Flow Properties and Fracture in Disordered Media

Xiaodong Zhang

January, 1996

A thesis submitted for the degree of Doctor of Philosophy of the Australian National University
Declaration

The work presented in this thesis is the result of original research carried out by myself, in collaboration with others, while enrolled as a Doctor of Philosophy student in the Department of Applied Mathematics, Research School of Physical Sciences and Engineering, the Australian National University. To the best of my knowledge, none of the work presented in this thesis has been submitted to any other university or educational institute for any degree.

Xiaodong Zhang
To my parents
Acknowledgement

The work for this thesis was undertaken at the Department of Applied Mathematics, Institute of Advanced Studies, Australian National University, with financial assistance from an Overseas Postgraduate Research Award, an ANU Ph. D. Scholarship and a scholarship from ANU Tech Pty Ltd. I would like to thank the Department and the Research School of Physical Science for having provided very good working environment. I would also like to thank PCRF for generous allocation of the supercomputing time and massive data storage, without which the simulations and analysis necessary for the completion of this thesis would otherwise be impossible.

I would like to thank my supervisors, Dr. M. A. Knackstedt, Dr. S. Marcelja, Dr. S. Hyde and Prof. B. W. Ninham. In particular I owe my thanks to Dr. M. A. Knackstedt who encouraged my independence in pursuing ideas. More importantly his ideas and contributions set the collaborative research on a firm physical basis. I would like to thank him for proof-reading this thesis, the readability of the latter is much improved by his massive effort. As departmental head, Prof. Barry W. Ninham has played an important role during the period of my study in ANU, his intellect originally attracted me to the ANU.

The research presented in the second part of the thesis was undertaken in collaboration with researchers in Melbourne: Prof. D. Y. C. Chan, Mathematics Department of Melbourne University; Dr. L. Paterson and Dr. S. Painter, Petroleum Engineering Division, CSIRO, Melbourne. I would like to thank them for their suggestions.

I must thank my fellow students and researchers for providing an interesting working atmosphere. In particular I would like to thank Diana, Jonathan, Tim, Erica, Tony, Kathryn.

I wish to thank my wife, Yi-Qing, whose support has been invaluable.
Abstract

The thesis consists of two broad aspects of studies using simulation methods: fluid flow in porous media and across fractal surfaces; fracturing phenomena in heterogeneous media.

In the first part of this thesis, we study single-phase steady fluid flow in three-dimensional porous media and across surfaces of self-affine roughness and fractal aggregates using the lattice gas automata method. We have investigated the permeability of porous materials with physically realistic randomness and quantify the effect of porosity and pore size distribution on the permeability of a model porous solid. We have measured the various microscopic parameters associated with pore geometry and used in various phenomenological models. We have considered the validity of various phenomenological models used in practice to relate flow properties of porous media. We have also considered the problem of the relationship between the electrical conductivity of a fluid saturated porous medium and the permeability of the same system. Difference between two measures over a range of porosities have been studied. We have studied the effect of surface roughness on the transport properties of the crack. The deviation from the classical cubic law for the flow rate is attributed to the surface roughness. We have also studied the steady fluid flow around the DLA clusters. The universal behaviour of hydrodynamic screening force distribution of DLA clusters is found.

In the second part of this thesis, the fracturing phenomena in two- and three-dimensional heterogeneous media are extensively studied using simulation. Comparisons between 2D and 3D simulations are made. The effect of heterogeneity on the resultant fracture network and fracture surfaces is discussed. The fracture surface roughness is measured and correlated to the extent of disorder in material properties. A percolation method is proposed and used for study of the effect of heterogeneity on transport properties in geological media. The results hint at the drastic effect of incorporation of realistic heterogeneity on the properties of fluid flows in natural porous media.
List of Publications


Contents

I  Lattice Gas Automata and its Application to Fluid Flow in Porous Media 5

1  Introduction 6

1.1  Lattice Gas Automata and its Implementation 9

1.2  Outline of lattice gas method and theory 11

1.3  Lattice Gas Automata Models 12

1.4  Implementation of LGA 16

1.4.1  Stepwise Algorithms for the Lattice Gas Automata 17

1.4.2  CM2 architecture and Implementation of Collision Table 18

1.4.3  Propagation of Particles and Boundary Conditions 20

1.4.4  Physical aspects on the LGA simulation setup 20

2  Permeability of Fluid Saturated Random Porous Media 23

2.1  Introduction 23

2.1.1  Pore geometry and simulations of permeability 25

2.2  Result and discussion 27

2.2.1  Random versus periodic media 27

2.2.2  Comparison to Empirical theory 31
## CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3 Bidisperse Media</td>
</tr>
<tr>
<td>2.4 Conclusion</td>
</tr>
<tr>
<td><strong>3</strong> Direct Evaluation of Length Scales and Structural Parameters associated with Flow in Porous Media</td>
</tr>
<tr>
<td>3.1 Introduction</td>
</tr>
<tr>
<td>3.2 Simulation and model porous media</td>
</tr>
<tr>
<td>3.3 Recovering the length scales of hydrodynamic interest</td>
</tr>
<tr>
<td>3.4 Conclusion</td>
</tr>
<tr>
<td><strong>4</strong> Direct Measurement of Electrical and Hydraulic Tortuosity in Porous Solids</td>
</tr>
<tr>
<td>4.1 Introduction</td>
</tr>
<tr>
<td>4.2 Simulation</td>
</tr>
<tr>
<td>4.3 Visualization of Flow Pathways</td>
</tr>
<tr>
<td>4.4 Evaluation of Electrical and Hydraulic Tortuosity</td>
</tr>
<tr>
<td>4.5 Conclusion</td>
</tr>
<tr>
<td><strong>5</strong> Fluid flow across fractal structures</td>
</tr>
<tr>
<td>5.1 Introduction</td>
</tr>
<tr>
<td>5.2 Flow in a Single Fracture with Fractal Surfaces</td>
</tr>
<tr>
<td>5.2.1 A comparison between hydrodynamic properties of flat surface and fractal surface</td>
</tr>
<tr>
<td>5.2.2 Permeability of single cracks</td>
</tr>
<tr>
<td>5.3 Hydrodynamics of Flow over a Fractal Aggregate</td>
</tr>
</tbody>
</table>
CONTENTS

5.3.1 Scaling properties of DLA hydrodynamics force spectrum ......................................................... 75
5.3.2 Determining the spectrum of singularities $f(\alpha)$ ............................................................. 78
5.3.3 Relationship between the frictional coefficient and Reynolds number ........................................ 80
5.4 Conclusion .......................................................................................................................................... 81

II Fracture in Heterogeneous Media ........................................................................................................ 83

6 Modelling Fracture Phenomena in Heterogeneous Media .................................................................. 84

6.1 Introduction ....................................................................................................................................... 84
6.2 Resistor network model for study of fracture phenomena ............................................................ 89
  6.2.1 The Resistor Network Model .................................................................................................. 90
6.3 Implementation of Network Model on CM5 ................................................................................. 92
6.4 Simulation ......................................................................................................................................... 93
  6.4.1 Lattice geometry and boundary conditions ............................................................................ 94
  6.4.2 Criterion for detection of catastrophic point ........................................................................... 95

7 Simulation of Fracture in Heterogeneous Media .................................................................................. 100

7.1 The statistical description for disorder of material properties ..................................................... 100
7.2 Simulations ..................................................................................................................................... 104
7.3 Discussions ..................................................................................................................................... 104
  7.3.1 The macroscopic conductivities when system ruptures ......................................................... 104
  7.3.2 Fracture morphology ............................................................................................................... 106
  7.3.3 Cluster size distribution in fracture network ........................................................................... 110
CONTENTS

7.4 Evolution of crack size distribution ....................................................... 114
7.5 Conclusion .................................................................................................. 118

8 The Scaling Properties of Fracture Surface Roughness 120
8.1 Background ............................................................................................... 121
8.2 Simulation .................................................................................................. 122
8.3 Result and Discussion ............................................................................. 124
8.4 Conclusion .................................................................................................. 129

9 Percolation in Geological Material 130
9.1 Model of geological media ....................................................................... 130
9.2 Percolation simulation and discussion .................................................... 134
9.3 Conclusion .................................................................................................. 139

10 Conclusion 140
10.1 Part I: Simulational studies on flow in porous media ......................... 140
10.2 Part II: Fracture in heterogeneous media .............................................. 142

A Implementation of Laplacian solver 146

B Parallel algorithm for identifying bond clusters 149
Part I

Lattice Gas Automata and its Application to Fluid Flow in Porous Media
Chapter 1

Introduction

In the first part of this thesis, I shall describe a computational study of transport phenomena associated with single phase flow in complex geometry. Problems addressed include steady-state flows in porous media of various configurations and flows across complex surfaces and fractal aggregates. The complex behaviour of these systems will be studied with a new computational method based on lattice gas automata.

Single and multi-phase fluid flow and gas flows in porous solids are of wide interdisciplinary concern. Knowledge of flow characteristics in porous solids strongly impact on oil and gas production, the disposal of hazardous wastes, ground-water flow and transport and reaction in porous catalysts. In many applications, the permeability of a porous solid is the physical parameter of primary interest. Despite numerous theoretical investigations, attempts to predict permeability from measurable properties of porous solids are often in error by an order of magnitude or more.

The slow flow of a single fluid in a porous solid can be described at the macroscopic scale by the phenomenological Darcy equation, which in one dimension is given by

\[ \nu = -\left(\frac{k}{\mu}\right) \frac{dp}{dx} \]  \hspace{1cm} (1.1)

where \( \nu \) is the volumetric flow rate per unit area, \( \frac{dp}{dx} \) is the applied pressure gradient, \( \mu \) is the fluid viscosity and \( k \) the permeability of the medium. The physical basis underlying Eqn. (1.1) is well understood. What still remains unknown is how the
permeability, a hydraulic conductivity coefficient which depends only on the porous medium itself and not the fluid, can be predicted from measurable rock properties. This question has been tackled in different ways.

Phenomenological approaches attempt to correlate permeability with other more easily measurable, macroscopic rock properties such as porosity and conductivity. However, these methods provide little insight into how the flow properties depend on the microscopic structure of the pore space. Another approach is to derive macroscopic transport coefficients from the microstructure of the porous medium. This necessarily entails a simplified representation of the pore space, e.g. as a bundle of capillary tubes. These approaches have not led to an understanding of the relationship between the flow in a porous medium and the microscopic morphology of the medium.

