MONet Community Science Meeting – Introduction to X-ray CT imaging

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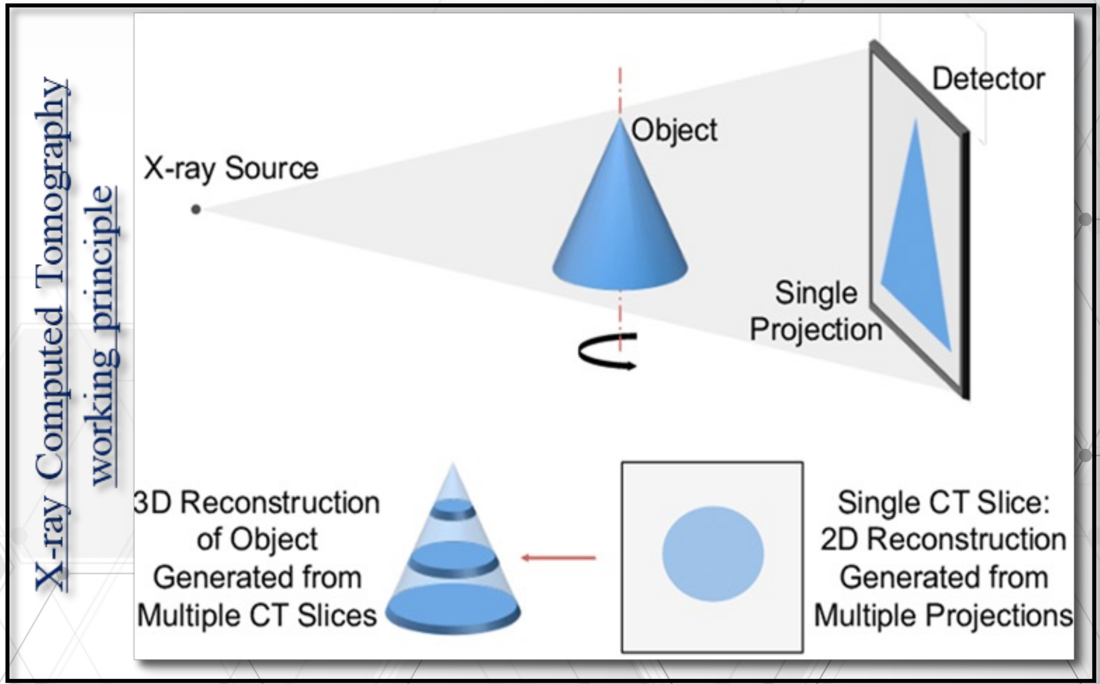
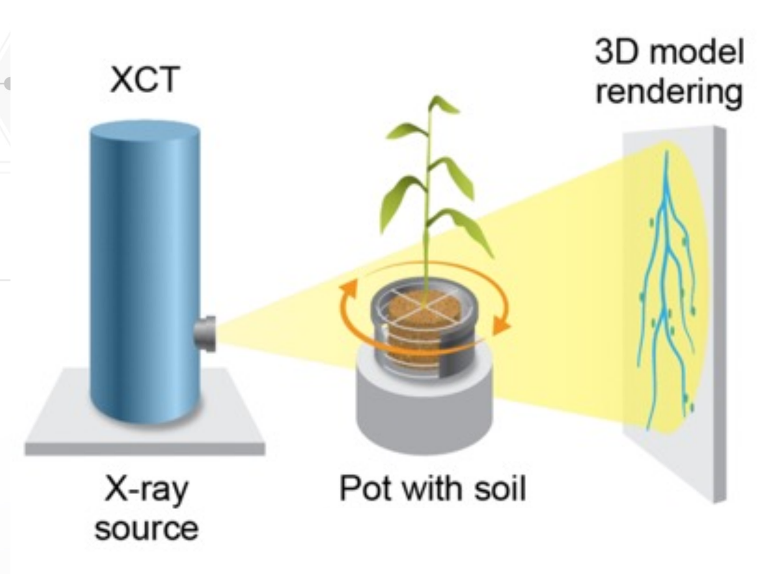




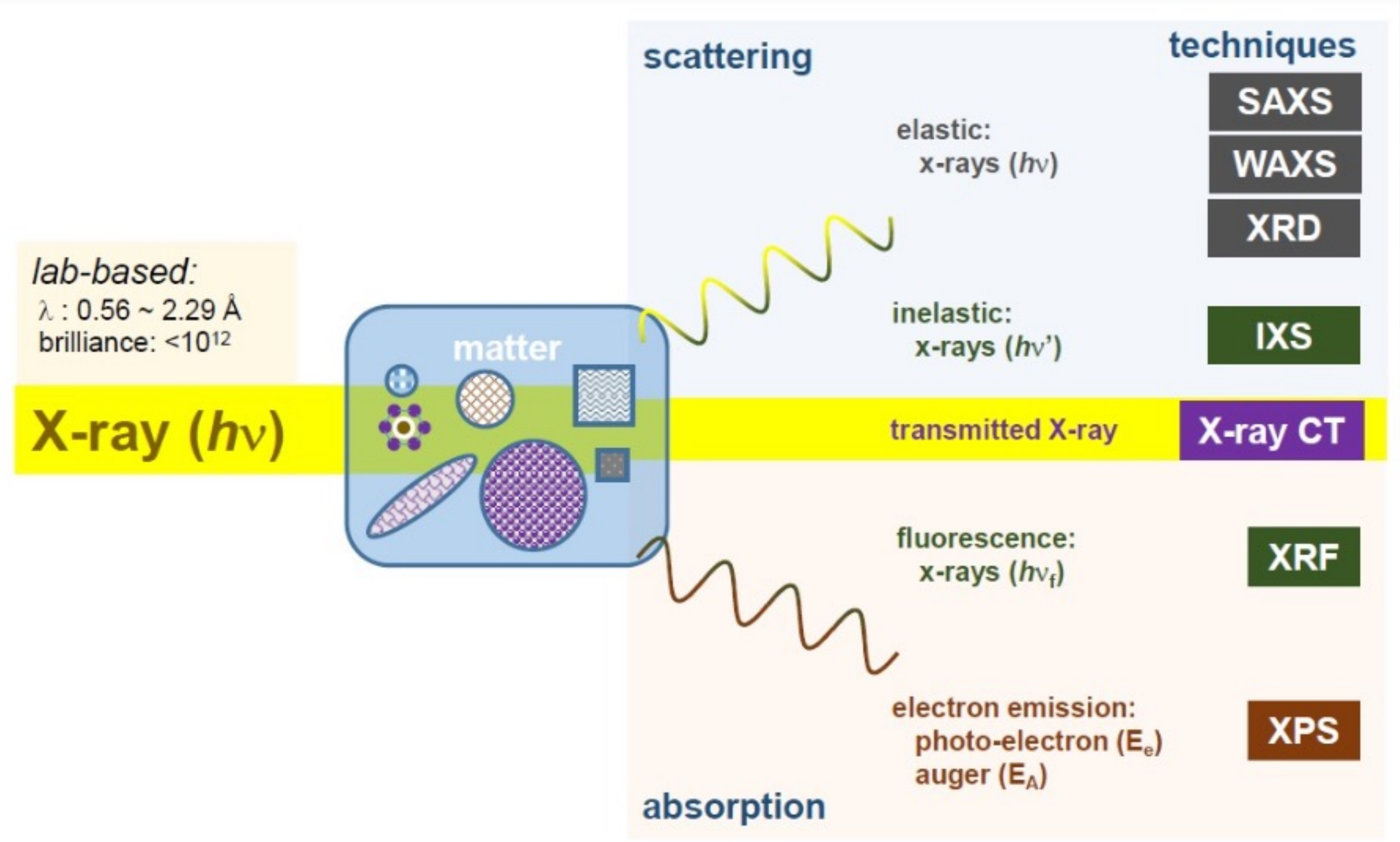
Outline

- Fundamentals of X-ray Computed Tomography (XCT)
- Information XCT can provide
- Examples for use of XCT-based 3D information
- References

What is X-ray Computed Tomography?

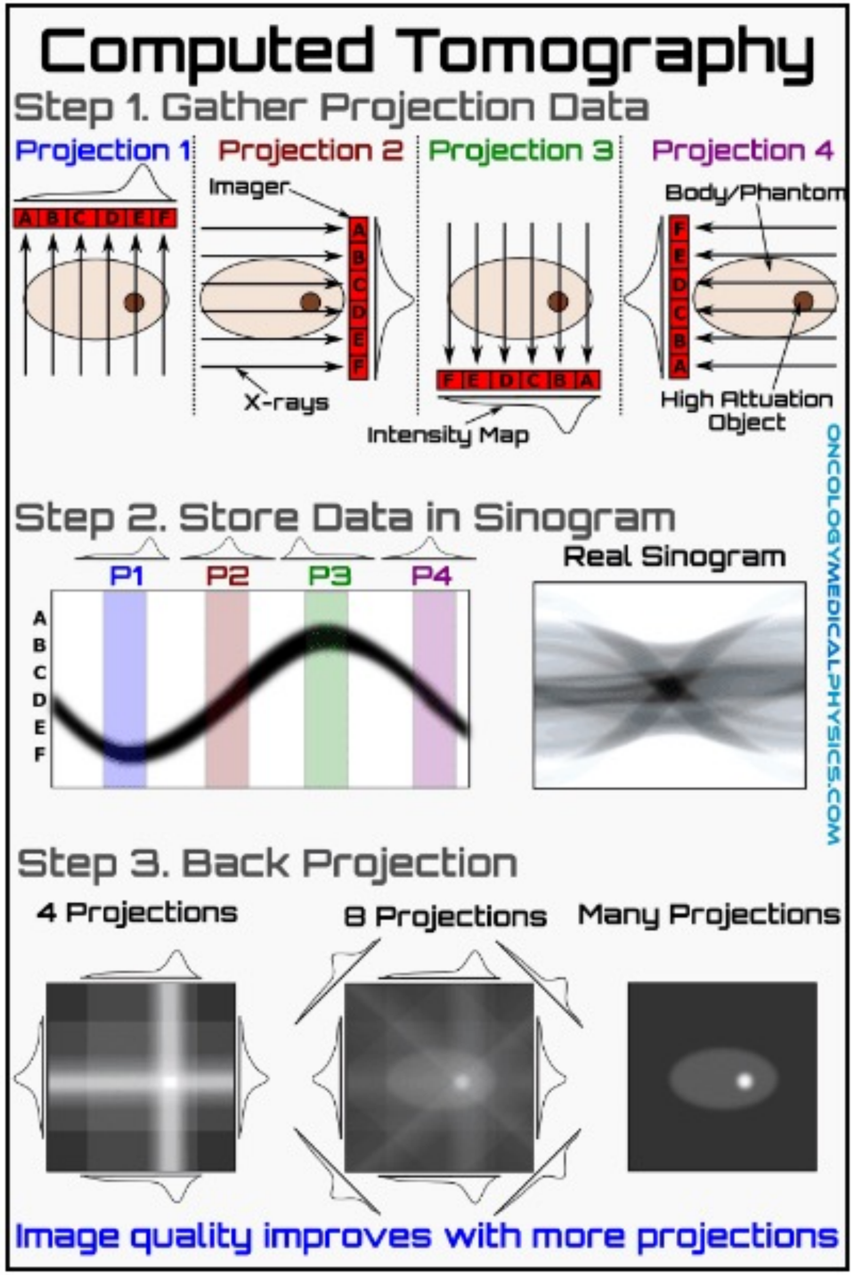
- Non-destructive x-ray imaging to examine/visualize the internal microstructure of objects
- Output: a series of radiographs computationally reconstructed as 3D volume (CT)
- Materials are differentiated in image data based on their electron density (x-ray absorption); difference in x-ray absorption results in different gray level (color) intensity in the image

Fundamentals: Interaction of x-rays with matter – absorption vs. transmission



https://www.ntu.edu.sg/facts/home/research-focus/x-ray-cluster

Fundamentals: CT theory of operation



- X-ray source emits an x-ray beam that hits the sample at a given angle.
- The part of the beam that passes through the sample is intercepted by a detector.
- The detector converts the photon generated signal into an electronic signal.
- The electronic signal of each detector element at each angular position is assembled in a computer and a sinogram is generated.
- The sinogram is converted into a CT image using either filtered back projection or iterative reconstruction.

