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Master's Thesis Proposal

Stochastic reconstruction of porous media from voxel data

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Part I

Introduction

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

Motivation II

- A specific requirement stemming from the SF 880 project is to generate a computer model of a porous material with a random microstructure and spanning a given volume, such that it can be used in flow simulations (i.e. the generated structure has the same effective physical properties as that of a given physical sample and also has a microstructure that is statistically similar to that of the given physical sample)
- The above requirement is also in line with a longstanding goal in materials science, which is to establish relationships between specific geometrical features of the microstructure and particular effective properties of the material



[Kutscher, 2016]

Motivation III

This thesis aims to help in addressing the previously mentioned requirement 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, relationships between the effective properties such as permeability, conductivity etc. of a porous medium and its microstructure

Goals I

- To establish relationships between effective properties (such as permeability) of a given porous material and its microstructure which can be divided into the following subgoals:
 - To study the relationship between different microstructural descriptors and the effective material properties through simulation on simple reference structures (random overlapping ellipses or circles etc.) and identify the relevant descriptors affecting the property of interest
 - To statistically characterise the geometry of the given porous material's microstructure using the identified descriptors. For example, to capture from the given voxel data
 - Pore size distribution



[Torquato, 2013]

Goals II

- Clustering/connectedness
- Pore-solid interface curvature
- To reconstruct the given porous material in 3D based on the identified descriptors
- 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

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 connectivity

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 $\omega = \prod_{i=1}^X (n_i^{k_i^2})$



[Torquato, 2013]

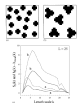
Microstructural descriptors V

- 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

- C_2 and local percolation probability was relatively better b/w reconstruction and reference images for the case of M_n and $C(z)$ 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

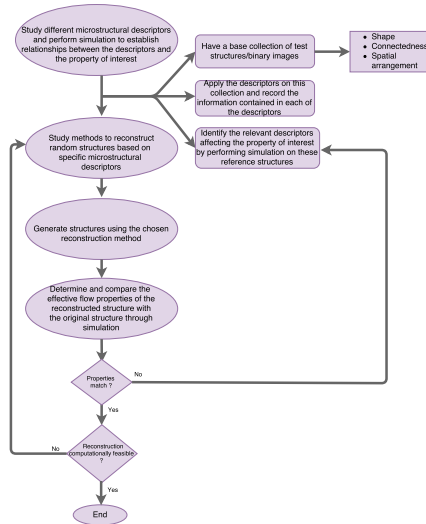
State of the art: Reconstruction studies V

- 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



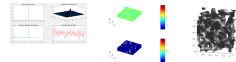
Preliminary Work I

- 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.



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