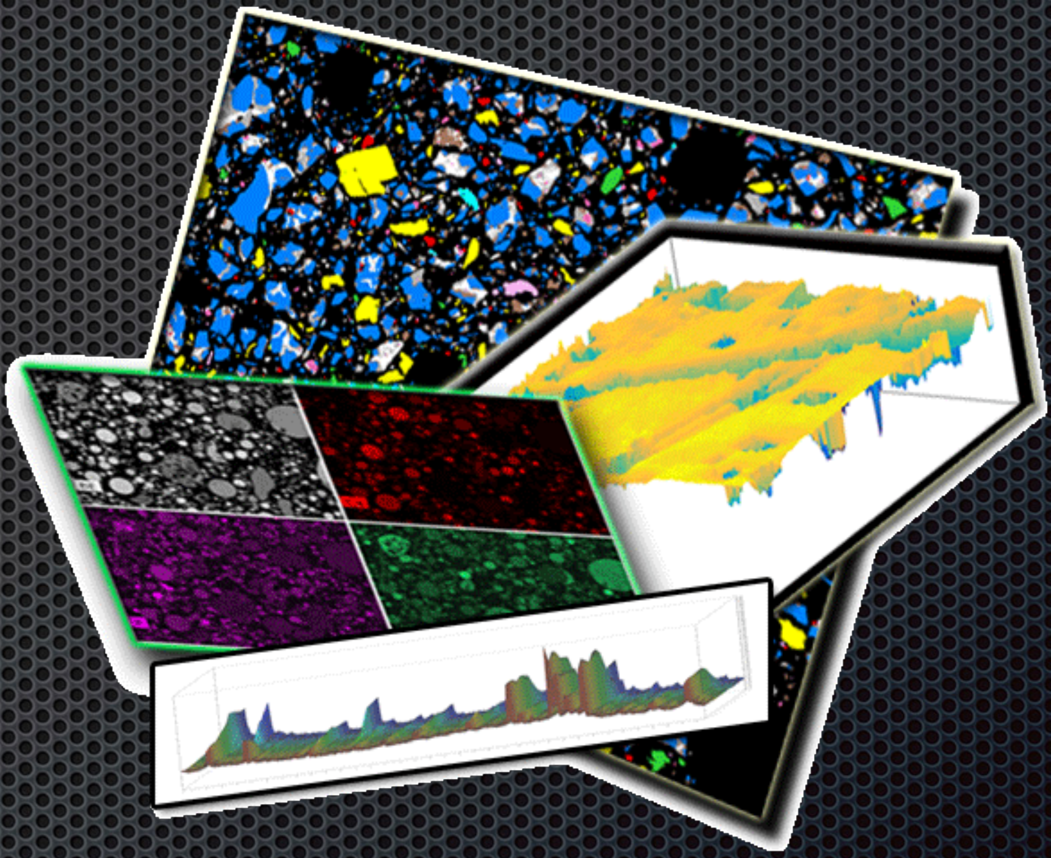
Using Characterization Data to Model Microstructure & Properties

Jeff Bullard



Cement Characterization Workshop, 2018

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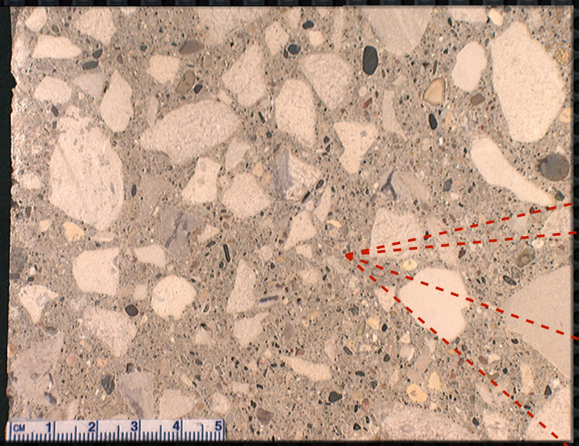
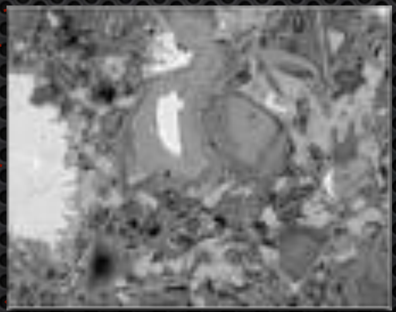
Background

We want to understand and predict the properties of concrete materials, including its early-age performance and service life





Performance of concrete depends on the properties of the cement binder component

Properties of cement binder

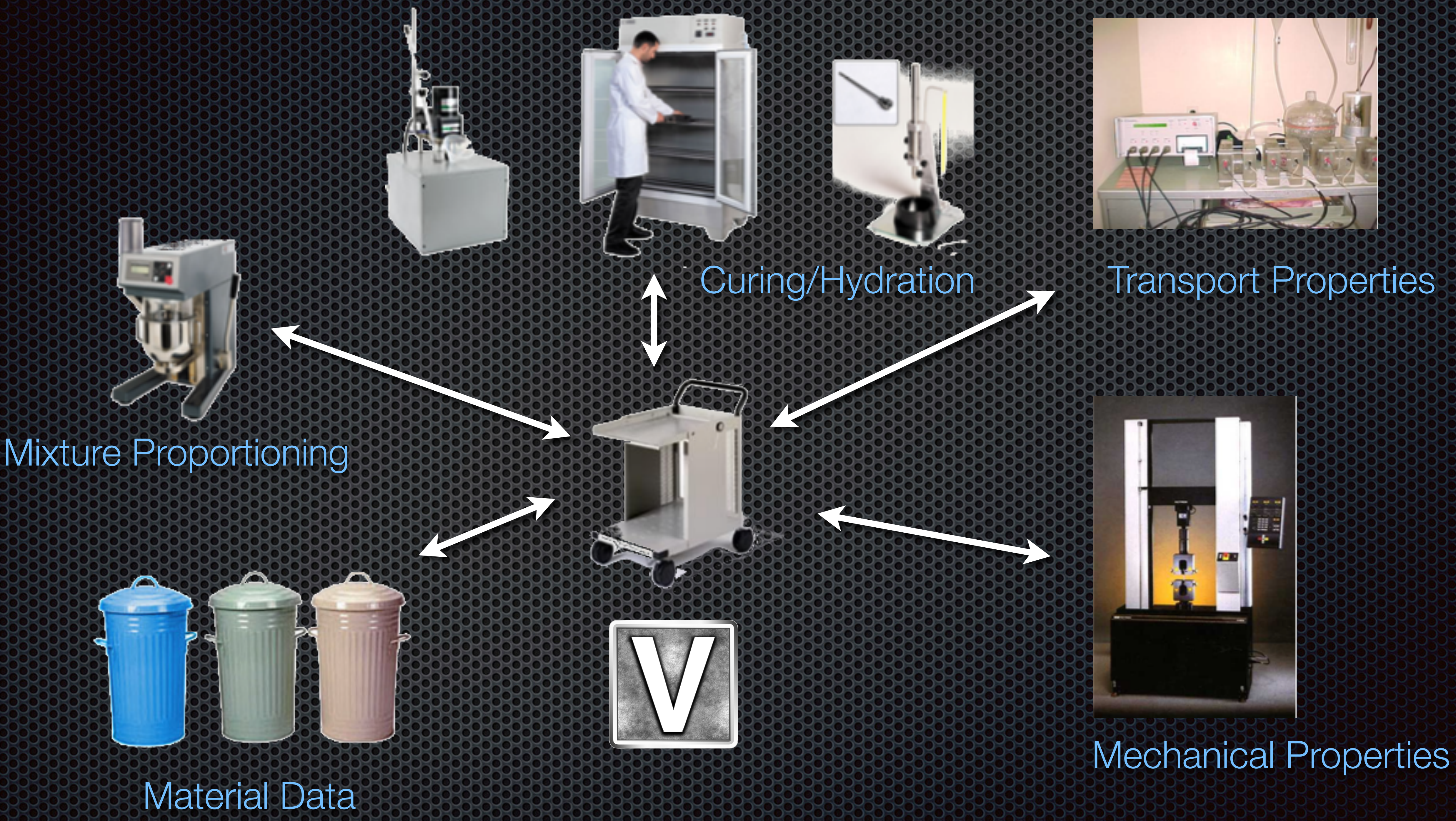
- change continuously in time
- depend on its proportioning, chemistry, microstructure, and nanostructure