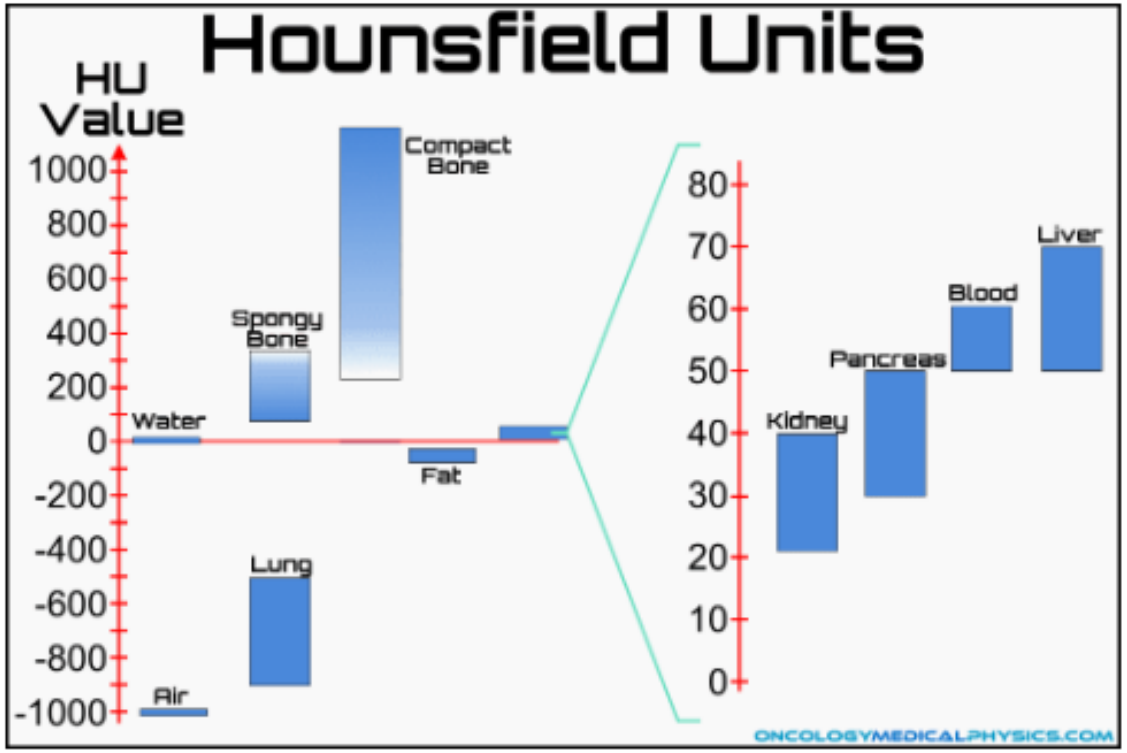
https://oncologymedicalphysics.com/ct-design-and-operation/

Fundamentals: What do CT scans actually “measure”?

Hounsfield Units

CT images are essentially maps of the linear attenuation coefficient (μ) of each voxel. The linear attenuation coefficient is measured in units of *Hounsfield Units* sometimes also called *CT numbers*:

$$HU_{(x,y,z)} = 1000\frac{\mu_{(x,y,z)} - \mu_{water}}{\mu_{water}}$$



- Linear attenuation coefficient, μ, is the percentage of a beam attenuated per unit path length. For kilovoltage energy beams passing through material, the linear attenuation coefficient is dominated by the Compton interaction.

$$\mu = \frac{1}{x} \cdot ln(\frac{I_0}{I_x})$$

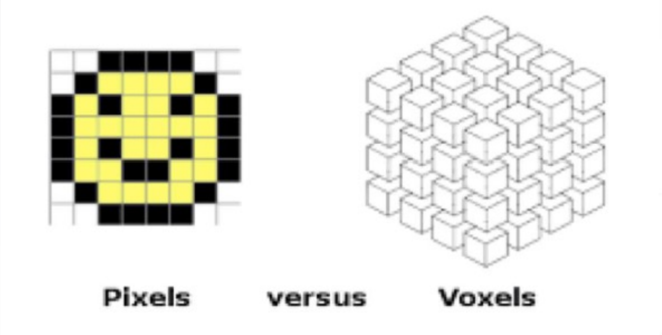
- I_0 is the initial intensity of the beam
- I_x is the intensity of the beam after passing through x distance of material
- x is the length of material traversed

- Since the Compton interaction is proportional to Z (and number of electrons), the linear attenuation coefficient is approximately proportional to the physical density.

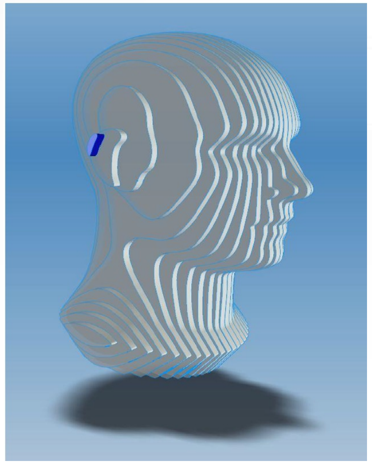
https://oncologymedicalphysics.com/ct-design-and-operation/

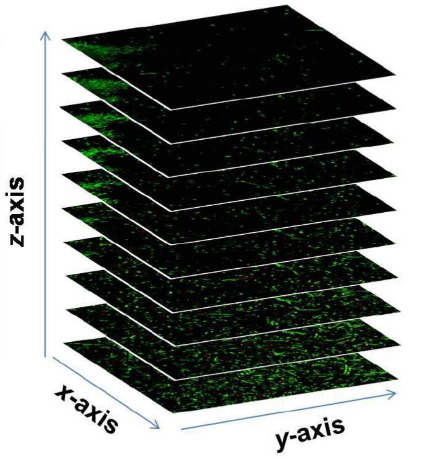
Fundamentals: A few key terms

- Voxels (size), volume data

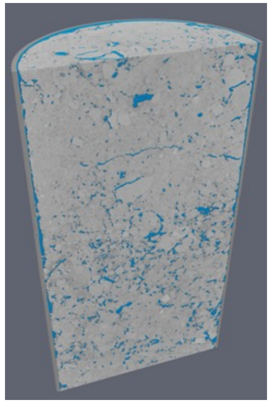


- Slices/stacks



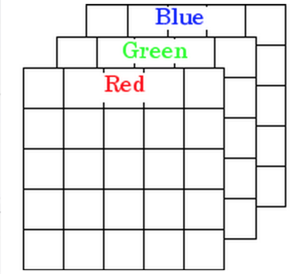


- Segmentation

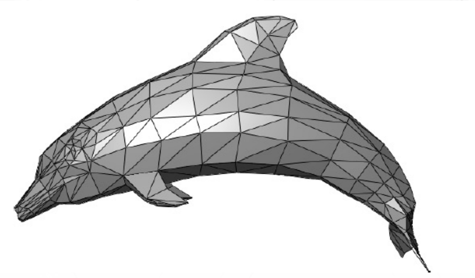


- Gray-scale vs. RGB

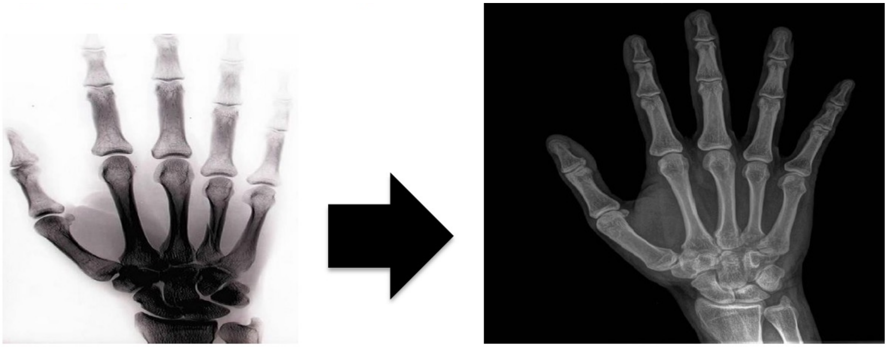
88	82	84	88	85	83	80	93	102
88	80	78	80	80	78	73	94	100
85	79	80	78	77	74	65	91	99
38	35	40	35	39	74	77	70	65
20	25	23	28	37	69	64	60	57
22	26	22	28	40	65	64	59	34
24	28	24	30	37	60	58	56	66
21	22	23	27	38	60	67	65	67
23	22	22	25	38	59	64	67	66



