3D Aggregate Shape Analysis and Parking Model

E.J. Garboczi, NIST, Boulder, CO

J.W. Bullard, NIST, Gaithersburg, MD

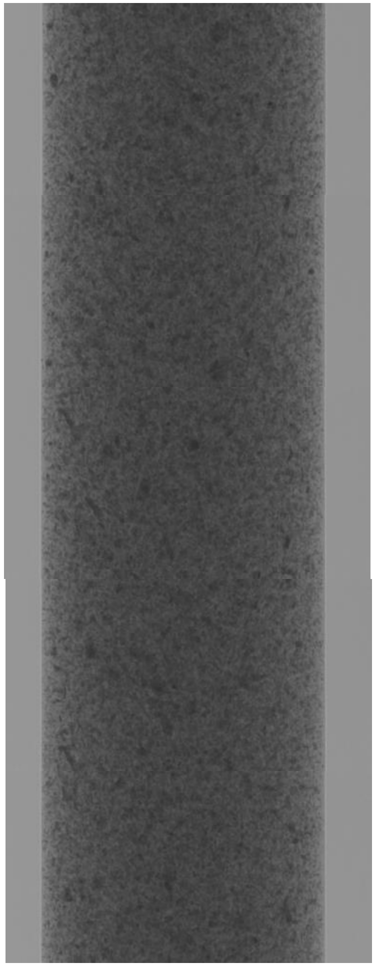
Y. Lu, Boise State University, Boise, ID

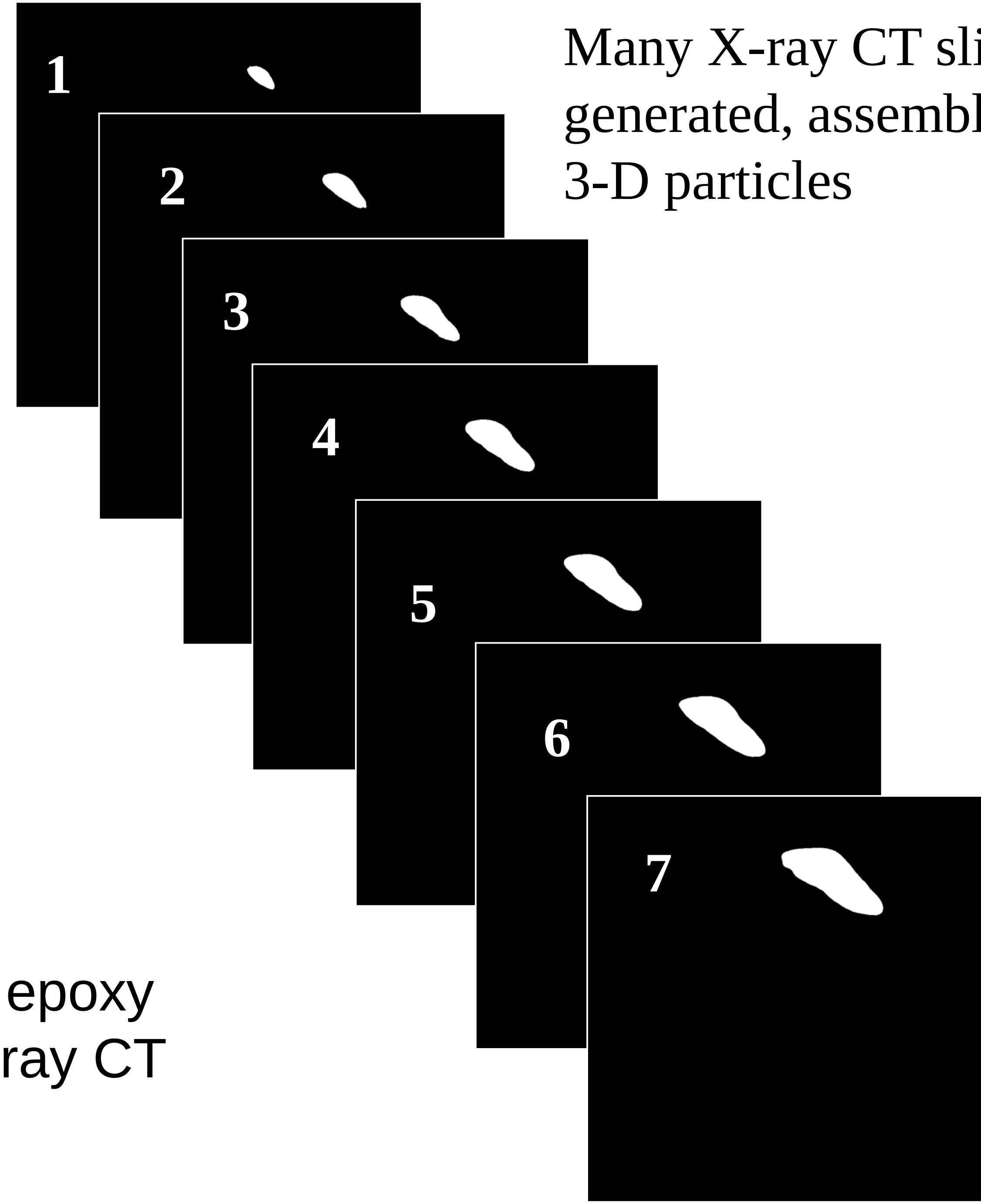
Z. Qian, Delft Technical University, Delft, Netherlands

Why particle shape analysis?

- Unbound aggregates:
  - Packing density, mechanical strength of beds
- In concrete:
  - Rheology of fresh concrete, early-age strength
- General applications:
  - Size measurement – laser diffraction, sieve analysis, high speed photography/image analysis, sedimentation
  - Initial reactivity of powders via specific surface area
  - State of health of cells/tumors, healthy vs. unhealthy, benign vs. malignant
  - Retroreflectivity of glass beads in road marking paints

