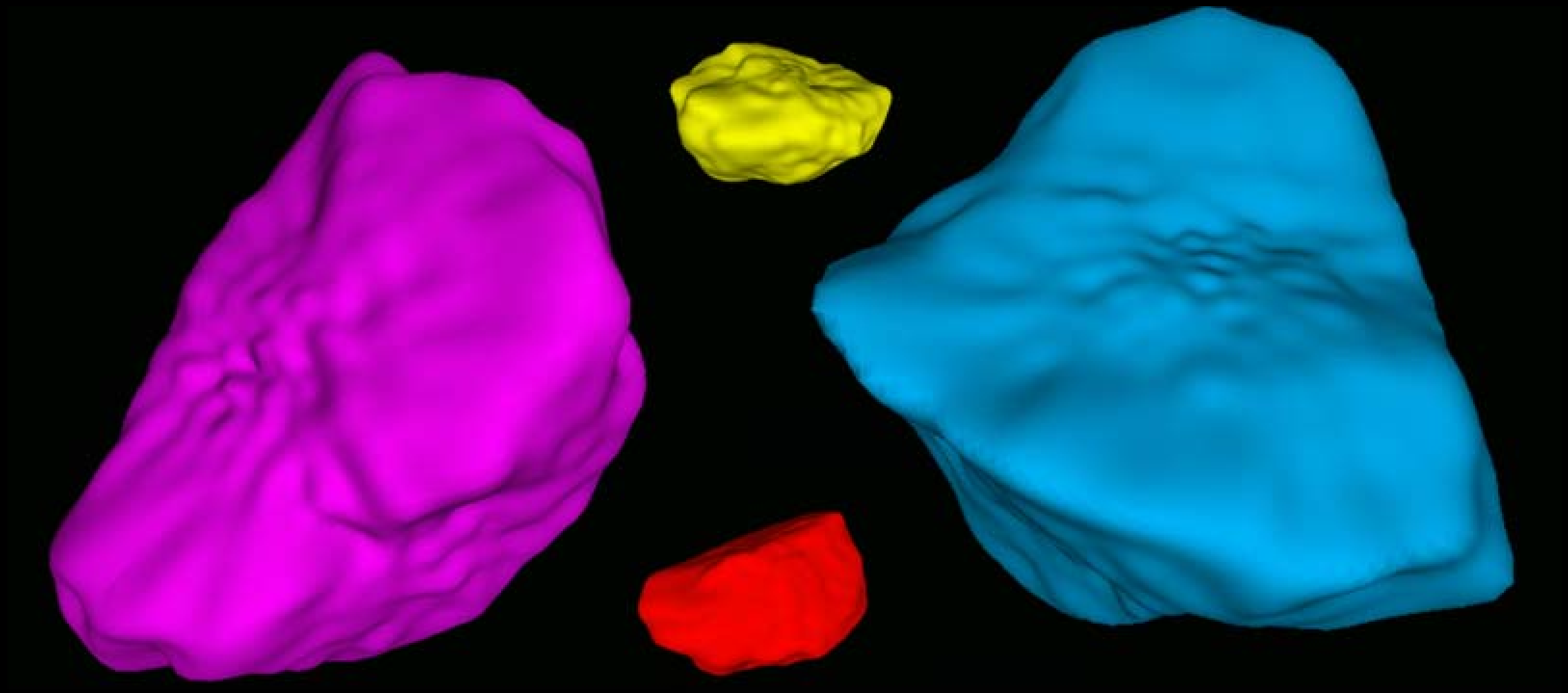
VIRTUAL CONCRETE

Ed Garboczi
National Institute of Standards and Technology
Gaithersburg, Maryland



Prediction of concrete performance

Gaithersburg, MD

NIST

Boulder, CO

- 1901-1988 National Bureau of Standards
- Now: National Institute of Standards and Technology, Dept. of Commerce
- The nation's measurement laboratory
- Basic research and technical input for standards development in existing and emerging industries

Inorganic Materials Group

- Purpose: Facilitate innovation in inorganic construction materials
  - Improved materials science basis (computational and experimental) for accelerated tests and performance-based standards

- Part of the Building and Fire Research Laboratory (BFRL)

Virtual Concrete in a Nutshell

- Physical tests on concrete require large amounts of material and long times (~ 28 days)

- **Idea**: Provide computer models with a virtual representation of the material and simulate the results of physical tests

- **Applications**:
  1. Design of new materials
  2. Supplant QA testing
  3. Understanding

The Virtual Cement and Concrete Testing Laboratory (VCCTL)

- Materials science-based
- Based on accurate material characterization
- **Prediction** of performance attributes

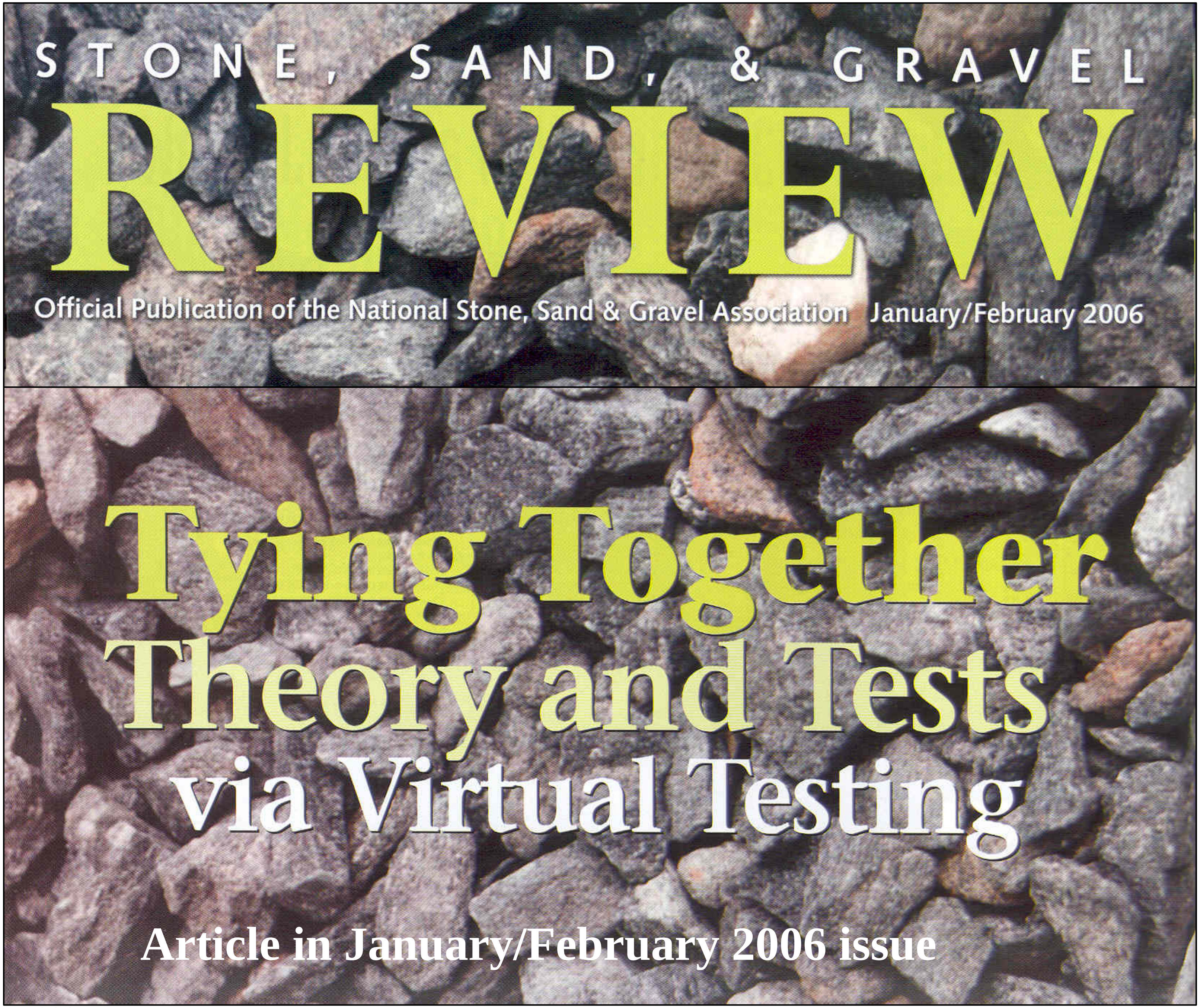
VCCTL™ 7.0

Virtual Cement and Concrete Testing laboratory

Driving Forces for VCCTL Research

- Industrial needs
  - New materials and new admixtures
  - Controlling and predicting durability and other properties, e.g., workability, stiffness, strength

- Concrete is complicated physically and chemically
  - Rise of computational materials science of concrete at NIST
  - Modern revolution in computer technology


STONE, SAND, & GRAVEL

REVIEW

Official Publication of the National Stone, Sand & Gravel Association January/February 2006

Tying Together Theory and Tests via Virtual Testing

Article in January/February 2006 issue

VCCTL Consortium: 8th Year

VDZ

PCA

Cement

National Stone, Sand & Gravel Association

Aggregates

NIST

National Institute of Standards and Technology

Admixtures

BASF The Chemical Company

Sika

GRACE Construction Products

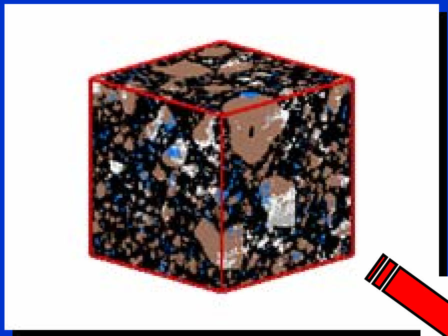
MAPEI

TURNER-FAIRBANK HIGHWAY RESEARCH CENTER

Florida Department of Transportation

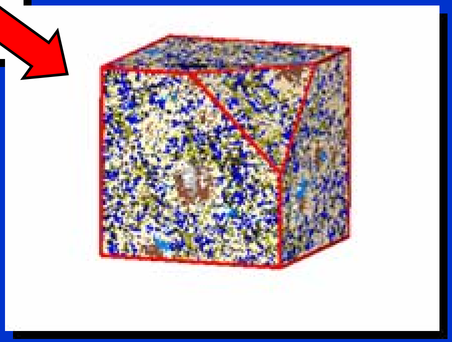
Concrete

VCCTL



3D Virtual
Cement Paste

Simulate Hydration
Reactions to Evolve
Microstructure



Hydration Properties

- Heat of hydration
- Chemical shrinkage
- Setting time

Mechanical Properties

- Elastic moduli
- Compressive strength

Degradation Behavior

- Leaching
- Sulfate attack

Transport Properties

- Formation factor
- Transport factor

Project Vision

- ***Computer-design concrete just like structural engineers computer-design structures***
  - **Make the VCCTL an effective tool for cement, aggregate, admixture, and concrete companies to optimize the use of existing and new materials for existing and new requirements**
  - **Widespread educational tool – every civil engineer will have used eVCCTL in their materials courses, just like they all learn finite element packages**

VCCTL analogy

- **Virtual** Testing Laboratory acts just like a **physical** testing laboratory
- Databases replace material hoppers and bins
- Material mixing models replace mixers
- Quantitative algorithms replace instrumented testing machines
- Software interface replaces lab cart

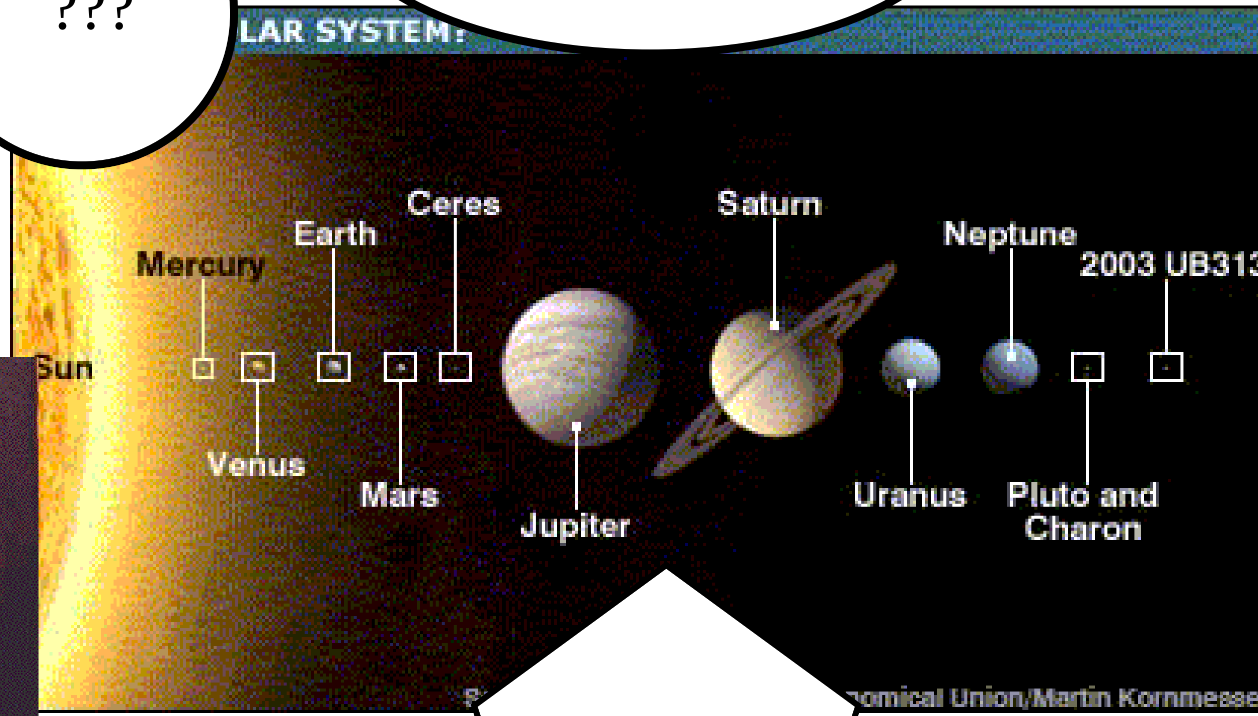
movie

A classic case of (good) experiment and (good) theory

Masses of observational data!!

???

???!!!!!

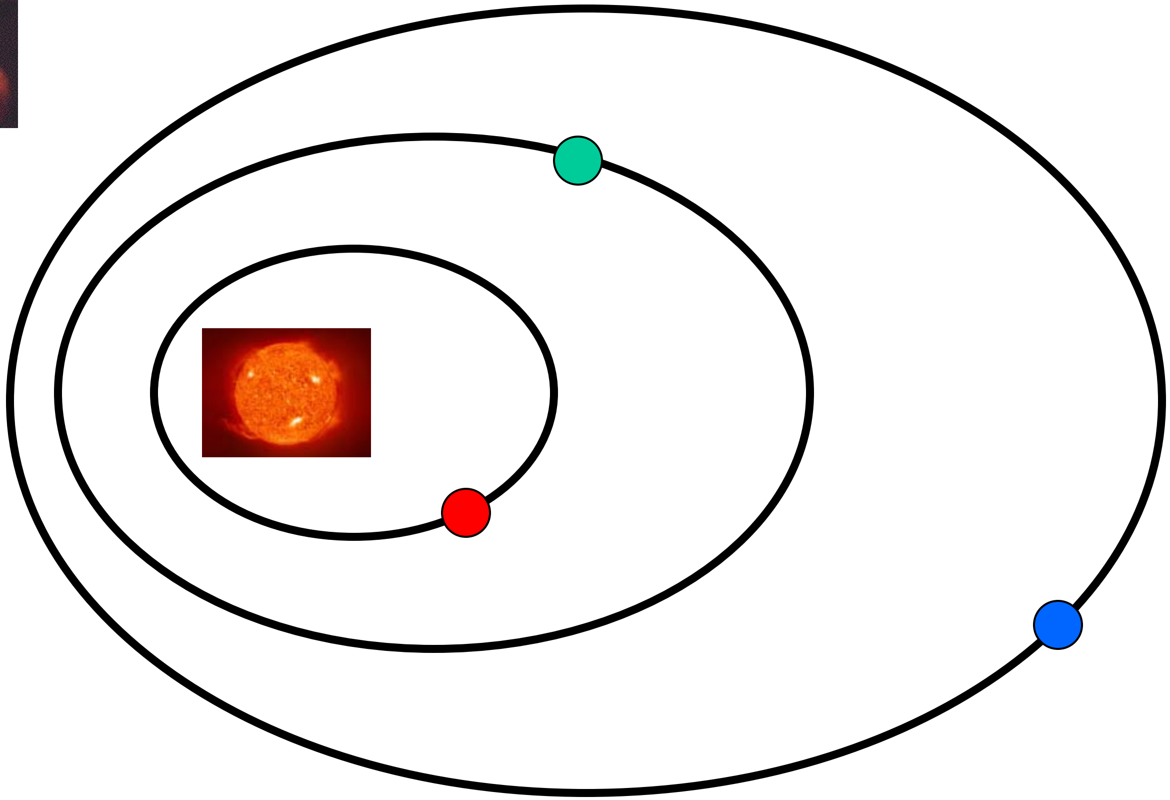


Johannes Kepler

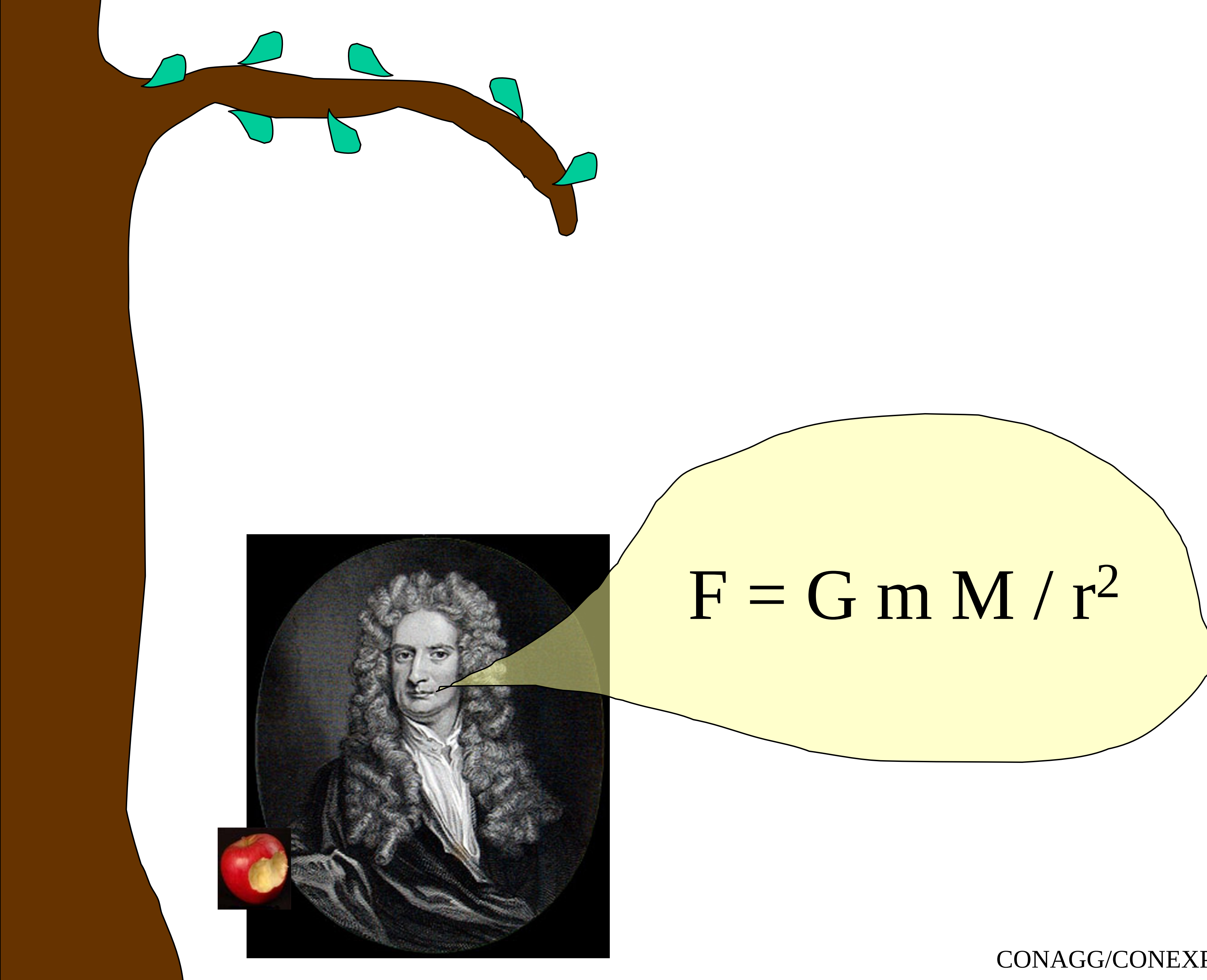
???

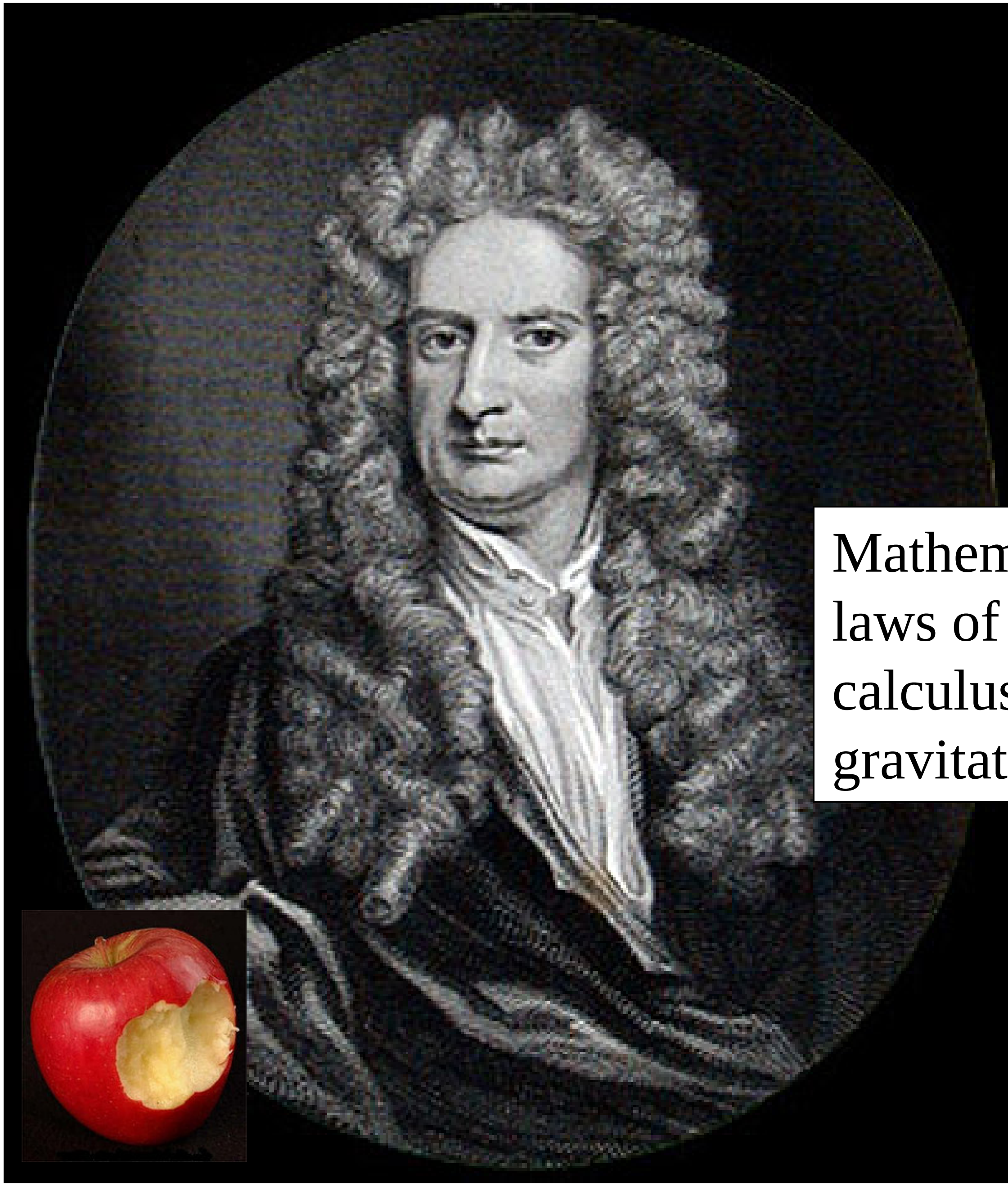
Mathematical fitting of data – years of effort

Three laws of planetary motion, mathematically formulated



Sir Isaac Newton


$F = G m M / r^2$



Mathematical derivation of three laws of planetary motion, using calculus and law of universal gravitation

Current status of concrete

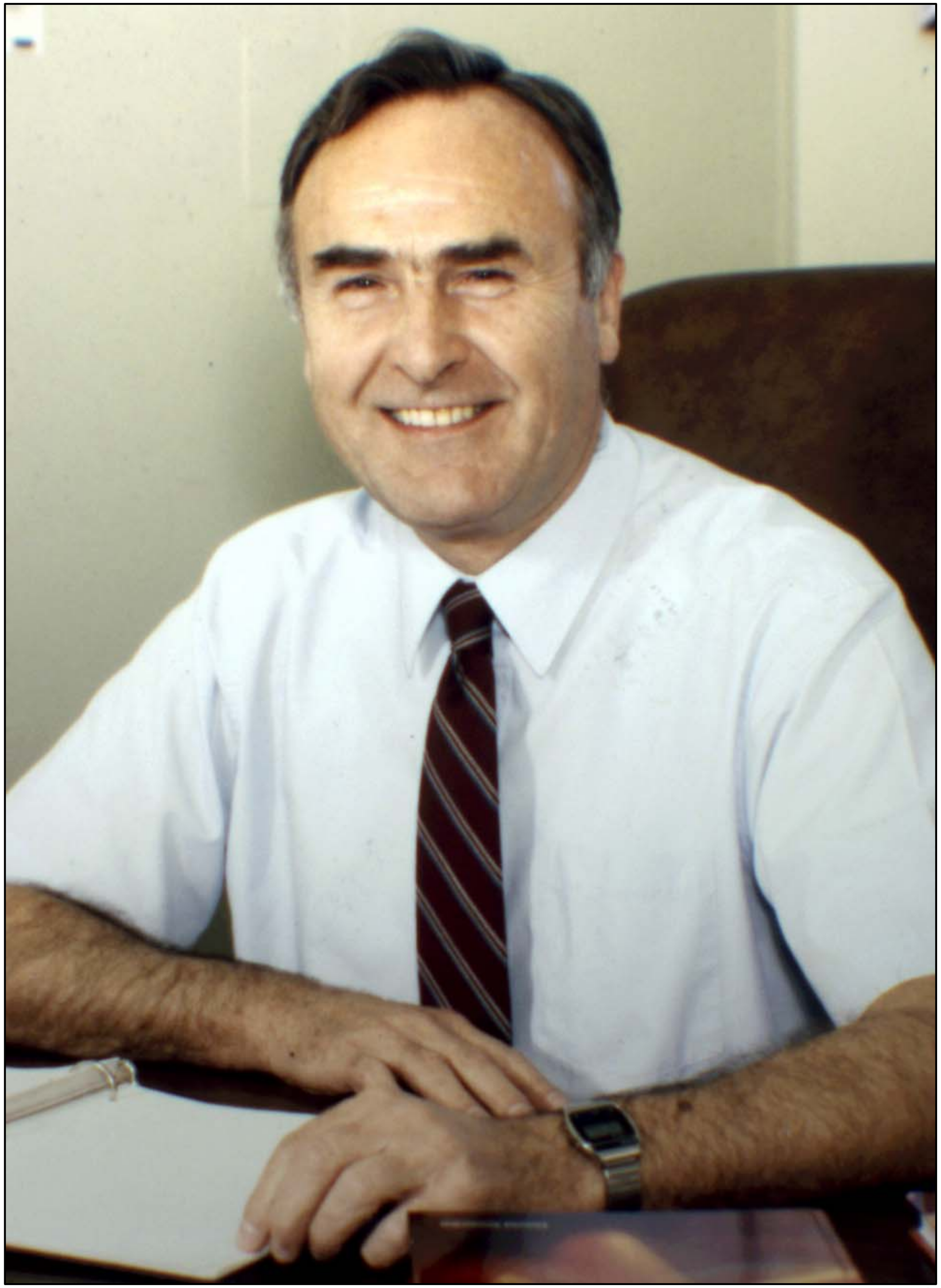
Too many empirical standard tests

- Example of durability (e.g., ASR)
  - bars and baths and uncontrolled mechanisms, oh my!
  - "acceleration" is totally empirical
- Typical test
  - make (big) bars and drop them into bucket of concentrated "bad stuff"
  - use various temperatures
  - measure length change every so often, one at a time
  - after six months, do for another six months because answer is not clear; **repeat** (endlessly)

Appropriate status for concrete

- Correct "theory" is the basics of chemistry and physics expressed through computer models = computational materials science
  - Empirical standard tests are not much use for computational materials science – measurements!
- Kepler-Newton scenario is experimental and computational materials science working together synergistically
  - This is really the only way to solve the difficult problems facing us in this difficult material
- This approach was put forth by Dr. Geoffrey Frohnsdorff →→→→

A visionary scientist and leader: Dr. Geoffrey Frohnsdorff (1928-2006)