Waste-stream materials

Cement powder

Water

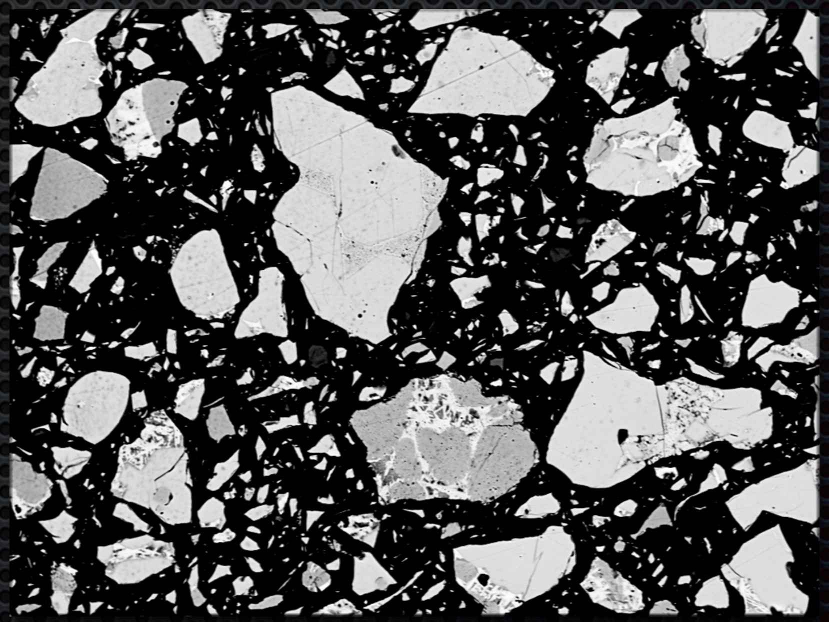
VCCTL Software



Digital Image Modeling

What we would like to reproduce accurately in 3D image:

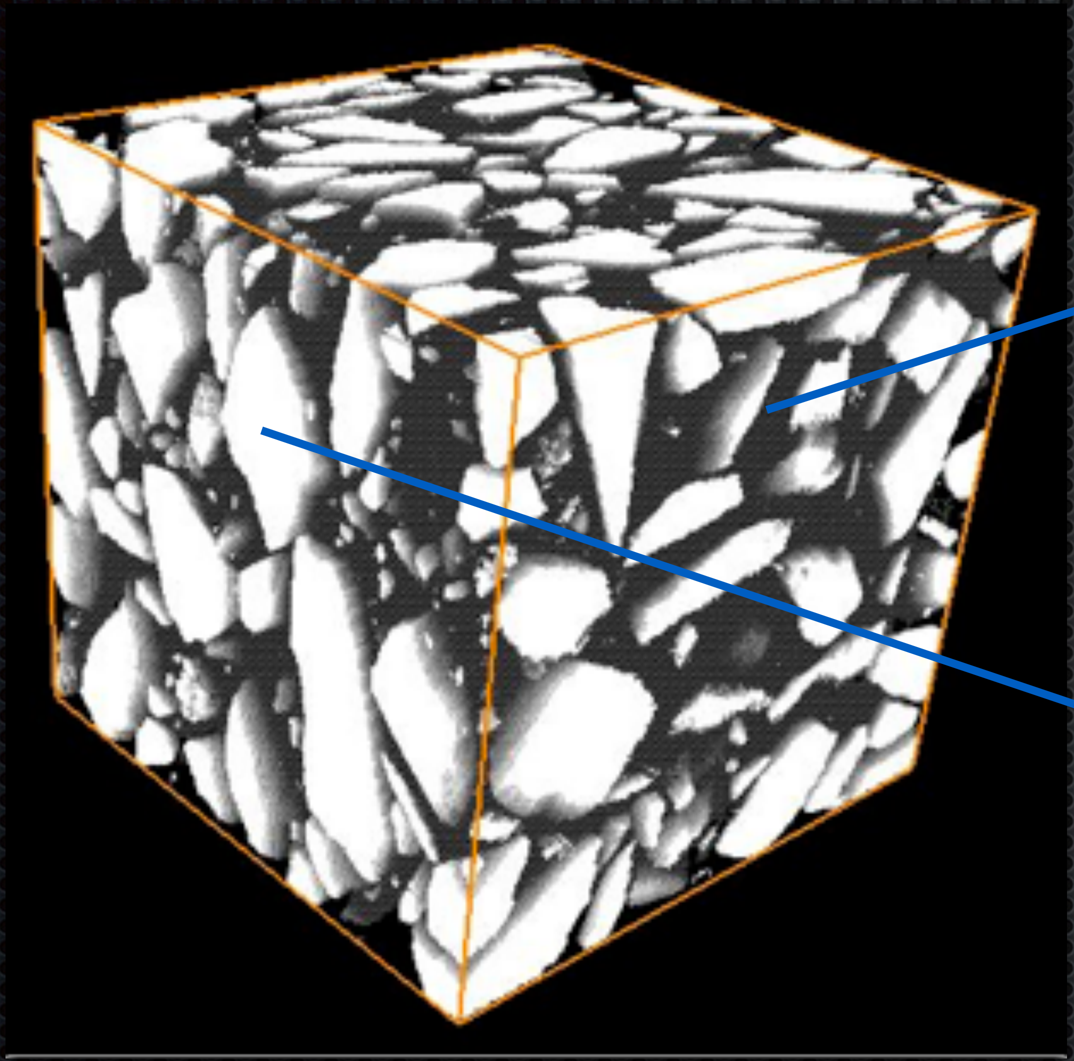
- Phase volume fractions
- Phase surface area fractions
- Phase correlations in space
- Particle size distribution
- Particle shape, if available



From a 2D image?

3D Particle Shape

X-ray µCT:

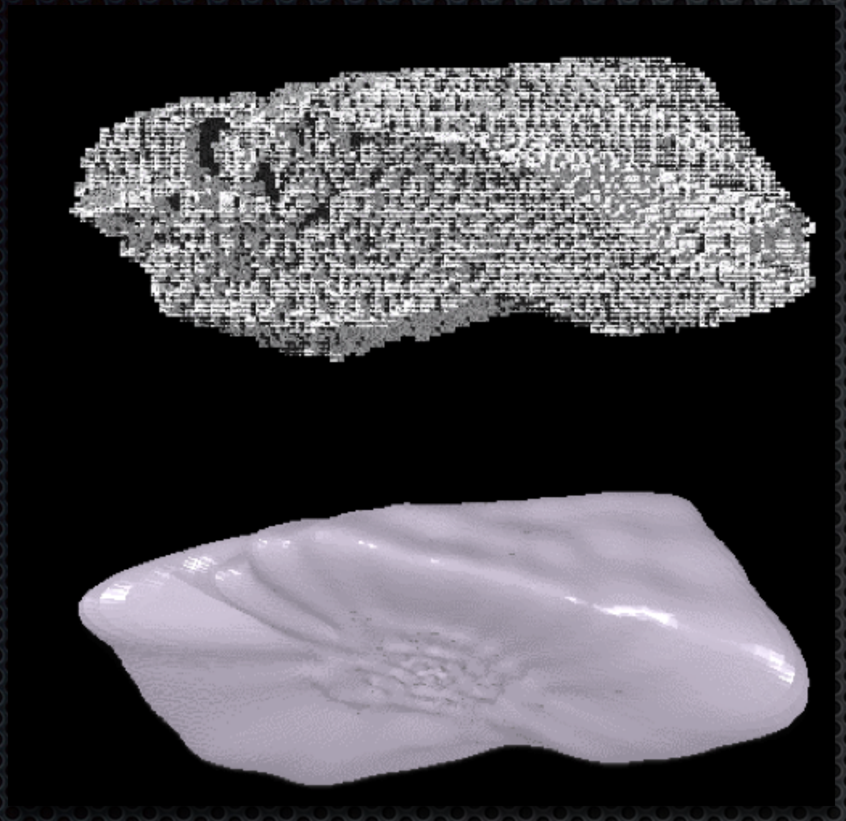


E.J. Garboczi and J.W. Bullard, *Cem. Concr. Res.* 34 [10] 1933-1937 (2004)