- Note: Software package for shape analysis = TSQUARE, in development at NIST

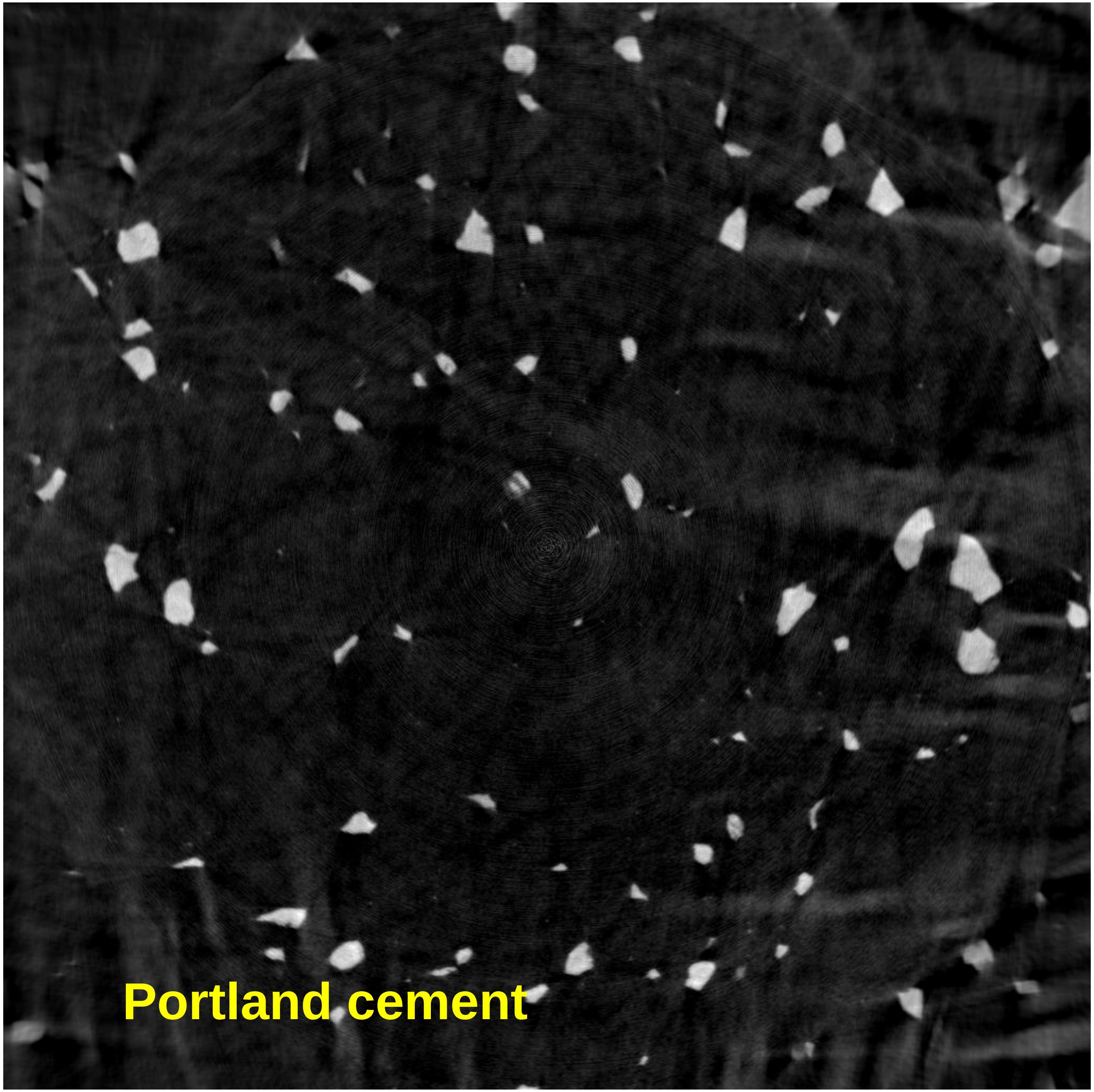


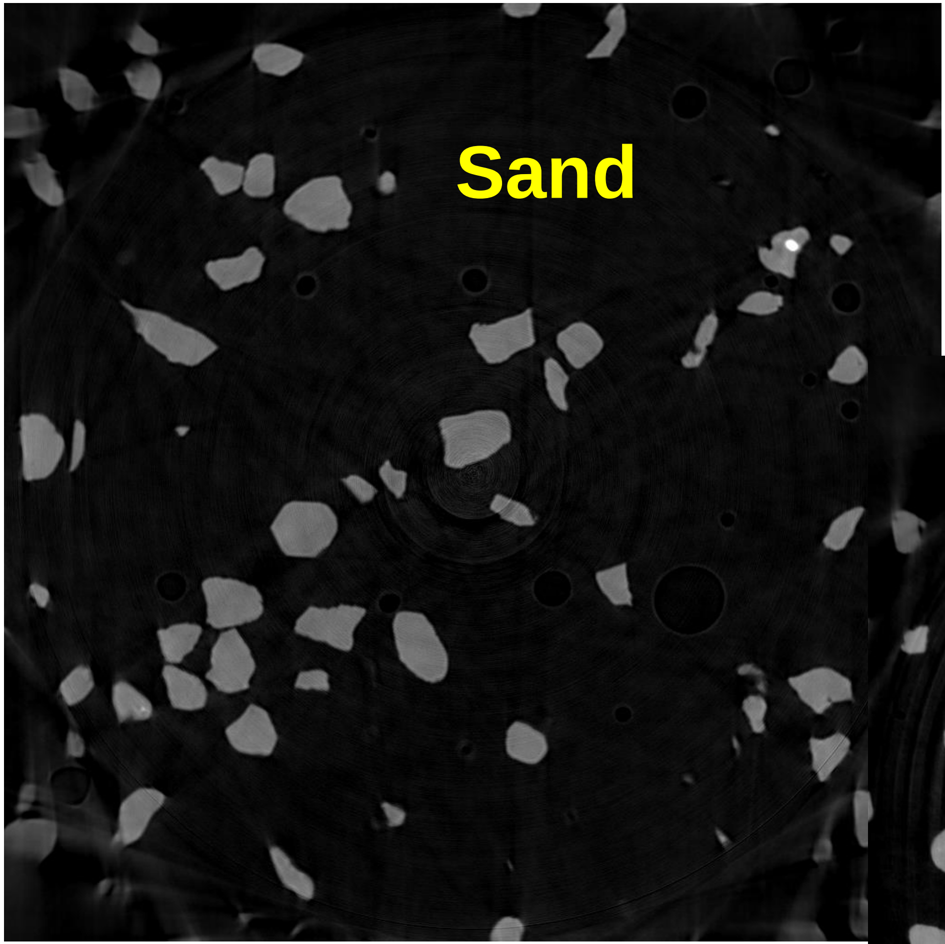


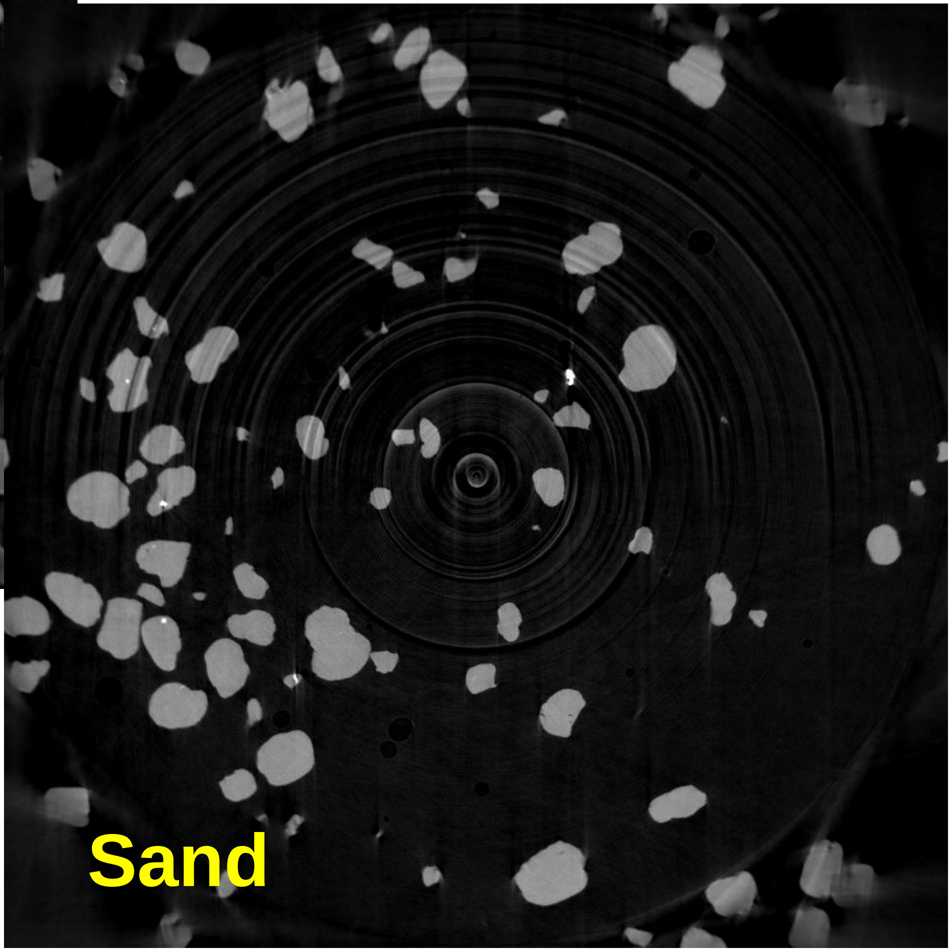
Many X-ray CT slices generated, assemble into 3-D particles