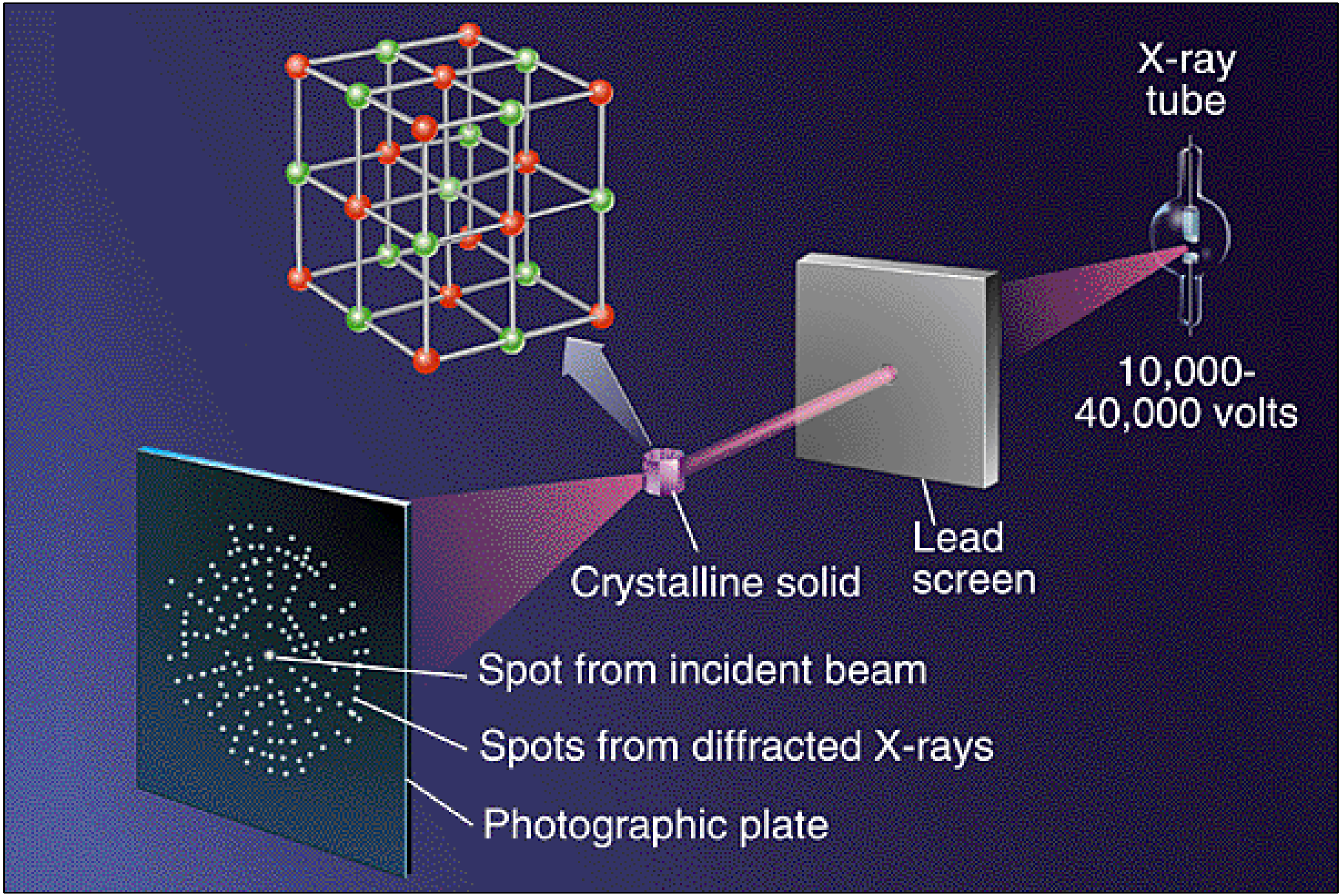
Materials science approach

- Characterization
- If models are to be more successful, then better characterization of starting materials needs to be done
  - Cement
  - Aggregates

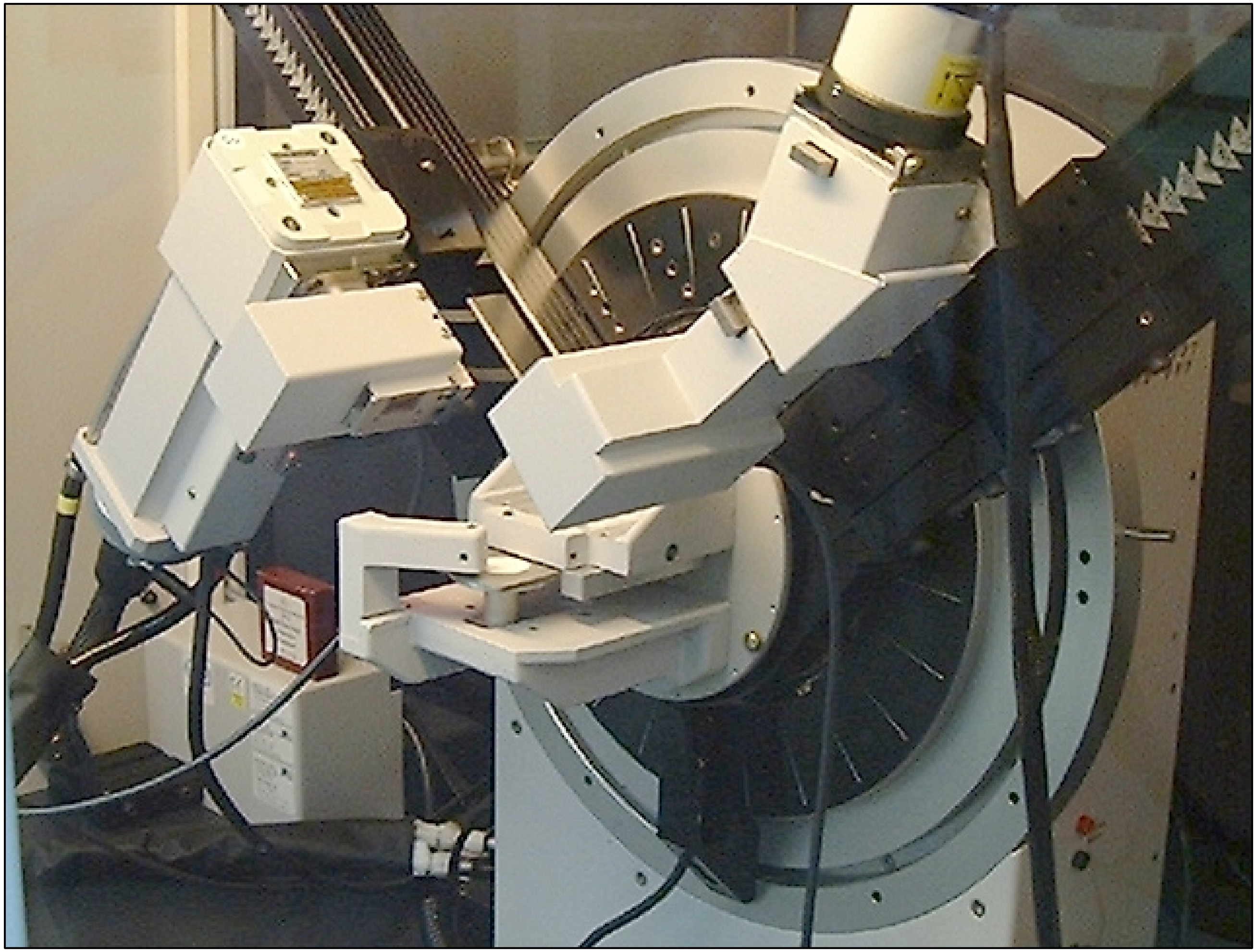
Length scales to remember

- One thousandth of a meter = one millimeter (mm) – typical medium fine sand grain
  - 25 mm in an inch
- One thousandth of a millimeter = one micrometer (μm) – average hair thickness and microfine aggreate is about 50 μm, average cement particle is about 20 μm
  - 25 μm in a mil (thousandth of an inch)
- One thousandth of a micrometer = one nanometer – five water molecules lined up in a row

X-ray Diffraction



X-ray Diffraction for Cement

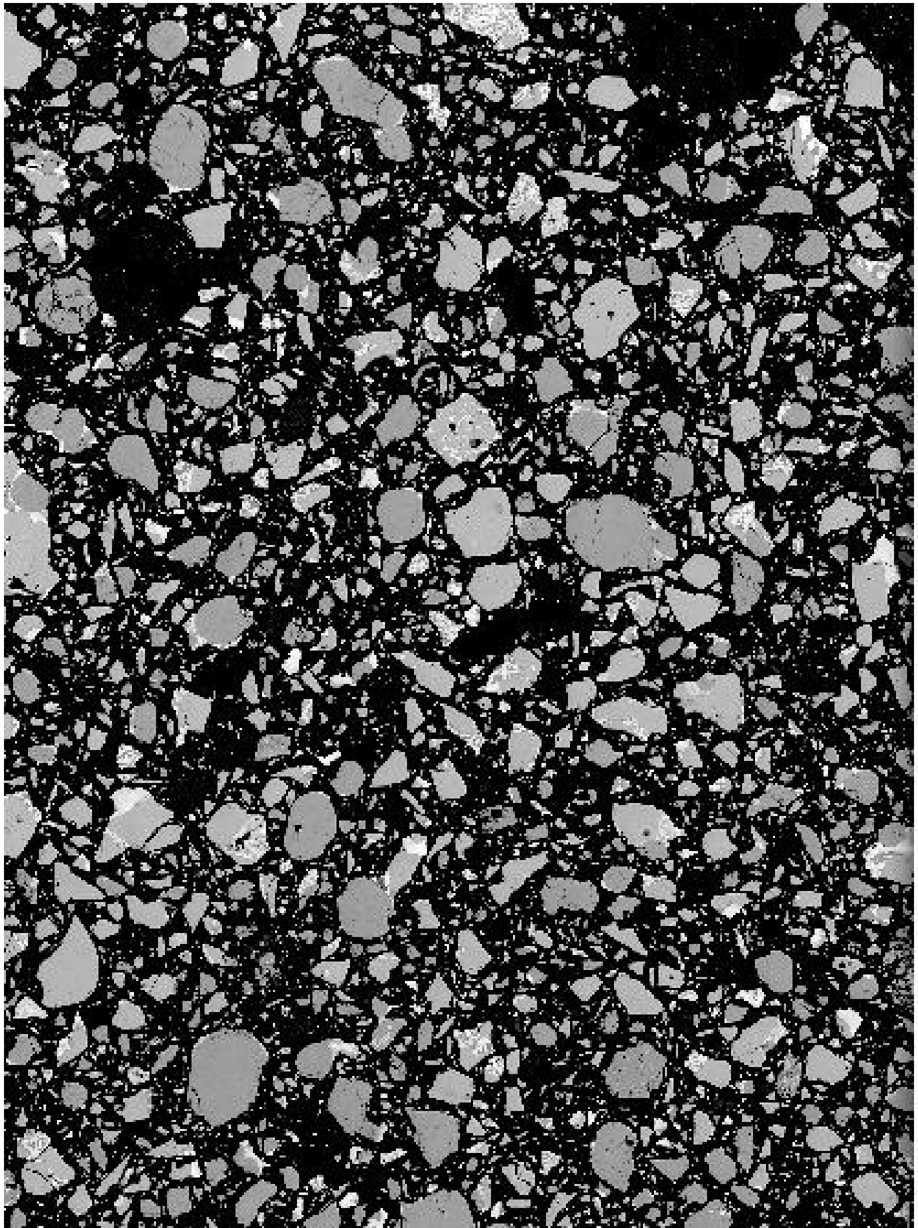


Ten or so different crystals making up cement, new nethod enables all their patterns to be extracted

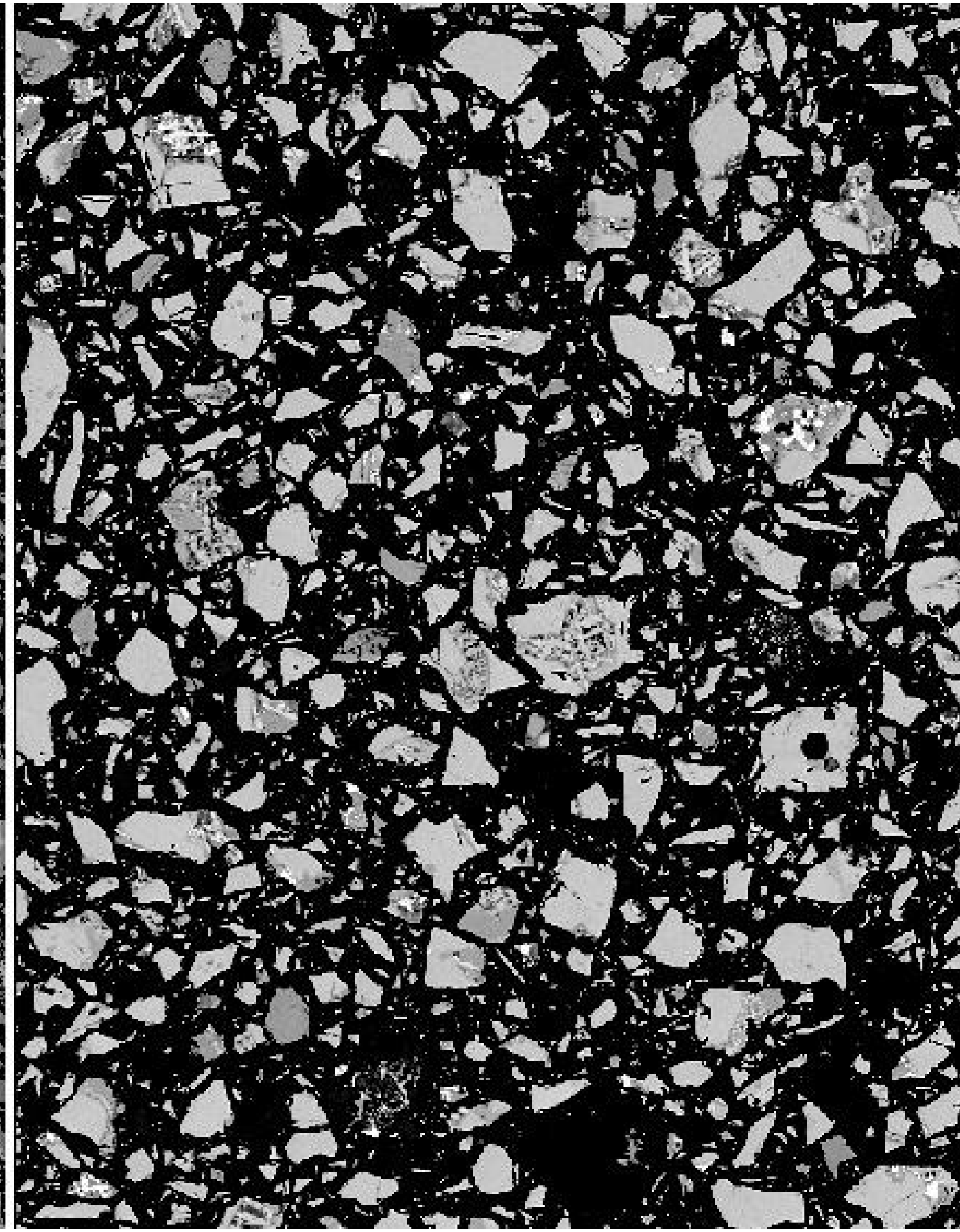
Rietveld method, first devised for high temperature superconductors

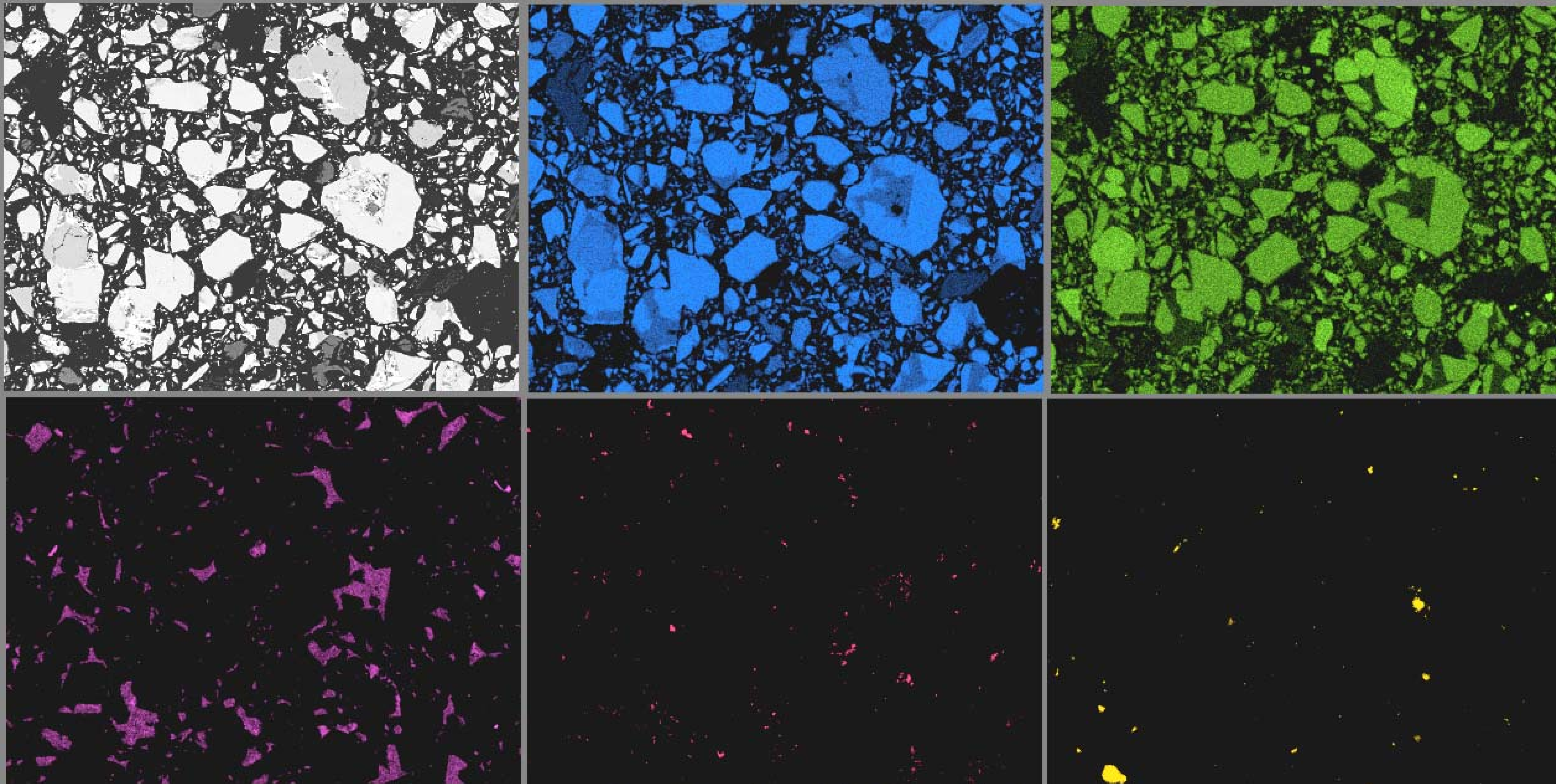
Scanning Electron Microscopy

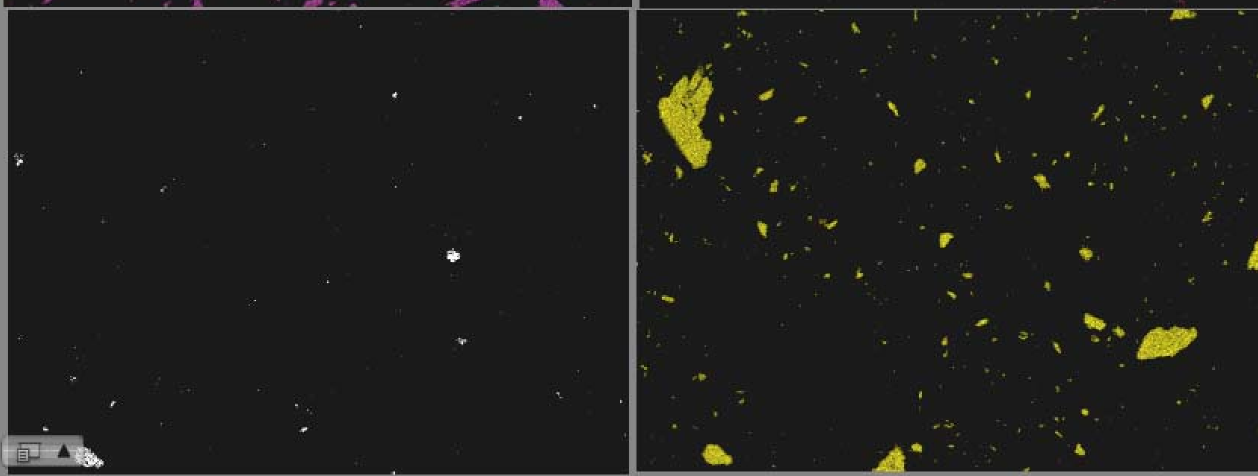
Portland Cement 1



Portland Cement 2







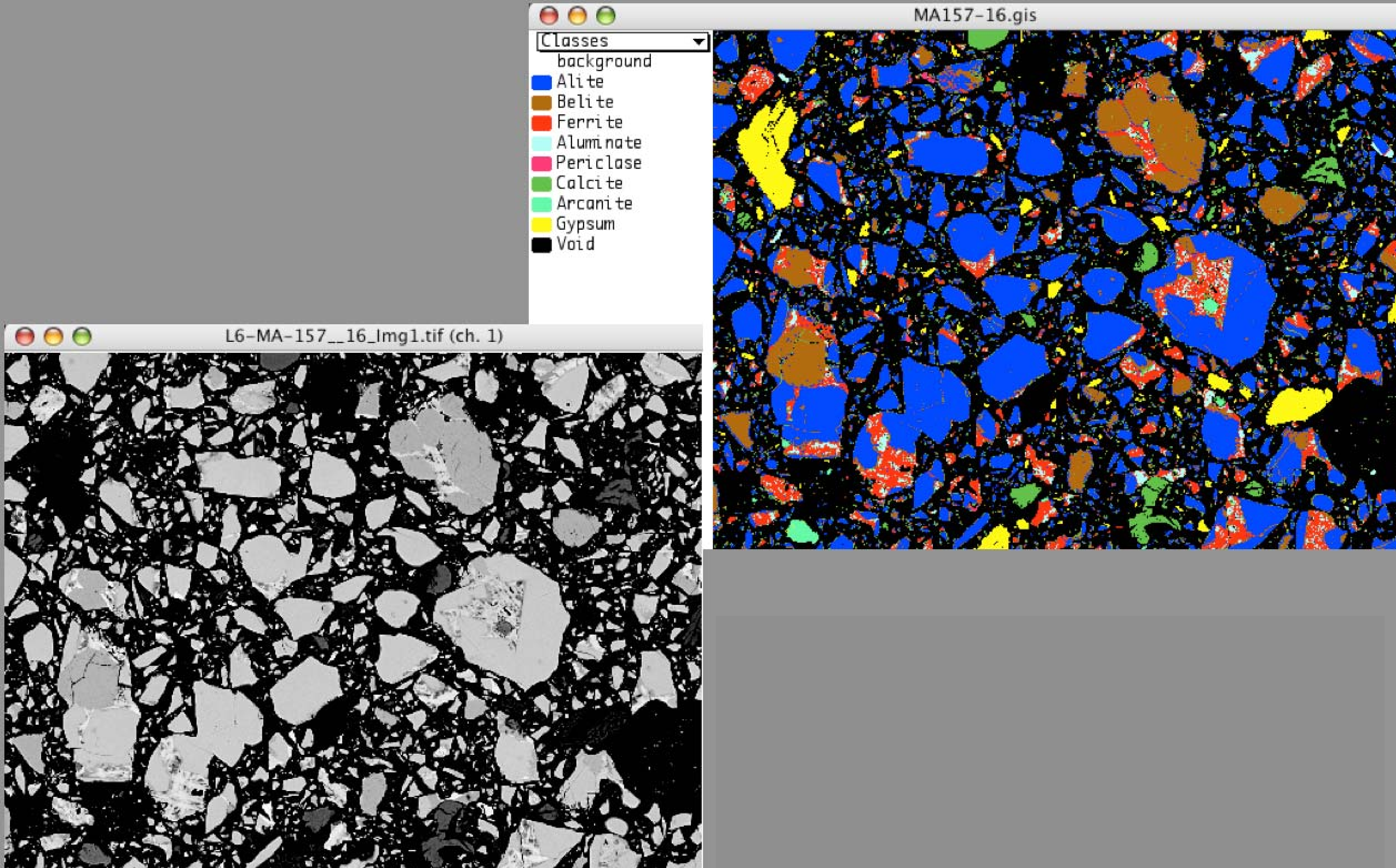
Examine Raw Data

-phase ID

-image quality

-Identify key images

BE, Al, Mg, K, Na, S

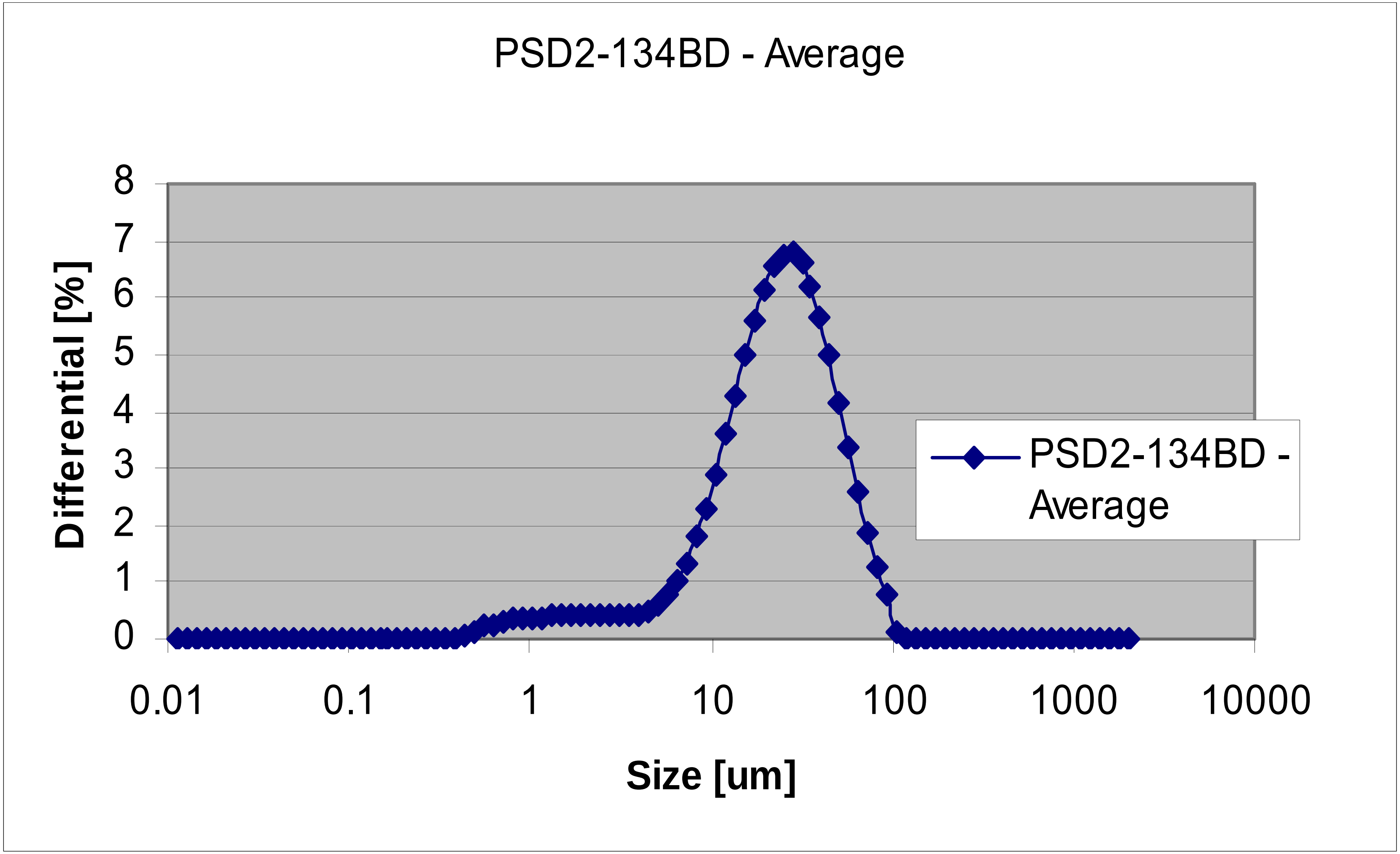


MA157-16.gis
Classes
background
Alite
Belite
Ferrite
Aluminate
Periclase
Calcite
Arcanite
Gypsum
Void
L6-MA-157__16_Img1.tif (ch. 1)

Particle size analysis

Laser shines through powder, approximately measures the size by how the light scatters off the particles

(useful for cement through microfines up to 1 mm diameter sand)



PSD2-134BD - Average
Differential [%]
8
7
6
5
4
3
2
1
0
0.01
0.1
1
10
100
1000
10000
Size [um]
PSD2-134BD - Average

X-ray microcomputed tomography

- X-ray micro CT
  - 3-D air void structure in mortars
  - Particle shape for cement, sand, gravel
  - Microstructure of fire-protective materials for protecting steel frames in fires
  - Pore structure for foamed thermal insulation materials for houses
  - Roundness of glass beads for reflective lines on roads
  - Particulates in explosives to help detect terrorists

