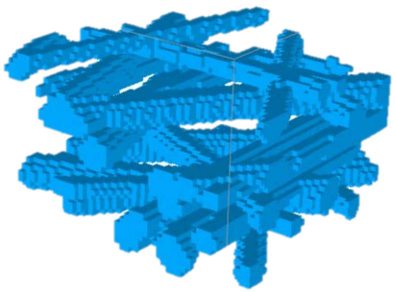


3. Track Particles

How Cake Filtration is Simulated



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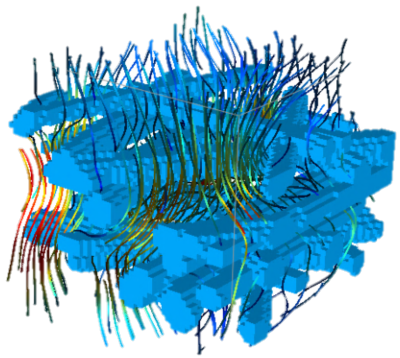

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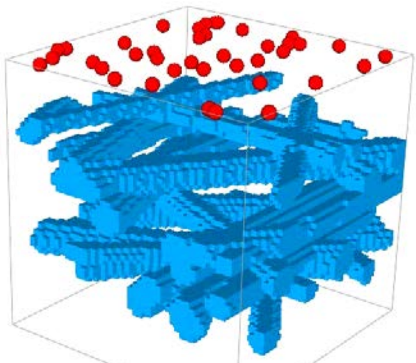

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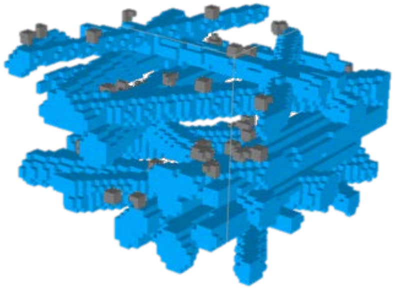
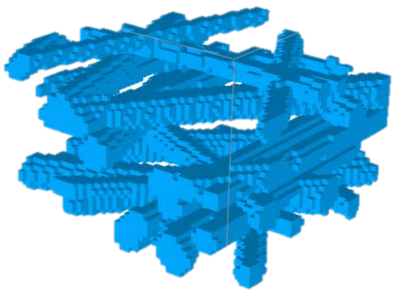


4. Deposit Particles

How Cake Filtration is Simulated



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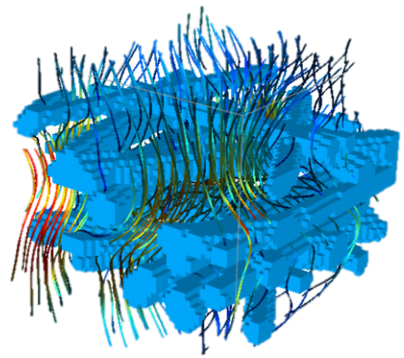

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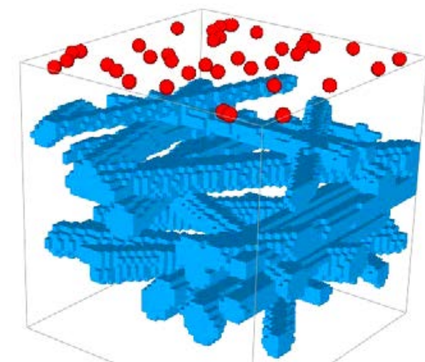

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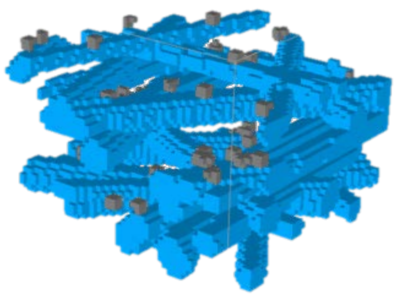

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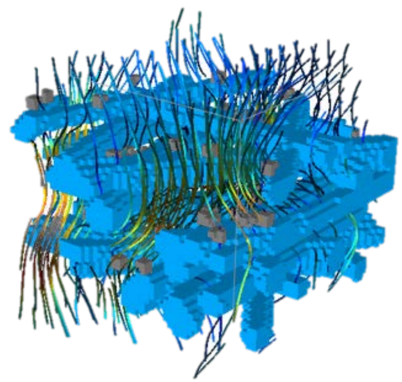
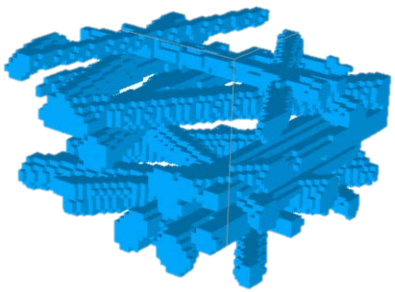


5. Flow Field

How Cake Filtration is Simulated



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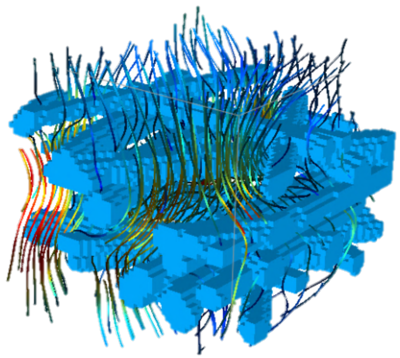

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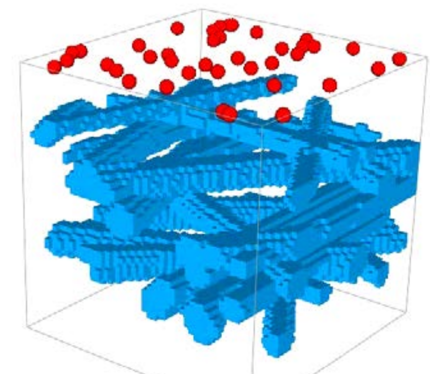

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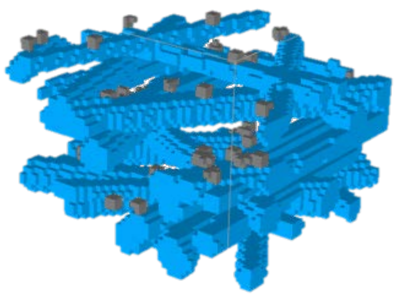