Embed particles in epoxy cylinder, scan in X-ray CT instrument

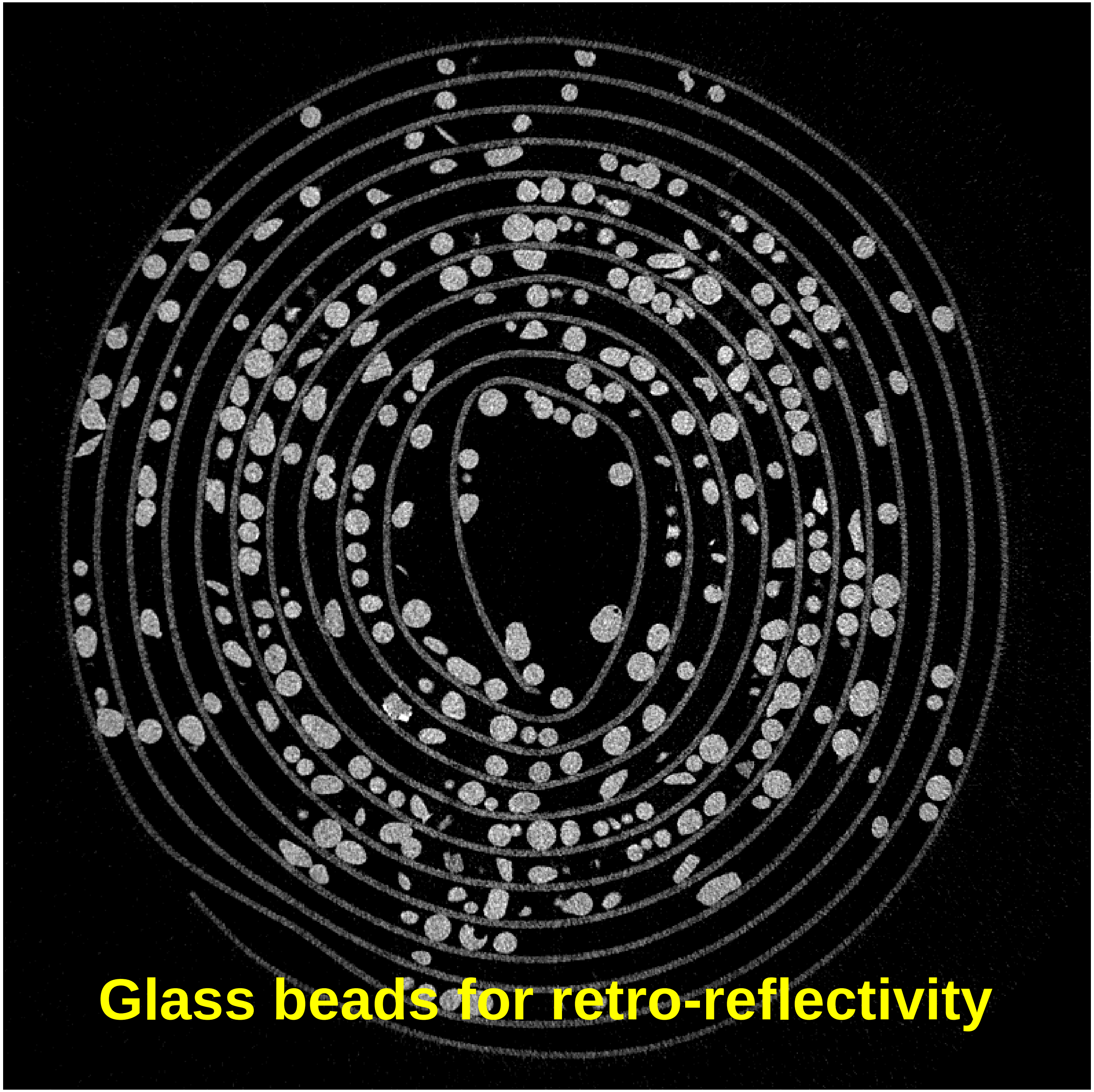
Two X-ray CT units

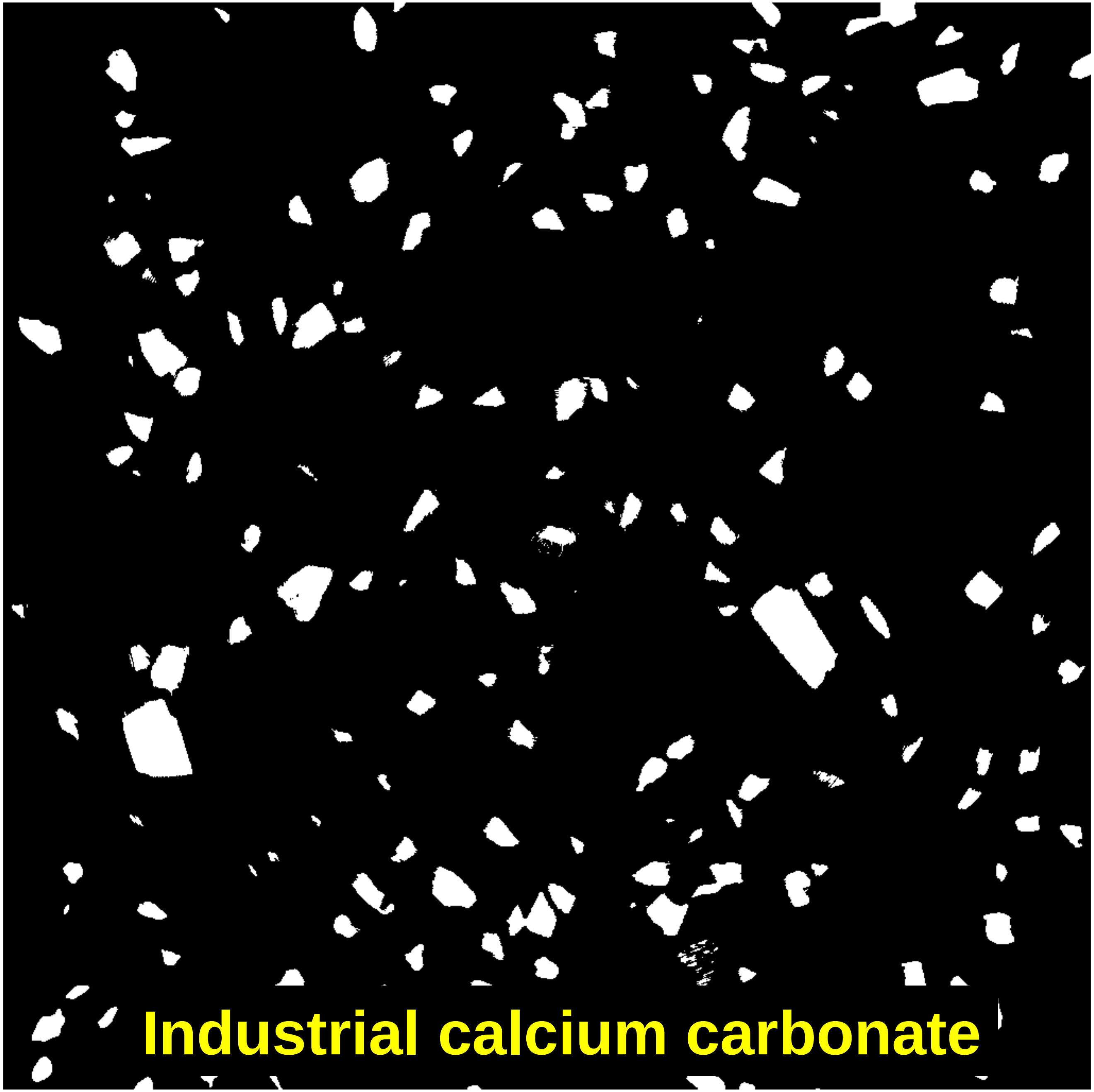

Portland cement

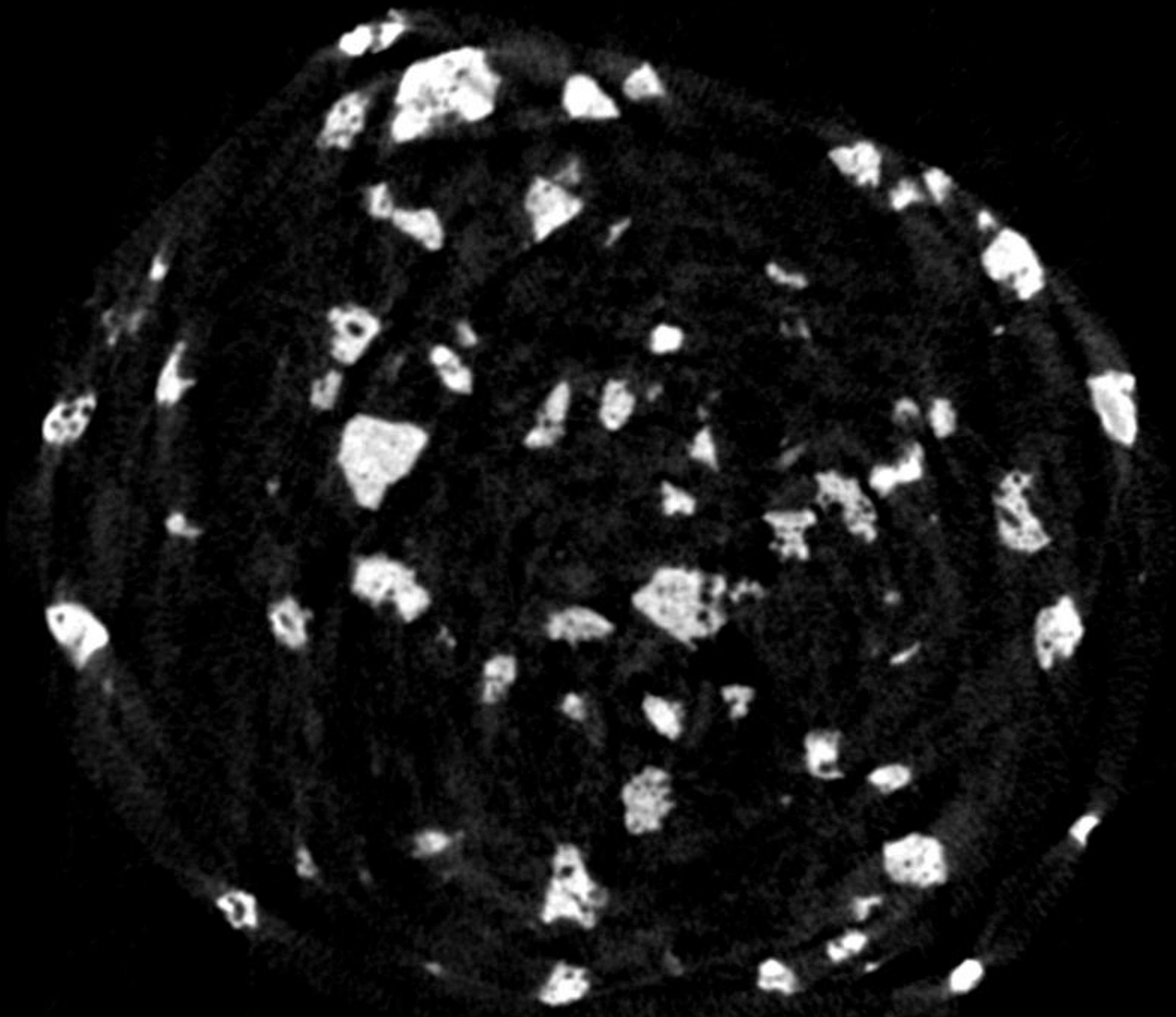

Sand


Sand

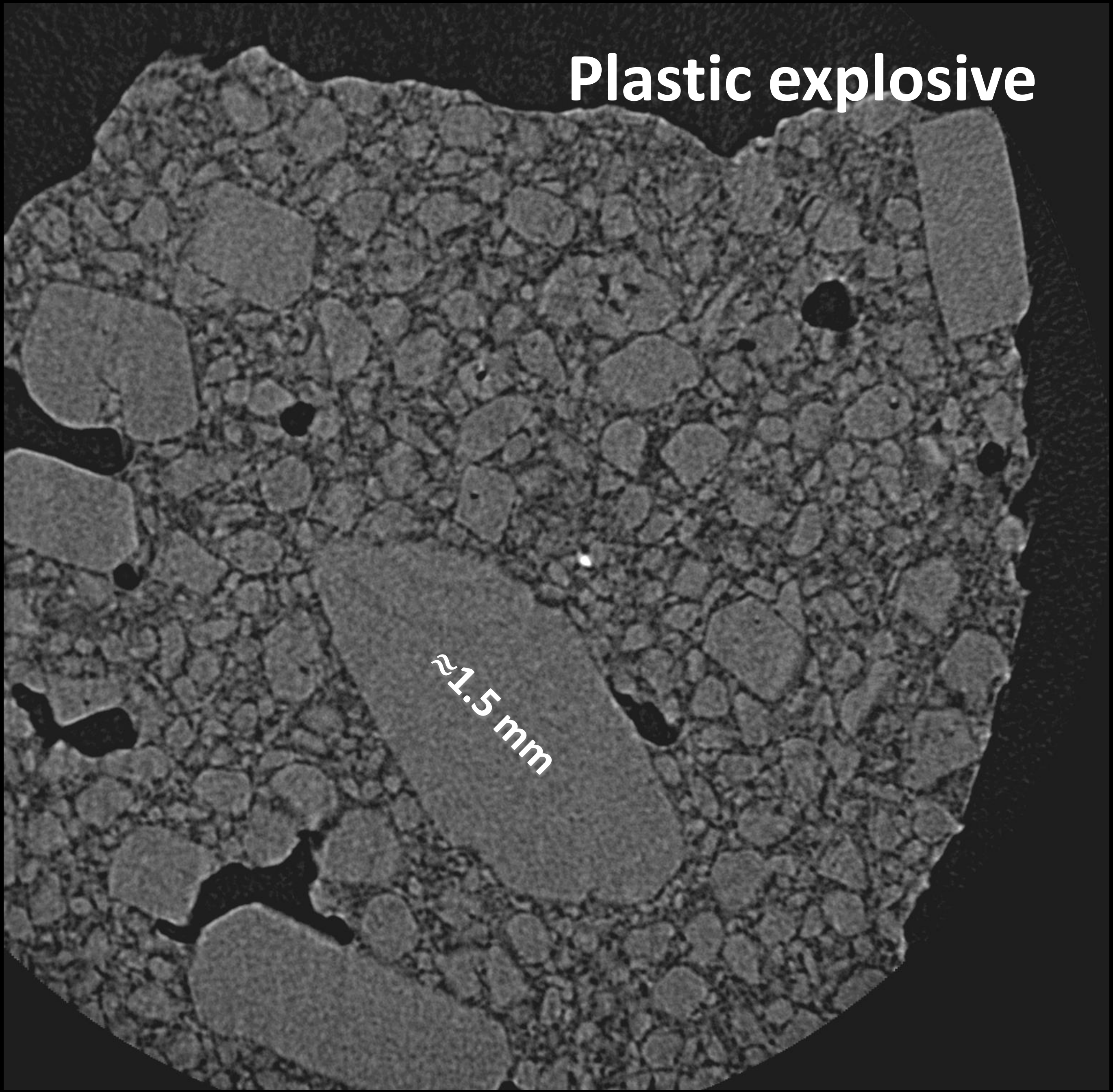

Blast furnace slag


Glass beads for retro-reflectivity


Industrial calcium carbonate

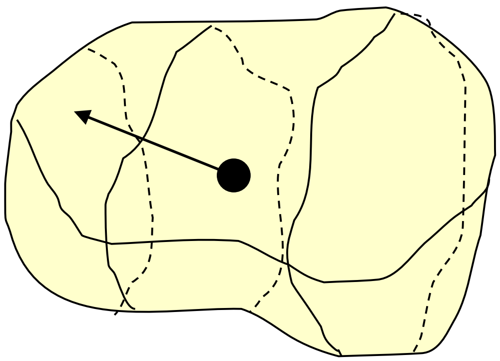


> 300 μm simulated lunar soil particles

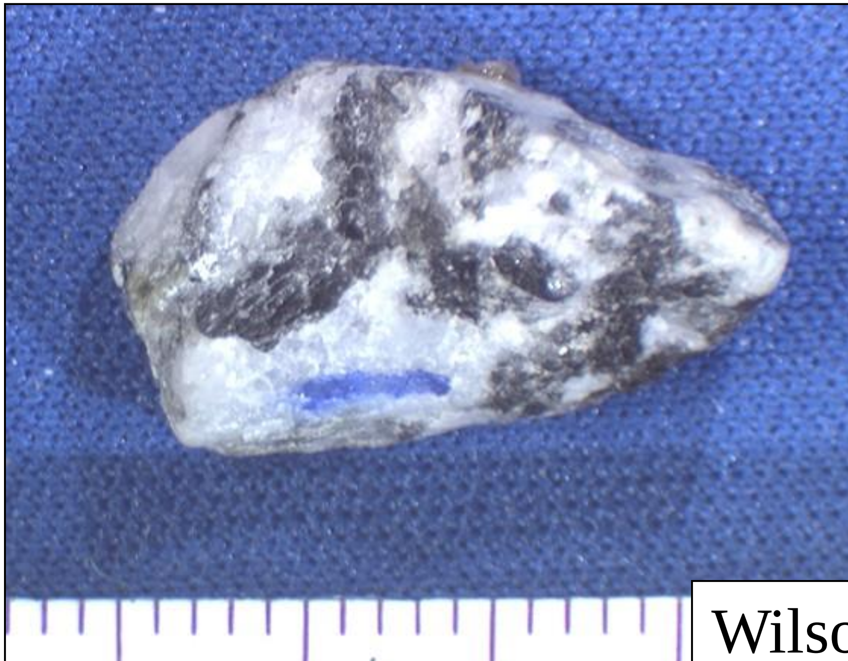

Plastic explosive
≈1.5 mm

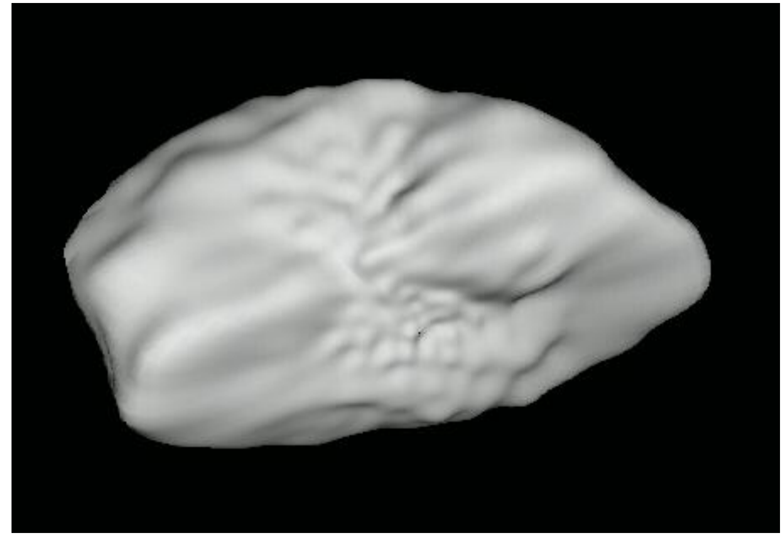
Spherical harmonic analysis and X-ray CT

- Define $r(\theta, \phi)$ from center of mass to surface

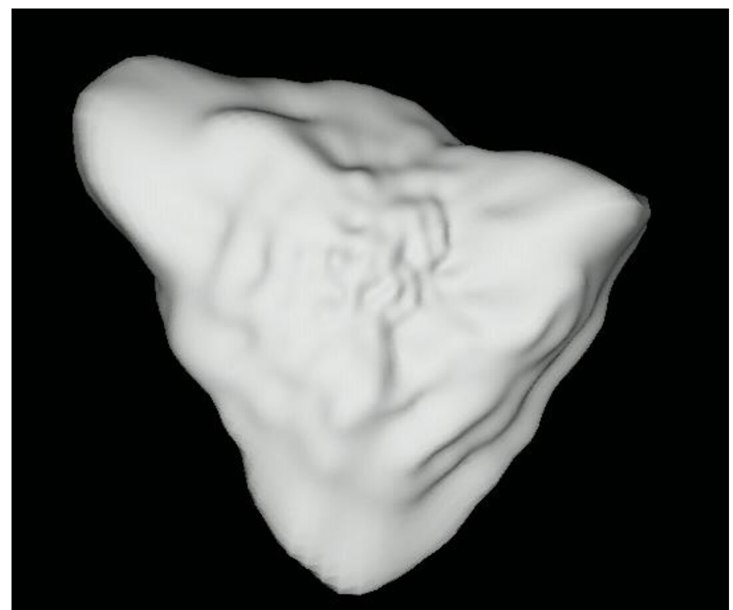


- Compute $r(\theta, \phi) = \Sigma_{n,m}\, a_{nm}\, Y_n^{\,m}(\theta, \phi)$
- $Y_n^{\,m}$ = spherical harmonic function
- Comprehensive mathematical characterization of shape, $n \approx 20$, $-n < m < n$
- *All shape and size information for particle is in the $(n+1)^2$ coefficients*