X-ray microcomputed tomography

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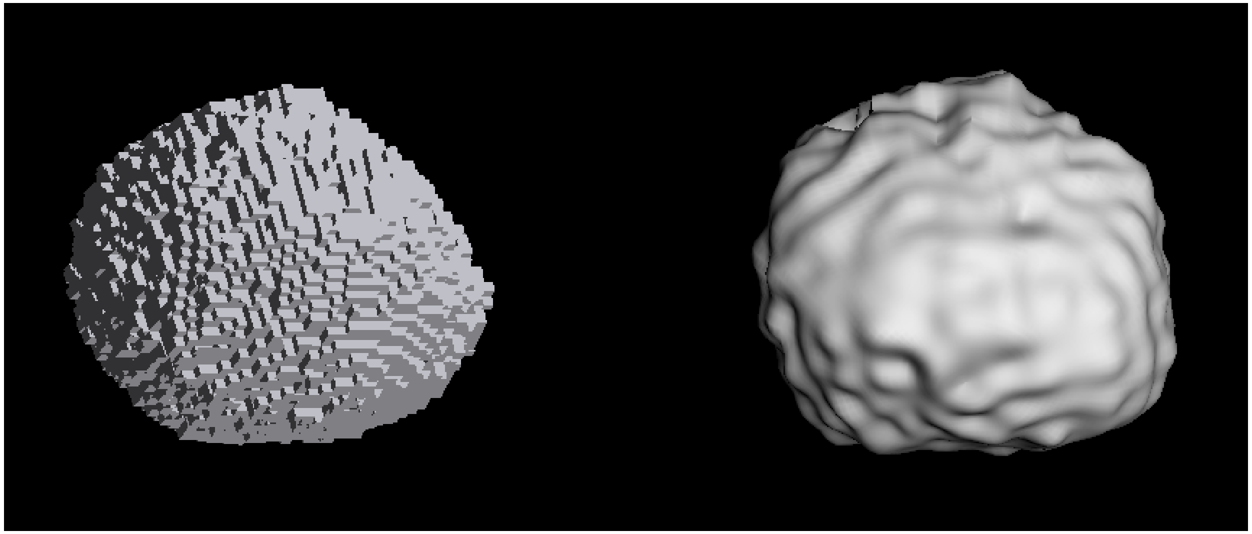
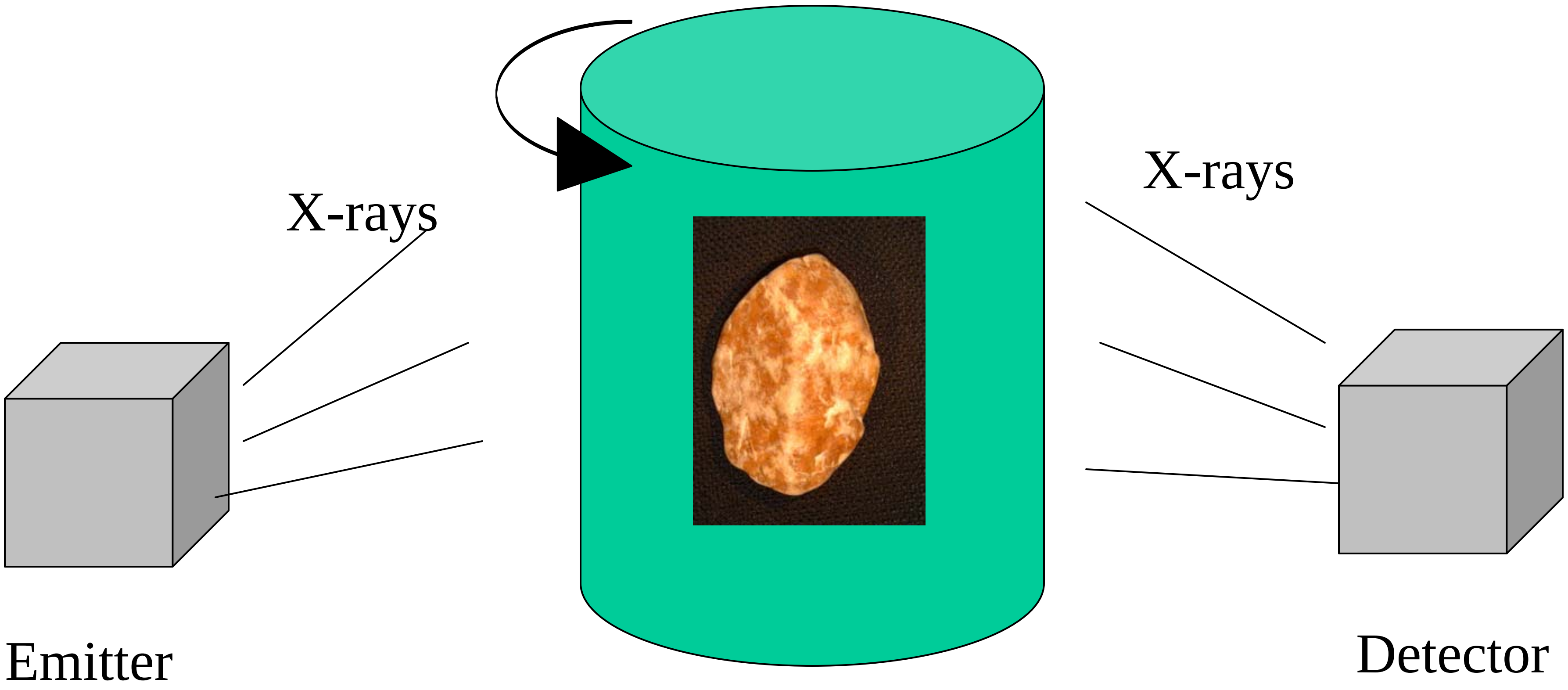
  - Roundness of glass beads for reflective lines on roads
  - Particulates in explosives to help detect terrorists

Particle Shape

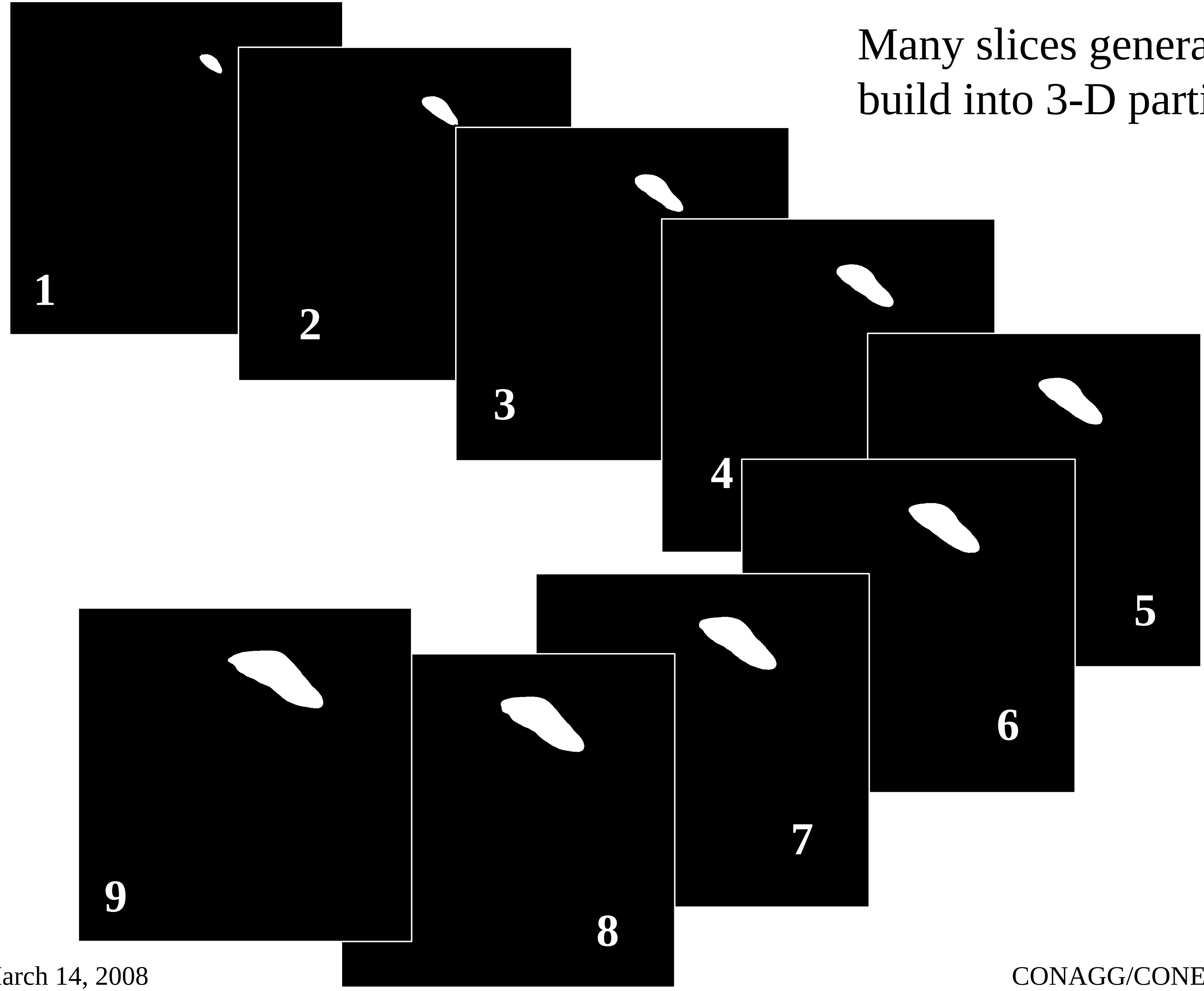
- Applications: cement, sand, gravel, cancer tumors, lunar soil

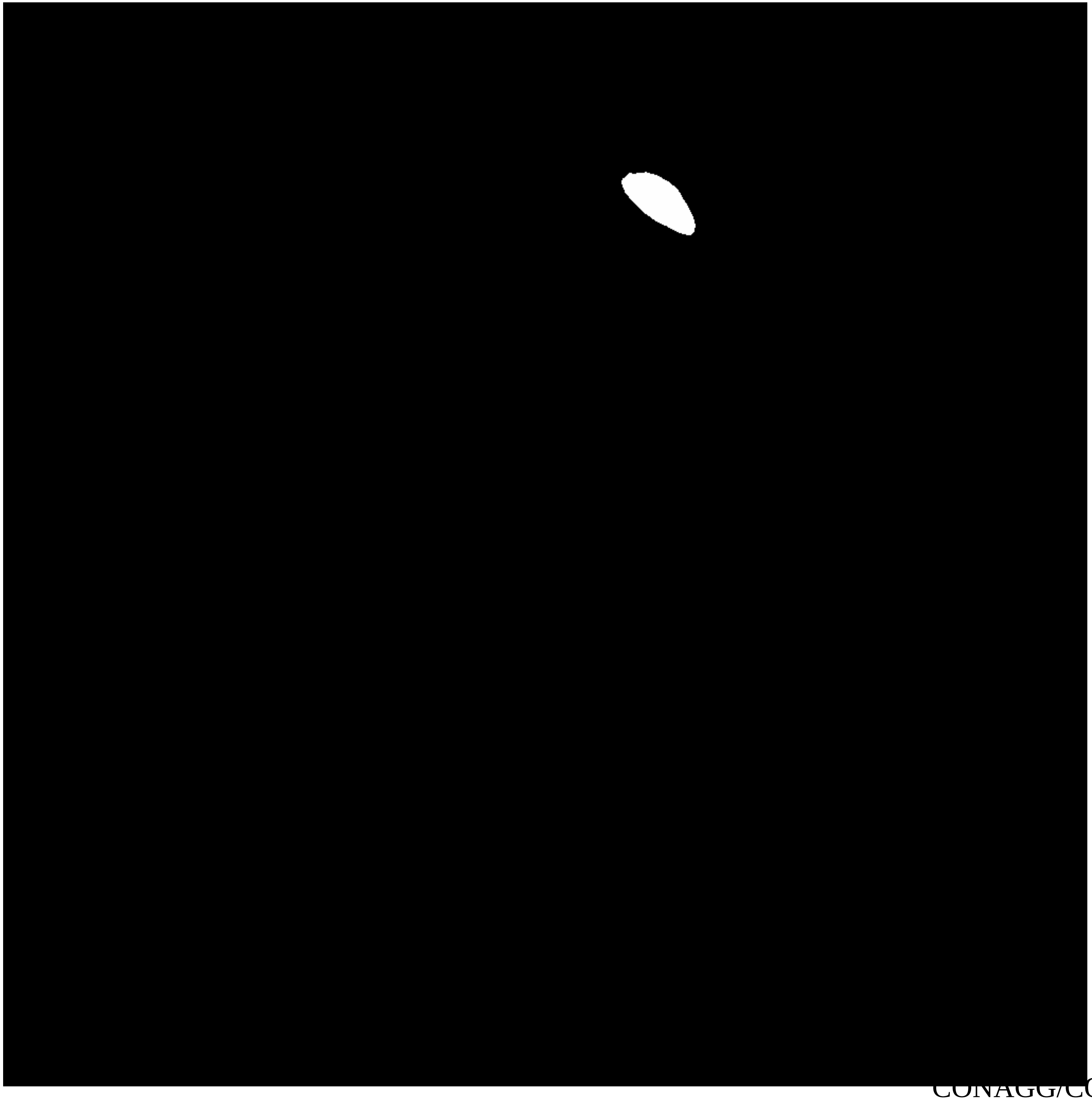


Acquire surface points with X-ray computed tomography



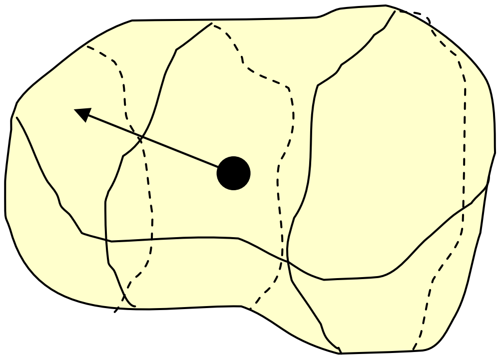
Many slices generated, build into 3-D particle



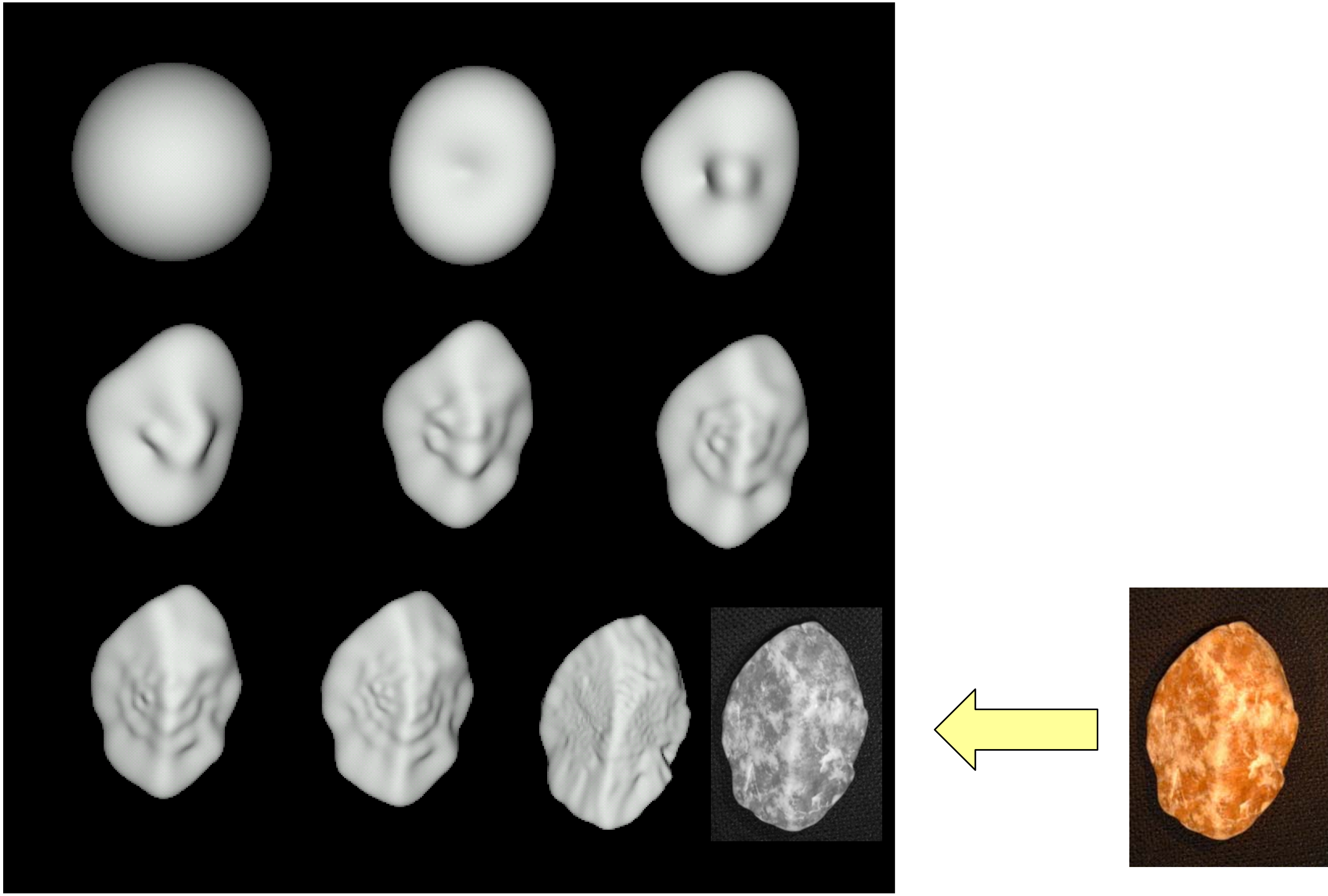


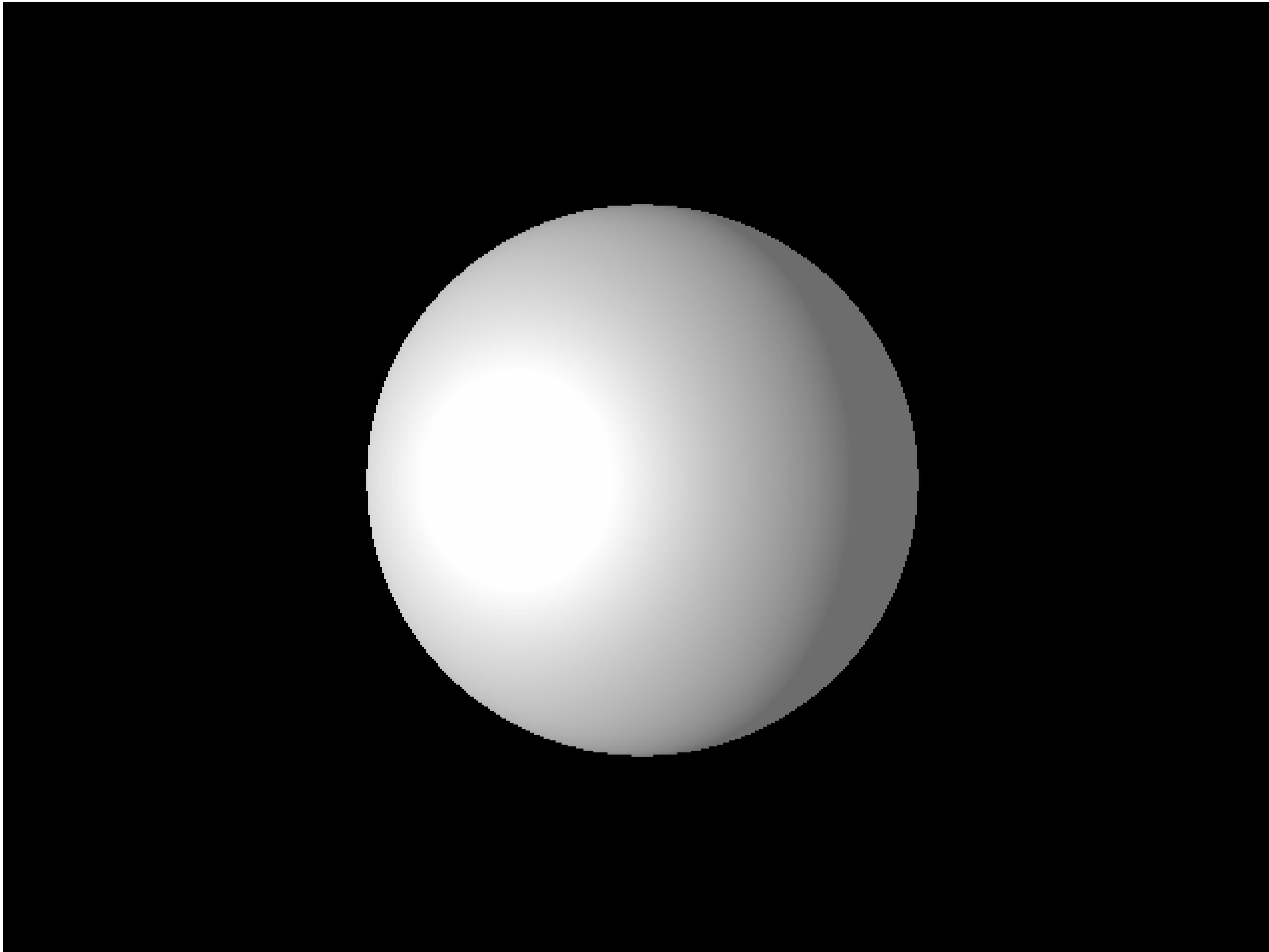
Spherical harmonic analysis

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

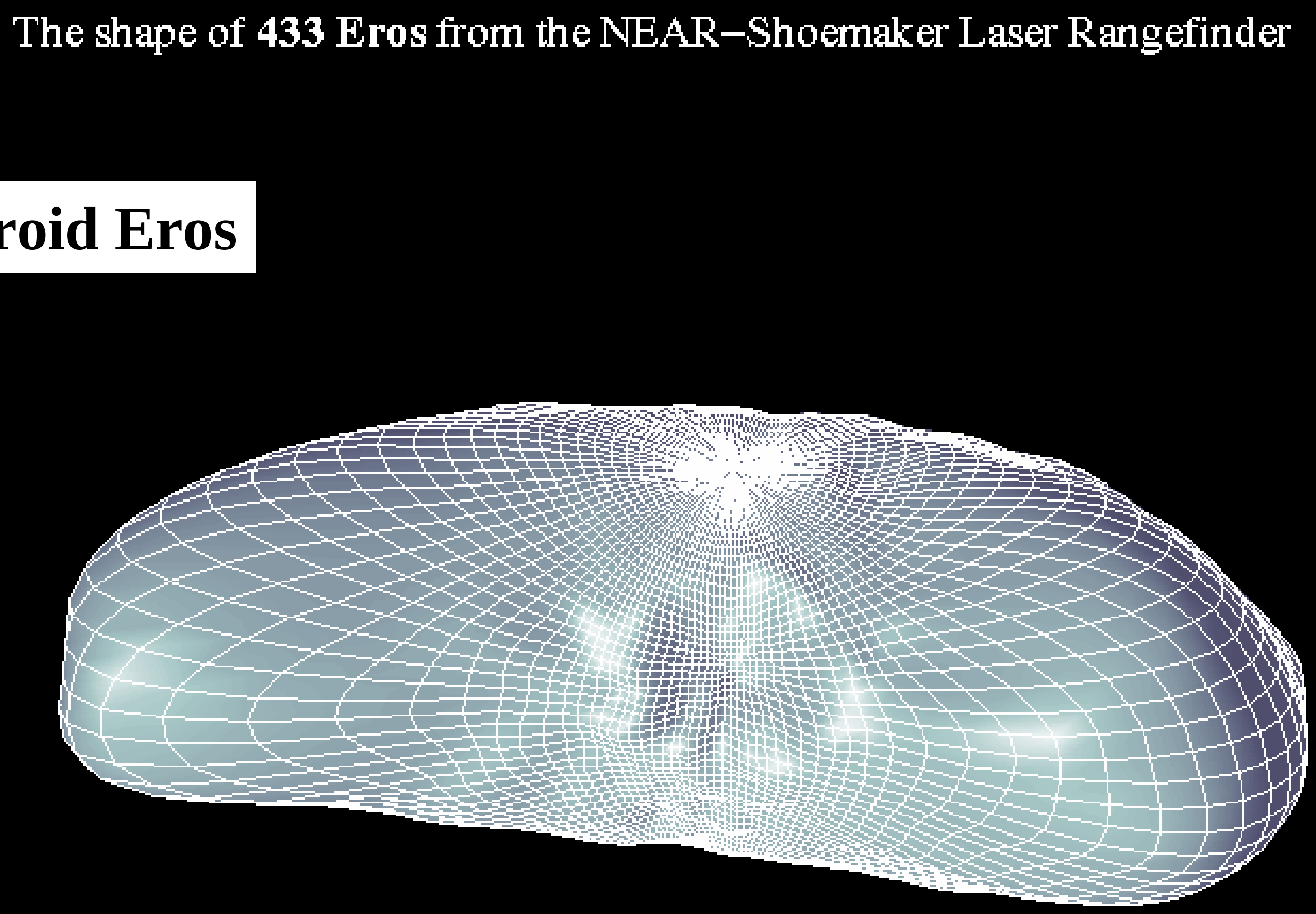


- Compute $r(\theta, \phi) = \Sigma_{n,m}\, a_{nm}\, Y_n^m(\theta, \phi)$
- Y_n^m = spherical harmonic function

