Continuing Development of Micro-Scale Simulation Methods for DPFs

Mark Stewart

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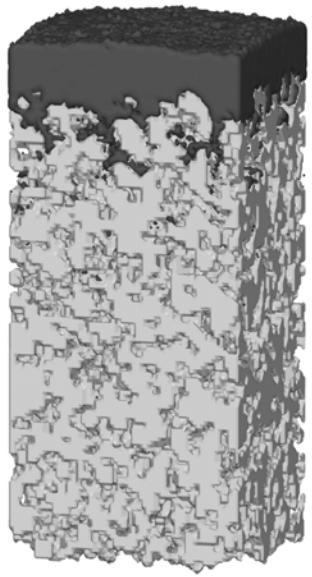
Strategies for improved DPF systems

- Better estimates of DPF state
  - Real-time measurement
  - Estimation via simple models
  - Systems that promote extensive and reproducible regeneration
- Improved filter materials
  - Lower average back-pressure
  - Better ash storage
  - Enhanced regeneration with lower energy requirements

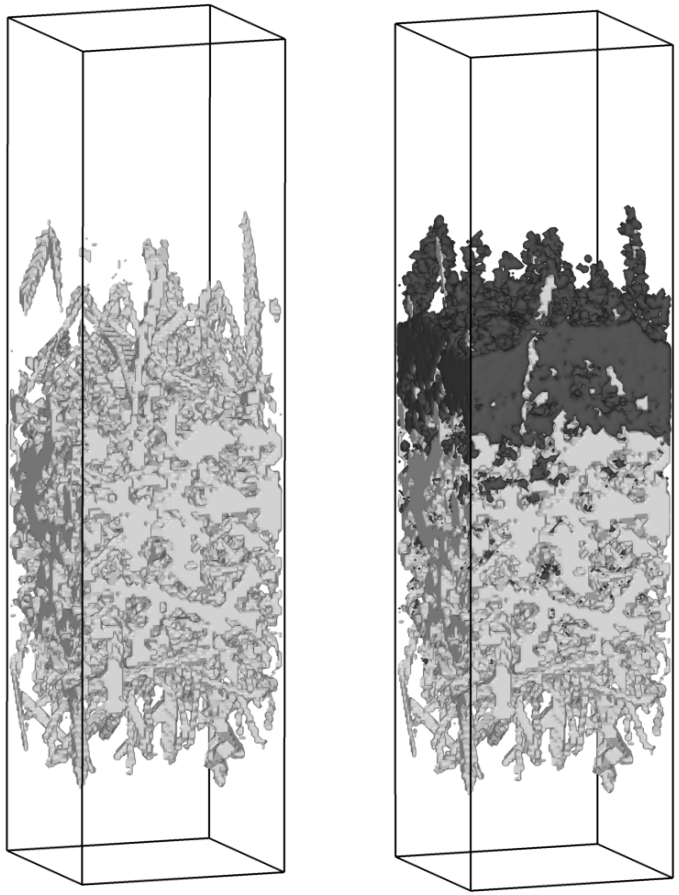


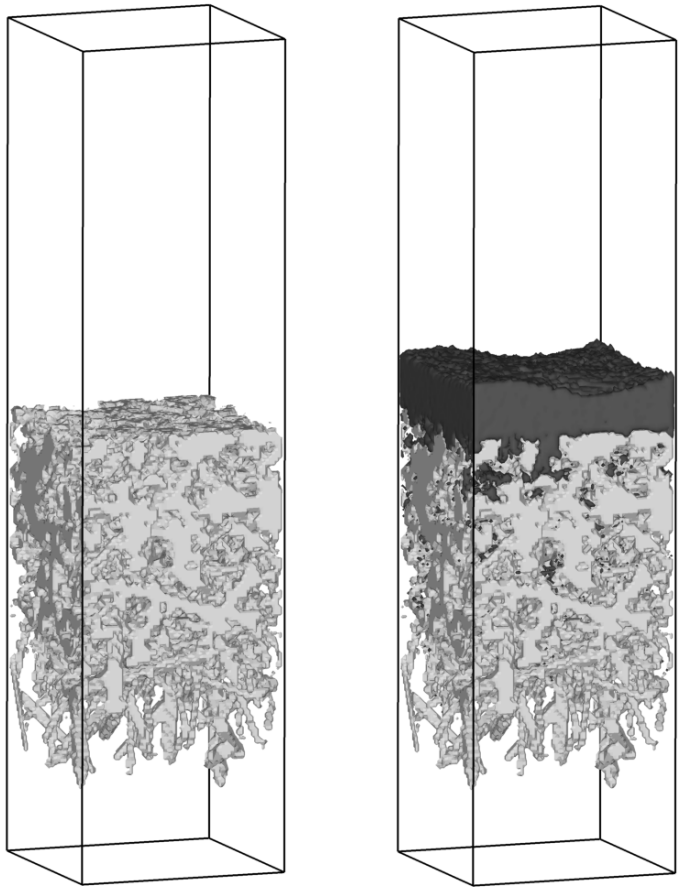
Address through better understanding of pore-scale mechanisms

Example application: analysis of filtration mechanism in Dow Automotive ACM filters