Extract individual particles

3D Particle Shape

Shape characterized by spherical harmonic analysis:



E.J. Garboczi, *Cem. Concr. Res*. **32** [10] 1621-1638 (2002)

(or any engineering math book)

$$r(\theta,\phi) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} a_{nm} Y_n^m(\theta,\phi)$$

Legendre polynomials

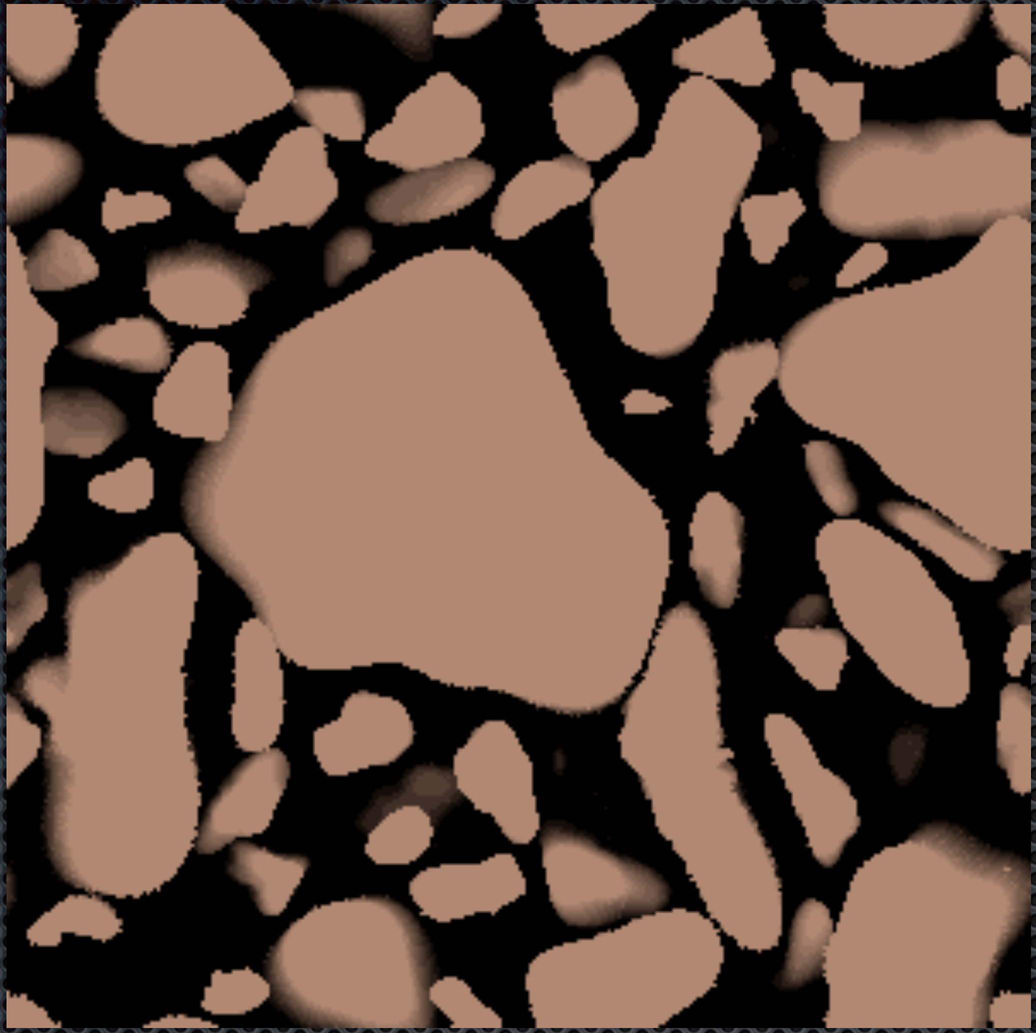
$$Y_n^m(\theta,\phi) = \sqrt{\frac{(2n+1)(n-m)!}{4\pi(n+m)!}} P_n^m(\cos(\theta))\, e^{im\phi}$$

$$a_{nm} = \int_0^{2\pi}\int_0^{\pi} d\phi\, d\theta\, \sin(\theta)\, r(\theta,\phi)\, Y_n^{m*}$$

Solve for SH coefficients, and store in a database for thousands of particles

Retrieve the set $\{a_{nm}\}$ for a given particle shape and choose arbitrary Euler angles θ,ϕ to reproduce the particle using the top equation

3D Particle Shape



Reproduces desired shape distribution

Reproduces desired size distribution

Reproduces desired solid volume fraction, usually to within ± 10^{-4}

Next: Multiphase particles

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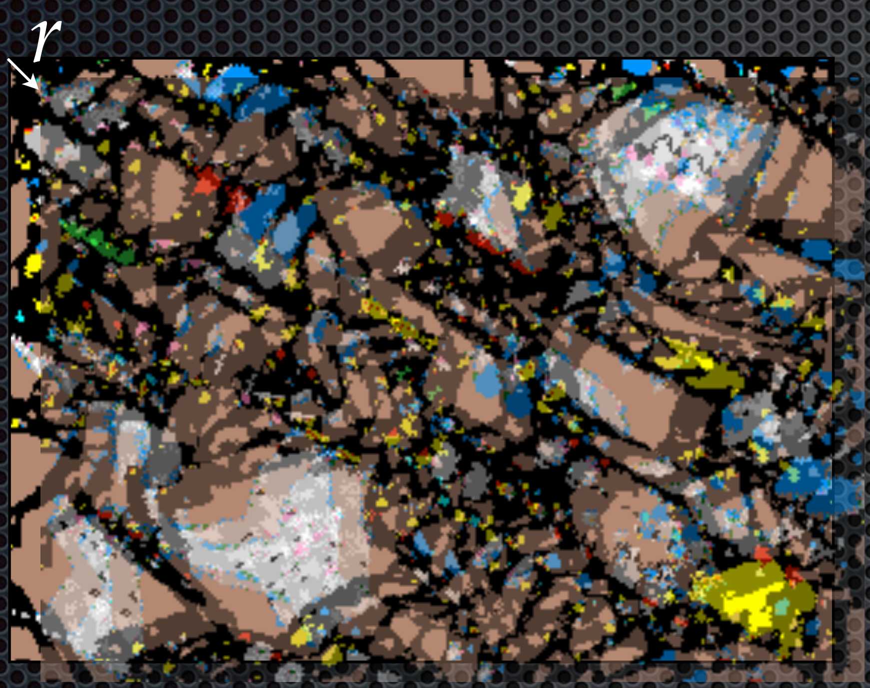
Multiphase Particles

We want to distribute the clinker phases among particles in a spatially realistic way, at least statistically.

To do so, first measure two-point correlation functions on different phases or collections of phases in segmented SEM image:

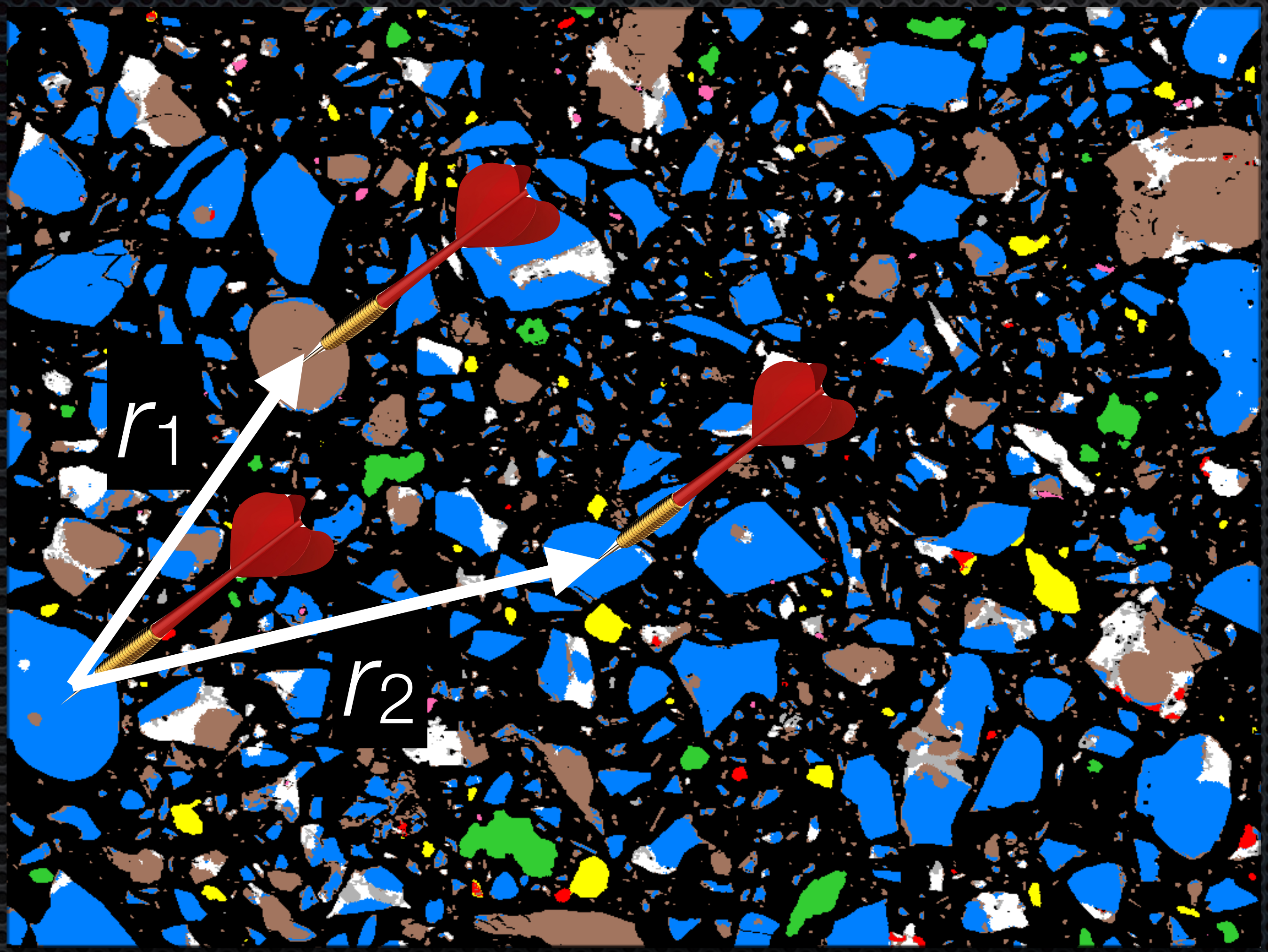


$$S_{2,i}(r) = \int_{-\infty}^{\infty} f_i(x+r)\, f_i(x)\, dx$$

where $f_i(x) = 1$ if phase i is located at x, and $f_i(x) = 0$ otherwise.

Equivalent to overlaying a displaced image on an original and measuring the overlapping areas of the same phase for different displacements.

Multiphase Particles



$S_2(r)$ = Probability that second dart lands in same phase as the first dart

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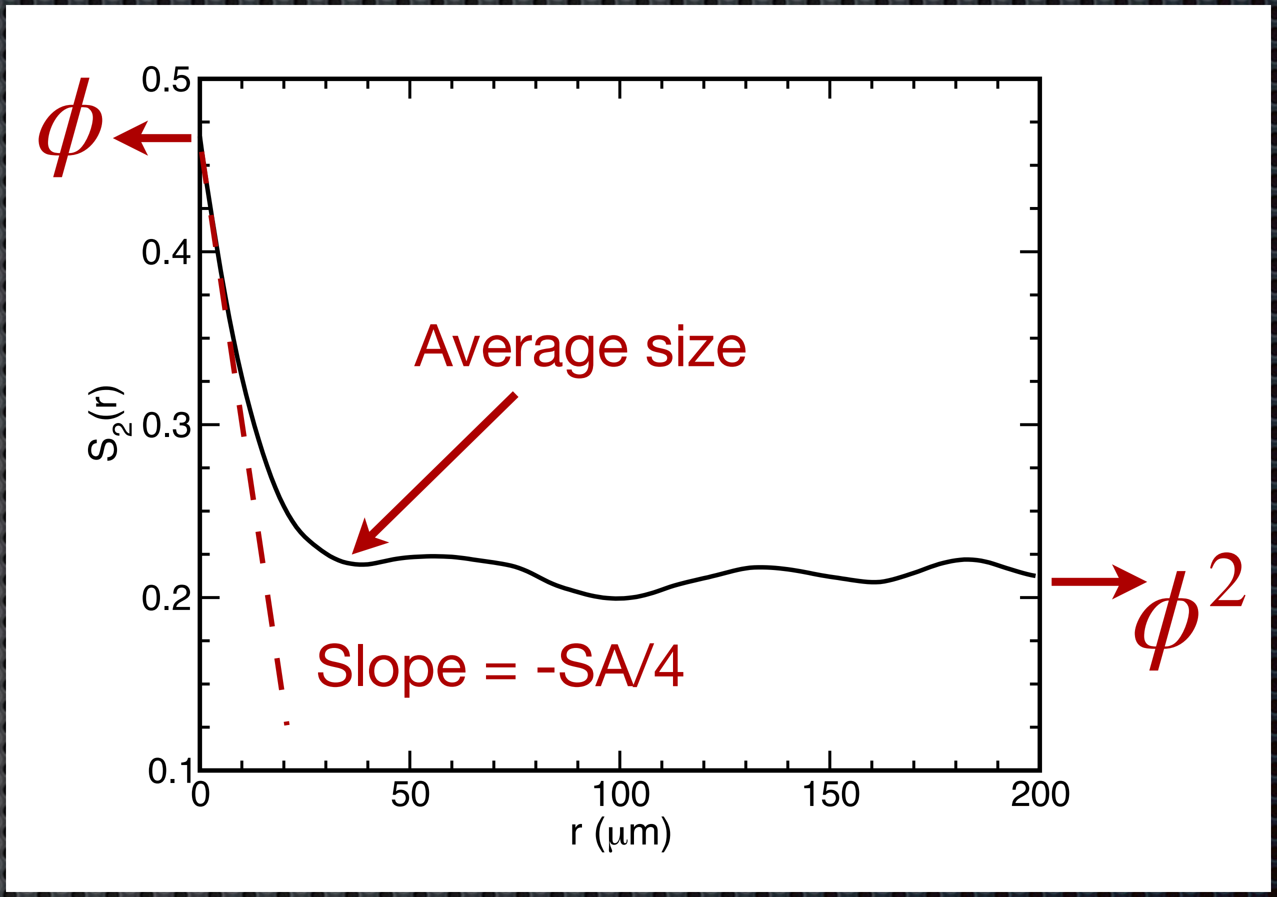
Multiphase Particles

Features of S_2:

- $S_2(0)$ = vol frac
- $S_2(\infty)$ = (vol frac)^2
- Slope at r = 0 is -1/4 of the specific surface area
- First minimum is average domain size
- Is the same in 2D and 3D for homogeneous, isotropic structures!



We can use S_2 measured on 2D images to construct 3D images with the same statistical features

J.G. Berryman and S.C. Blair, *J. Appl. Phys.* **60** [6] 1930-1938 (1986)

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Multiphase Particles

1. Make a 3D box of desired size populated with Gaussian noise
2. Filter the Gaussian noise image with $S_{2,i}(r)$ to create a correlated noise image corresponding to distribution of a phase i
3. Overlay the correlated noise image onto the generic particle image, applying the correlated noise only within the particles (this is done in the distrib3d function of the C program `genmic.c`)

