



MONet Community Science Meeting – Data tutorial on XCT

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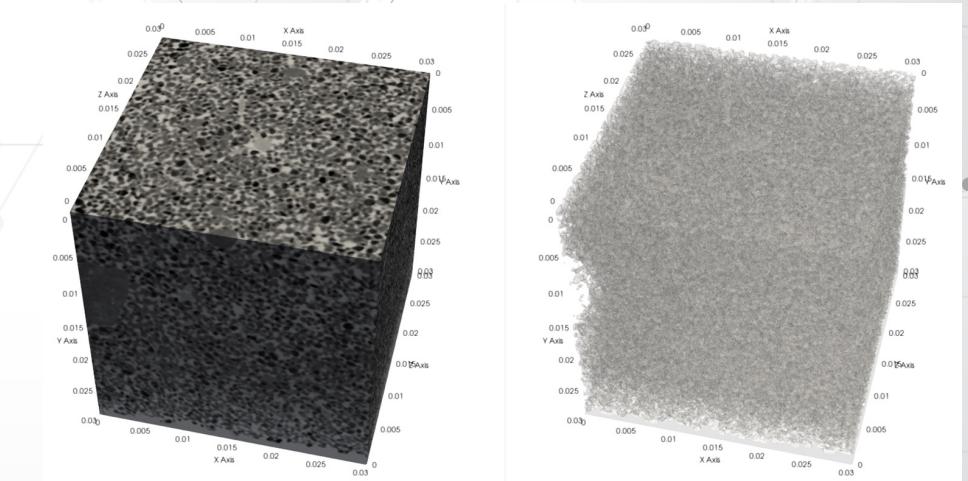
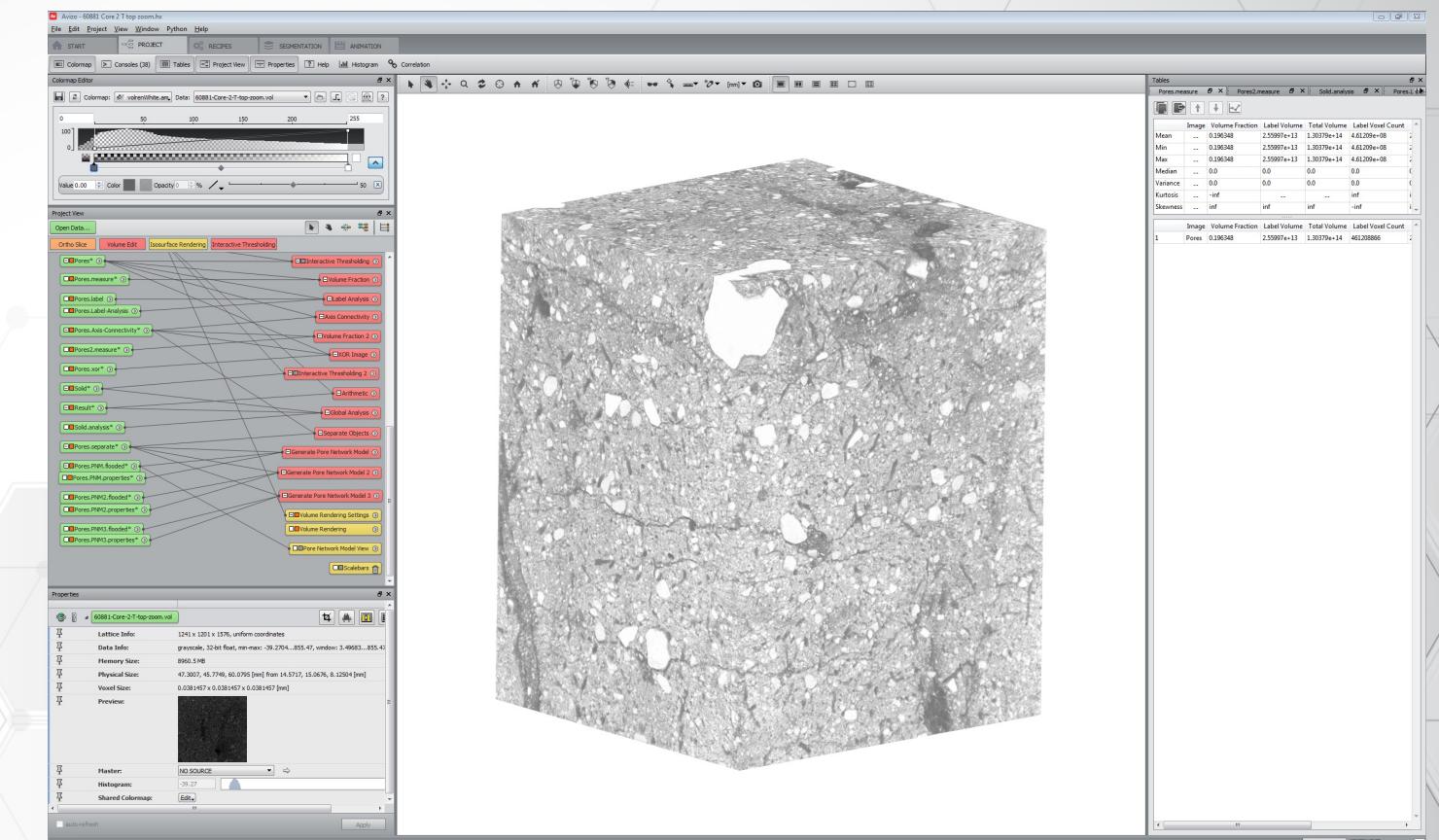
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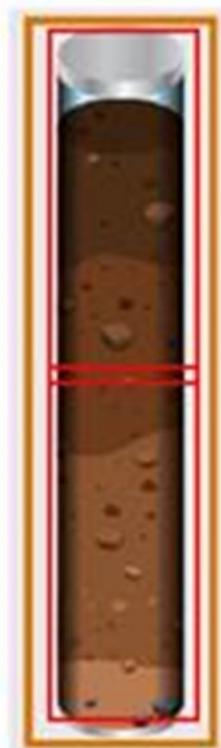
Nov 7, 2023



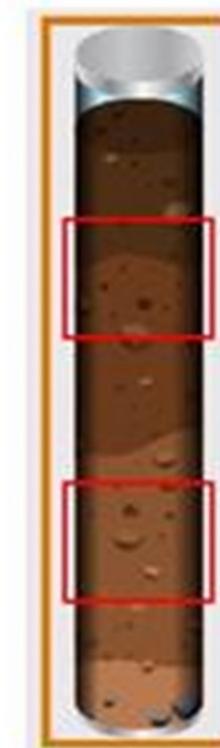
- Data types from XCT for MONet
- How do we get these: workflow
- A walk-through of our MONet-specific data analysis of soil porosity: creating/processing the raw data, other processing steps, segmentation, analyses
- Other data output formats/options, software used
- How this data can be used (examples including modeling)

Scanning protocol

Low resolution XCT
scans collected on
whole core in 2
tiles
(82.5 microns voxel
size)

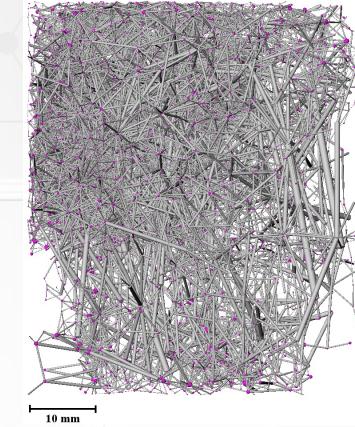
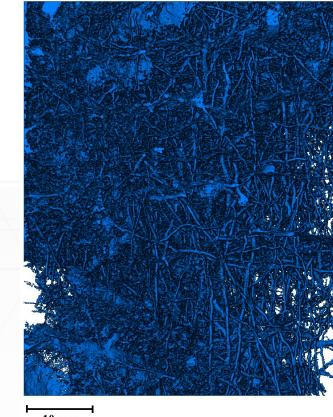
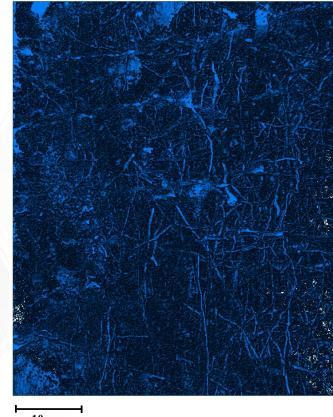
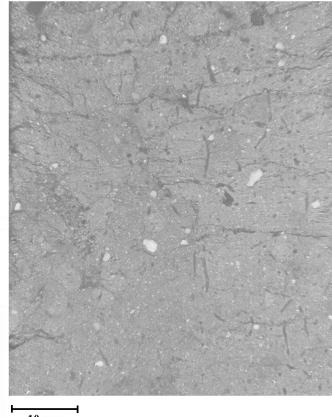
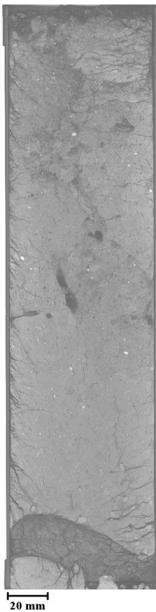


High resolution XCT
scans collected on
top and bottom
sections
(38.2 microns voxel
size)



Data types for MONet

- **Image data:**



- **Numerical data:**

- Pore size
- Pore volume fraction
- Pore connectivity
- Pore size distribution

- Bulk density
- Permeability
- Flow rate
- Tortuosity

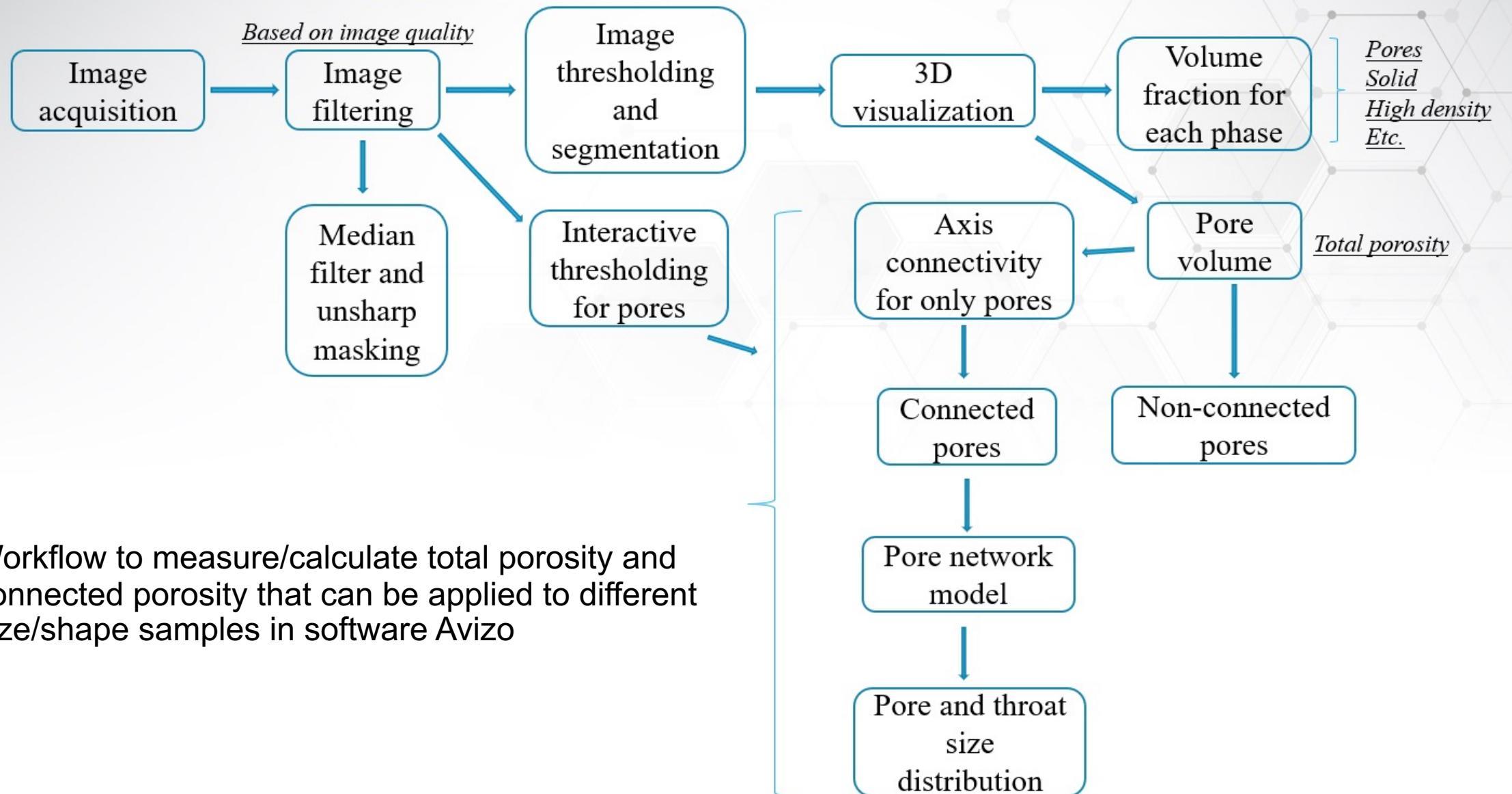
Data types for MONet: Numerical porosity data

Numerical data:

- Pore size
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- Pore connectivity
- Pore size distribution
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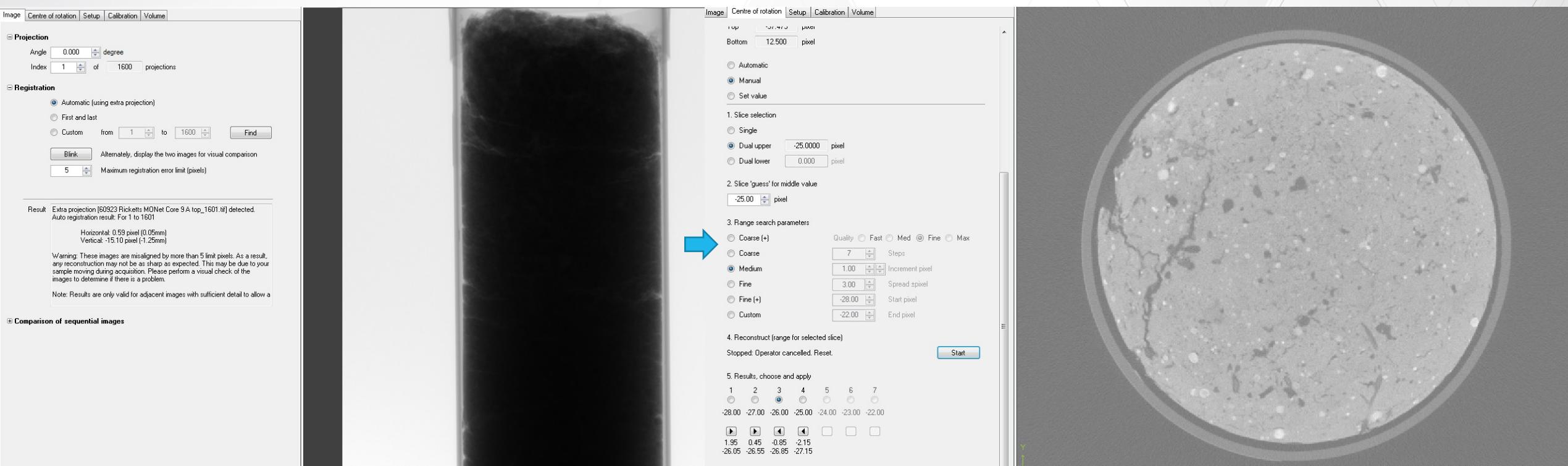
A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
1						volume (m³)	Area (mm²)	Area Fract	Diameter (mm)				volume (m³)	Area (mm²)	Area Fract	Diameter (mm)	
2						0.000555	0.031101	4.07E-09	0.101964				Mean	0.001985	0.054057	1.45E-08	0.069619
3	Pores	0.085973				5.55E-05	0.004371	4.07E-10	0.047327				Min	5.55E-05	0.004371	4.07E-10	0.047327
4						0.000222	0.015275	1.63E-09	0.075128				Max	9249.336	190975.9	0.067838	26.04379
5						0.00444	0.187809	3.26E-08	0.203928				Median	9.22E-05	0.007635	6.76E-10	0.059606
6						0.006994	0.320421	5.13E-08	0.237267				Variance	15.13321	6446.432	8.14E-10	0.001437
7	Pores.Axis	0.067838				0.050177	1.23785	3.68E-07	0.457617				Kurtosis	5658180	5658176	5658182	69404.55
8						0.0005	0.031401	3.66E-09	0.098445				Skewness	2378.692	2378.691	2378.693	90.81248
9						0.000111	0.008209	8.14E-10	0.059629								
10	PNM in Z					9249.34	190975.9	0.067838	26.0438								
11	k [µm²]	k [d]	TotalFlow	Tortuosity		0.006328	0.2437	4.64E-08	0.229482								
12	14197.26	14385.37	141710.1	1.353234		0.025144	1.01731	1.84E-07	0.363479								
13						0.000555	0.036606	4.07E-09	0.101964								
14						5.55E-05	0.004371	4.07E-10	0.047327				frequency count				
15	PNM in Y					0.000444	0.02565	3.26E-09	0.094655				(mm)				
16	k [µm²]	k [d]	TotalFlow	Tortuosity		5.55E-05	0.004371	4.07E-10	0.047327				0-0.1			945303	
17	71.17569	72.11877	1257.678	1.808984		0.048179	1.67739	3.53E-07	0.45146				0.1-0.2	0.1		92624	
18						5.55E-05	0.004371	4.07E-10	0.047327				0.2-0.3	0.2		7860	
19						0.0005	0.030019	3.66E-09	0.098445				0.3-0.4	0.3		1727	
20	PNM in X					0.000222	0.015041	1.63E-09	0.075128				0.4-0.5	0.4		558	
21	k [µm²]	k [d]	TotalFlow	Tortuosity		0.000666	0.042052	4.89E-09	0.108353				0.5-0.75	0.5		370	
22	368.3572	373.2379	5184.799	1.582346		0.001443	0.080395	1.06E-08	0.140207				0.75-1	0.75		84	
23						0.000111	0.008438	8.14E-10	0.059629				1to5	1		47	
24						5.55E-05	0.004371	4.07E-10	0.047327				5to10	5		0	
25						5.55E-05	0.004371	4.07E-10	0.047327				10to25	10		0	
26	wet bulk d	2.06034				0.0005	0.029642	3.66E-09	0.098445				25to50	25		1	
27						5.55E-05	0.004371	4.07E-10	0.047327				>50	50		0	
28						0.000167	0.011742	1.22E-09	0.068258								
29						0.000111	0.008506	8.14E-10	0.059629								
30						5.55E-05	0.004371	4.07E-10	0.047327								
31						0.000111	0.008438	8.14E-10	0.059629								
32						5.55E-05	0.004371	4.07E-10	0.047327								
33																	

