Technische Universität Braunschweig

Master's Thesis Proposal

Stochastic reconstruction of porous media from 2D images

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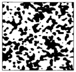
Part I

Introduction

Goals

- To statistically characterise the geometry of the porous material's microstructure. For example, to capture from the 2D images
  - Pore size distribution
  - Clustering/connectedness
  - Pore-solid interface curvature
- To reconstruct the porous material in 3D based on the microstructural descriptors obtained in the above step
- To obtain effective physical properties (such as permeability) of the reconstructed material by performing flow simulation and to compare it with that of the original material



[Torquato, 2013]

Motivation I

- The geometry of the microstructures of porous materials is random in nature (nature of the manufacturing processes - Chemical Vapour Deposition and Freeze Casting, random natural processes - rocks, soil etc.)
- Effective material properties such as structural and flow properties etc. depend on the material's microstructure
- Longstanding goal is to establish relationships between specific geometrical features of the microstructure and particular effective properties of the material

Motivation II

This thesis aims to help in addressing this longstanding goal through the following

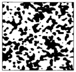
- Generating via computer random structures of porous media, which are statistically similar to physical samples, for use in computer simulations
- Establishing, with the help of these simulations, a link between the effective properties such as permeability, conductivity etc. of a porous medium and it's microstructure

Part II

Literature Review

Microstructural descriptors I

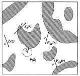
- These descriptors attempt to capture the following features in a microstructure
  - Shapes
  - Sizes of these shapes
  - Spatial distribution
  - Connectivity



[Torquato, 2013]

Microstructural descriptors II

- List of descriptors
  - N point correlation functions
    - N cornered polygon randomly tossed into the structure
    - Spatial arrangement of the structure
  - Surface correlation functions
    - surface-surface and surface-void
    - Spatial arrangement of the solid-pore interface with respect to itself and the interface with respect to the void
  - Lineal path function L(z)
    - Random lines tossed into the structure that lie wholly within a given phase
    - Crude information on connectedness (for different lengths of lines)
    - Tail of L(z) gives information on the largest features of the image corresponding to a particular phase



[Torquato, 2013]

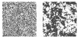
Microstructural descriptors III

- Chord length density function
  - Lines from one point in the interface to another such that the lines are wholly within a single phase
  - Crude information on connectedness as in the lineal path function
  - Crude information on sizes of a given phase
- Pore size function
  - The Probability $P(\delta)d\delta$ of inserting a sphere/circle of radius (δ) into the structure in a given phase
  - Pore size function for a 3D structure cannot be obtained from a single 2D image unlike the previously mentioned descriptors
  - Crude information on connectedness of a given phase
- 2 point cluster function
  - Same as 2 point correlation function but with the additional requirement that both the points must lie within the same cluster
  - Provides information on connectivty

Microstructural descriptors IV

- 2 point cluster function for a 3D structure cannot be obtained from a single 2D image

- Minkowsky functionals for 2D (d+1 functionals)
  - $M_0 = \int_A d^2r$ gives volume fraction of a given phase
  - $M_1 = \frac{1}{2\pi} \int_{\partial A} dr$ gives total perimeter of the interface
  - $M_2 = \frac{1}{2\pi^2} \int_{\partial A} \frac{1}{R} dr$ gives the Euler characteristic which gives information on the connectedness of the structure
- Entropy descriptors
  - Entropy $S(\kappa) = k_b \ln \Omega(\kappa)$, where $\omega = \prod_{i=1}^{\chi} \binom{k^2}{n_i}$



[Torquato, 2013]

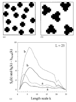
Microstructural descriptors V

- Spatial inhomogeneity measure

$$S_\Delta(\kappa) = \frac{S_{max}(\kappa) - S(\kappa)}{\kappa}$$

- Spatial complexity measure

$$C_\lambda(k) = \frac{[S_{max}(\kappa) - S(\kappa)][S(\kappa) - S_{min}(\kappa)]}{\kappa[S_{max}(\kappa) - S_{min}(\kappa)]}$$



[Piasecki, 1999]

Reconstruction methods

- Truncated Gaussian fields
  - Quick reconstruction
  - Can reproduce only the two point correlation function and the volume fraction
- Simulated annealing with random pixel swapping
  - Can reproduce any number of correlation functions
  - Slow as all the correlation functions need to be recomputed after each swap
  - Related methods include
    - Simulated annealing with object swapping instead of pixel swapping
    - Multi-grid hierarchical nearest neighbor based reconstruction
    - Multipoint statistics method
    - Dilation erosion method
    - Hybrid stochastic optimisation tool (genetic algorithm, simulated annealing and tabu-list)

State of the art: Reconstruction studies I

- Reconstructions based on different combinations of descriptors
  - S_2 and $L(z)$ versus S_2 and $P(\delta)$ [Manwart, 2008]
    - Both the combinations give similar information with respect to total fraction of percolating cells (probability of finding a cell of given length and porosity that is percolating in all three directions) and mean survival time.
    - $L(z)$ and S_2 combination reproduces $P(\delta)$ too.
    - Connectivity (total fraction of percolating cells/local percolation probability (probability of finding a cell of given porosity that is percolating in all three directions) and permeability (function of porosity, mean survival time and fraction of percolation cells)) is not reproduced for both combinations. The combinations give around 50% percolating cells fraction but original structure is fully (99%) percolating.