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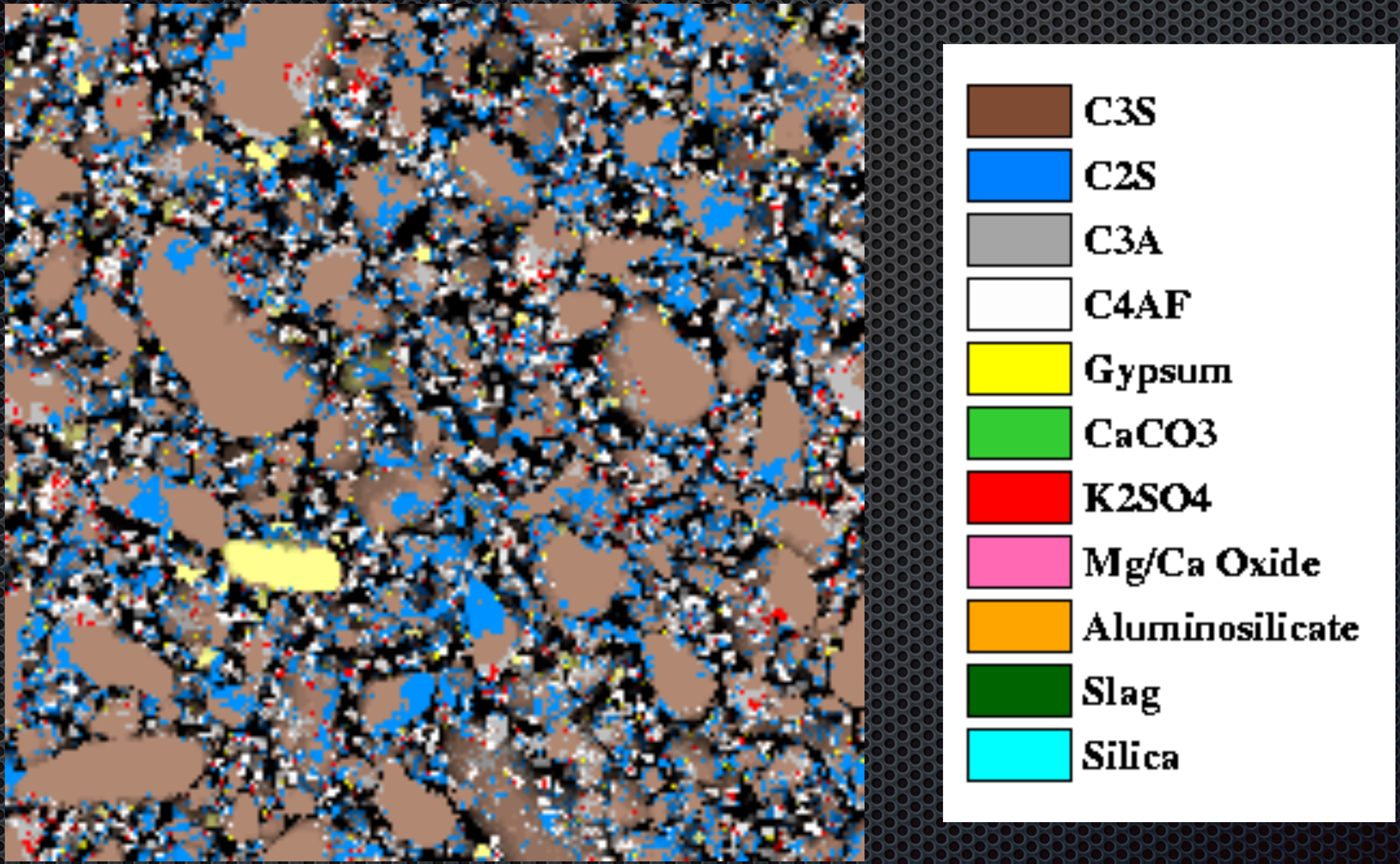
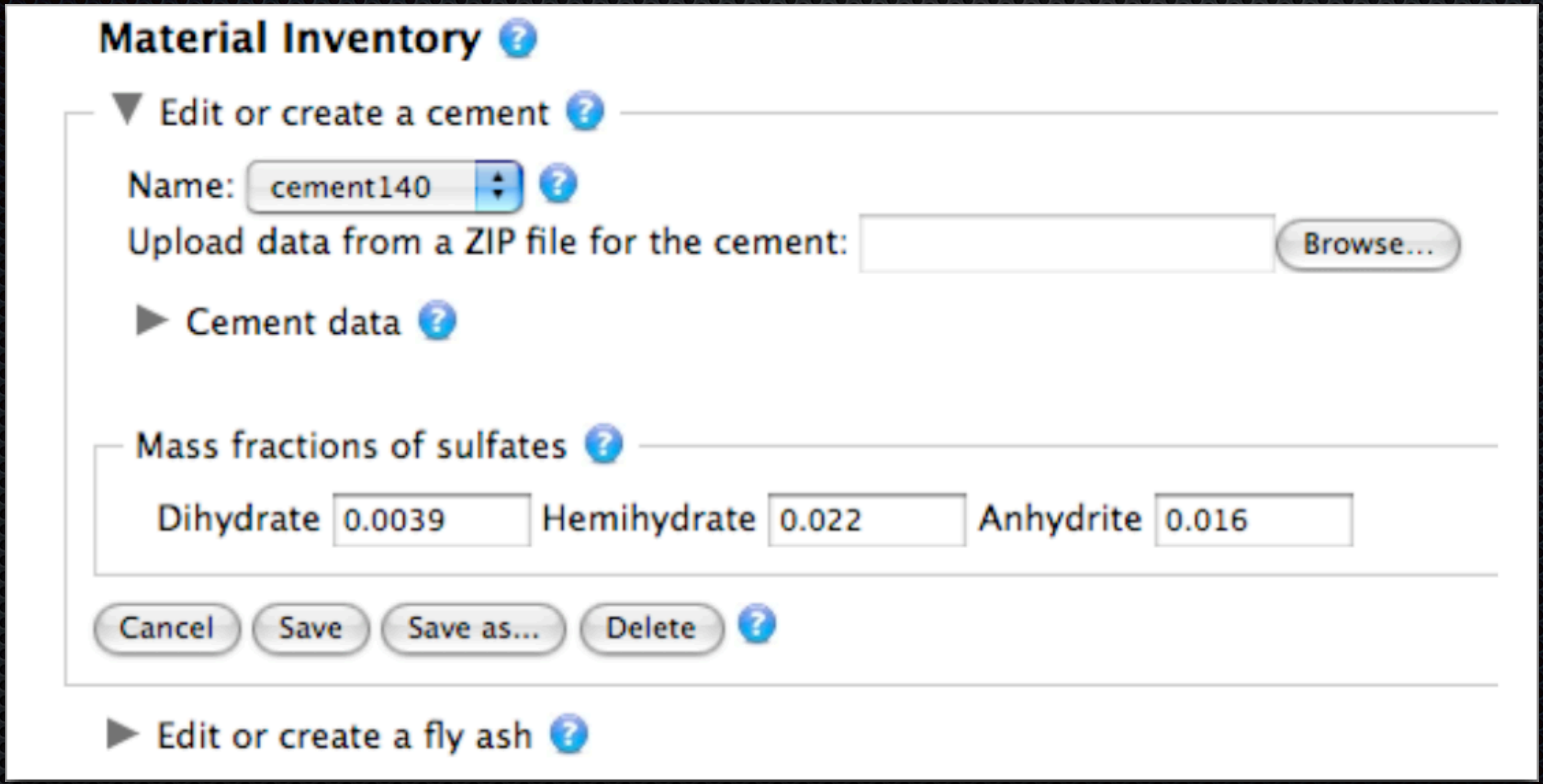
Multiphase Particles

4. Because correlation structure is dependent on which phase is considered, execute the algorithm in five passes:
    a. separate into silicates and aluminates/alkali sulfates, then
    b. separate aluminates and alkali sulfates
    c. separate silicates into C_3S and C_2S, then
    d. separate aluminates into C_3A and C_4AF
    e. separate alkali sulfates into K_2SO_4 and Na_2SO_4
5. After each pass, use a surface smoothing algorithm between the two modified phases until correct surface area is obtained. This is done in the function sinter3d in the C program **`genmic.c`**