Baseline

Surface Crystals Removed





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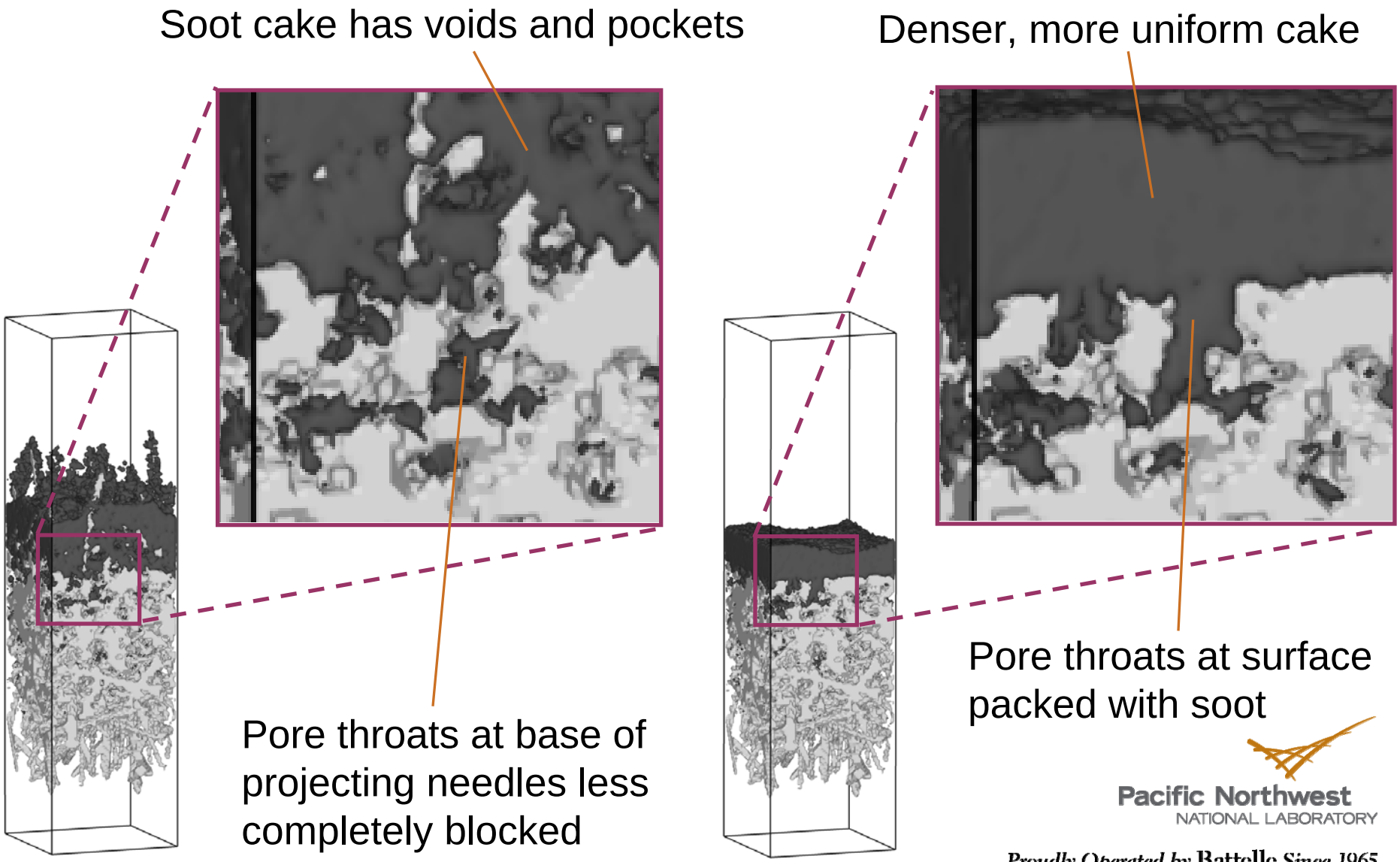
Close-ups of simulated soot deposits with and without projecting needles



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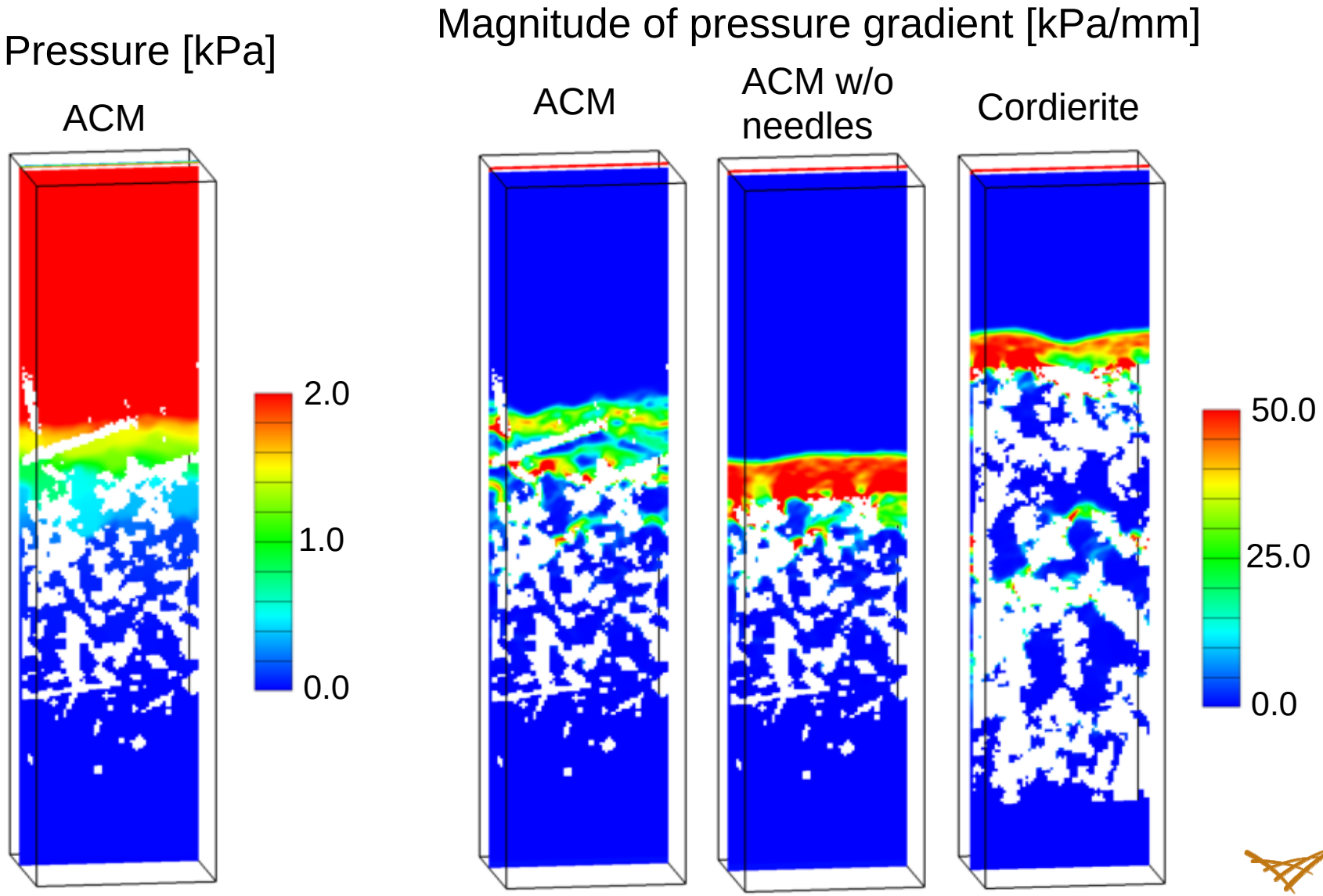
Effect of needles on soot cake consistency