A study of fluid flow in porous media should be based on the assignment of a realistic microscopic geometry to the medium. Due to the complexity of the network structure, the conventional approach of discretizing the continuum Navier-Stokes equations requires a large computational effort to realize an accurate treatment of the flow properties and to account for the complex boundary conditions associated with the pore geometries. The advances in computational fluid mechanics based on lattice gas automata (LGA), in effect, a discrete solution of the Navier-Stokes equations, provides a new efficient method to study flow in realistic porous solids.

LGA are discrete analogues of molecular dynamics, in which particles with discrete velocities populate the links of a fixed array of lattice sites. An exclusion principle is imposed so that no more than one particle of a given site can have a given momentum state. The configuration of sites evolves in a sequence of discrete time steps. An important feature of the lattice gas approach is that all operations are purely discrete, local and logical; ideal for high speed simulation on parallel computers. A second feature of the method is its flexibility. In lattice gas models boundary conditions are very easy to implement. The application of the lattice gas method to the study of fluid flow in porous media is particularly promising because of the ease
with which complicated boundary conditions can be implemented. From the microscopic transport equations for the particle distribution functions, the Navier-Stokes equation can be obtained using a Chapman-Enskog expansion. The continuum fluid properties are derived from large scale averaging of the LGA solution of the transport equations. The application of LGA methods have primarily been applied to study of flow problems in two dimensions. In this thesis we have extensively studied three dimensional problems. Despite the discrete nature of the method, this model is capable of exhibiting rich macroscopic complexity such as turbulence [1]. Moreover rigorous comparisons between theoretical predictions and lattice gas simulations have also been reported with impressive results [2]. There have been a few previous applications of the lattice gas method to the study of single phase flow in porous media [3]. This previous work has concentrated on proof-of-principle studies, demonstrating for example the emergence of Darcy's law at low flow velocities.

The specific problems I have investigated using the LGA approach are:

- Permeability of random porous media in three dimensions: we use a lattice gas approach to investigate the permeability of porous materials with physically realistic randomness. Earlier lattice gas studies of the permeability of a porous media have been limited to homogeneous (ordered) systems and systems of high porosity. However, real porous media often exhibit low porosity and a widely varying pore/inclusion size distribution. The lattice gas approach has been used to quantify the effect of porosity and pore size distribution on the permeability of a model porous solid.

- Permeability/conductivity relation in porous media: The conductivity of porous solid is often used as a measure of its permeability. A long standing and unsolved problem is to understand the relationship between the electrical conductivity of a fluid saturated porous medium and the permeability of the same system. Although various empirical relationships between the two properties have been suggested, none is successful over the entire range of the porosities or range of pore size distributions. Computational determination of the permeability
and conductivity for various pore size distributions and porosities have allowed comparisons with the existing empirical relationships.

- Drag Forces around complex obstacles and fractal aggregates: The drag force exerted by a steady flow on a submerged obstacle is characterized in terms of the hydrodynamic radius of the obstacle. The LGA simulation have been carried out to measure the drag force on the Diffusion Limited Aggregate (DLA) clusters. As colloidal particles flocculate irreversibly, they form aggregates which exhibit fractal structure. The aggregates have a very low density when compared with bulk matter, yet they are very effective at screening hydrodynamic forces. The quantitative nature of the force depletion around a fractal structure is important since these materials are often used for their screening properties (e.g. as thickeners in fluids). Fractal aggregates are known to exhibit a large spread of drag forces on the flowing fluid, leading to unique mass transport properties onto and off the aggregate (e.g., in a controlled release mechanism). Previous hydrodynamic studies of flow about the fractal aggregates were limited to small aggregates and to approximate solutions of the hydrodynamics equations. The simulation study on this subject using LGA have analyzed and the distribution of the hydrodynamic forces over rigid fractal object investigated.

- Fluid flow across self-affine surfaces (single fractures): conventionally in studies of underground reservoirs, the fracture surfaces are modelled as perfectly smooth. Flow in a single fracture is modelled as flow between parallel flat plates. The LGA simulation study on fluid flow across rough surfaces shows that the incorporation of a realistic description of the fracture surfaces leads to important differences in fluid flow properties.

## 1.1 Lattice Gas Automata and its Implementation

We begin with a brief description of the lattice gas methodology. It is well known that two fluids with rather different microscopic structures can have the same macroscopic
behaviour because the form of the macroscopic equations is entirely governed by the microscopic conservation laws and symmetries. Such observations have led to a new simulation strategy for fluid dynamics: fictitious micro-world models obeying discrete cellular automata rules have been found. Two- and three-dimensional fluid dynamics are then recovered in the macroscopic limit [4, 5]. Cellular automata, originally introduced by von Neumann and Ulam [6], consist of a lattice of squares, each site of which can have a finite number of states; the automaton evolves in discrete steps, the sites being simultaneously updated by a deterministic or nondeterministic rule.

The interest in cellular automata (CA) algorithms for fluid flow simulation, known as Lattice Gas Automata (LGA), dates back to 1986 when Frisch, Hasslacher and Pomeau (FHP) discovered a simple lattice gas that can be used to simulate two-dimensional Navier-Stokes flow [4]. Soon after this discovery, d'Humières, Lallemand and Frisch presented a similar lattice gas model for three-dimensional flow, based on the four-dimensional face-centered hypercubic (FCHC) lattice [7]. Although other models have been proposed since, none of those model has become as popular as the FHP model and FCHC model.

LGA in the present context is a discrete solution of the Navier-Stokes equations [8]. The lattice gas method allows one to describe macroscopic flow phenomena using large-scale averaging, but most importantly, it also provides detail crucial to the understanding of relationships between the volume-averaged parameters used in the study of flow in porous media. Before the early 90’s, most LGA studies of flow focused on analyzing physical properties (e.g., viscosity, compressibility) [9, 10, 11, 12, 13]. As a result, the basic theory for these models has been well developed and verified by numerical experiments [14, 15, 16, 17]. More recently, lattice gas studies of flow in porous media have been considered, but these have been primarily limited to two dimensional flows [18, 19, 20, 21]. Previous applications of the lattice gas method to the study of single phase flow in porous media in three dimensions [22] has concentrated on proof-of-principle studies, demonstrating for example the emergence of Darcy’s law at low flow velocities [1]. Another study compared the lattice Boltzmann
1.2 Outline of lattice gas method and theory

Lattice gases are distinct from ordinary gases by having only a discrete set of particle velocities. In the simple lattice gases that are of interest for flow simulation, particles of unit mass move synchronously from one node of lattice to a nearest neighbour node and collide with other particles arriving at that node. This means there are as many different velocities as there are nearest neighbours to a node. For a given velocity one particles is allowed at a given node at a given time. This means that for a lattice gas with \( n \) different velocities \( c_1, ..., c_n \) the state of each node is defined by \( n \) bits \( s_1, ..., s_n \), each bit indicating whether particle with corresponding velocity is present at the node or not. The absence of a particle with a given velocity is called a hole.

For the simulation of Navier-Stokes flow it is essential that mass,

\[
\sum_i s_i, \tag{1.2}
\]

and momentum,

\[
\sum_i s_i c_i, \tag{1.3}
\]

are conserved in collisions[4]. For a given velocity set, the algorithm is defined by the collision rules, i.e. the rules that specify for any given initial state (of incoming particles) what the final, after-collision, state of a node will be. By changing these rules it is possible to vary the properties (e.g. the viscosity) of the gas within a certain range[10].

With a few adaptations, routine statistical physics can be applied to lattice gases to relate the microscopic rules to macroscopic properties. A survey of results from statistical analysis of single-phase models can be found in [7, 12, 10, 8]. Statistical analysis of lattice gases starts by considering the probability density fields \( N_i \), each of
which represents the ensemble-averaged number of particles with velocity $c_i$ per node as a function of space and time. From the conservation of mass and momentum at nodes – two equations, representing mass and momentum balance – can be derived,

$$\partial_t \rho + \nabla \cdot \rho \mathbf{u} = 0 \tag{1.4}$$

$$\partial_t \rho \mathbf{u} + \nabla \cdot \Pi = 0 \tag{1.5}$$

where $\rho$ and $\mathbf{u}$ are the density and velocity of the gas, $\sum_i N_i$ and $\sum_i N_i c_i$ respectively. $\Pi$ is the momentum flux density tensor,

$$\Pi = \sum_i N_i c_i c_i \tag{1.6}$$

given a lattice with sufficient symmetry, the momentum flux density tensor in two dimensions turns out to be equal to

$$\Pi_{\alpha\beta} = g \rho \mathbf{u}_\alpha \mathbf{u}_\beta + \frac{\rho}{2}[c^2 - g u^2] \delta_{\alpha\beta} - \eta [\partial_\alpha u_\beta + \partial_\beta u_\alpha - \nabla \cdot \mathbf{u} \delta_{\alpha\beta}] \tag{1.7}$$

This is the momentum flux density tensor of a perfect Navier-Stokes gas with viscosity $\eta$ and pressure $\rho [c^2 - g u^2]/2$ except for the factor $g$. The factor $g$ should be unity for a physical continuum system; it may be tuned to unity by varying the collision rules [9]. It has been shown however that the term $g u^2$ in the pressure term becomes irrelevant for the velocity field in the incompressible limit.