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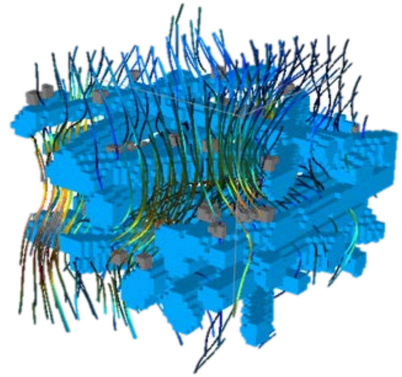

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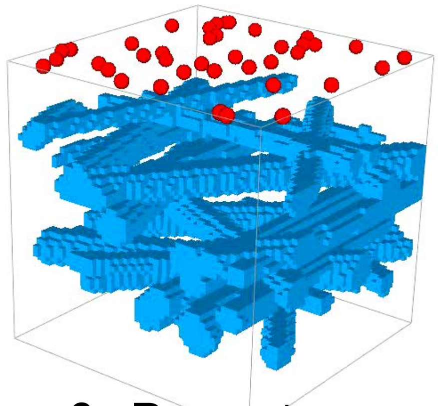
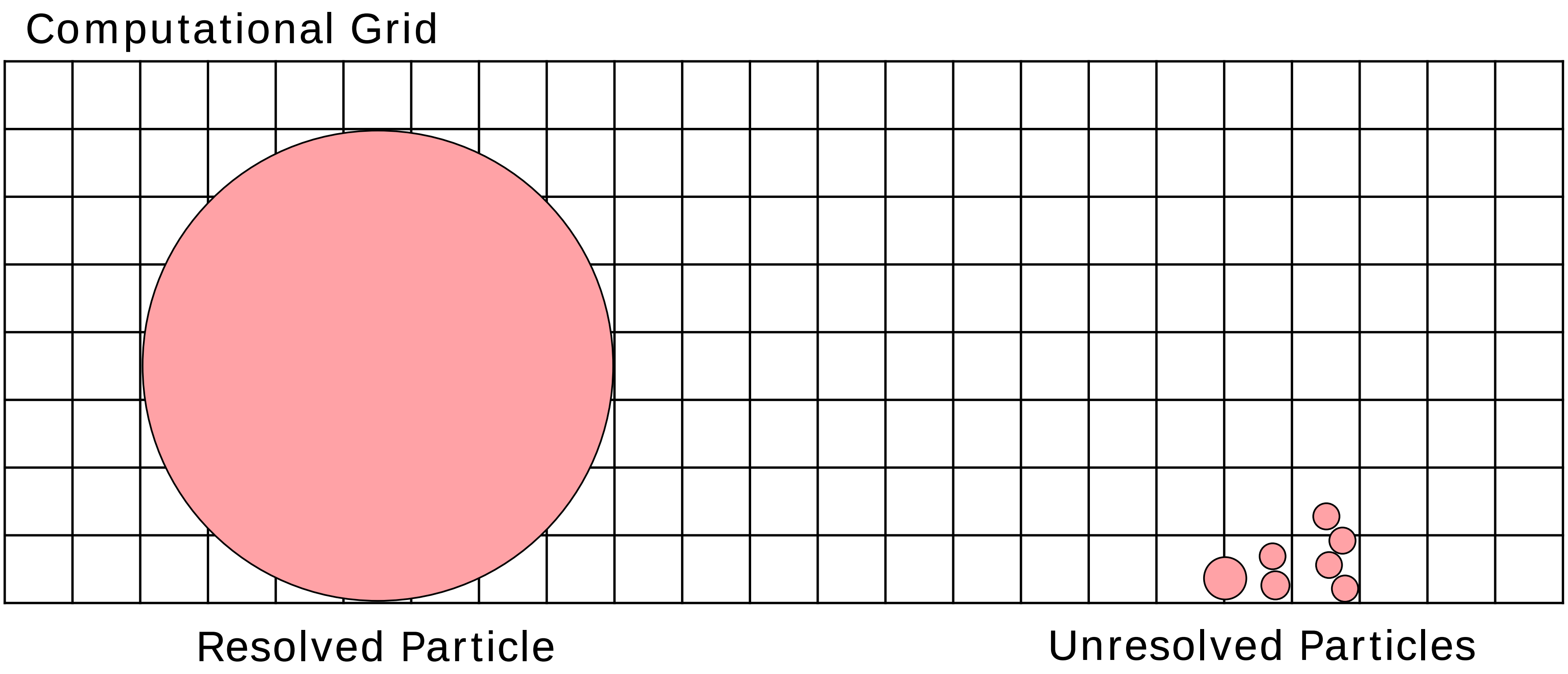