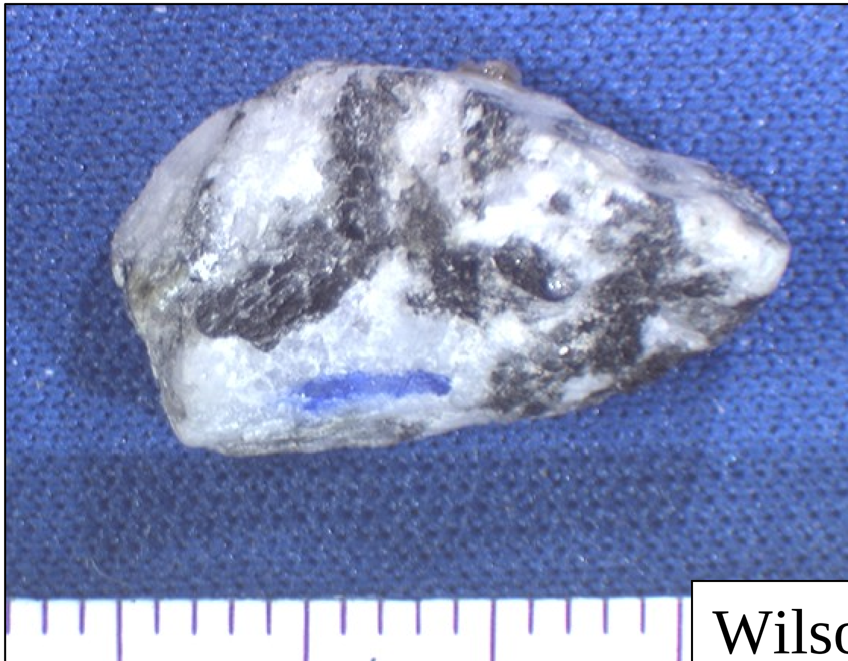


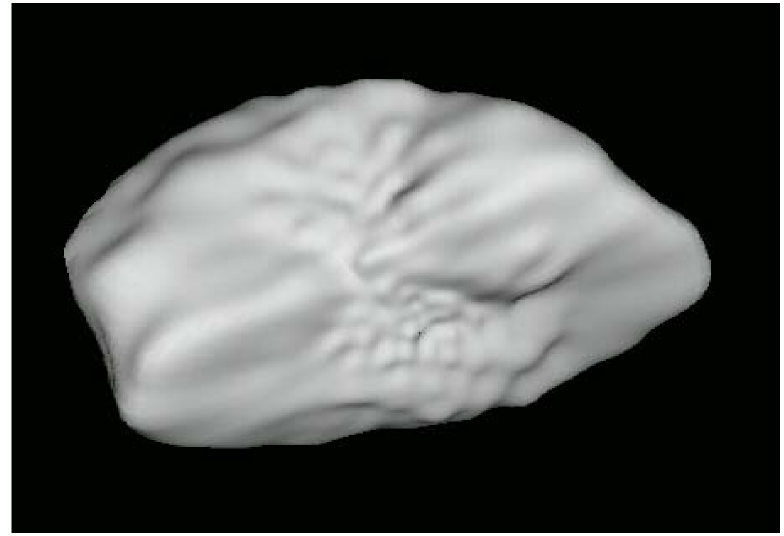


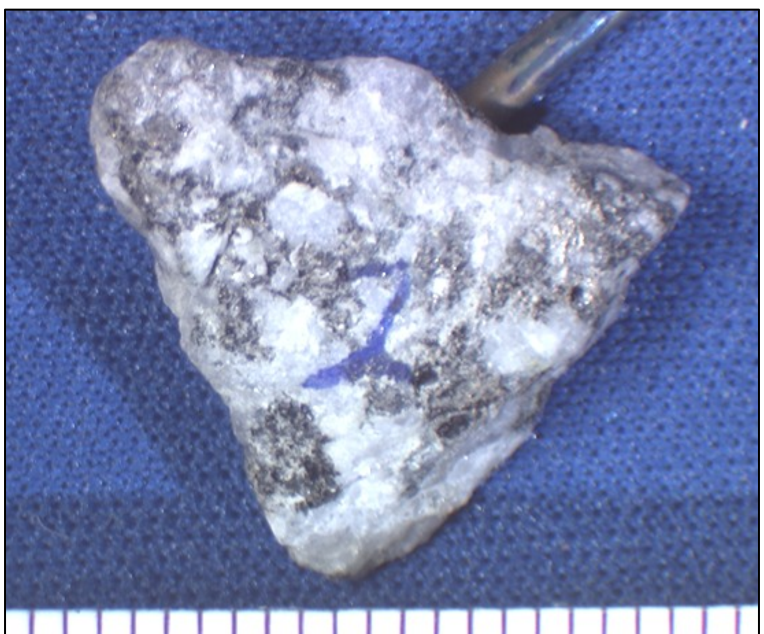
Asteroid Eros

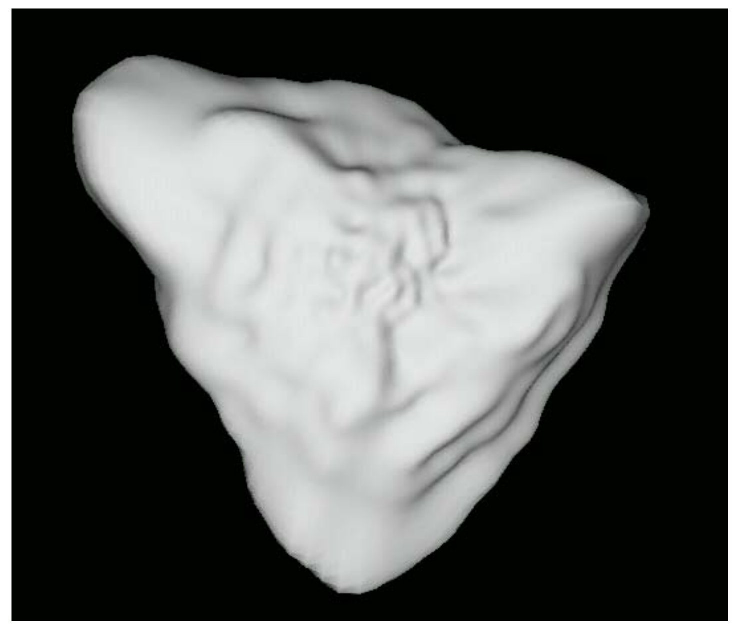


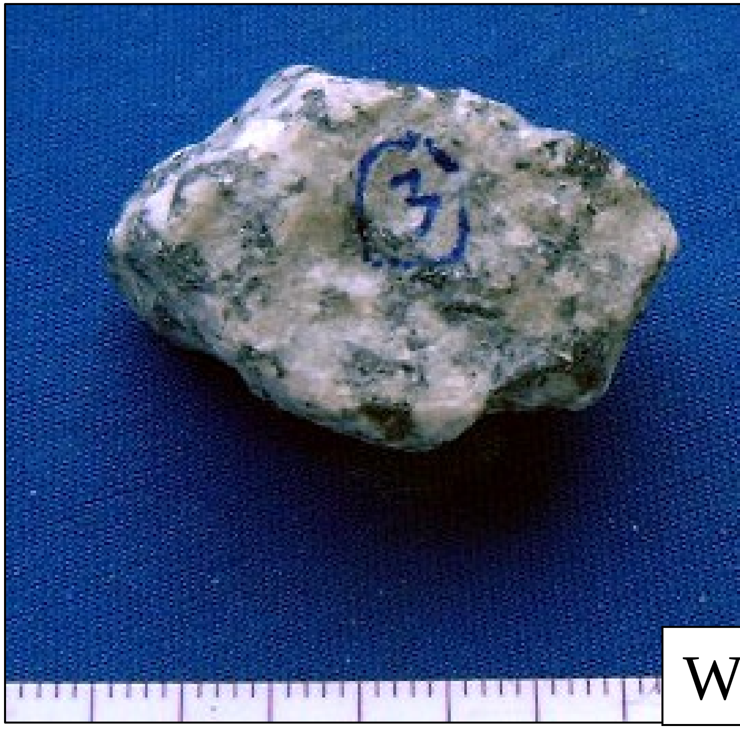
Wilson 0.5 in - #1,2

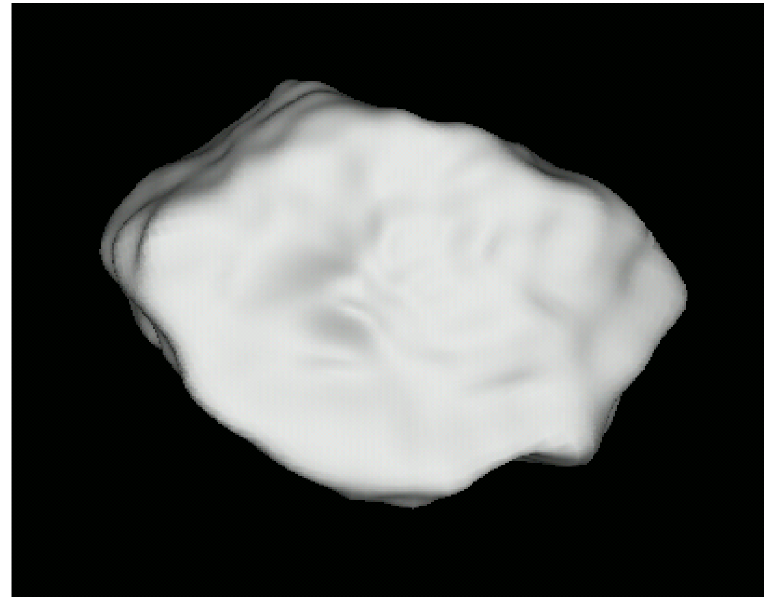




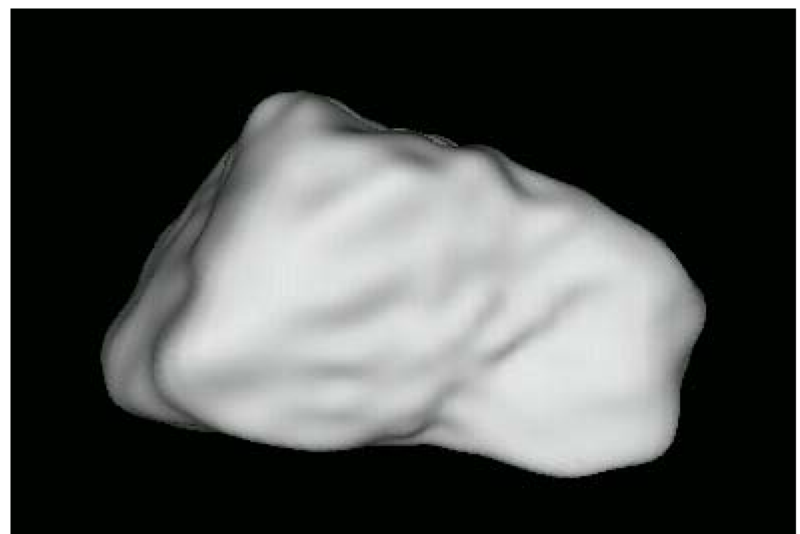


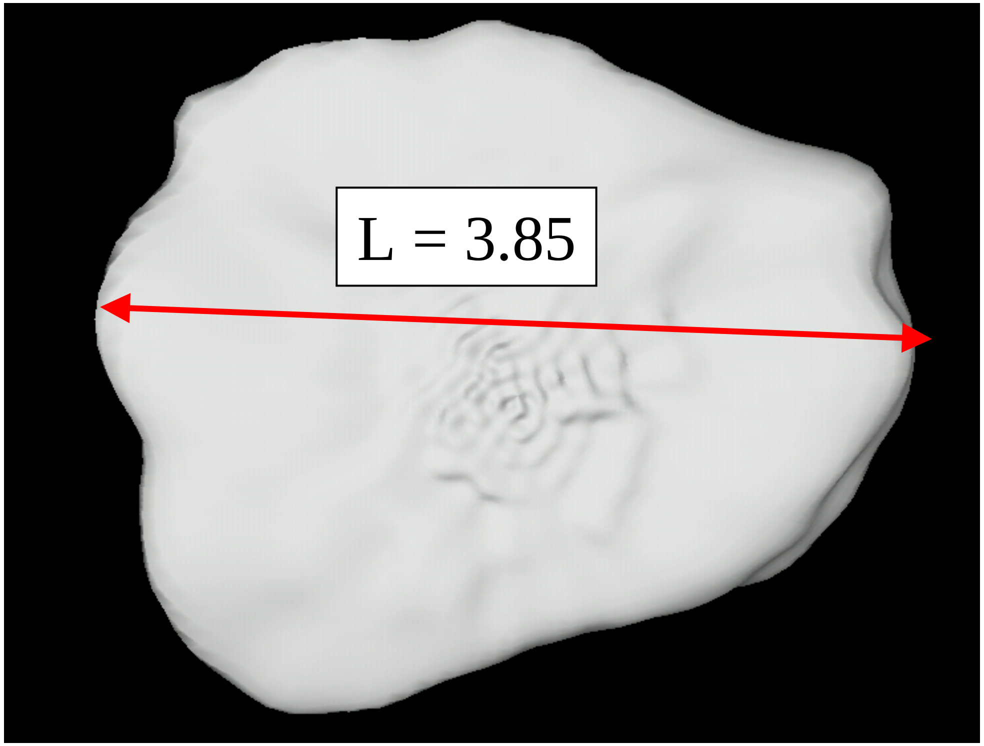


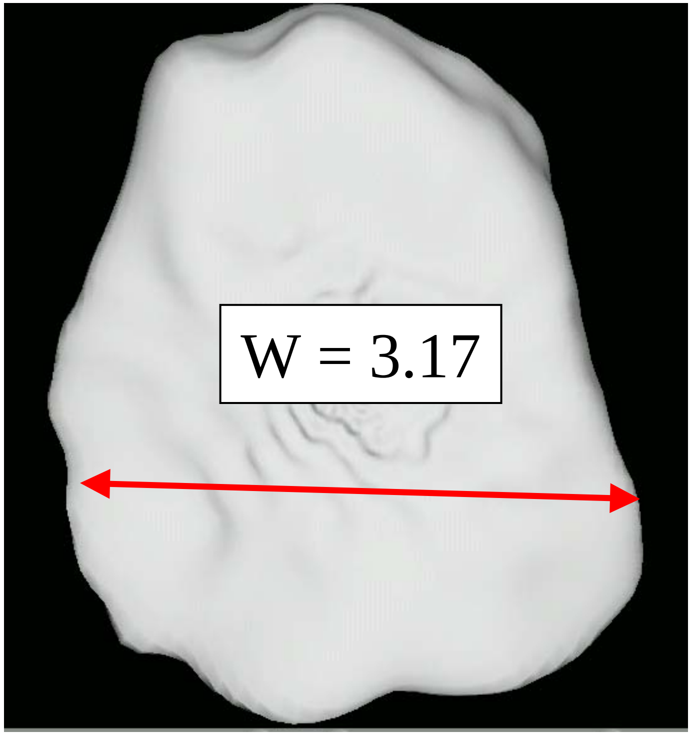


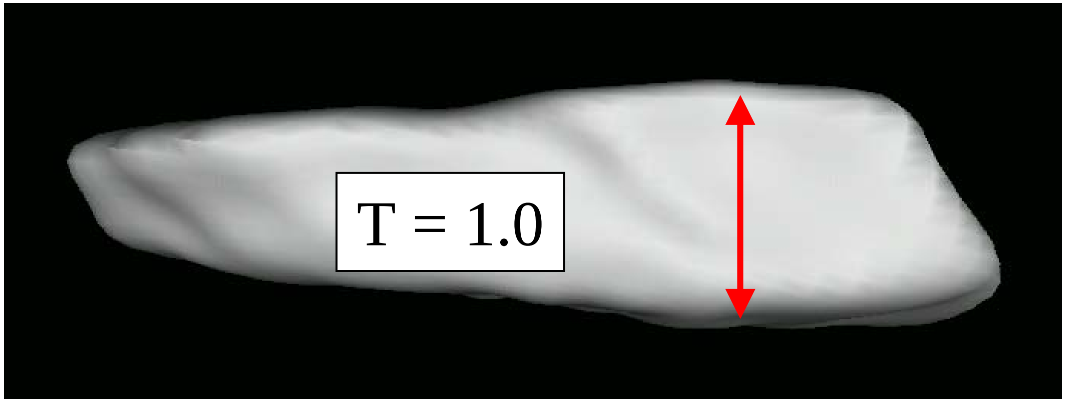


Wilson 0.75 in - #3,4





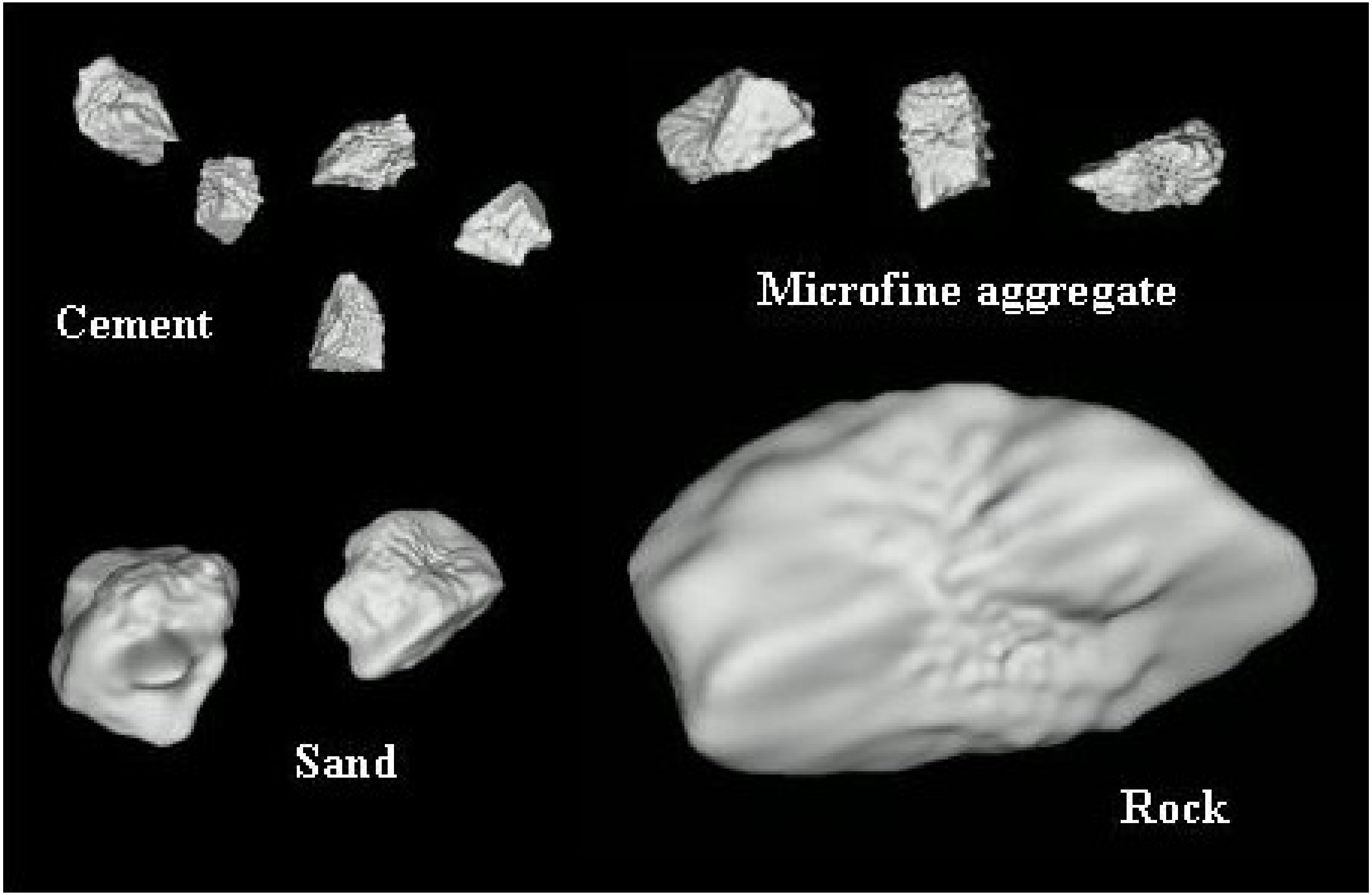




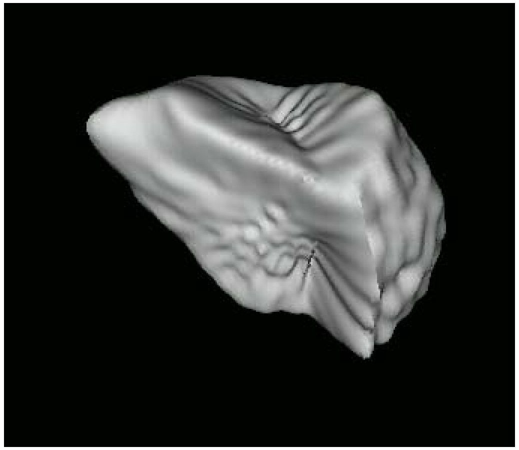
ASTM D 4791
L = length
W = width
T = thickness

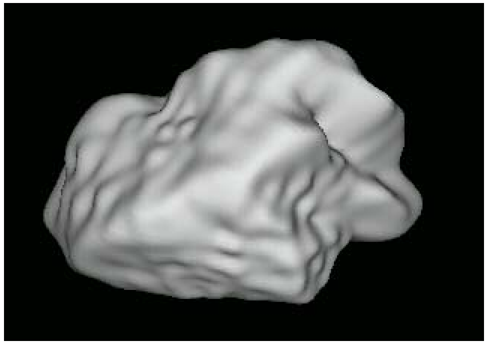
Wilson Rocks	Measured				Model			
	V (mm^3)	L	W	T	V (mm^3)	L	W	T
0.5 in – 1	696.5	2.4	1.4	1	709.1	2.3	1.4	1
0.5 in – 2	651.1	3.3	2.5	1	666.9	3.3	2.7	1
0.5 in – 3	887.6	1.7	1.5	1	892.5	1.6	1.4	1
0.5 in – 4	976.8	2.6	1.5	1	992.9	2.4	1.4	1
0.5 in – 5	777.6	1.5	1.2	1	787.8	1.6	1.2	1
0.5 in – 6	607.7	1.9	1.4	1	613.6	1.9	1.4	1
0.75 in – 1	7250	1.8	1.2	1	7350	1.8	1.2	1
0.75 in – 2	4480	2.1	1.6	1	4367	2.2	1.6	1
0.75 in – 3	6611	1.7	1.3	1	6592	1.6	1.2	1
0.75 in – 4	7798	1.8	1.3	1	7817	1.7	1.3	1
0.75 in – 5	4502	2.2	1.6	1	4443	2.2	1.6	1
0.75 in – 6	3329	2.3	2.2	1	3268	2.4	2.3	1