### 1.3 Lattice Gas Automata Models

The lattice gas methods for hydrodynamic system was originally proposed by Hardy et al. (HPP)[24, 25] on a square lattice in two dimensions. But there are serious problems in the square lattice, spurious momentum conservation and anisotropy of the stress tensor. The important contribution made by Frisch et al. [4] was to show that a hexagonal lattice gas model has an isotropic stress tensor and has greatly reduced the spuriously conserved quantities. The basic 2D lattice gas model introduced by Frisch,
Hasslacher and Pomeau (FHP) consists of identical particles on a hexagonal lattice with lattice unit $c = 1$. All particles have the same mass and they reside only on the sites of the hexagonal lattice. There are six different particle momentum states at each lattice site, associated with the directions $e_a = [\cos(2\pi a/6), \sin(2\pi a/6)], a = 1, ..., 6$. An exclusion rule is imposed so that no more than one particle at a given site can have a given momentum state. There are two microscopic updating processes at each discrete time step: advection and collision. Figure 1.1 illustrates how the FHP lattice gas evolves. In the advection process, a particle in state $e_a$ moves from its present site to the nearest neighbour site in the direction $e_a$; all particles have the same speed (= 1) and the same kinetic energy. In the collision process, particles at each site are redistributed among the six momentum states at the same site in such a way that the total particle number ($\equiv \sum_{a=1}^{6} N_a$), and the total mass, momentum and energy conservation is equivalent to mass conservation for this model. The evolution of FHP system can be described by the following microscopic equation:

$$N_a(x + e_a, t + 1) = N_a(x, t) + \Lambda_a$$  \hspace{1cm} (1.8)
where $\Lambda_a$ represents the collision operator, which includes the creation or annihilation of a particle in momentum state $e_a$ and only depends on the information at the site $x$ at time $t$. The collision operation has the form:

$$\Lambda_a = \sum_{s, s'} (s' - s) P(s \rightarrow s') \prod_j N_j^{s_j} (1 - N_j^{s_j})^{1-s_j}$$

where $s = (s_1, s_2, ..., s_6)$ and $s'$ represent the local states before and after collision. $P(s \rightarrow s')$ is the transition probability from state $s$ to $s'$.

Mass and momentum conservation are satisfied if

$$\sum_{a=1}^{6} \Lambda_a = 0, \quad (1.10)$$

and,

$$\sum_{a=1}^{6} e_a \Lambda_a = 0. \quad (1.11)$$

The fluid density and momentum are defined as follows:

$$n(x, t) = \sum_a f_a(x, t) \quad (1.12)$$

$$f(x, t) = n\nu = f_a(x, t)e_a \quad (1.13)$$

where

$$f_a(x, t) = < N_a(x, t)> \quad (1.14)$$

and $< \cdots >$ denotes an ensemble average.

If the microscopic collision transition probability $P(s \rightarrow s')$ satisfies the semi-detailed balance condition then,

$$\sum_s P(s \rightarrow s') = 0 \quad (1.15)$$

then one can prove that collisions will make the system approach a local equilibrium, described by a Fermi-Dirac distribution:

$$f_a = \frac{1}{1 + e^{\alpha + \beta e_a \nu}} \quad (1.16)$$
where $\alpha$ and $\beta$ are Lagrange multipliers determined by mass and momentum conservation.

Assuming infinite size and time for evolution for the system, one obtains the continuum version of the kinetic equation:

$$\partial_t f_a + a_a \cdot \nabla f_a = \Omega_a$$  \hspace{1cm} (1.17)

where $\Omega$ is the collision operation obtaining by replacing $f_a$ for $N_a$ in $\Lambda$. After ensemble averaging the microscopic equation and using the Chapman-Enskog expansion, it can be shown that the $FHP$ system approximates the following fluid equations:

$$\partial_t n + \nabla \cdot (n\mathbf{v}) = 0$$  \hspace{1cm} (1.18)

$$\partial_t (n\mathbf{v} + \nabla \cdot [ng(n)\mathbf{v}]) = -\nabla p + \mu \nabla^2 (n\mathbf{v})$$  \hspace{1cm} (1.19)

$$p = \frac{1}{2}[n - g(n)\mathbf{v}^2].$$  \hspace{1cm} (1.20)

As discussed above, the dependence of $g(n)$ causes a non-Galilean effect. In practice, by tuning the collision operator, $g(n)$ is scaled to unity. The incompressible Navier-Stokes equations are recovered only in the low-Mach-number limit when time and pressure and viscosity are rescaled by the factor $g$ for constant-density problem.

The four-dimensional face-centered-hypercubic lattice (FCHC) was proposed by d’Humières et al.\cite{8} to simulate three-dimensional problems. The four-dimensional model was chosen because no three-dimensional single-speed lattice model yields an isotropic stress tensor to fourth order in the velocity. The $FCHC$ is the simplest lattice to meet the required symmetry requirement. The $FCHC$ lattice is the set of all points on the integral lattice for which the sum of the coordinates is even. Each lattice site has 24 nearest neighbours that are a distance $\sqrt{2}$ away. Particle collisions in each site can involve up to 24 particles and conserve mass and momentum. The velocity of a particle at site $x$ can be defined as $e_a, a = 1, 2, ..., 24$. A periodic condition for the fourth dimension is used, henceforth, leading to a pseudo-FCHC model. In
case of pseudo-\textit{FCHC} model, one simulates the 3D system on a 4D lattice which is only one lattice unit into the 4th dimension. The figure 1.2 gives an illustration of the \textit{FCHC} lattice.

\section*{1.4 Implementation of LGA}

The advantage of LGA is the simplicity in its algorithm, which is completely discrete, local and logical. The algorithm involves only integer operations. In 2D models, the implementation is fairly straightforward and simple due to the fact that the set of collision rules for various 2D models are very small. In 3D simulations, the implementation is relatively straightforward. The major complication is due to the size of collision tables which makes memory management problematic.
1.4 Implementation of LGA

1.4.1 Stepwise Algorithms for the Lattice Gas Automata

Before discussing the detailed implementation of the collision table, I shall summarize briefly the general stepwise algorithm for LGA.

The micro-dynamical evolution of lattice gas automata is described by the following equation:

\[ N_a(x + e_a, t + 1) = N_a(x, t) + \Lambda_a \]  

(1.21)

\( N_a(x, t) \) denotes the particle population in momentum state \( e_a, a = 1, 2, \ldots, n \) on site \( x \) at time step \( t \); \( \Lambda_a \) denotes the collision operator,

\[ \Lambda_a = \sum_{s, s'} (s' - s) P(s \rightarrow s') \prod_j N^{s_j}_j (1 - N^{s_j}_j)^{1-s_j} \]  

(1.22)

where \( s = (s_1, s_2, \ldots, s_n) \) and \( s' \) represent the local states before and after collision. \( P(s \rightarrow s) \) is the transition probability from state \( s \) to \( s' \).

The collision operator can be implemented as a table to look up for an integer with a given input integer. Here the input integer is defined as a bit-wise indicator of, in the case of the FCHC lattice, 24 bits in length, each bit carrying the population information 0 or 1 for a momentum state \( e_a \) associated with the lattice site \( x \). In lattice gas automata, the momentum state is associated with the link on the lattice, therefore, the position of \( i \)th bit in the input integer can be used as an index to a list of the momentum states \( (e_a, a = 1, 2, \ldots, n) \) associated with the lattice site.

The LGA automata evolves in following steps,

- collision - the bitwise particle population information on all the links to a node are collected and arranged into an integer (incoming state); the latter is used as an index into the collision table to look for the set of all the possible outgoing states associated with the index integer; one of the possible resultant states will be selected and it carries the population of particle on all the links indicated by the 0 or 1 on the corresponding bits.
1.4 Implementation of LGA

- advection - the resultant integer state after collision are read. The bit information is transmitted to the nearest neighbour site along the link denoted by the position of the corresponding bit in the after-collision integer state, to update the population information at the nearest neighbour site on the corresponding link.

1.4.2 CM2 architecture and Implementation of Collision Table

The LGA hydrodynamic simulations discussed in this thesis were performed on the Connection Machine 2 (CM2) at PCRF\textsuperscript{1} at ANU. Before we discuss the implementation of LGA on CM2, we first discuss the CM2's architecture. The CM2 available at ANU is a SIMD\textsuperscript{2} parallel computer consisted of 16,384 processors in 512 groups. Each group consists of 32 physical processors. One SUN 4/690 main-frame is used as the front-end to CM2 and one SUN 4/690 as the DJM\textsuperscript{3} master together with a third SUN 4/690 main-frame managing the massive parallel data storage device. The memory is distributed among the processors, each physical processor has a 262,144 bits memory and total amount of memory avail for a 16K processor partition is 4,294,967,296 bits\textsuperscript{4}.

The CM2 is in many aspects an ideal machine for the lattice gas automata simulation. The lattice structure can be mapped onto the machine memory in a well-defined manner. Problematic, in the case of the \textit{FCHC} lattice, is the size of the full collision table. In the simplest case with no rest particles, the full collision contains $2^{24} = 16,777,216$ entries. One entry in the table takes up 24 bits of physical memory; then the whole table would take up the $24 \times 2^{24} = 402,653,184$ bits. The input state, as a 24-bit integer can directly be used as the address to index the table. The full collision table can in principle therefore be implemented by spreading it across all processors.

\begin{flushleft}
\textsuperscript{1}The Parallel Computing Research Facility.
\textsuperscript{2}SIMD is the abbreviation for Single-Instruction-Multiple-Data.
\textsuperscript{3}DJM is the abbreviation for Distributed Job Manager.
\textsuperscript{4}The bit is a natural unit of memory for the CM2 parallel machine
\end{flushleft}
Unfortunately the inter-group communication (the communication between physical groups of processors) is slow on CM2 (in principle, about $10^2$ times slower than the communication from within the same physical group). In order to optimize the implementation of LGA on CM2, it is important that this kind of inter-group communication be used sparingly. In practice, to store the collision table in a group of physical processors and to access from within the same group will optimize the pattern of communication for table-lookup. Unfortunately, a group of 32 physical processors has a maximum of 64MBits of memory. A full collision table of 400MBits is obviously too large by an orders of magnitude.

A large effort has been made by various research groups to construct the reduced collision table and various reduction algorithms have been reported[26, 10, 11, 27]. The general strategy of the reduction algorithms is that the collision table is invariant under duality (exchange of particles and holes), then one can extend the definition of species by including also the dual states. With the collision table reduced in such a way, the table look-up follows the following steps:

- Find the deputy state $\hat{s}$ of $s$ and the isometry $I$ which transforms $s$ to $\hat{s}$;
- Look up the reduced table to obtain the output state $\hat{s}'$ corresponding to $\hat{s}$;
- Apply the inverse isometry $I^{-1}$ to $\hat{s}'$ to obtain the output state $s'$.

Further reduction of the collision table is possible with various emphasis on different aspect of physics. I used J. A. Somers and P. C. Rem's reduced collision with no rest particles [28, 10] for my simulation to single phase flow in porous media.