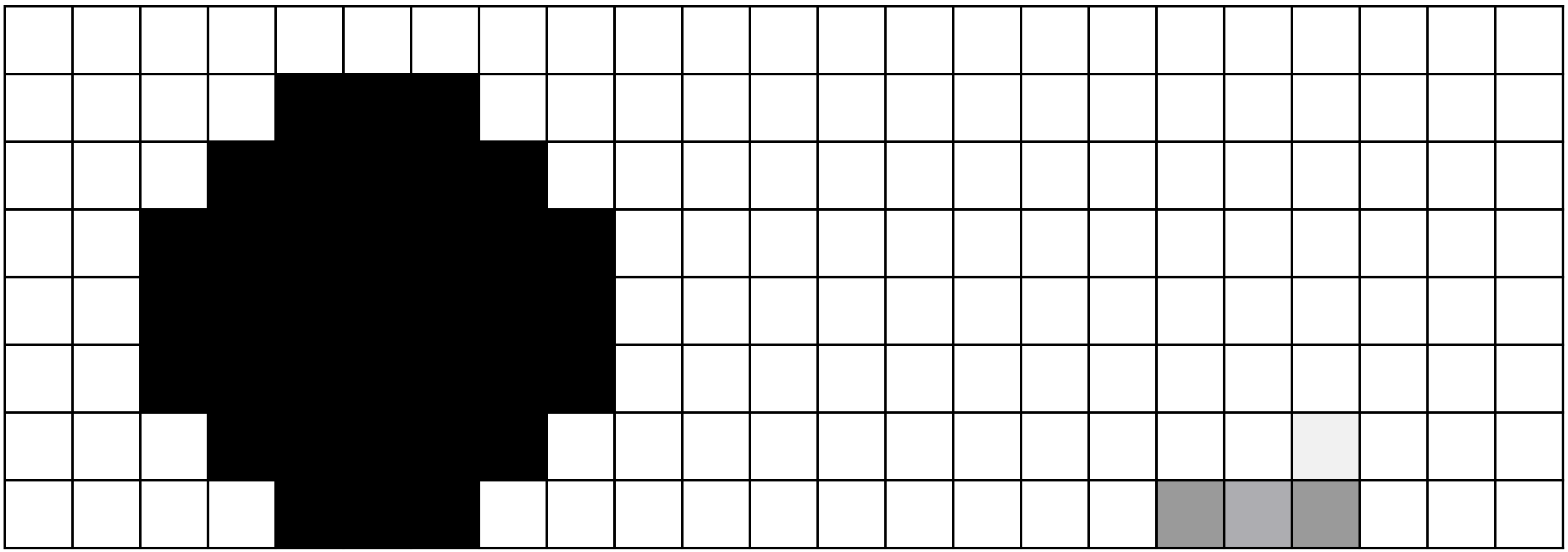
6. Repeat …

Computational Grid, Resolved & Unresolved Particles



Discretization of Resolved and Unresolved Particles

Computational Grid



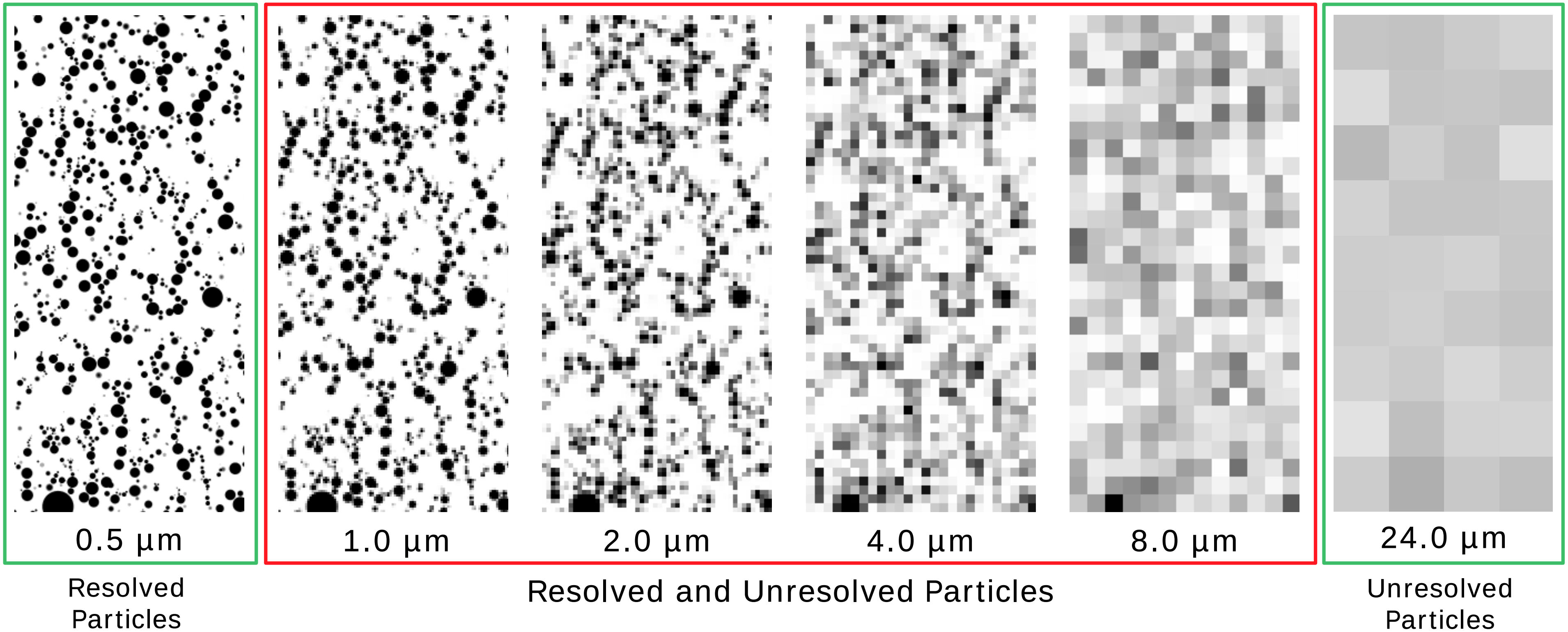
Resolved Particle

Empty/Solid Cells

Unresolved Particles

Porous Cells

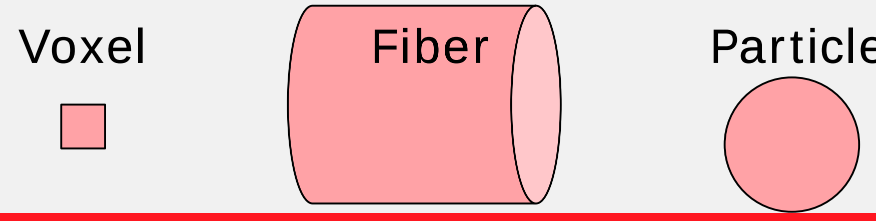
Mixed Resolved & Unresolved Particles for Varying Resolutions



SVF from resolved 3d simulation (voxel length 0.5µm) upscaled by post-processing.

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

Resolved Particles



- Voxels are solid or empty

- Stationary incompressible Navier-Stokes equation

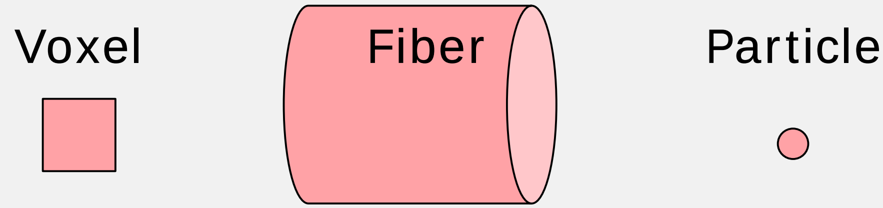
$$-\mu\Delta\vec{u} + \rho(\vec{u}\cdot\nabla)\vec{u} + \nabla p = 0, \qquad \nabla\cdot\vec{u} = 0$$

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)

Unresolved Particles



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

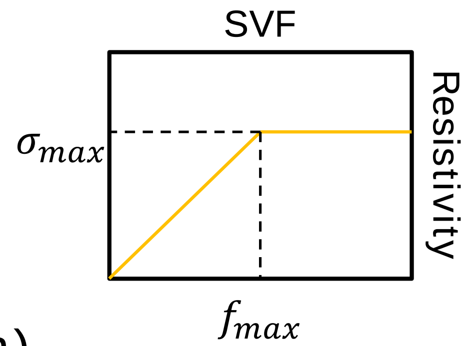
$$-\mu\Delta\vec{u} + \rho(\vec{u}\cdot\nabla)\vec{u} + \frac{\mu}{\kappa}\vec{u} + \nabla p = 0, \qquad \nabla\cdot\vec{u} = 0$$