Data analysis workflow



Data reconstruction

- Create 3D volume data from the individual projections
- We use CT Pro 3D (X-Tek software suite by Nikon)

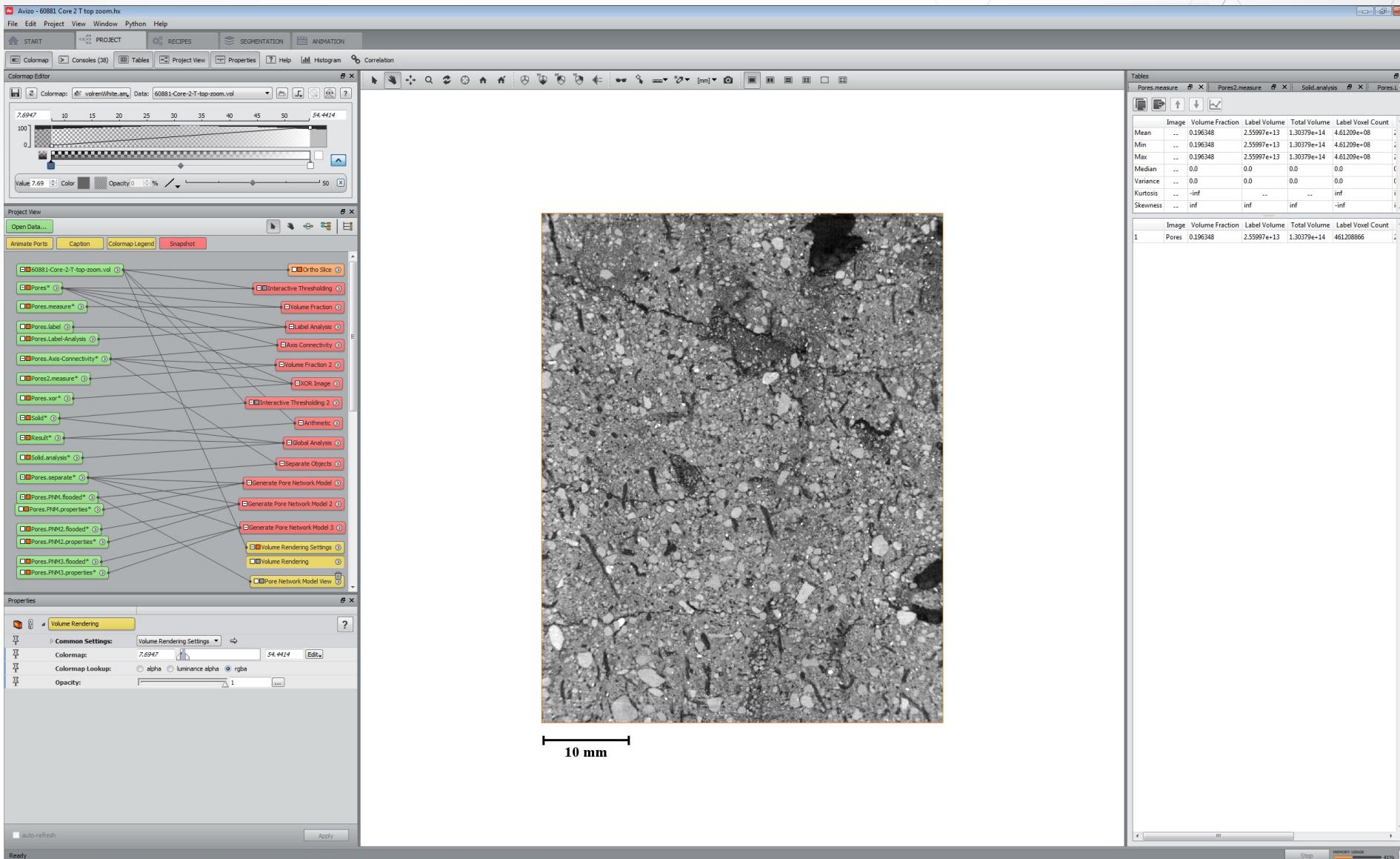


Data processing

- Importing reconstructed data into Avizo (Thermo Fisher)
- Image cropping (as necessary)
- Filtering (as necessary)
- Segmentation – see next
- Pore volume/size analysis
- Pore network analysis
- Visualization

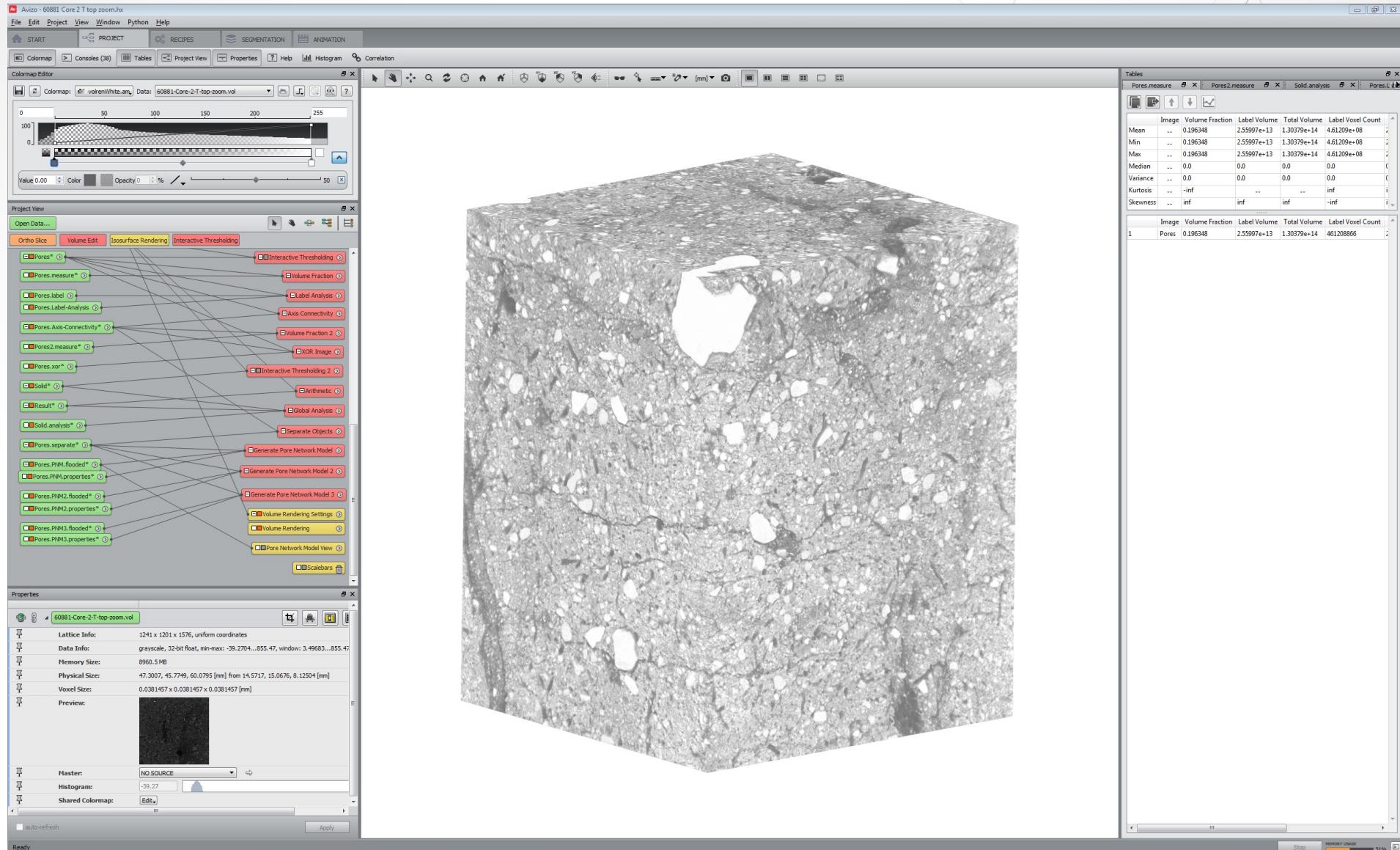
Importing the image

Reconstructed data read in as VGI volume (2D slice shown)



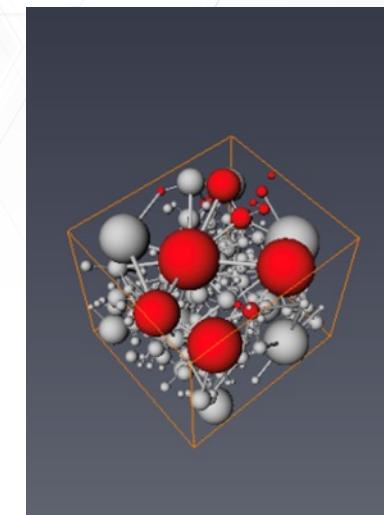
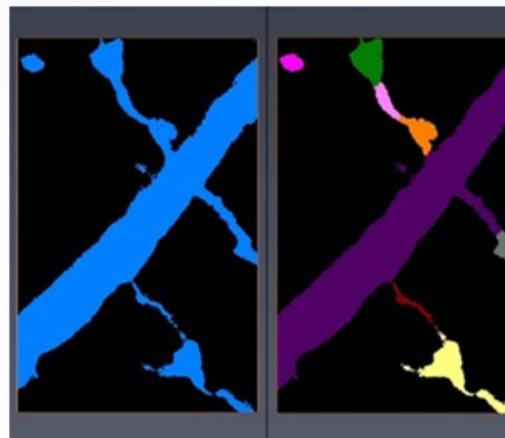
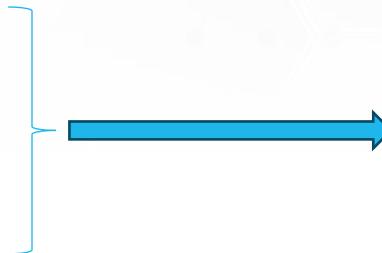
Visualization as 3D volume

Initial look at the raw data as 3D volume



Porosity analysis – major steps

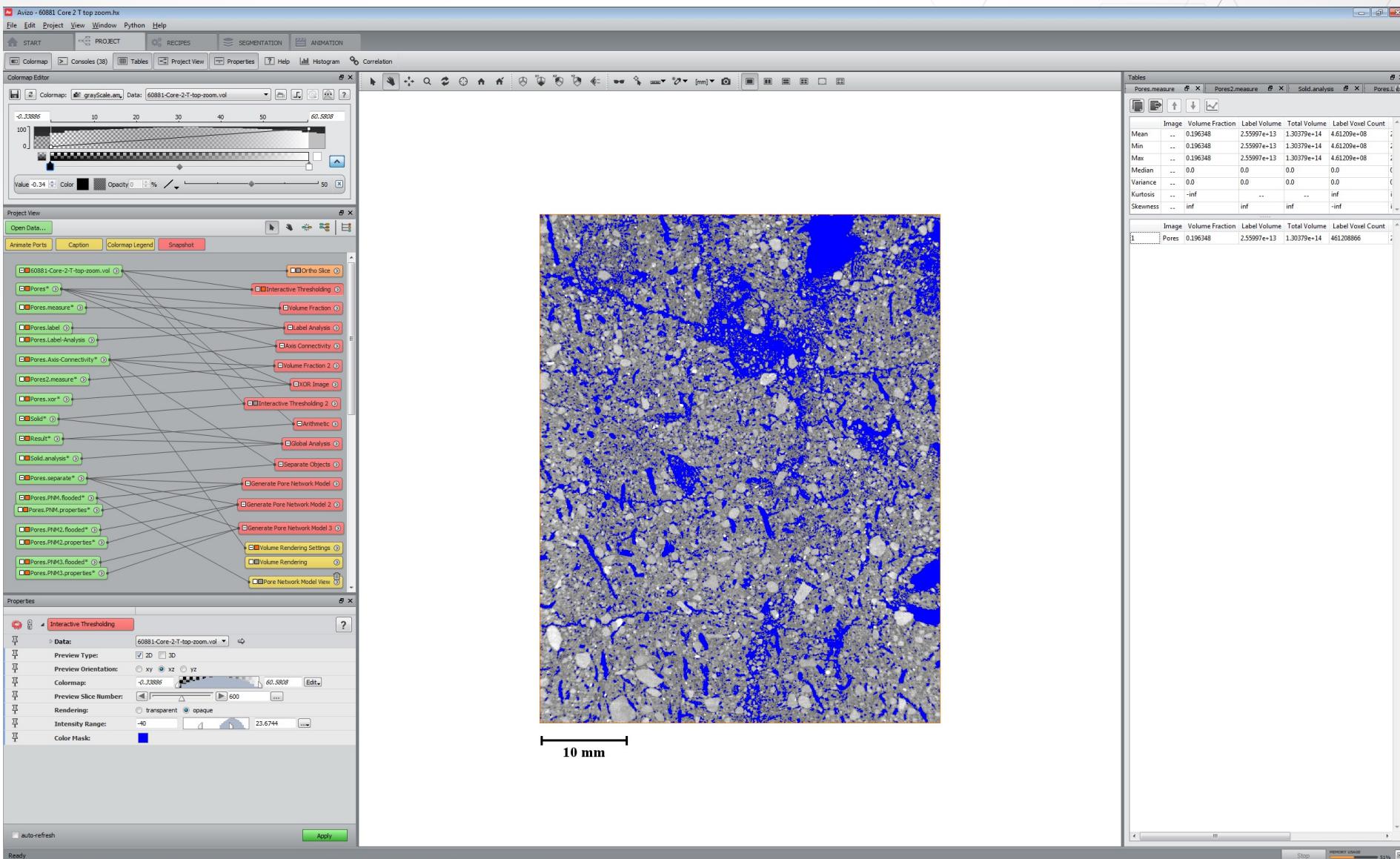
- Thresholding
- Volume fraction
- Measurement to calculate results
- Data analysis
- Pore network module (PNM-Xpore)



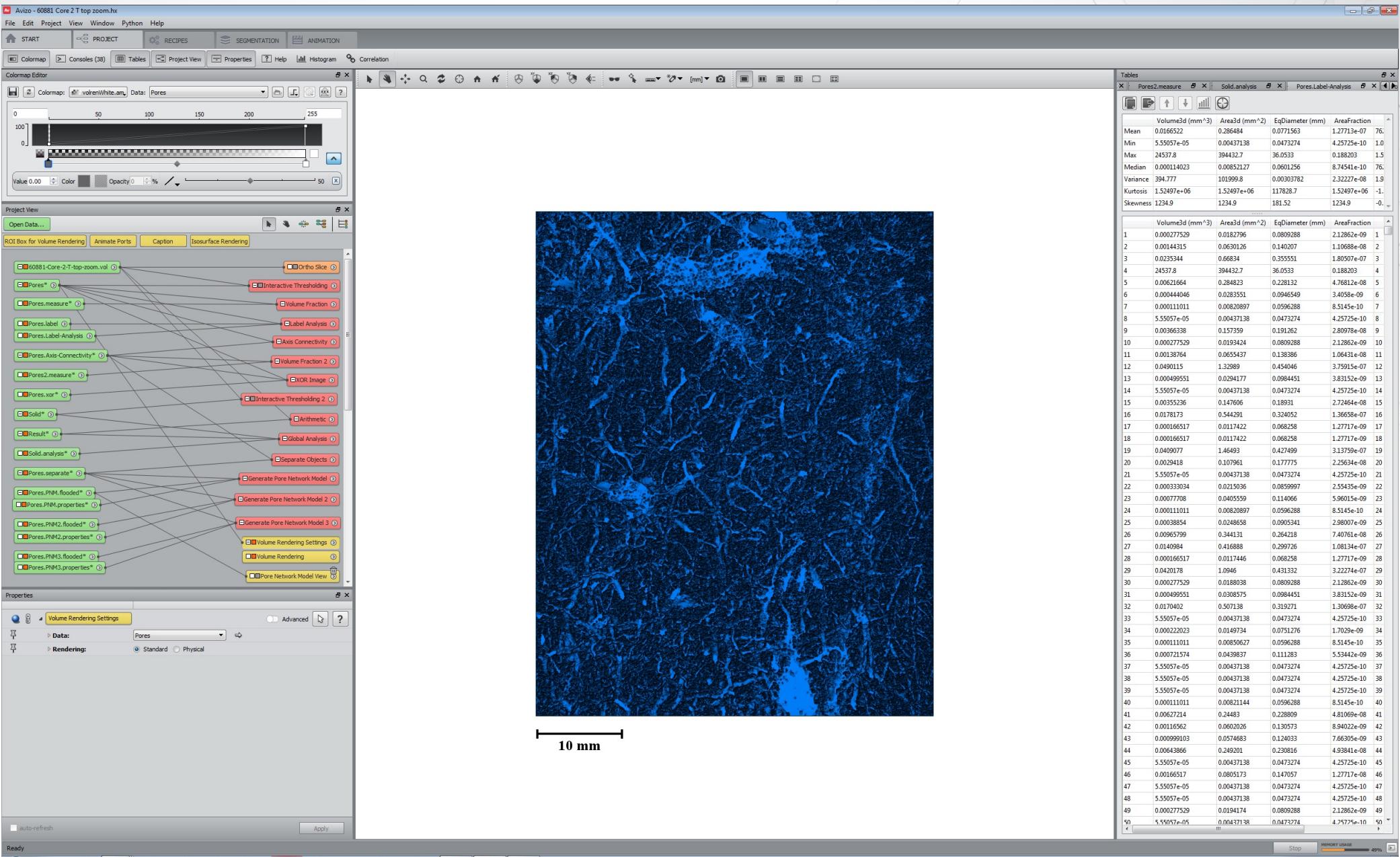
Pore ID	Volume	Area	EqRadius
1 0	0.0780605	1.22915	0.265123
2 1	0.361577	3.40463	0.441947
3 2	0.138114	1.8833	0.320664
4 3	0.00145212	0.0639127	0.0702487
5 4	0.00497395	0.150073	0.105894
6 5	0.0012192	0.0690542	0.0662717
7 6	0.227738	2.95732	0.378834
8 7	0.0133606	0.86959	0.147231
9 8	0.537073	4.36064	0.504253
10 9	0.09510395	0.147367	0.106802
11 10	0.392412	3.24608	0.454169
12 11	0.00184743	0.110051	0.076119
13 12	0.703226	4.66303	0.551656
14 13	0.0356269	0.617245	0.204125
15 14	0.00127244	0.0578862	0.0672227
16 15	0.0140633	0.953941	0.149738
17 16	0.000535062	0.0344628	0.0503623