Somers' reduced collision contains 106496 entries. The table now requires less than 32MBits in a group of 32 processors on CM2 (the total memory of 32 processors is 64MBits)—favourable for storage within groups of processors on the CM2. As memory per group is 1 MByte, this leaves enough memory per processor to store other information—for example, the state of lattice, structural information etc.
1.4 Implementation of LGA

The collision table look-up phase is the most time-consuming phase throughout the simulations as it involves the application of isometries, a search in the reduced collision table and application of reverse isometries. To speed up the table look-up, the table is in fact stored in a way that it is shared with the group of 32 physical processors; 1 bit of an entry (now a 32-bits long integer) in the table is stored in a processor within the group, the position of which corresponds to the position of the bit in the integer. An algorithm was developed to allow the collaborative look-up among the processors which is much more efficient than the conventional way. Programming in a mixture of C*, a superset of general C for parallel programming on Connection Machines, and CM assembly insured the efficiency of this frequently used part of the program. When the simulation runs at a configuration of $32 \times 32 \times 64$ in the relaxation phase (no statistical data is accumulated in this phase), it reached the 2.1GFlops, which was approximately 60% of the designer's peak speed for this machine.

1.4.3 Propagation of Particles and Boundary Conditions

The advection step of the LGA is easy to simulate on the CM2 due to its SIMD structure. The particles - bitwise information - are propagated to its nearest neighbouring lattice site along the link. In this phase, simple grid communication in parallel format is used 24 times to update the population information on all the links associated with each node. Extra caution has been taken to make sure that the transferred bit information sets the corresponding bit of the status integer on the recipient site.

1.4.4 Physical aspects on the LGA simulation setup

Boundary conditions

An important feature for the LGA method is that boundary conditions are very easy to implement. Total reflection of particles at a solid boundary corresponds to, on a macroscopic scale, a no-slip boundary condition; specular reflection of particles gives
1.4 Implementation of LGA

a macroscopic *free-slip* boundary condition. Arbitrary complex solid boundaries can be modelled by appropriate arrangements of boundary cells. The *no-slip* boundary condition shown in figure 1.3(a) is used throughout the simulations.

![Diagram of boundary conditions](image)

Figure 1.3: a) non-slip boundary condition; b) the slip-boundary condition.

**Mean free path problem in the LGA simulation**

Considerations in lattice gas studies are the assessment of the range of parameters in which the lattice gas solution gives a faithful representation of the hydrodynamic equations. In this respect, a crucial parameter is the size of the open pores. If the pore size is so small that it becomes comparable to the mean free path of the particles, then true macroscopic fluid behaviour will not necessarily be produced within the pores [22]. The average density for the typical lattice gas runs were $\frac{1}{8}$ per lattice link, which gives us a mean free path of approximately 1.4 lattice units. Sahimi and Stauffer [29] contend that in order that the LGA results approach the continuum limit, the mean size of obstacles must be at least twice the mean free path of the simulation. For all the simulations, the resultant data used in this thesis, it is made sure that the smallest cross-section area in the model porous material on the lattice on the actively flow path is, e.g. for the porous flow simulation, 3×3 in lattice units.
1.4 Implementation of LGA

Physical data retrieval

To create a pressure gradient across the channel, we use a uniform forcing condition at the inlet of the channel. The fluid flow velocity profile is introduced at the inlet of the channel with a prescribed macroscopic fluid velocity. At every automaton step, particles arriving at the inlet are rearranged. They are repositioned to uniform distributed among all inlet nodes. The overall local fluid velocity maintained at the prescribed macroscopic value; the latter is done by resampling the particle velocity to a probability distribution given by expanding the Fermi-Dirac distribution to the second order of the local fluid speed. Due to the perturbation applied to the particles at the inlet, the local fluid behaviour in regions near the inlet and outlet (periodic boundary conditions for between inlet and outlet) of the channel are under the effect of the forcing rule. For a 64 x 64 x 128 lattice, the pressure bias is applied elongated dimension z at z = 0. To eliminate possible artifacts caused by the forcing rule at the inlet, we measure the macroscopic quantities only in the central part of the channel, where 32 ≤ z ≤ 95.

Statistical methods are used to obtain macroscopic quantities. Time averaging is used to reduce noise as we are interested in the detailed flow structure for steady state flow in arbitrary porous media. The system was allowed to equilibrate for 8,000 (or more if necessary) steps and measurements were taken from 2,000 steps. It was verified that 8,000 steps is more than adequate for most systems for fluid flow with a biased inlet velocity profile to reach equilibrium. Local flow information (e.g. local drag measurements on obstacles) was consistently obtained within 2,000 steps of measurement in the lattice gas scheme with very small relative errors. Increasing the number of steps for measurement of macroscopic physical quantities made no notable improvement to the statistical quality of the data.
Chapter 2

Permeability of Fluid Saturated Random Porous Media

In this chapter, the lattice gas automata is used to evaluate the permeability of simple three-dimensional porous media over a wide range of the porosity. Media with both random and periodic arrays of obstacles are studied. Flow and structural properties of the medium are obtained at a microscopic scale. Comparing the results for flow in random and periodic media illustrates the strong effect randomness has on the flow properties of porous media. Predictions of the permeability of porous media are compared to popular empirical models. The Kozeny equation is shown to give good agreement with the permeability of the periodic media over the full range of the porosities studied. The Blake-Kozeny and Rumpf-Gumpte models correlate well with the random monodisperse media data. For more complex media we show that use of the empirically based models may lead to large errors in the permeability prediction.

2.1 Introduction

The problem of fluid flow and transport in a wide variety of porous media is of great theoretical and practical interest[30, 31, 32]. Important examples include flows in
sedimentary rock, packed beds and catalysts. Of particular interest in the study of flow is the determination of the fluid permeability of a saturated porous material. The fluid permeability $k$ is defined by the Darcy equation written here in differential form:

$$v = -\frac{k}{\mu} \nabla P$$

(2.1)

where $v$ is the volumetric flow, $P$ the hydrostatic pressure and $\mu$ the fluid viscosity. While the physical basis underlying the Darcy equation is well understood [33], what remains unknown is how the permeability, which is dependent only on the structure of the porous medium, can be predicted from other porous media properties. It is clear that the property of permeability should be linked to other properties of the porous medium — internal surface area, porosity, pore size distribution, etc. — since all such properties are manifestations of the geometrical arrangement of the pores.

Empiricism, aided by dimensional analysis and theoretical considerations, has been the most prevalent way to model flow in disordered porous media[30, 34]. Empirical correlations typically use well defined properties of porous medium such as the internal surface area and the porosity. Unfortunately general correlations do not exist for all types of porous media. Therefore most models contain other factors that are either very difficult to measure directly, or are vaguely identified with geometrical quantities. Most are however nothing more than undetermined factors used in order to make the data fit the desired equations. The problem with empirical approaches is that the substantiation of the empirical equation is impossible—most contain at least two parameters which have to be determined by independent means in order to perform a valid check of the theory. Moreover, the parameters are in most cases poorly defined quantities and often can only be measured indirectly. Lattice gas automata (LGA)[35, 36] offers a promising approach to the understanding of single-phase flows in porous media.

LGA in the present context is a discrete solution of the Navier Stokes equations[8]. The lattice gas method allows one to describe macroscopic flow phenomena using large-scale averaging, but most importantly, it also provides detail crucial to the
understanding of relationships between the volume-averaged parameters used in the study of flow in porous media. To date, lattice gas studies of flow in porous media has been primarily limited to two dimensional flows[18, 19, 29, 37]. Previous applications of the lattice gas method to the study of single phase flow in porous media in three dimensions[22] has concentrated on proof-of-principle studies, demonstrating for example the emergence of Darcy’s law at low flow velocities[1]. One study compared the lattice Boltzmann result for random porous media to various rigorous variational bounds and to the Kozeny-Carman model[23].

In this chapter, the study is concentrated on fluid flow in porous media in random and periodic media in three dimensions using LGA. Comparing the results for flow in random and periodic media illustrates the strong effect randomness has on the flow properties of porous media. The permeability of random and periodic porous media are simulated over a large range of porosity. The other structural properties of a porous medium (e.g. the porosity, the internal surface area, etc.) used commonly in empirical relationships are directly determined. Comparison between the predictions of commonly used empirical flow models and lattice gas predictions is made. Finally, we consider more complex random media (mono- and bi-disperse inclusions) and compare the simulations with empirical equations.

2.1.1 Pore geometry and simulations of permeability

In the present work, the porous medium is placed within a channel with fixed solid walls. The channel dimensions are 128 sites along the flow direction with a cross-sectional area 64x64. At the solid boundaries a no-slip boundary condition is applied to the fluid.

The periodic media are built within cubes of size 16x16x16 within the channel. In each of these cubes two identical (smaller) cubic obstacles are placed along a diagonal of the cube; the two inner cubes sit at diagonally opposite corners of the larger cube. To achieve various porosities, the size of the two obstacles are varied. Overlap of the
inner cubes is allowed.

The first type of random media are constructed by randomly depositing cubic obstacles of side length 4 in lattice unit within the channel. The model random porous media is constructed systematically by stepping through the lattice randomly placing obstacles of size $4 \times 4 \times 4$ with probability $1 - \phi$ within the lattice, i.e. no overlapping was allowed. A wide range of porosities were realized by varying the number of obstacles placed within the channel. In the second case we allow overlapping of obstacles to occur. In these two cases, no measurable difference in properties is observed (see Section 2.3).

To create a pressure gradient across the channel, a uniform forcing condition is implemented at the inlet of the channel. The fluid flow velocity profile introduced at the inlet has a prescribed macroscopic fluid velocity ($u = 0.2$). At every automaton step, particles arriving at the inlet are rearranged: the particles are uniformly redistributed among all inlet nodes; the overall local fluid velocity maintained at the prescribed macroscopic value $u$ which is done by populated the lattice links to a probability distribution derived by an expansion of Fermi-Dirac equation to second order of local fluid speed $u$.