κ: permeability

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:

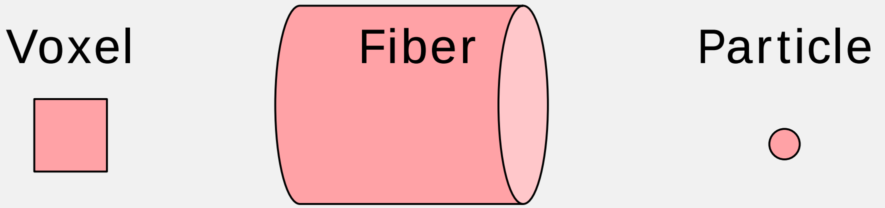
$$\sigma = \frac{\mu}{\kappa} = \begin{cases} \frac{f}{f_{max}}\sigma_{max} & \text{for } 0 < f < f_{max} \\ \sigma_{max} & \text{for } f_{max} \le f \le 1 \end{cases}$$



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

and σ_{max} (maximal flow resistivity)

Unresolved Particles



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

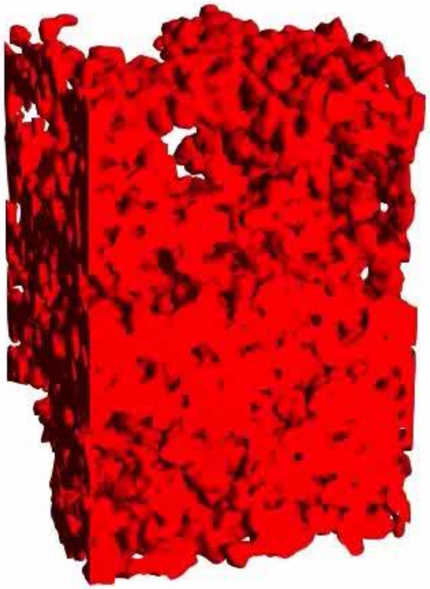
Unresolved Particles

Voxel

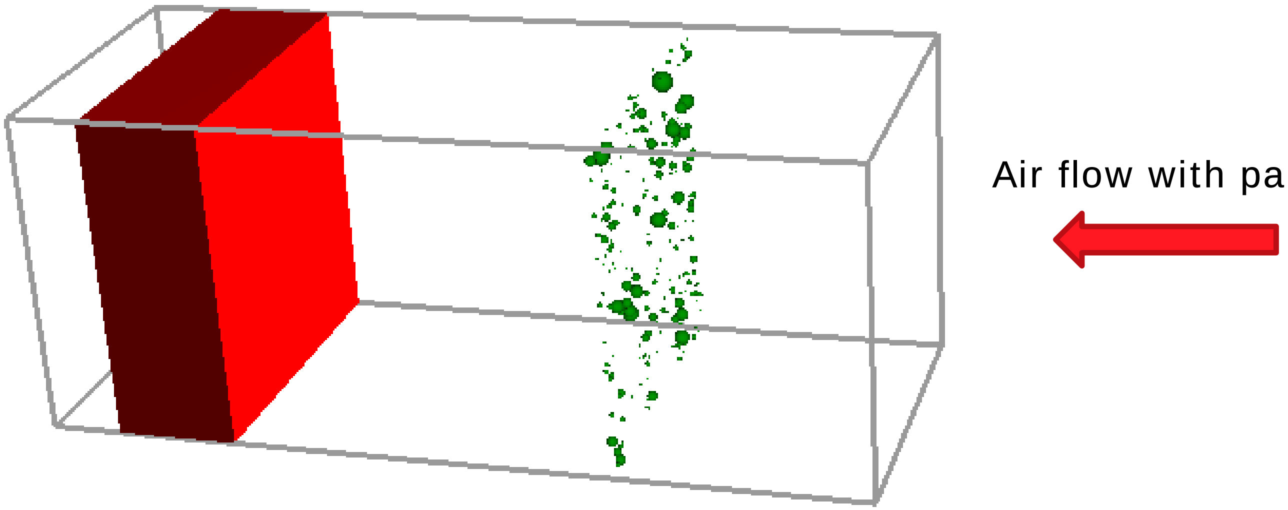
Fiber

Particle

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



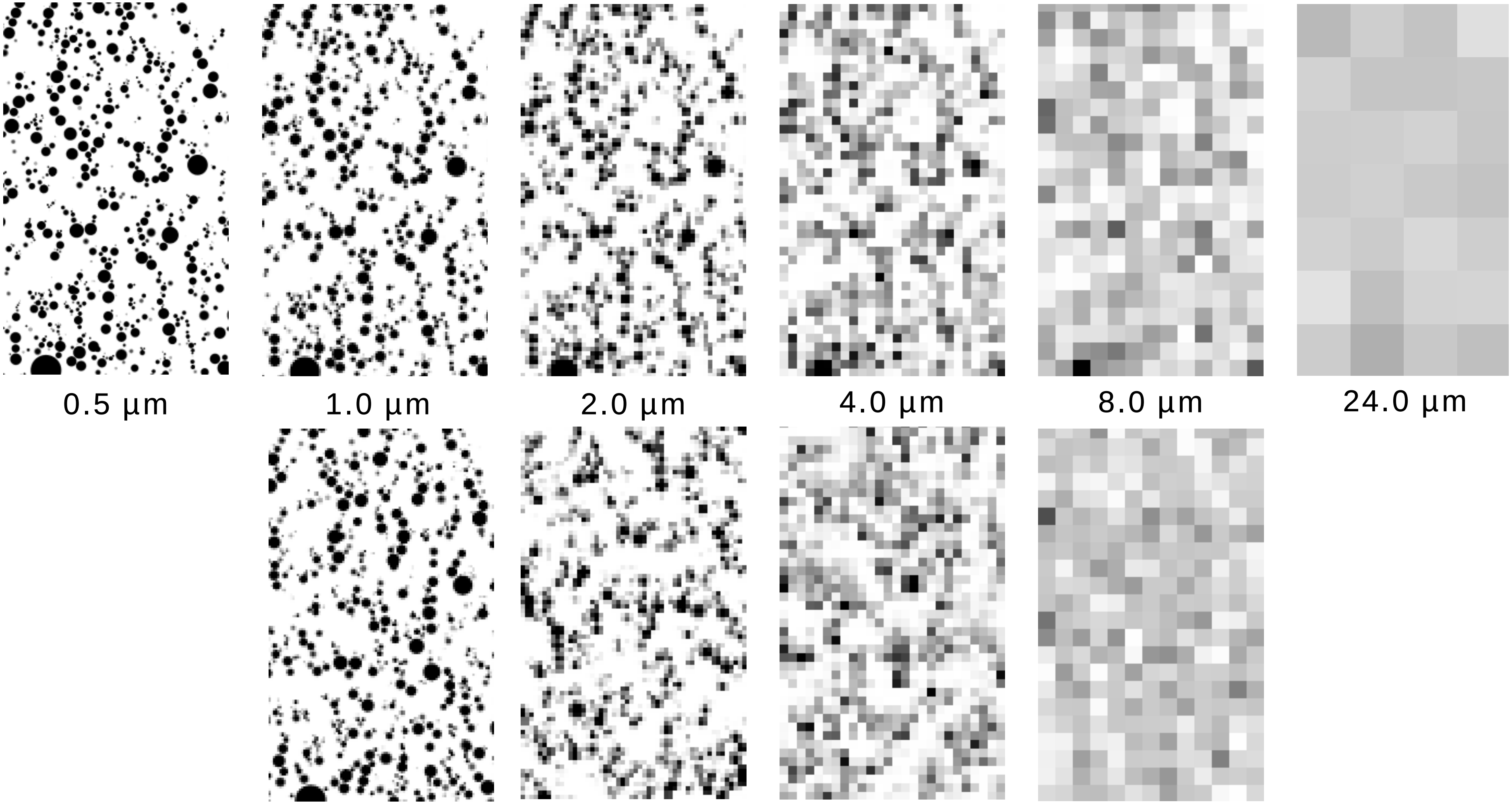
Simulation Setup



- 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

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

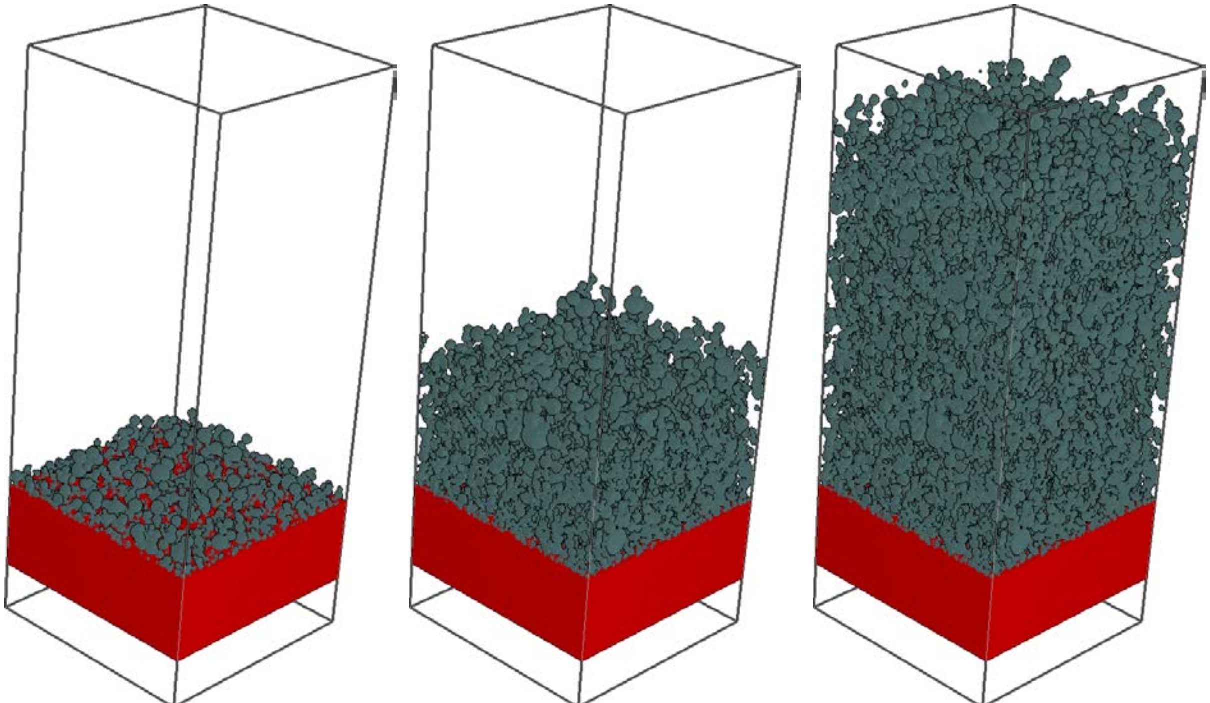
SVF=0 (empty)

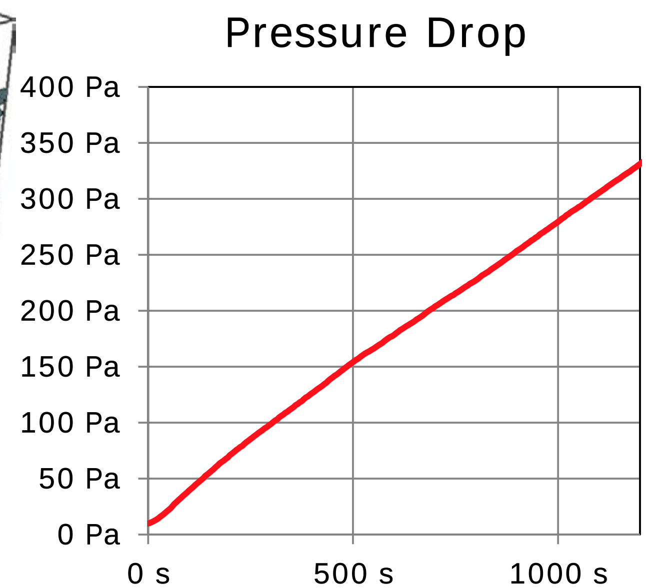
0<SVF<1 (porous)

SVF=1 (solid)