Image segmentation

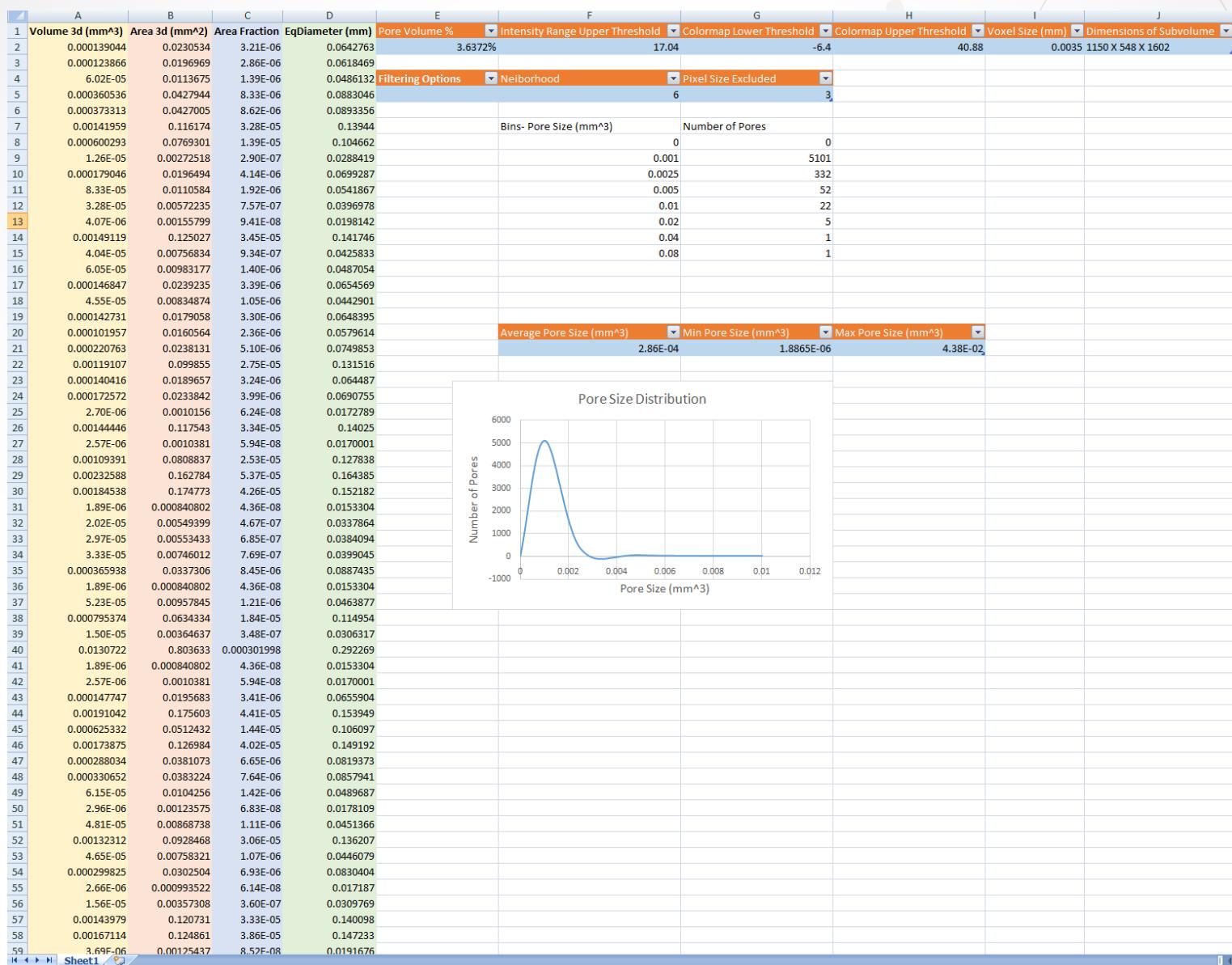
Thresholding image for segmentation (manual or auto thresholding)



Porosity analysis – calculation of porosity numbers

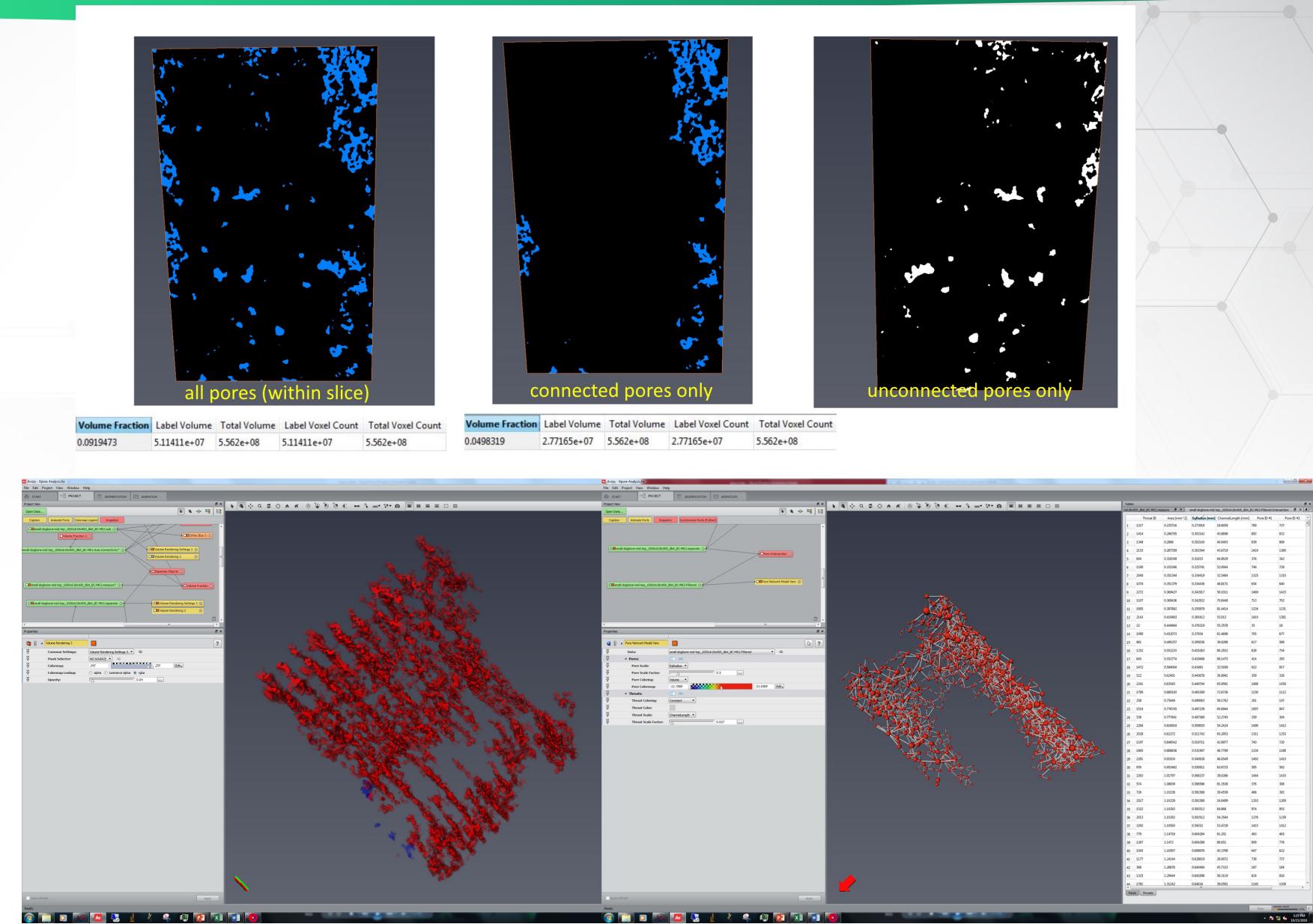


Porosity analysis – additional analysis

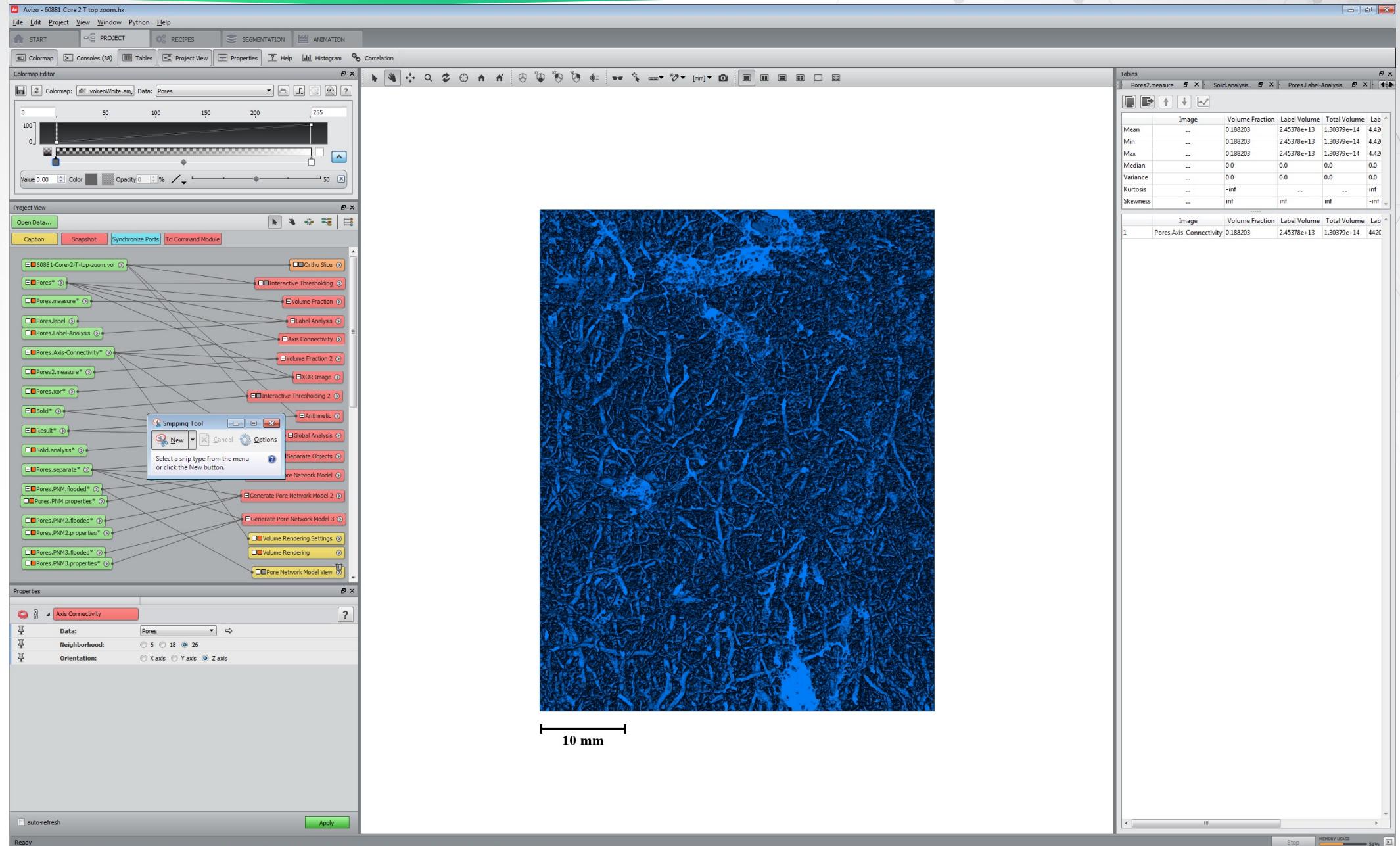


Pore Network Modeling (PNM) – major steps

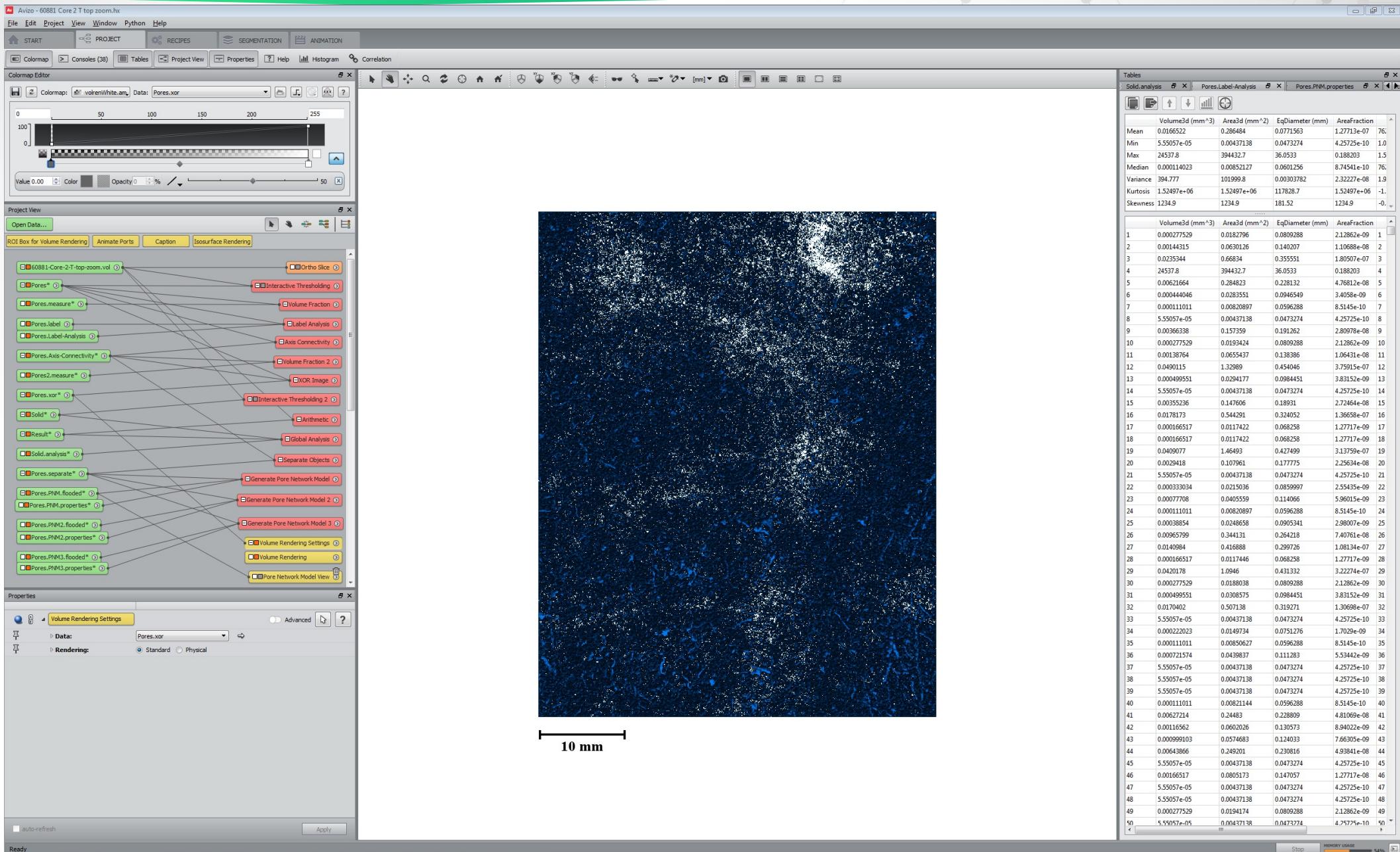
- Thresholding
- Axis connectivity
- Volume fraction
- Image subtraction
- Separate objects
- Pore Network Model