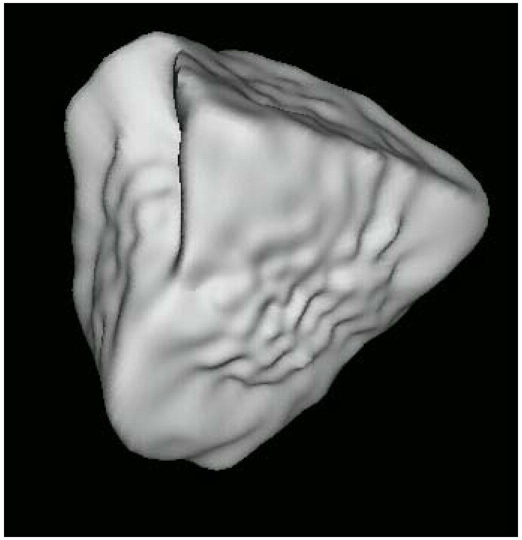
Shape results



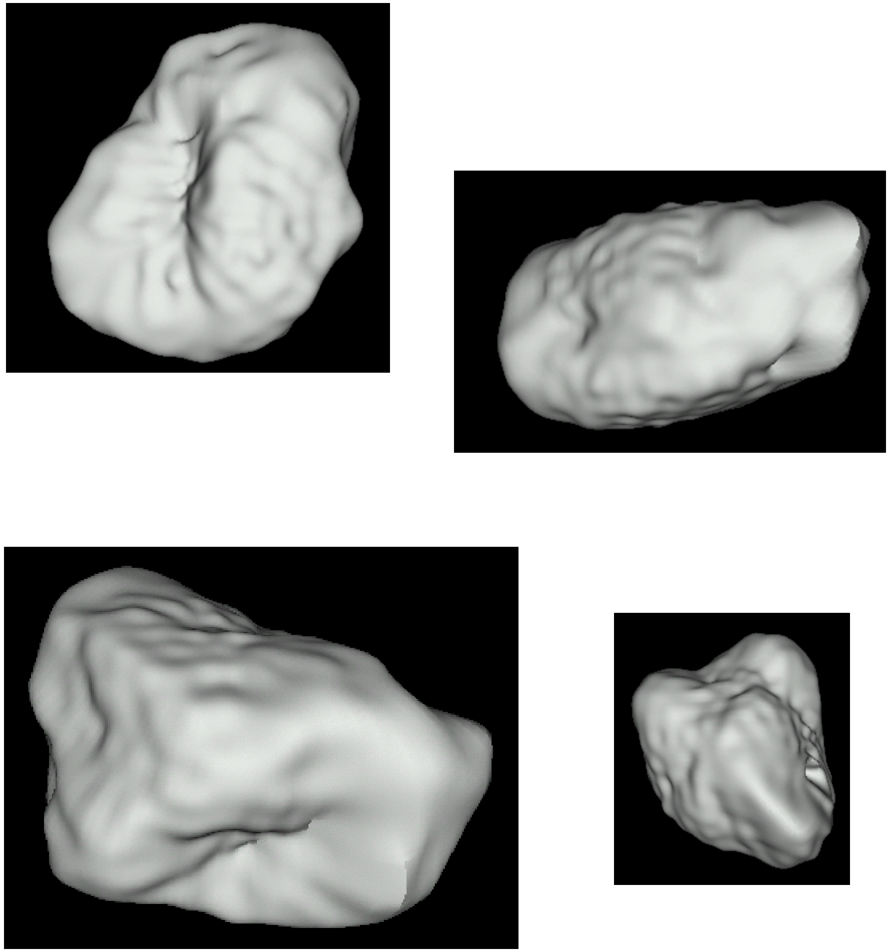
AMRL coarse limestone





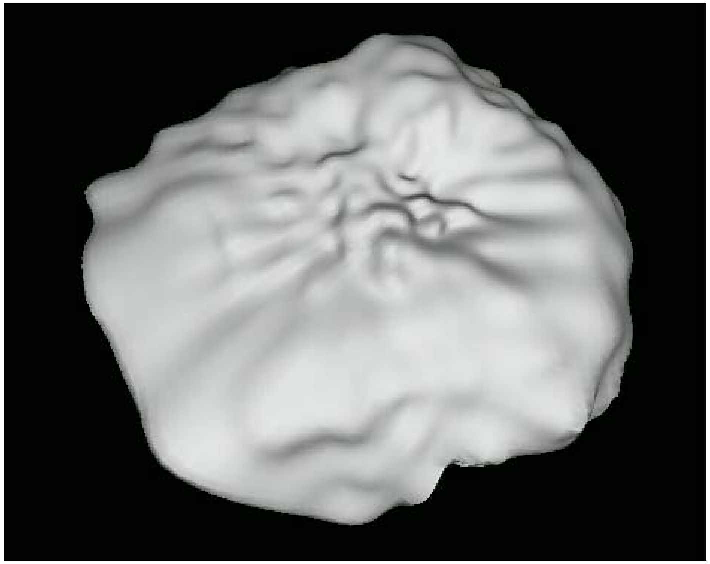


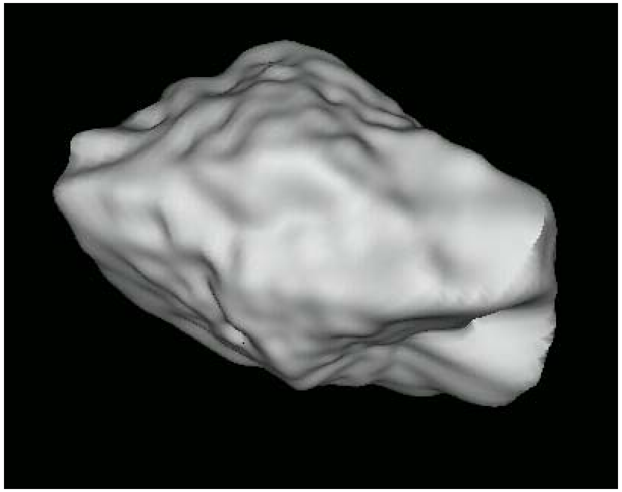
European standard sand



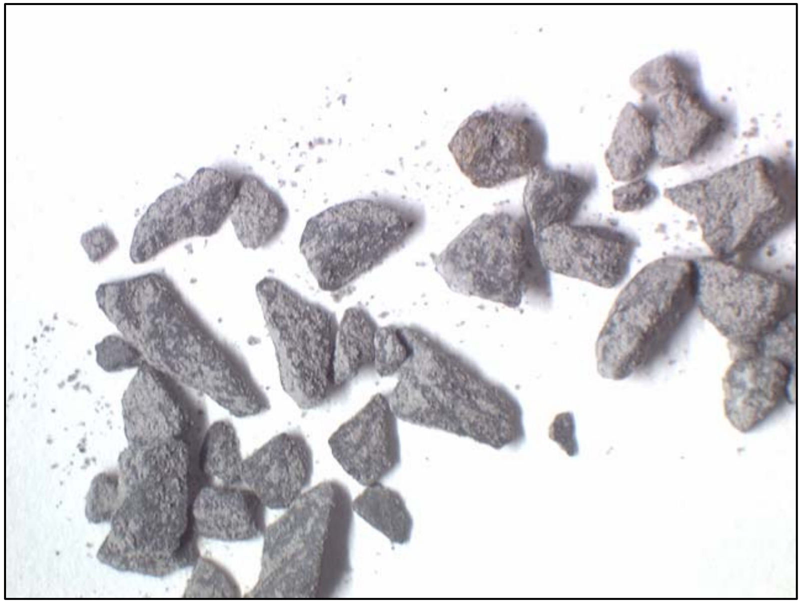
Coarse aggregate from France

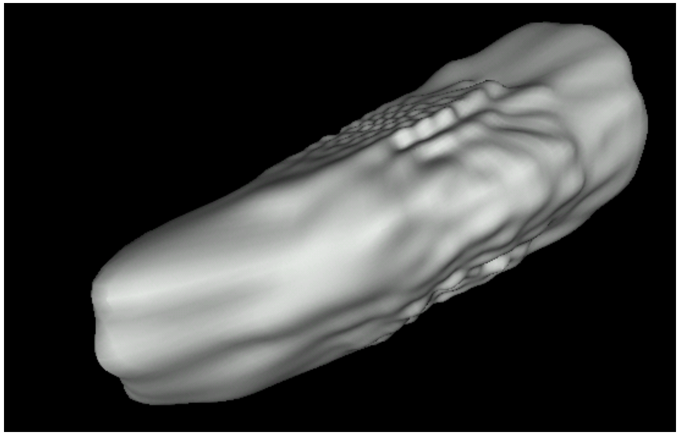
mm scale

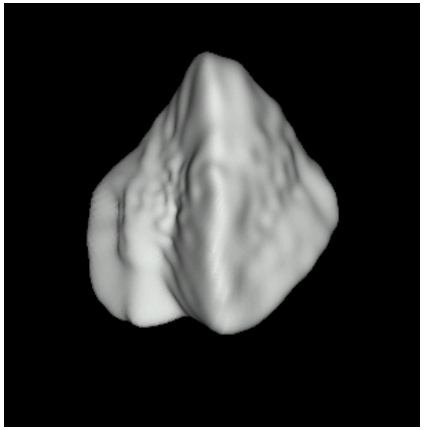


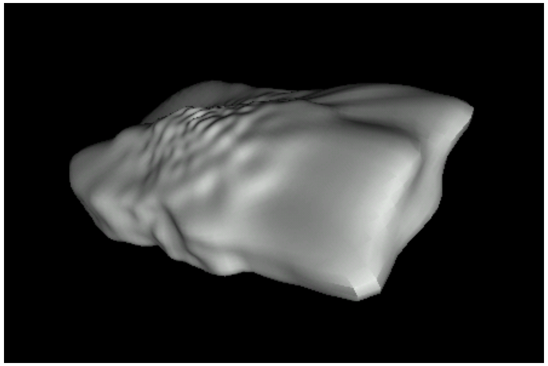


Fine aggregate for hot-mix asphalt

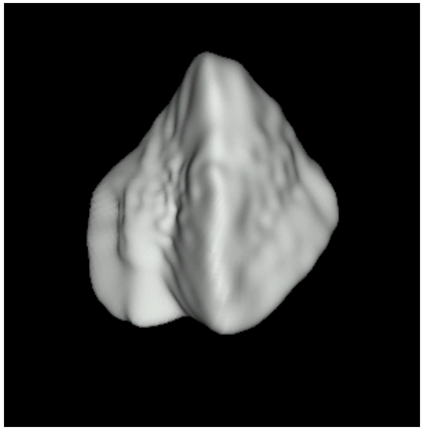


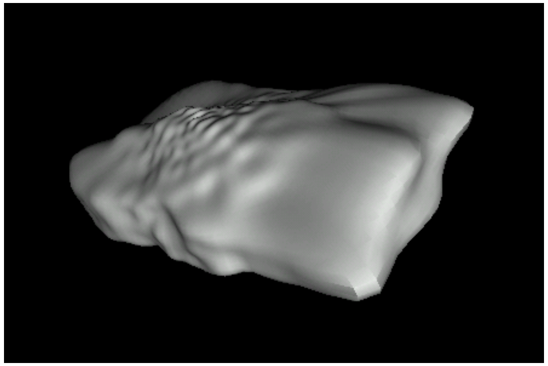




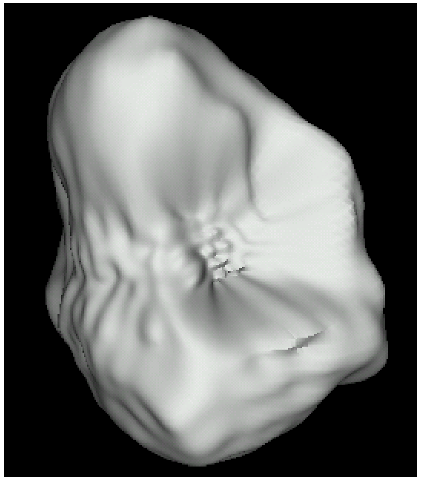


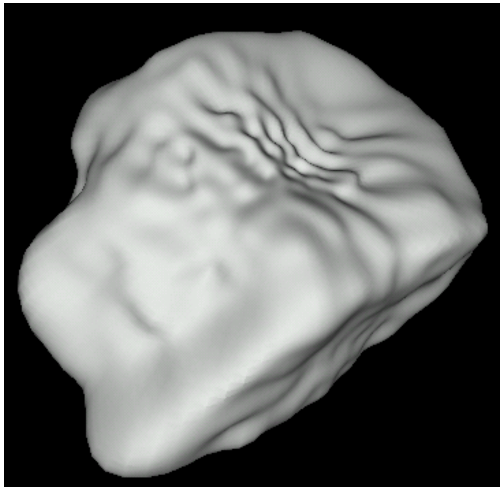
Fine aggregate for hot-mix asphalt





ASTM C-33 sand



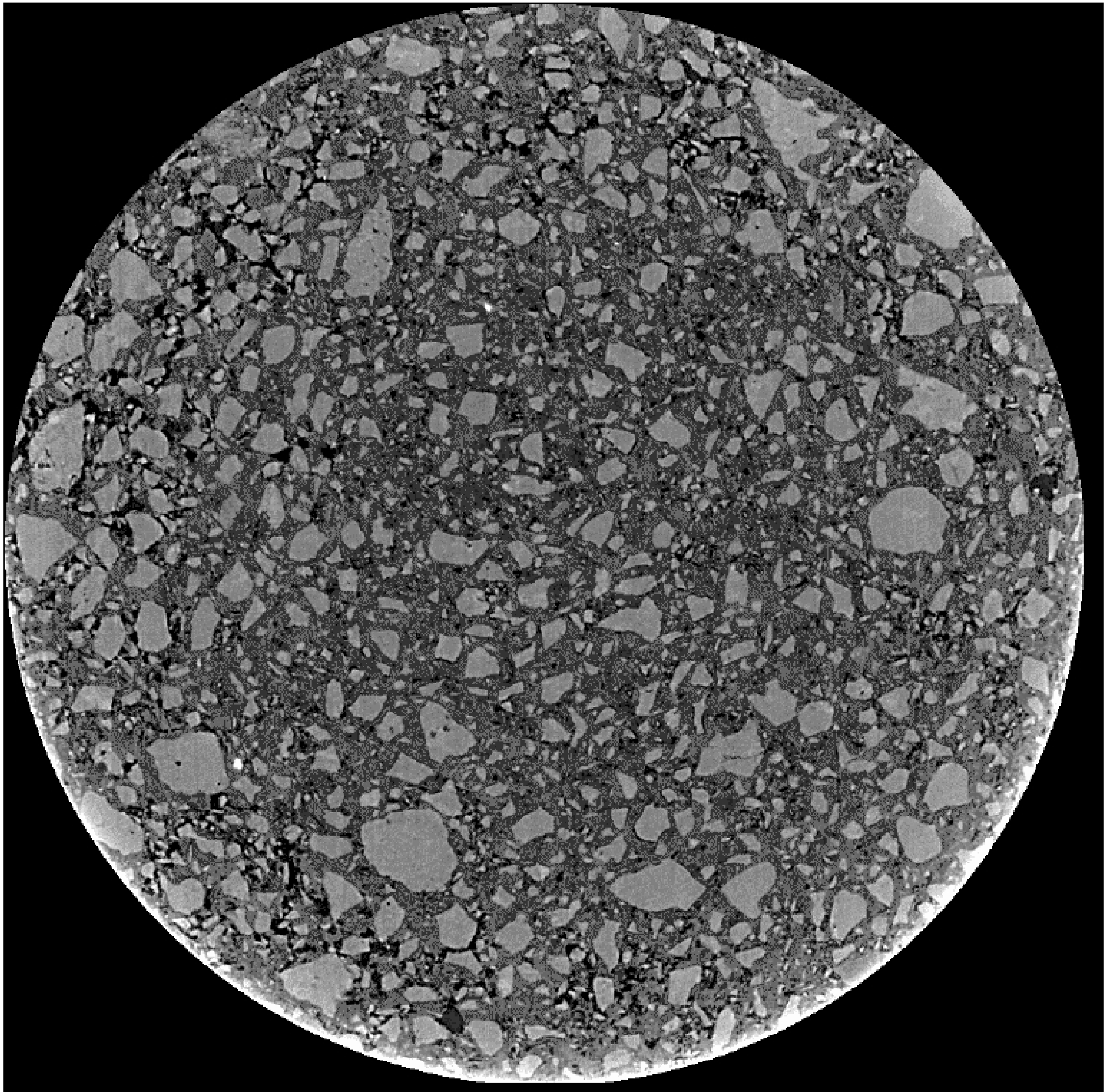


W-5					0.0
W-4				0.0	0.0
W-3			0.3	0.2	0.0
W-2		4.5	1.4	0.6	0.0
W-1	63.4	27.1	2.2	0.0	0.0
	L-1	L-2	L-3	L-4	L-5

ASTM C-33 sand
for concrete

W-5					0.0
W-4				0.0	0.0
W-3			0.5	1.3	0.0
W-2		8.5	8.9	3.8	0.0
W-1	32.4	37.4	6.7	0.4	0.2
	L-1	L-2	L-3	L-4	L-5

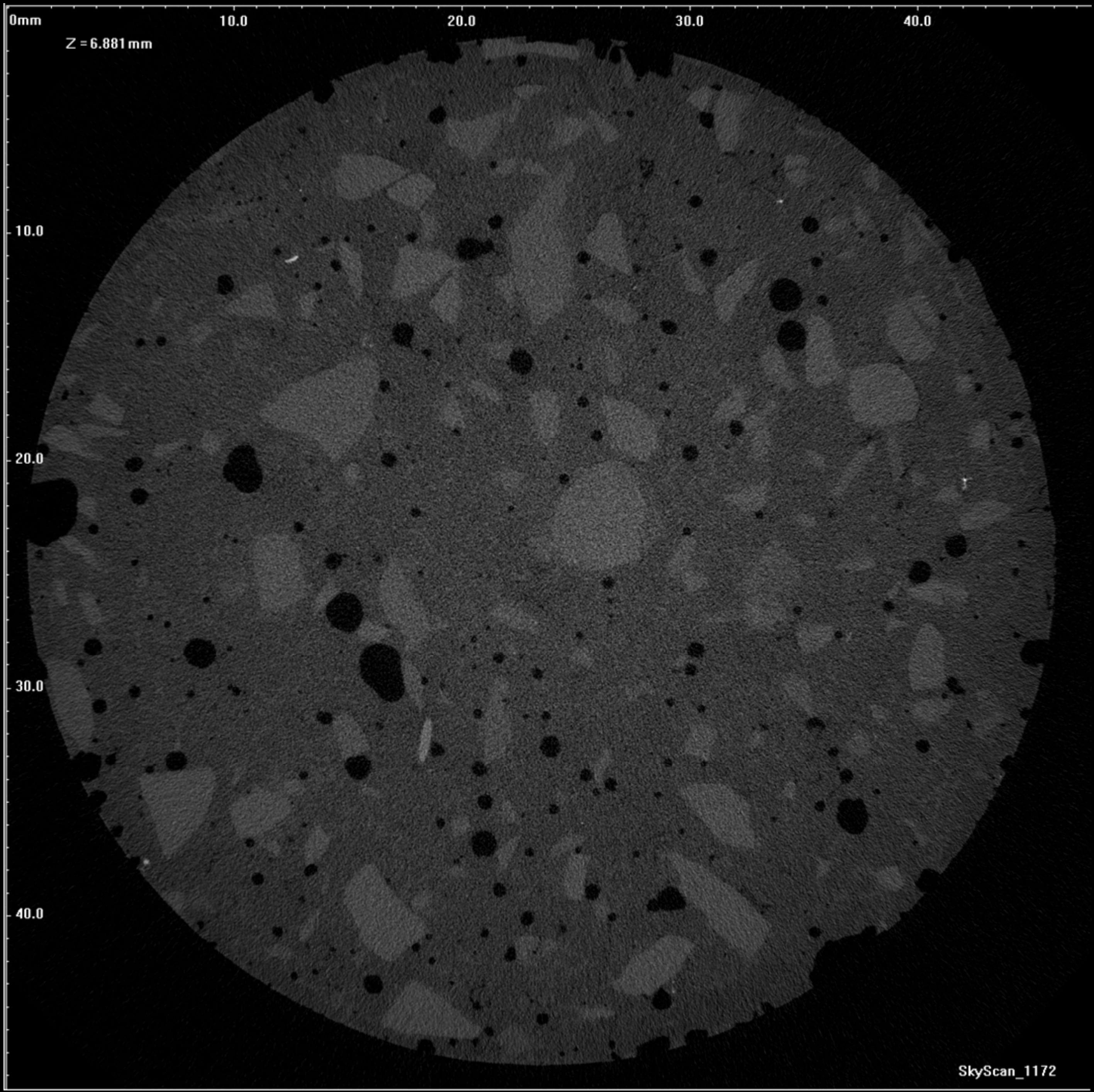
Sand for hot-mix asphalt



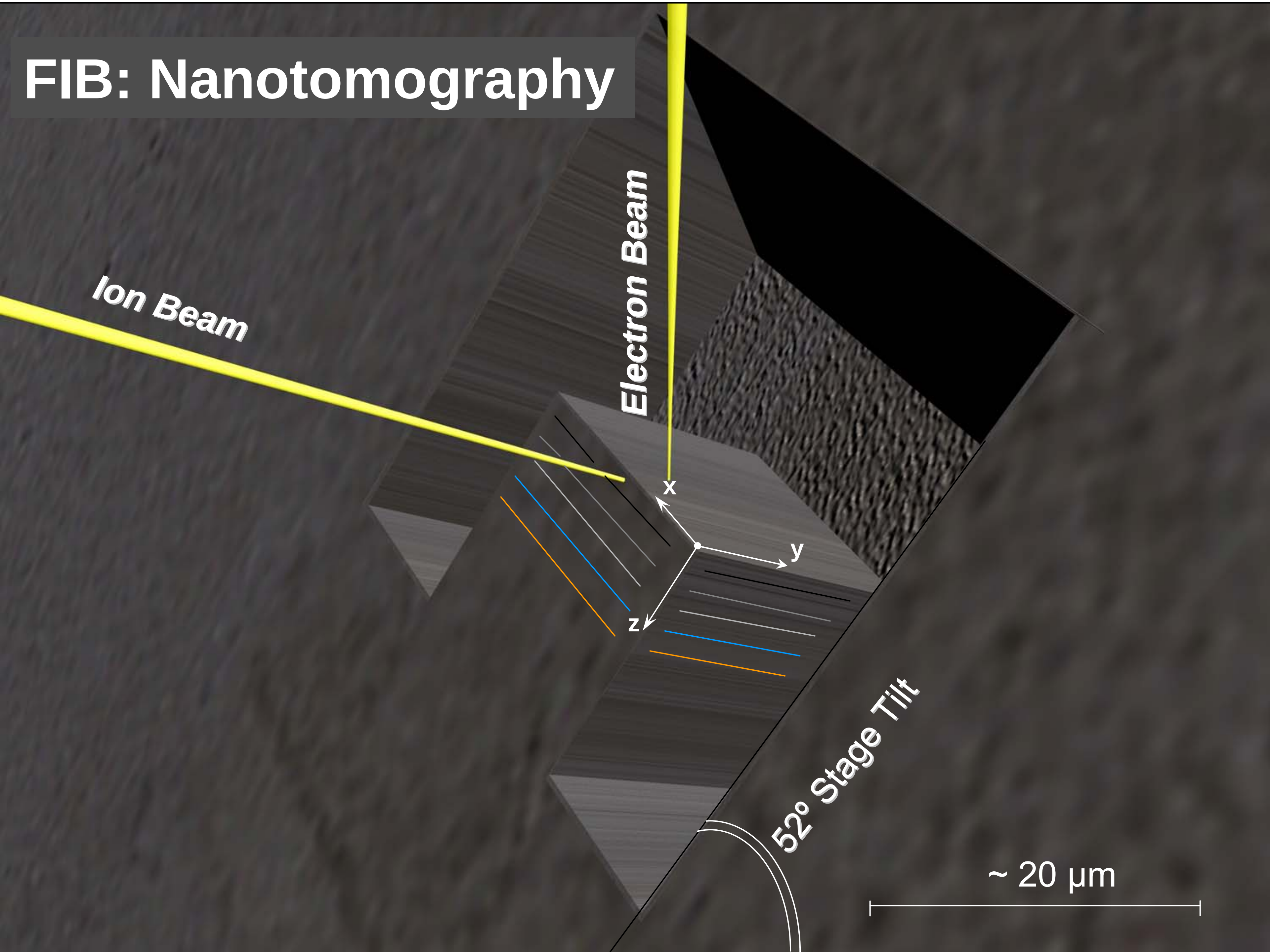
0.3 w/c, 48 h hydration time

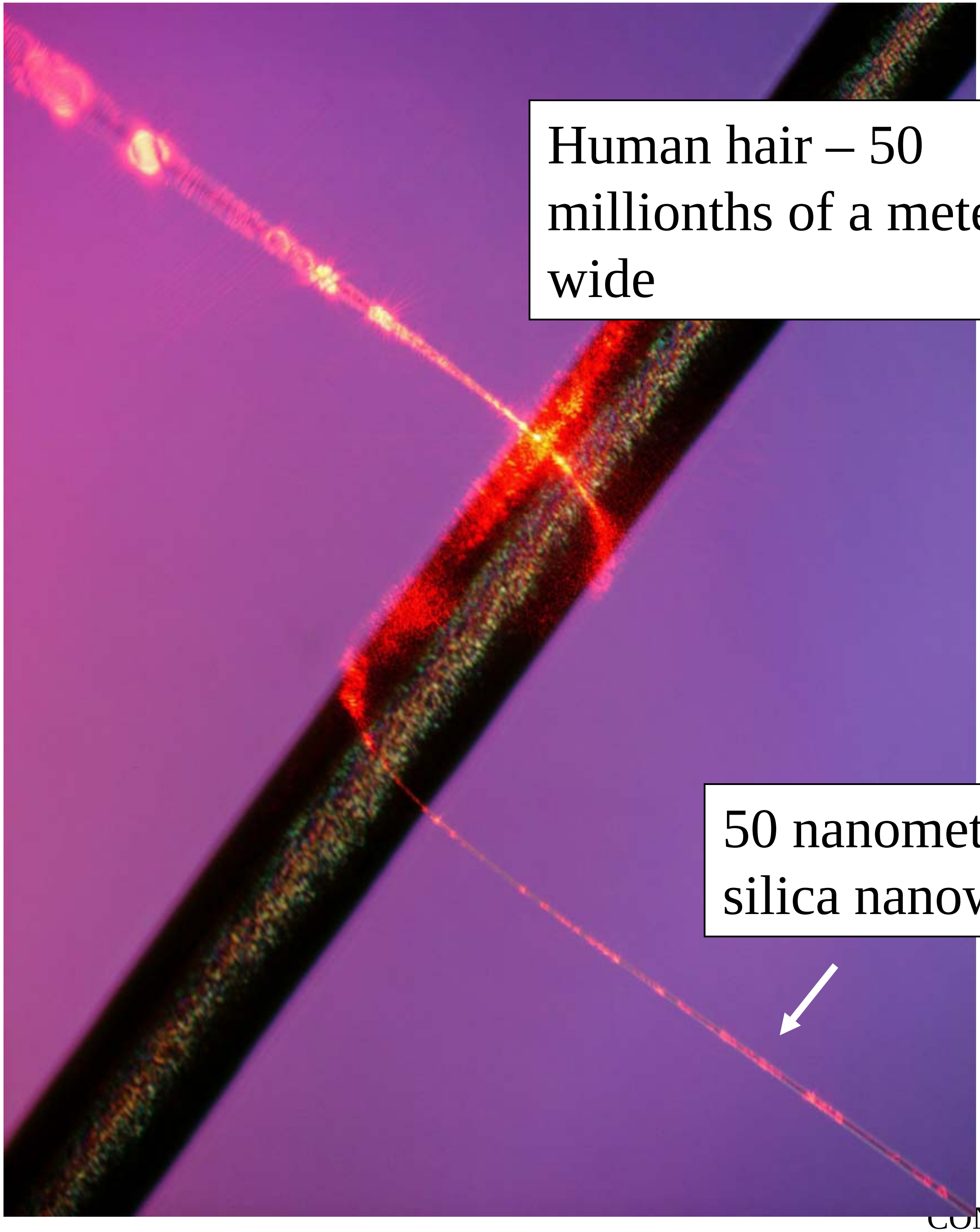
From the Visible Cement Database, visiblecement.nist.gov

1 micrometer/pixel

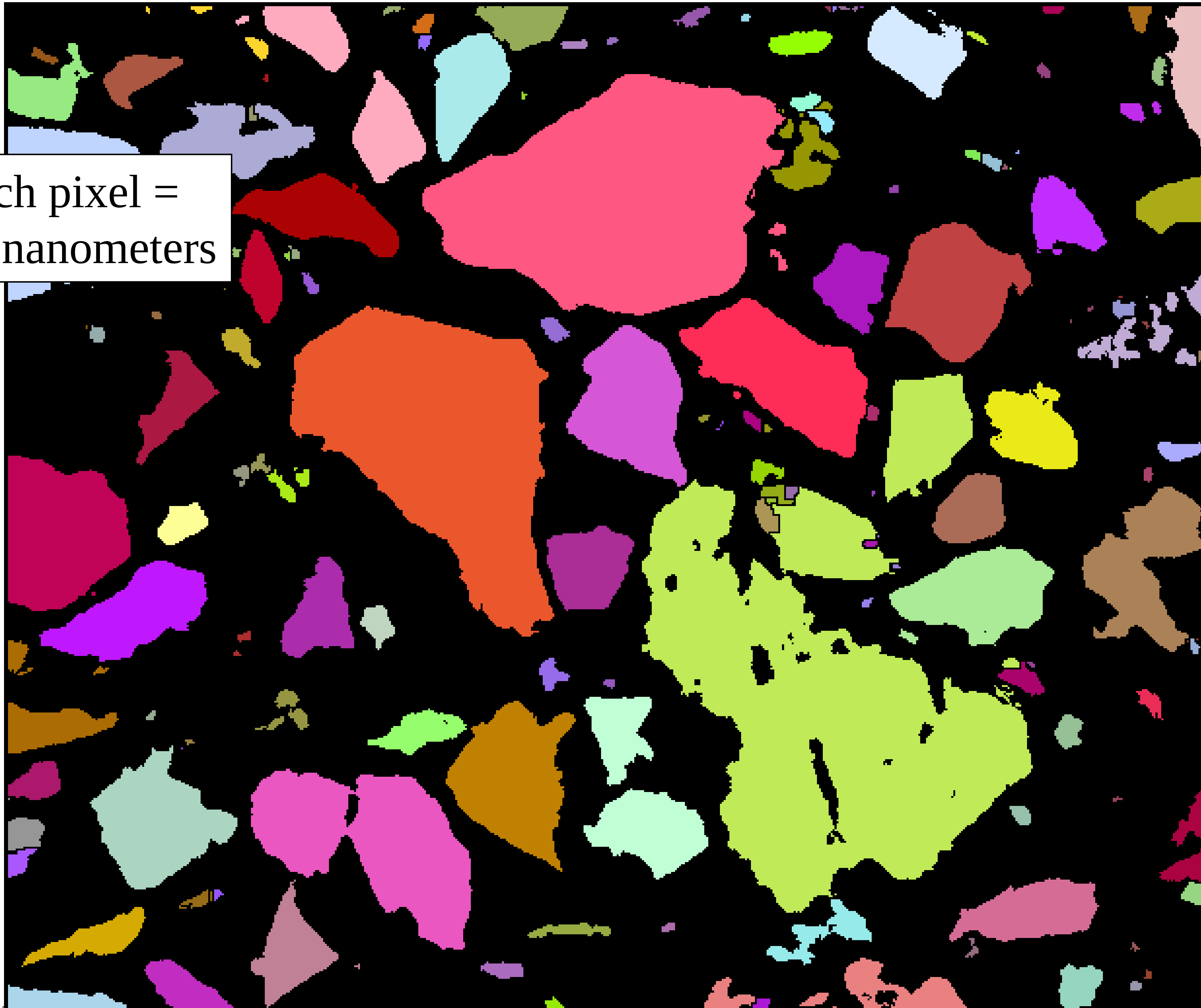

0mm
10.0
20.0
30.0
40.0
Z = 6.881 mm
10.0
20.0
30.0
40.0
SkyScan_1172

FIB: Nanotomography




Human hair – 50 millionths of a meter wide
50 nanometer-wide silica nanowire


Human hair – 50 millionths of a meter
50 nanometer-wide silica nanowire

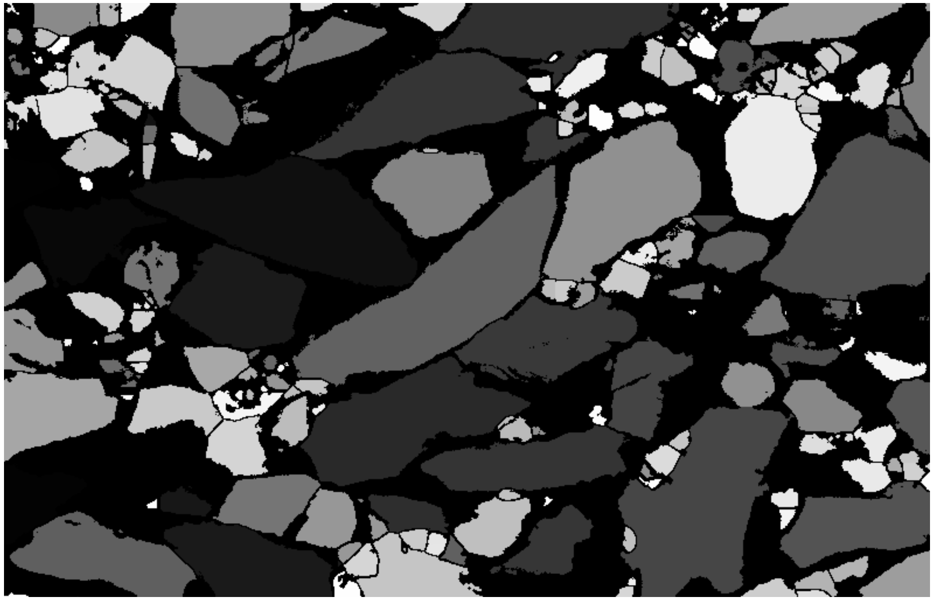

Each pixel =
25 nanometers

Fib-SEM cement images from Sika

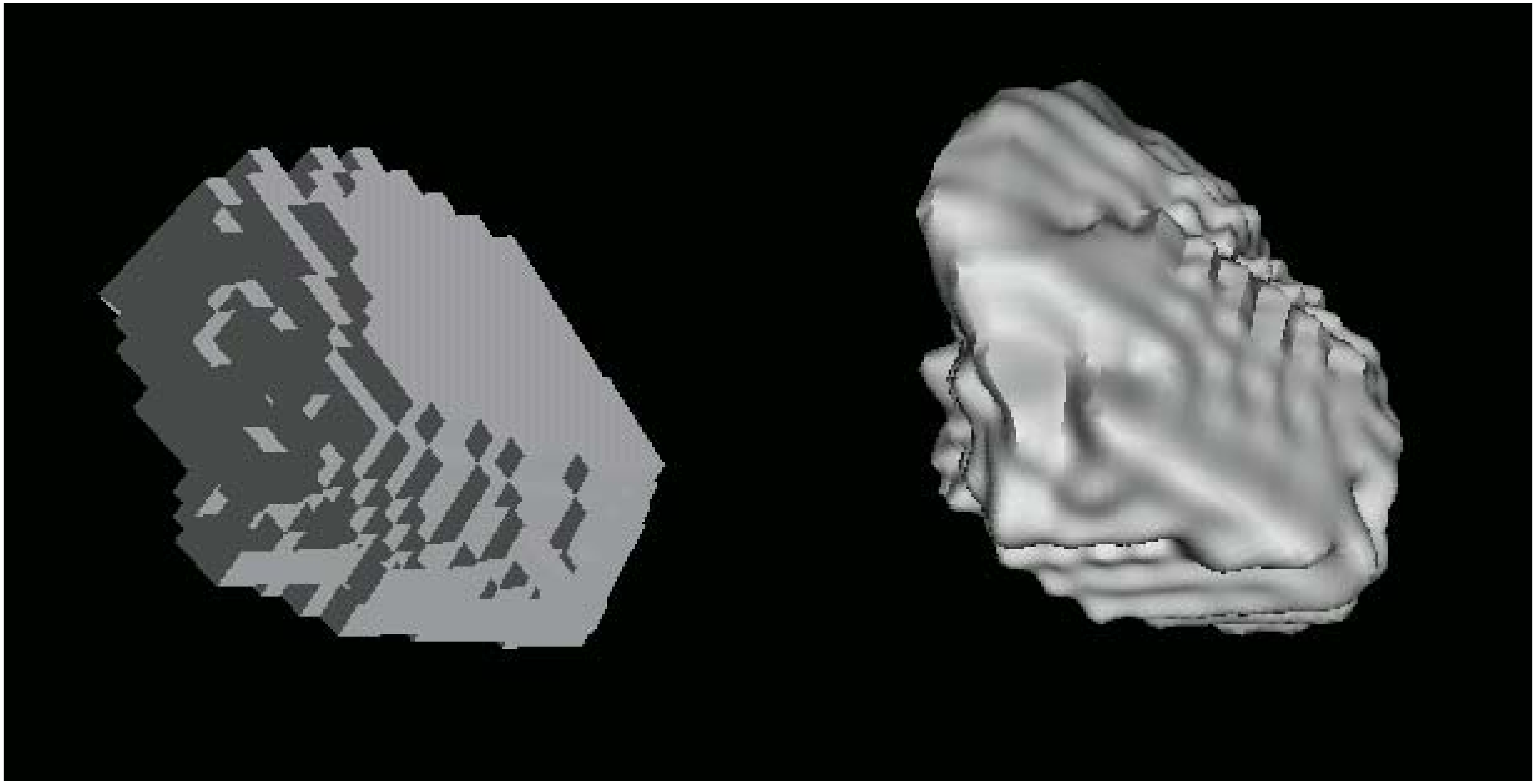
- Particles retrieved from dual fib images
- 1665 particles reconstructed
- Equivalent spherical diameters from 0.47 μm to 6.1 μm
- Fib images done