Time averaging is used to reduce the noise in the detailed flow structure for steady state flow in arbitrary porous media. The system was allowed to relax for 8,000 automaton steps and measurements were taken from 8,000 to 10,000 steps. It was verified that 8,000 steps is more than adequate for fluid flow with a biased inlet velocity profile to reach equilibrium. Local flow information was consistently obtained within 2,000 steps of measurement in the lattice gas scheme with very small relative errors. Increasing the number of steps for measurement of macroscopic physical quantities made no notable improvement to the statistical quality of the data.
2.2 Result and discussion

2.2.1 Random versus periodic media

Simulations were performed at thirteen different porosities for the periodic media and fifteen different porosities for the random media. For each porosity at least four runs were performed. The error in the measurement of the permeability data for the periodic media is smaller than the size of the symbols shown in Fig. 2.1. The error bars in the random data are primarily due to fluctuations in the porosity. Randomly placing obstacles on the lattice with probability \((1-\phi)\) leads to variations in the measured porosity of the medium. Fluctuations in the data are also due to the inevitable fluctuations in the pore geometry, particularly at lower porosities.

Figure 2.1: The permeability of random and periodic porous media as a function of porosity. \((\triangle)\) Periodic Medium and \((\oplus)\) Random Medium.
Figure 2.2: 2D slices of the 3D flow paths for flow in the periodic medium at a porosity of 40%. The macroscopic flow direction is from left to right. The snapshots are four continuous layers along the x direction for $z \in [40,83]$ and $y \in [10,53]$. (a) $x=47$ – here the local overlapping of obstacles creates a more disordered flow pattern. (b) $x=48$ – one lattice unit from overlapping pattern, here well-defined flow pattern begins to take form. (c) $x=49$ – Development of well defined flow paths. (d) $x=50$ – flow pattern is fully developed.
Figure 2.3: Snapshots of the 3D flow in random porous medium. Orientations are (a) along and (b) perpendicular to the macroscopic flow direction. Local velocities are of the same magnitude in (a) and (b) illustrating the strong effect of local disorder. Note the circulation evident in the pores in the lower region of both figures.
2.2 Result and discussion

A direct comparison can be made between the flow properties of porous media with random and periodic obstacles. Snapshots of the microscopic flow configurations in Fig. 2.2 and 2.3 illustrate the strong effect that randomness has on the flow properties. The snapshots both show flow at a porosity of 40%. First we illustrate differences in local flow properties.

In the case of a spatially periodic system, in Fig. 2.2, the pore space exhibits a predictable configuration, and the flow occurs through quite well defined channels. However since the periodic media is constructed by placing obstacles at diagonals of a volume element allowing overlapping of obstacles (Fig. 2.2(a)) one can observe regions of the flow following more disordered path, with large lateral velocities.

Unlike the spatially periodic system, in the random media, flow meanders throughout the medium, i.e., large connected obstacles are present and large regions can be seen where there is little flow. In Fig. 2.3(a) it shows a snapshot of the flow along the macroscopic flow direction; the Fig. 2.3(b) gives a snapshot of a cut orthogonal to flow. Comparing the Fig. 2.3(a) and (b) one notes the magnitude of the lateral and tangential flow velocities are similar. This illustrates the strong effect that the random geometry has on the flow paths. Interestingly, the snapshot of the flow paths in random media exhibits circulation within pores, indicating the presence of dead-end pores.

The permeability of the two media are measured as a function of the porosity. The permeability of the random media is compared with the permeability of the periodic system in Fig. 2.1. One notes that at large values of the porosity the permeabilities of the two systems are similar. However, as the porosity decreases, the differences become marked. At porosities of 40%, the permeabilities do not resemble one another at all. The random media exhibits a smaller permeability by nearly one order of magnitude than that of the periodic media. Measurement of permeability for random media with non-overlapping and overlapping obstacles shows no distinguishable difference. This indicates that a spatially periodic system, used by many to model disordered porous media [38], is not an appropriate model of disordered porous
media—particularly at intermediate to low values of porosity.

### 2.2.2 Comparison to Empirical theory

Empiricism, aided by dimensional analysis and theoretical considerations, has been the most prevalent way to model flow in disordered porous media. These methods have proved particularly useful in the case of packs of fairly uniform and isometric particles. Initially comparison of the lattice gas data with these simple models will indicate whether the lattice gas solution reproduces quantitatively the correct flow properties of porous media. Further work on more complex media will test the prediction of these empirical methods on more general media.

![Figure 2.4: The specific surface of random and periodic porous media as a function of porosity. (◊) Periodic Medium. (—) Random Medium.](image)
Figure 2.5: The permeability of random and periodic porous media as a function of porosity. (Δ) Periodic Medium. (+) Random Medium. The lines are the prediction of the Kozeny-Carman equation with the measured $S_0$ shown in Fig. 2.4. Using Eqn. (2.2), both Random (—) and Periodic (---) predictions overestimate the simulation results.

The simplest empirical approaches are based on the idea of conduit flow. The Kozeny-Carman theory is today a widely accepted explanation for the permeability as conditioned by the geometrical properties of a porous medium. The Kozeny theory represents the porous medium by an assemblage of channels of various cross-sections, but of a definite length. The Navier-Stokes equations are solved simultaneously for all channels passing through a cross-section normal to the flow in the porous medium. The permeability is expressed in terms of the specific surface, $S_0$ of the porous medium, defined as the wetted pore surface per solid (non-porous) volume of
2.2 Result and discussion

Figure 2.6: The permeability of the random porous media as a function of porosity. The line indicates the prediction of the Blake-Kozeny model. An excellent match is evident.

The bed, and the porosity, $\phi$, by

$$k = \frac{1}{5} \phi^3 / S_0^2 (1 - \phi)^2.$$

(2.2)

The parameter $S_0$ can be obtained directly and simply in the lattice gas scheme for both periodic and random systems. In Fig. 2.4 it shows the specific surface as a function of porosity for the periodic and random media. In Fig. 2.5 the comparison between the prediction of the Kozeny-Carman theory with the simulation data for both the periodic and the random media are made. The theory is in good agreement for periodic media. By replacing the constant in Eqn. (2.2) by $\frac{1}{7}$ the simulation data for periodic media would match the Kozeny-Carman prediction perfectly. Zick and Homsy [39] found that the Carman prediction was within 15% of the results for periodic arrays of spheres in periodic media for porosities greater than 0.5 in
agreement with our results. The prediction of Eqn. (2.2) for random media is not satisfactory, however: in particular it diverges from the LGA data at low porosity. In the literature there is frequent disagreement between the experimentally measured permeability and the permeability as predicted by the Kozeny-Carman equation. Our results show that Kozeny-Carman equation overestimates permeabilities.

An empirical equation that has resulted in excellent correlations for flow in random porous media, particularly at low porosities, is the Blake-Kozeny model[40]. In this model the specific surface is related to the average particle size within the packed beds, defined as $D_p$. Defining the mean particle diameter $D_p$ as the diameter of the hypothetical sphere with the same $S_o$ as the medium, one can express $D_p = \frac{S_o}{S_o}[41]$. 

Figure 2.7: The permeability of the random porous media as a function of porosity. The (—) indicates the prediction of the Blake-Kozeny equation; the (— --) shows the prediction of the Rumpf-Gumpte equation.
Coupled with a small change in the constant, the equation reads:

\[ k = \frac{D_p^2 \phi^3}{150 (1 - \phi)^2}, \]  

(2.3)

The comparison of the prediction of the Blake-Kozeny equation with the experimental data is shown in Fig. 2.6. The Blake-Kozeny equation is in remarkable agreement with the lattice gas results for a wide range of porosity. Only at the lowest porosities does one see a noticeable difference between the Blake Kozeny theory and the simulations result.

While the empirical approaches described above assume the flow of the fluid is through an imaginary capillary with structure related to the physical structure of the porous medium, a purely phenomenological theory avoids any assumption of that nature. A phenomenological permeability model based on general dimensional analysis of the porous media flow problem due to Rumpf and Gumpte [42] has enjoyed success. Rumpf and Gumpte studied systems of uniform random packs consisting of various distributions of spherical particle size over the range of porosities from 0.35 to 0.70, for low Reynolds number. The relationship derived by the phenomenological approach for the permeability reads:

\[ k = \frac{D_p^2}{5.6K \phi^5.5} \]  

(2.4)

where \( K \) is a constant determined by the distribution of spherical sizes of the random packs. For narrow distributions of pack sizes, as in the present case, \( K = 1.00 \). Comparing our data with this relationship for the random packs in the porosity range 0.2 – 0.7 gives excellent agreement — even at lower porosities (see Fig. 2.7). The excellent agreement of our LGA data with proven empirical relationships for monodisperse media is further evidence of the utility of LGA for flow in porous problems. We next consider the question of how well the common empirical equations predict properties of more complex media.
Most porous media are not made up of monodisperse grains, but are instead made up of a range (often very broad) of grain sizes. The pore geometry of non-monodisperse media is more complex and more difficult to enumerate. Flow properties can again be correlated to empirical methods. In practice the matching has been poor. We consider the effect of varying grain size on the flow properties of random porous media.

Figure 2.8: The permeability of random and periodic porous media as a function of porosity. (Δ) periodic medium; (+) random medium with no overlaps; (◇) random mono-disperse 1:1 media with overlaps; (◊) with error bars 2:1 bi-disperse media with overlaps. The difference is not distinguishable between the permeability of mono-disperse random media with overlaps and that of the random media with no overlaps.
media. In particular, a simulation study on the permeability of bi-disperse random porous media is discussed in this section.

We construct random bidisperse media in a similar manner to the random monodisperse media. The two obstacle sizes used are cubic obstacles of side length 4 and 8. Again the overlap of obstacles is allowed. For the monodisperse and bidisperse model media, caution has been taken to insure that the dimension in any specific pore in the medium is not less than 4 lattice units.

Fig. 2.8 shows the difference in the permeability of mono- and bi-disperse media. The permeability of the random bidisperse media sits between the curves for periodic and mono-disperse random media. At higher porosities, the bidisperse permeability follows the periodic media; at the intermediate and low porosity region, it deviates from the periodic, but is consistently a factor of two or more greater than the permeability for random mono-disperse media.

Figure 2.9: The permeability of random bidisperse porous media. (◊) denotes the simulation results. All curves give the fit by Black-Kozeny equation (Eqn. (2.3)) with the modified $D_{p,eff}$ by Eqn. (2.5)(— • • • —), Eqn. (2.6)(— • —) and Eqn. (2.7)(— — — • • • •).
2.3 Bidisperse Media

Figure 2.10: The permeability of random bidisperse porous media. All curves give the fit by Rumpf-Gumpte equation (Eqn. (2.4)) with the modified $D_{p,\text{eff}}$ by Eqn. (2.5)(— • • • —), Eqn. (2.6)(— • —) and Eqn. (2.7)(—— — — —).