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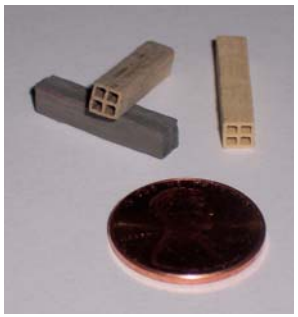
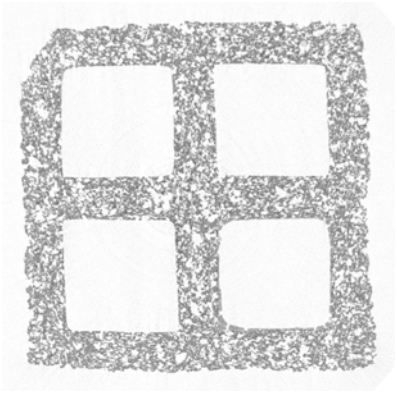
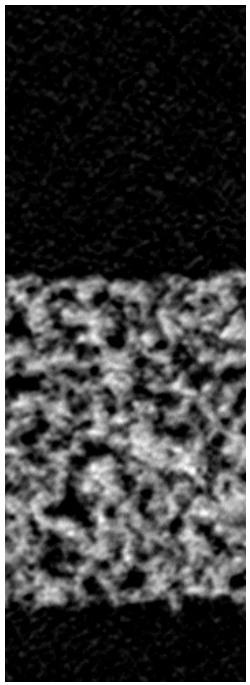
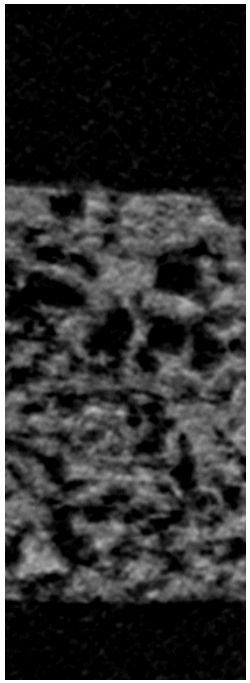
Toward more faithful reconstructions of filter microstructure: micro X-Ray CT scans







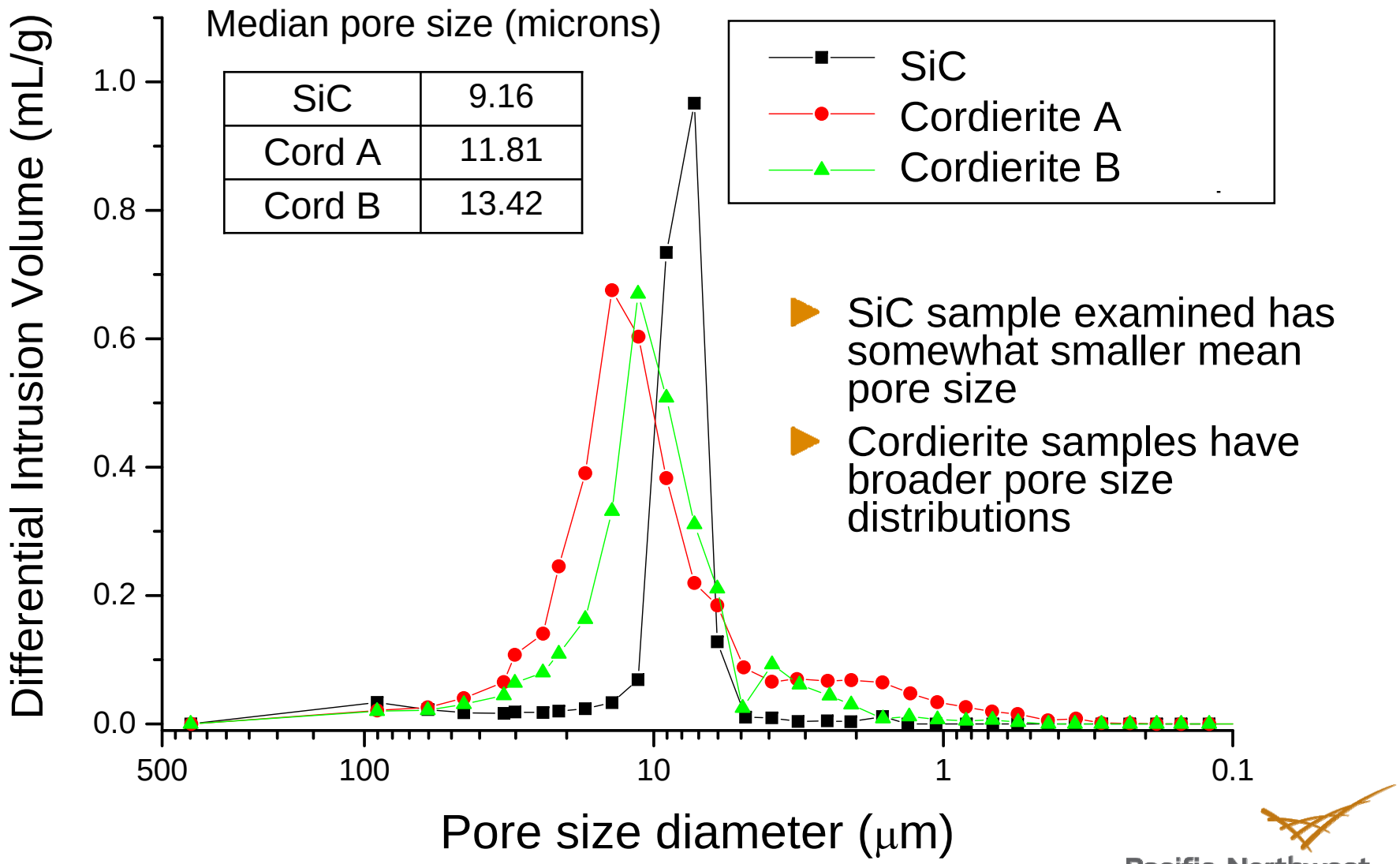
SiC



Cordierite

- Several samples scanned
- Thousands of images per sample
- 1.6 micron resolution
- Higher resolutions are possible for smaller volumes
- Quick method to obtain relatively detailed 3D microstructures
- Some artifacts may be present
- Grayscale images must be thresholded for conversion to boundary sets