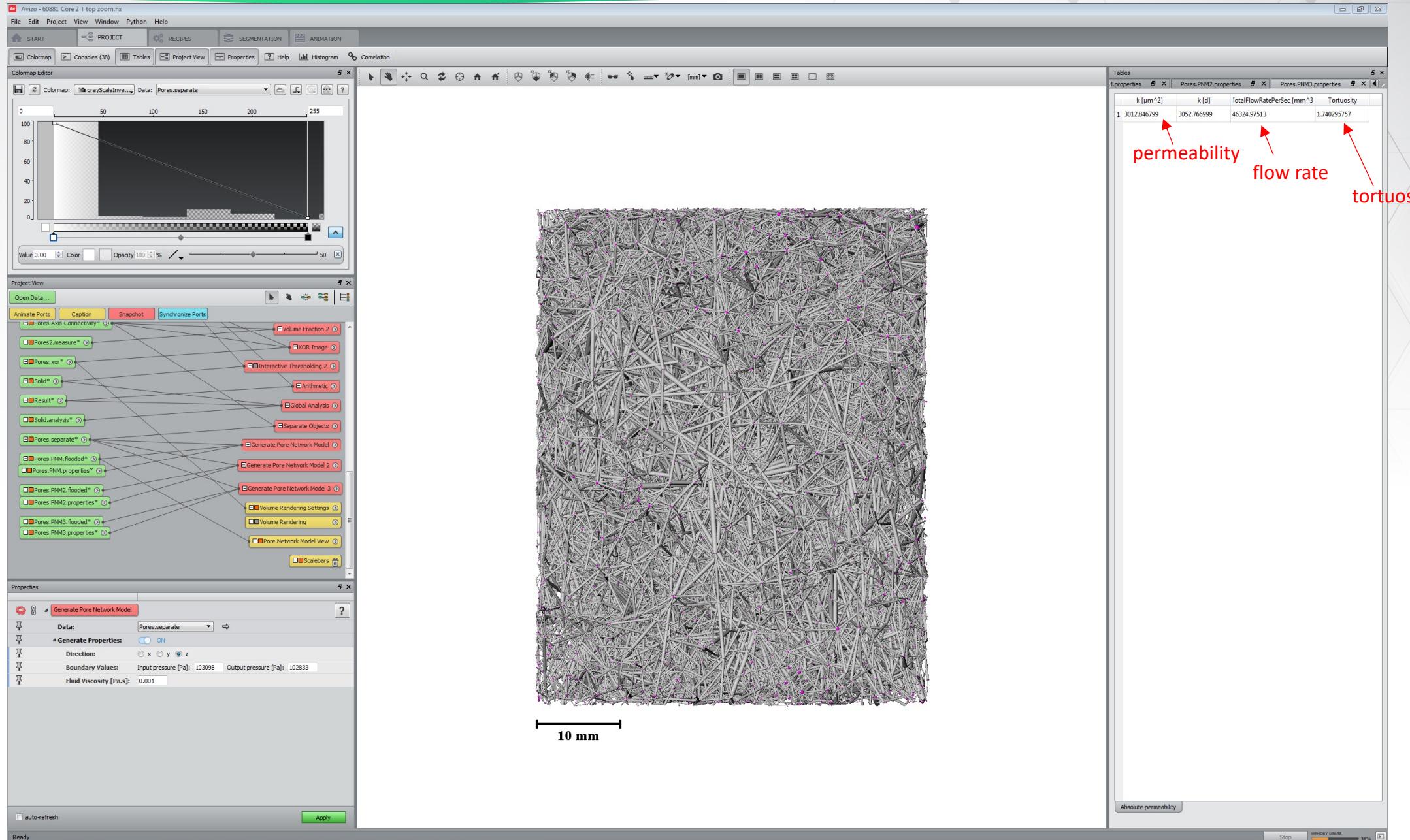
Pore Network Modeling – Axis connectivity



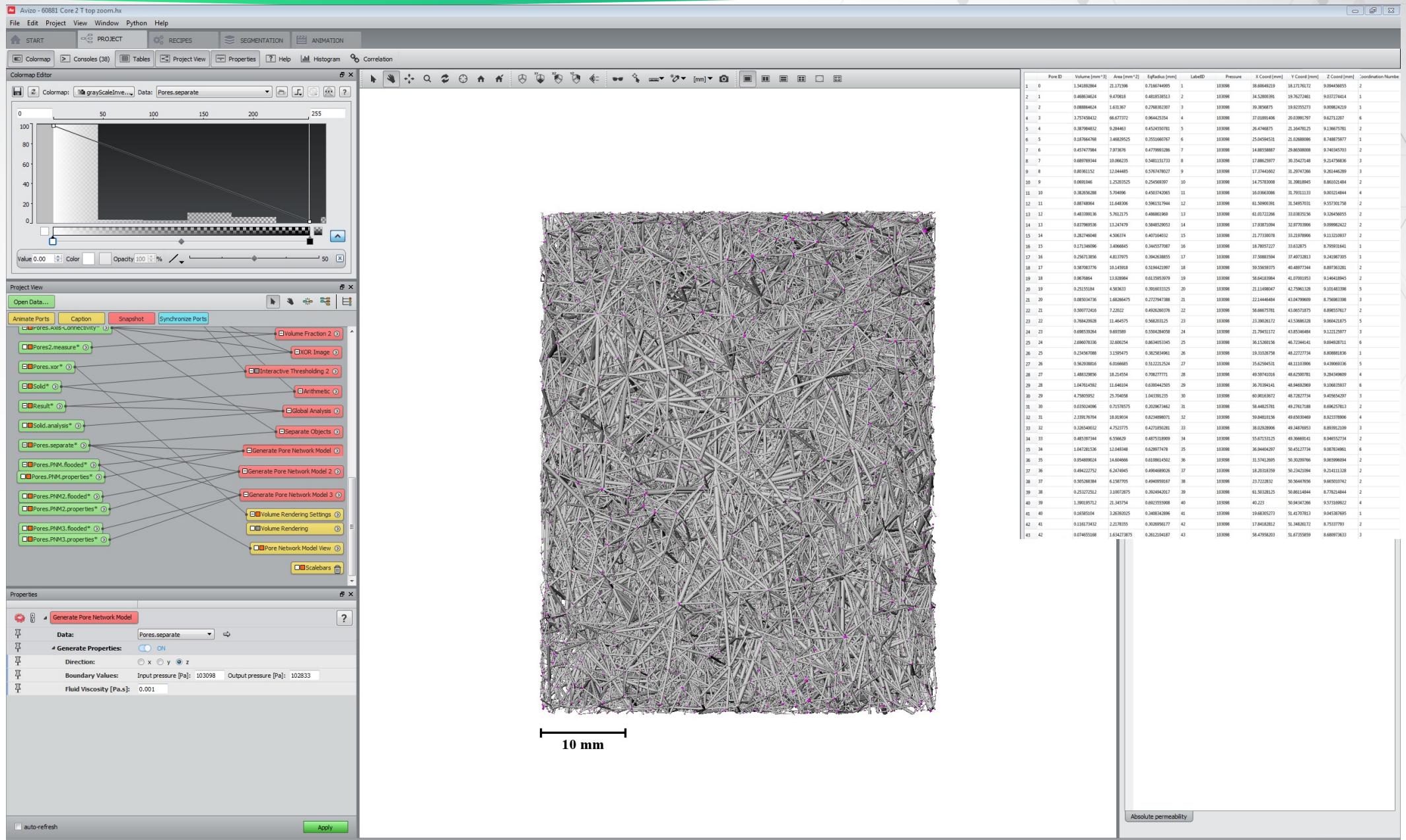
Pore Network Modeling – Volume fraction (unconnected vs connected)



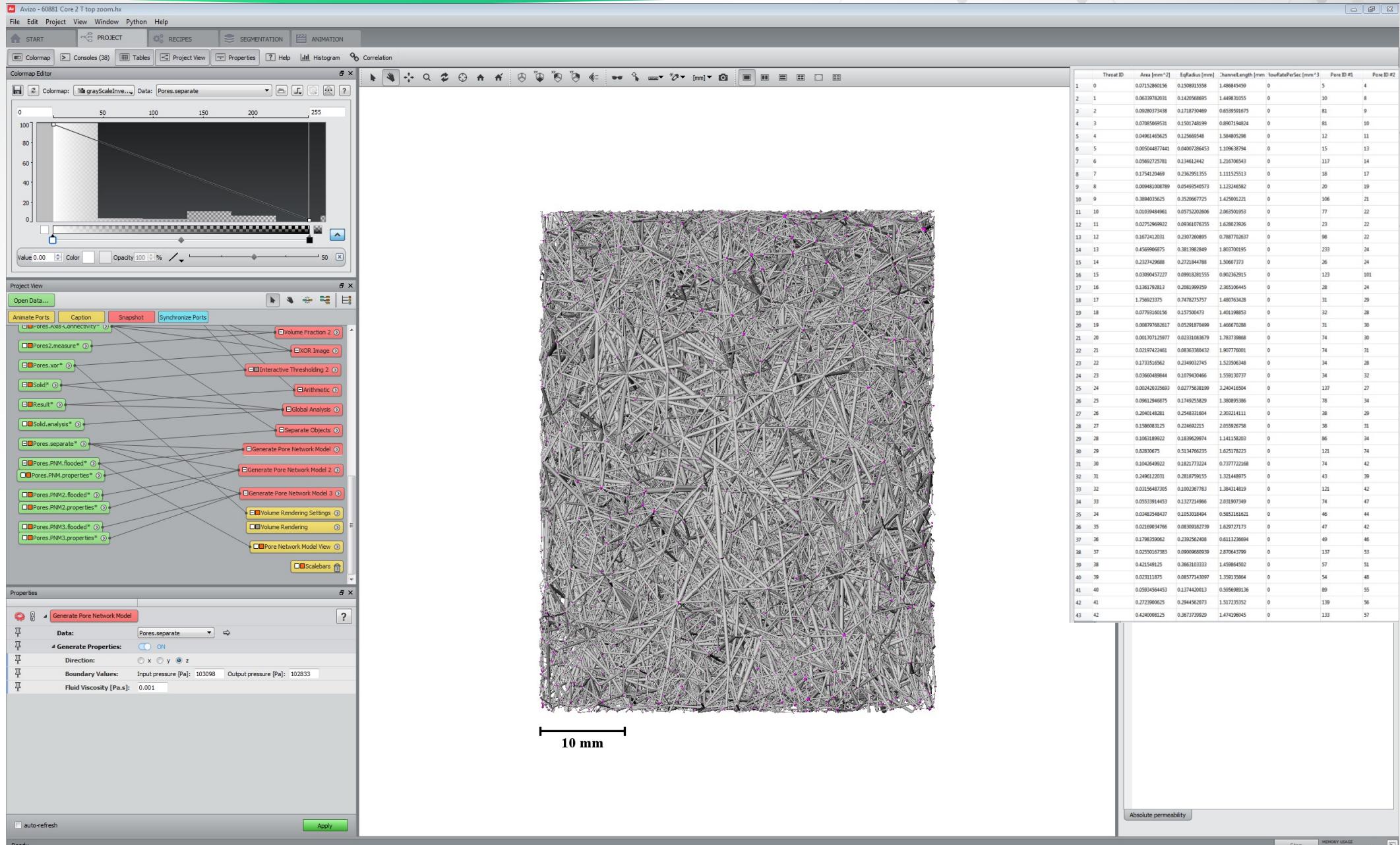
Pore Network Modeling – Calculation of results



Pore Network Modeling – Calculation of results



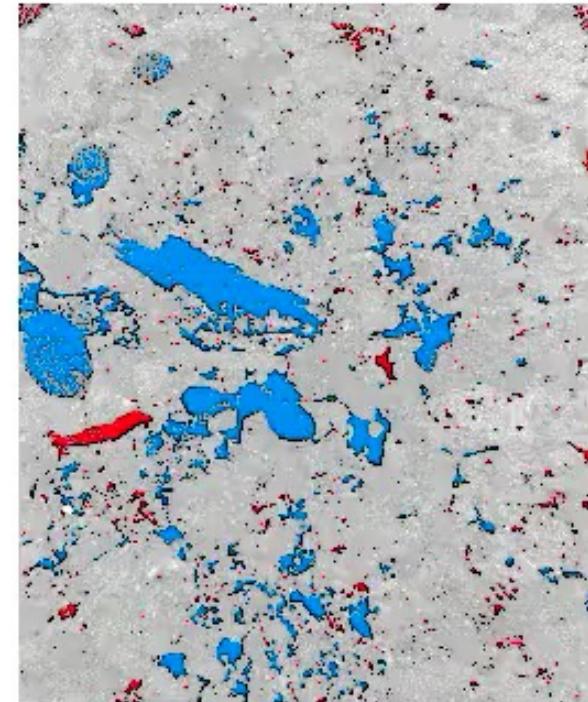
Pore Network Modeling – Calculation of results



Other data output options

- **Image data:**

- Animations
- Mesh
- STL file (3D printing)
- ...



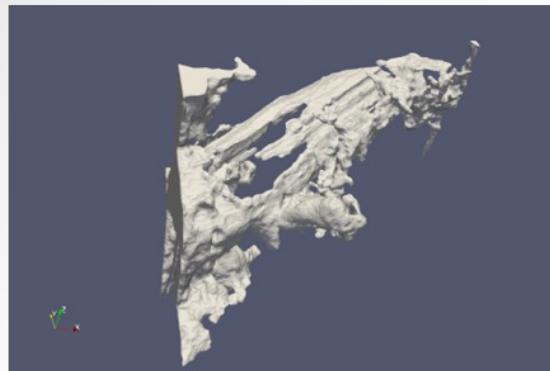
- **Numerical data:**

- Pore throats
- Pore coordination numbers

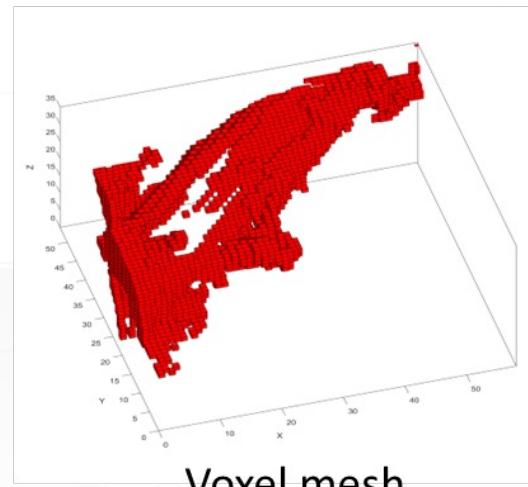
- Visual Graphics Studio, Dragonfly (license)
- ImageJ/Fiji, ParaView (free)
- Modeling:
 - OpenPNM:
 - <https://openpnm.org/>
 - <https://github.com/PMEAL/OpenPNM>
 - PoresPy:
 - <https://porespy.org/>
 - PFLOTTRAN:
 - <https://www.pflotran.org/>
 - OpenFOAM:
 - <https://www.openfoam.com/>

How this data can be used: Example 1 – Flow & transport modeling

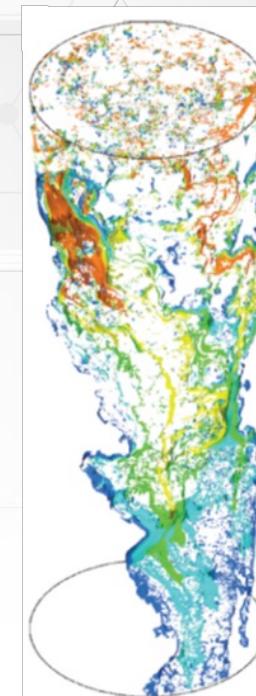
- Incorporate XCT segmented data to build flow and transport model