Attempts to predict permeability by the Black-Kozeny equation (Eqn. 2.3) and Rumpf-Gumpte equation (Eqn. 2.4) for media of various inclusion size have been made by assuming an effective particle size $D_{p,\text{eff}}$. In Perry’s handbook [43], it is suggested that $D_{p,\text{eff}}$ be defined as:

$$\frac{1}{D_{p,\text{eff}}} = \frac{P_4}{D_{p,4}} + \frac{P_8}{D_{p,8}}. \quad (2.5)$$

Two other natural descriptions would include:

$$D_{p,\text{eff}}^2 = P_4 D_{p,4}^2 + P_8 D_{p,8}^2, \quad (2.6)$$

$$D_{p,\text{eff}} = P_4 D_{p,4} + P_8 D_{p,8}. \quad (2.7)$$

In the above equations, $D_{p,4}$ and $D_{p,8}$ is the particle size $D_p$ for cube side length 4 and 8 correspondingly and $P_4$ and $P_8$ are the corresponding weight densities for the two sizes of cubes. Here $P_4 + P_8 = 1$. As shown in Fig. 2.9 and Fig. 2.10, no
2.3 Bidisperse Media

Figure 2.11: The permeability of random bidisperse porous media as a function of porosity. The curve gives the fit by Eqn. (2.2) with the measured specific surface $S_0$.

A satisfactory fit is found for either Black-Kozeny or Rumpf-Gumpte equations across the entire range of porosities studied; For lower porosity, Eqn. (2.5) gives a better fit; For higher porosity, Eqn. (2.6) gives a good agreement. The Kozeny-Carmen equation (Eqn. (2.2)) with the measured specific surface $S_0$ overestimates the permeability at low porosity region and underestimates in the high porosity region (see Fig. 2.11).

These results indicates that the parametrization of the Black-Kozeny and Rumpf-Gumpte equations are not adequate. They are simply empirical fits valid primarily for mono-disperse media. More extensive simulation studies on the effect of various geometric factors including the ratio of large to small obstacles, a continuous range of obstacle size, varying the shape of obstacles and incorporation of anisotropicity will lead to a more comprehensive understanding of flow in random porous medium.
2.4 Conclusion

I have shown that the lattice gas method is a fast and efficient numerical scheme to study flow in complex three dimensional porous media. With LGA, one can study flow in periodic and random porous media. Comparing the results for flow in random and periodic media illustrates the strong effect randomness has on the flow properties of porous media. We consider the validity of different phenomenological models used in practice to relate flow properties of porous media. As has been noted before, the Kozeny-Carman equation is in good agreement with the data for flow in periodic media [39]. The Blake-Kozeny and Rumpf-Gumpte models give excellent fits to the monodisperse random media results. The quantitative agreement between the lattice gas solution and the empirical equations for both random and periodic media indicates the strength of the method in the study of porous media flows. For more complex media we show that use of the empirically based models leads to large errors in the permeability prediction.

Relating the permeability to other macroscopic properties of a porous medium has to date been chiefly empirical. The lattice gas method allows one to describe macroscopic flow phenomena using large-scale averaging, but more importantly, can provide microscopic detail crucial to the understanding of relationships between the volume-averaged parameters. The LGA solution allows the direct evaluation of these properties of porous medium. In the next chapter we extend this study to evaluate various other parameters (e.g. tortuosity) commonly introduced into empirical models to ascertain their relevance to flow in porous media.
Chapter 3

Direct Evaluation of Length Scales and Structural Parameters associated with Flow in Porous Media

In this chapter, we shall discuss the work via LGA aimed at directly evaluating the flow and structural properties of three-dimensional random porous medium at a microscopic level. The length scale associated with the pore structure and the geometric factor accounting for pore shape, connectivity, and tortuosity used in empirical models are independently measured. It is shown that the empirical models greatly underestimate the effect of the structure of the medium on flow properties. The tortuosity, in particular, is shown to have a much larger effect than accounted for by empirical models.
3.1 Introduction

It is clear that the property of permeability $k$, defined by phenomenological Darcy equation (Eqn. 1.1), should be linked to other properties of the porous medium — internal surface area, porosity, pore size distribution, etc. — since all such properties are manifestations of the geometrical arrangement of the pores (see Chapter 2). However, to uncover the relationships is possible only if one is able to understand exactly how all these properties are conditioned by the geometrical properties of the pore system. To date the understanding of the relationship between media properties and the permeability has been poor. A direct approach to finding relationships between the various properties of random porous media has been limited to establishing empirical relationships, as flow properties could not be measured directly. LGA provides a method to directly evaluate the flow and structural properties used in the derivations of common empirical relationships.

As discussed in Chapter 2, in hydraulic radius models the porous medium is assumed to be equivalent to a conduit, the cross section of which has an extremely complicated shape, but, on average, a constant area. The theories all make use of the fundamental observation that the permeability, in absolute units, has the dimensions of length squared. It is argued that a length should be characteristic for the permeability of a porous medium. This length is called the hydraulic radius $R_h$. In analogy with laminar flow through tubes we define the average pore or seepage velocity $v_p$ in the flow channels by:

$$v_p = \frac{\Delta P c R_h^2}{L_e \mu}, \quad (3.1)$$

where $L_e$ is the average path length for flow and $c$ is a shape factor associated with the channel cross section. The pore velocity and the macroscopic velocity $v$ defined in equation 1.1 are related by $v_p = \frac{v L_e}{\phi L}$. The division of $v$ by $\phi$ is used to define an average interstitial velocity. The multiplication by $\frac{L_e}{L}$ is a correction for the fact that a hypothetical fluid particle used in the macroscopic flow equations and flowing with the macroscopic velocity $v$ covers a length $L$ in the same time as an actual fluid
Combination of the preceding two equations and Darcy's Law gives:

\[ k = \frac{c}{(\frac{L}{L_c})^2} R_h^2 \phi \]  

(3.2)

This is the basic form of all hydraulic radius theories, differing only in the method of calculating the mean square hydraulic radius and in the definition of the geometric factor \( \frac{c}{(\frac{L}{L_c})^2} \). It is useful to rewrite equation 3.2 as,

\[ k = k_0 \ell^2 \phi \]  

(3.3)

where \( \ell \) is the length scale associated with the pore structure and \( k_0 \) is the geometric factor accounting for pore shape, tortuosity, connectivity, etc. and is a function of the pore geometry only.

The problem with the hydraulic radius approach is that the substantiation of the empirical equation is impossible. The length scale \( \ell \) and the geometrical parameter \( k_0 \) have to be determined by independent means in order to perform a valid check of the theory. In principle one requires a method to determine the macroscopic flow parameters, while providing information about the local flow configuration. LGA is capable of solving this problem.

The LGA method and the simple implementation of complex boundary conditions allows the direct evaluation of various flow and microstructural properties used in hydraulic radius models. In the present chapter, we will discuss the direct measurement of these microstructural properties, in particular, the hydraulic tortuosity.

### 3.2 Simulation and model porous media

The LGA simulation is again performed on identical media to those described in Chapter 2. The random media are constructed by systematically stepping through the lattice and randomly placing obstacles of size \( 4^3 \) with probability \( 1 - \phi \) within the lattice, i.e. no overlapping is allowed. As discussed in Chapter 1, in order that
the LGA results approach the continuum limit, the mean size of obstacles must be at least twice the mean free path of the simulation[29]. It is ensured therefore that the smallest cross-section area of the pores is 4×4.

3.3 Recovering the length scales of hydrodynamic interest

In Chapter 2, we have compared the predictions of various hydraulic radius models with the LGA simulation results. The comparison between the empirical models and simulation results are summarized in Fig. 3.1. The differences shown in Fig. 3.1 between the empirical models and simulation results are attributed to that the empirical models ignore a very strong effect that pore geometry has on flow in porous media. In this section, we will discuss the measurement of the variation with porosity of the length scale parameter \( \ell \) defined by the pore structure and the geometrical parameter \( k_0 \) describing the pore shape, tortuosity and connectivity directly using LGA. The tortuosity, in particular, is shown to have a much larger effect than accounted for by these models.

Before discussing the simulation results and compare it with the various empirical equations, it would be interesting to recover the length scales parameters \( \ell \) and geometrical parameter \( k_0 \) associated with the empirical equations.

Among the hydraulic radius theories, the Kozeny theory enjoys much success[30]. The permeability is expressed in terms of the specific surface, \( S_0 \) of the porous medium, defined as the wetted pore surface per solid (non-porous) volume of the bed, and the porosity, \( \phi \), by

\[
k = (c)\left(\frac{\phi}{S_0(1 - \phi)}\right)^2 \phi.
\]

(3.4)

where \( c \), the Kozeny constant, a dimensionless number approximately equal to \( \frac{1}{2} \), is dependent only on the flow cross-section. In the Kozeny theory, by analogy to equation 3.4, the length scale \( \ell \) is equivalent to the hydraulic radius, defined as \( \ell = \)
3.3 Recovering the length scales of hydrodynamic interest

Figure 3.1: Summary of the comparisons (see Chapter 2) between hydraulic theories and simulation data. The curves are the prediction of the empirical equations: Kozeny (-----), Kozeny-Carman (· · · · ), and Blake-Kozeny (− − − − ).

\[ R_h = \frac{\phi}{S_0 (1 - \phi)} \text{, and the geometrical factor is given by } k_0 = c. \]  

The surface property \( S_0 \) can be evaluated directly from the LGA simulation as discussed in Chapter 2. In Fig. 3.1 we can see the prediction of this theory is not satisfactory.

Empirical attempts to establish correlations between properties of porous media are futile unless additional parameters are introduced. A parameter often invoked is the tortuosity. Tortuosity is related to the fact that the actual flow path of the fluid is greater than the apparent path length across the medium. As the Kozeny equation neglects the tangential component of the velocity, the equation is extended by introducing the tortuosity \( \Upsilon \) as an undetermined factor. This leads to the expression

\[ k = \left( \frac{c}{\Upsilon} \right) \left( \frac{\phi}{S_0 (1 - \phi)} \right)^2 \phi. \]  

\[ (3.5) \]
3.3 Recovering the length scales of hydrodynamic interest

To date the tortuosity could not be directly measured. It has therefore been largely used as an additional arbitrary parameter relating the theoretically predicted permeability to the measured permeability.