Resolved Particles
Caught On First Touch

Resolution 0.5µm



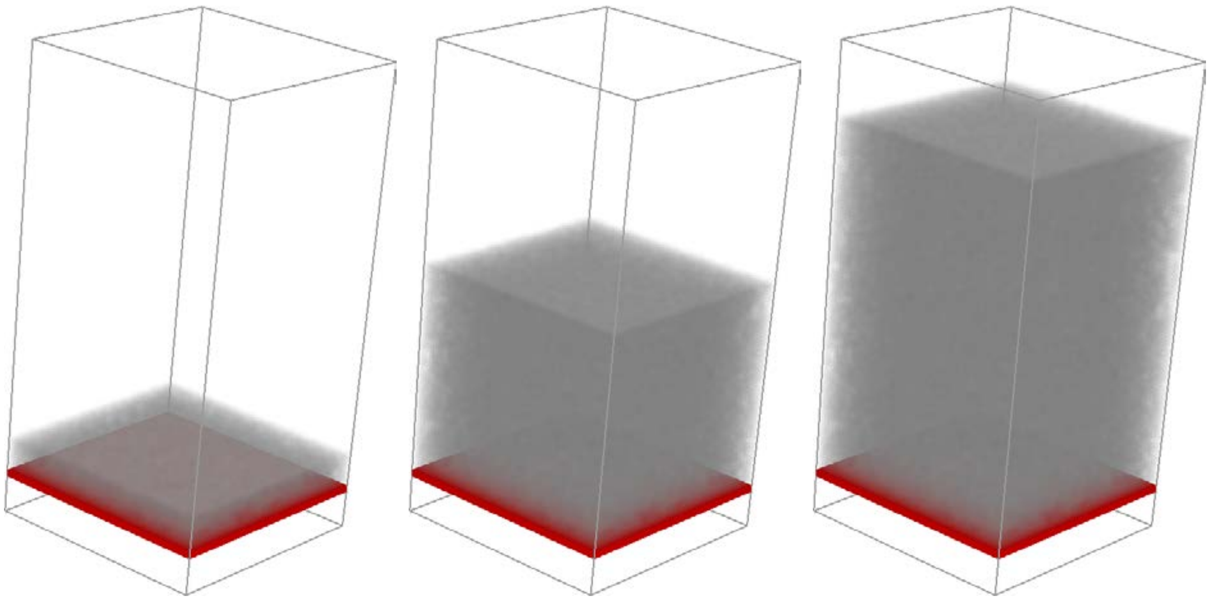


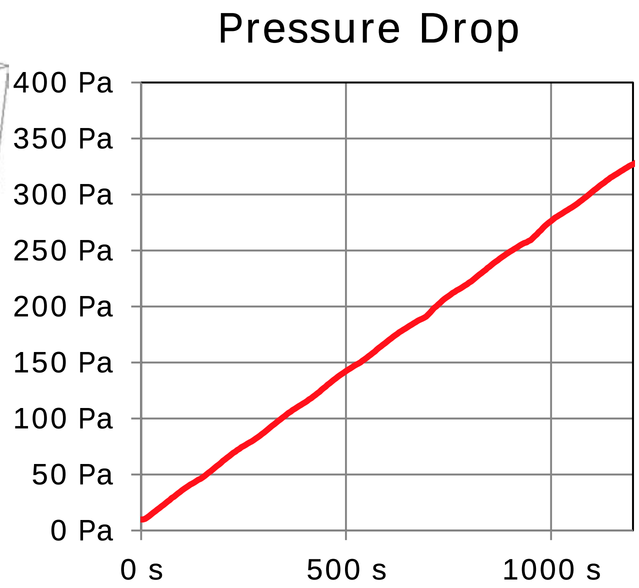
Result:

- 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

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	14.34
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

Results for Partially Resolved Particles with Parameters for Unresolved Particles

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0.5 µm	solid/empty	solid/empty	0.1953	14.40

Solidity too low
Need higher f_{max}

Results for Partially Resolved Particles with Parameters for Unresolved Particles

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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}

Quick Parameter Fitting

Resolution 4 µm

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

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
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

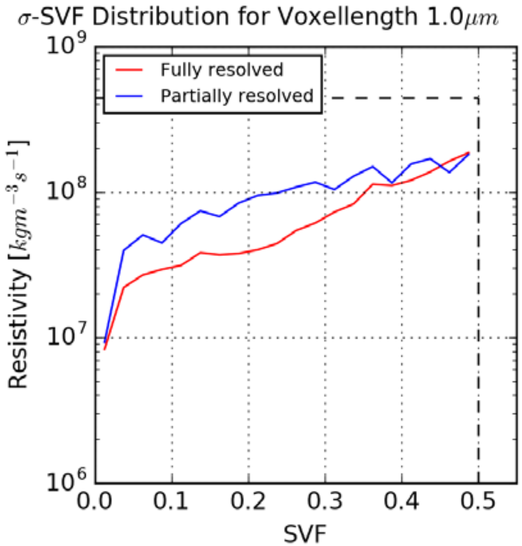
Resolution	Input Parameters		Resulting Cake	
	f_{max}	σ_{max} [10^6 kg/m³s]	Solidity	Flow Resistivity [10^6 kg/m³s]
24 µm	0.1953	14.4	0.2027	14.3
8 µm	0.1953	20.19	0.1967	14.4
4 µm	0.2956	56.34	0.1904	13.5
2 µm	0.4600	170.00	0.1949	13.8
1 µm	0.5000	441.50	0.1928	15.2
0.5 µm	solid/empty	solid/empty	0.1953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

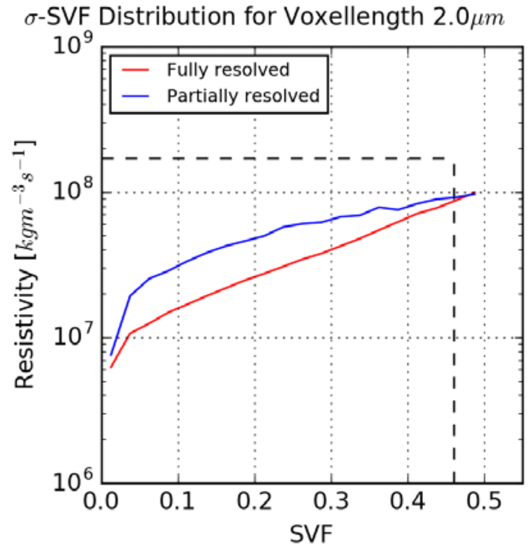
Questions:

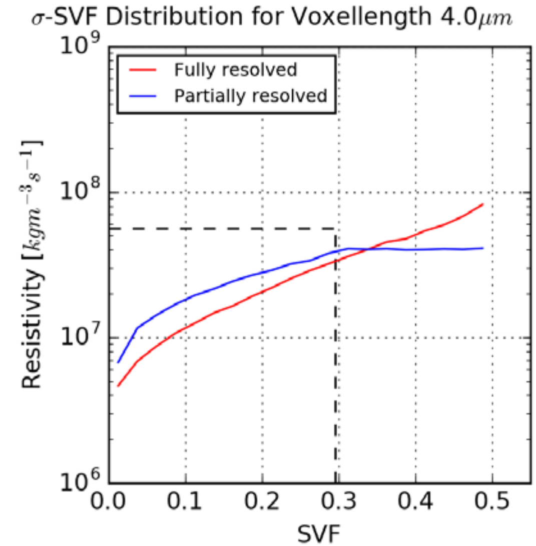
- Do *local solidity* and *local flow resistivity* distributions match for resolved and mixed resolution computations?