XCT image with connected pores



Voxel mesh



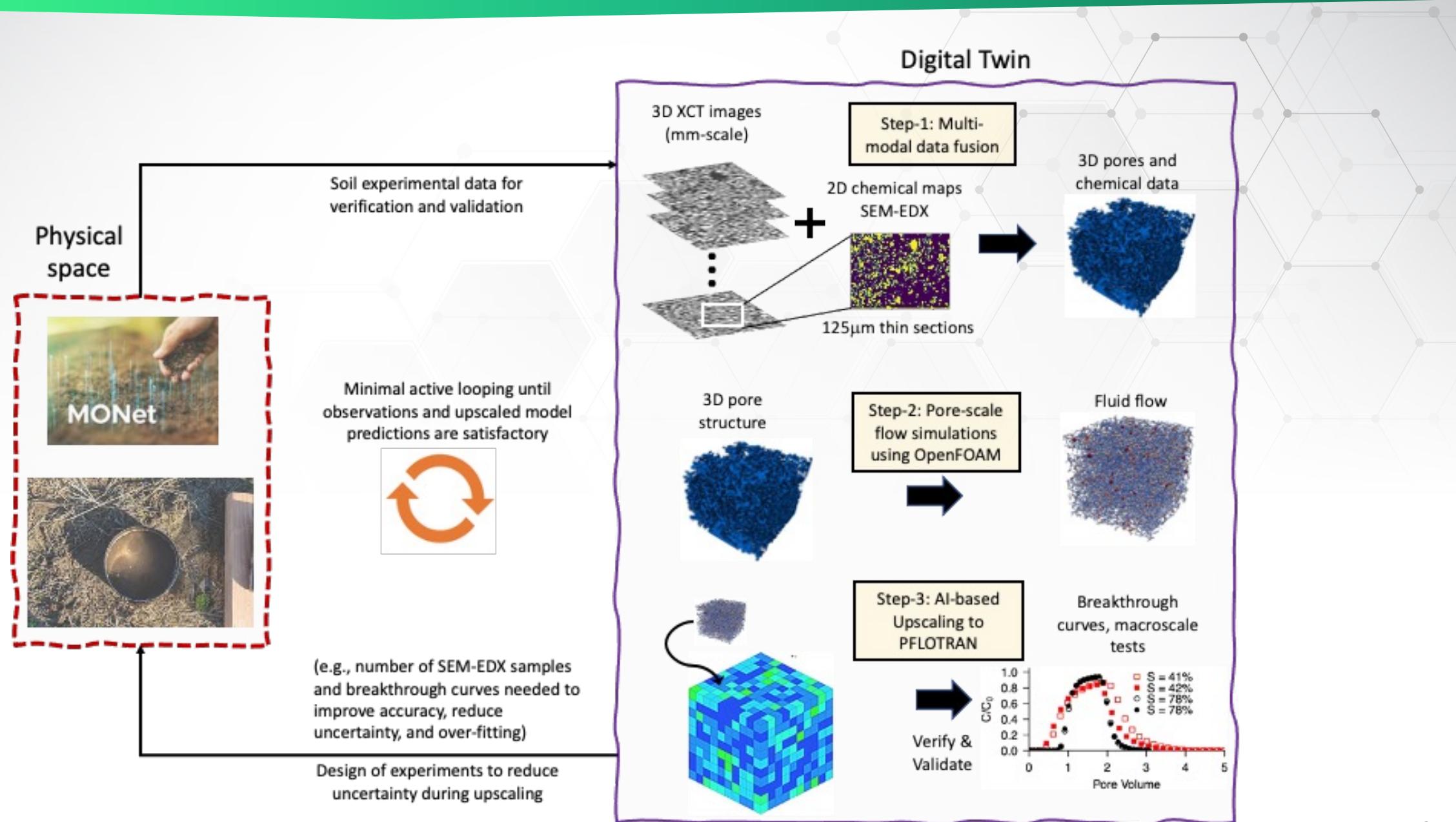
CFD model

Image from
Scheibe et al., 2014
WRR

- TETHYS

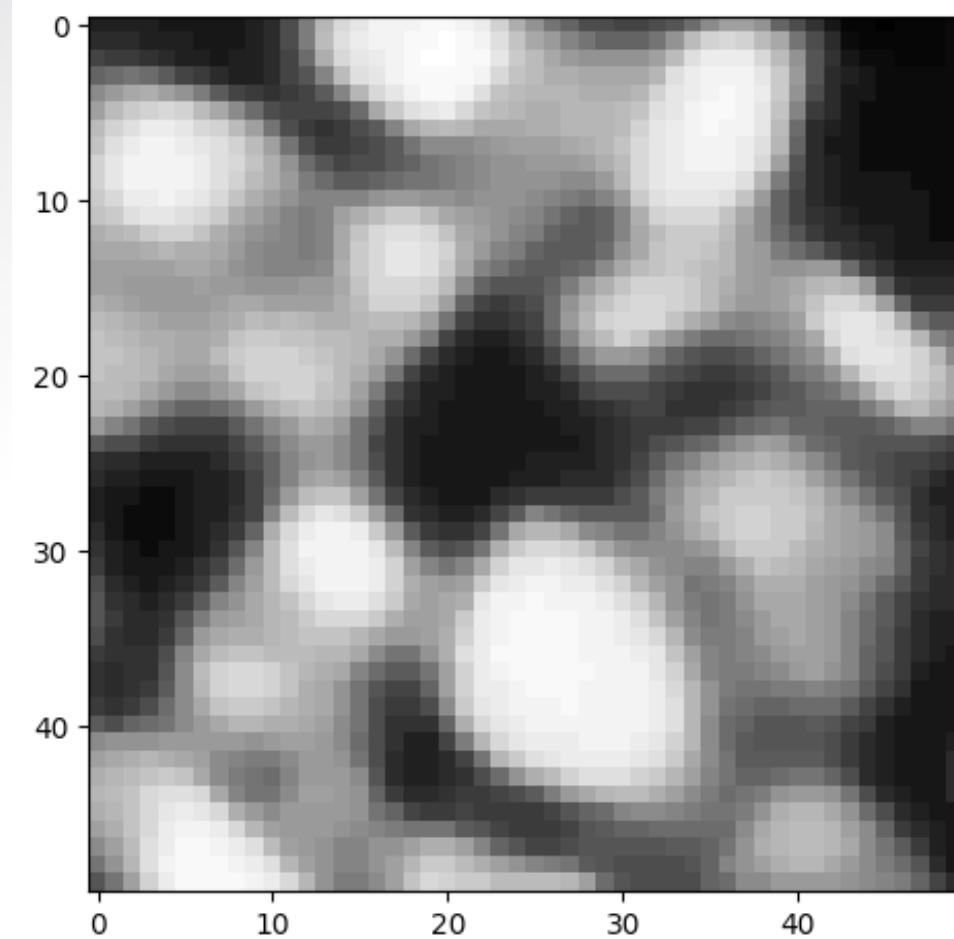
- Multiphase simulation – VOF (volume of fluid) method
 - Multiple immiscible fluids.
 - Fluids surface tension and contact angle.
- Reaction engine – BIOGEOCHEM (Fang et al. 2003)
 - Individual species specified (aqueous, solid, gas, mobile, immobile).
 - Reactions: Equilibrium, Kinetic (forward/backward) or user defined.
 - Needs more robust testing and validation

How this data can be used: Example 2 – XCT to PFLOTRAN (work-in-progress)



How this data can be used: Example 2 – XCT to PFLOTRAN (work-in-progress)

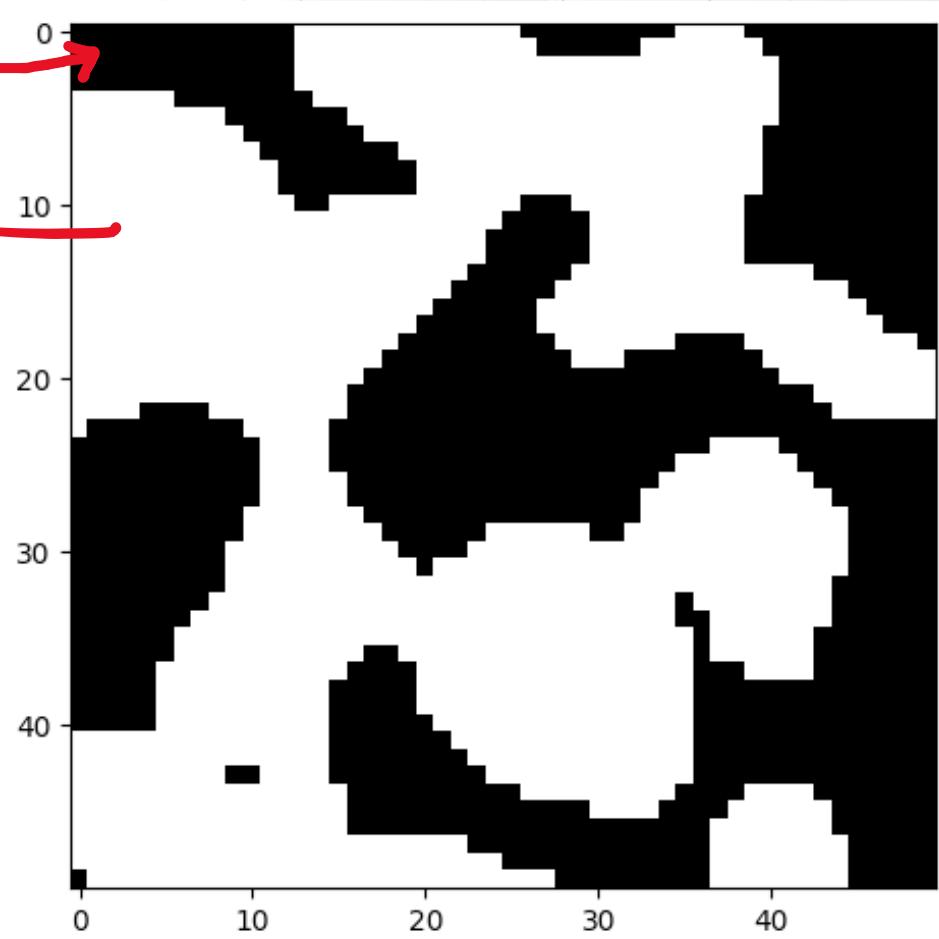
Raw XCT image (sub-set)



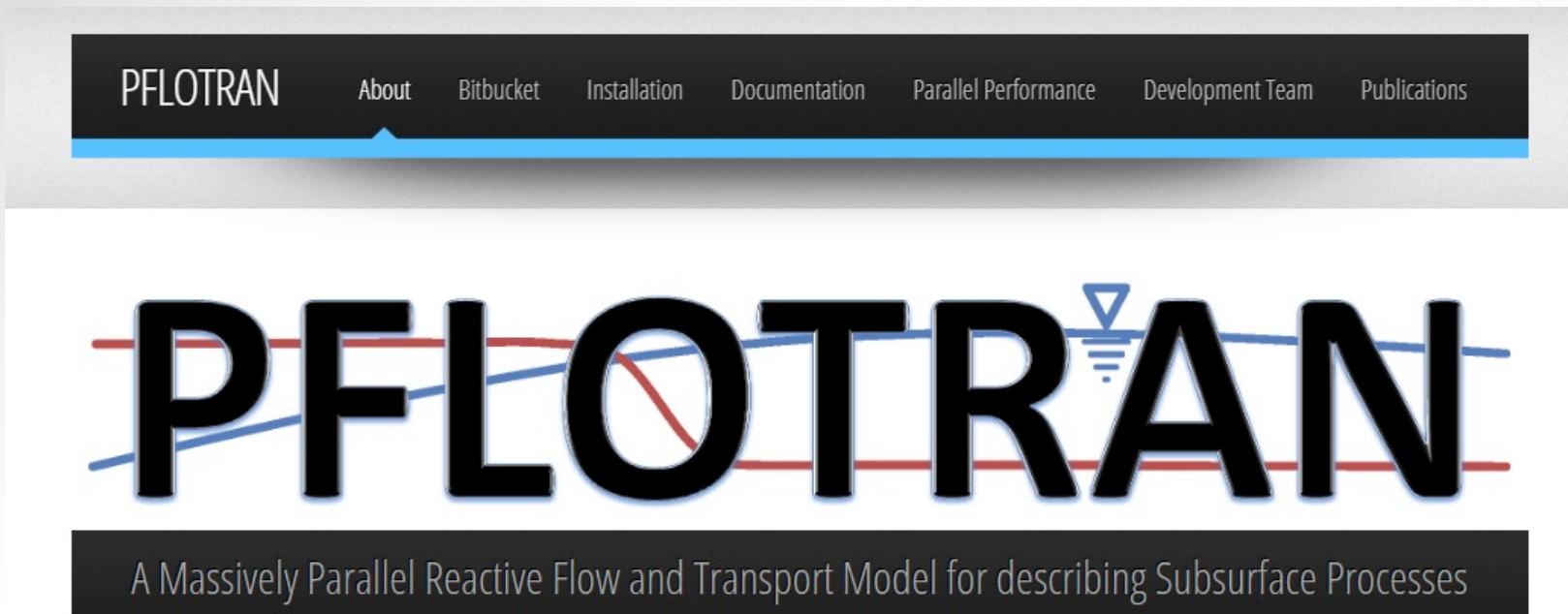
Assign
material
properties
(e.g.,
permeabil-
ity,
porosity)



Segmented XCT image (sub-set)



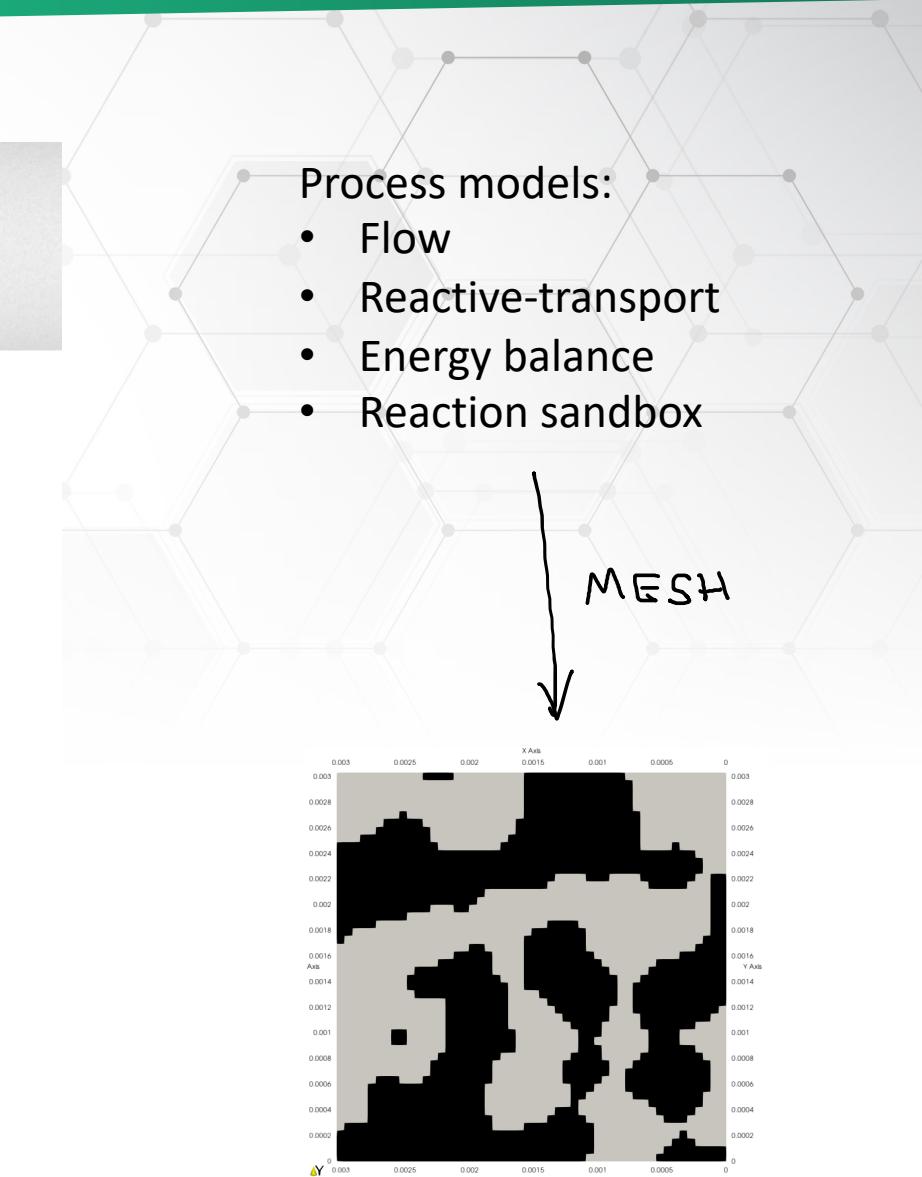
How this data can be used: Example 2 – XCT to PFLOTRAN (work-in-progress)



The screenshot shows the PFLOTRAN website. The header includes a navigation bar with links: PFLOTRAN, About, Bitbucket, Installation, Documentation, Parallel Performance, Development Team, and Publications. Below the header is a large logo with the word "PFLOTRAN" in bold black letters. The letter "O" contains a stylized water drop icon with red and blue lines. A subtitle below the logo reads: "A Massively Parallel Reactive Flow and Transport Model for describing Subsurface Processes".

What is PFLOTRAN?

PFLOTRAN is an open source, state-of-the-art massively parallel subsurface flow and reactive transport code. PFLOTRAN solves a system of generally nonlinear partial differential equations describing multiphase, multicomponent and multiscale reactive flow and transport in porous materials. The code is designed to run on massively parallel computing architectures as well as workstations and laptops. Parallelization is achieved through domain decomposition using the PETSc (Portable Extensible Toolkit for Scientific Computation) libraries. PFLOTRAN has been developed from the ground up for parallel scalability and has been run on up to 2¹⁸ processor cores with problem sizes up to 2 billion degrees of freedom. PFLOTRAN is written in object oriented, free formatted Fortran 2003. The choice of Fortran over C/C++ was based primarily on the need to enlist and preserve tight collaboration with experienced domain scientists, without which PFLOTRAN's sophisticated process models would not exist. The reactive transport equations can be solved using either a fully implicit Newton-Raphson algorithm or the less robust operator splitting method.



How this data can be used: Example 2 – XCT to PFLOTRAN (work-in-progress)

```
1 # Description: Reaction Sandbox Simple (A + B --> C + D)
2 # Number of reaction network parameters: D = 7
3 # Sobol-based GSA: N * (2D+2) samples for first and second-order indices
4
5 =====
6 SIMULATION
7   SIMULATION_TYPE SUBSURFACE
8   PROCESS_MODELS
9     SUBSURFACE_TRANSPORT transport
10    MODE GIRT
11  /
12  /
13 END
14 =====
15
16 SUBSURFACE
17
18 ===== constraints =====
19 # modify these initial concentration
20 CONSTRAINT initial
21   CONCENTRATIONS # [mol/L]
22     Aaq 1.d-3 F
23     Baq 5.d-4 F
24     Caq 1.d-10 F
25     Daq 1.d-10 F
26     Eaq 1.d-10 F
27  /
28   IMMOBILE # [mol/m^3 bulk]
29     Xim 1.d-4
30     Yim 1.d-10
31  /
32 END
33
34 ===== chemistry =====
35 CHEMISTRY
36   PRIMARY_SPECIES
37     Aaq
38     Baq
39     Eaq
40     Caq
41     Daq
42  /
43   IMMOBILE_SPECIES
44     Yim
45     Xim
46  /
```

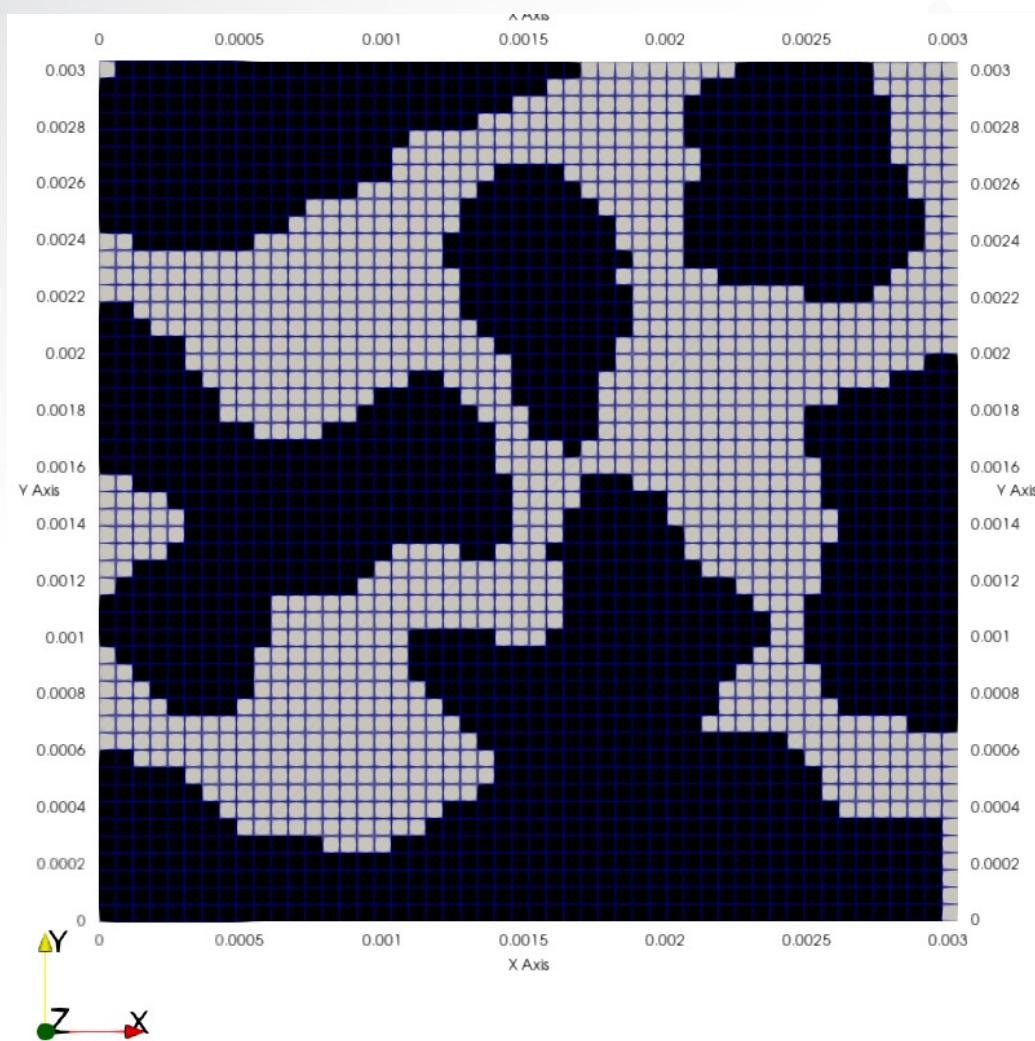
Carbon degradation modeling using PFLOTRAN