Multiphase Particles



VCCTL Software



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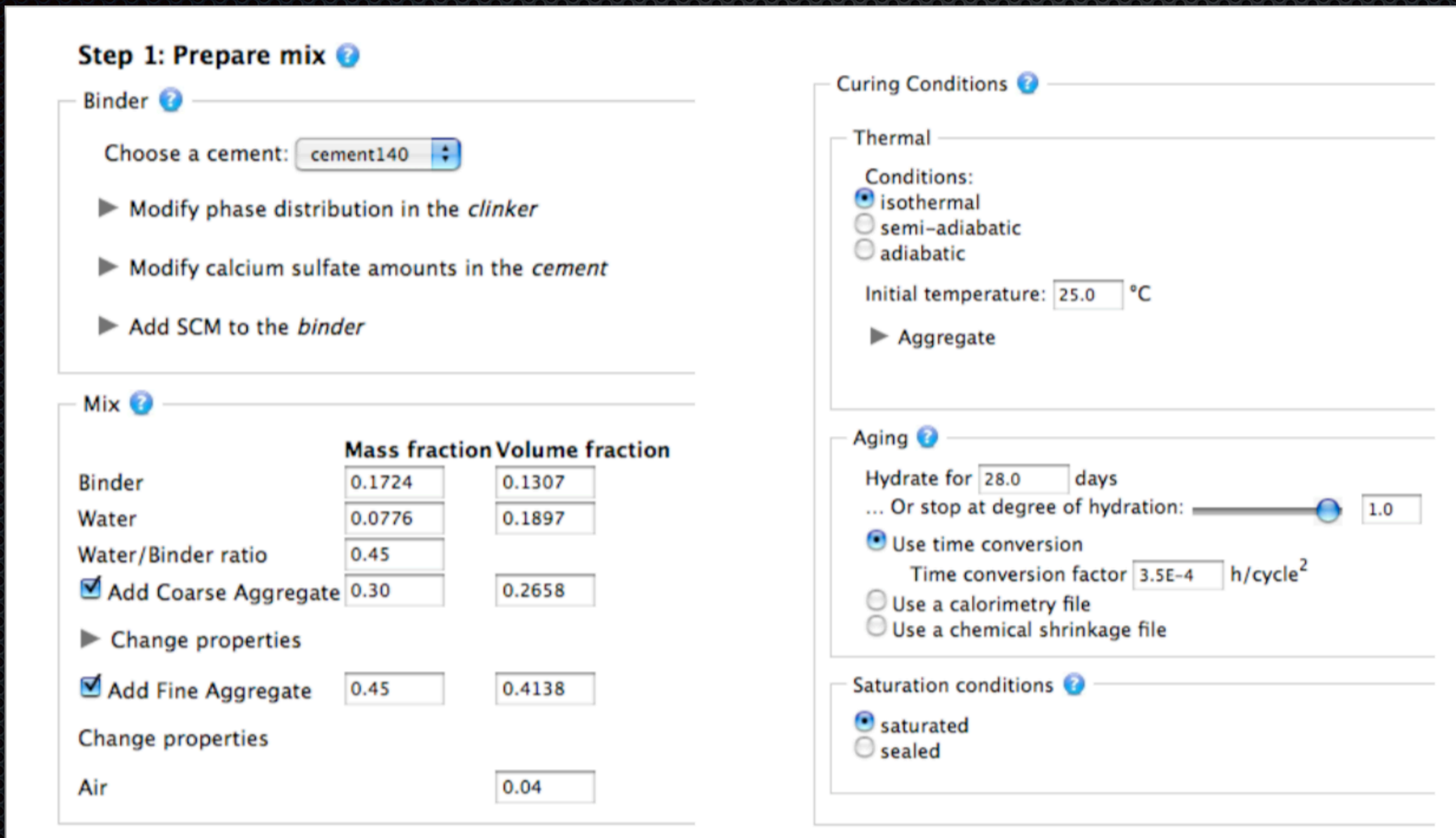
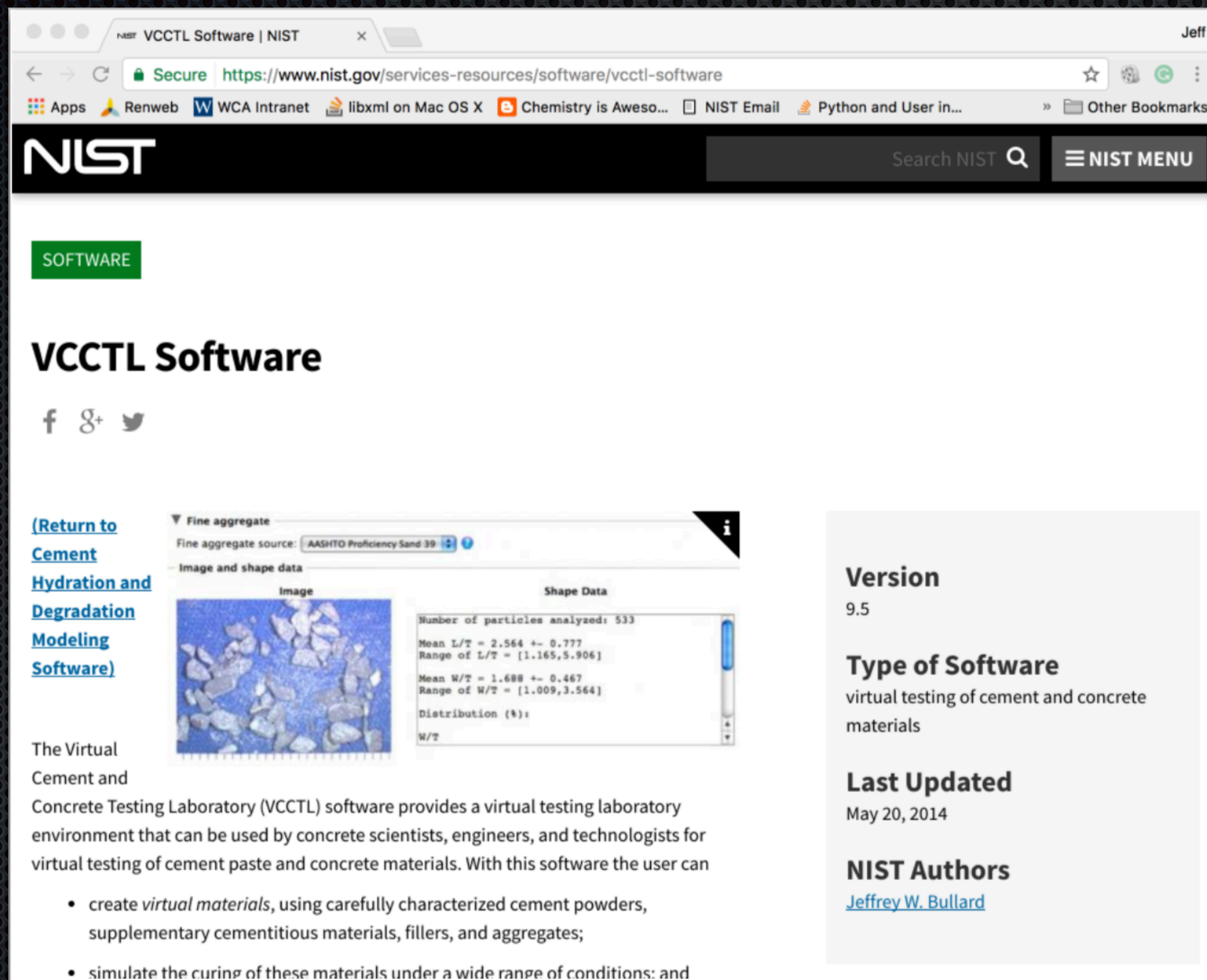
VCCTL Software