Mercury porosimetry data



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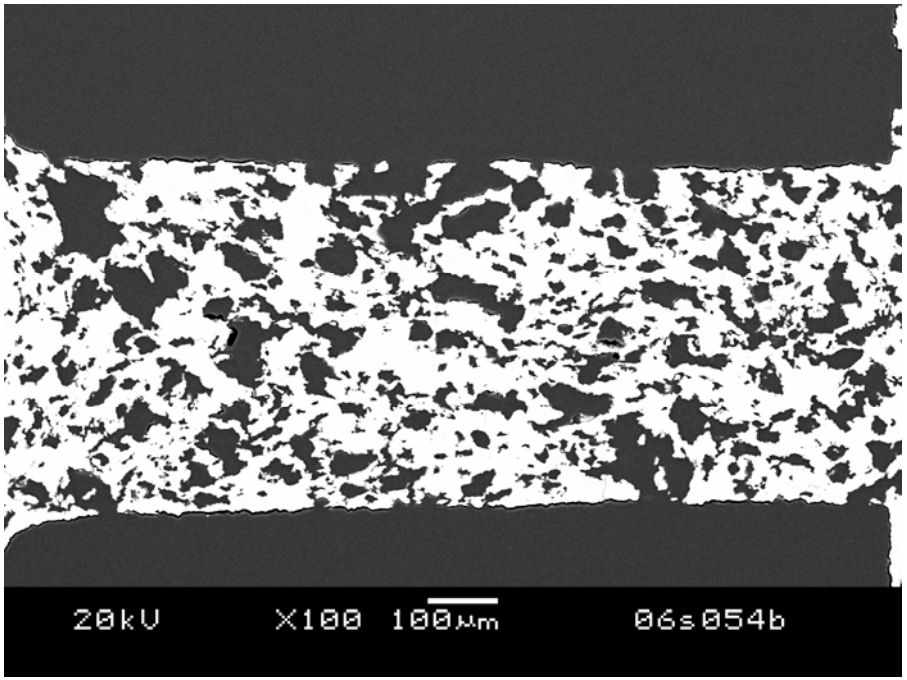
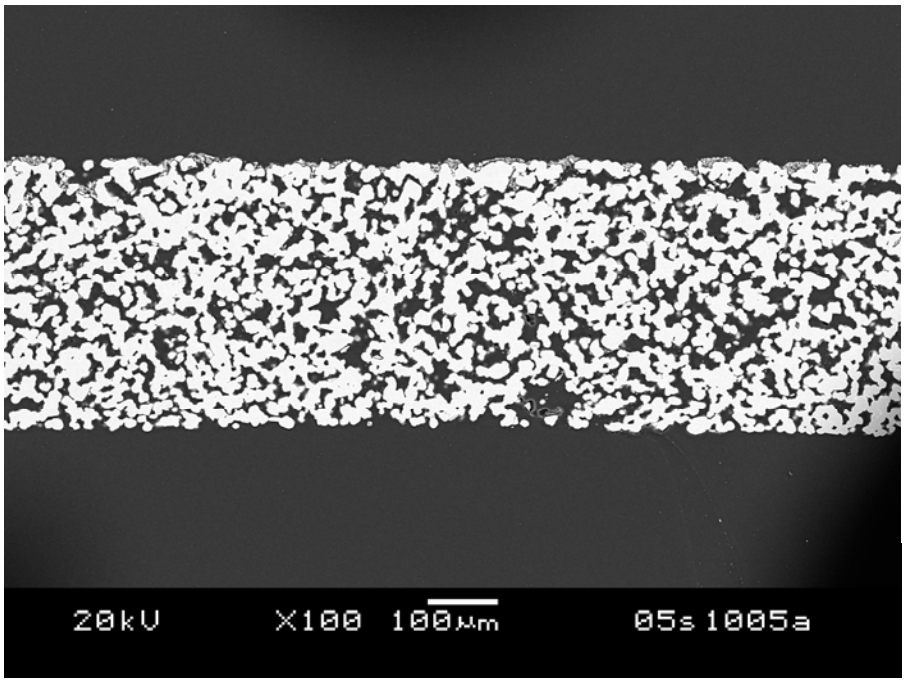
Estimation of properties from 2D SEM images



