Goal: Stochastic reconstruction of porous media from 2-D images to match the macroscopic flow/transport properties of the physical material sample whose 2-D images were used.

1) Which specific flow/transport properties need to be matched ? 2) Use sensitivity analysis or any other means to check how specific flow/transport properties depend on different microstructural descriptors. Involves doing fluid simulation. 3) If possible, To establish a link between the microstructural descriptors and the macroscopic properties. 4) Representative elementary volume 5) efficient method to generate random structures based on certain microstructural descriptors. 6) Get the actual information content (physical meaning) from each microstructural descriptor.

Steps:

- Study different microstructural descriptors - learn what we can learn from them.
  - Have a base library of structures to check the influence of these descriptors.
    - What kind of structures do we want to have - ellipses, circles, completely random, ... ?
  - Check and record the application of all of these descriptors on each of these structures.
  - Get the understanding as to what kind of features are captured by each of the descriptors.
- In parallel, determine which flow properties need to be matched.
- Study methods to construct random structures based on specific microstructural descriptors.
  - If possible, make a more efficient method.
- Generate structures with this chosen reconstruction method and perform fluid simulation.
  - In parallel, find the specific fluid properties that need to be matched.
  - Identify the structural parameters on which these fluid parameters depend like surface area, volume fraction of porosity etc. and then determine which micro-structural props. are important to capture these parameters.
- Check how the simulation outputs vary for structures based on the identified structural parameters.

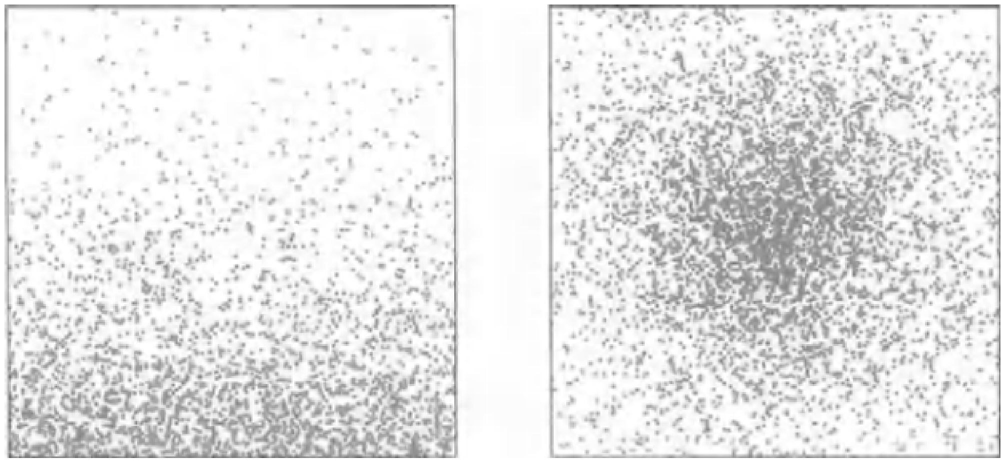

Figure 1: 2 cases of non homegenity [Torquato]

1 Random structures classification

- Statistically homogeneous - n point correlation functions are not dependent on the absolute positions but only relative positions. Fix the origin at say bottom left and check n-point correlation functions for different parts of the image. They must be same for all the parts.
- Statistically isotropic - S_2 can be obtained by averaging random lines from your 3-d image (if line is sufficiently large) and S_3 can be obtained by averaging random planes from your 3-d image. Rotate the image and the n-point correlation functions must be the same for all angles of rotation.

2 Microstructural descriptors

Attempting to capture the microstructural features such as phase volume fractions, surface areas of interfaces, orientations, sizes, shapes, spatial distribution of the phase domains and connectivity of the phases etc.

- Random media of arbitrary microstructure
  - N-point probability functions: Statistically describe the microstructure. Corners of a n-cornered polygon randomly tossed lie in a given phase.
    - Derivative of 2 point correlation function as r tends to zero is proportional to the specific surface for 3d (pore-solid interface area per unit volume) if image is isotropic.

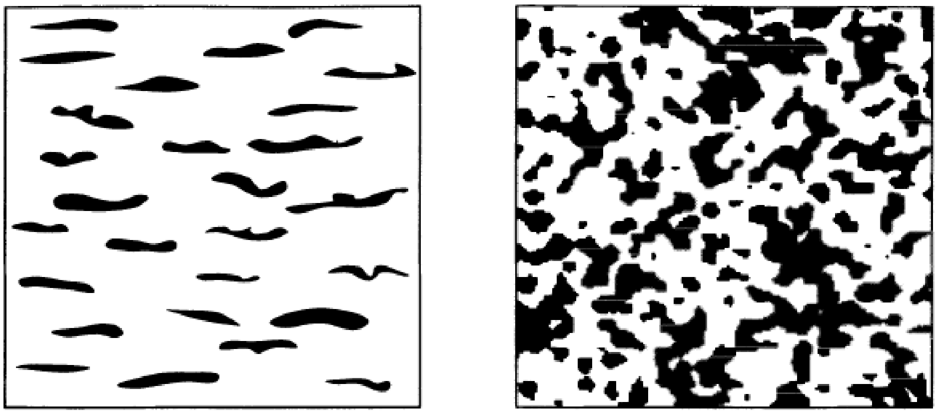

Figure 2: Non isotropic versus isotropic media [Torquato]