VCCTL Software



MicroChar

Analyzing Segmented Microstructure Images

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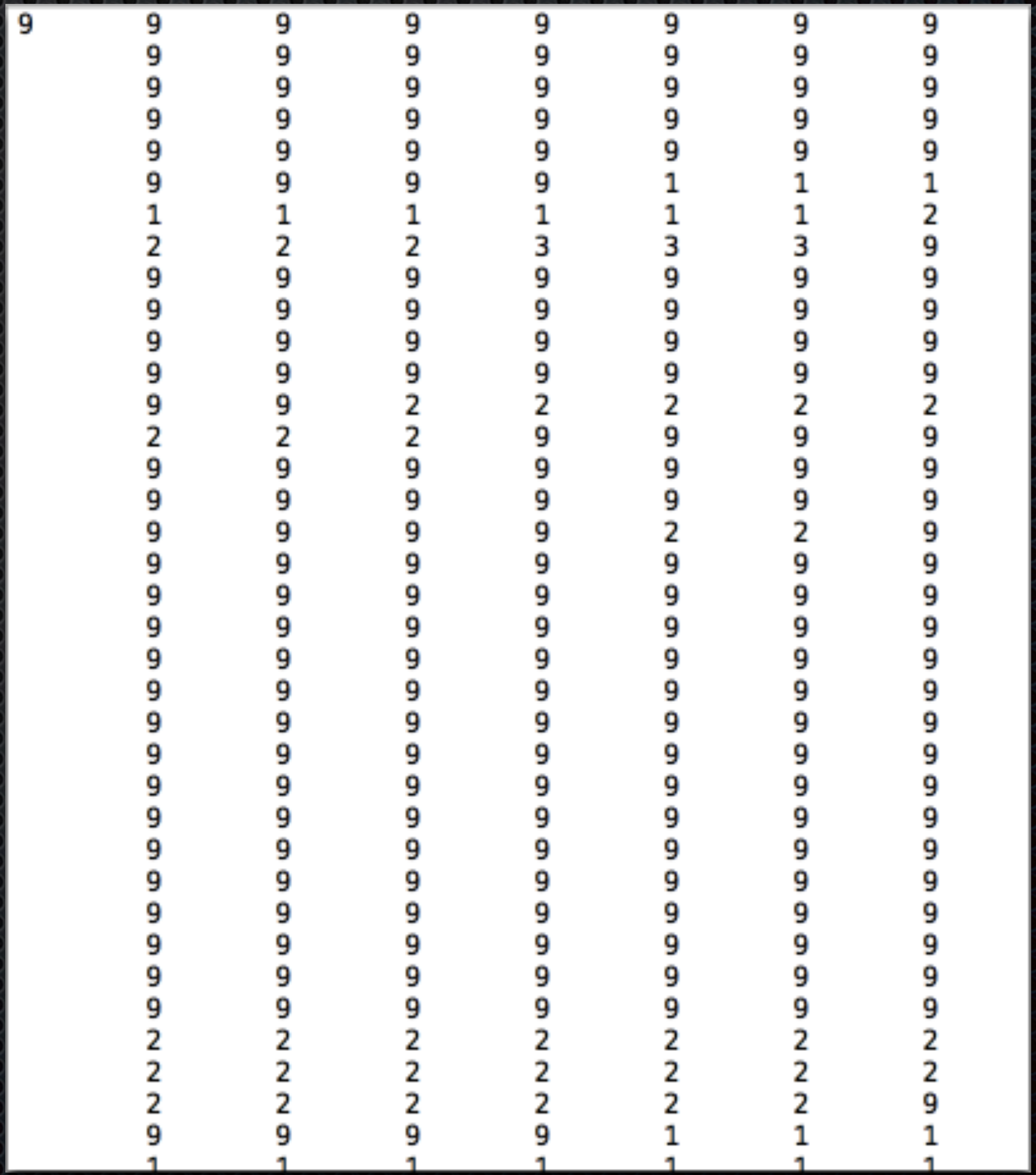
What you need…

- An indexed image of a segmented micrograph (clinker or cement)
- Knowledge of the phase assigned to each index (1 = alite, … 9 = void)



9	9	9	9	9	9	9	9
	9	9	9	9	9	9	9
	9	9	9	9	9	9	9
	9	9	9	9	9	9	9
	9	9	9	9	9	9	9
	9	9	9	9	1	1	1
	1	1	1	1	1	1	2
	2	2	2	3	3	3	9
	9	9	9	9	9	9	9
	9	9	9	9	9	9	9
	9	9	9	9	9	9	9
	9	9	9	9	9	9	9
	9	9	2	2	2	2	2
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	9	9	9	9	9	9	9
	9	9	9	9	9	9	9
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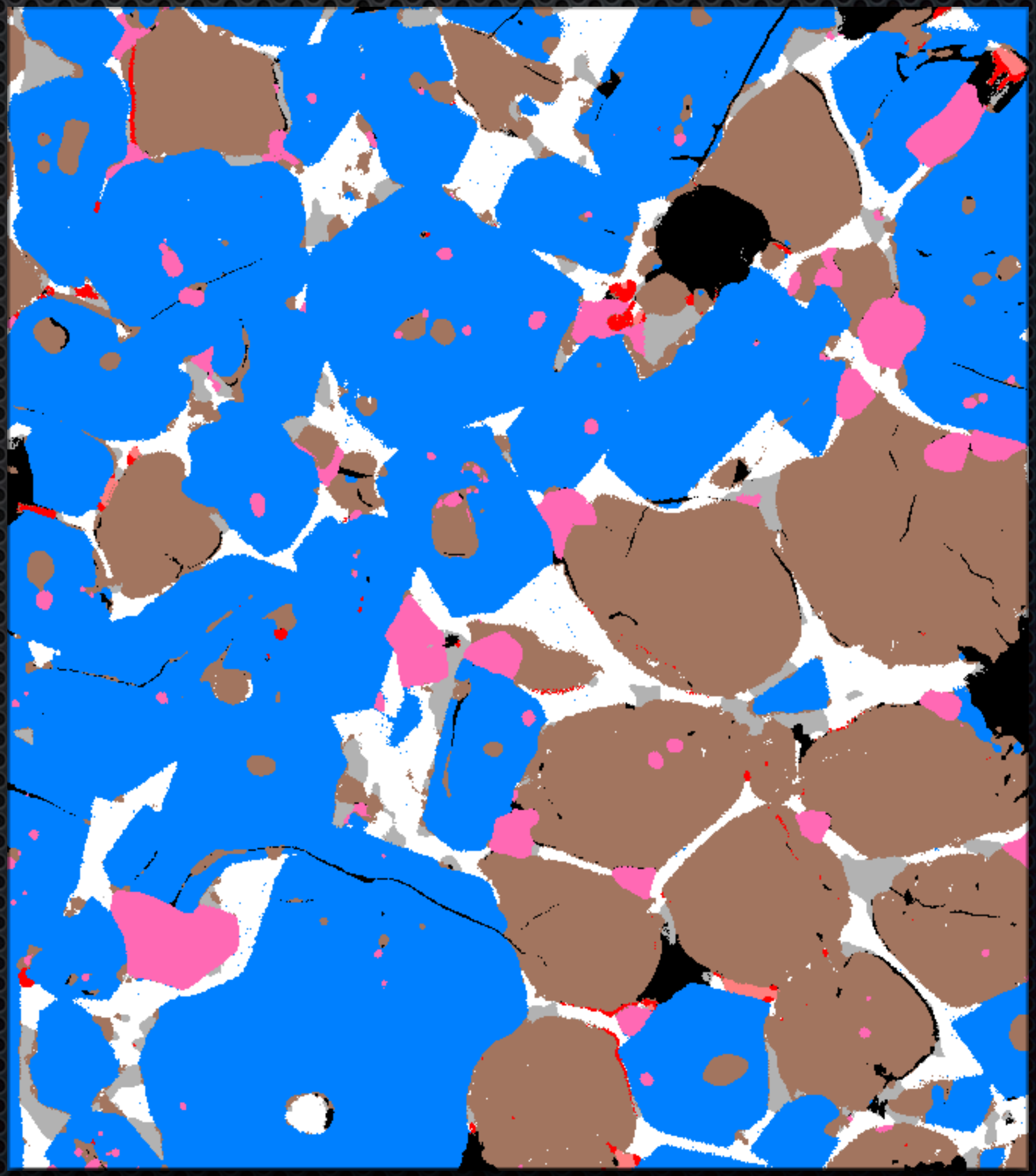
	9	9	9	9	9	9	9
	2	2	2	2	2	2	2
	2	2	2	2	2	2	2
	2	2	2	2	2	2	9
	9	9	9	9	1	1	1
	1	1	1	1	1	1	1

What MicroChar Does (1)

- Removes interior voids and cracks (clinker only)
- Counts pixels to get area of each phase
- Divide counts by total to get *area fraction* of each phase
- Area fraction = *3D volume fraction* if microstructure isotropic