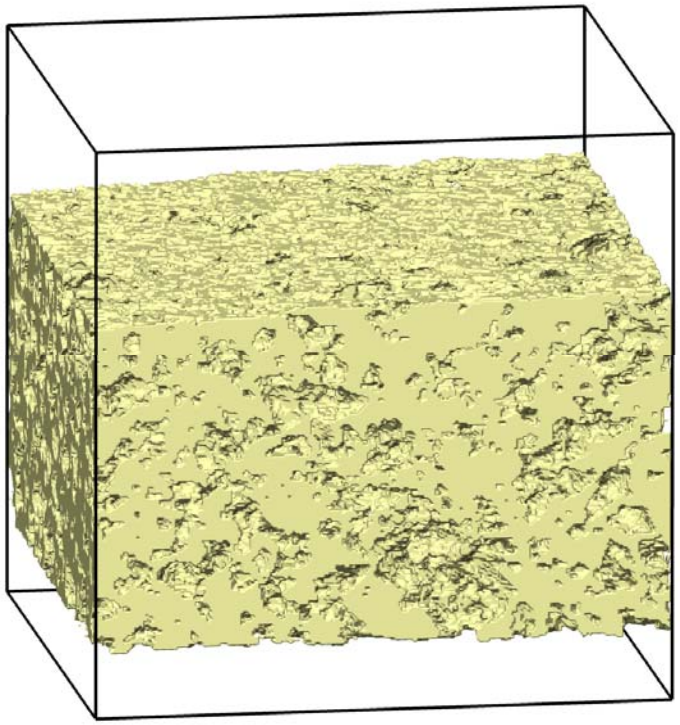
Cordierite

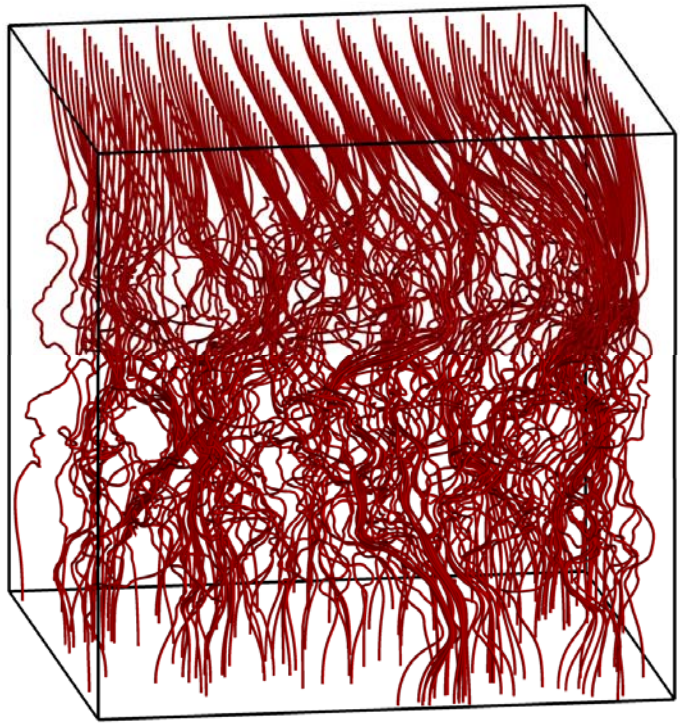


Silicon Carbide

- Higher resolution and better contrast than X-Ray CT
- Difficult to know a-priori how many images are necessary to estimate a property like porosity