- Process models:
- Flow
 - Reactive-transport
 - Energy balance
 - Reaction sandbox

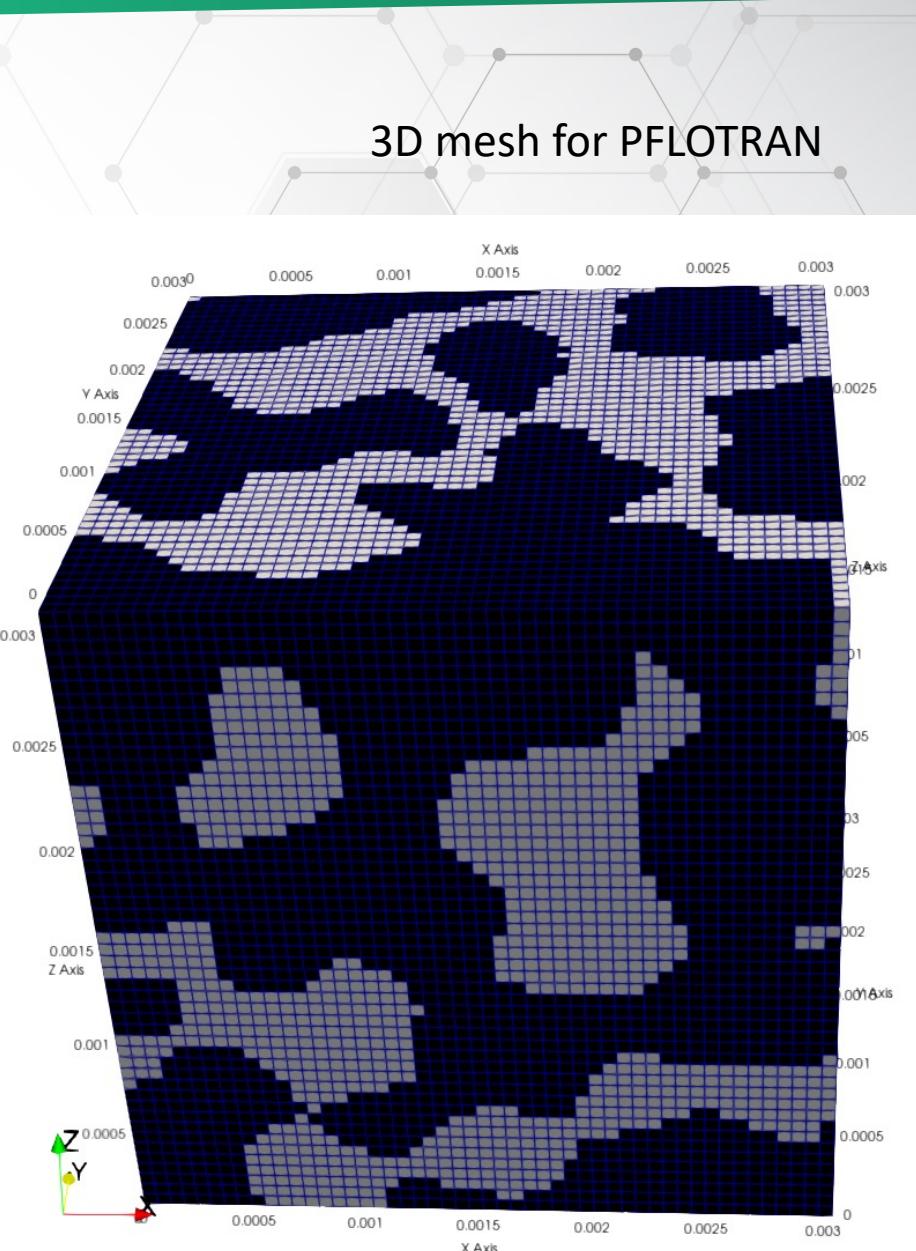
Example:
PFLOTRAN
input deck
for numerical
simulations

How this data can be used: Example 2 – XCT to PFLOTRAN (work-in-progress)

2D view of the mesh for PFLOTRAN

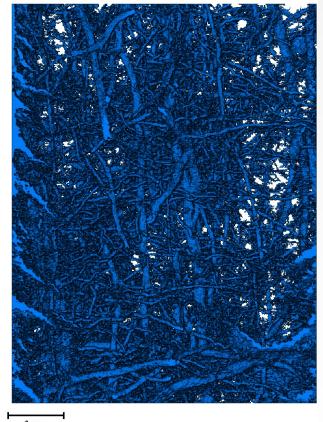


3D mesh for PFLOTRAN

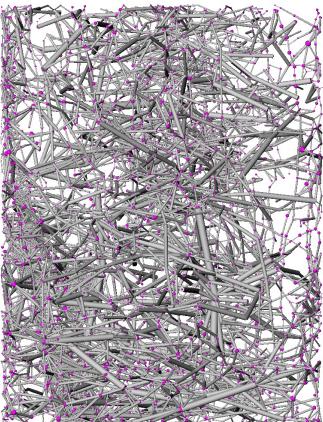


How this data can be used: Example 3 – Pore network modeling

XCT (AVIZO)

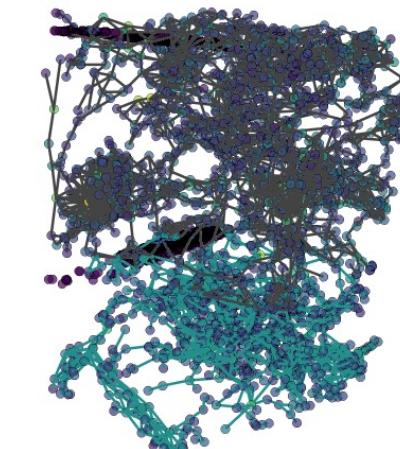
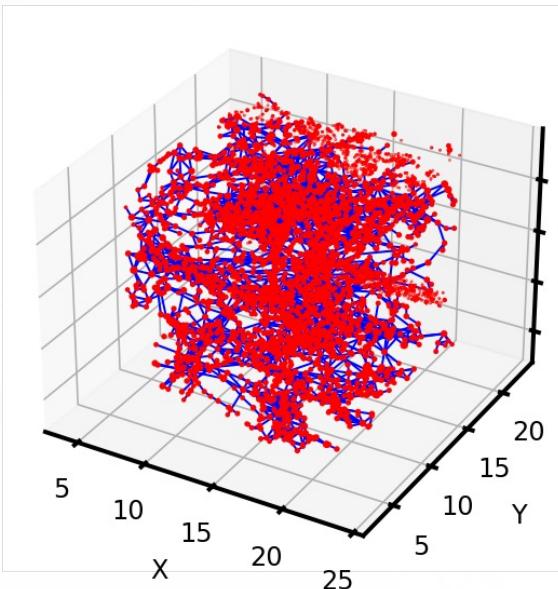


Connected pores



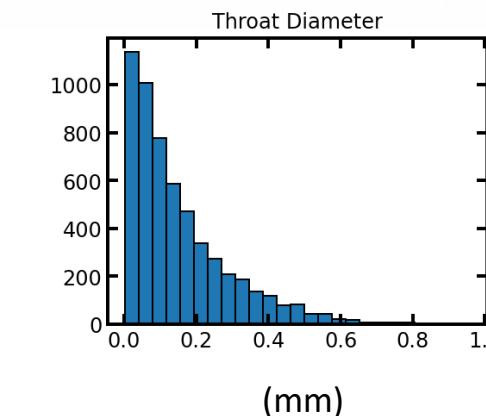
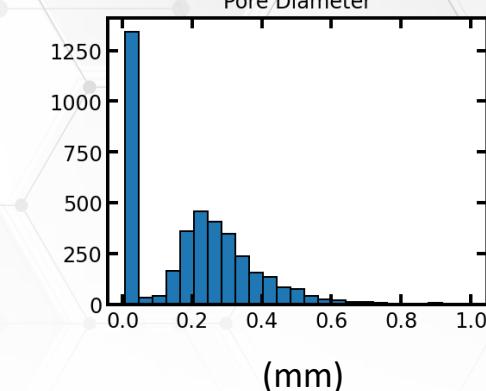
Pore Network Model

OpenPNM

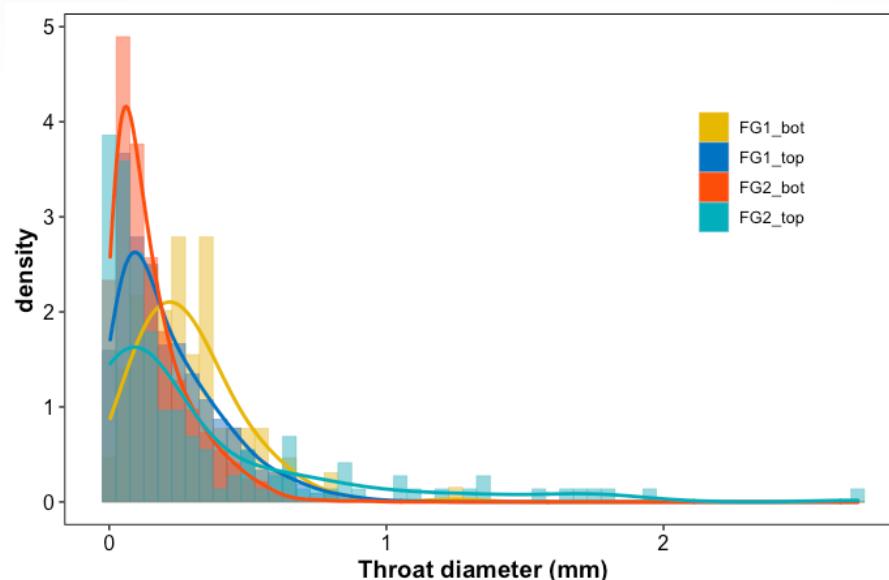
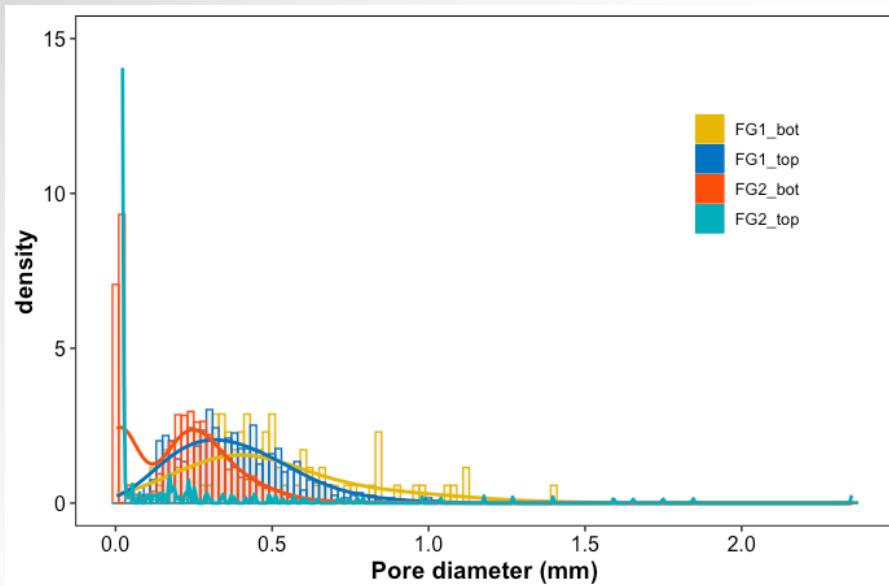


Reconstructed pore network

Probability distribution functions



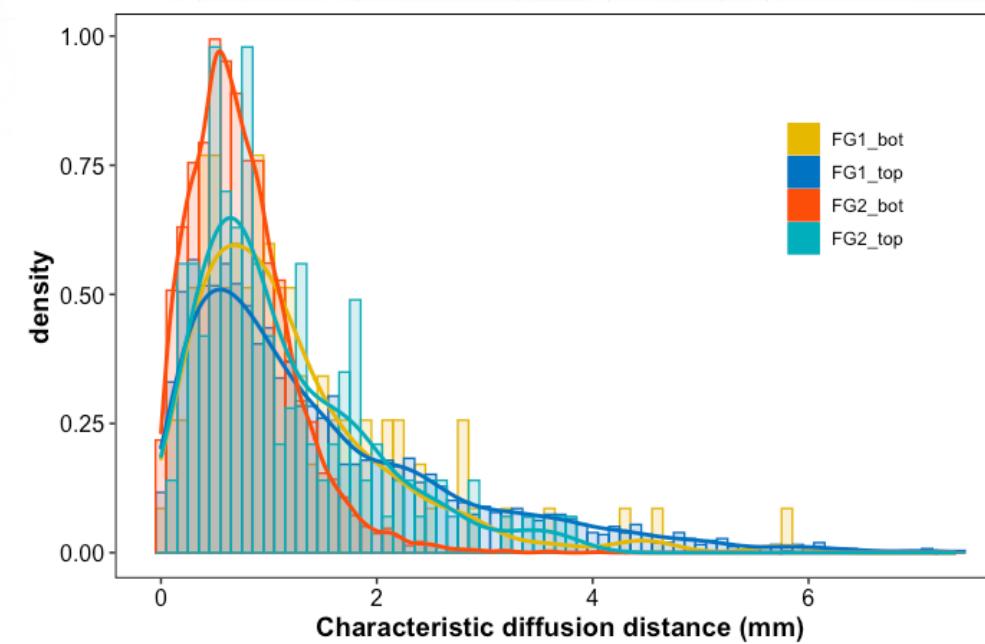
Example 3 - Geometry of pore network informs probability distribution functions (PDFs)



- Diffusion length calculated from pore diameter

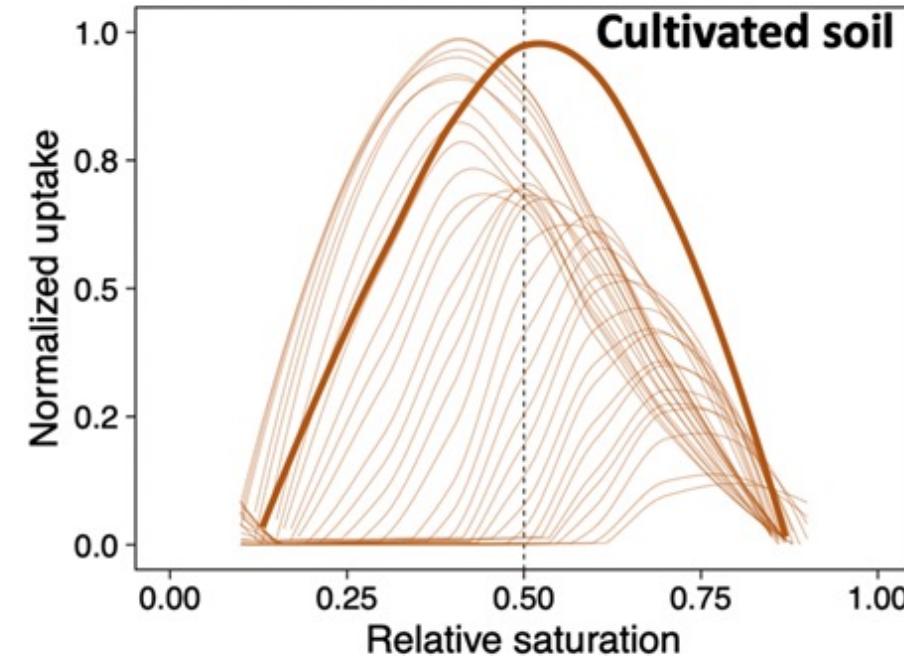
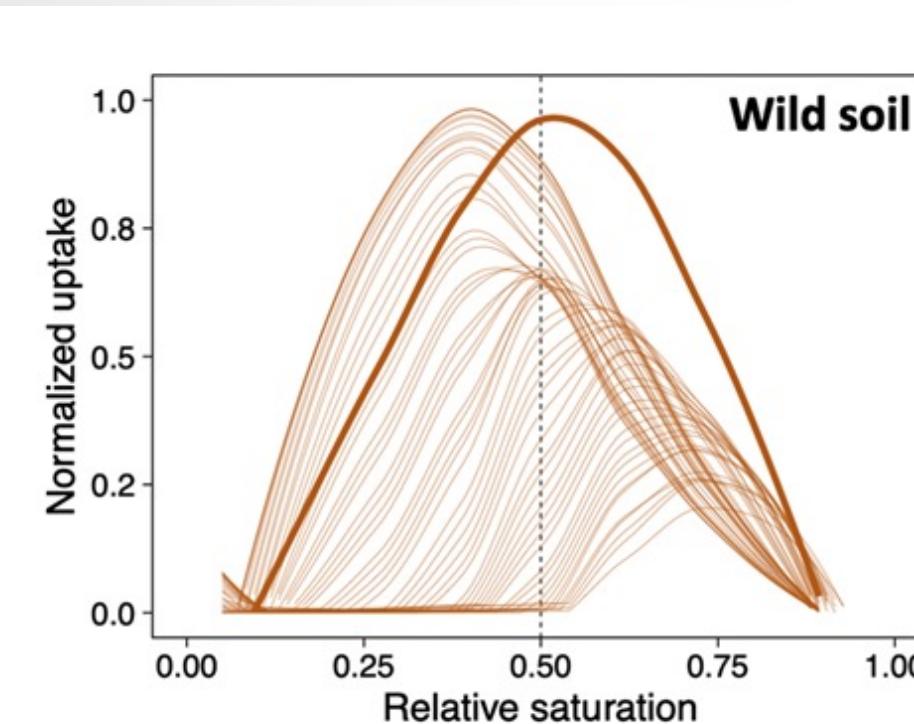
$$L_{i,j} = L - (r_{pore,i} + r_{pore,j})$$

- Longer diffusion length for Cultivated soil due to its finer pore sizes and less pore connectivity



Example 3 - Implementation of porosity and SOM information in reactive transport modeling

Diffusion limited SOM decomposition kinetics



Soil respiration as normalized C uptake vs relative soil saturation compared for a “wild” and a cultivated soil. Soil respiration appears reduced in the cultivated soil relative to the “wild” due to reduced pore network connectivity.