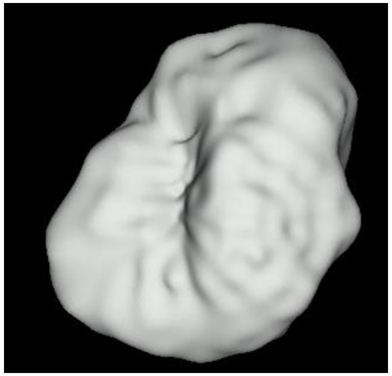


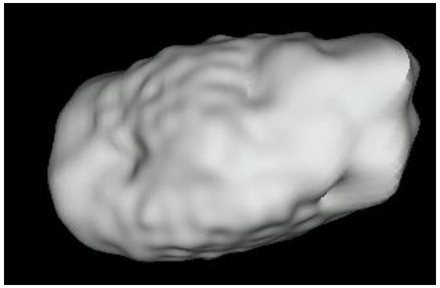


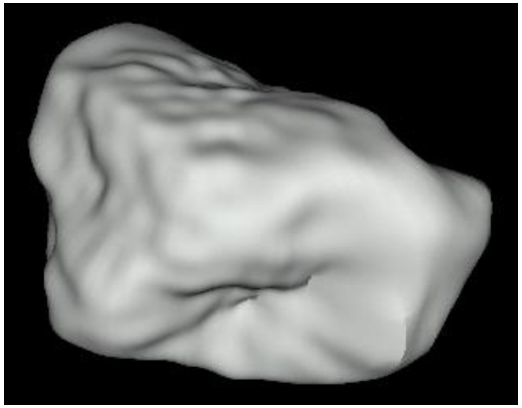
Wilson 0.5 in - #1,2

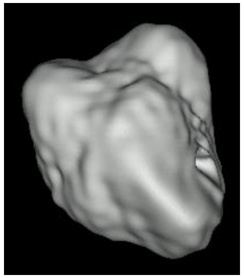


European standard sand

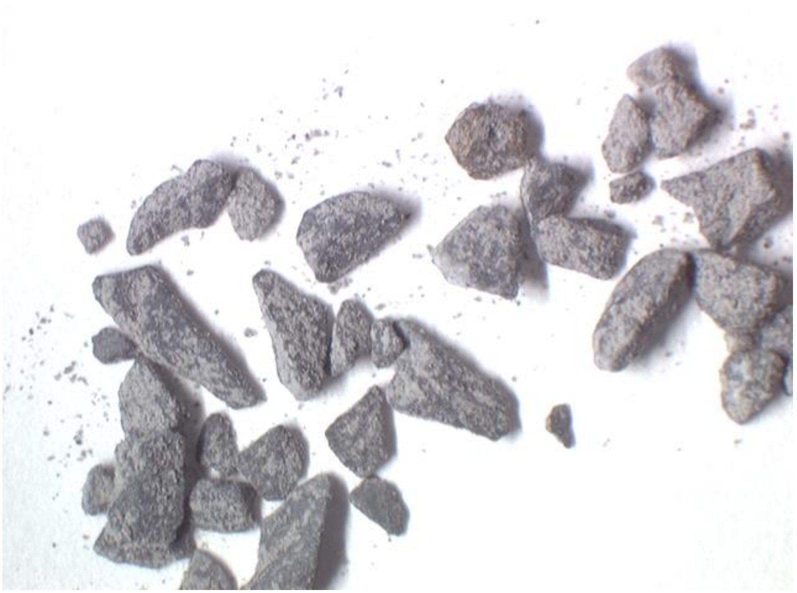


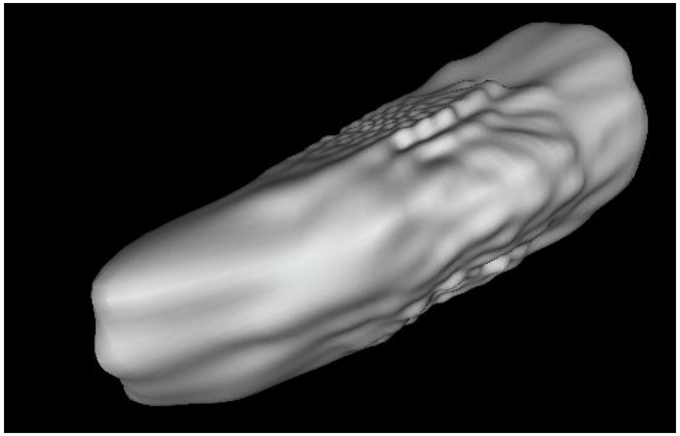


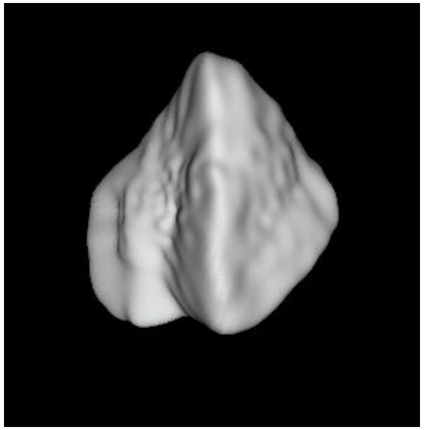


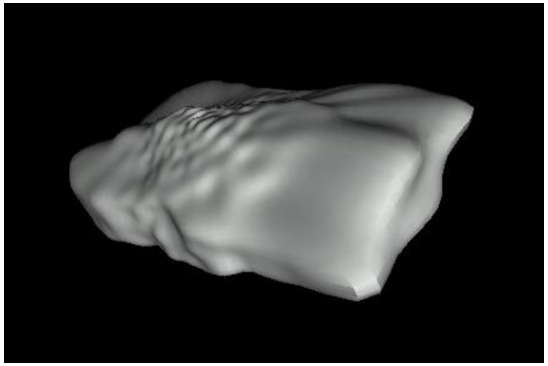


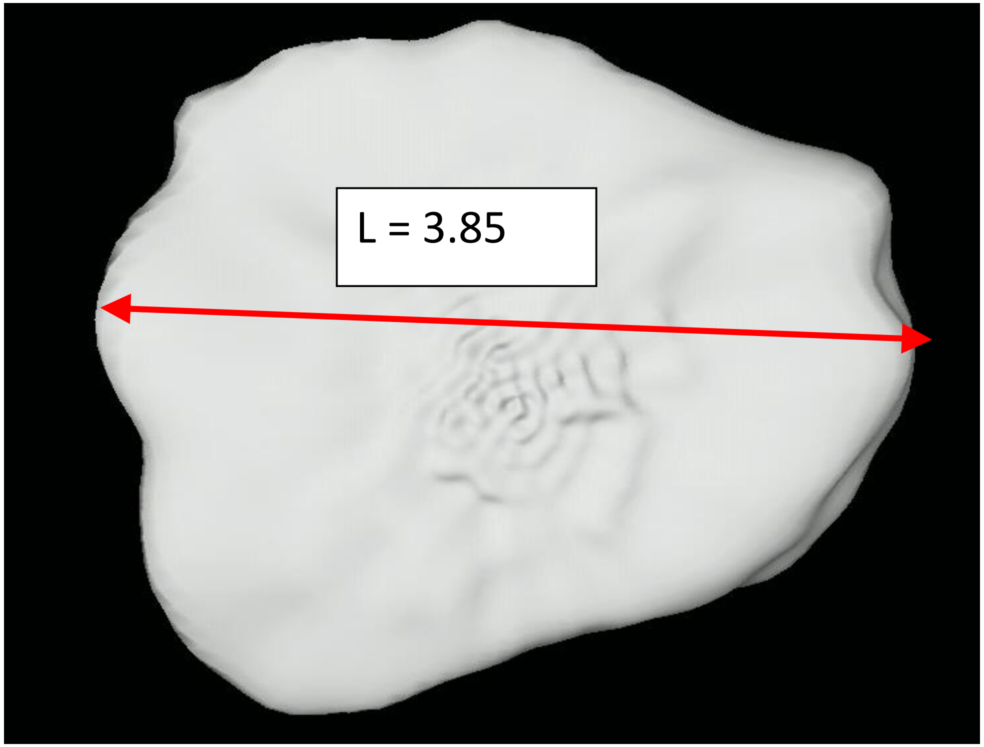
Fine aggregate for hot-mix asphalt

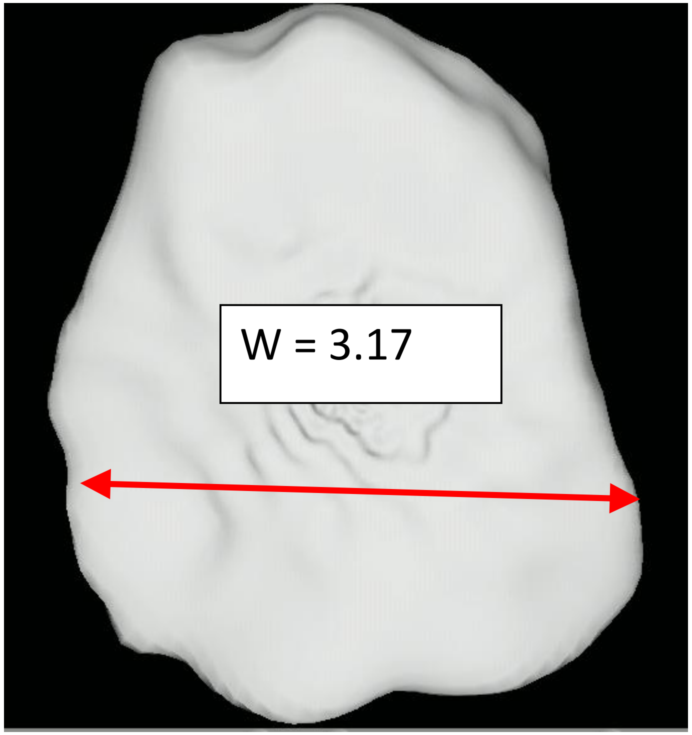


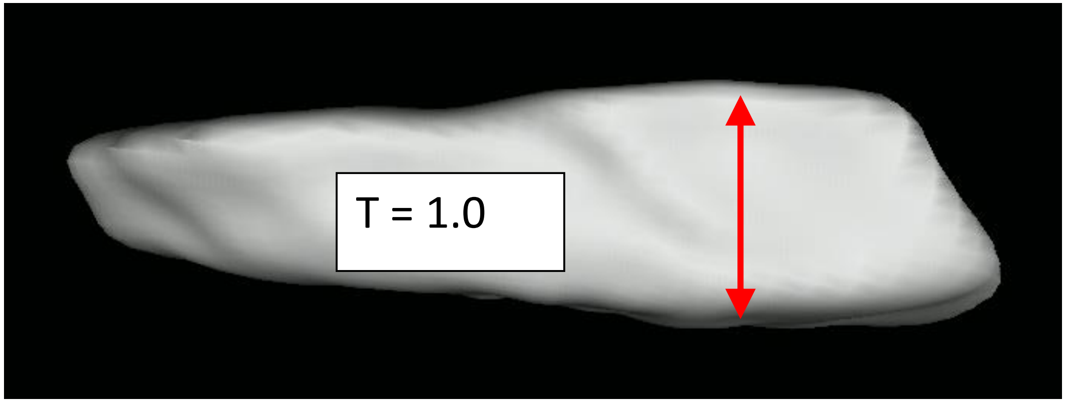










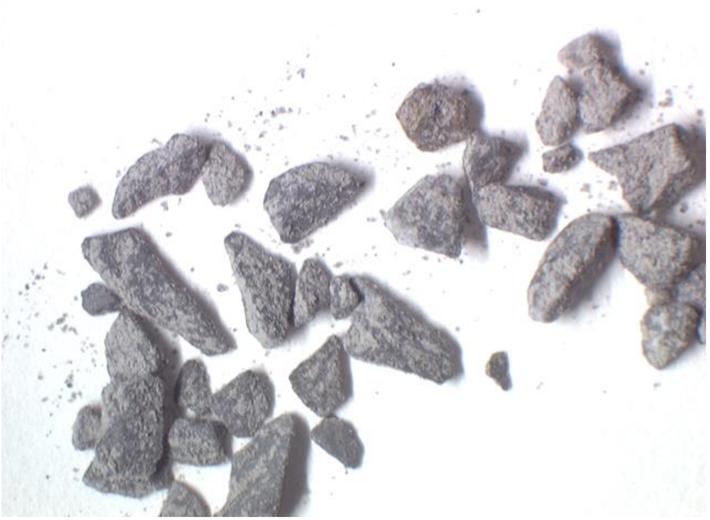


Rock denoted by
3.85 - 3.17 - 1 (L-W-T)