Carman[44] first realized the need to introduce a geometrical parameter similar to the tortuosity into the Kozeny theory. By fitting experimental data on packed beds he determined the best value of the tortuosity $\Upsilon \approx \frac{5}{2}$. The Kozeny-Carman relation discussed in Chapter 2 is thus given by:

$$k = \left(\frac{1}{3}\right)(\frac{\phi}{S_0(1-\phi)})^2 \phi.$$  \hspace{1cm} (3.6)

The prediction of the model is shown in Fig. 3.1. The theory is in reasonable agreement with the data at higher porosities.

![Figure 3.2: Comparison of the length scale $\ell$ (in lattice gas units) defined by the different empirical models plotted as a function of porosity.](image)

(□) Hydraulic radius, $\ell = \frac{\phi}{S_0(1-\phi)}$:  (△) $\ell = \frac{\phi D_p}{\sigma(1-\phi)}$.  

...
As noted in Chapter 2 excellent correlations for flow in random porous media, particularly at lower porosities, is given by the Blake Kozeny equation[40]. We remind the reader of the derivation of this equation. In this model, the specific surface of the porous medium is related to the average particle size within the medium. Defining the mean particle diameter $D_p$ as the diameter of the hypothetical sphere with the same $S_0$ as the medium, one can express $D_p = \frac{6}{S_0}[41]$. This approximation, coupled with a slight change in the geometric factor $k_0$ to $\frac{6}{25}$ \((\tau = \frac{25}{12})\), gives:

$$k = \left(\frac{6}{25}\right)(\frac{D_p}{6(1-\phi)})^{2\phi}.$$  \hspace{1cm} (3.7)

The comparison of the prediction of the Blake-Kozeny equation with the experimental data has been shown also in Fig. 3.1. The length scale $\ell$ in the Blake-Kozeny model is given by $\ell = \frac{\phi D_p}{6(1-\phi)}$. It is difficult to justify that the length scale based on the mean particle size $D_p$ is a more meaningful measure of the length scale of a porous media than the hydraulic radius[45]. Large differences in the two length scales are evident at lower porosity. A plot of the magnitude of the length scales defined by Eqn. (3.4) and (3.7) is given in Fig. 3.2.

The parameter $k_0$ accounts for the connectedness, pore shape, coordination and tortuosity of the flow paths. The lattice gas method enables one to determine the tortuosity of a random media, and thus directly measure the structure factor $k_0$ of the medium.

From the LGA simulations, the volumetric flow speed at each node within the pore space of the medium is known. To determine the tortuosity of the medium we record all streamlines ($>2000$) crossing every lattice node along an inlet plane. We then trace the streamlines through the medium until they pass across a chosen outlet plane. The integral length, $L_i$, of the $i$th streamline is measured. The streamline tortuosity $T_i$ is then defined by $T_i = \frac{L_i}{L_f}$ where $L_f$ is the macroscopic distance between the up-stream and down-stream planes. The number of steps it takes to move along the streamline is recorded as $t_i$. As the overall volumetric flow varies greatly from one streamline to another, we do not define the tortuosity factor by simply averaging over the N streamlines $\sum_{i=1}^{N} T_i/N$. We choose instead to weight the streamline tortuosities
3.3 Recovering the length scales of hydrodynamic interest

by the overall volumetric flow associated with the streamline, which is proportional to $t_i^{-1}$. We therefore define a macroscopic tortuosity factor $T \equiv T_L$ of our random media as,

$$T = \frac{t_i^{-1}T_i}{\sum_{i=1}^{N} t_i^{-1}}.$$ 

All of the popular hydraulic radius theories assume the structure factor $k_0$ is approximately constant over a wide porosity range. For example, Carman determined experimentally that the best value for the tortuosity factor is $\frac{5}{2}$ for the range of porosity $0.90 \leq \phi \leq 0.25$[44]. The Blake-Kozeny equation assumes $\Upsilon = \frac{25}{12}$. Our determination of the tortuosity factor $T$ as a function of porosity is shown in Fig. 3.3. According to the definition of $k_0$ the tortuosity $\Upsilon$ of the medium should be given by $T^2$. Based on this definition we find that $\Upsilon$ varies from 1.0 at porosities near 0.90 up to values greater than fifty at porosities less than 0.40. Clearly the models do not correctly account for the strong effect of the structure of the medium. The quantities $T$ and $T^2$ have been defined by various authors as the true tortuosity of the medium. We

Figure 3.3: The tortuosity factor $T \equiv T_L$ as a function of porosity.
Figure 3.4: Kozeny theory prediction with the two definitions of the tortuosity $\Upsilon$ defined in the literature. (-----) shows the prediction of the original Kozeny theory ($\Upsilon = 1$). The two other curves show the prediction of equation 3.4 with the tortuosity $\Upsilon$ given by: $\Upsilon = T$ (-----) and $\Upsilon = T^2$ (---------).

believe that the actual value will lie somewhere between these values [46]. We show in Fig. 3.4 the Kozeny theory prediction by equation 3.5 with our direct determination of $\Upsilon$. The introduction of either definition of $\Upsilon$ greatly improves the prediction of the Kozeny theory.

In the literature there is frequent disagreement between the experimentally measured permeability of a porous sample and the permeability as predicted by the Kozeny-Carman equation. Authors often make a controversial claim that higher sample tortuositities are experienced in the experimental samples than are accounted for by theory[47]. The results discussed here support these claims, particularly at
lower porosities.

That the hydraulic radius concept gives an excellent match to the data with a correct evaluation of the tortuosity is a confirmation that this remarkably simple concept known to be a good approximation under turbulent flow conditions is valid for study of creeping flow in porous media. The results of our study show however that the approximation used in most hydraulic radius theories, that the tortuosity can be considered approximately constant over a wide range of the porosity, is incorrect. The geometrical parameter associated with the tortuosity of the medium has a marked effect on the flow properties of porous media. The Blake-Kozeny equation, which matches the data very well, does not predict a change in the structural factor $k_0$ over all porosities, in clear contradiction to the results of this study. The success of this model is due to the circumstance that the approximation $S_0 = 6/D_0$ corrects in the same manner as an increasing tortuosity for lower porosities and is not based on a more meaningful measure of the length scale associated with the pore structure.

3.4 Conclusion

Relating the permeability to other macroscopic properties of a porous medium has to date been chiefly empirical. The lattice gas method allows one to describe macroscopic flow phenomena using large-scale averaging, but more importantly, provides microscopic detail crucial to the understanding of relationships between the volume-averaged parameters. As direct extention of this work, it is important to ascertain which parameters in the determination of macroscopic flow properties in more general porous media are most meaningful, i.e. the effect of particle shape and size on the permeability of unconsolidated media. In these cases the empirical models have difficulty defining meaningful parameters to characterize shape and packing structure.
Chapter 4

Direct Measurement of Electrical and Hydraulic Tortuosity in Porous Solids

In this chapter, I shall discuss the comparison of the direct evaluation of the fluid-flow field with electrical conductivity of model three dimensional random porous medium at a microscopic level. It allows a direct test of the popular assumption that fluid-flow and electrical current follow equivalent flow paths in sedimentary rocks. Visualization of the fluid-flow and electric-current streamlines within identical porous samples show this assumption is incorrect. The tortuosity factors, characterizing the geometry of the flow paths associated with fluid-flow and electrical current transport, are directly evaluated. Fluid-flow tortuosity is systematically larger than the electrical tortuosity, and can differ by as much as an order of magnitude at lower porosities.

4.1 Introduction

Fluid flow and electrical current transport in porous media are governed by similar macroscopic laws which state the proportionality between a driving force and the
resultant flow. In fluid flow, the average flow velocity $v$ under a pressure gradient $\nabla \cdot P$ is governed by Darcy's law, as follows;

$$v = -\frac{k}{\mu} \nabla \cdot P,$$

where $\mu$ is the fluid viscosity. The analogous defining equation for the electrical conductivity of the same porous rock, where the saturating fluid is a conductor and the solid phase is an insulator, is Ohm's law;

$$J = -\sigma \nabla \cdot V,$$

where $J$ is the current density, $\sigma$ is the measured rock conductivity and $\nabla \cdot V$ is the potential gradient.

Both processes are described by the same equation and the flow characteristics are controlled by the volume of the pore space rather than the rock matrix. Due to the close correlation between the two processes it is commonly assumed that ions flowing through the rock under a potential gradient follow the identical flow paths to fluid flowing under a pressure gradient. This assumption has been questioned recently[48]. Direct verification of this approximation is difficult. The flow pathways for electrical and hydraulic fields must be determined by independent means in order to perform a valid check on the approximation. Detailing the local conductivity and fluid-flow configurations on the same porous samples seems impossible. The implementation of our lattice gas methods [3] have been shown to be capable of solving these problems. We directly evaluate the fluid-flow and electrical conductivity of three dimensional random porous medium at a microscopic level. This allows a direct test of the popular assumption that fluid-flow and electrical current follow equivalent flow paths in sedimentary rocks. Visualization of the fluid-flow and electric-current streamlines within identical porous samples show the assumption is incorrect. The tortuosity factors, characterizing the geometry of the flow paths associated with fluid-flow and electrical current transport, are directly evaluated. The hydraulic tortuosity $T_h$ ranges from one to greater than fifty at porosities less than 30%. The electrical tortuosity $T_e$ ranges from one to ten. $T_e$ exhibits systematically lower values than $T_h$ on identical
samples over a wide range of porosities. The difference $\frac{\eta}{\eta_c}$ can be as large as an order of magnitude at lower porosities. This analysis clearly shows that the assumption of equivalent flow paths for fluid-flow and electrical current in sedimentary rocks is incorrect.

4.2 Simulation

The simulation for evaluating the hydraulic tortuosities are performed on CM2 as described in Chapter 1 and Chapter 3. A minimum of four simulations are performed for each porosity and over thirty porosities are studied. The full local fluid flow velocities at equilibrium are recorded and used for the analysis of fluid flow pathways.

Evaluating the conductivity of identical porous media requires the solution of the Laplace equation the three dimensional system. A finite difference scheme is used to approximate the field. A CM5/CMSSL iterative solver with conjugate gradient methods have been extensively used to solve the system on a 32 node CM5. For details, refer to Appendix A. Local information of current flow across the system are obtained and used for analysis of the electrical current pathways.