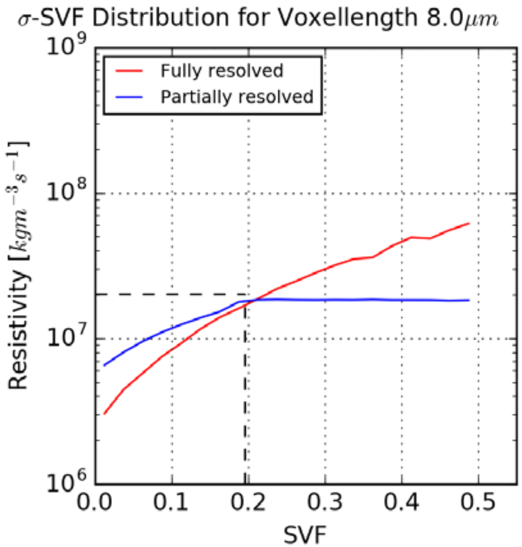
- Can we estimate f_{max} and σ_{max} from just a single resolved cake filtration simulation?
  - Reduce estimation effort from three to one simulation
  - Develop a theory or provide a data base with effective parameters depending on particle size distribution and grid resolutions

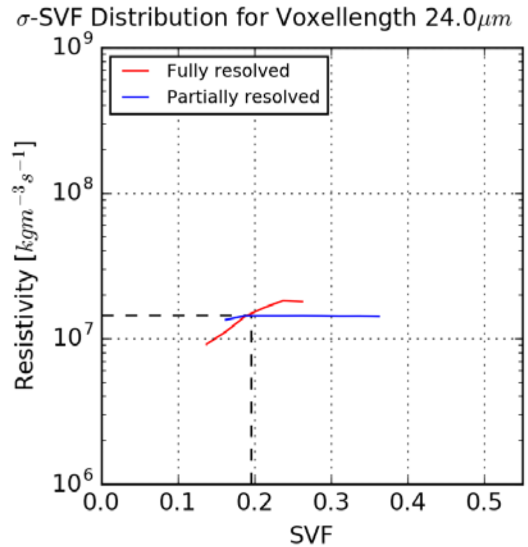
Comparison of σ – SVF Distribution





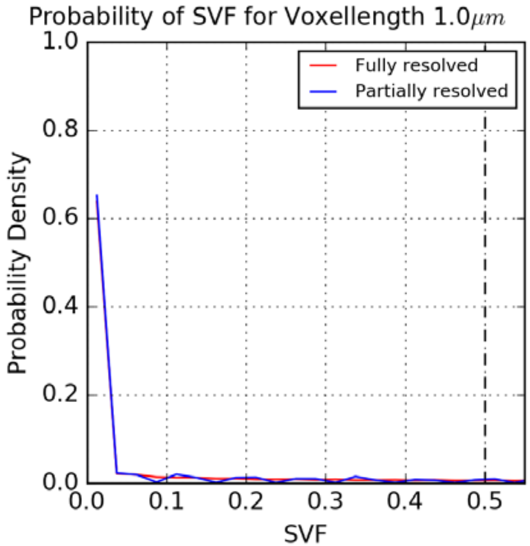


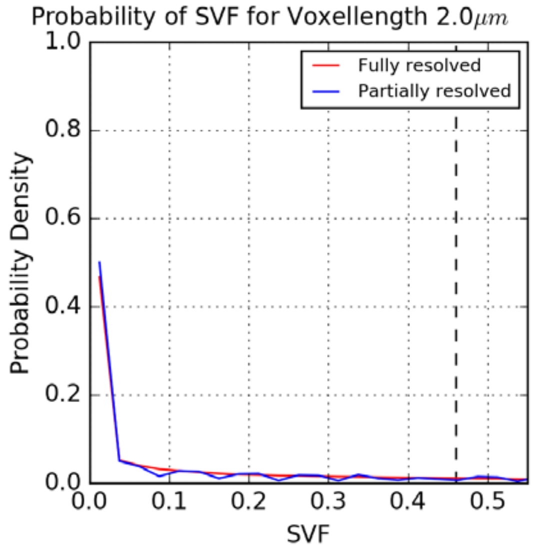


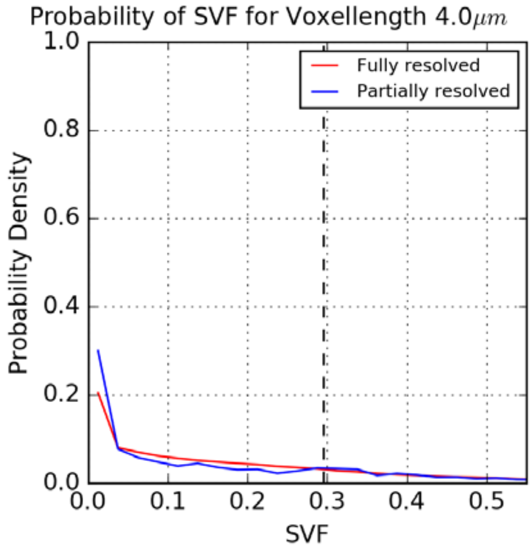


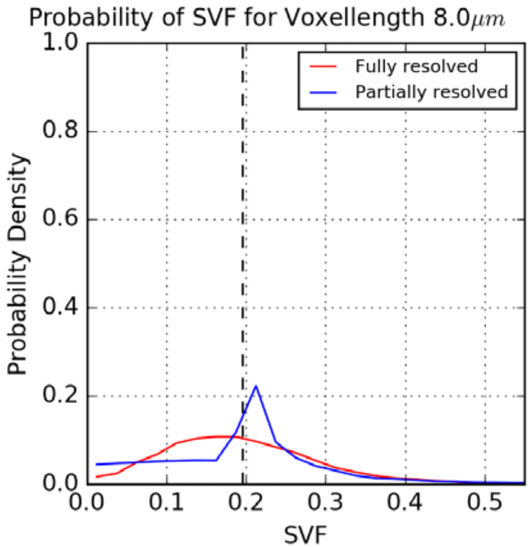
- σ-SVF Distribution of fully and partially resolved particles match
- If f_{max} is known then we can estimate σ_{max}