European standard sand

W-5					0.0
W-4				0.0	0.0
W-3			0.3	0.0	0.0
W-2		2.6	1.2	0.2	0.0
W-1	72.7	22.7	0.3	0.0	0.0
	L-1	L-2	L-3	L-4	L-5

W-5					0.0
W-4				0.0	0.0
W-3			0.4	1.1	0.0
W-2		8.3	8.3	3.6	0.0
W-1	33.6	38.2	6.2	0.2	0.2
	L-1	L-2	L-3	L-4	L-5



Sand for hot-mix asphalt

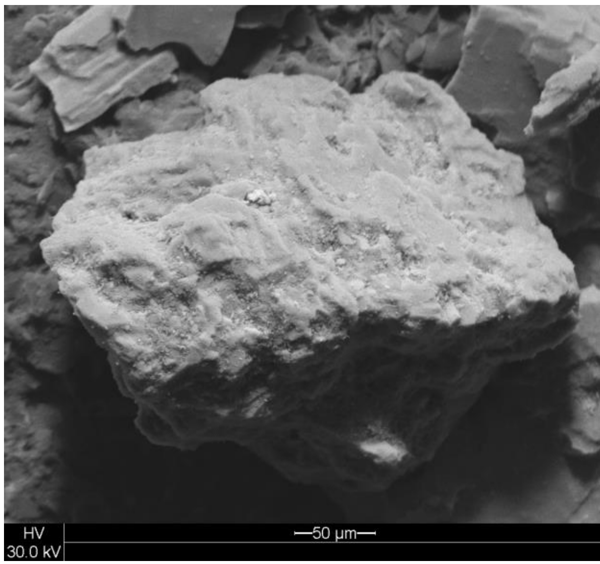
Potential ASTM standard

- ASTM Committee D04.51
- Initially for “sand” – size between 0.5 mm and 5 mm
  - Will supplement existing procedure ASTM D4791-10 for coarse aggregates
- Standard procedures for making cylindrical samples – sand embedded in epoxy
- Suggested X-ray CT scanning procedures, minimum pixel size needed
- Automated image analysis and particle analysis procedures
- End result will be a file, importable into a spreadsheet program, of 3D particle geometrical/shape data
  - Original mathematical description via spherical harmonic coefficients, will also be available for further user-specific data analysis

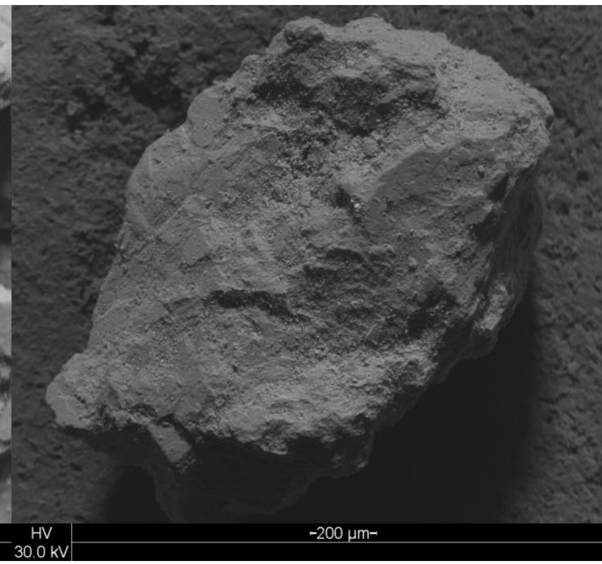
Size-shape scaling

- Rock from single source
  - Granite Rock Wilson quarry in California, collaboration with Michael Taylor
  - Crushed and screened
- Size of rocks from 20 µm – 40 mm, judged by ASTM sieve analysis
- Particle samples from different sieves used to prepare X-ray CT samples
- Scanned and shape analysis – 58 000+ particles
- Separated into three size classes:
  - 0.0175 mm to 0.24 mm, 0.24 mm to 3.29 mm, and 3.29 mm to 45.1 mm
  - **Particle shape parameters remained essentially unchanged, within uncertainty, for three size classes**