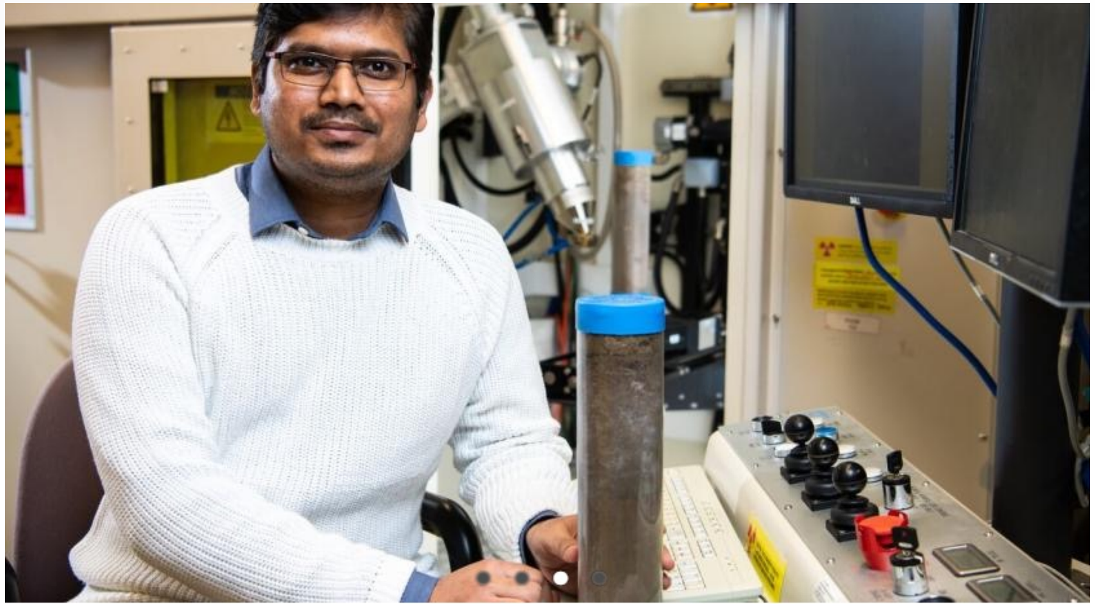
- Mesh

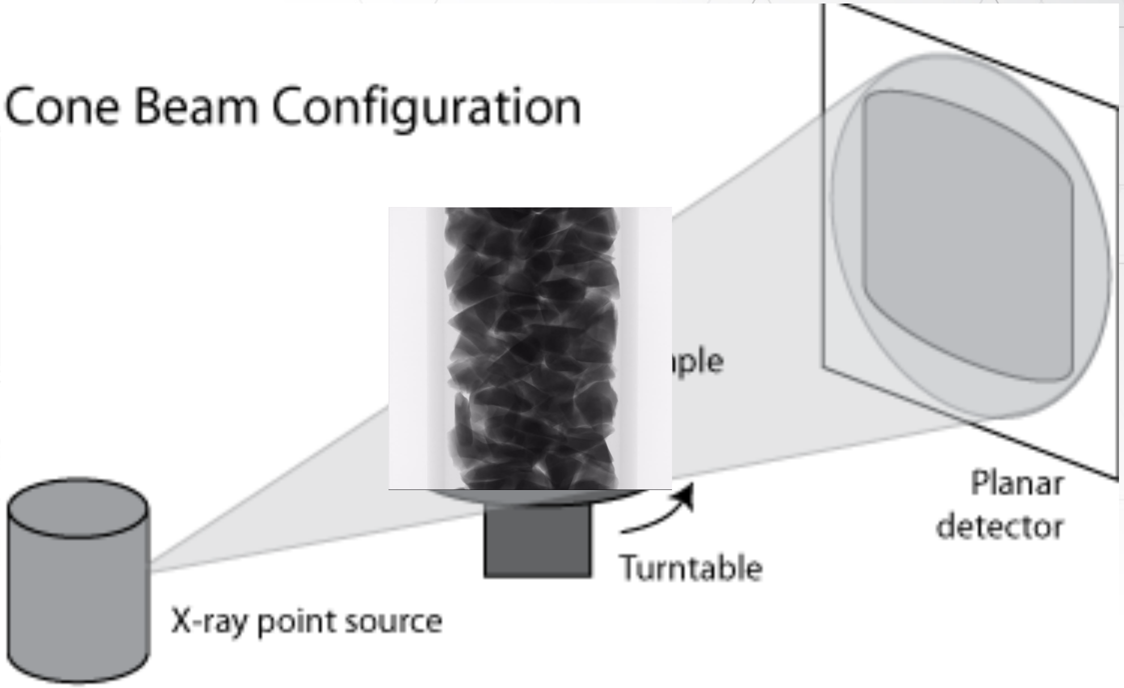


- Radiograph



Fundamentals: How does our x-ray CT work?





http://serc.carleton.edu/images/research_education/geochemsheets/techniques/_1172960774.png

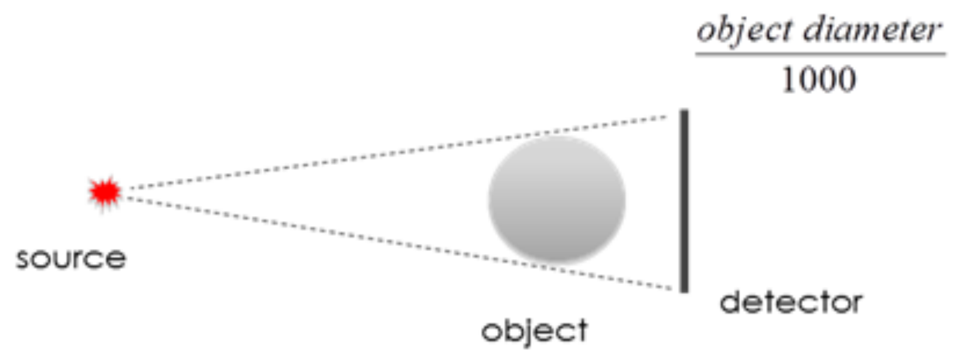
https://www.emsl.pnnl.gov/science/instruments-resources/x-ray-computed-tomography

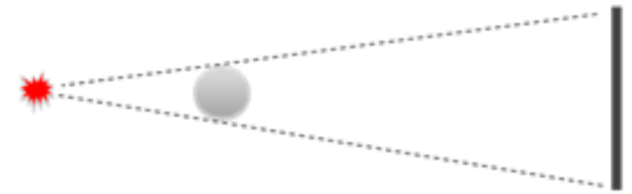
Fundamentals: Imaging conditions

- X-ray source options (power):
  - 225-kV fixed tube (high resolution)
  - 320-kV fixed tube (high penetration)
- Wavelength/E options:
  - reflection target with Ag, Cu, Mo, and W options, filter kit (Ag, Al, Cu, Sn)
- Detector:
  - Area: 40 x 40 cm^2, 2000 x 2000 pixels, 0.2 mm pixel pitch
  - 32/16-bit digitization options
  - ~0.3 – 4 second integration
  - Circular trajectory (Feldkamp-Davis-Kress (FDK) cone beam reconstruction)
- Variable Magnification (M)
  - Object can move between source and detector
  - M ~1 to ~40
- Data collection – Minutes to hours
  - Exposure time (286ms-2s), projections (3142), frames (1-16)
  - Continuous motion *vs* “stop and shoot” shuttle mode (ring-artifact minimization)

Fundamentals: Image resolution

- Spatial resolution or phase contrast?
- Depends on:
  - Sample size / region of interest (sample to source distance – spatial resolution)
  - X-ray power (spatial resolution)
  - X-ray energy, component densities (density resolution/phase contrast)





A Couple Rules:
- Collect projections as object rotates through 360-deg
- Must see full width of object in each projection

- Focal-spot size limits high magnification (and high power)

$$resolution \approx \sqrt{\frac{d_d^2 + \left[d_s(M-1)\right]^2}{M^2}}$$

d_s is the source spot size

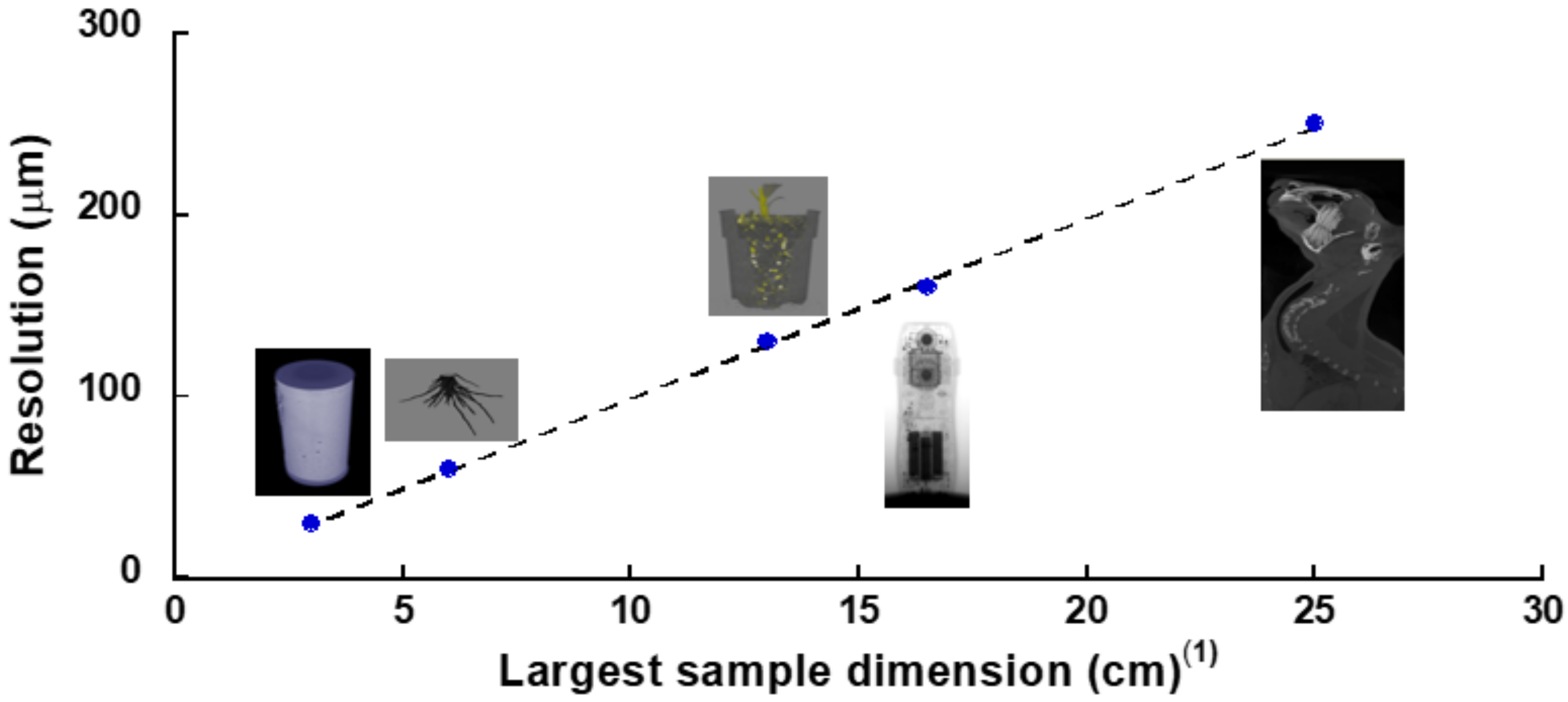
d_d is the detector spot size

M is the magnification

- Focal-spot size changes with power

Tube	Min focal spot	Max focal spot
225kVp fixed	3micron at 3W	100micron at 225W
225kVp rotating	5micron at 3W	30micron at 300W
320kVp	20x40micron at 6W	300x40micron at 320W