by Lorenz Holzer

at EMPA

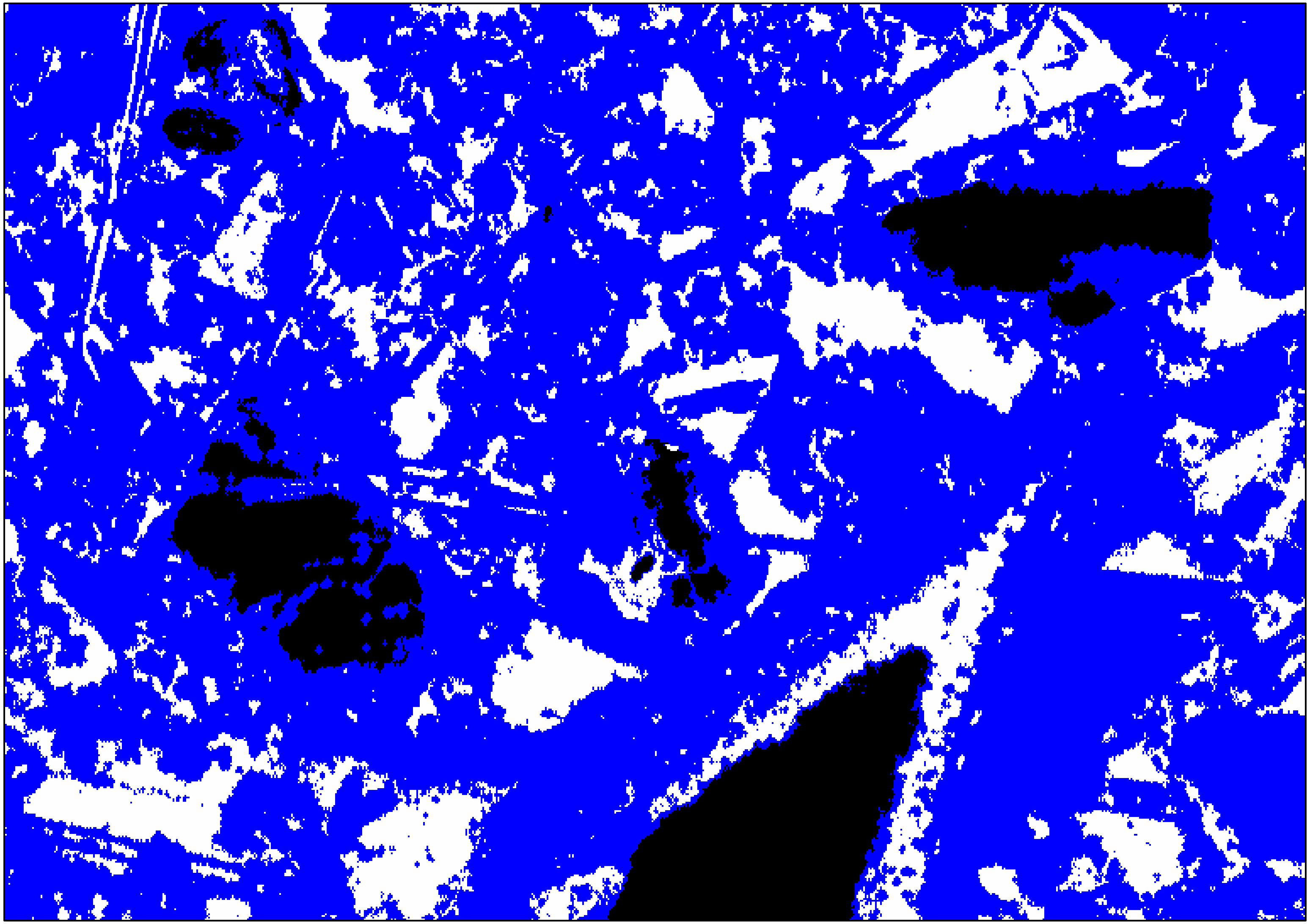


0.53 μm equivalent spherical diameter

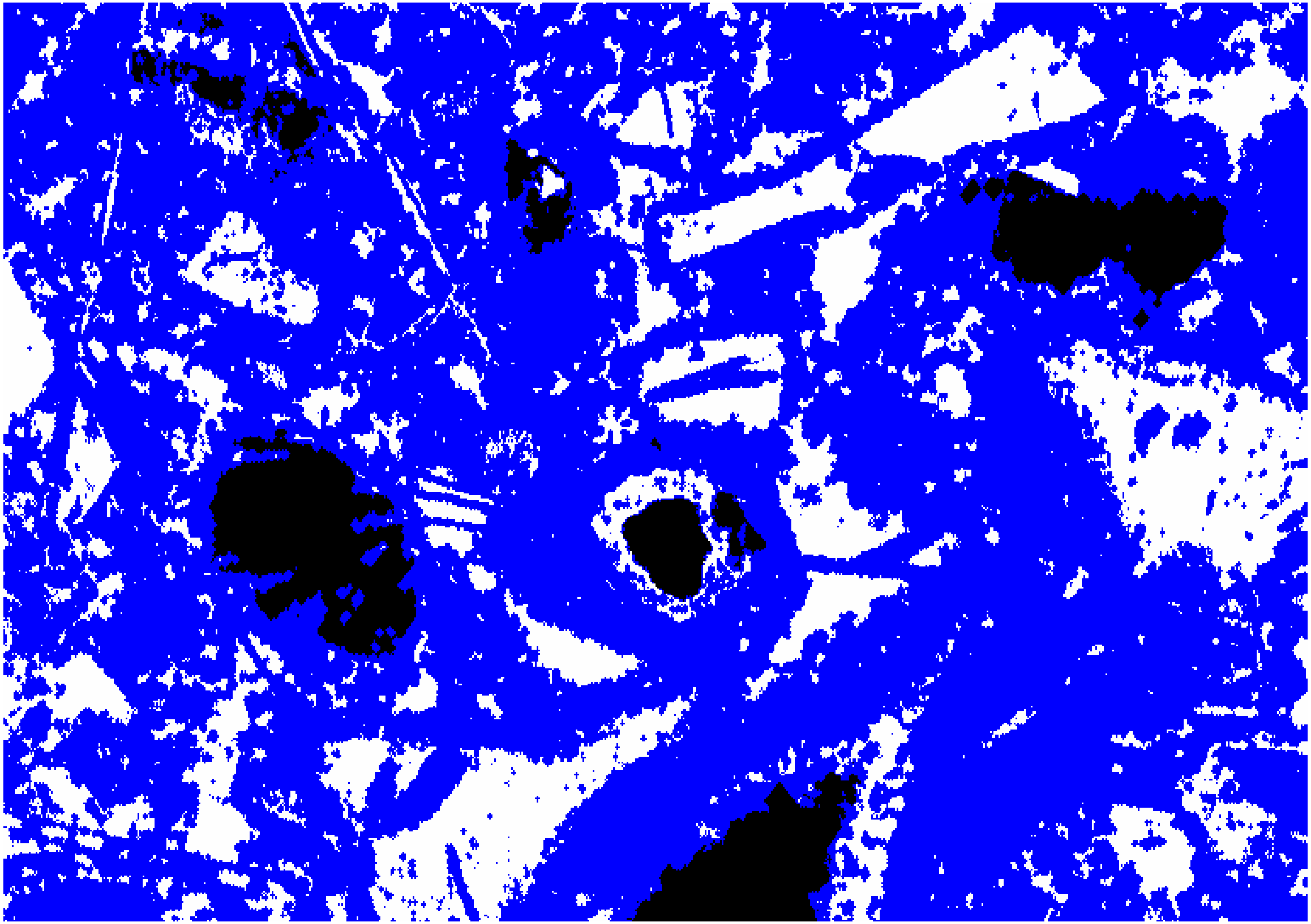


Direct from fib-SEM imaging

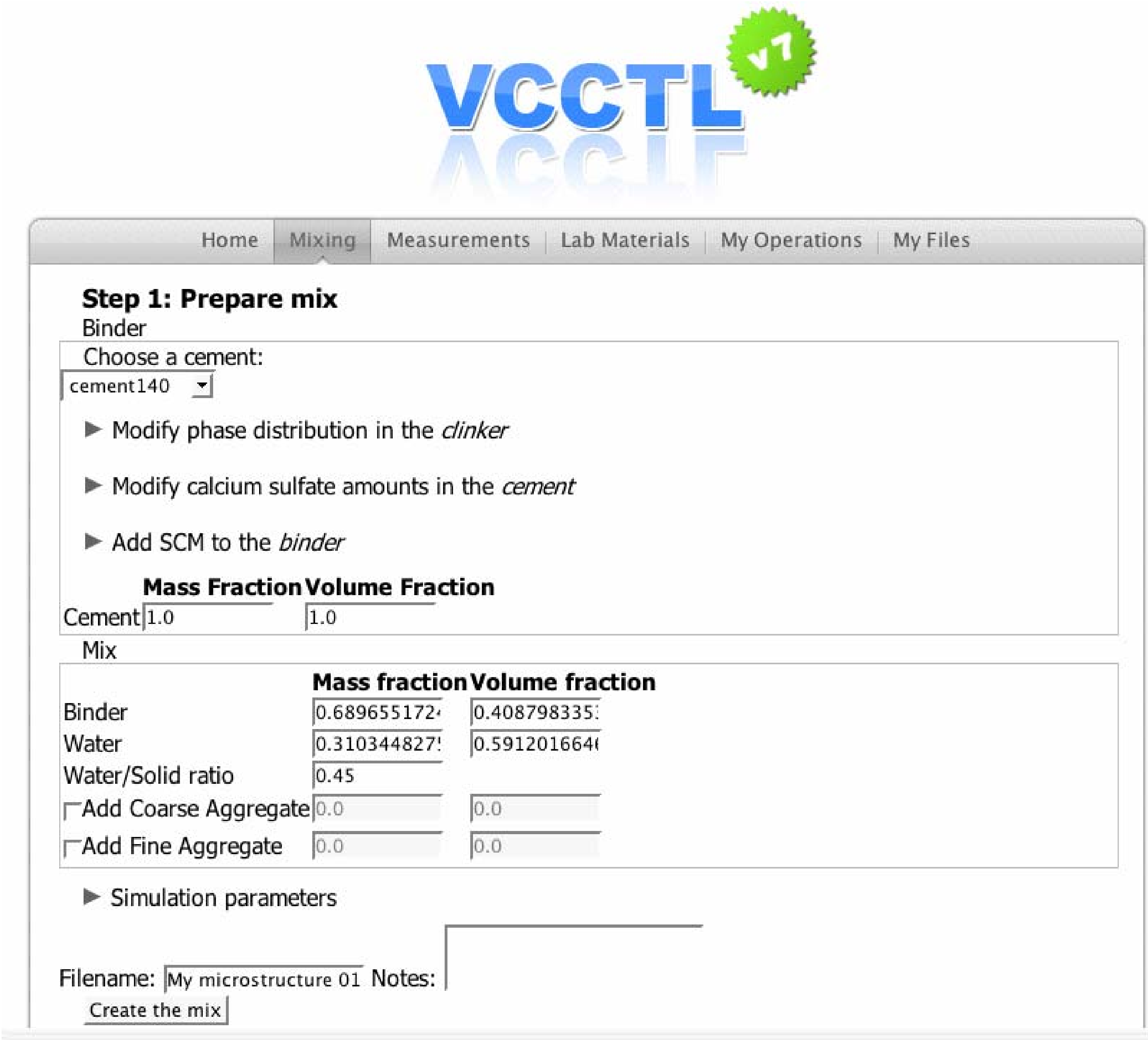
Reconstructed with spherical harmonic functions

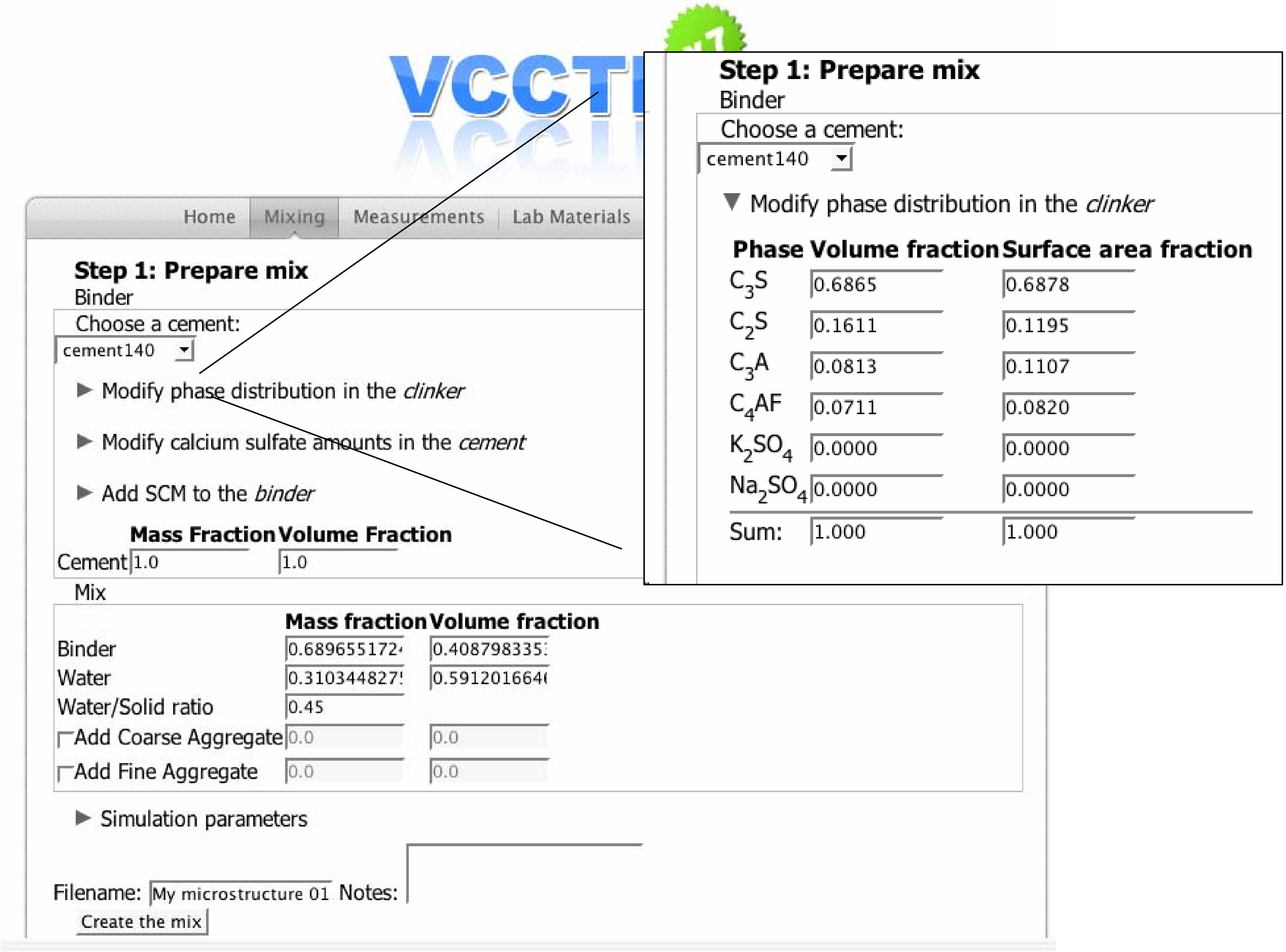


60 nm pixel size, 46 µm x 32 µm
Black = cement, white = pore, blue = hydration products
(Holzer et al.)

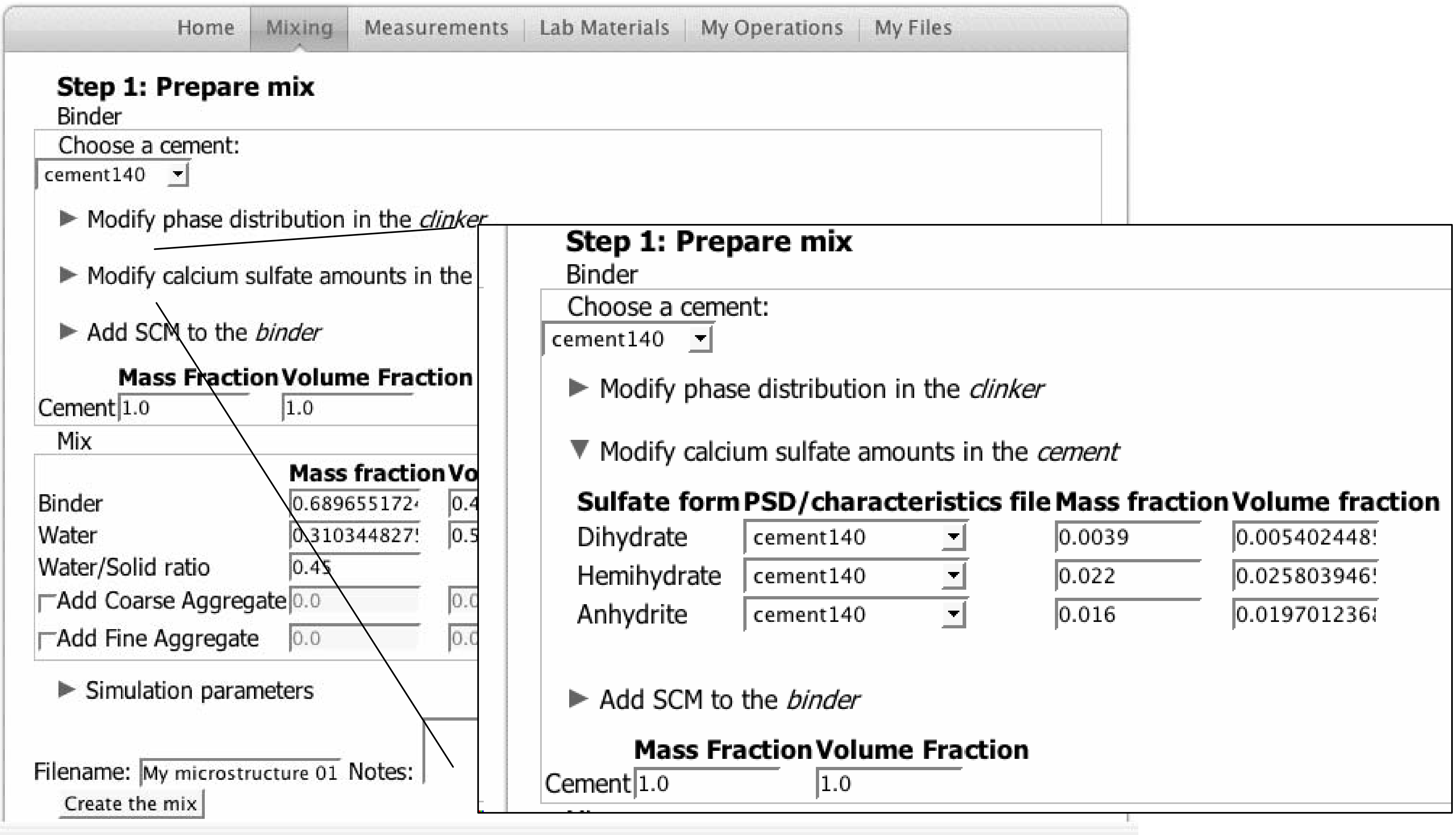


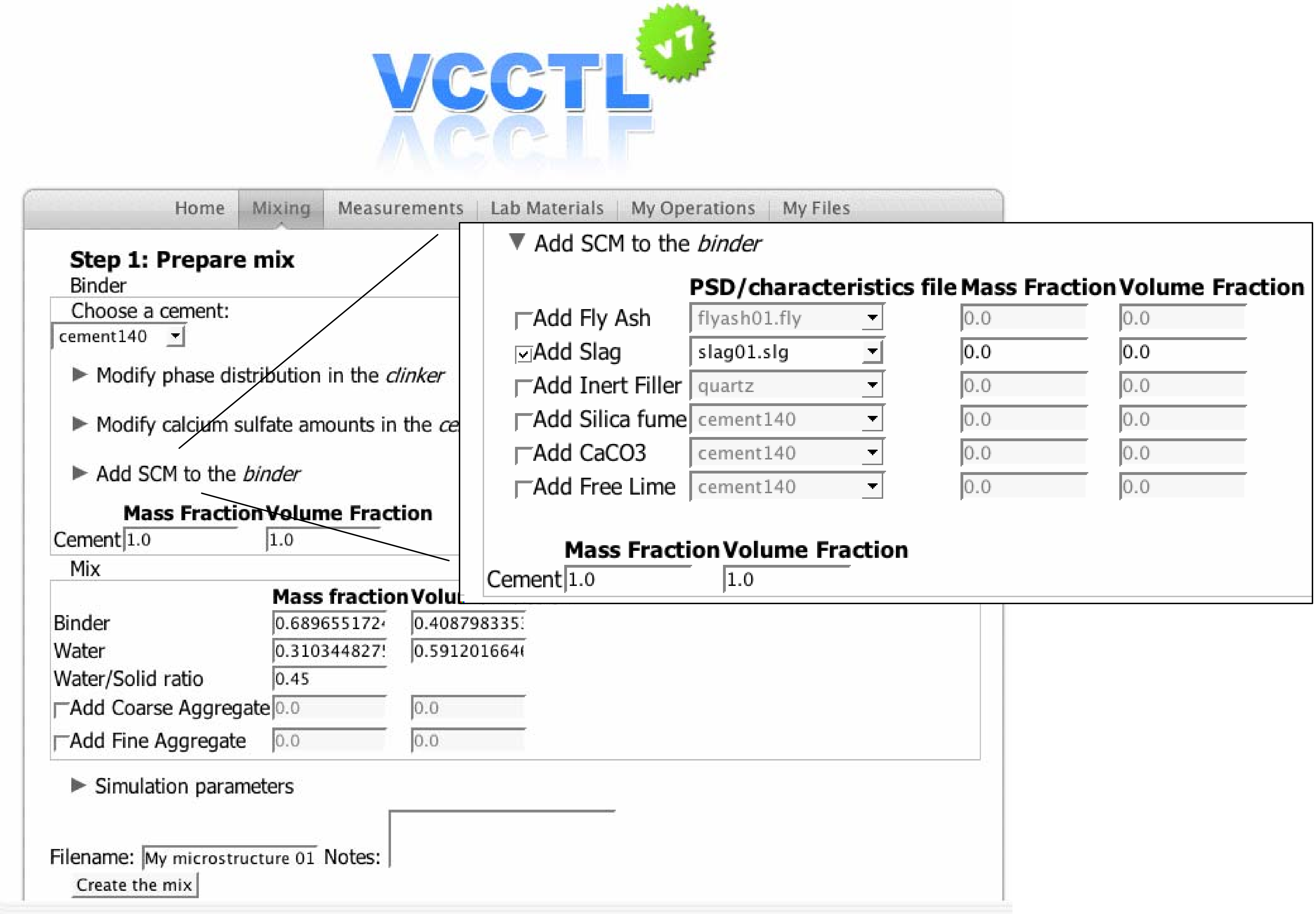
Virtual Concrete

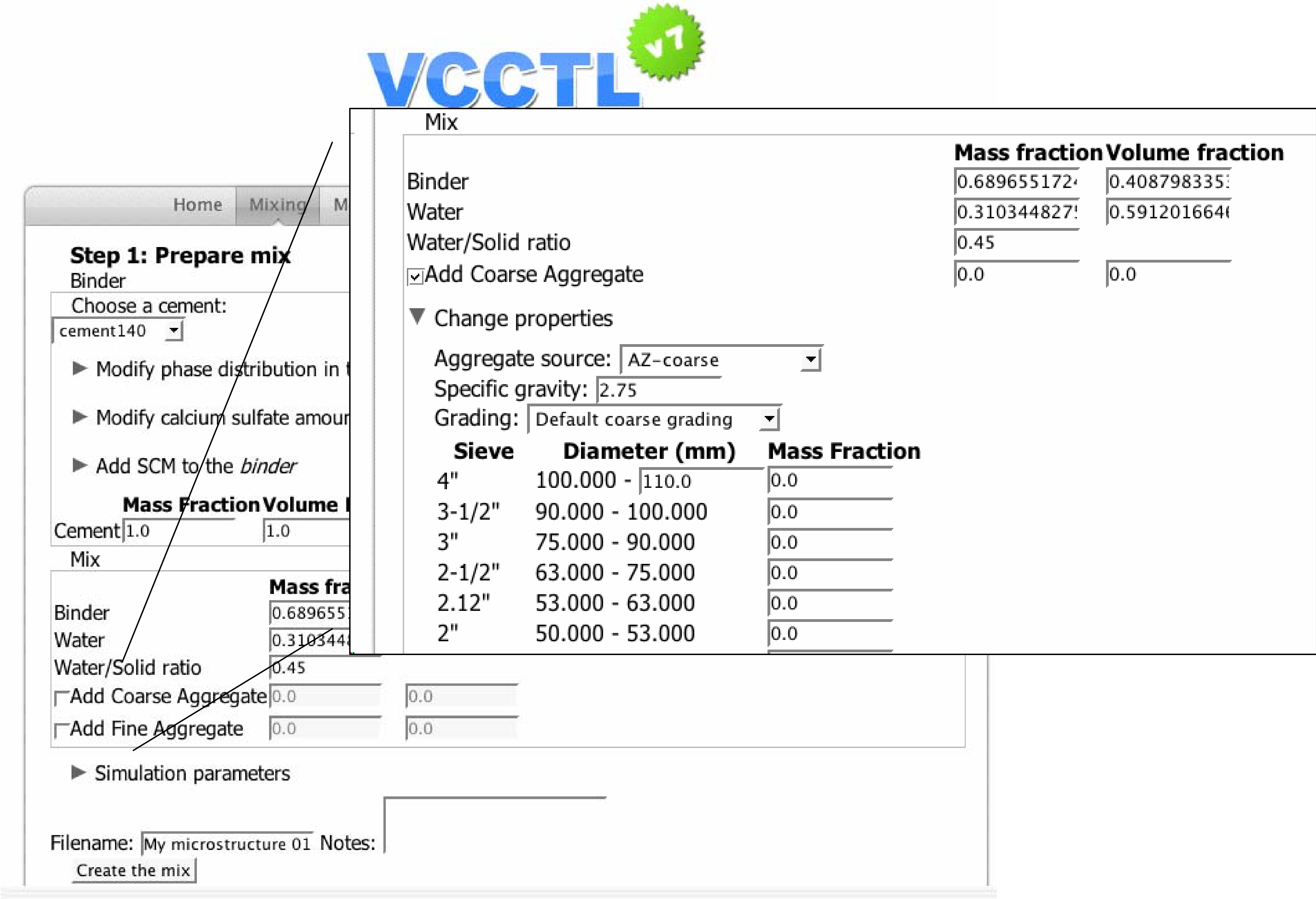

VCCTL v7
Home
Mixing
Measurements
Lab Materials
My Operations
My Files
Step 1: Prepare mix
Binder
Choose a cement:
cement140
Modify phase distribution in the clinker
Modify calcium sulfate amounts in the cement
Add SCM to the binder
Mass Fraction
Volume Fraction
Cement 1.0 1.0
Mix
Mass fraction
Volume fraction
Binder 0.689655172 0.408798335
Water 0.310344827 0.591201664
Water/Solid ratio 0.45
Add Coarse Aggregate 0.0 0.0
Add Fine Aggregate 0.0 0.0
Simulation parameters
Filename: My microstructure 01
Notes:
Create the mix


VCCTL
Home
Mixing
Measurements
Lab Materials
Step 1: Prepare mix
Binder
Choose a cement:
cement140
Modify phase distribution in the clinker
Modify calcium sulfate amounts in the cement
Add SCM to the binder
Mass Fraction Volume Fraction
Cement 1.0 1.0
Mix
Mass fraction Volume fraction
Binder 0.689655172 0.408798335
Water 0.310344827 0.591201664
Water/Solid ratio 0.45
Add Coarse Aggregate 0.0 0.0
Add Fine Aggregate 0.0 0.0
Simulation parameters
Filename: My microstructure 01 Notes:
Create the mix
Step 1: Prepare mix
Binder
Choose a cement:
cement140
Modify phase distribution in the clinker
Phase Volume fraction Surface area fraction
C3S 0.6865 0.6878
C2S 0.1611 0.1195
C3A 0.0813 0.1107
C4AF 0.0711 0.0820
K2SO4 0.0000 0.0000
Na2SO4 0.0000 0.0000
Sum: 1.000 1.000

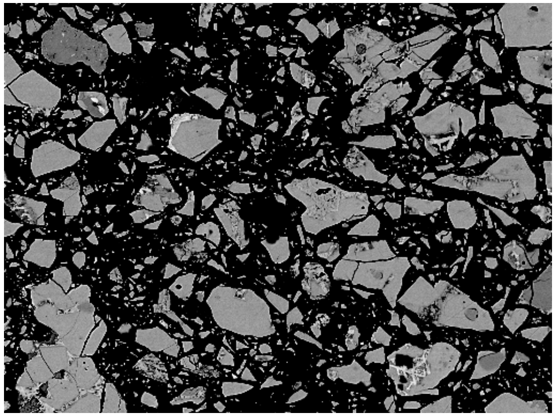
VCCTL v7

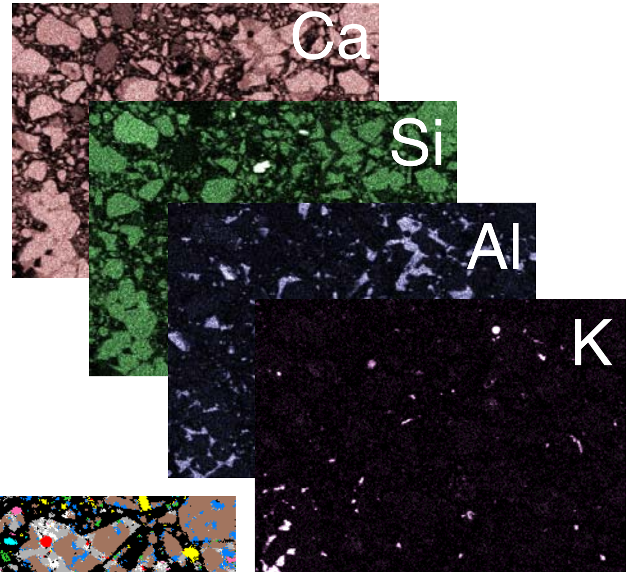

Home
Mixing
Measurements
Lab Materials
My Operations
My Files
Step 1: Prepare mix
Binder
Choose a cement:
cement140
Modify phase distribution in the clinker
Modify calcium sulfate amounts in the cement
Sulfate form
PSD/characteristics file
Mass fraction
Volume fraction
Dihydrate
cement140
0.0039
Hemihydrate
cement140
0.022
Anhydrite
cement140
0.016
Add SCM to the binder
Mass Fraction
Volume Fraction
Cement
1.0
1.0
Mix
Mass fraction
Binder
Water
Water/Solid ratio
0.45
Add Coarse Aggregate
Add Fine Aggregate
Simulation parameters
Filename:
My microstructure 01
Notes:
Create the mix


VCCTL v7
Home
Mixing
Measurements
Lab Materials
My Operations
My Files
Step 1: Prepare mix
Binder
Choose a cement:
cement140
▶ Modify phase distribution in the clinker
▶ Modify calcium sulfate amounts in the ce
▶ Add SCM to the binder
Mass Fraction Volume Fraction
Cement 1.0 1.0
Mix
Mass fraction Volu
Binder 0.689655172 0.408798335
Water 0.310344827 0.591201664
Water/Solid ratio 0.45
Add Coarse Aggregate 0.0 0.0
Add Fine Aggregate 0.0 0.0
▶ Simulation parameters
Filename: My microstructure 01 Notes:
Create the mix
▼ Add SCM to the binder
PSD/characteristics file Mass Fraction Volume Fraction
Add Fly Ash flyash01.fly 0.0 0.0
Add Slag slag01.slg 0.0 0.0
Add Inert Filler quartz 0.0 0.0
Add Silica fume cement140 0.0 0.0
Add CaCO3 cement140 0.0 0.0
Add Free Lime cement140 0.0 0.0
Mass Fraction Volume Fraction
Cement 1.0 1.0

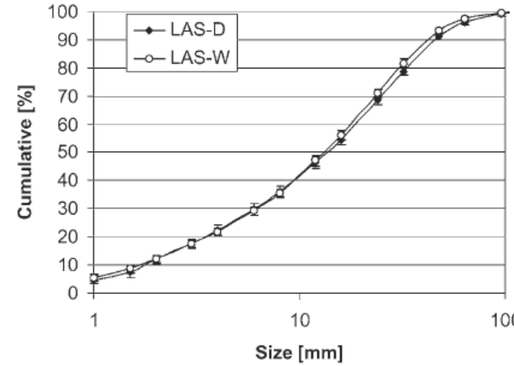

VCCTL v7
Home
Mixing
Step 1: Prepare mix
Binder
Choose a cement:
cement140
Modify phase distribution in t
Modify calcium sulfate amour
Add SCM to the binder
Mass Fraction
Volume f
Cement 1.0 1.0
Mix
Binder 0.689655
Water 0.310344
Water/Solid ratio 0.45
Add Coarse Aggregate 0.0 0.0
Add Fine Aggregate 0.0 0.0
Simulation parameters
Filename: My microstructure 01
Notes:
Create the mix
Mix
Mass fraction
Volume fraction
Binder 0.689655172 0.408798335
Water 0.310344827 0.591201664
Water/Solid ratio 0.45
Add Coarse Aggregate 0.0 0.0
Change properties
Aggregate source: AZ-coarse
Specific gravity: 2.75
Grading: Default coarse grading
Sieve
Diameter (mm)
Mass Fraction
4" 100.000 - 110.0 0.0
3-1/2" 90.000 - 100.000 0.0
3" 75.000 - 90.000 0.0
2-1/2" 63.000 - 75.000 0.0
2.12" 53.000 - 63.000 0.0
2" 50.000 - 53.000 0.0

SEM/BSE Image...

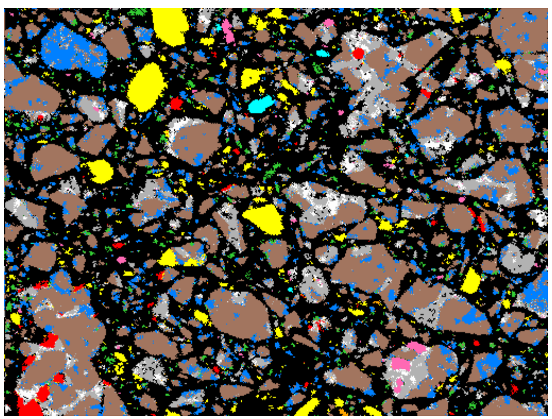




... X-ray element maps ...

