Generation of 2-D Porous Media for a Study of Macroscopic Properties

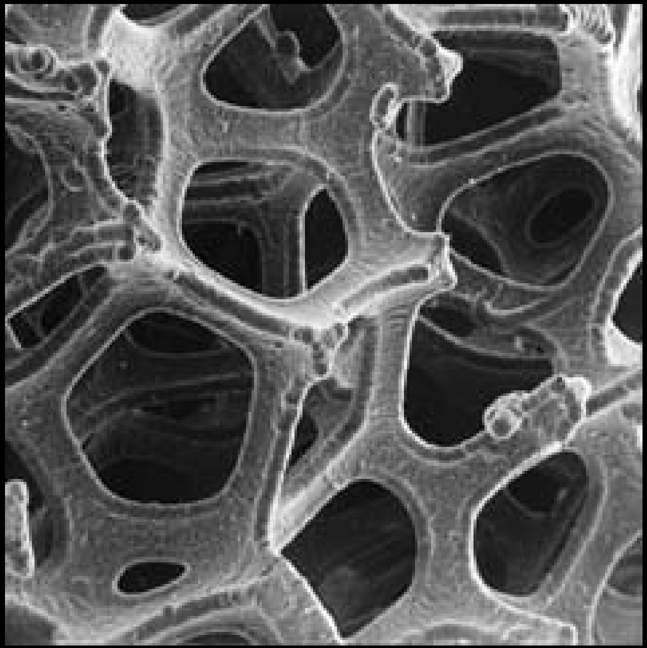
Frank Petruzielo
Advisor – Jerry Seidler

Overview

- Why are porous media interesting?
- What is morphological information and what type of morphological information do we study?
- How do we reconstruct 2-D porous media?
- What insight will studies of the 2-D media give us with respect to macroscopic properties?

Porous Media

- Any solid possessing pore space
  - Foam, soil, bones, and concrete
- We look at a 2-D lattice that consists of two phases
- What can we learn from studying the structure of these materials?

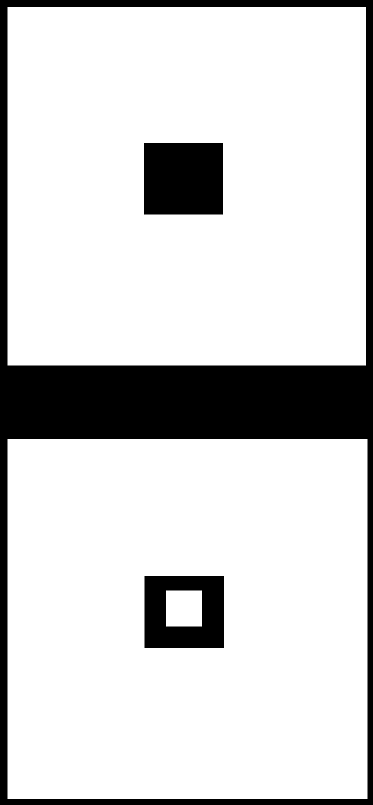


Morphological Information

- Pertains to the physical shape, form, or structure of a substance
- Different measurements include the two-point auto-correlation function, the lineal-path function, the chord-length distribution function and the Minkowski functionals.

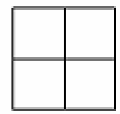
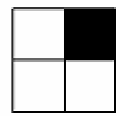
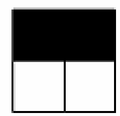
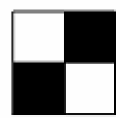
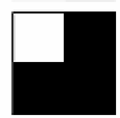
Minkowski Functionals

- For a two-phase material in 2-D, describe the area and Euler characteristic of a particular phase, as well as the boundary length between the two phases



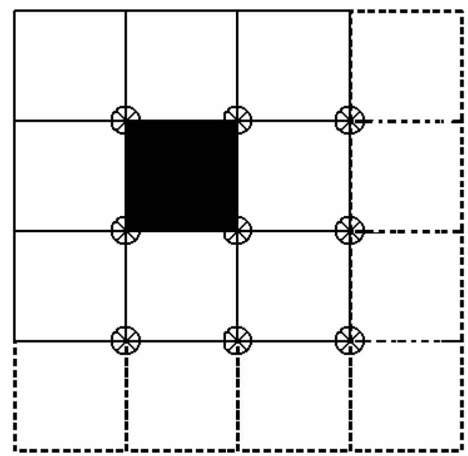
Iterative Calculation of Functionals

- Define some base structure to calculate Minkowski functionals using an additive method
- Correct for over-counting and normalize