3D reconstructions for flow and filtration simulations

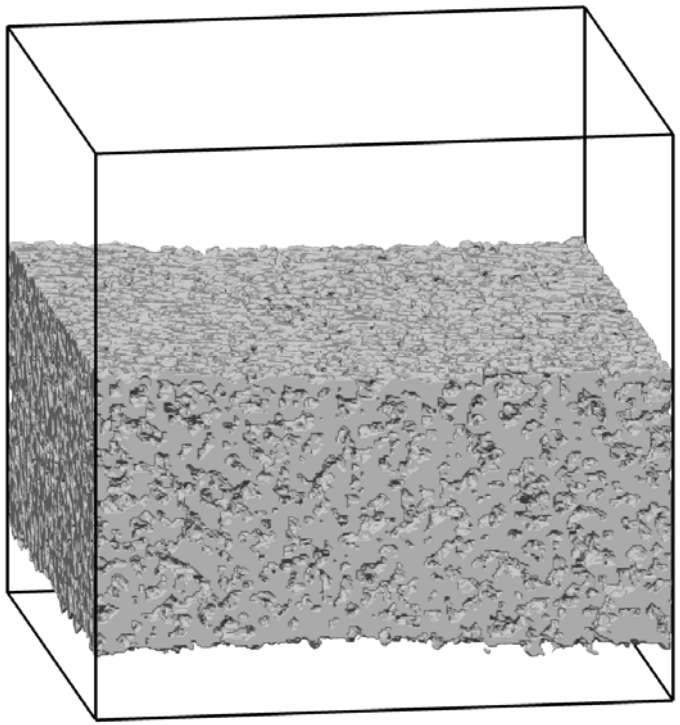


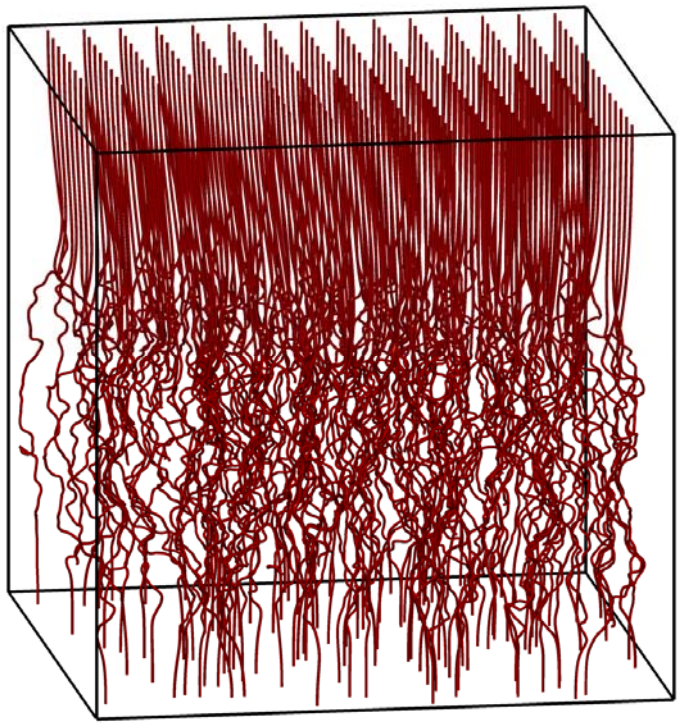


Cordierite reconstruction

Thresholded for wall porosity of roughly 0.39

3D reconstructions for flow and filtration simulations

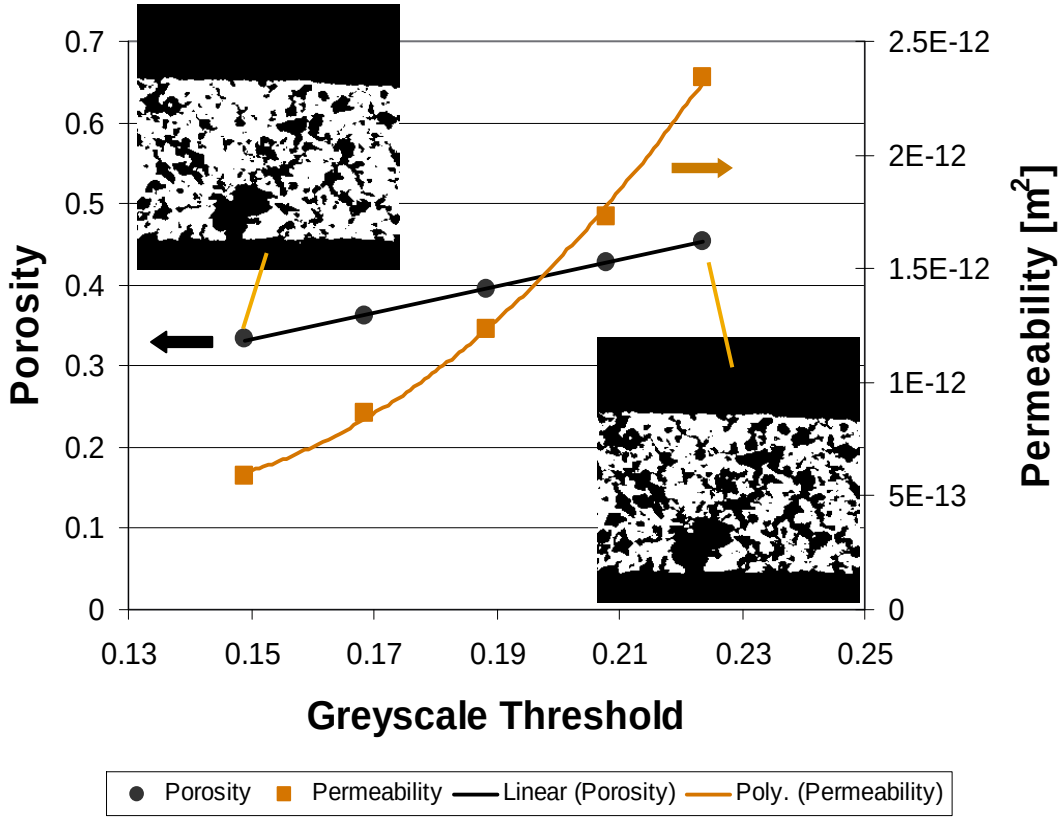




Silicon carbide reconstruction

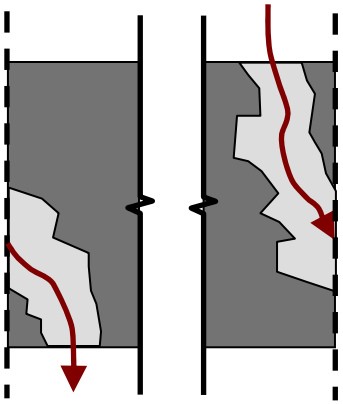
Thresholded for wall porosity of roughly 0.37

Relationship between grayscale threshold values, porosity, and predicted permeability

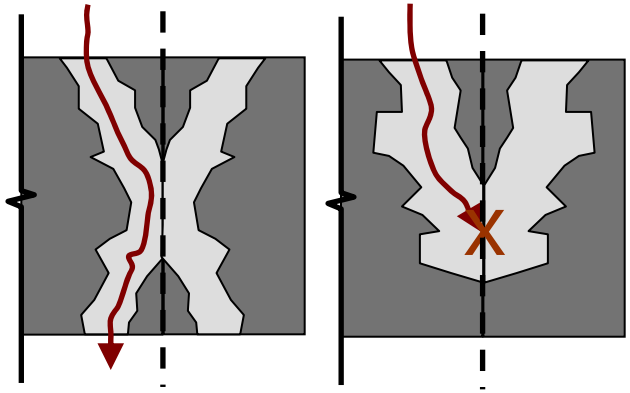


- Results shown are for a cordierite sample
- Original data with 1.62 micron resolution coarsened to 3.24 microns
- Linear relationship between porosity and threshold value
- Second order relationship between threshold value (affects both porosity and pore size) and predicted permeability

Effects of side boundaries



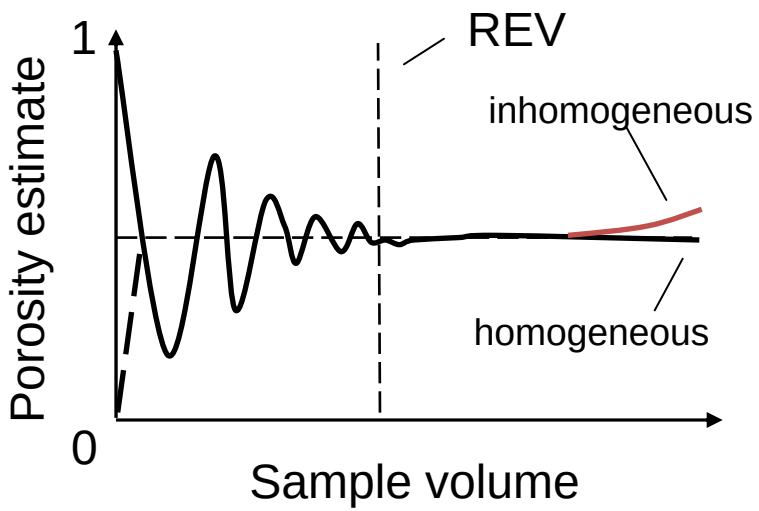
Periodic boundaries – can use with stochastic reconstructions

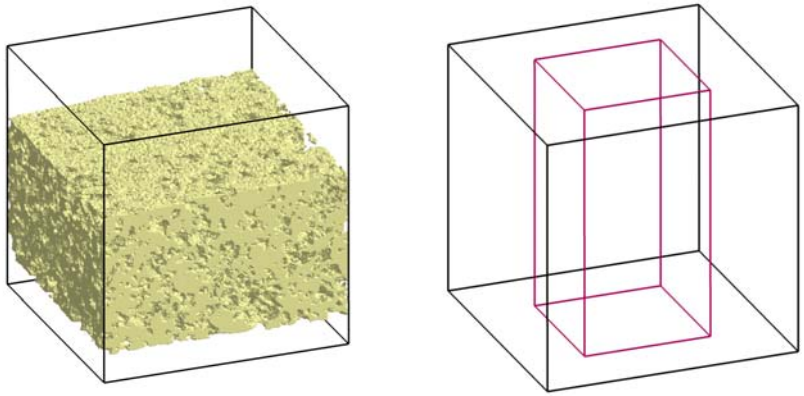


Slip boundaries – must use with reconstructions from real images

- Periodic boundaries are practical with stochastic reconstructions from statistical data
- "Slip" or "reflection" boundaries must be used at the edges of geometries reconstructed from real images
  - Emulate a mirror image pore geometry on other side of plane
  - Can affect connectivity of pores
  - Result: Larger volume needed to represent pore structure