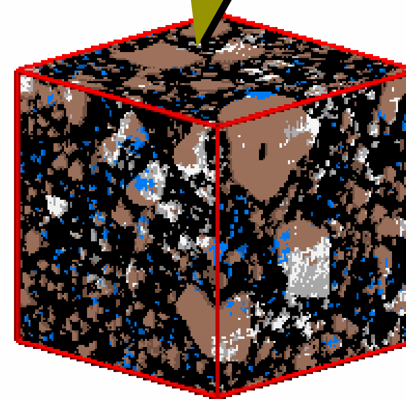


... Particle Size Distribution ...



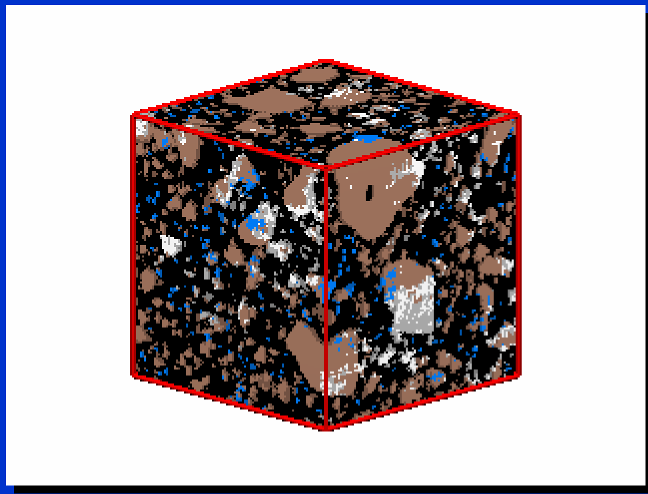
... segment image into **phases** ...

Measure autocorrelation functions on majority phases

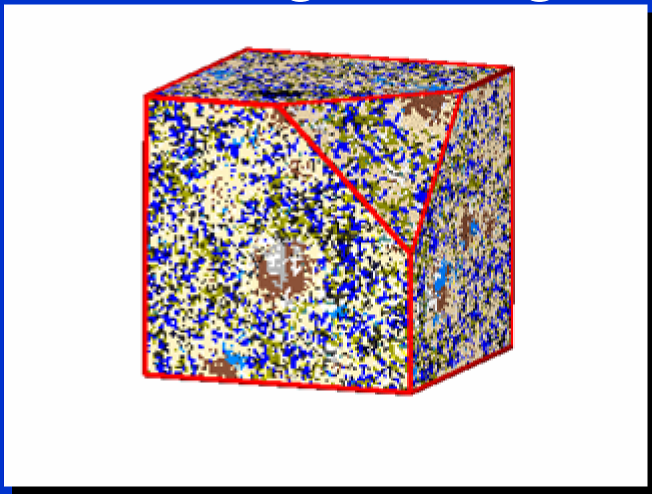


Elastic Properties of Cement Paste

Virtual Cement



Cure to given age

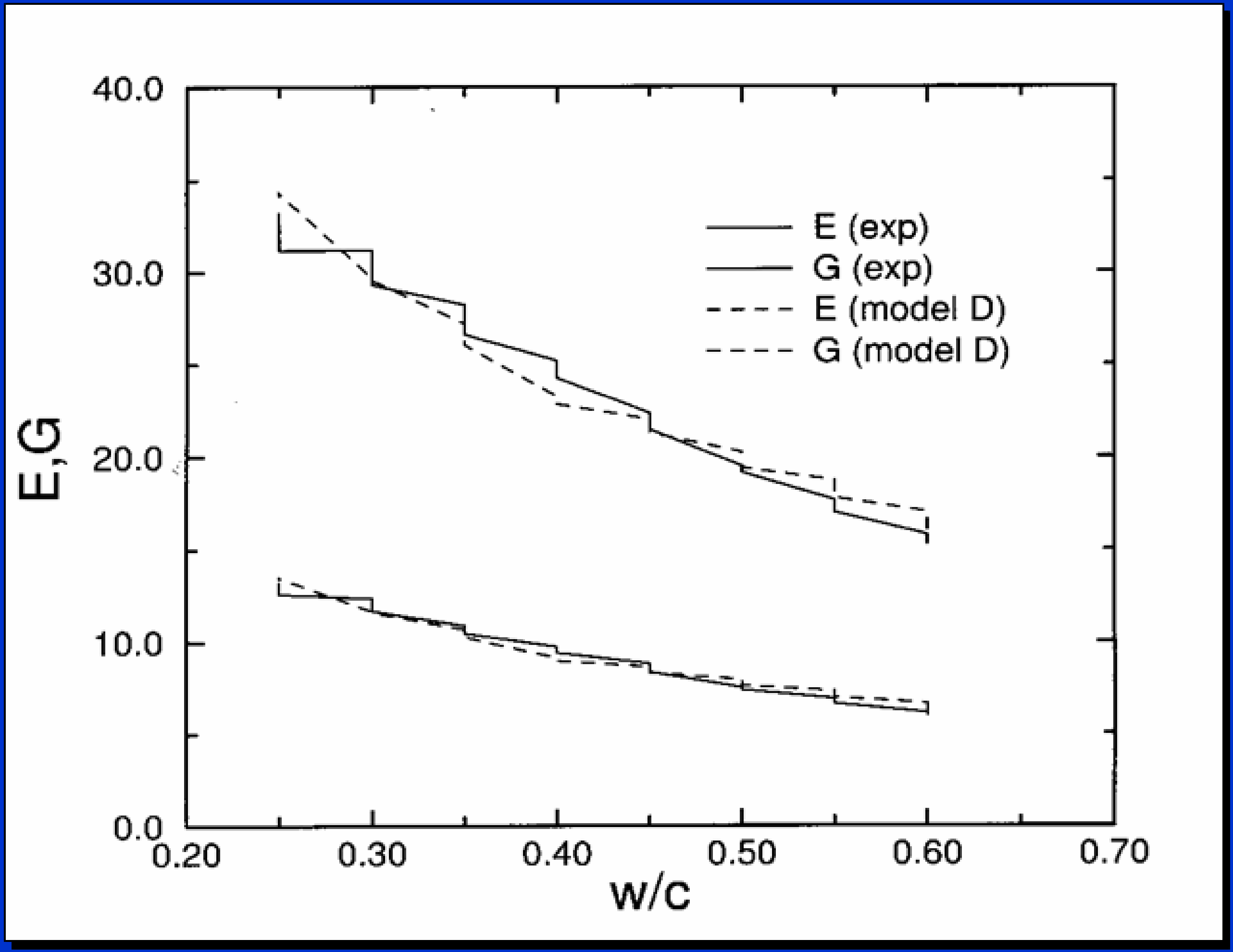


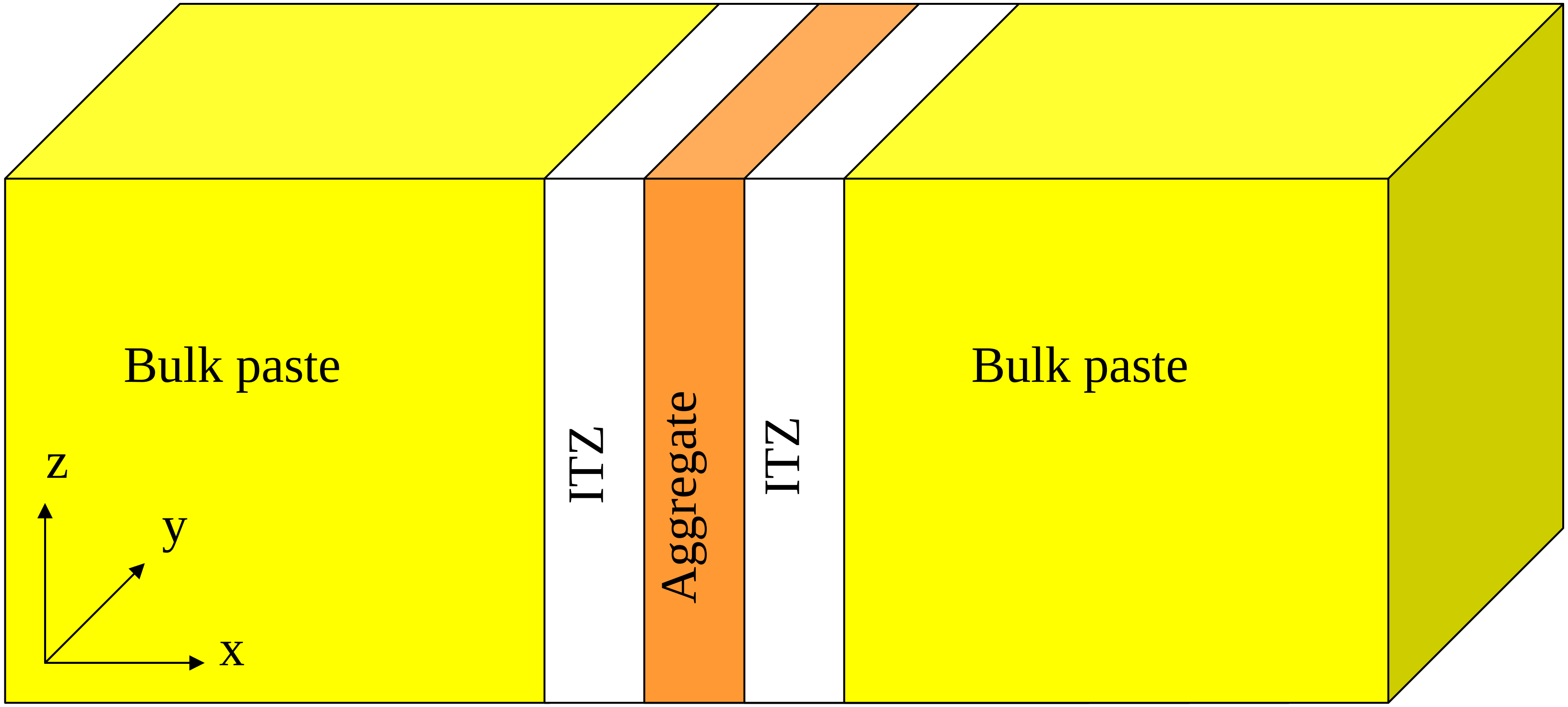
Finite Element Model:

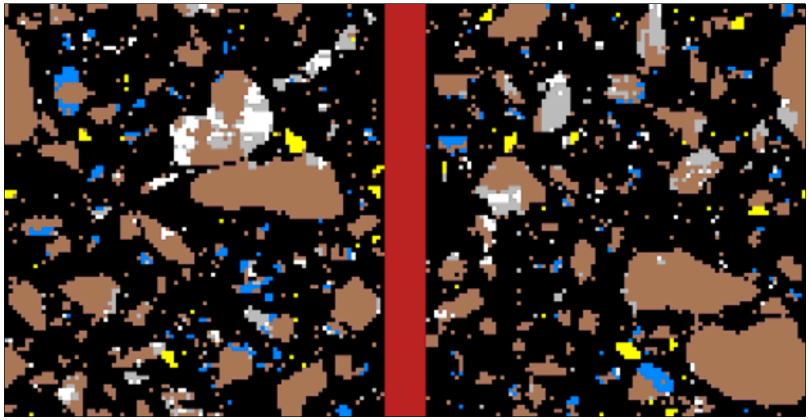
- input phase moduli
- input microstructure

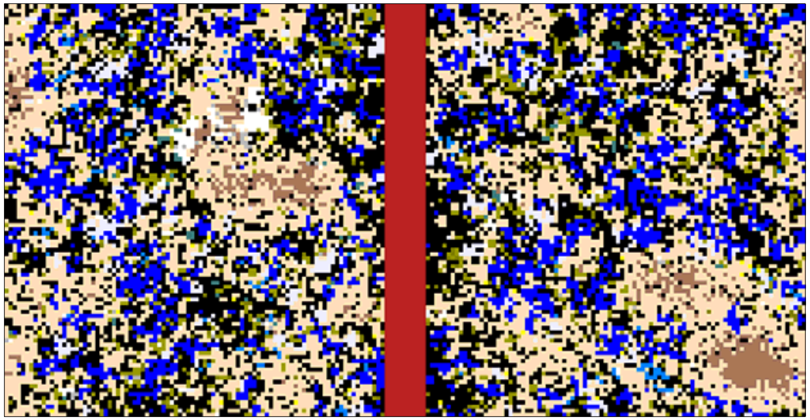
Output Paste Elastic Moduli

Cement Paste Elastic Moduli



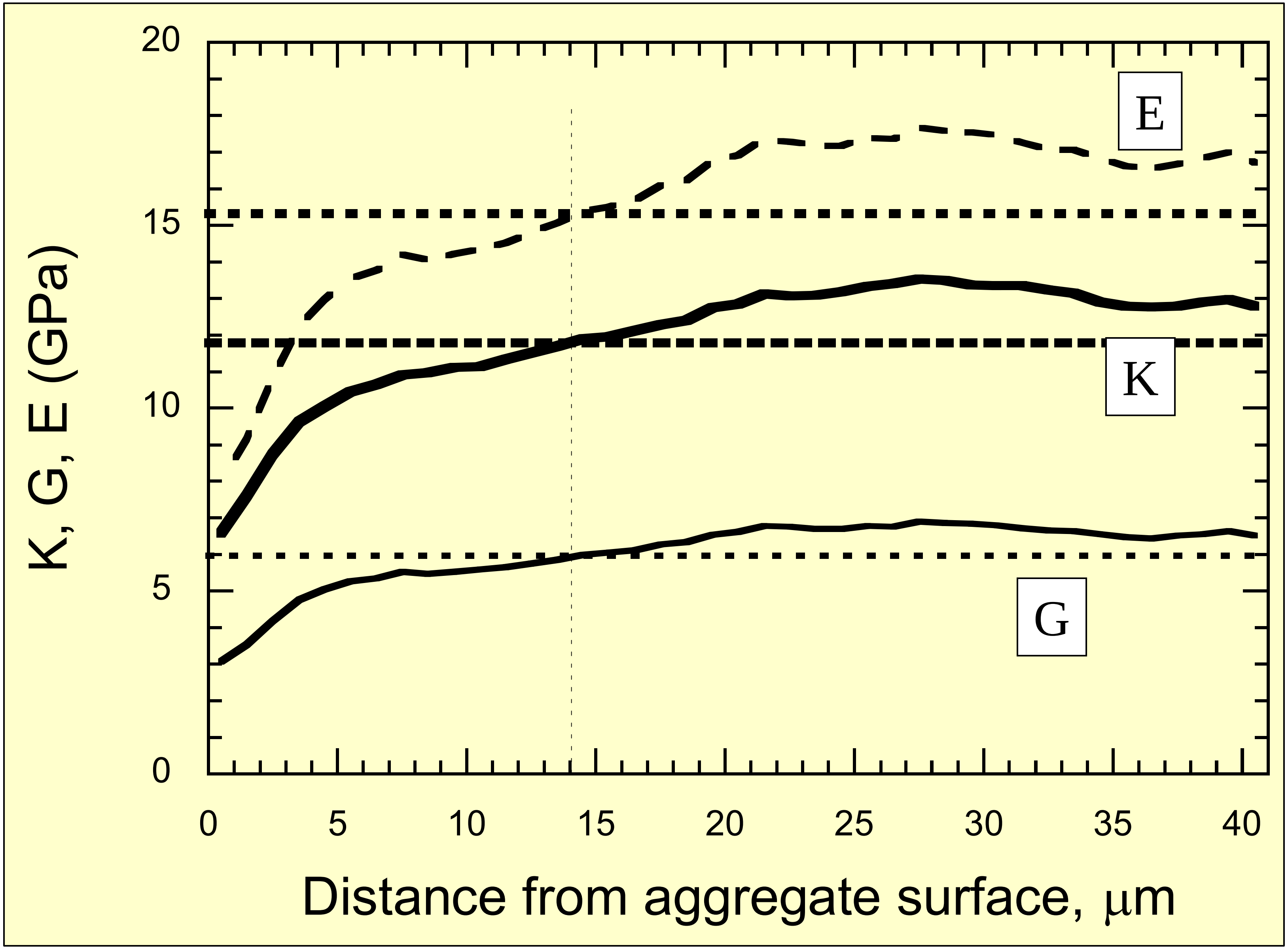




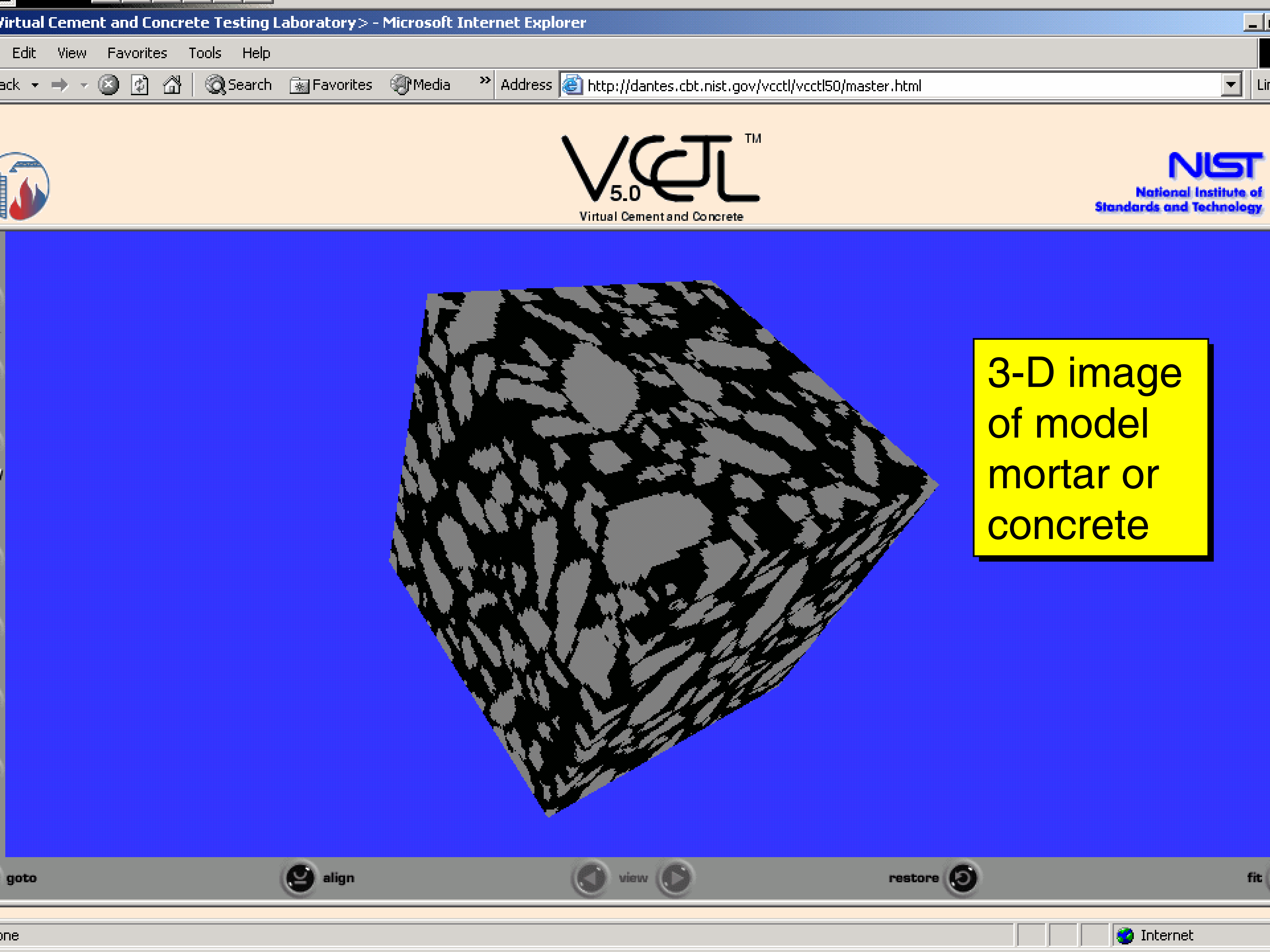


w/c = 0.6 α = 0.0

w/c = 0.6 α = 0.83



0.5 w/c, concrete

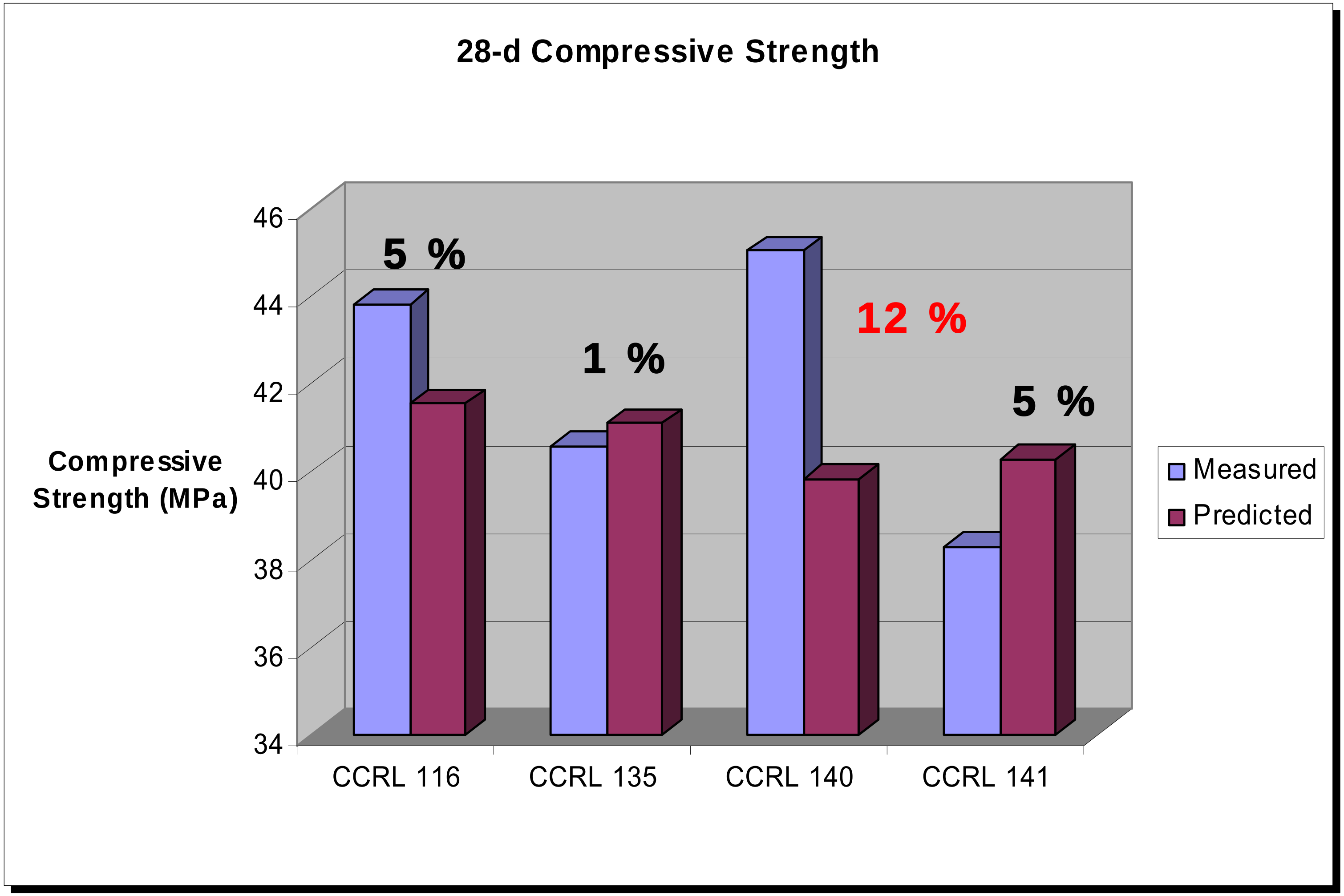

Virtual Cement and Concrete Testing Laboratory> - Microsoft Internet Explorer
Edit View Favorites Tools Help
Search Favorites Media
Address http://dantes.cbt.nist.gov/vcctl/vcctl50/master.html
VCCTL 5.0 TM
Virtual Cement and Concrete
NIST
National Institute of Standards and Technology
3-D image of model mortar or concrete
goto
align
view
restore
fit
Internet

Module for Mechanical Properties of Concrete

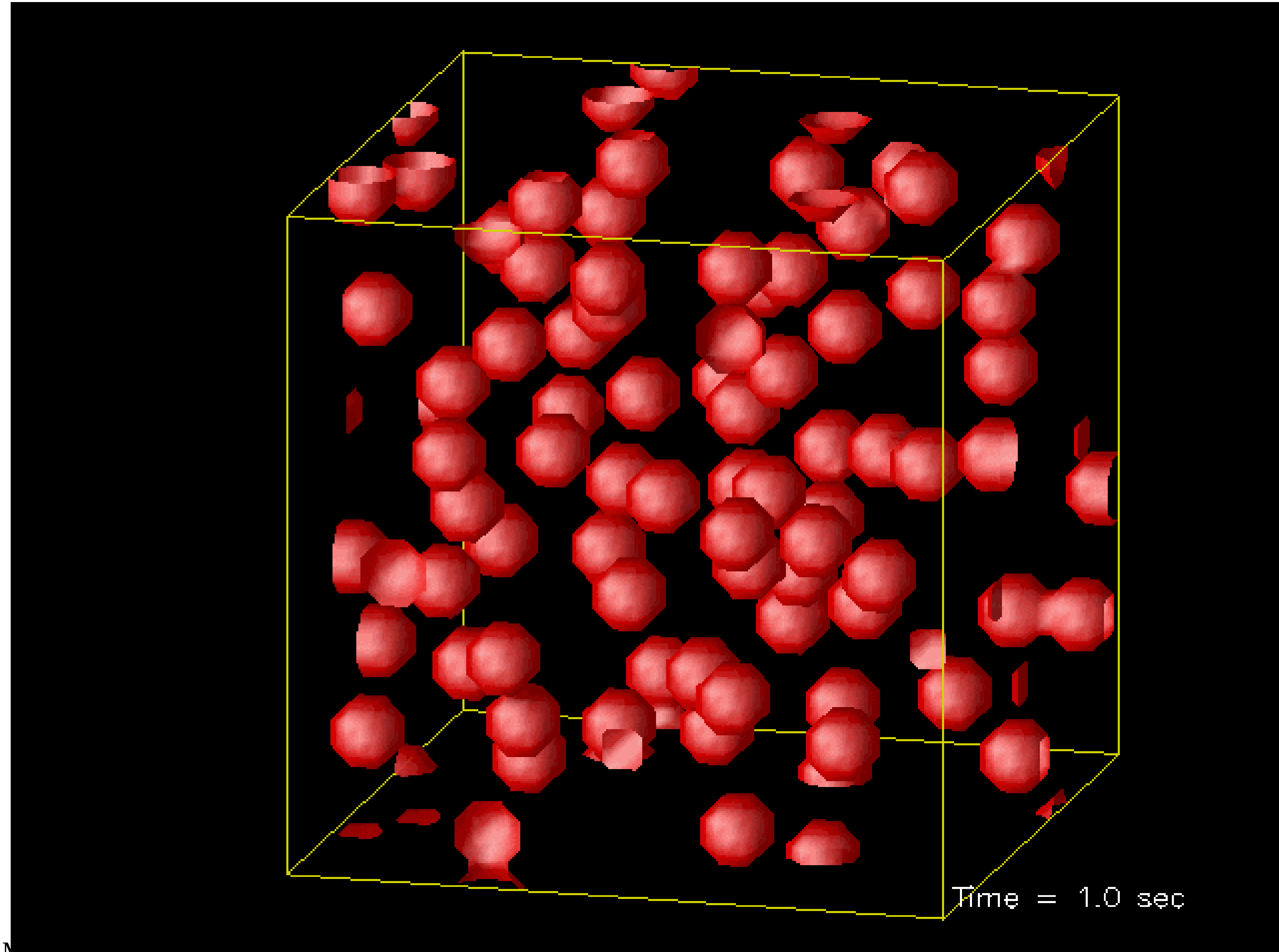
Moduli and Strength of Concrete

- Concrete has structure over many length scales
- Too computationally intensive to handle as a finite element problem
- Alternative: Effective Medium Theory (EMT)
  – Provides estimate of **elastic moduli** of mortar and concrete
  – Requires information on the mix parameters and elastic properties of each component
- With the elastic moduli calculated, **compressive strength** is estimated using empirical correlations between strength and the moduli.