Fundamentals: Image resolution *vs* sample size

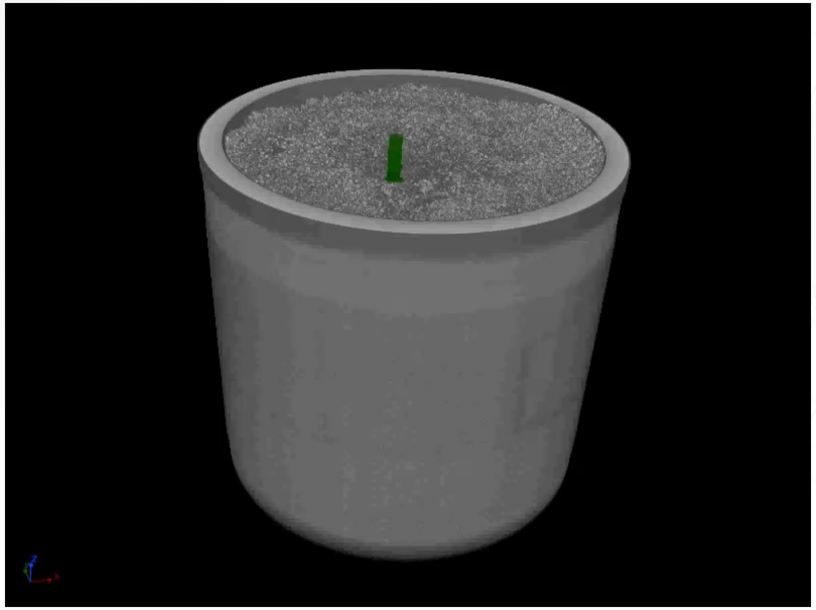


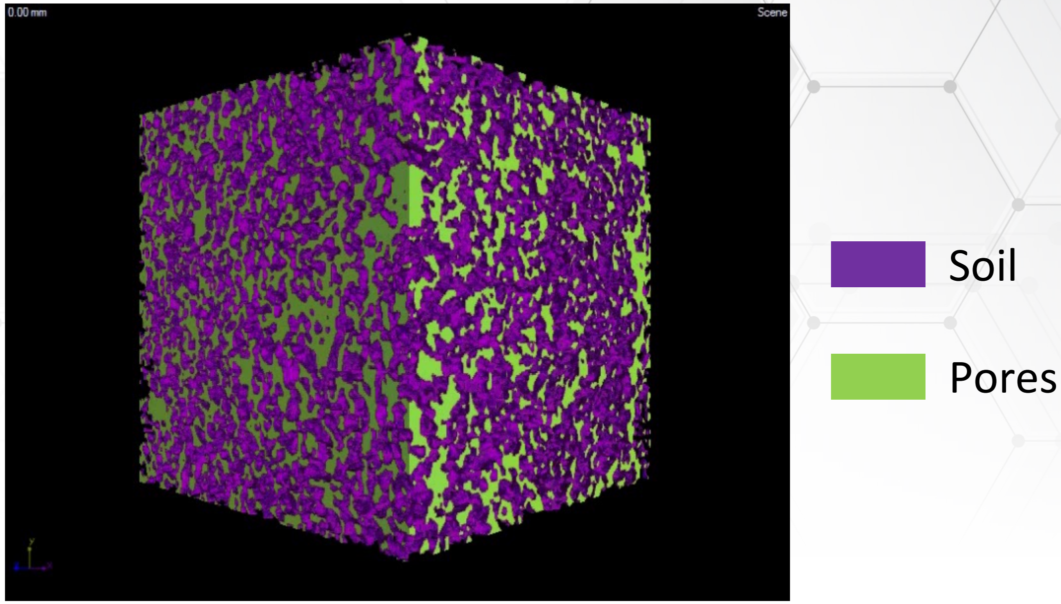
Sample	Size (cm)	M	Distance from X-ray Source	Voxel Size	Resolution	X-ray Power (W)
A scan of a small cement cylinder	1 x 1 x 3	13.1 X	66.4 mm	15.3 µm	30 µm	38.8 W
A scan of the roots of a small potted grass plant	4.5 x 4.5 x 6	6.7 X	136.1 mm	31.3 µm	60 µm	16.2 W
A scan of a small ficus plant, with both plant and roots visible	13 x 13 x 13	3.0 X	286.5 mm	65.7 µm	130 µm	12.3 W
A scan of a handheld telephone	7 x 7 x 16.5	2.4 X	361.3 mm	83 µm	160 µm	37.5 W
A scan of a rabbit in a plastic bucket	25 x 25 x 14	1.6 X	539.8 mm	124 µm	250 µm	32.4 W

Information content in CT images: A couple of examples

Provides a computer model of the 3-dimensional internal structure of samples:

Smith et al., Nature Communications 8: 1335 (2017)





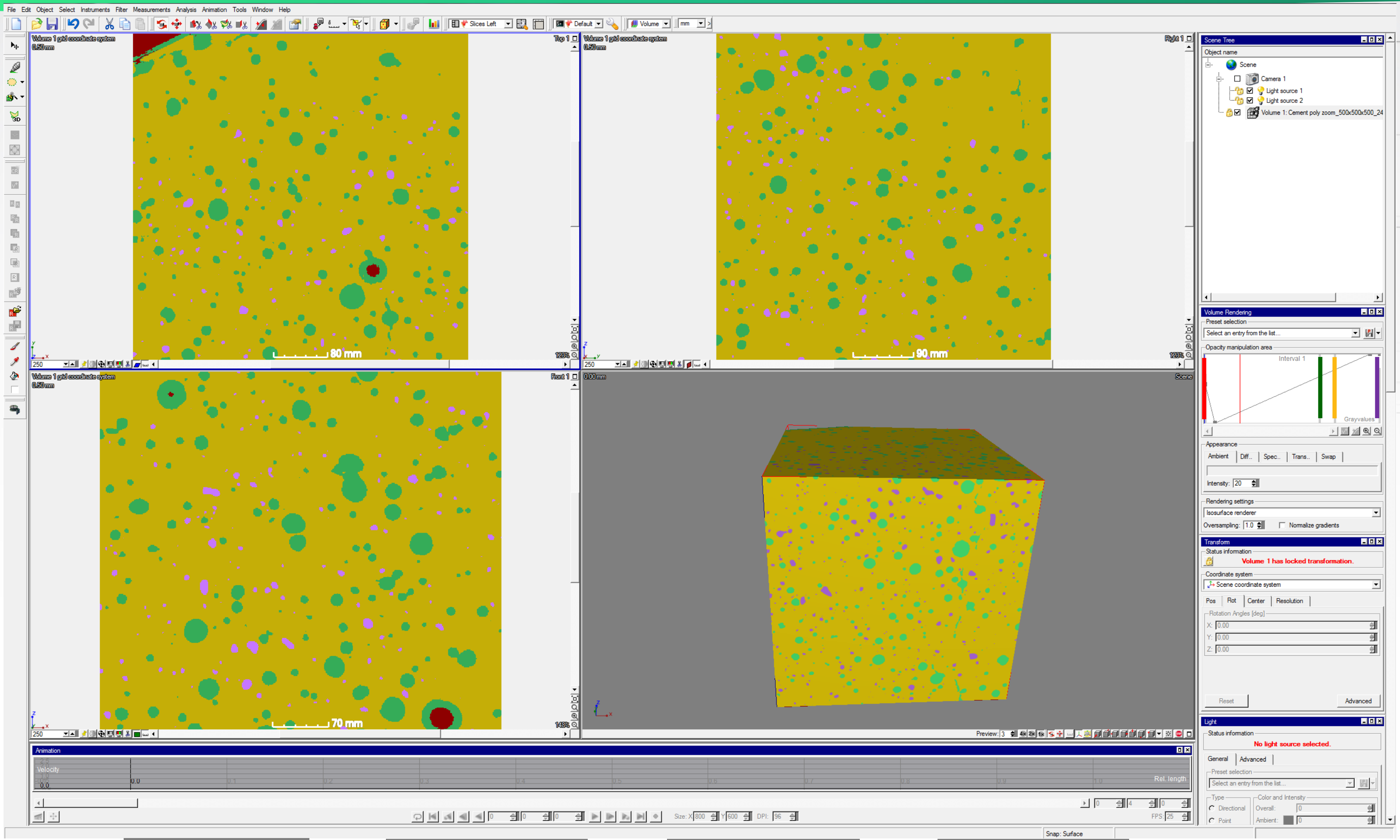
Segmentation of root architecture from whole plant:

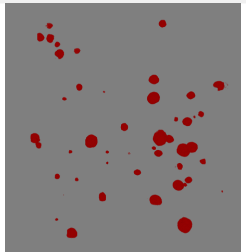
- Mapping root structure to drought, CO_2, temperature etc.
- Computation of root volume, surface area, diameter, etc.

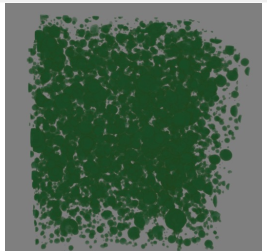
Pore structure of intact soil core:

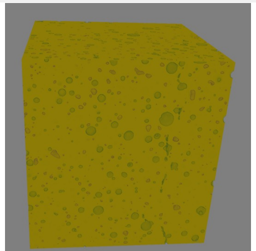
- How soil wetting patterns depend on pore structure and flow direction
- How porosity directs transport of water, microbes, minerals, etc.