Blasted/crushed rock from 20 µm – 40 mm

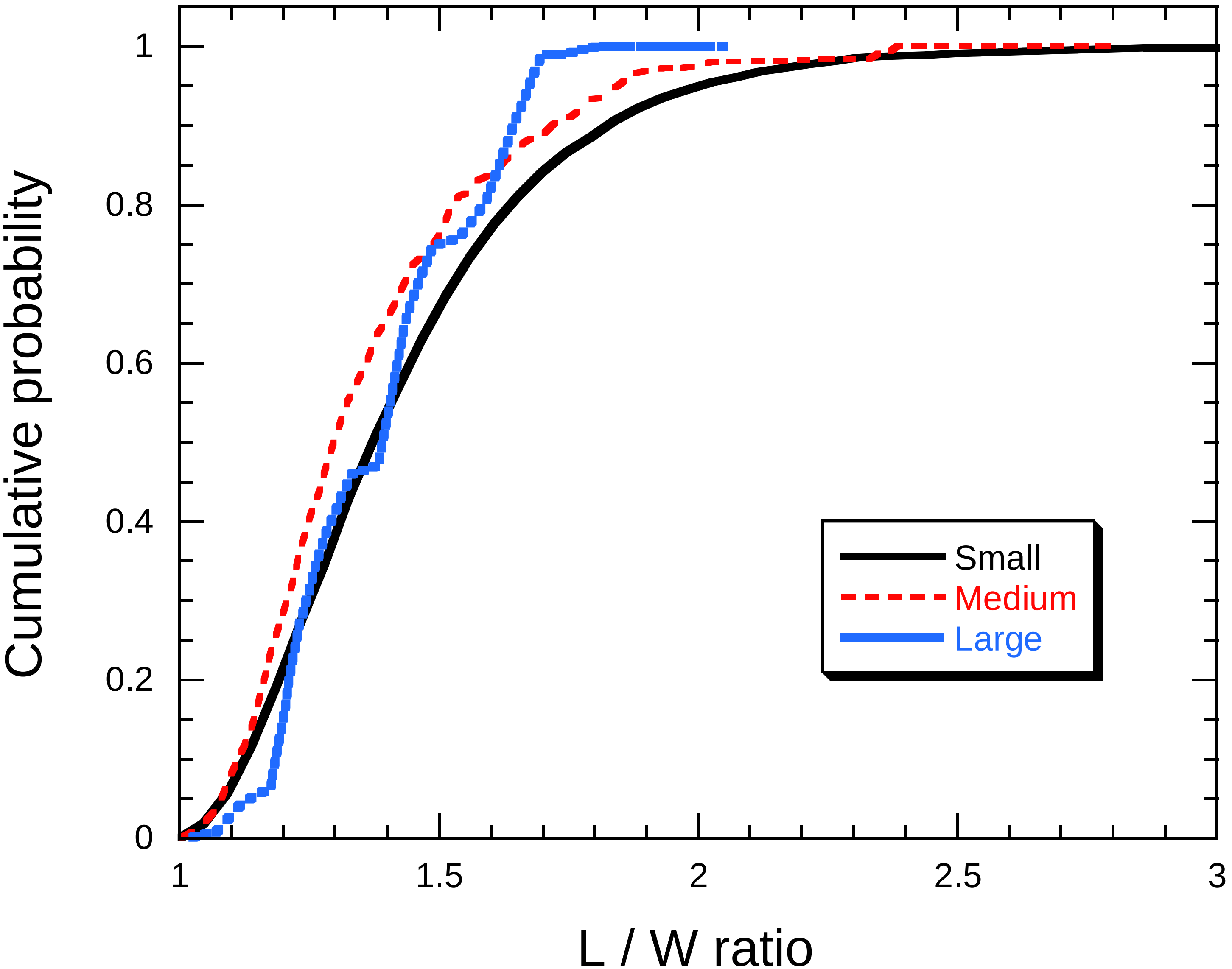


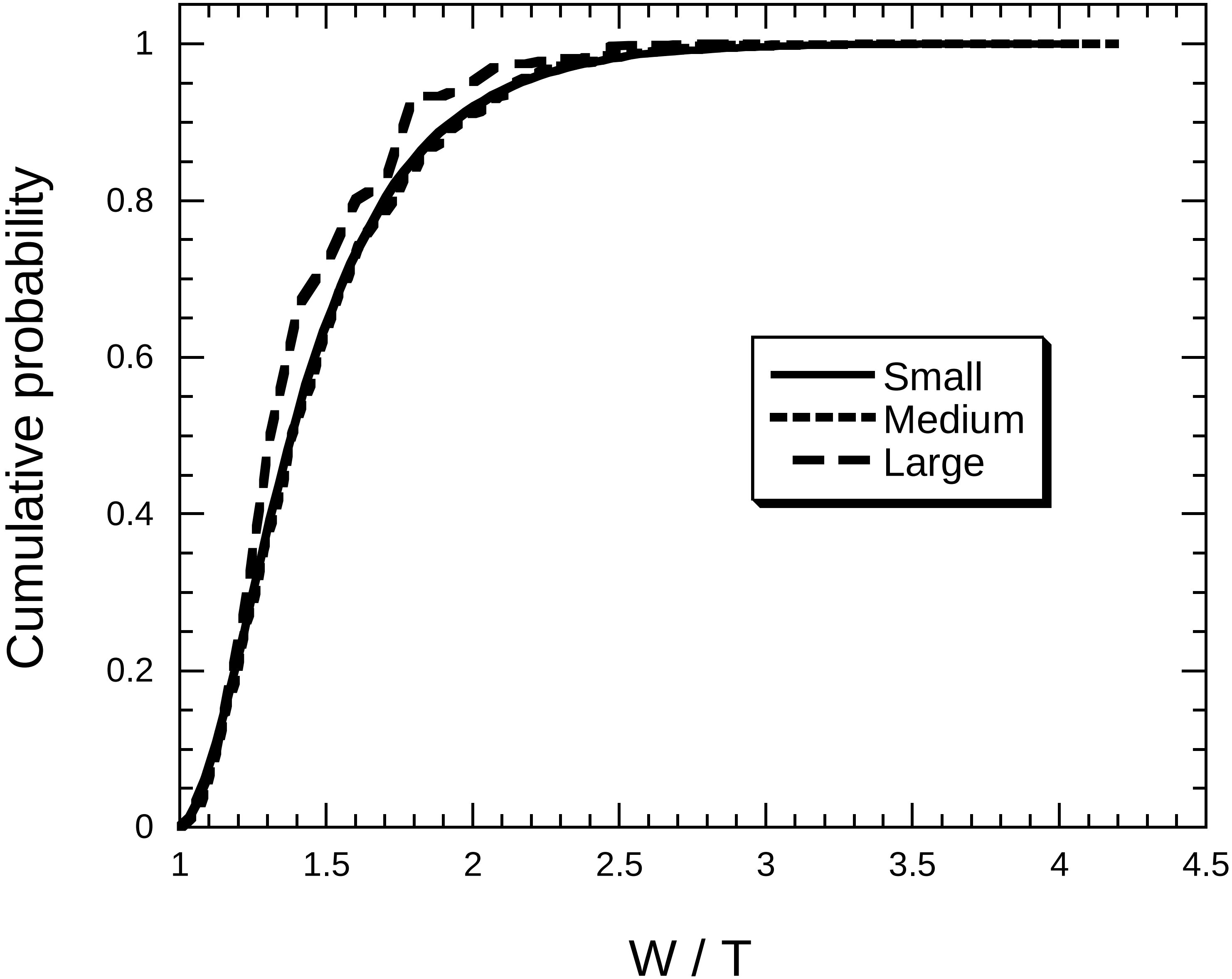
360 micrometers



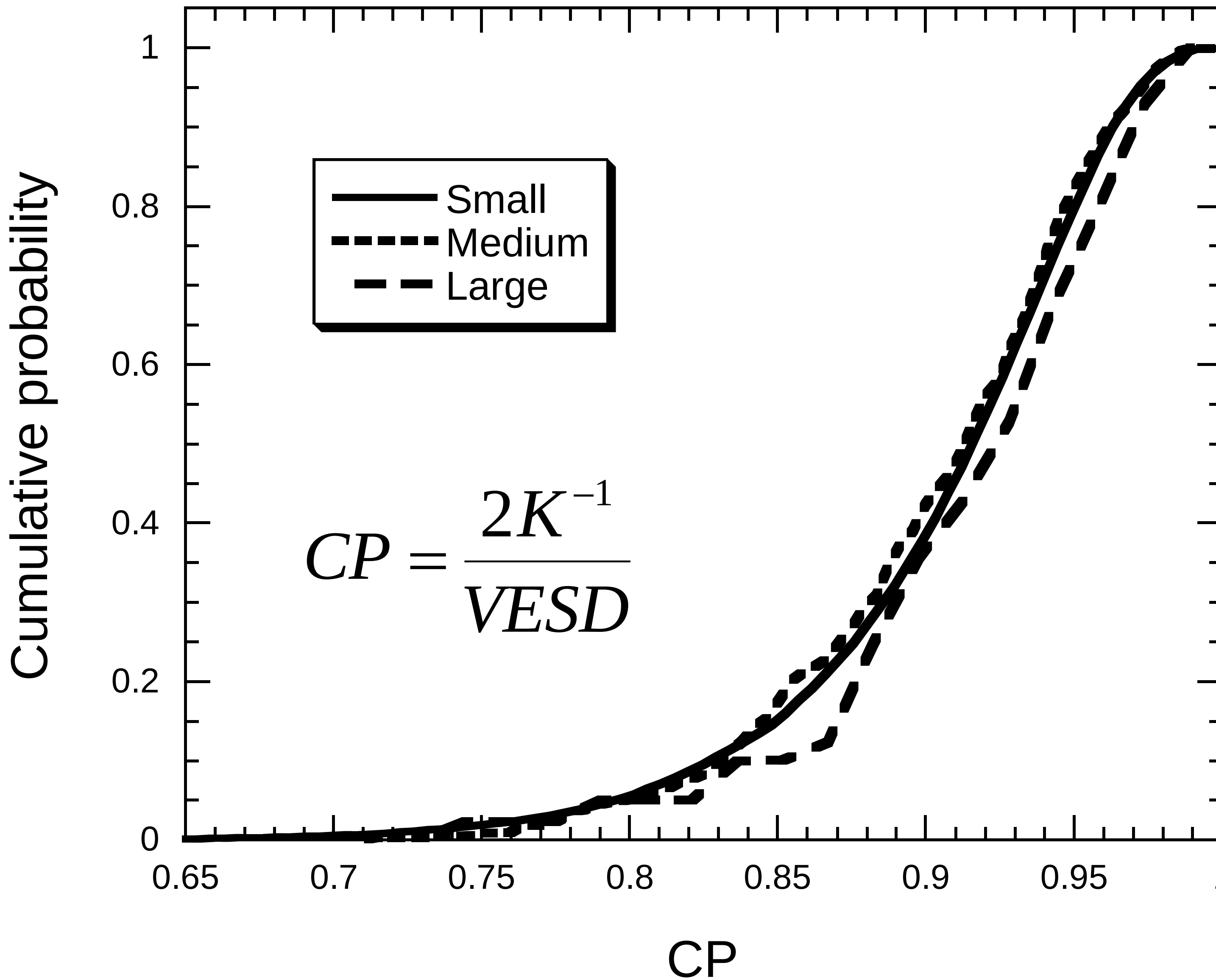
1.8 mm

11 mm


Cumulative probability
1
0.8
0.6
0.4
0.2
0
1
1.5
2
2.5
3
L / W ratio
Small
Medium
Large



Cumulative probability
W / T
0
0.2
0.4
0.6
0.8
1
1
1.5
2
2.5
3
3.5
4
4.5
Small
Medium
Large



K^{-1} = Inverse of integrated curvature, VESD = diameter of sphere with equal volume

PSD graphs

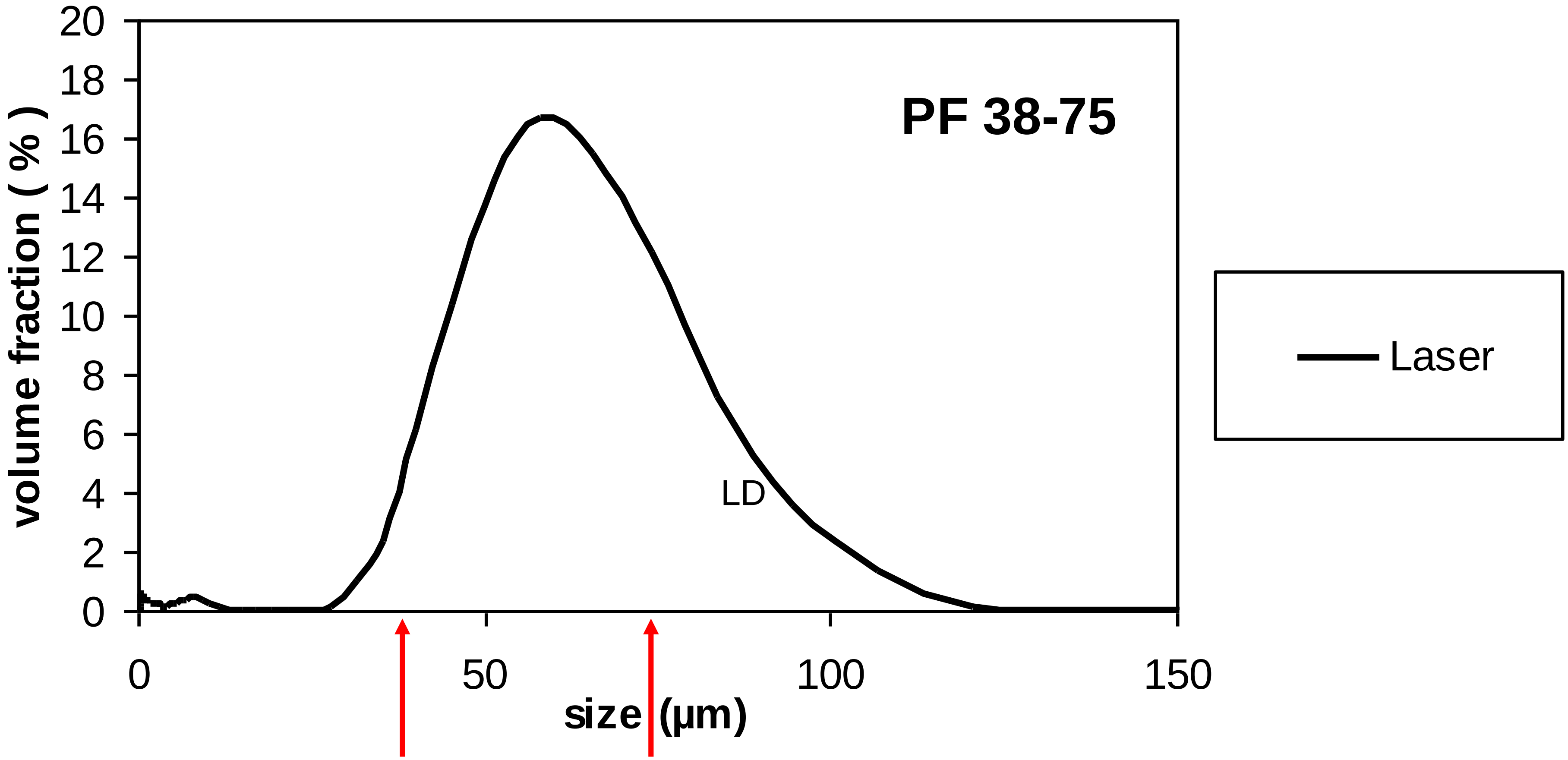
- Particle size distribution graphs are always presented as
  - “size” on the x-axis
  - volume fraction or mass fraction (same for homogeneous material) on the y-axis

Question: what length should be used to characterize the “size” of the particle? Is it even possible to do so with a one-parameter model?

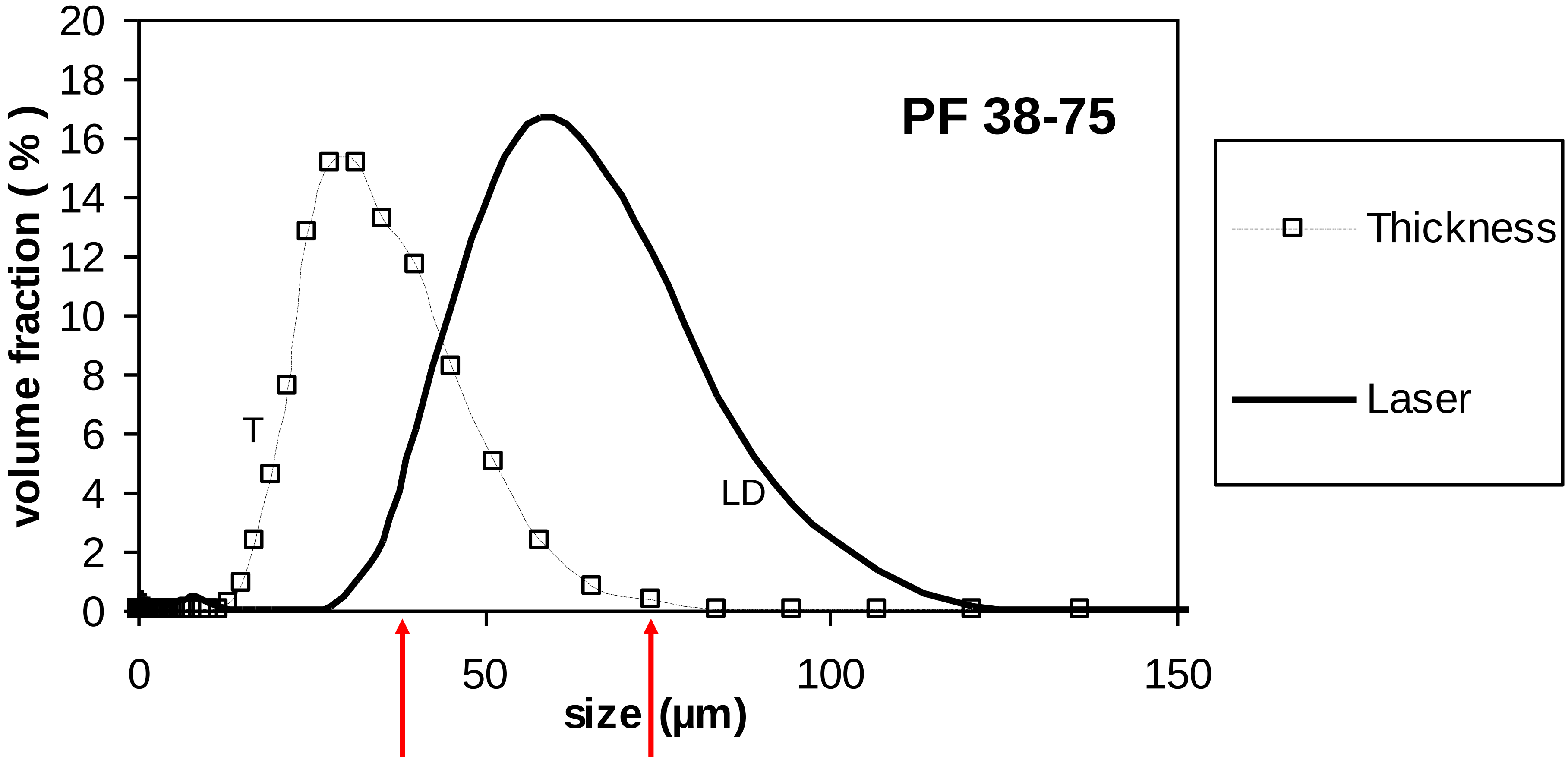
Use various X-ray CT computed “size” quantities