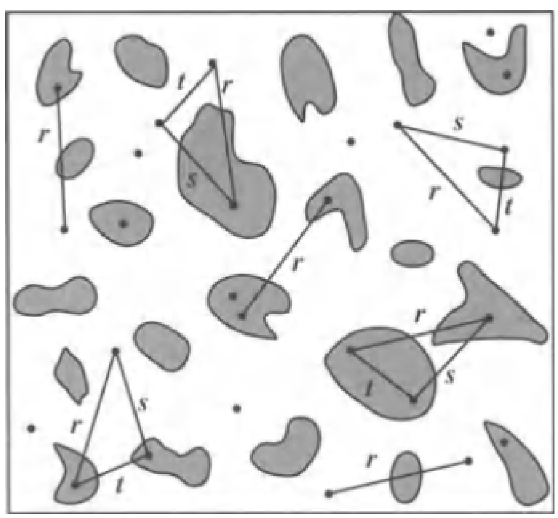

Figure 3: 1,2 and 3 point correlation functions [Torquato]

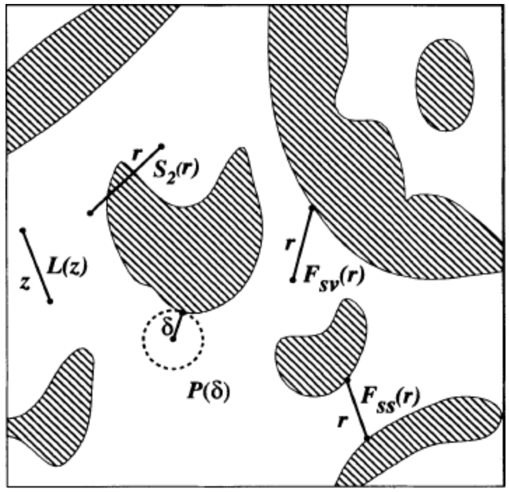

Figure 4: Pore size distribution and surface correlation functions [Torquato]

$$\left.\frac{dS_2}{dr}\right|_{r=0} = \begin{cases} -\frac{s}{2}, & d=1 \\ -\frac{s}{\pi}, & d=2 \\ -\frac{s}{4}, & d=3 \end{cases}$$

- surface correlation functions: Surface correlation functions contain information about the random pore-soild interface and are of basic importance in the trapping and flow problems. It gives us info. on the spatial arrangement of the interface with respect to itself and also the spatial arrangement of the interface with respect to one of the phases (By surface-surface and surface-void correl funcs)
  * Surface correlation function gives information on the interface. You have surface-surface and surface-void correlation functions (surface (actually boundary line in 2-d and surface in 3-d) here means the interface between pore and solid).
- lineal-path function - L(z) - probability that an entire line segment of length z lies within a given phase when randomly thrown in a sample.
  * Gives the connectedness information along lines.
  * L(0) gives the porosity
  * Tail of z gives the information on the largest lines in the image.
- chord-length density function
  * lines from interfaces to interfaces
- pore-size functions

    * the probability of inserting a sphere/circle (2d/3d) of radius δ into the system $P(\delta)d\delta$
    * Pore size function for a 3D system cannot be obtained from a 2D system like in the previously defined micro-structural descriptors.
    * Gives crude information on 3D connectedness for a given phase.
  - Percolation and cluster functions such as the 2 point cluster function C_2. Corresponds to S_2 but both points must lie in the same cluster.
    * Cluster function for 3D cannot be found using 2D images as it is intrinsically a 3D property.

- Random particle dispersions (Particles of one phase randomly dispersed in another phase like platelet cells in blood)
  - nearest-neighbor functions
  - point/q-particle correlation functions
  - surface-particle function
- Other microstructural descriptors
  - Minkowsky functionals
  - D34 descriptor
  - Entropy descriptor

3 Stochastic reconstruction

Currently two methods:

- Joshi, Quibler and Adler approach - Gaussian random field based reconstruction technique. To reconstruct realizations of statistically homogeneous and isotropic random media from the associated two-point correlation functions [En-Yu Guo, 2013].

  Other related methods are "phase recovery method" (Based on a vector of 2 point correlation functions for each phase in a multi-phase heterogeneous material), multi-point method (to use all n-point correlation functions to reconstruct a portion of the image (size of this portion is obtained from the correlation length calculation)), Raster-path method makes the multi-point method more efficient.
  - Well studied
  - Less computation cost
  - Only reproduce S_2 and porosity.

- Stochastic optimisation technique (Rintoul and Torquato 1997b, Yeong and Torquato l998a)

  Other related methods are the dilation erosion method (to achieve required connectivity in filamentary structures with just using S2 function thereby improving computational time but retaining connectivity info), multi-grid hierarchical nearest neighbour based reconstruction, object swapping method using an initial grain size distribution instead of porosity and using only S_2 to perform reconstruction.

  – Can reproduce as many micro-structural descriptors as needed.
  – High computational cost.

4 References

4.1 Estimating effective material properties of random media

- Transport - Diffusion coefficient (Brown 1955, Prager 1963b, Beran 1968, Torquato 1980, Milton 1981a, Phan-Thien and Milton 1982, Torquato 1985a)
- Effective elastic moduli (Beran 1968, McCoy 1970, Dederichs and Zeller 1973, Kroner 1977, Willis 1981, Milton 1982, Milton and Phan-Thien 1982, Torquato 1997)
- fluid permeability (Prager 1961, Weissberg and Prager 1970, Berryman and Milton 1985, Rubinstein and Torquato 1989)

4.2 Microstructural descriptors

- General properties of microstructures - (Frisch and Stillinger (1963) and Torquato and Stell (1982, 1983a))