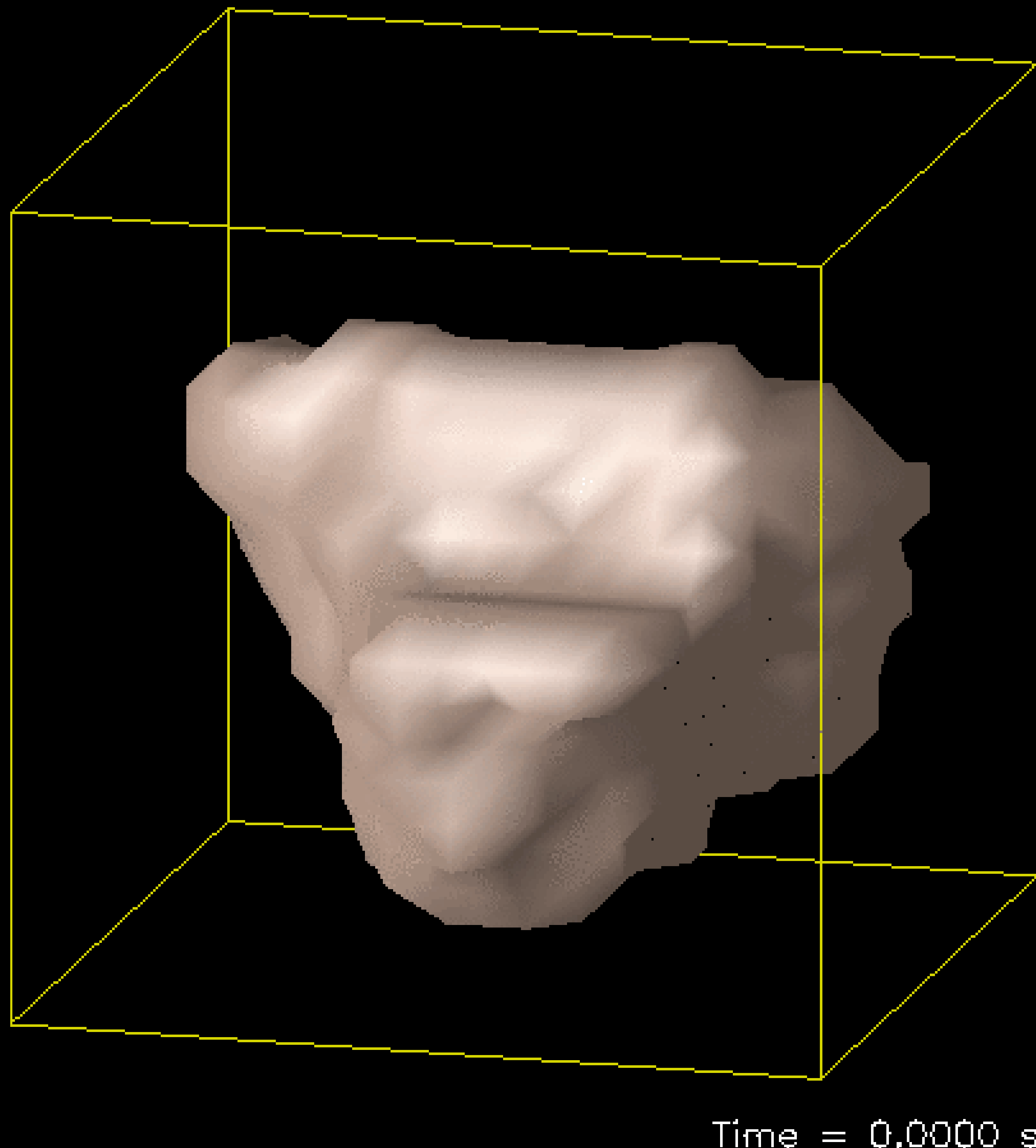
Moduli and Strength of Mortar



Lime particles reacting (20 micrometers in size) using HydratiCA – a new generation hydration model


Time = 1.0 sec

Reactions at Nanoparticle Surfaces (50 nm in size) using HydratiCA


Time = 0.0000 s

Concrete rheology (flow) modeling

- Fresh concrete! Shape of aggregates plays a big role
- Concrete – coarse aggregate suspended in mortar matrix
- Mortar – sand suspended in cement paste matrix
- Cement paste – cement particles suspended in water+liquid admixtures
- Need to model at each level, at the scale of the suspended particles
- Difficulties – random shape particles, dense suspension (e.g., particles come close together), interparticle forces (mainly in cement paste), non-Newtonian fluid matrix
- Dissipative particle dynamics – invented in Europe, greatly developed at NIST

Advances

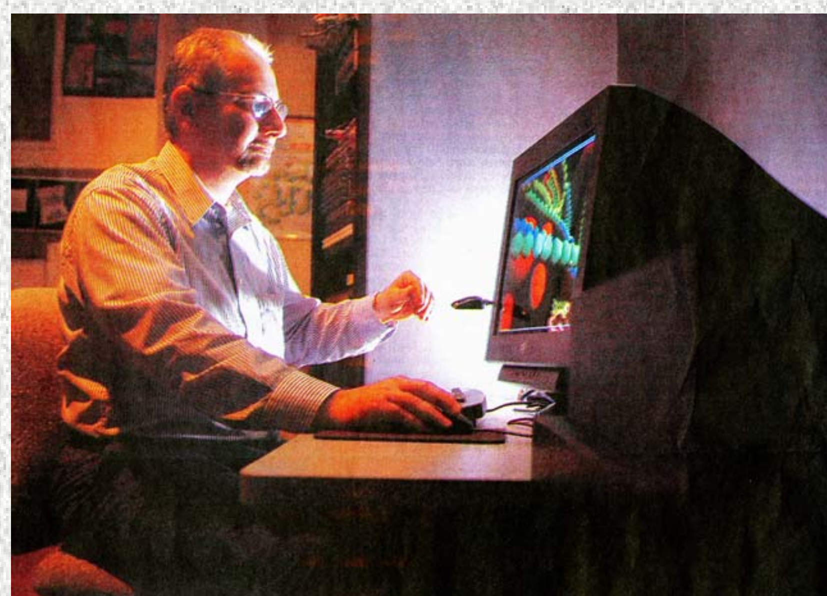
- Massively parallel computations – lots of time on lots of processors
- Supercomputer time awarded for concrete flow:
  - considered worthy of major time on some of the nation's fastest computers
  - considered a problem of national interest
  - considered to be a "grand challenge" computational problem
- 3/06 to 8/07 – 1,000,000 CPU hours on NASA Columbia supercomputer
- 2008 – 200,000 more hours for rheology, 200,000 hours for cement hydration
- 11/07 to 11/10 – 750,000 hours per year on DOE Argonne Blue Gene supercomputer
- Models now accurately handle real-shape particles with surface forces and non-Newtonian matrix fluid

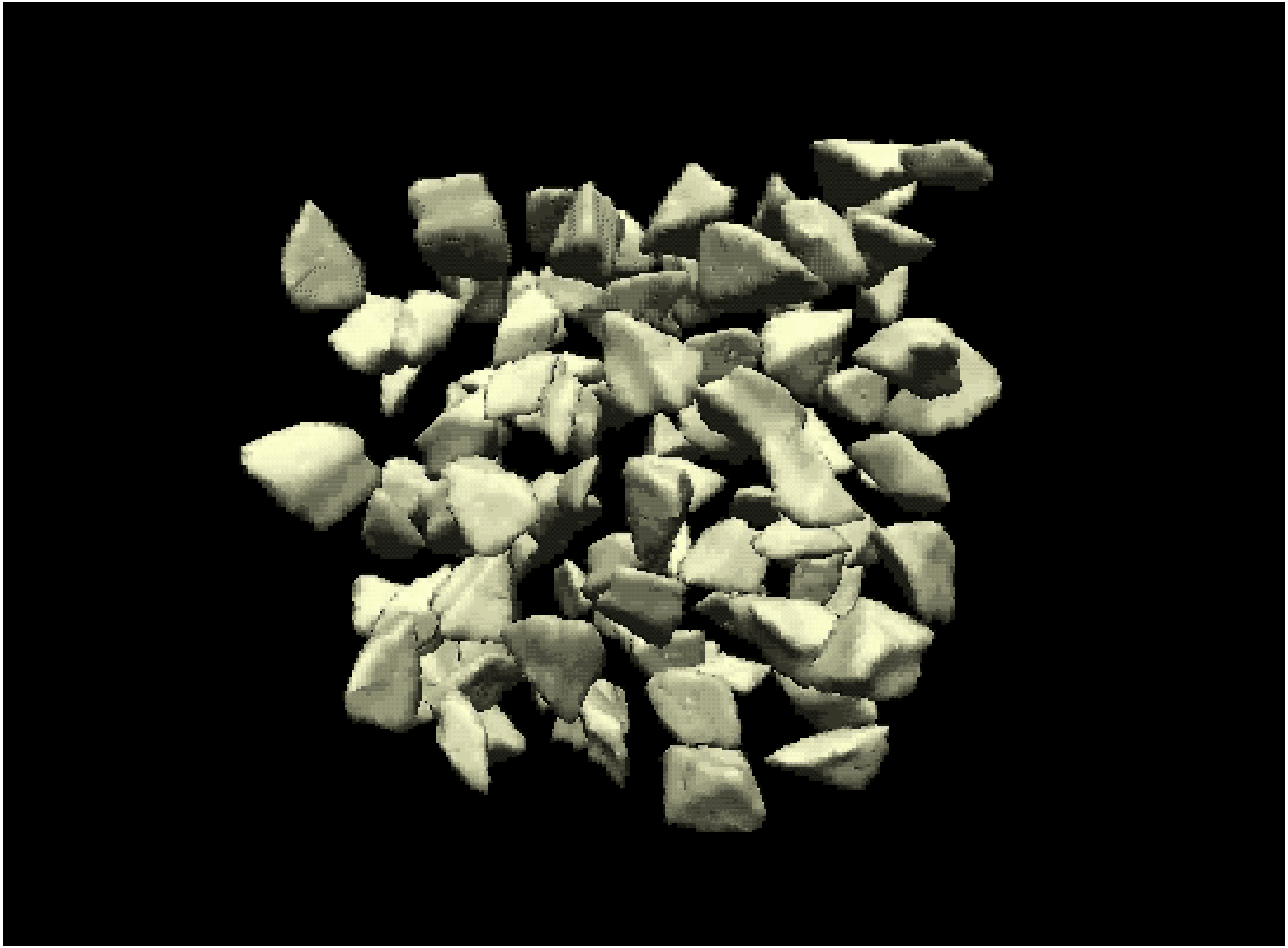
THE BALTIMORE SUN

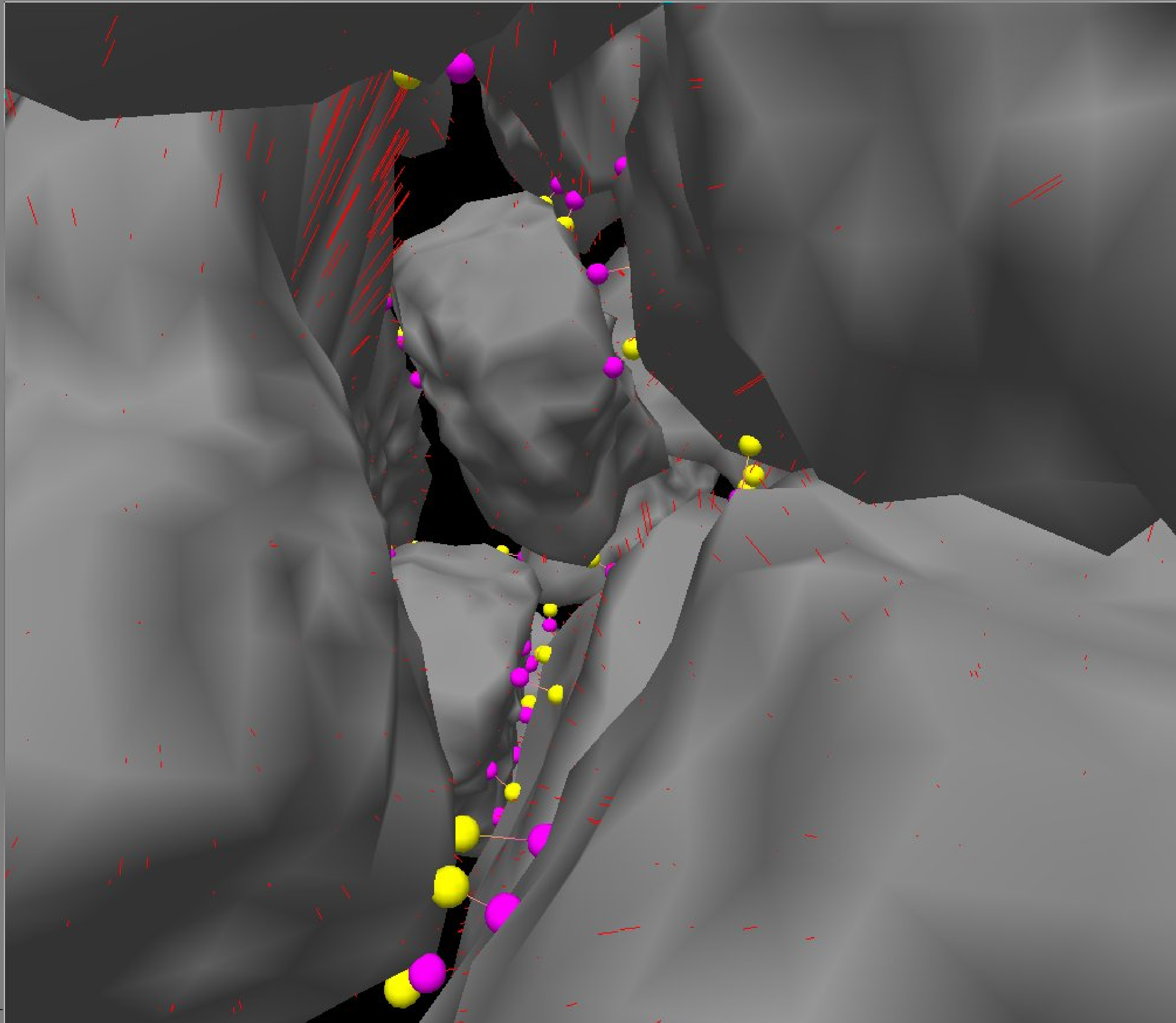
March 24, 2006

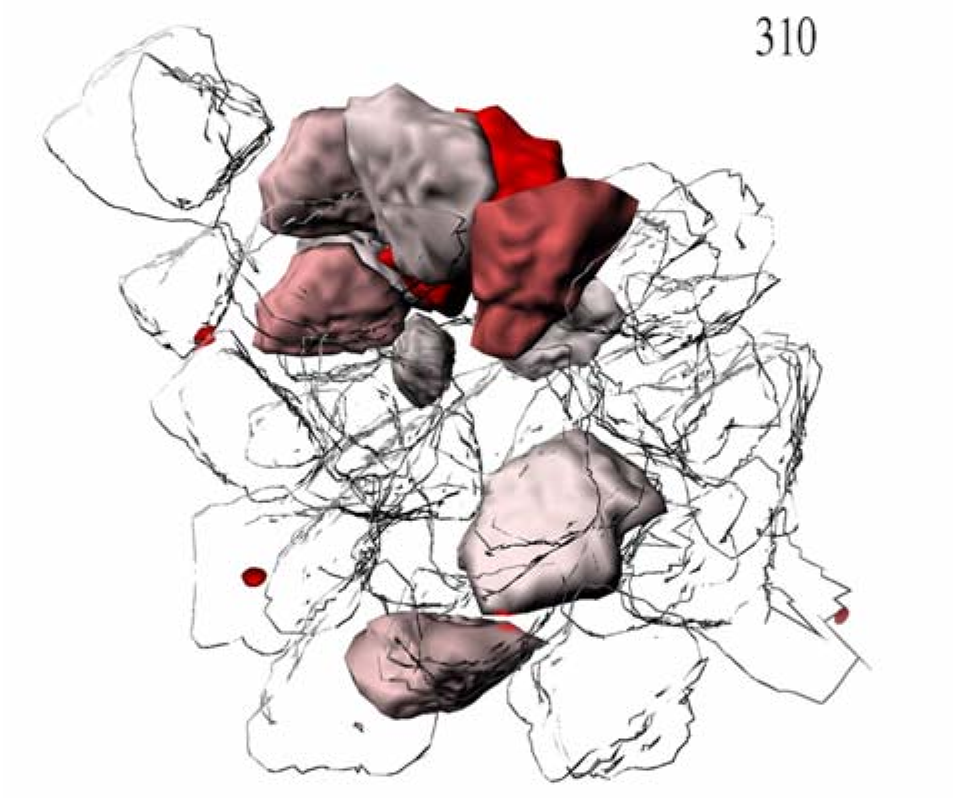
Mix masters try to crack code for construction

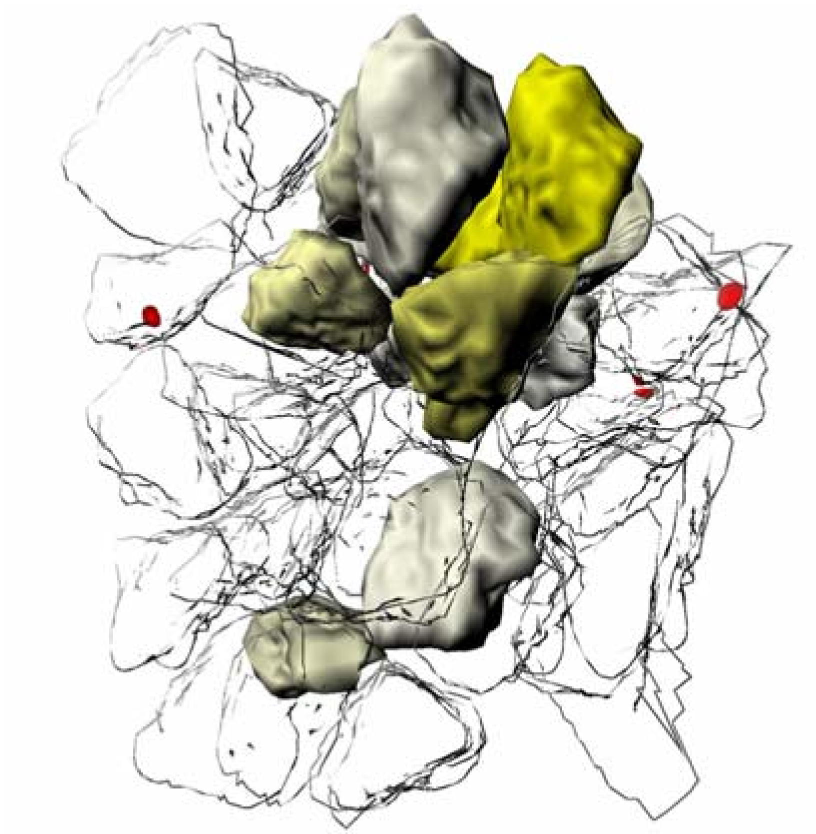
Researchers are borrowing a million hours of processor time from NASA to analyze how concrete is combined—and to find the right recipe for building success

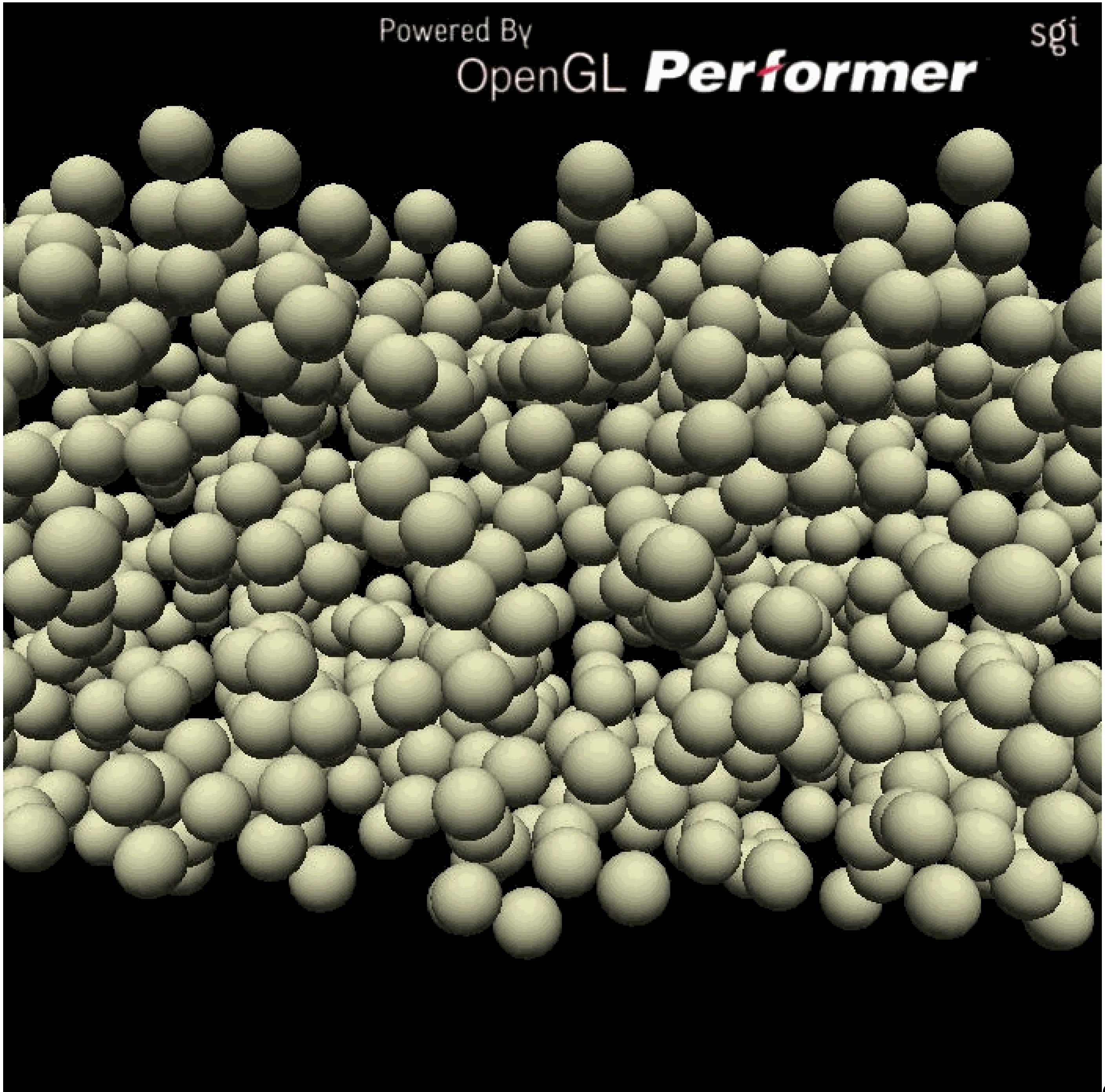







310




Powered By
OpenGL Performer
sgi

Multi-scale approach to experimental rheology

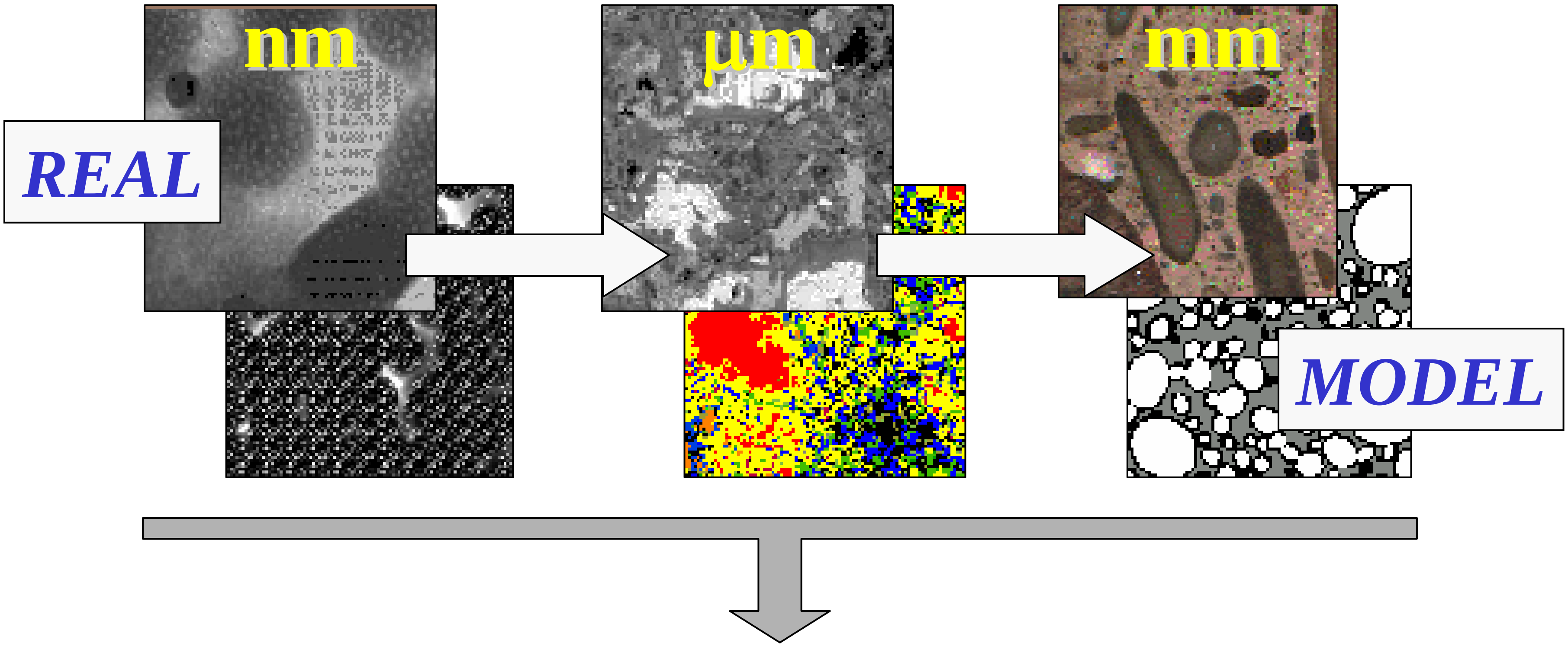
Cement paste (Micro)

Mortar (Milli)

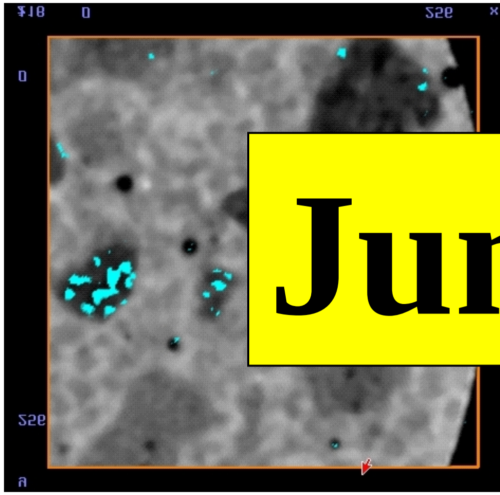
Concrete (Macro)

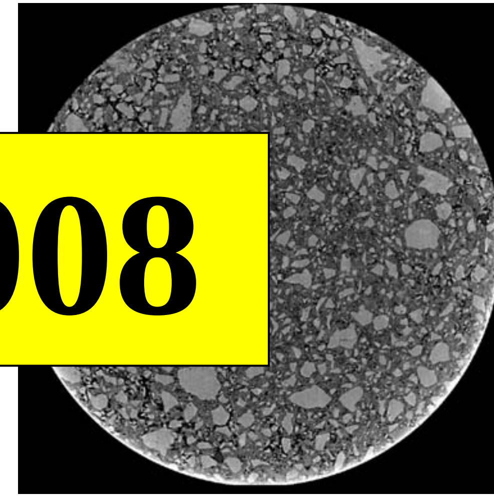
Modeling and Measuring the Structure and Properties of Cement-Based Materials

http://ciks.cbt.nist.gov/monograph/



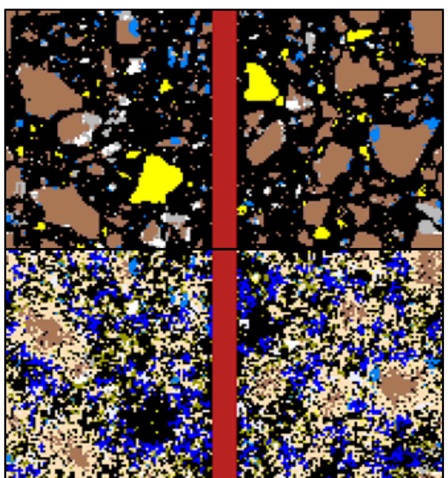
12,000+ users from 90+ countries per month

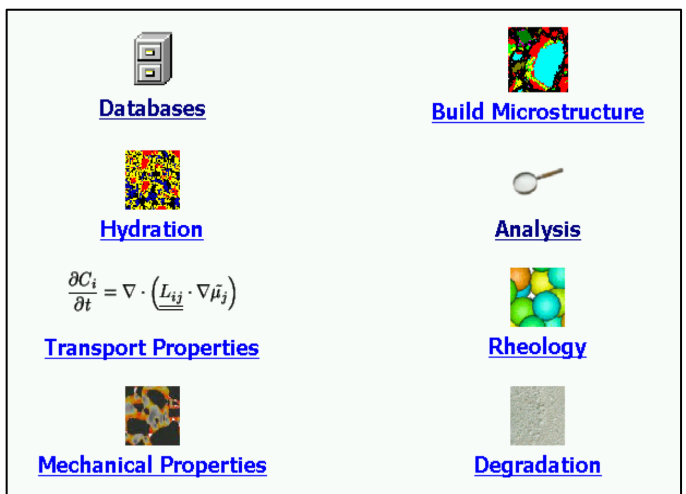




June 16-19, 2008

18th ACBM/NIST Computer Modeling Workshop June 25-27, 2007





Building a user community

- Educational version of VCCTL: **eVCCTL**
  - Improved, user-friendly interface
  - Web server application
  - Should be available sometime in 2008

- Hopefully widely-used by students and faculty and others who want to try out these ideas

Prospectus

- You have to characterize concrete materials well in order for models to perform well
- Basic foundations of virtual concrete have been “poured”
- There is a lot to look forward to, in many ways!
  – Characterization and simulation of supplementary cementitious materials (e.g., fly ash, blast furnace slag, metakaolin, silica fume)
  – Increasing number of processors on a desktop means that quicker and better simulations can become more and more accessible to the average user
  – National shape database of coarse and fine aggregates and cement

Nanotechnology of portland cement concrete and asphaltic concrete

Three basic questions that must be answered first

- Do you understand the appropriate physical/chemical mechanisms and microstructure at the nano-scale, so that you can, with knowledge, affect them?
- Are you ingenious enough to generate effects at the nanoscale?
- How can you tell you if made a difference?
  - Macro measurements
  - Micro/nano measurements

An approach to avoid

- Take a bottle of “nano-gee-whiz” off the shelf
- Add to your concrete or asphalt
- Poof! Nanotechnology!

Nanotechnology is considered "high-tech" for a good reason:

It requires deep knowledge of the system considered - at the nano-scale - in order to be able to intelligently design - at the nano-scale!

The only way to make good use of nanotechnology in concrete and asphalt materials science is to do more fundamental research!