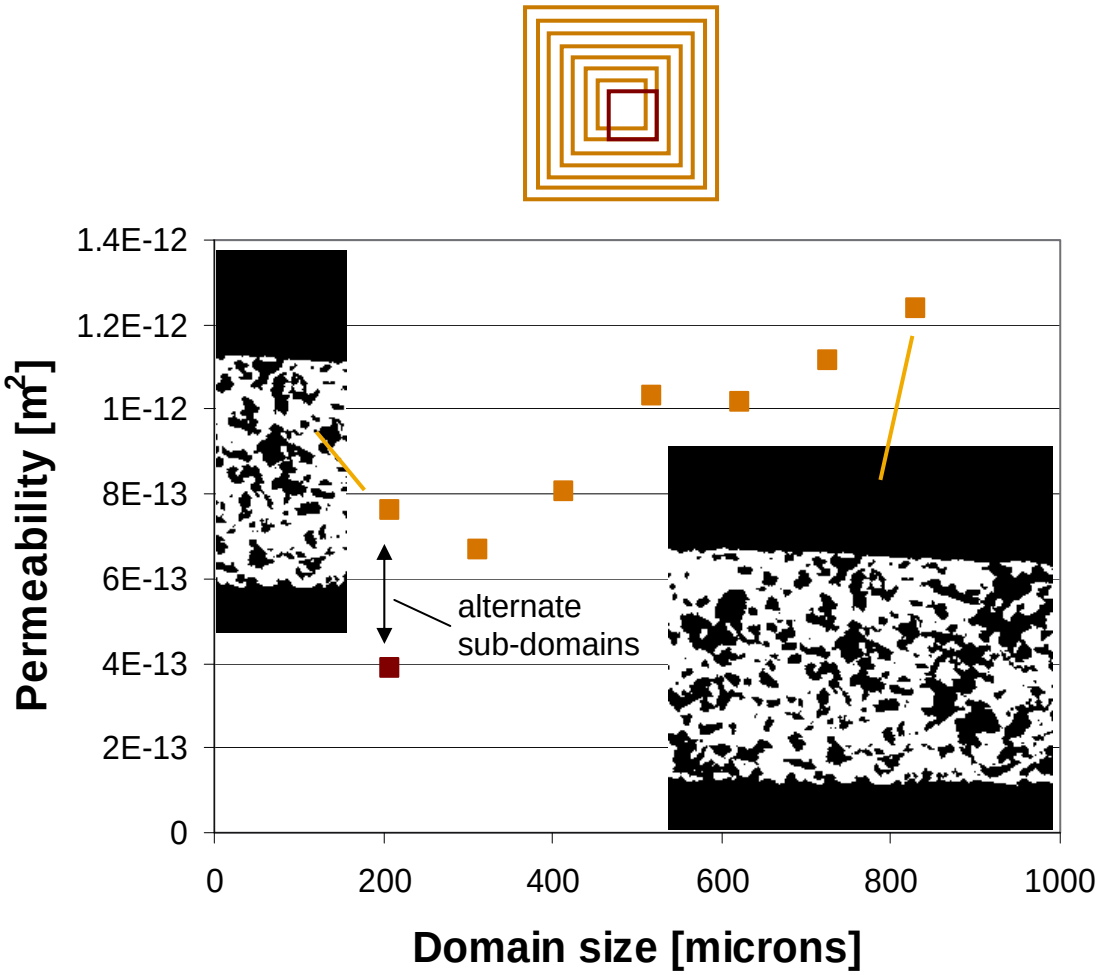
Representative Elementary Volume (REV)





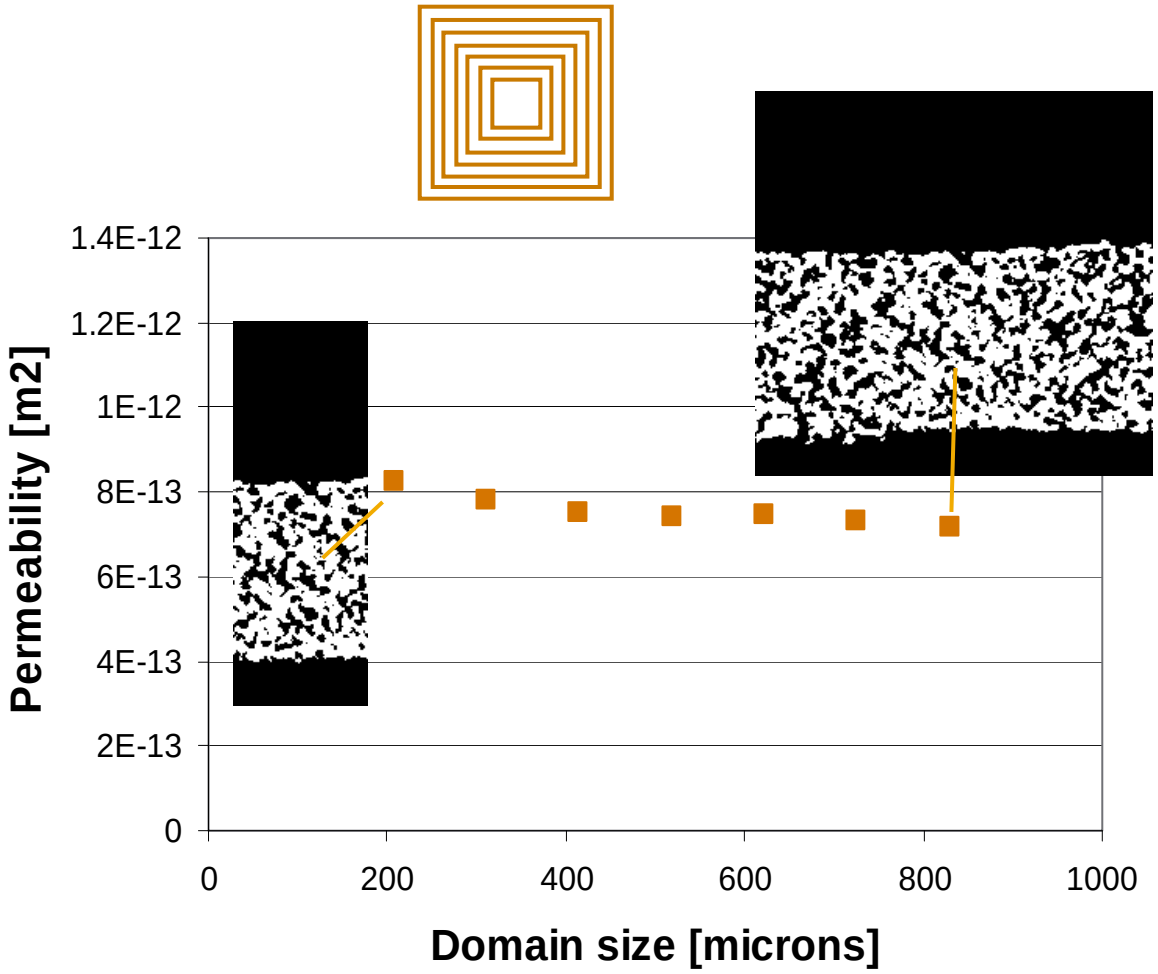
- Concept described by Jacob Bear in Dynamics of Fluids in Porous Media (1972)
- Accurate estimates of ‘macroscopic’ parameters can be made when the volume of material becomes large enough to average out variations in the porous medium
- For micro-scale studies of filter media, it would be valuable to have some idea of the size of a REV, especially for properties such as permeability and filter efficiency
- Flow simulations were carried out with various sub-volumes of filter reconstructions with 3.2 micron resolution