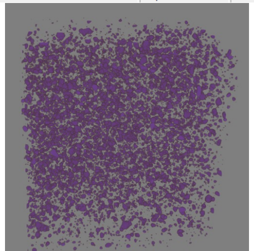
Information content in CT images: Component visualization by segmentation





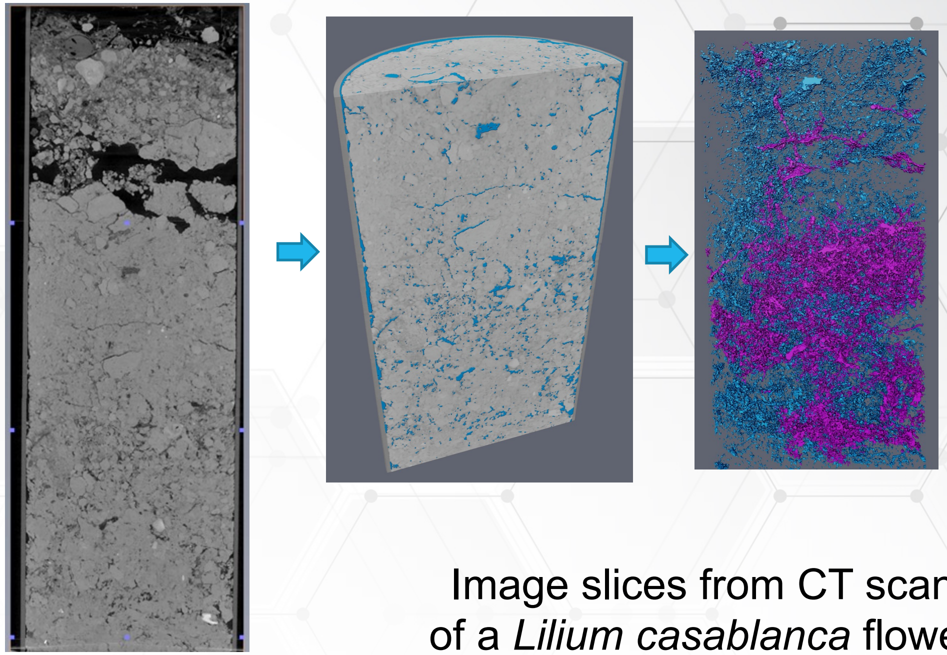


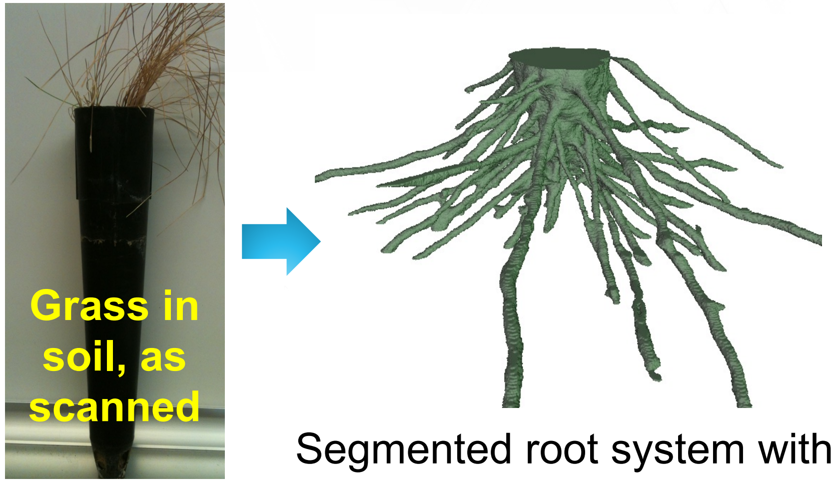




Information content in CT images: Image forms and visualization options

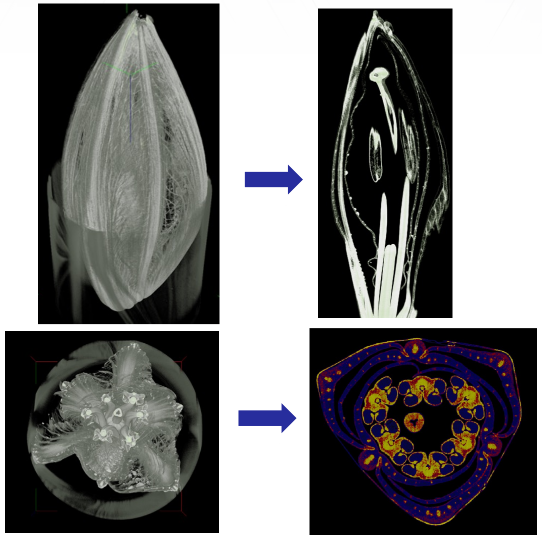
- Image options:
  - Digital radiographs
  - From full CT (volume data): image slices, image stacks, 3D rendering, videos
  - Color, component transparency, and slicing planes can be added to show/ emphasize elements in 3D reconstructions
  - .vol/.raw files, tiff or other formats, avi, etc.





Segmented root system with the soil virtually removed

Image slices from CT scan of a *Lilium casablanca* flower

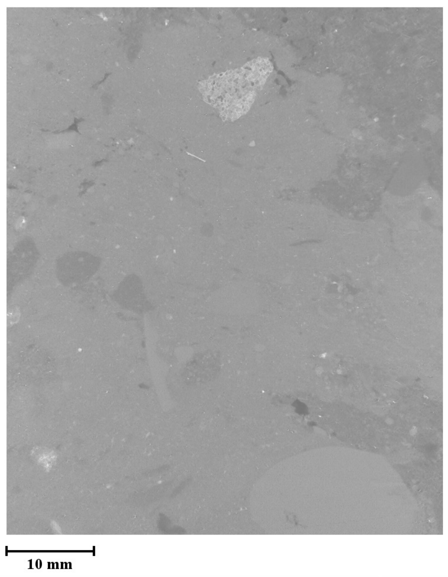


Example 1: Soil pore network characterization for MONet

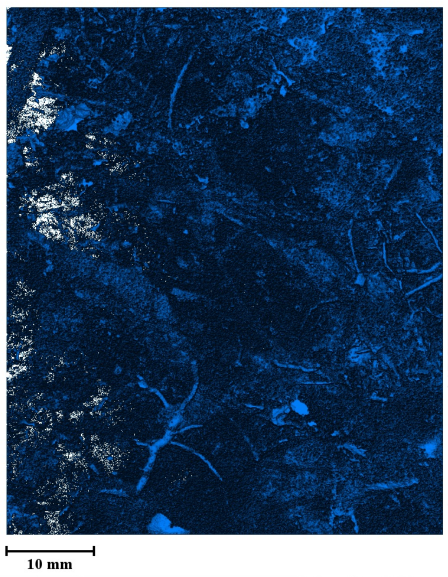
Soil is a challenging, multicomponent system

Cropped volume:

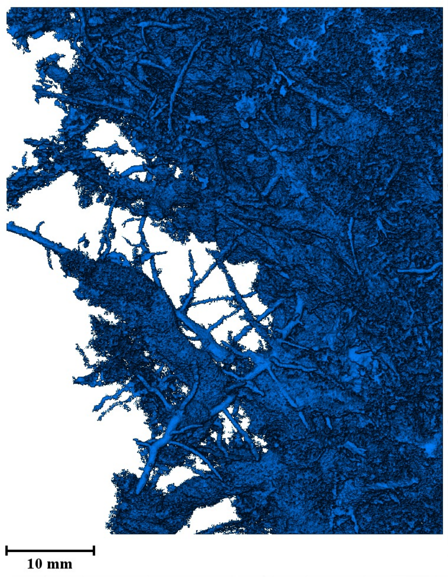
50x45x60 mm



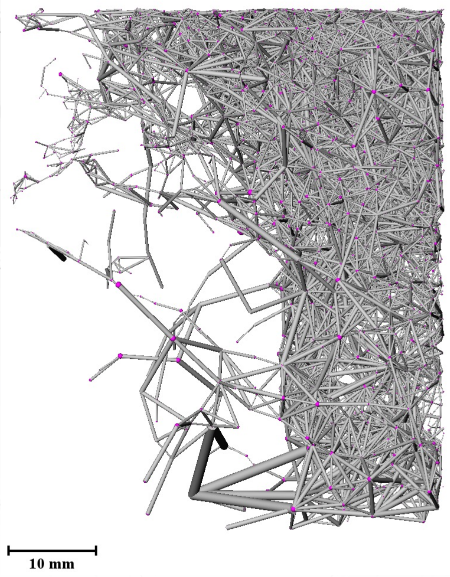
Reconstructed, cropped volume



Visualizing all pores



Connected pores only



PNM

- 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 mm^3

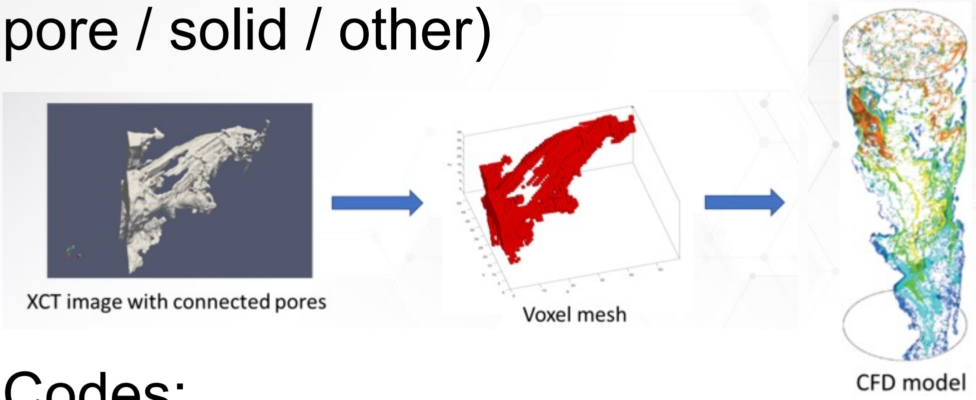
Pore Network Model in Z-direction

- Absolute permeability: 601.66 μm^2
- Total flow rate: 6016.31mm^3
- Tortuosity: 1.64

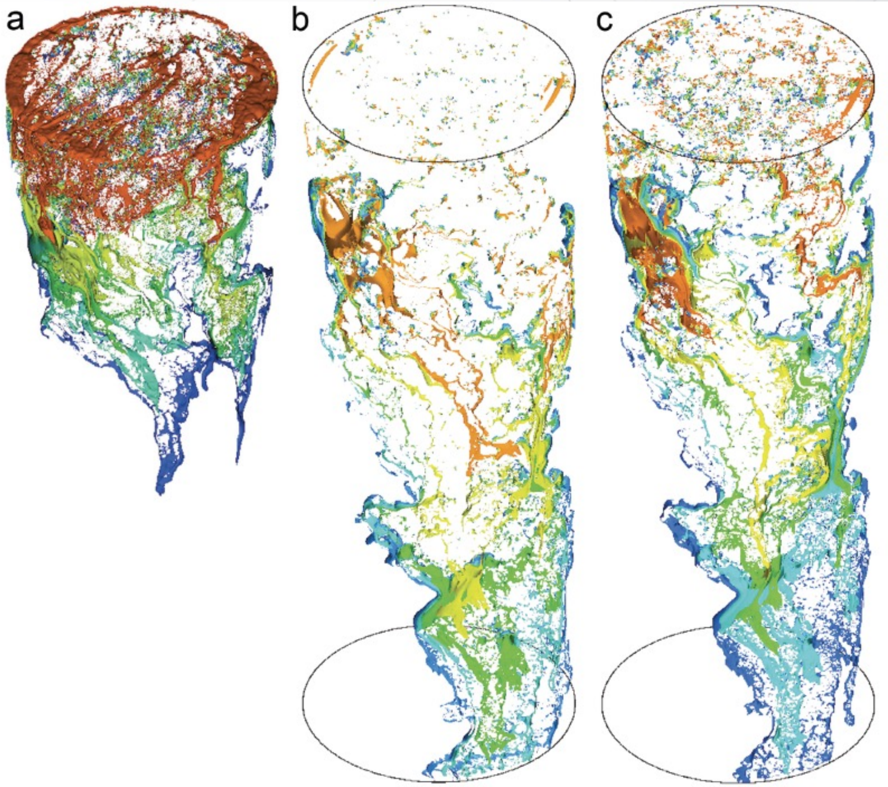
Input pressure: 103098 Pa,
Output pressure: 102833 Pa,
Fluid viscosity: 0.001 Pa·s