	Area	Boundary	Euler
	v_0	v_1	v_2
	0	0	0
	1	2	1
	2	2	0
	2	4	2
	3	2	-1
	4	0	0

Example – Minkowski Functionals

- Totals are consistent with values obtained by visual inspection



	Area	Boundary	Euler
	v_0	v_1	v_2
	1	2	1
	1	2	1
	0	0	0
	1	2	1
	1	2	1
	0	0	0
	0	0	0
	0	0	0
	0	0	0
Sum	4	8	4
Total	1	4	1
Normalized	1/9	4/9	1/9

Reconstructing Two-Phase Porous Media

- Cannot directly generate samples
- Use MCMC method to indirectly generate samples with desired values
  - Gibbs sampler
  - Metropolis-Hastings algorithm

Gibbs Sampler

- Produces sample indirectly when generations from conditional distributions are possible
- Advantages
  - easy to implement
  - convergence guaranteed
- Disadvantage
  - conditional distributions are not always available

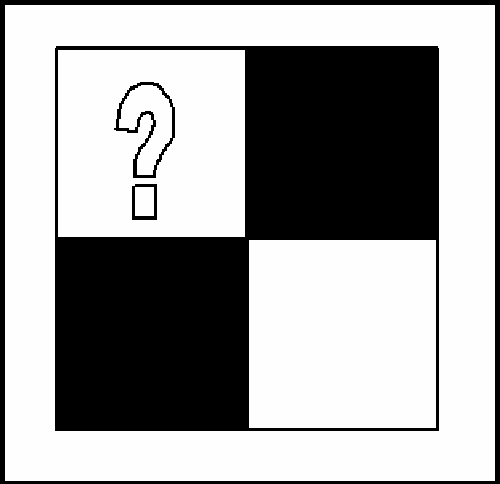
The Specifics

- Want to sample from all structures consistent with a set of functionals
- Consider $\pi(\vec{S})$ and

$$\pi_i(S_i) = \pi(S_i \mid \vec{S}_{-i})$$

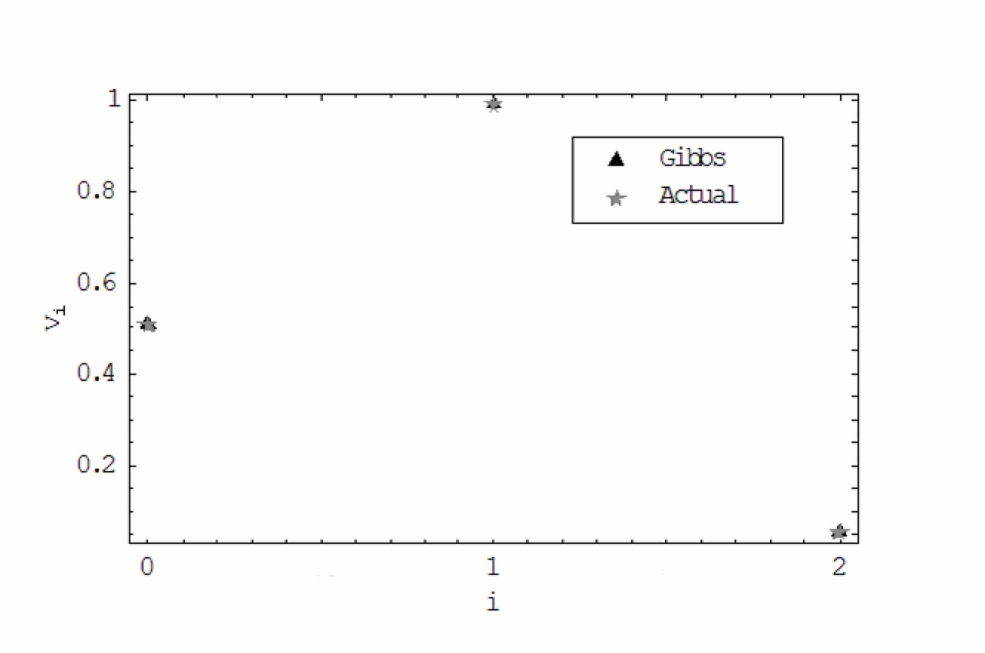
- Assume independence of 2-by-2 structures
- Probability of a point switching to phase one given S_j, S_k is

$$\Pr(p_{r,c} = 1 \mid S_j, S_k) = \frac{s_j}{s_j + s_k}$$



Results of Gibbs Sampler

- Able to reproduce functionals for a random lattice because of independence of lattice points
- Cannot reproduce functionals for a lattice that is not random because of correlations between lattice points