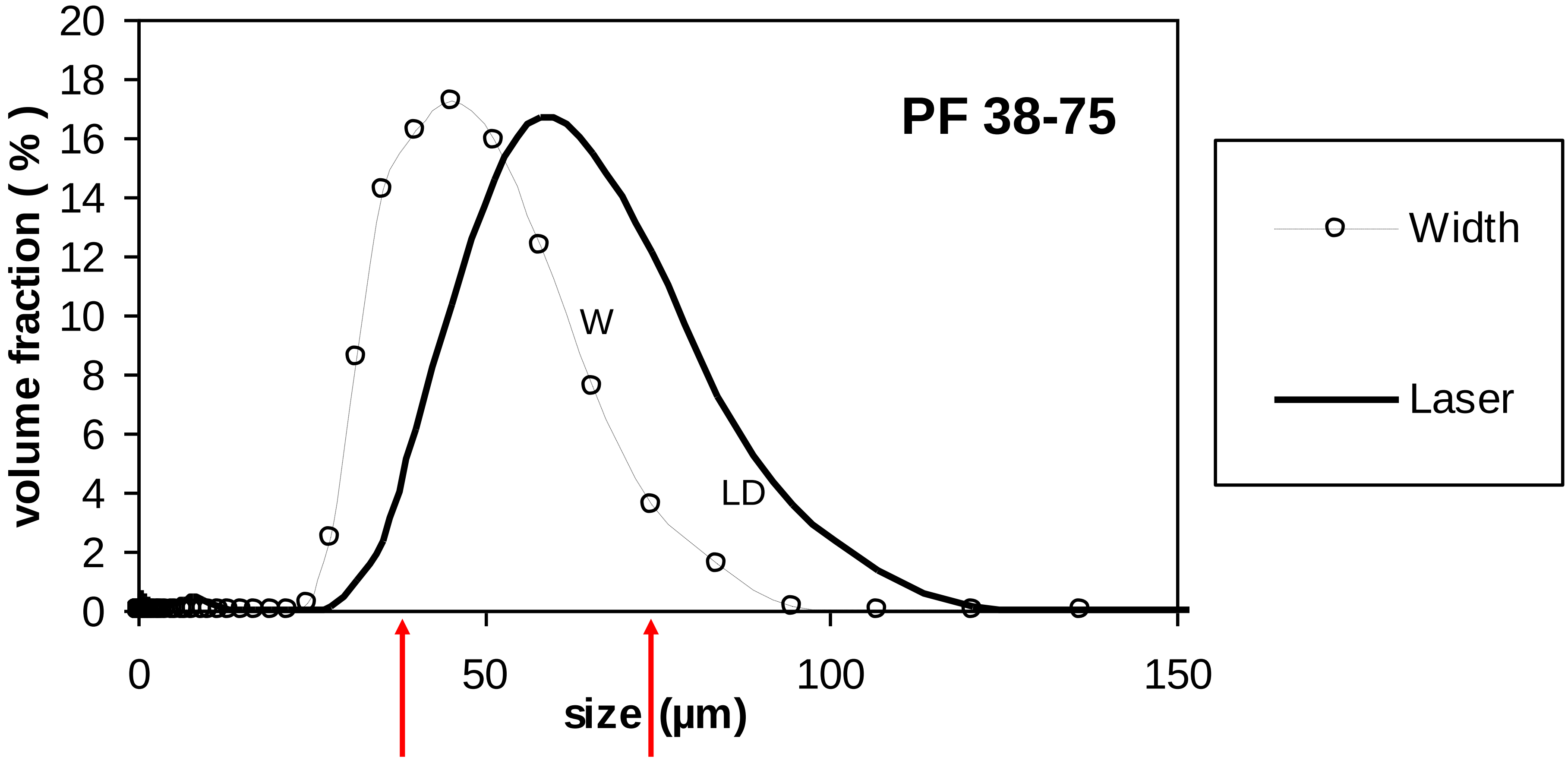
Microfine aggregate

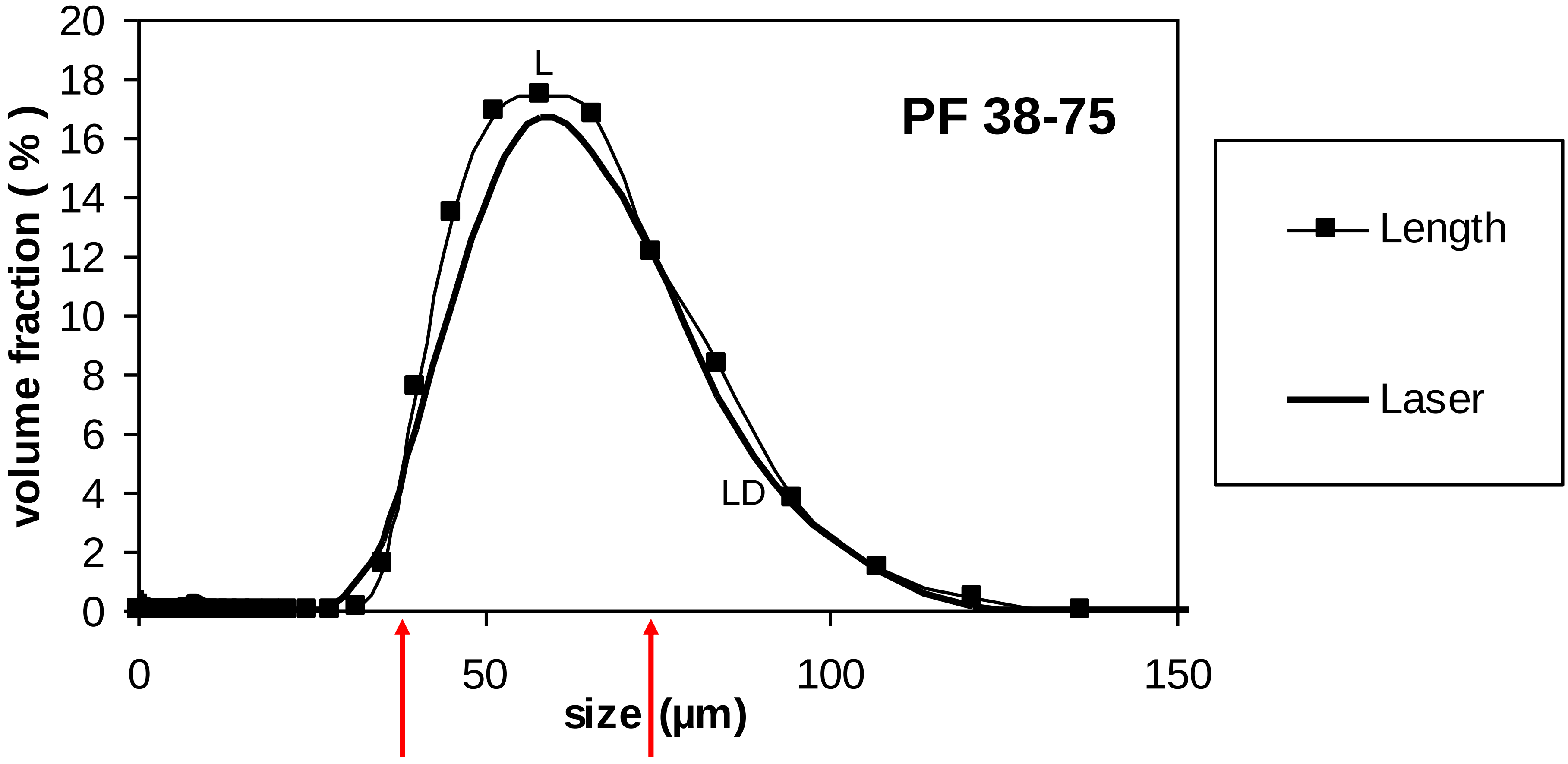
- Do X-ray CT plus spherical harmonic analysis, calculate L, W, and T
- Construct PSD using L, W, or T as the “size” variable
- Carry out laser diffraction experiments
- “Size” is diameter of a sphere with equal diffraction patterns
- Compare laser diffraction with various constructed histograms, see which, if any, of LWT compares best with laser diffraction “size”



Question: Why does graph go well outside the 38 μm and 75 μm sieve limits?


PF 38-75
volume fraction (%)
20
18
16
14
12
10
8
6
4
2
0
T
LD
0
50
100
150
size (µm)
Thickness
Laser

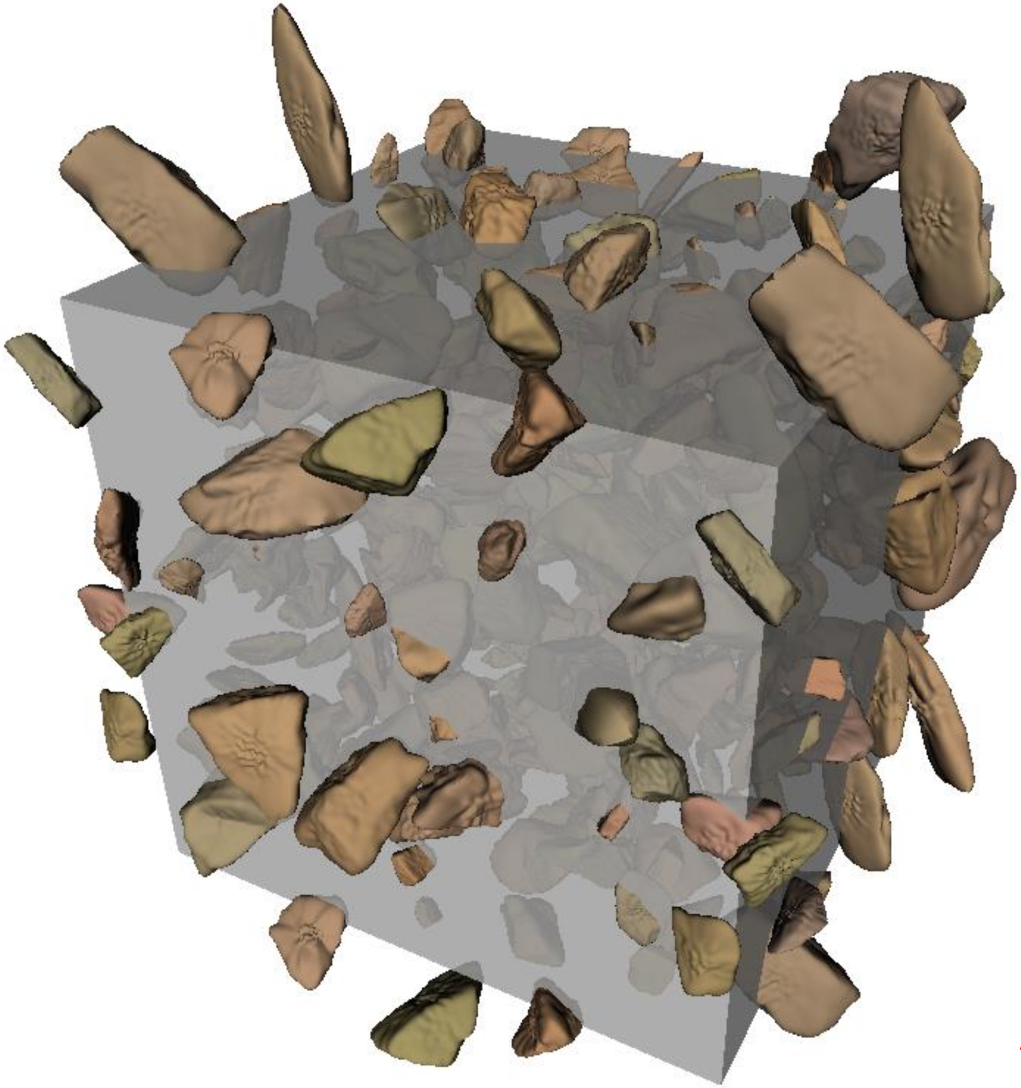

PF 38-75
volume fraction (%)
size (µm)
W
LD
Width
Laser
0
2
4
6
8
10
12
14
16
18
20
0
50
100
150