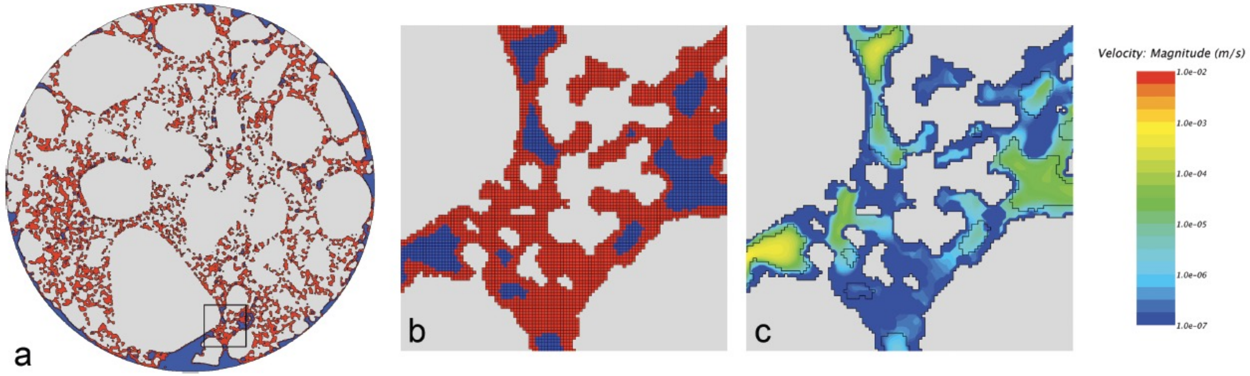
Example 2: Using soil pore structure data in direct simulation

- Computational Fluid Dynamics (CFD) modeling: fluid flow modeled using Navier-Stokes equations
- Explicit discretization of pore space - can directly use XCT data (segmented into pore / solid / other)



- Codes:
  - **Tethys** (PNNL-developed, Bill Perkins; includes batch geochemical reaction solver)
  - CGS (Oregon State Univ., Dr. Sourabh Apte / PNNL, Bryan He)
  - OpenFOAM (open-source CFD code; https://www.openfoam.com/)

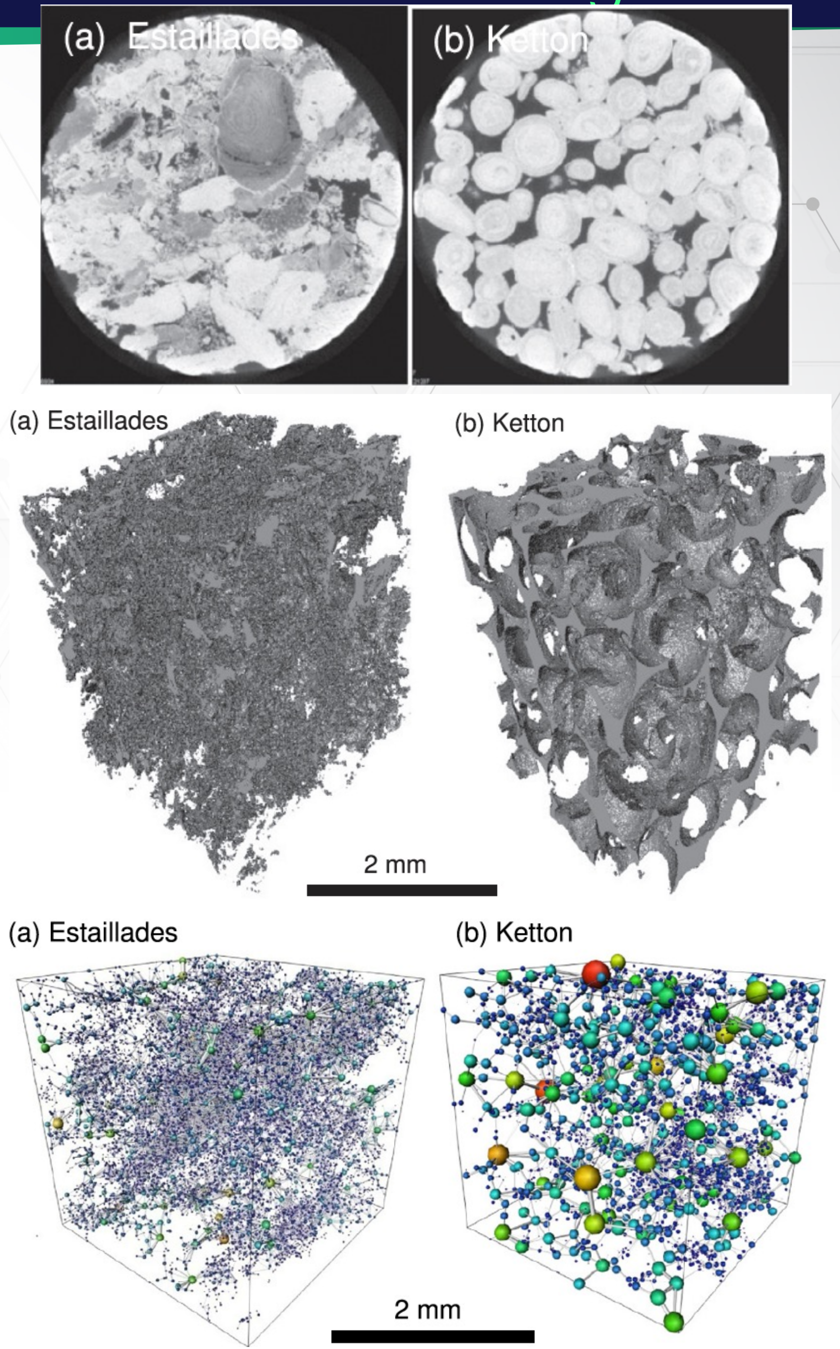




Scheibe et al. / Water Resources Research 51 (2015) 1023-1035

Example 3: Using soil pore structure data in pore network modeling

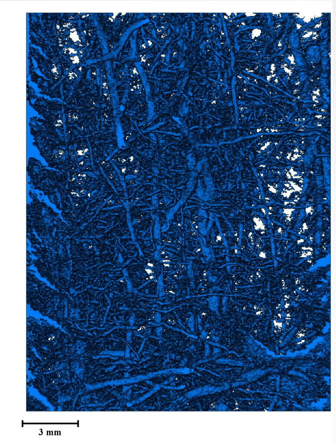
- Pore topology (e. g. from XCT) abstracted into connected system of pore bodies and pore throats with idealized geometries (e. g. spheres, cylinders)
- Solve flow (Darcy's Law + continuity eqn.) and transport equations for pore network
- Codes:
  - **AVIZO** (https://www.thermofisher.com/us/en/home/electron-microscopy/products/software-em-3d-vis/avizo-software.html; XCT analysis and permeability estimation using built-in PN model - Anil K. Battu and Tamas Varga, PNNL)
  - **OpenPNM** (https://openpnm.org/; diffusion modeling - Jianqiu Zheng, PNNL)



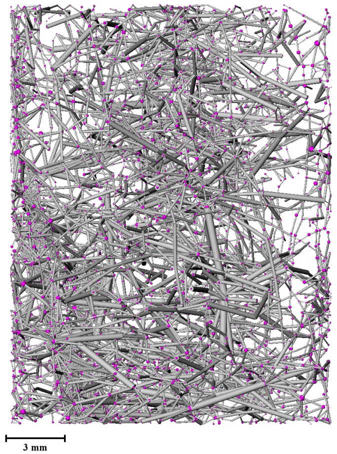
M.J. Blunt et al. / Advances in Water Resources 51 (2013) 197–216

Example 3: OpenPNM enables pore network queries, manipulations and reactive transport modeling

XCT (AVIZO)