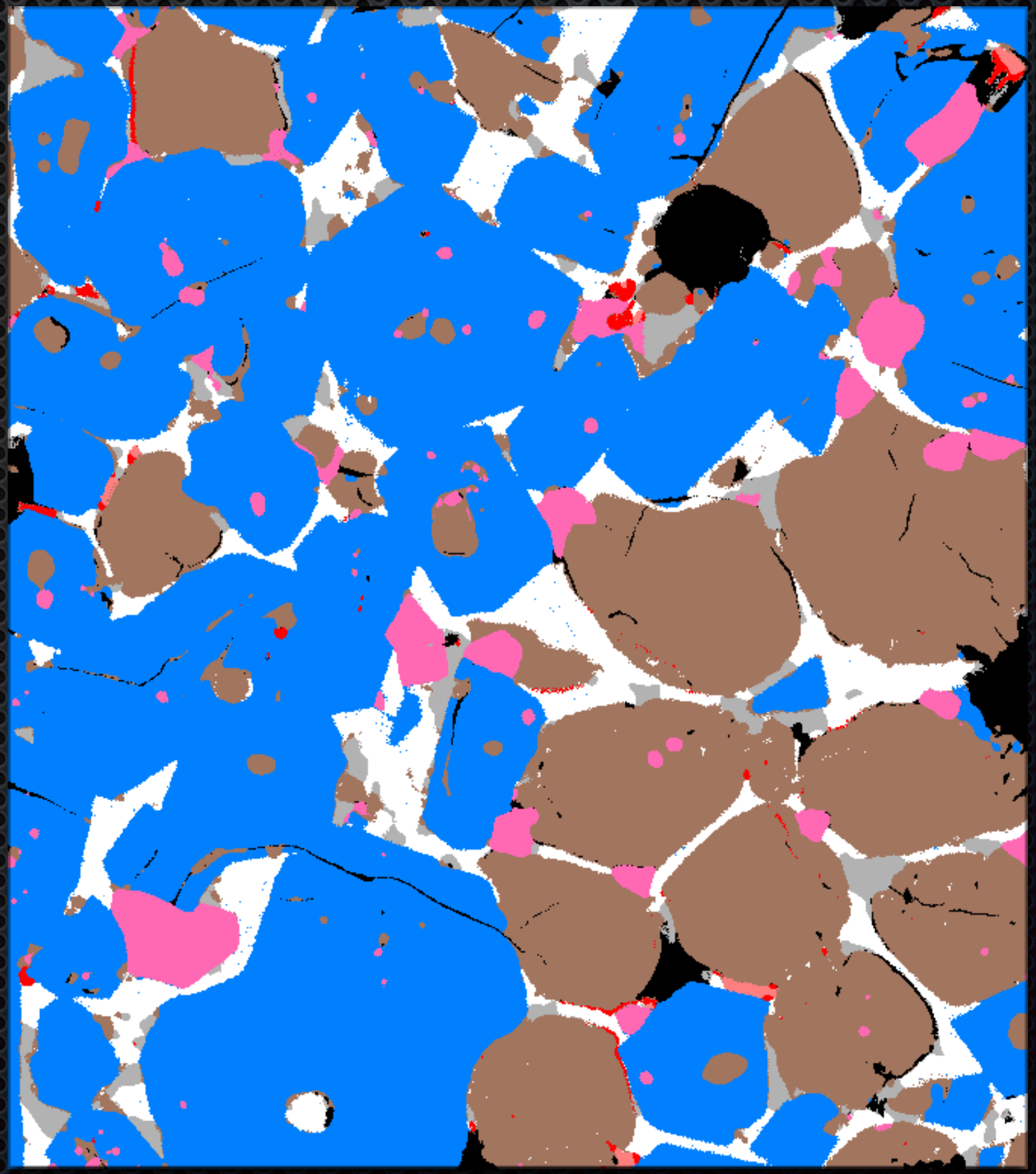
What MicroChar Does (2)

- Multiplies each phase volume fraction by the published value of its density to get *scaled mass*
- Divide each scaled mass by total mass to get phase *mass fractions*

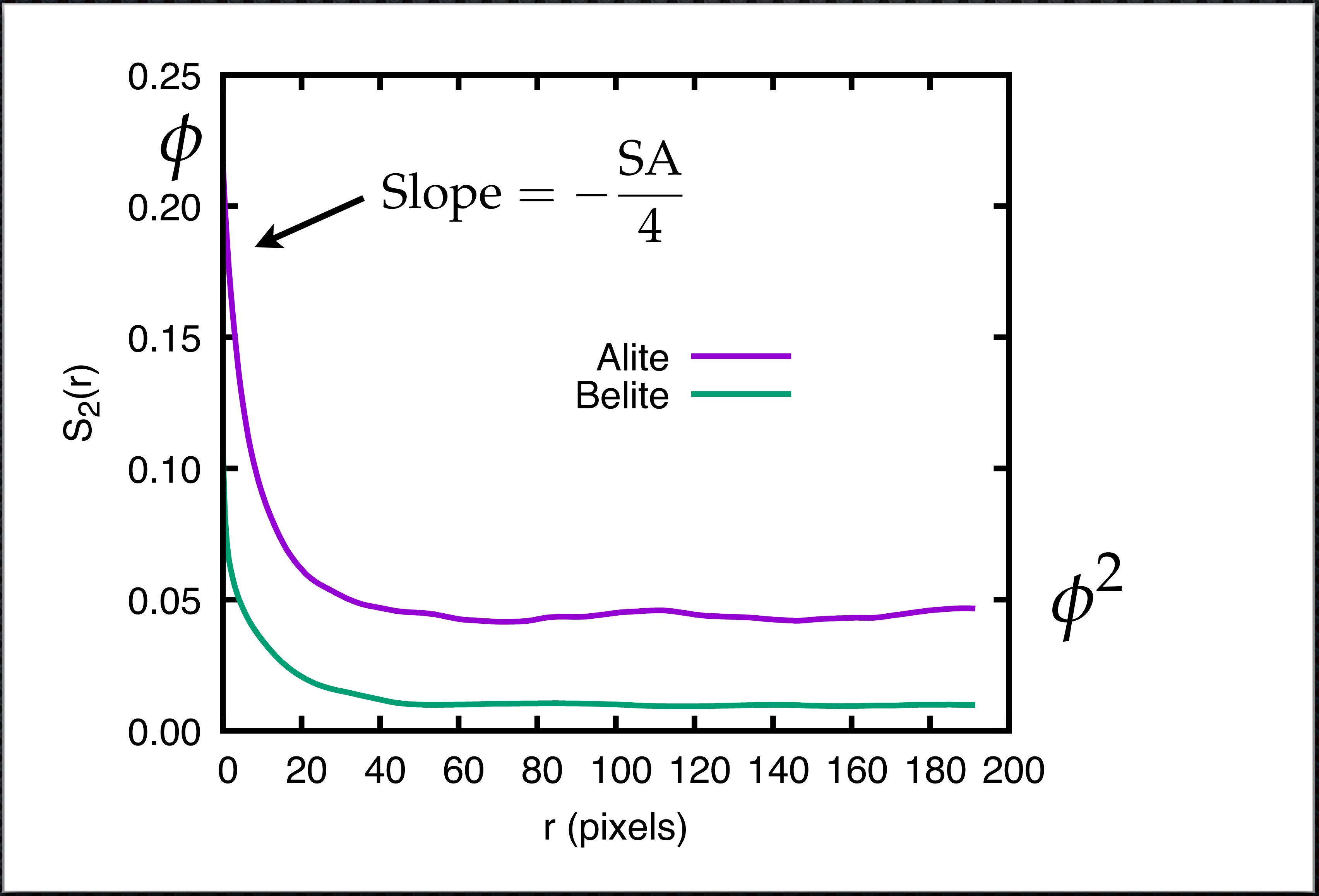
Phase	Formula	Density ($kg\,m^{-3}$)
Alite	C_3S	3210
Belite	C_2S	3280
Aluminate	C_3A	3038
Ferrite	C_4AF	3730
Arcanite	K_2SO_4	2662
Thenardite	Na_2SO_4	2680
Gypsum	$CaSO_4 \cdot 2\,H_2O$	2320
Lime	CaO	3310
Calcite	$CaCO_3$	2710
Periclase	MgO	3780
Am. Silica	SiO_2	2650

What MicroChar Does (3)

- For each phase, count number of its pixels that are next to a different phase (border), to get the phase's scaled perimeter
- Divide each scaled perimeter by the total scaled perimeter to get each phase's *perimeter fraction*
- Perimeter fraction = *3D surface area fraction* if microstructure isotropic



Autocorrelation Functions (Optional)



MicroChar Download