References

- Avizo: <https://www.thermofisher.com/us/en/home/electron-microscopy/products/software-em-3d-vis/avizo-software.html>
- ImageJ/Fiji: <https://imagej.nih.gov/ij/download.html> and <https://fiji.sc/>
- Modeling:
 - OpenPNM:
 - <https://openpnm.org/>
 - <https://github.com/PMEAL/OpenPNM>
 - PoresPy:
 - <https://porespy.org/>
 - PFLOTRAN:
 - <https://www.pfotran.org/>
 - OpenFOAM:
 - <https://www.openfoam.com/>

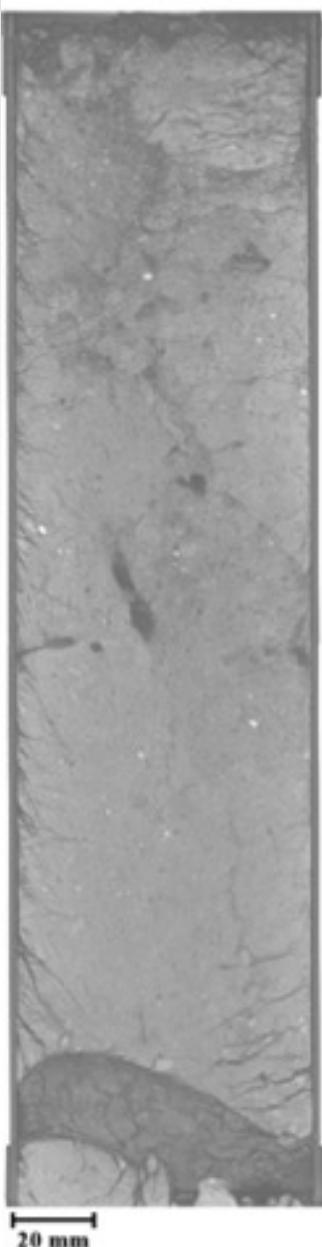
Questions?



Extras



Our methodology to estimate bulk density from CT data



Estimate of bulk density is based on formula from Tanaka *et al.*, *Earth Planets Space*, **63**, 103–110, 2011:

$$HU = \frac{1000(\mu - \mu_w)}{\mu_w},$$

where HU means Hounsfield Units, μ is the grey value of a given voxel and μ_w is the grey value of water for our scan. μ_w was obtained from finding the average grey value of water in a previous scan with similar conditions. Then we used *HUs* to estimate the bulk density for a given pixel through the formula

$$\rho = \frac{0.677}{1000} HU + 1.0756.$$

Finally, we averaged the bulk densities for all pixels that are soil or pore (excluding wall porosity) to find the overall average bulk density of the scan.

Wet bulk density: $\approx 1.50 \frac{g}{cm^3}$

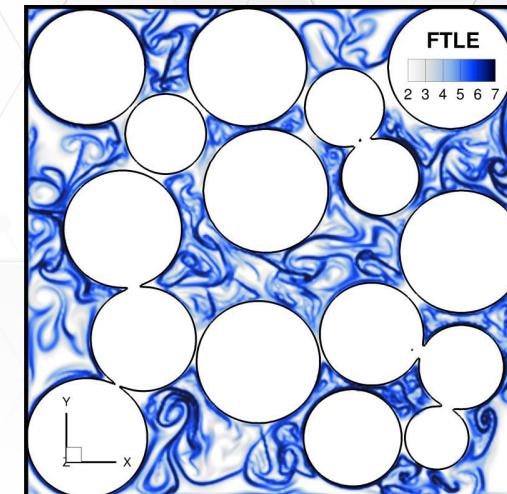
CFD - A bigger picture

Objective: Address the critical gap in our ability to translate molecular understanding and data to parameters for ecosystem-scale reactive transport models.

1. Spatial heterogeneity:

E.g., How convective water flow distributes soluble nutrients through the heterogeneous pore space?

- A direct visualization of 3D distribution with temporal evaluations
- A full spectrum of data set for detailed analysis

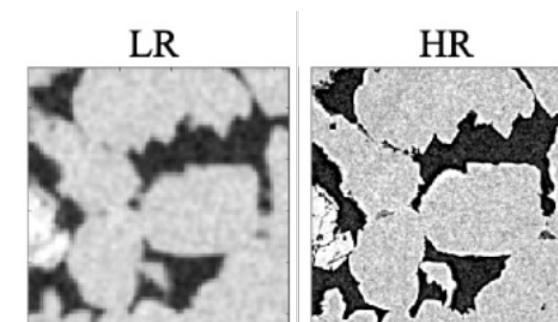


Finn 2013
Thesis

2. Spatial resolution:

Overall porosity measured from XCT data differs from that obtained in lab measurement

- Micro-continuum approach (*Scheibe et al., 2014 WRR, Soulaine et al., 2017 JFM*)
- Multi-resolution simulation framework (*Fukami et al. 2018 JFM*)
- Identify key spatial scales for specific physical/chemical/biological processes



Jackson et
al. 2022
PRApplied

CFD - Upscaling

Question: How to translate the pore-scale dataset to reach-scale simulations?

1. **Volume averaging:** equations that are valid for a particular phase can be spatially smoothed to produce equations valid everywhere
(Whitaker 1996; Soulaine et al., 2017 JFM; Wood, He and Apte, 2020 ARFM)

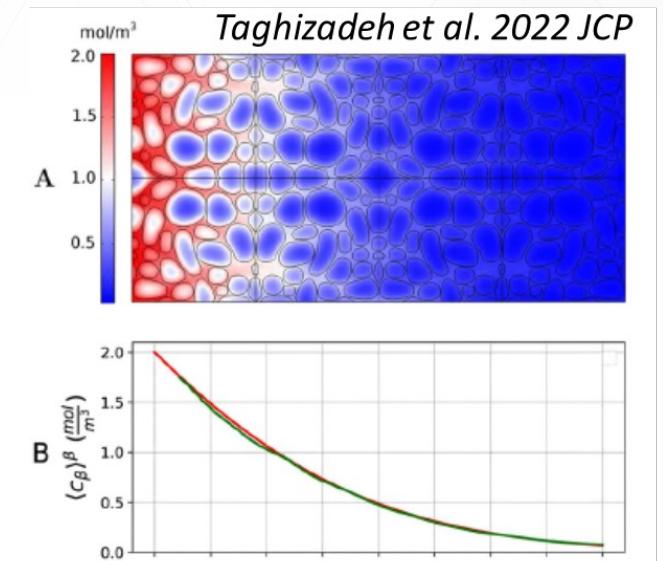
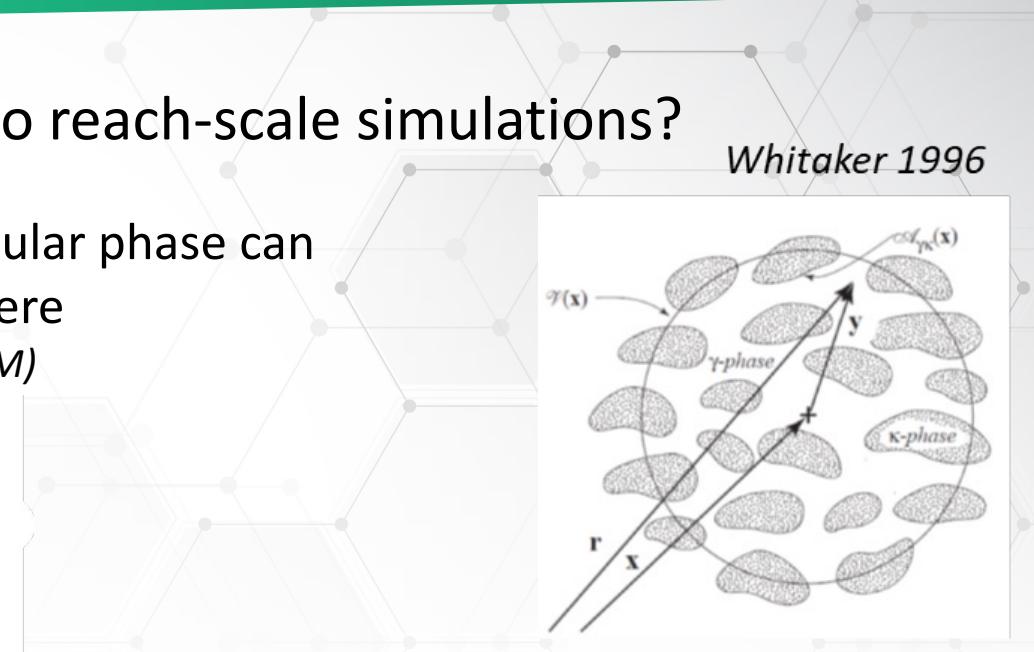
The volume average theorem for any quantity ψ in the fluid (γ) phase:

$$\langle \psi_\gamma \rangle = \frac{1}{V} \int_{\mathbf{r} \in \mathcal{V}_\gamma(\mathbf{x})} \psi_\gamma(\mathbf{r}) dV(\mathbf{r})$$

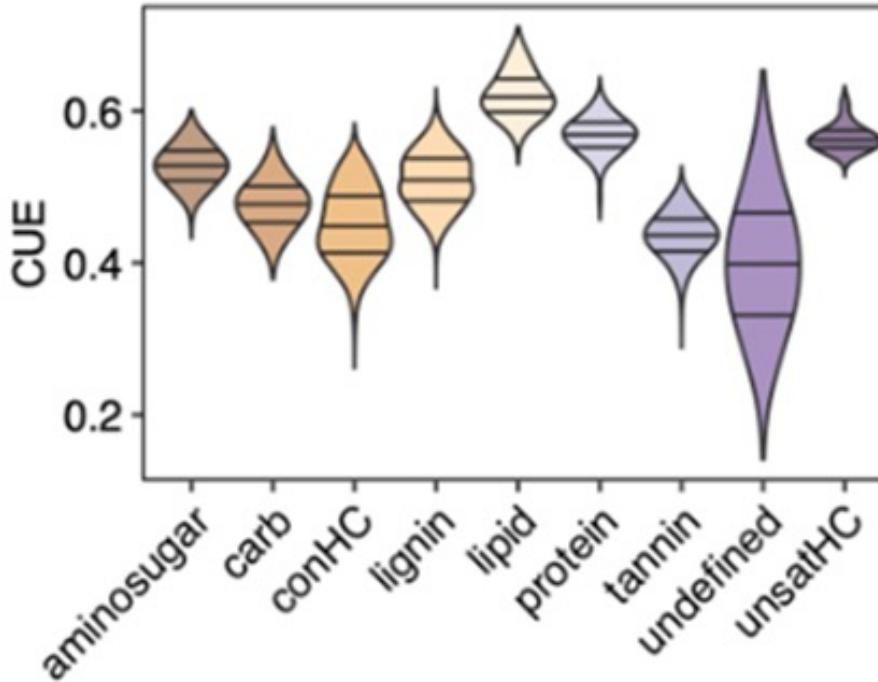
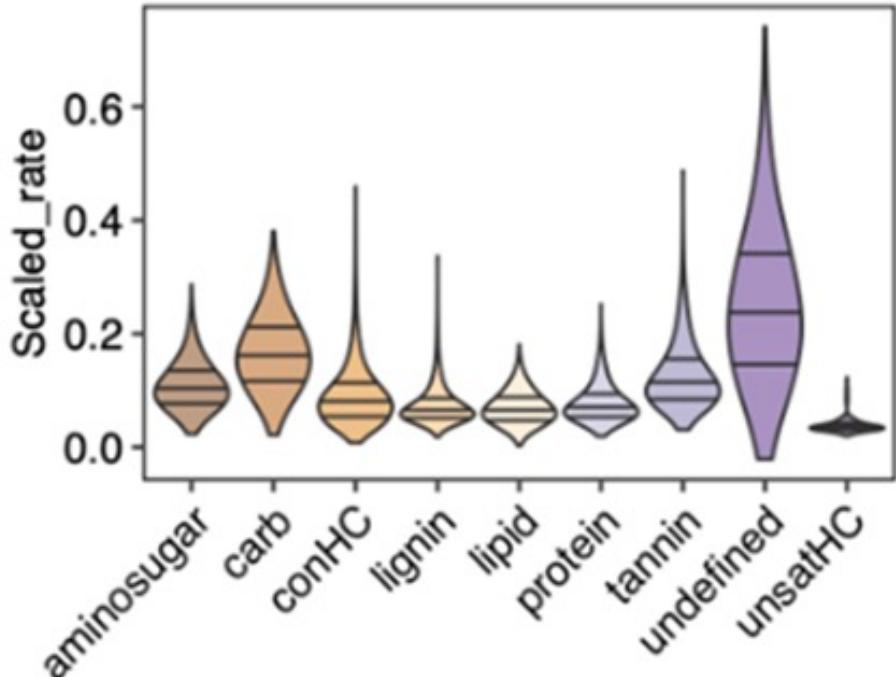
where V is the total volume in the averaging domain.

2. **Machine learning approach** (Taghizadeh et al. 2022)

- Use a combination of formal upscaling and data-driven machine learning for explicitly closing a nonlinear transport and reaction process in multiscale tissues.
- Utilize the datasets generated from high-resolution and the multi-resolution pore-scale simulations to train the ML networks to solve the nonlinear upscaling problem.



Example 2 – Connection to chemical information

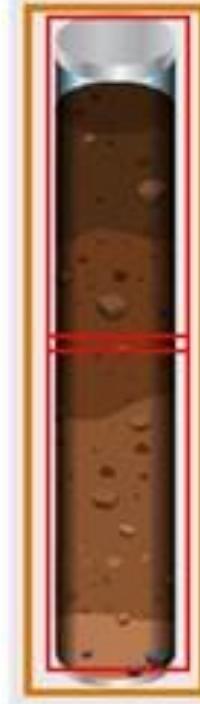


Scaled rate and carbon use efficiency (CUE) were calculated based on molecular information on SOM from FTICR-MS data. Variations in SOM properties can lead to differences in the rate and efficiency of decomposition.

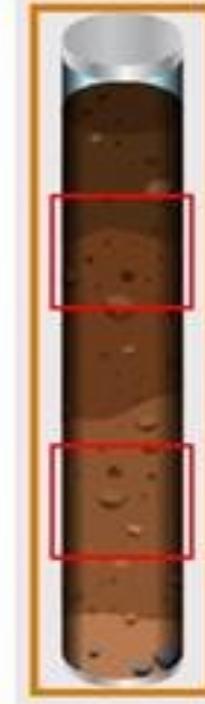
XCT analysis on a typical MONet soil core at EMSL

Tamas Varga

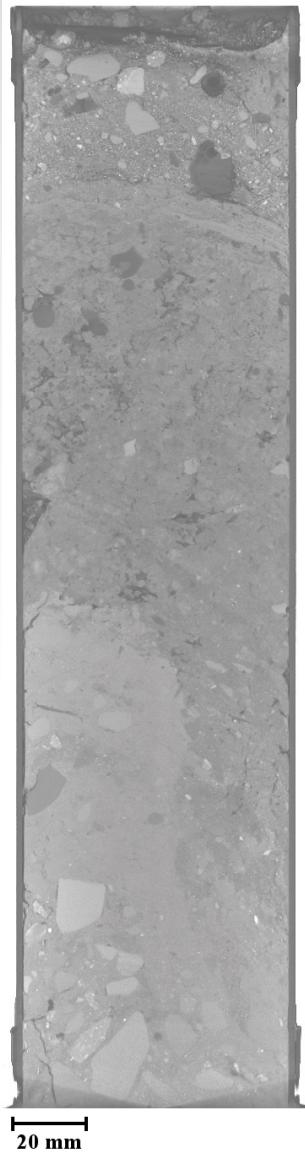
Low resolution XCT
scans collected on
whole core in 2
tiles
(82.5 microns voxel
size)



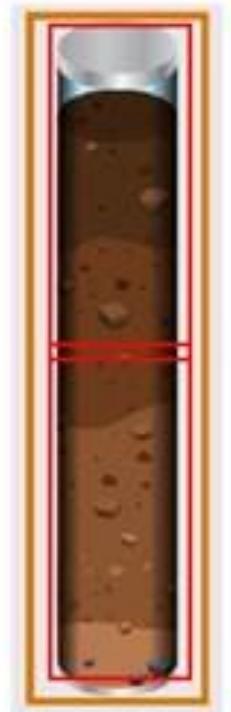
High resolution XCT
scans collected on
top and bottom
sections
(38.2 microns voxel
size)



Whole core (merged low-resolution data on top and bottom sections)



*Tomographic image of
whole core in XZ
plane view*



The two lower-resolution (82.5 micron voxel size, estimated spatial resolution 165 microns) scans are used to get the overall image of the whole 1-ft tall core. This image has been stitched together from two tiles as suggested in the title.