REV study for cordierite



- Alternate sub-domains on the small end illustrate how estimates of the macroscopic parameters vary depending on location
- General upward trend in permeability as more pores are included
- Trend still has not leveled out in the largest domain examined: roughly 0.8 mm square of filter wall area ~1.7E7 computational cells

REV study for silicon carbide



- Far less variation than cordierite – suggests that reasonable estimates can be made with far smaller geometries
- Upward trend in permeability with domain size observed with cordierite is not evident at these scales – pore bodies are much smaller and tortuosity is lower

Observations on the cost of massively parallel computing

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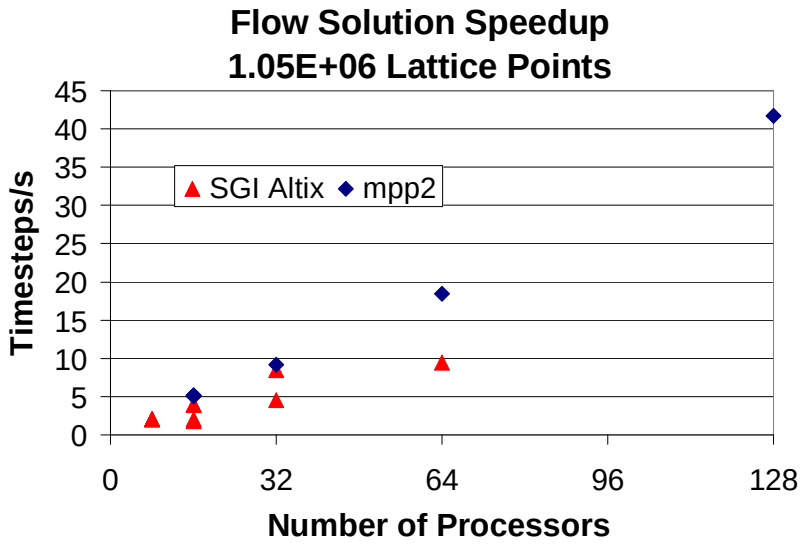
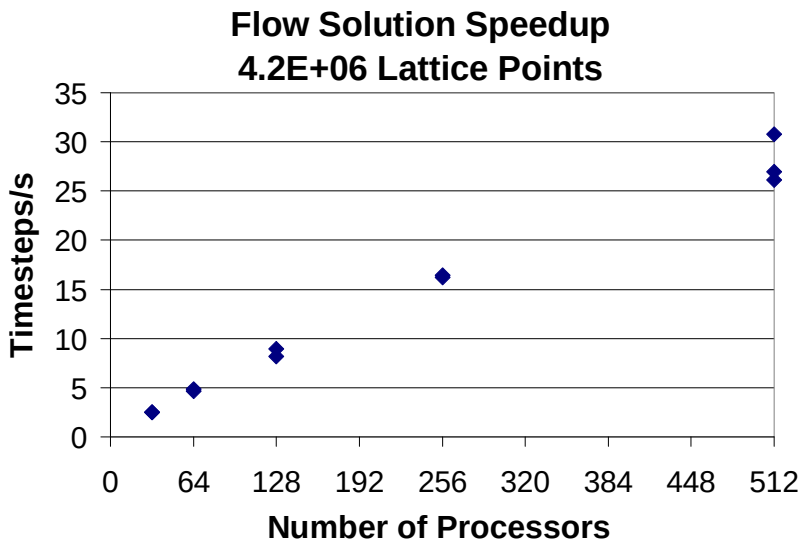
Five years ago:
Large runs on 128 processor shared memory HPC platform
64 bit Itanium chips
Price tag > $500 K

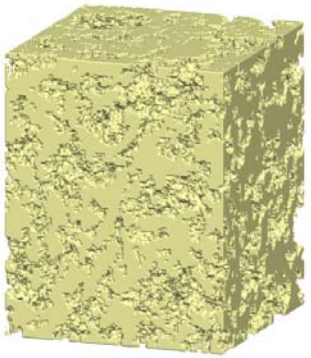
Today:
128 *core* cluster
Commodity quad-core Opteron chips
Price tag ~ $50 K

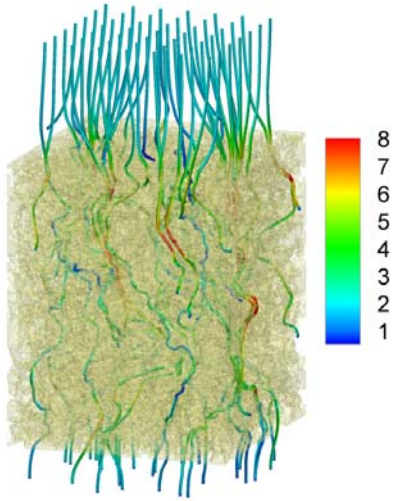
Cost roughly equivalent to that of a loaded 2009 4x4 diesel pickup with DPF & LNT

Scalability of lattice-Boltzmann method









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Summary

- First-principles micro-scale simulations of DPFs have been used to help provide qualitative insight into fundamental mechanisms
- Current focus is improvement of quantitative accuracy, especially back-pressure and filter efficiency as a function of loading
- X-ray CT data is being examined to improve the geometric representations used in pore-scale models
  - Good estimates of sample porosity are necessary for thresholding images
  - Cordierite may require significantly larger sample sizes to approach Representative Elementary Volumes than granular substrates like SiC
- Large-scale production of multi-core processors will likely continue to make massively parallel computations more affordable. This means that analyses which are impractical today may be practical within a few years.

Future work

- Conclude study of necessary spatial resolution for good quantitative predictions of DPF permeability
- Validate filtration models by comparing to single fiber filtration data
- Examine micro-CT data for catalyzed filter substrates
- Conduct filtration studies with CT filter reconstructions
- Continue fundamental filtration studies using simple particle surrogates, lab-generated soot, and diesel soot

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