State of the art: Reconstruction studies II

- S_2 versus S_2 and $L(z)$ versus S_2 and $C(z)$ [Pant, 2016]
  - Effect of the above descriptors/combinations on diffusivity
  - Diffusivity is the rate of diffusion (movement of particles/heat/fluid due to a concentration gradient)
  - Diffusivity depends on porosity (was the same in reference and reconstructed images), bulk diffusivity (was treated as a constant) and tortuosity.
  - Diffusivity was found to depend on S_2 but S_2 cannot characterise diffusivity alone.
  - Diffusivity estimates improved both when $L(z)$ and $C(z)$ was used in addition to S_2 for reconstruction but only slightly.
  - Weak dependence of diffusivity on both $L(z)$ and $C(z)$. Expected as $L(z)$ and $C(z)$ give connectivity only along lines and not along curves.
- M_n versus $C(z)$ versus M_n and $C(z)$ [Vogel, 2010]

State of the art: Reconstruction studies III

- C2 and local percolation probability was relatively better b/w reconstruction and reference images for the case of $M_n andC(z)$ reconstruction and was very bad while using either of them alone
- Transport reproduction (in terms of breakthrough curve) was very good for the case of M_n and $C(z)$ and were slightly worse when either of them were used alone
- Transport properties were predicted almost perfectly even though C_2 and local percolation probability weren't a perfect match because the evaluated transport properties are not affected by small gaps in connectivity in the longer ranges.
- Long range connectivity will be important for predicting a property like permeability but it is not so important to predict the evaluated transport properties.

State of the art: Reconstruction studies IV

- Different reconstruction methods
  - Simulated annealing with object swapping instead of pixel swapping [Diogenes, 2009]
    - Object swapping using S_2 and a given pore size distribution was compared to pixel swapping using S_2, $C(z)$ and grain size distribution.
    - The resulting reconstructions were compared to check S_2, connected porosity (excluding porous areas which don't percolate), grain size distribution and permeability.
    - The object swapping method produced images with good connected porosity and permeability (for low porosity images) even though no connectivity related information was used during the reconstruction and it is faster than the pixel swapping method.

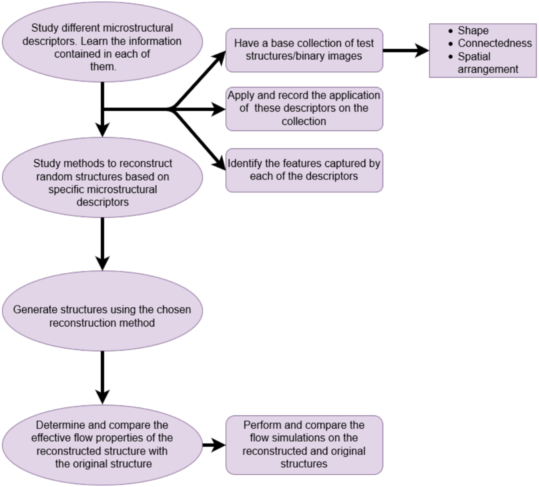
State of the art: Reconstruction studies V

- Dilation erosion method
  - S_2, L(z) and C_2 with simulated annealing is compared to S_2 with dilation-erosion
  - Dilation erosion is able to reproduce almost the same S_2, L(z) and C_2 even without using L(z) and C_2 during the reconstruction.
  - This works for filamentary structures only. It increases the probability of obtaining a percolating structure even though it is filamentary. Without dilation-erosion, this probability would be reduced.
  - Dilation thickness is arbitrary.

Part III

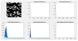
Approach

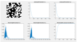
Approach


Study different microstructural descriptors. Learn the information contained in each of them.
Have a base collection of test structures/binary images
• Shape
• Connectedness
• Spatial arrangement
Apply and record the application of these descriptors on the collection
Identify the features captured by each of the descriptors
Study methods to reconstruct random structures based on specific microstructural descriptors
Generate structures using the chosen reconstruction method
Determine and compare the effective flow properties of the reconstructed structure with the original structure
Perform and compare the flow simulations on the reconstructed and original structures

Preliminary Work I

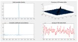
- Reviewed the state of the art in microstructural descriptors and reconstruction techniques
- Applied certain microstructural descriptors on a select library of structures

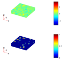




Preliminary Work II

- Produced a random field using the truncated gaussian method to match a given S_2 correlation function. Exponential correlation function in this case.
- Produced a random field using the Fourier transform technique to match a given correlation function.





References

C.Manwart, S.Torquato and R. Hilfer
Stochastic reconstruction of sandstones

Lalit M. Pant
Stochastic Characterization and Reconstruction of Porous Media

Hans-J. Vogel, Steffen Schlueter
On the reconstruction of structural and functional properties in random heterogeneous media

A. N. Diogenes, L. O. E. dos Santos, C. P. Fernandes, A. C. Moreira and C. R. Apolloni
Porous media microstructure reconstruction using pixel-based and object-based simulated annealing - comparison with other reconstruction methods

En-Yu Guo, Nikhilesh Chawla, Tao Jing, Salvatore Torquato and Yang Jiao
Accurate modeling and reconstruction of three-dimensional percolating filamentary microstructures from two-dimensional micrographs via dilation-erosion method

Salvatore Torquato
Random Heterogeneous Materials: Microstructure and Macroscopic Properties

R. Piasecki
Entropic measure of spatial disorder for systems of finite-sized objects