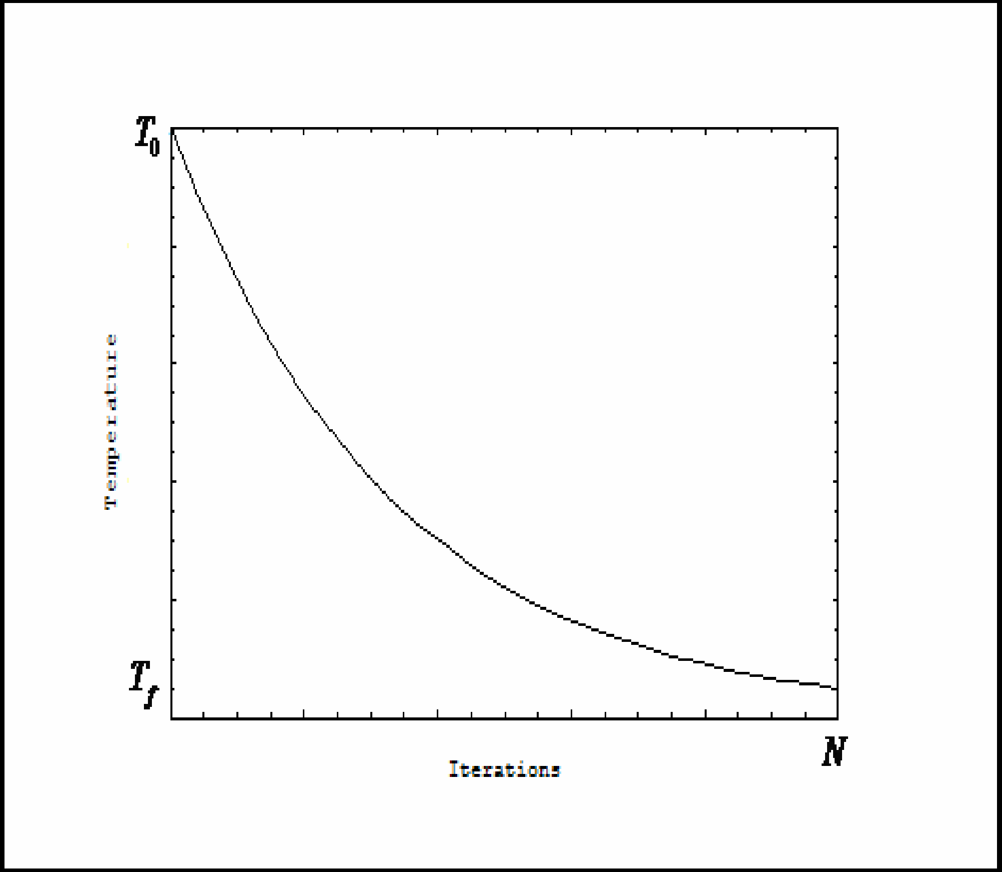


Metropolis-Hastings Algorithm

- Useful when non-iterative method of generating a sample from a distribution is not possible
- Modeled after physically cooling a substance until it is frozen into a state
- Advantages
  - Proven to work well
  - Fairly easy to implement
- Disadvantages
  - Convergence is not guaranteed
  - Many initial parameters