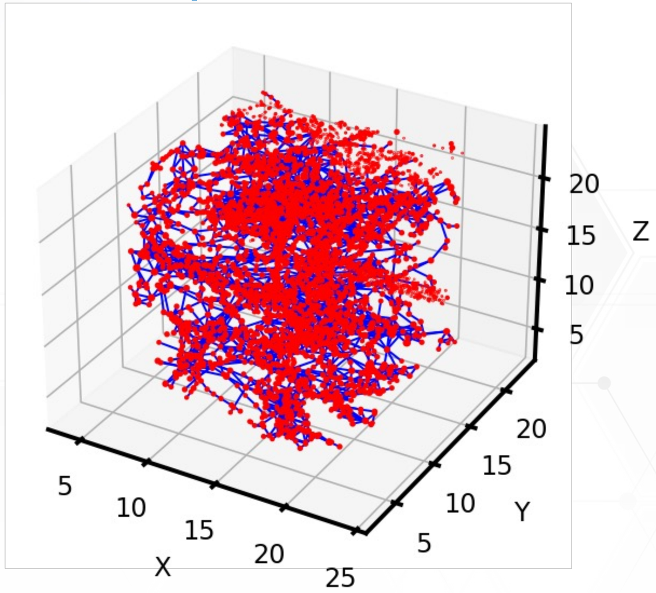


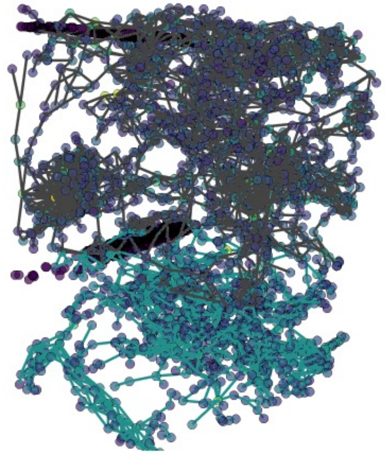
Connected pores



Pore Network Model

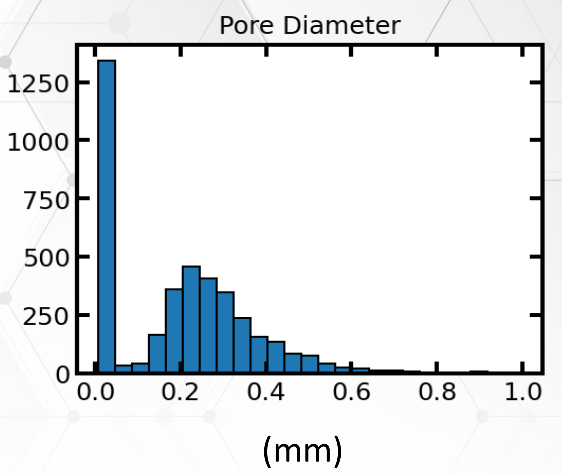
OpenPNM

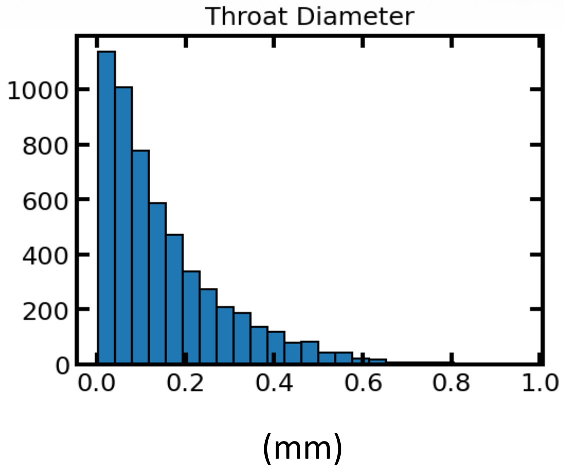




Reconstructed pore network

Probability distribution functions





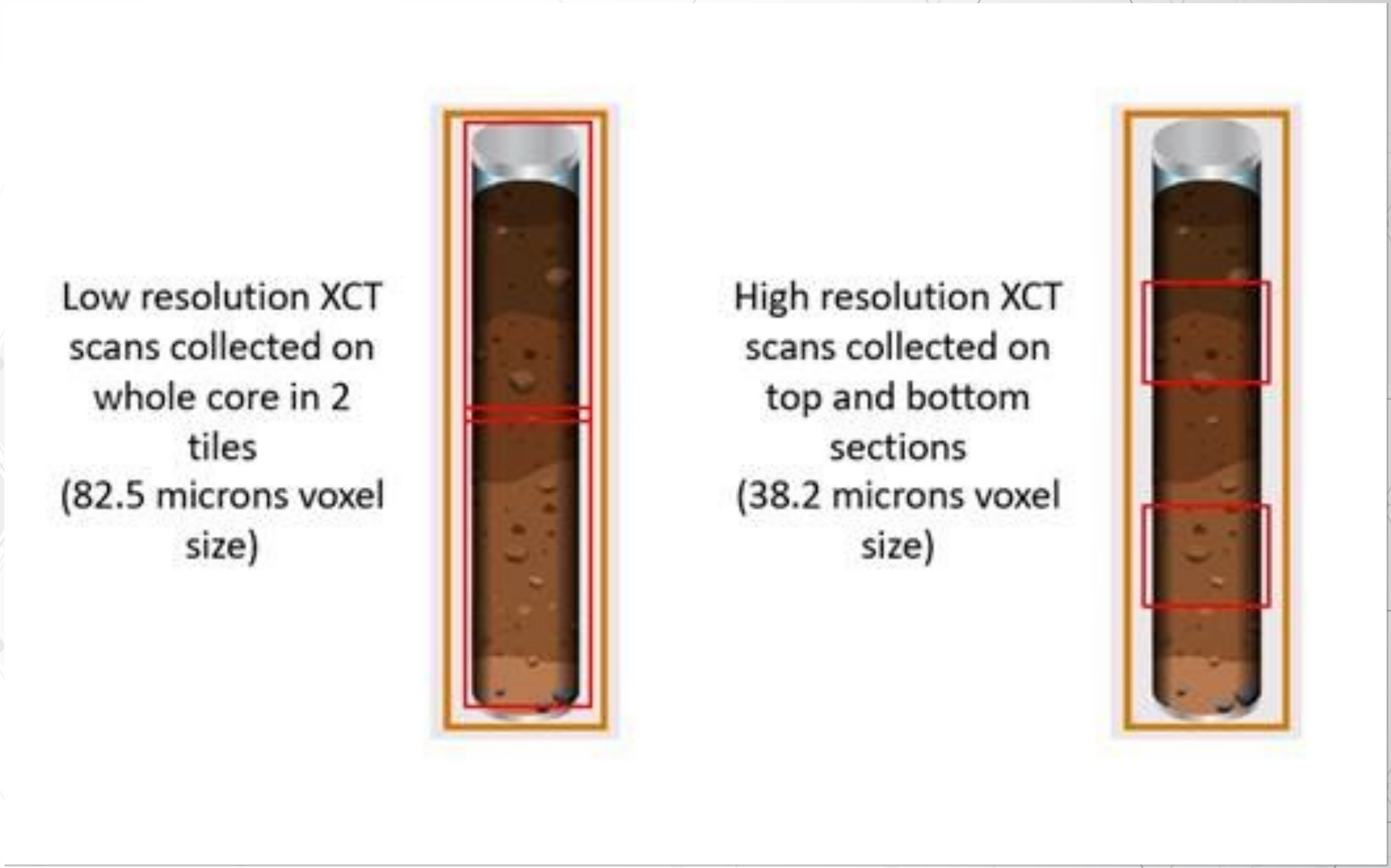
References

- Good summary of CT basics from UT Geosciences: https://www.ctlab.geo.utexas.edu/about-ct/
- EMSL instrument: https://www.emsl.pnnl.gov/science/instruments-resources/x-ray-computed-tomography
- FDK cone-beam reconstruction: Feldkamp, Davis, Kress, J. *Opt. Soc. Am. A*, 1(6), 612-619 (1984)
- XCT in soil science review: Taina, Heck, Elliot, *Canadian J. Soil Sci*., 88(1), 1-19 (2008)
- “MONet” perspective: Bowman, *et al*., *Front. Soil Sci*., 3:1120425 (2023)
- Soil paper out of a user project: Rooney, *et al*., *Geoderma*, 411: 115674 (2022)
- Soil structure library: Weller, *et al*., *Soil*, 8(2), 507–515 (2022)

Questions?

XCT analysis on a typical MONet soil core at EMSL

Tamas Varga



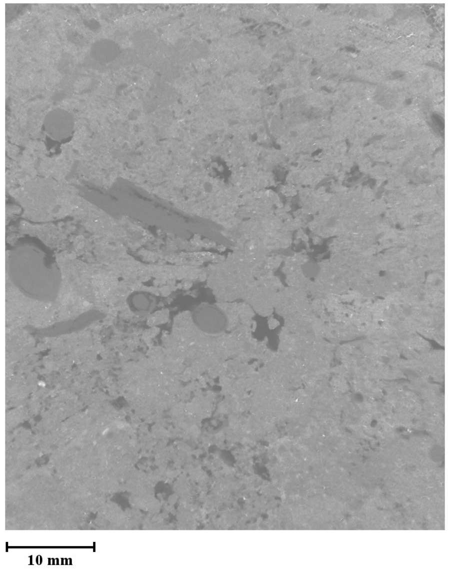
Whole core (merged low-resolution data on top and bottom sections)

Tomographic image of whole core in XZ plane view

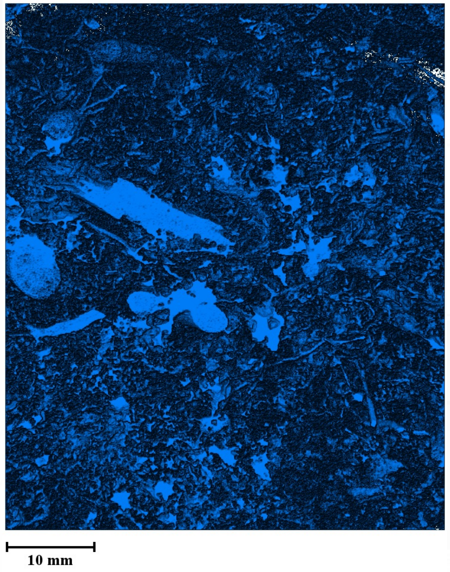
The two lower-resolution (82.5 micron voxel size, estimated spatial resolution 165 microns) scans are used to get the overall image of the whole 1-ft tall core. This image has been stitched together from two tiles as suggested in the title.

Scan conditions:
X-ray power: 105 kV and 325 μA
Projections: 1600
Frames/projection: 2
Exposure time: 500 ms
Filter: 0.5-mm Cu foil
Voxel size is 82.5 microns

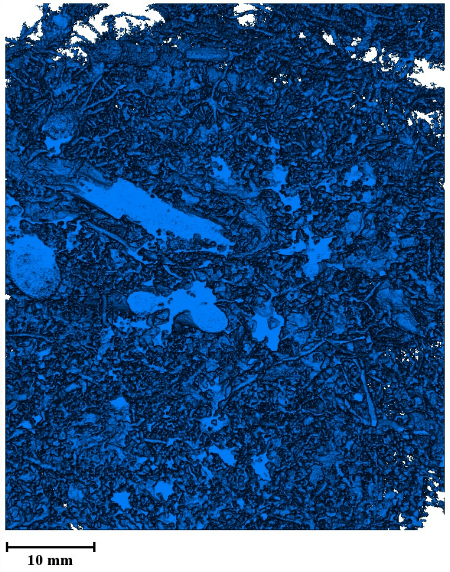
Higher-resolution scan (with 38.2-micron voxel size) on the top section of core



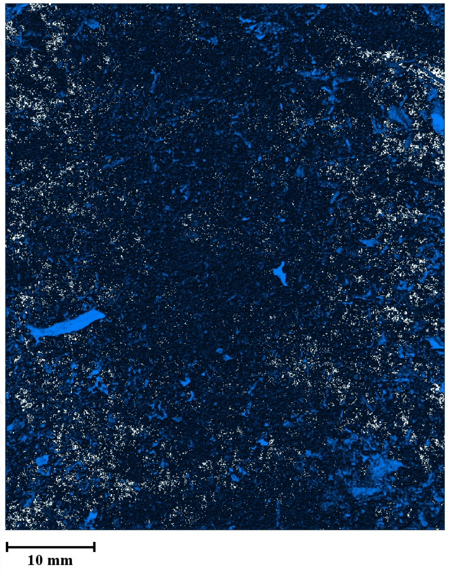
Reconstructed, cropped volume



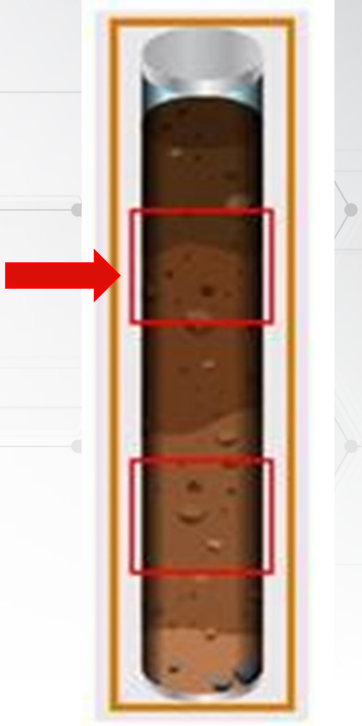
Visualizing all pores



Only connected pores



Only unconnected pores



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

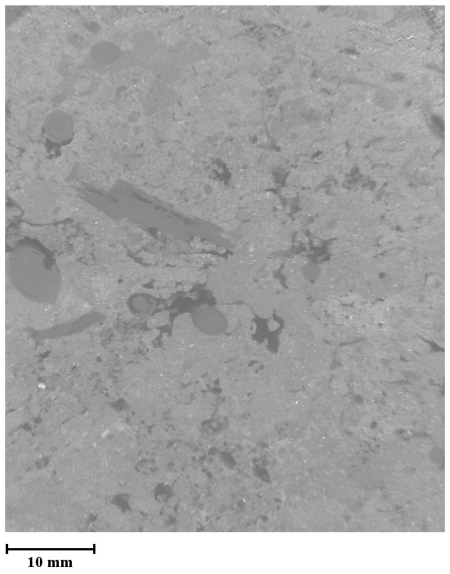
- Mean Pore size: 0.06448 mm
- Min Pore size: 0.047327 mm
- Max Pore size: 29.63071 mm
- Median Pore size: 0.047338 mm
- Variance Pore size: 0.001942 mm
- Mean Pore Volume: 0.005736 mm^3