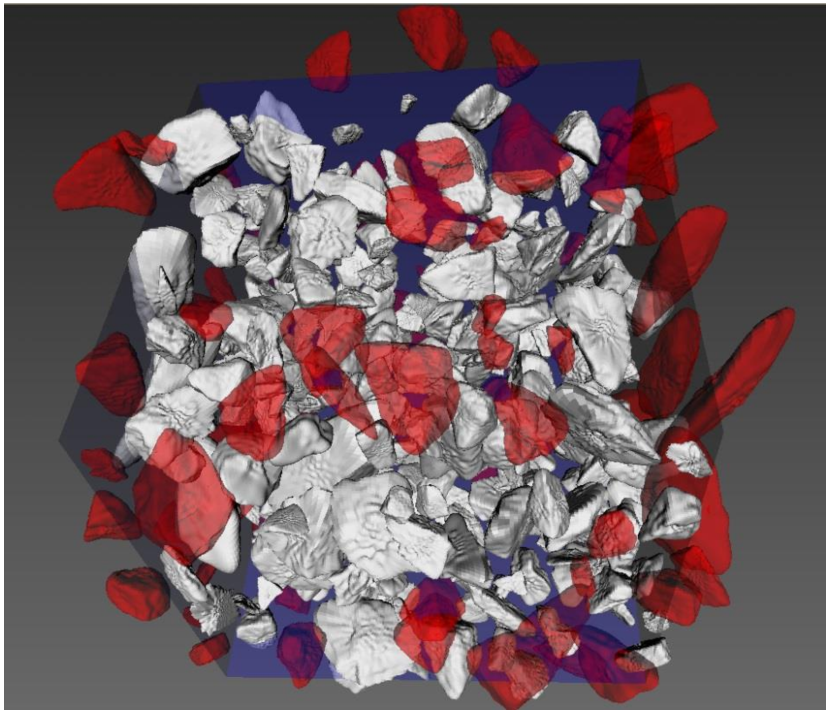

PF 38-75
L
LD
Length
Laser
volume fraction (%)
size (µm)
0
2
4
6
8
10
12
14
16
18
20
0
50
100
150

Anm model

- Places real particles randomly into a unit cell
- Cement in water matrix, sand in cement paste matrix, gravel in mortar matrix
- Geometrical model – can use as input into meshing and material models

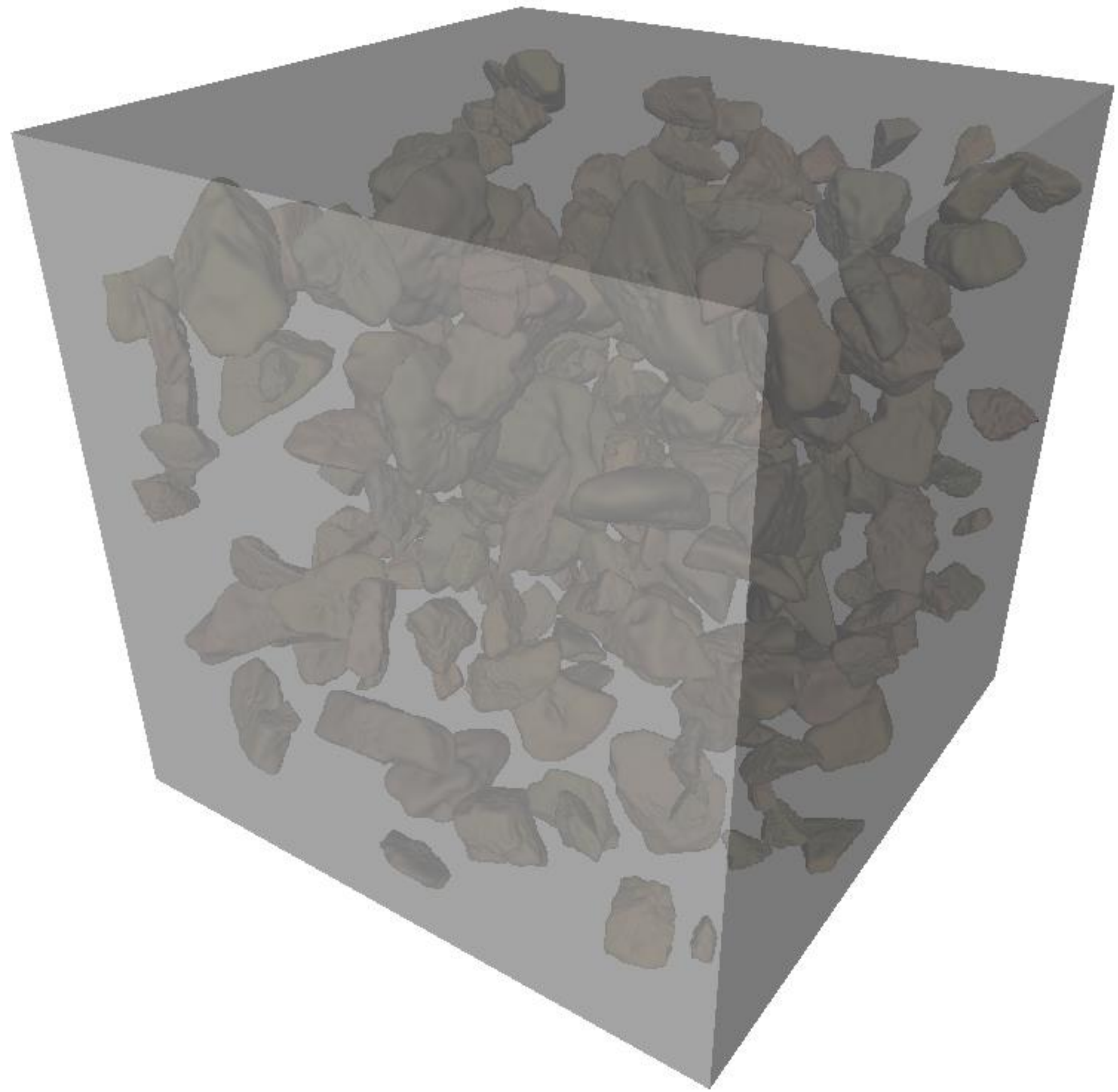
- Version 1 developed with Zhiwei Qian (Delft)
- Version 2 developed with Yang Lu and Stephen Thomas (Boise State University) and Jeff Bullard (NIST)
- Code not yet public, collaborators welcome – contact Yang Lu at Boise State, Civil Engineering or myself



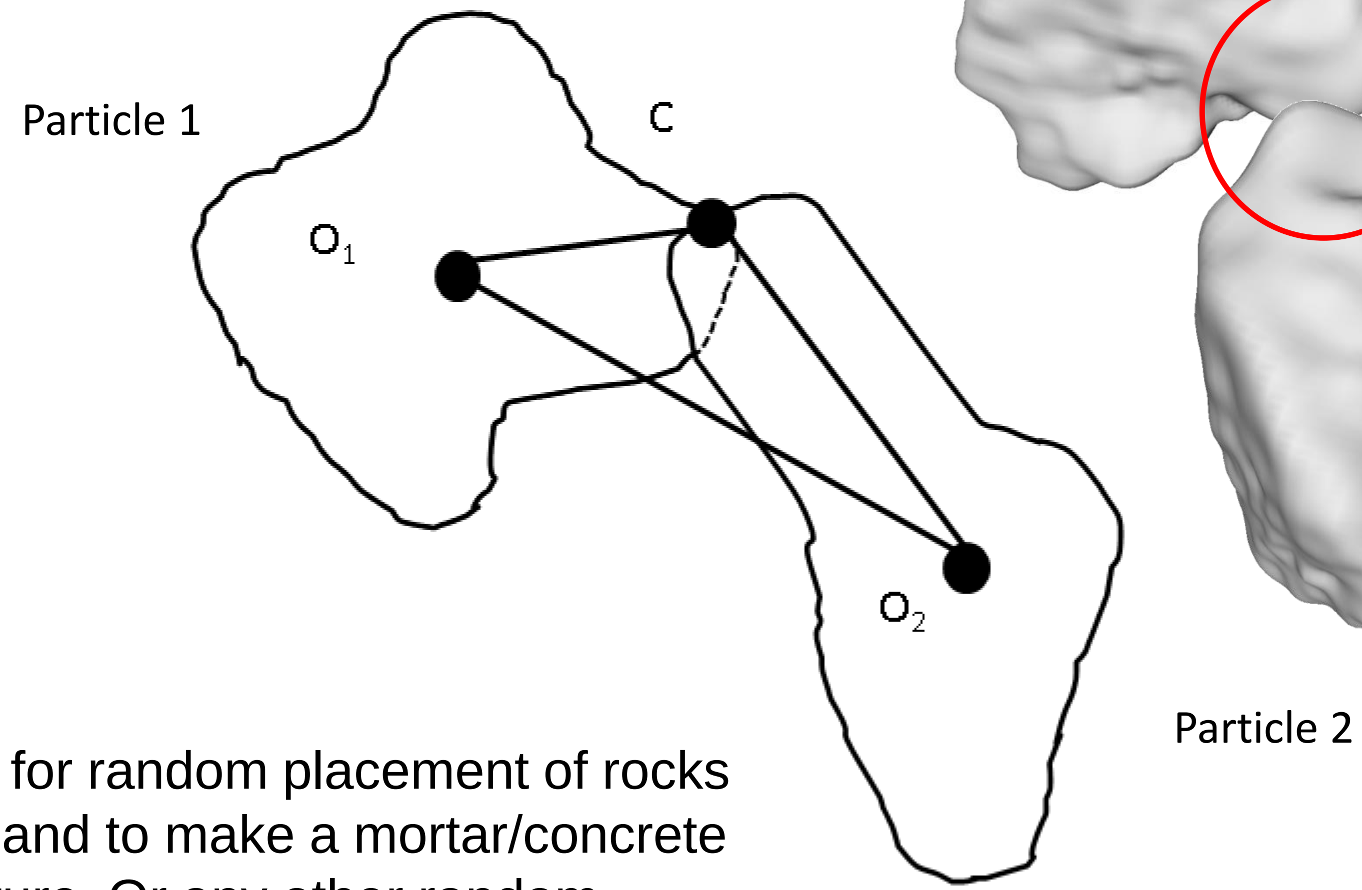


Anm model: Two mortars using periodic boundary conditions. Particles outside the box are periodic “ghost” particles.

Anm model - concrete



Overlap algorithm



Used for random placement of rocks and sand to make a mortar/concrete structure. Or any other random composite

Summary

- Blend of computational and experimental materials science is powerful for examining 3D particle shape
- Many collaborators…
- **Future work**: In collaboration with Jay Goguen (JPL) and Olga Gomez (Spain), have borrowed 2 g of actual lunar soil from NASA, will do shape characterization followed by light scattering computation, to better analyze light scattering from the moon and Mars