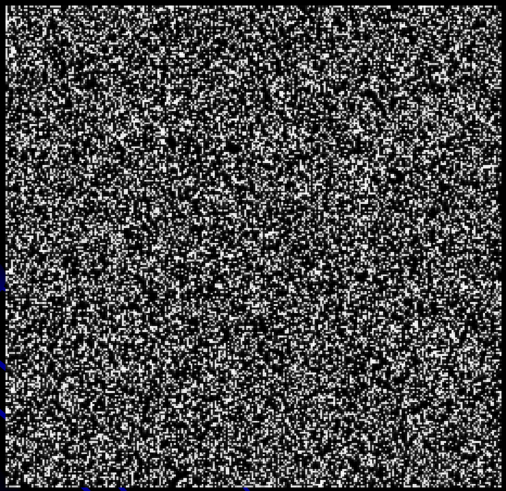
The Specifics

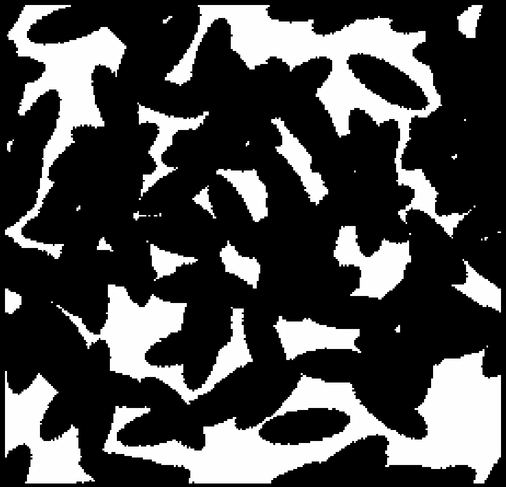
- $E = \sum_{i=0}^{2} (v_i^t - v_i^0)^2$
- $\Delta E = E' - E$
- $\Pr(\Delta E) = \begin{cases} 1, & \Delta E \le 0 \\ \exp(-\Delta E / T), & \Delta E > 0 \end{cases}$
- $T = T_0 \left(\frac{T_f}{T_0} \right)^{(i/N)}$



Results of Metropolis-Hastings Algorithm

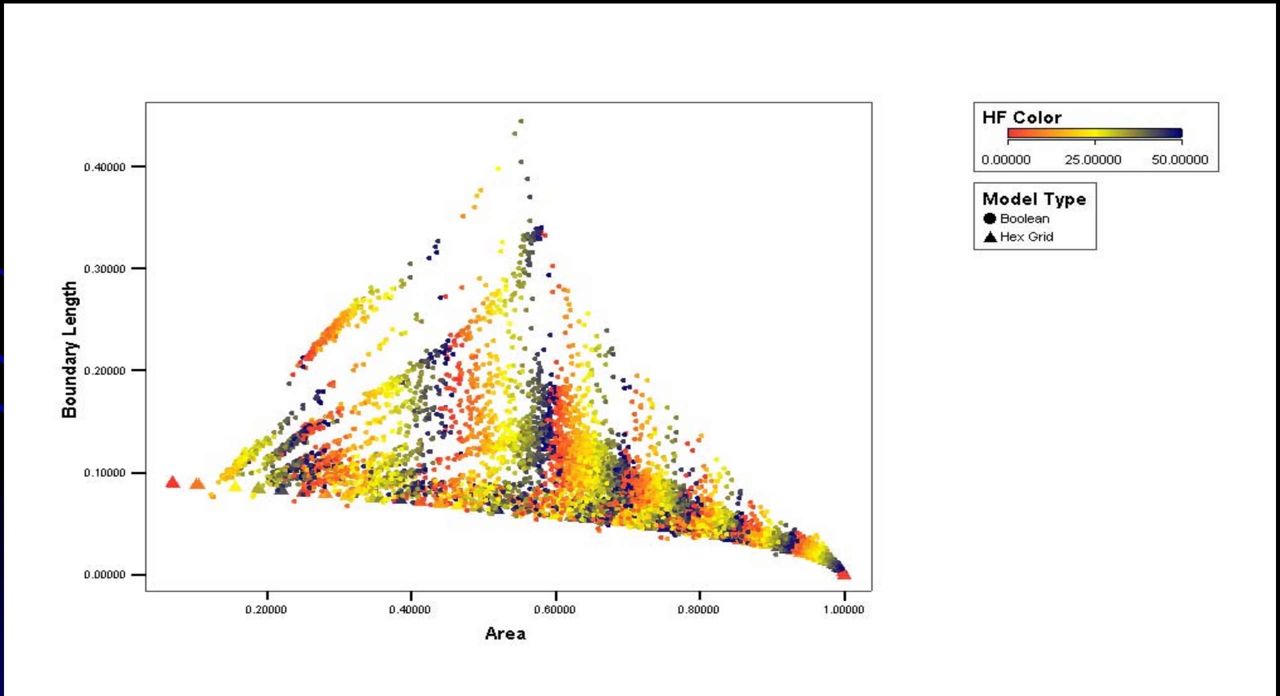
- Works for all possible Minkowski functionals regardless of correlations





Macroscopic Properties

- Can macroscopic properties be determined from limited morphological information?



Conclusion

- Metropolis-Hastings algorithm is effective for producing two-phase porous media in 2-D
- The generation of many samples with an array of values for the Minkowski functionals will enable the evaluation of the hypothesis driving this work

References and Acknowledgments

- 1. C. H. Arns, M. A. Knackstedt, and K. R. Mecke, Phys. Rev. Lett. **91,** 215506 (2003).
- 2. B. Lu and S. Torquato, Phys Rev. A **45,** 922 (1992).
- 3. S. Torquato, Phys. Rev. E **47,** 2950 (1993).

- I would like to thank Jerry Seidler for being such a helpful mentor and for coordinating the REU program
- I would like to thank Jake Englund and David Wu for their contributions to this project