Cropped volume size analyzed here:

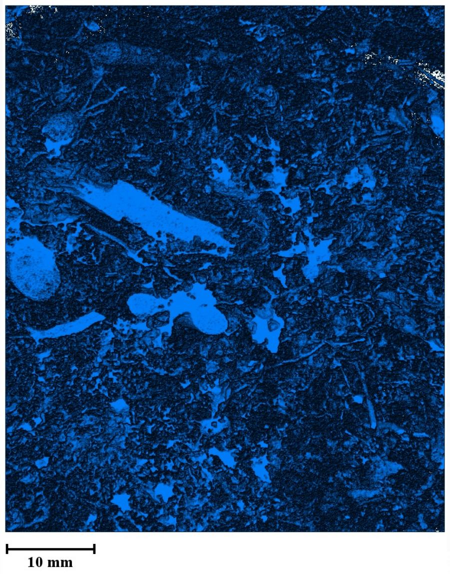
50x45x60 mm

XZ plane view, clip

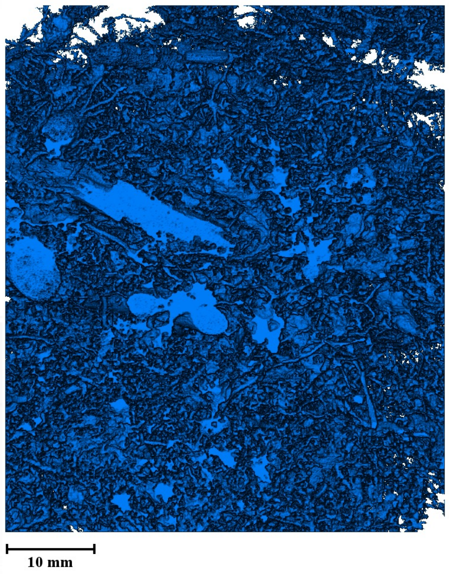
Pore network modeling (PNM) results on higher-resolution data from top section of core



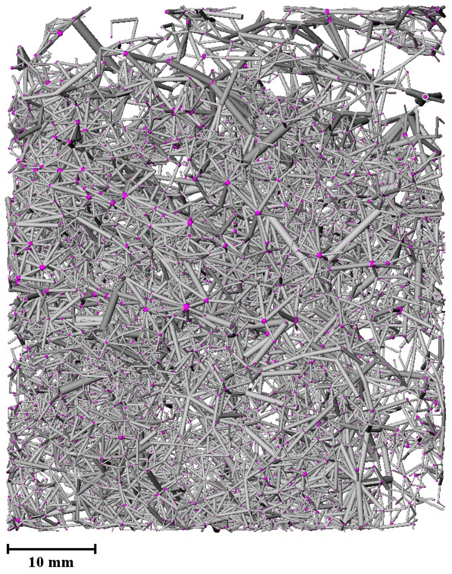
Reconstructed, cropped volume



Visualizing all pores



Only connected pores



PNM

Pore Network Model in Z-direction

- Absolute permeability: 109.69 µm^2
- Total flow rate: 1102.00 mm^3
- Tortuosity: 1.80

Pore Network Model in Y-direction

- Absolute permeability: 2882.55 µm^2
- Total flow rate: 50706.88 mm^3
- Tortuosity: 1.52

Pore Network Model in X-direction

- Absolute permeability: 379.04
- Total flow rate: 5450.30 mm^3
- Tortuosity: 1.76

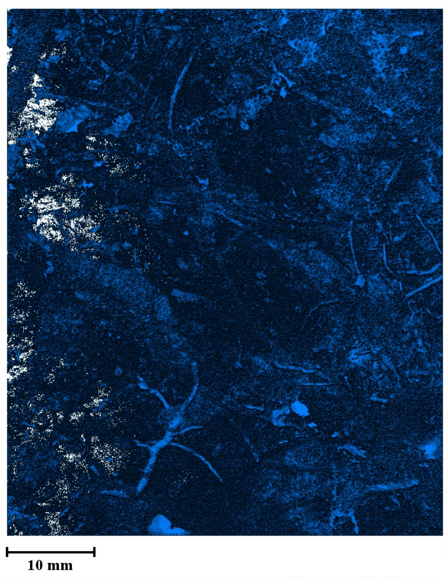
Input pressure: 103098 Pa,
Output pressure: 102833 Pa,
Fluid viscosity: 0.001 Pa.s

Cropped volume:

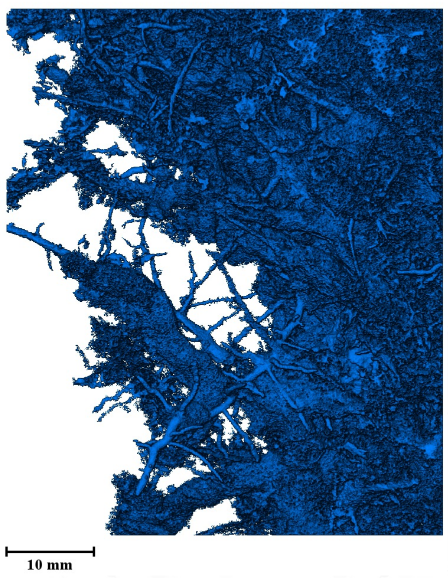
50x45x60 mm

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

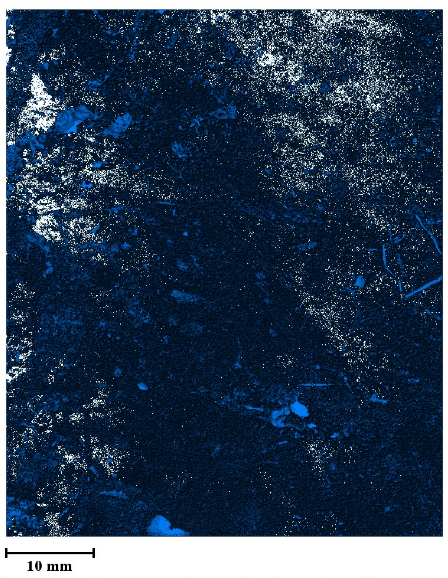
Raw volume



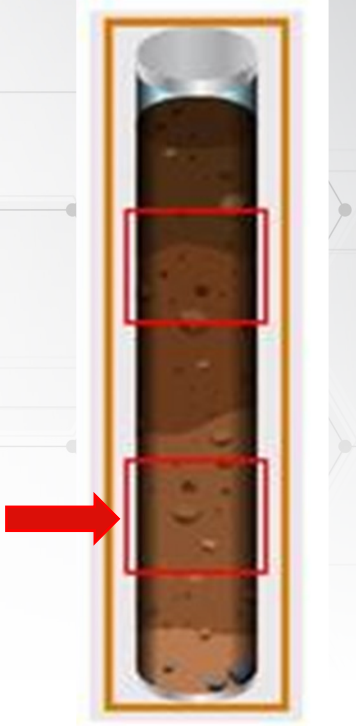
Visualizing all pores



Only connected pores



Only unconnected pores



- 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 mm^3

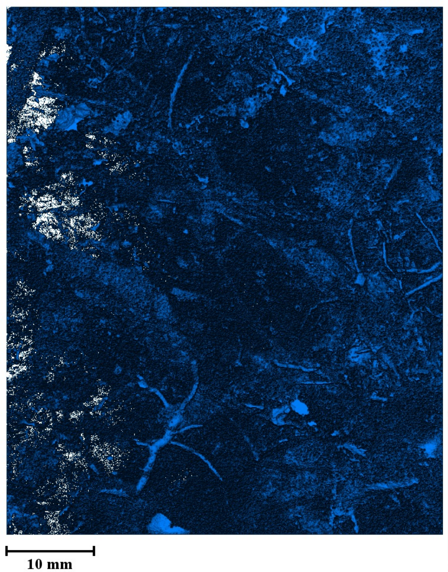
Cropped volume:

50x45x60 mm

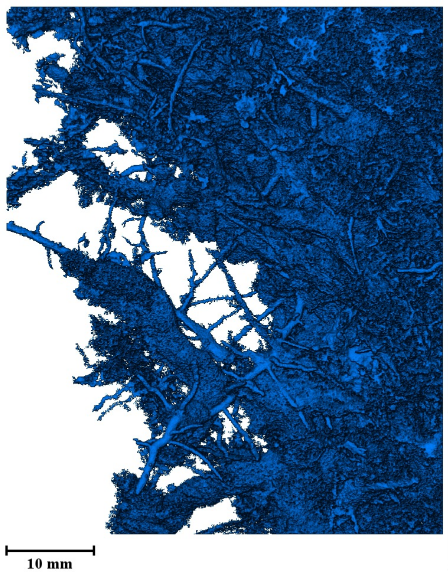
XZ plane view, clip

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

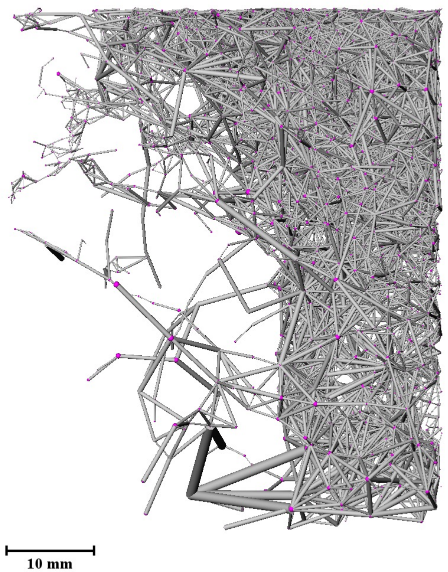
Raw volume



Visualizing all pores



Only connected pores



PNM

Pore Network Model in Z-direction

- Absolute permeability: 601.66 μm^2
- Total flow rate: 6016.31mm^3
- Tortuosity: 1.64

Pore Network Model in Y-direction

- Absolute permeability: 751.03 μm^2
- Total flow rate: 12886.47 mm^3
- Tortuosity: 1.60

Pore Network Model in X-direction

- Absolute permeability: 11.76 μm^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:

50x45x60 mm

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

Size (mm)	count
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

Size (mm)	count
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

Scan conditions for higher resolution scans:
X-ray power: 105 kV and 325 μA
Projections: 3142
Frames/projection: 2
Exposure time: 708 ms
Filter: 0.5-mm Cu foil
Voxel size is 38.2 microns