Scan conditions:

X-ray power: 105 kV and 325 μ A

Projections: 1600

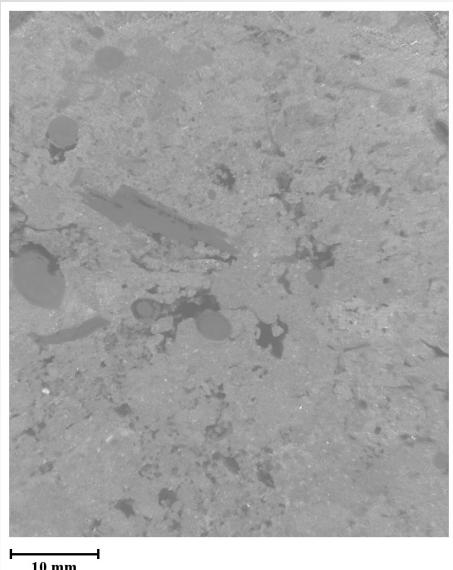
Frames/projection: 2

Exposure time: 500 ms

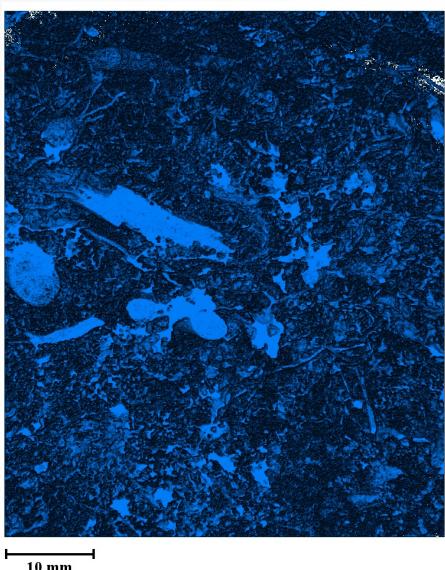
Filter: 0.5-mm Cu foil

Voxel size is 82.5 microns

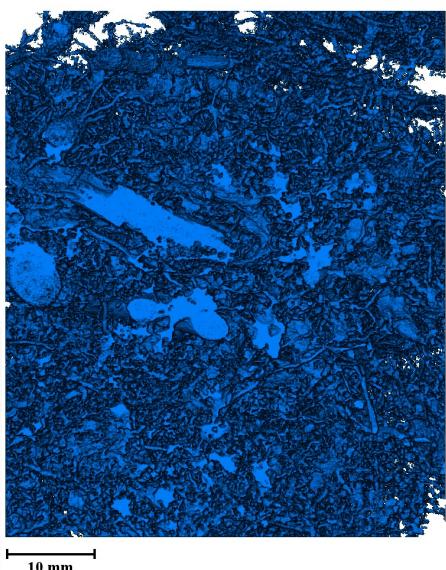
Higher-resolution scan (with 38.2-micron voxel size) on the top section of core



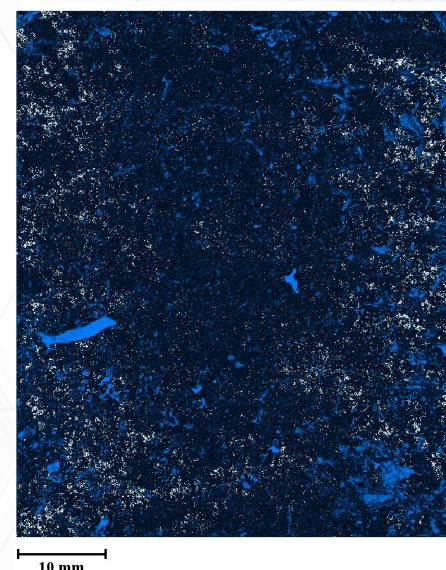
Reconstructed, cropped volume



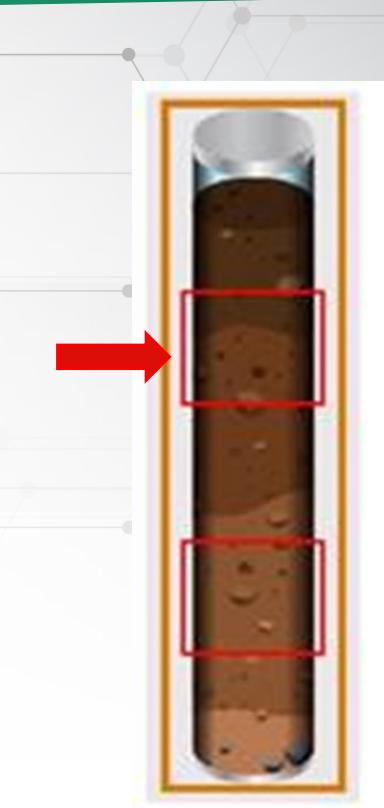
Visualizing all pores



Only connected pores



Only unconnected pores

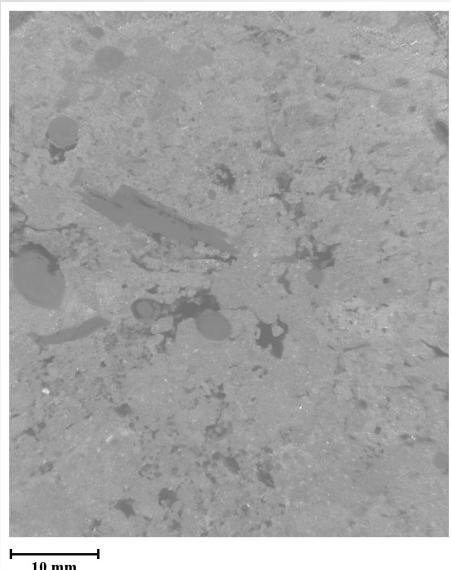


- Total Porosity: 10.97 %
- Connected Pores Percentage: 89.75 %
- Wet Bulk Density: $\approx 2.05 \frac{g}{cm^3}$

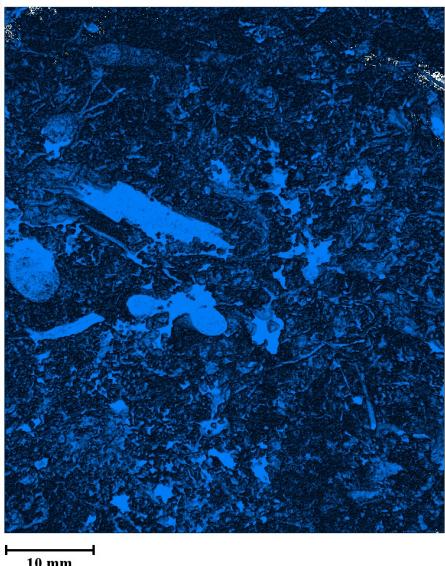
- Mean Pore size: 0.06448 mm
- Min Pore size: 0.047327 mm
- Max Pore size: 29.63071 mm
- Median Pore size: 0.047338 mm
- Variance Pore size: 0.001942 mm
- Mean Pore Volume: 0.005736 mm³

Cropped volume size analyzed here:
50x45x60 mm

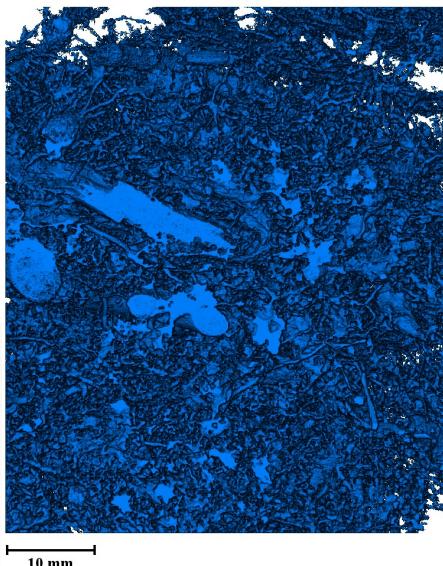
Pore network modeling (PNM) results on higher-resolution data from top section of core



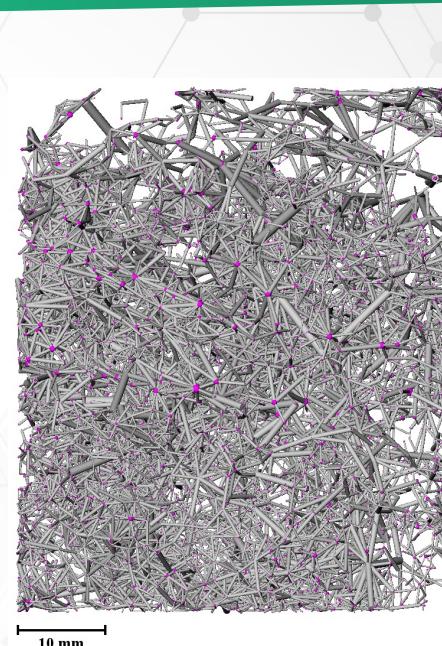
Reconstructed, cropped
volume



Visualizing all pores



Only connected pores



PNM



Pore Network Model in Z-direction

- Absolute permeability: $109.69 \mu\text{m}^2$
- Total flow rate: 1102.00 mm^3
- Tortuosity: 1.80

Pore Network Model in Y-direction

- Absolute permeability: $2882.55 \mu\text{m}^2$
- Total flow rate: 50706.88 mm^3
- Tortuosity: 1.52

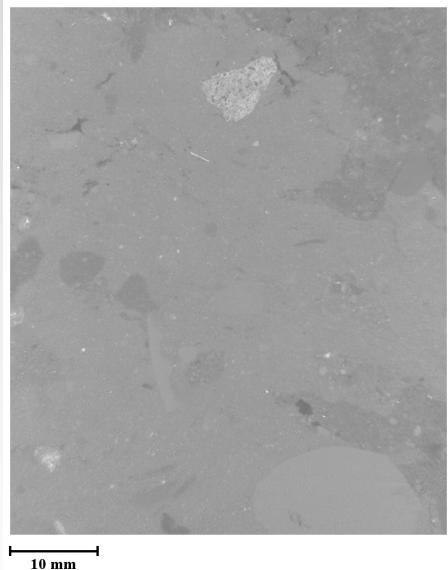
Pore Network Model in X-direction

- Absolute permeability: $379.04 \mu\text{m}^2$
- Total flow rate: 5450.30 mm^3
- Tortuosity: 1.76

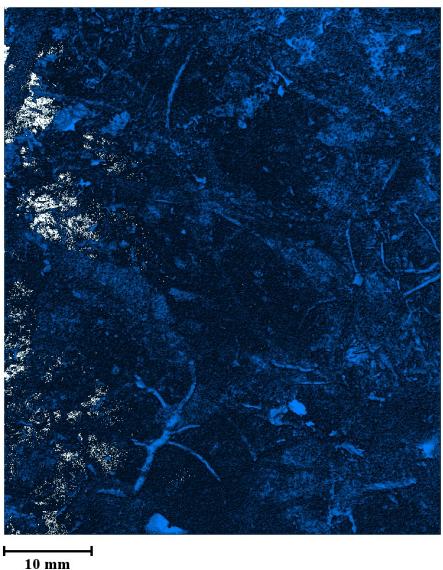
Input pressure: 103098 Pa,
Output pressure: 102833 Pa,
Fluid viscosity: 0.001 Pa.s

Cropped volume:
 $50 \times 45 \times 60 \text{ mm}$

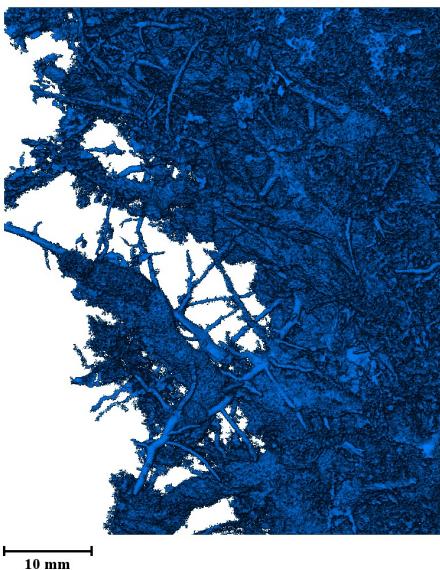
Higher-resolution scan (with 38.2-micron voxel size) on bottom section of core



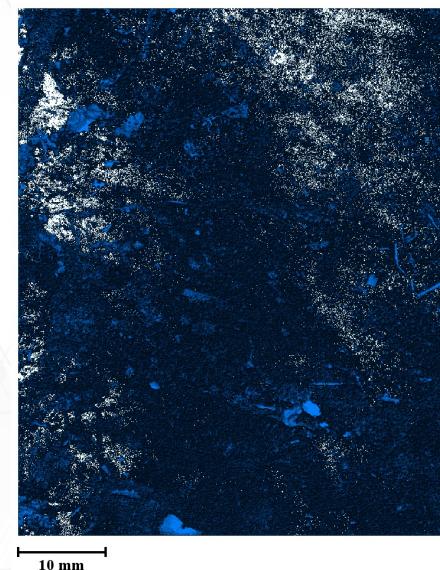
Raw volume



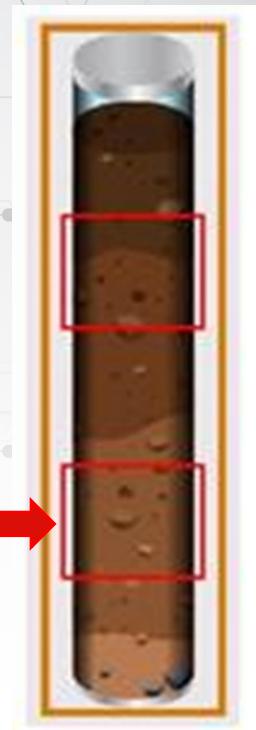
Visualizing all pores



Only connected pores



Only unconnected pores

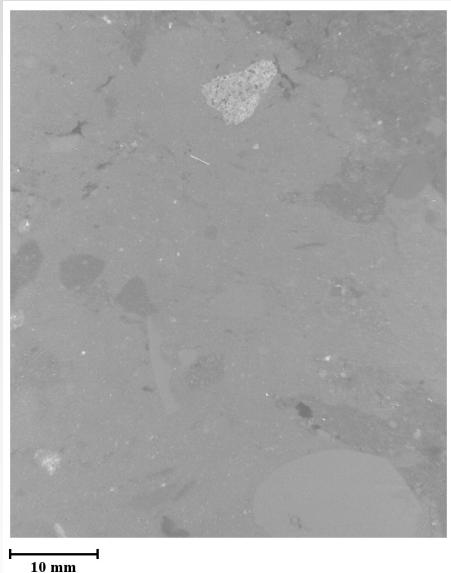


Cropped volume:
50x45x60 mm

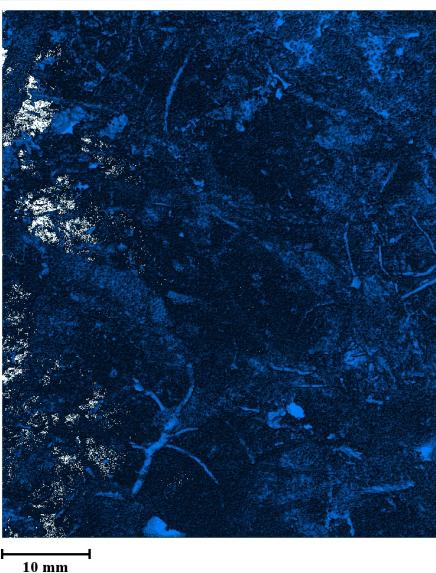
- Total Porosity: 10.22 %
- Connected Pores Percentage: 89.06 %
- Wet Bulk Density: $\approx 2.48 \frac{g}{cm^3}$

- Mean Pore size: 0.060224 mm
- Min Pore size: 0.047327448 mm
- Max Pore size: 28.8251591 mm
- Median Pore size: 0.047327455 mm
- Variance Pore size: 0.000824662 mm
- Mean Pore Volume: 0.002673 mm³

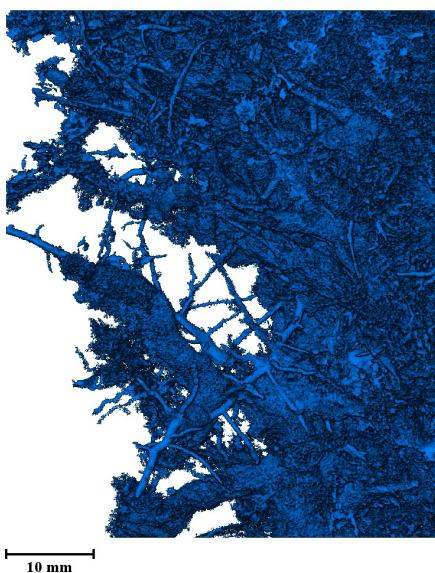
Pore network modeling (PNM) results on higher-resolution data from bottom section of core



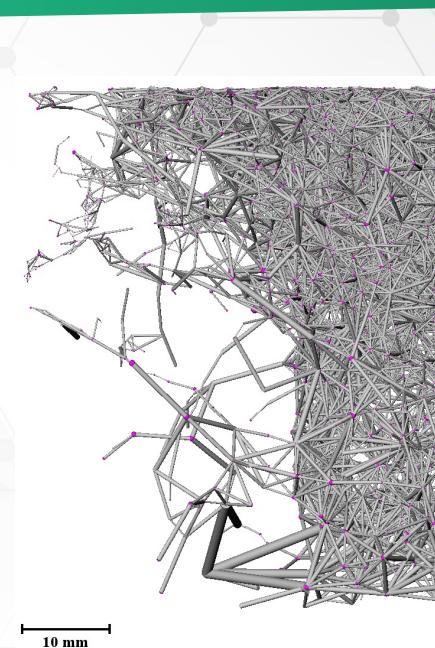
Raw volume



Visualizing all pores



Only connected pores



PNM



Pore Network Model in Z-direction

- Absolute permeability: $601.66 \mu\text{m}^2$
- Total flow rate: 6016.31 mm^3
- Tortuosity: 1.64

Pore Network Model in Y-direction

- Absolute permeability: $751.03 \mu\text{m}^2$
- Total flow rate: 12886.47 mm^3
- Tortuosity: 1.60

Pore Network Model in X-direction

- Absolute permeability: $11.76 \mu\text{m}^2$
- Total flow rate: 169.91 mm^3
- Tortuosity: 1.63

Input pressure: 103098 Pa,
Output pressure: 102833 Pa,
Fluid viscosity: 0.001 Pa.s

Cropped volume:
 $50 \times 45 \times 60 \text{ mm}$

Pore size distribution for top and bottom sections from high-resolution data

<u>Size (mm)</u>	<u>count</u>
0-0.1	979856
0.1-0.2	57796
0.2-0.3	6842
0.3-0.4	2186
0.4-0.5	923
0.5-0.75	693
0.75-1	172
1-5	105
5-10	0
10-25	0
25-50	1
>50	0

Top section

<u>Size (mm)</u>	<u>count</u>
0-0.1	1003966
0.1-0.2	41578
0.2-0.3	2282
0.3-0.4	431
0.4-0.5	143
0.5-0.75	124
0.75-1	22
1-5	26
5-10	1
10-25	0
25-50	1
>50	0

Bottom section