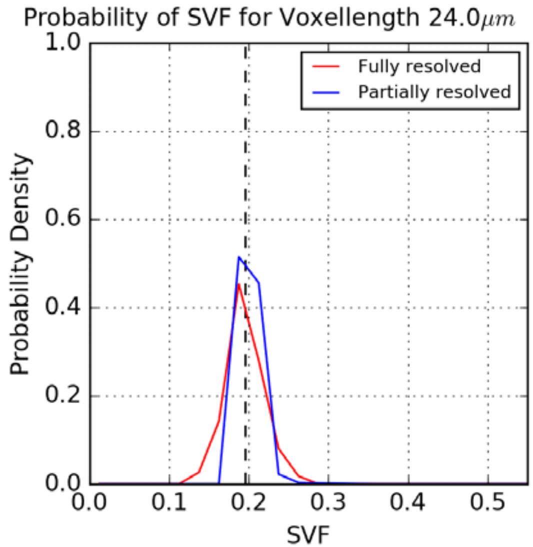
Comparison of SVF Probability Density





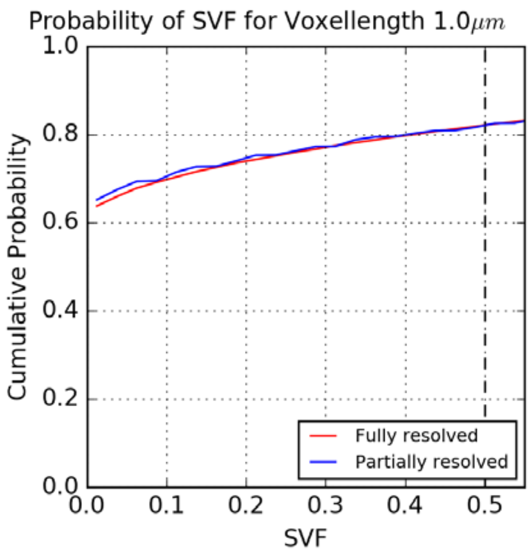


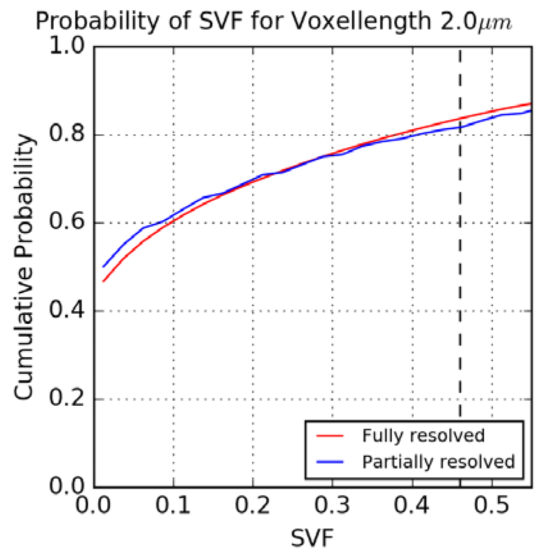


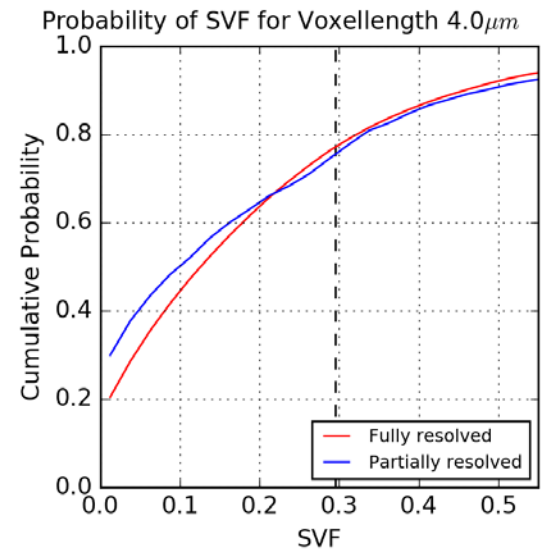


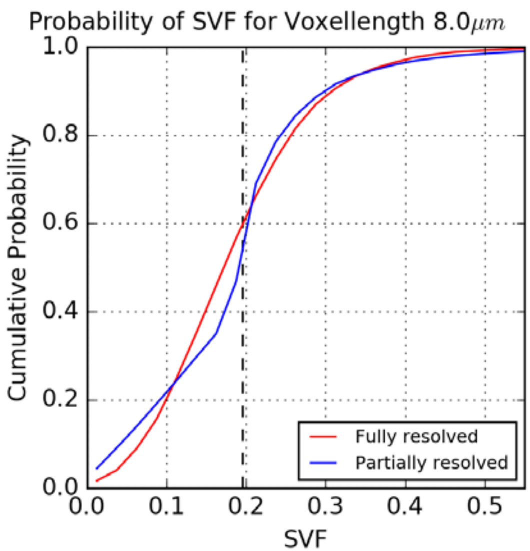
- SVF probability of fully and partially resolved particles match

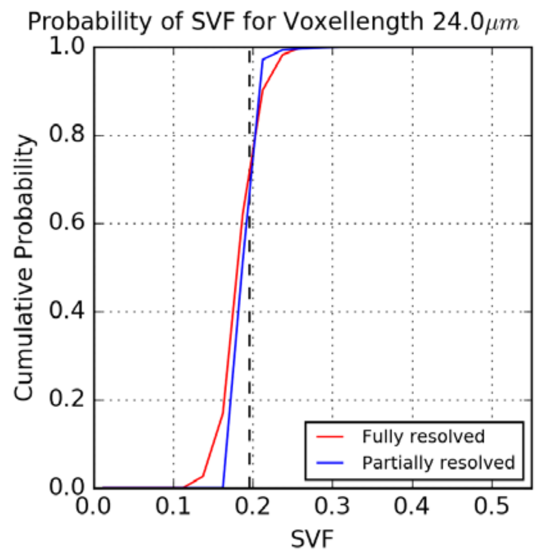
Comparison of SVF Cumulative Probability











- 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 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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