4.3 Visualization of Flow Pathways

From the simulations, the localized fluid-flow and local electrical current pathways are known at each node within the pore space of the medium. We can therefore trace all streamlines passing through the medium from a chosen inlet plane to an outlet plane. We show in Fig. 4.1 examples of streamlines for the flow and the conductivity fields at two porosities. Fig. 4.1(a) shows the fields for identical samples and identical initial positions chosen on the inlet plane. It is clear that the pathway for fluid flow is less direct than the pathway for electrical current. A difference between fluid and current streamlines is noticeable even at a high porosity $\phi = 0.50$. The differences are more abrupt for a lower porosity $\phi = 0.35$. Most sedimentary rocks exhibit porosities in the
Figure 4.1: Fluid flow and electrical current flow streamlines on porous media samples at different porosities. The thicker lines represent fluid flow pathways; the thinner lines electrical current pathways. (a) at porosity 0.50: the neighbouring positions chosen along the inlet plane for the streamlines shown are [10,31],[11,31] and [11,32]. The individual electrical streamline tortuosities $\frac{L_{\text{elec}}}{L}$ are 1.27, 1.33, and 1.32 and the hydraulic tortuosities $\frac{L_{\text{hyd}}}{L}$ are 1.62, 1.76, and 1.79. (b) at porosity 0.35: the variation in streamline length is more pronounced. The position along the inlet plane for the streamline shown is [24,24]. The electrical streamline tortuosity $\frac{L_{\text{elec}}}{L}$ is 1.75 and the hydraulic tortuosity $\frac{L_{\text{hyd}}}{L}$ is 4.2. (c) at porosity 0.35: this figure shows the streamline patterns orthogonal to the flow direction. More pronounced lateral flow is evident in the case of fluid flow than electrical current.
range $0.10 < \phi < 0.40$. Clearly the assumption of equivalent flow paths for fluid flow and electrical current is incorrect. A difference between hydraulic and current flow in porous media has been observed previously by David[48] from a critical path analysis on two-dimensional networks exhibiting a heterogeneous pore size distribution. The present results confirm that the flow paths for hydraulic flow and electrical current are different even in a homogeneous porous medium.

4.4 Evaluation of Electrical and Hydraulic Tortuosity

We now consider macroscopic measurements of the geometry of flow paths. In particular, the tortuosity factor is measured. As discussed in equivalent channel models, the whole pore space is approximated by a single straight channel, the size of which is given by the so-called hydraulic radius $R_h$, that is the ratio of the pore volume to the pore surface. The model deals with a scalar $T_h$, the hydraulic tortuosity factor, which provides a way to quantify the increased length of the actual fluid flow path compared to the apparent length in the direction of the driving force for fluid flow[30, 34, 47]. This definition of the tortuosity factor is rather vague and this parameter cannot be measured directly in laboratory or field experiments. A common approximation is to correlate this term using electrical conductivity measurements on the same rock saturated with an electrolyte[49, 50]. In the equivalent channel model one writes the permeability ($k$) and conductivity ($\sigma$) in the form:

$$k = \frac{\sigma_0 \phi}{T_h} R_h^2 \quad (4.3)$$

$$\sigma = \frac{\sigma_0 \phi}{T_e} \quad (4.4)$$

The common approximation for $k$ is based on using the easily measured factor $\frac{\phi}{T_e}$. 
as an estimate of \( \frac{\mu}{\eta} \). The flow paths in this approximation are implicitly assumed to be the same. From the Visualization in Fig. 4.1 we know this assumption is incorrect. From our simulation we measure the quantitative difference between \( T_h \) and \( T_e \). For the definition of the hydraulic tortuosity, we refer to section 3.3. The electric tortuosity of the medium is defined in a similar manner as for the hydraulic tortuosity – except that the field of local fluid velocity for tracing the hydraulic streamlines is derived from the averaging over 2,000 steps of lattice gas steps while the electric field for tracing out the electric current streamlines is derived from solution of the Laplacian equation with the boundary values set to unity and zero at the inlet and outlet planes, correspondingly. The local current field is derived from the electrical potential field and scaled to the velocity field of the tracers. This is an analogy of the velocity field for the fluid flow in the same porous medium on which the LGA simulation is performed. Similarly, one tracer is released from every lattice node along a chosen up-stream plane and advanced at the position-dependent velocity derived by interpolating the velocities on the nearest neighbouring lattice nodes. The trajectories (streamlines) of the tracers are traced through the medium until they pass across a chosen down-stream plane. The effective length, \( L_{\text{eff},i} \), of the \( i \)th streamline is measured. The streamline tortuosity \( T_{e,i} \) is then defined by \( T_{e,i} = \left( \frac{L_{\text{eff},i}}{L} \right) \) where \( L \) is the macroscopic distance between the up-stream and down-stream planes. The number of steps it takes to move along the streamline is recorded as \( t_i \). As the overall volumetric flow varies greatly from one streamline to another, we do not define the tortuosity factor by simply averaging over the \( N \) streamlines \( \sum_{i=1}^{N} T_{e,i}/N \). We choose instead to weight the streamline tortuosities by the overall volumetric flow associated with the streamline, which is proportional to \( t_i^{-1} \). We define the phenomenological electrical tortuosity factor \( T_e \equiv \left( \frac{L_{\text{eff}}}{L} \right)^2 \) of our random media as:

\[
T_e = \left[ \frac{\sum_{i=1}^{N} t_i^{-1} T_{e,i}}{\sum_{i=1}^{N} t_i^{-1}} \right]^2
\]  

(4.5)

Most equivalent channel theories assume the tortuosity \( T_h \) is approximately constant over a wide porosity range. For example, Carman determined experimentally that the best value for the tortuosity factor is \( \frac{3}{2} \) for the range of porosity \( 0.90 \leq \phi \leq 0.25[44] \).
Our determination of the tortuosity factor $T_h$ as a function of porosity is shown in Fig. 4.2. As discussed in Chapter 3 $T_h$ varies from one at porosities near 0.90 up to values greater than fifty at porosities less than 0.30.

From the conductivity simulations the local current at each node within the the pore space of the medium is also known. To determine the electrical tortuosity of the medium we again record all current 'streamlines' crossing every lattice node along the inlet plane. The trace of the streamlines through the medium allows a similar evaluation of $T_e$. The determination of the electrical tortuosity factor $T_e$ as a function of porosity is also shown in Fig. 4.2. We find that $T_e$ varies from 1.0 at porosities near 0.90 up to values of slightly less than ten at porosity of 0.30. The predicted tortuosity is well within the range of 'experimental' tortuosities for conductivity measurement on sandstones[34, 51] which ranged from 2 to greater than 10 for porosities less than
Fig. 4.2 highlights the large error incurred in assuming the tortuosity factor associated with fluid flow and electrical current are identical. Paterson[49] suggested that the error incurred from the approximation could be as large as a factor of two. The difference between the two macroscopic measures is up to an order of magnitude for porosities less than 30%. The analysis clearly shows that the macroscopic tortuosity factors for fluid flow and electrical current are not equivalent—particularly for porosities exhibited by sedimentary rock (\( \phi < 40\% \)). For porosities lower than those measured in this study one can only expect that the discrepancy between the two measures increases.

4.5 Conclusion

Fluid flow and electrical current transport are governed by similar macroscopic laws which state the proportionality between a driving force and the resultant flow. In this regard both problems are formally equivalent, and the conducting elements can be either electrical conductances or hydraulic conductances. It is tempting therefore to assume that the electrical current and fluid follow the same paths within porous material and so the tortuosity for the two processes is the same. Our analysis clearly shows that this approximation is incorrect — particularly for porosities exhibited by sedimentary rock.
Chapter 5

Fluid flow across fractal structures

5.1 Introduction

Flow and transport in systems with fractal and self-affine surfaces and boundaries are relevant to a wide variety of scientific and industrial problems. For example, natural porous media and rock contain a wide variety of pores and fractures with broad distributions of sizes and shapes. There is now experimental evidence [52, 53] that the internal surface of the pores and the fractures is very rough, and that the roughness obeys fractal statistics. Conventionally fracture surfaces were modelled as perfectly smooth, and flow in a single fracture was modelled as flow between parallel flat plates. Volumetric flow rate $Q$ is then given by, $Q = (w\delta^3 \Delta P)/(12\eta L)$, where $w$ is the width of the fracture and $\delta$ its aperture, $\Delta P/L$ is the pressure gradient along fracture, and $\eta$ is the viscosity of the fluid. Thus, according to this model $Q$ depends on the third power of $\delta$, and the permeability $K$ of the fracture varies as $\delta^2$. However, there is ample experimental evidence [54, 55, 56] for deviations from the cubic law, $Q \sim \delta^3$, which has been attributed to the roughness of the fracture surface. Attempts to quantitatively verify this prediction is problematic. Flow in a single fracture with a realistic shape cannot be solved analytically, and only numerical solutions of the problem can be obtained. The numerical methods used so far have been mostly based on discretizing the governing equations, the usual continuity and
5.1 Introduction

the Stokes’ equations, by a finite-difference or finite-element method and solving the resulting equations. If the effect of surface roughness of a fracture is to be taken into account, the grid has to be very refined near the surface and this requires prohibitive computations.

The problem of hydrodynamics of particles or aggregates dispersed or suspended in a fluid is a second example of a flow problem of considerable importance to a wide variety of natural or man-made systems including colloids, polymers, granular and composite materials and ceramics. Colloidal particles for example, flocculate irreversibly and form aggregates which exhibit a fractal structure. The aggregates have a very low density when compared with bulk matter, yet they are very effective at screening hydrodynamic forces. The quantitative nature of the force depletion around this mass fractal structure is important as these materials are used for these screening properties, e.g. as thickeners in fluids. The most important theoretical and practical problem is to predict the effective equilibrium and transport properties of these materials, from a knowledge of their microstructural mechanics. The microstructural mechanics entails the distribution of various forces acting on the particles, such as the hydrodynamic, Brownian, and interparticle forces, as well as the morphology or the microstructure of the particles. From the knowledge of microstructural mechanics, the physical properties of the particles and the fluid that surrounds them, and the location and motion of the boundaries of the system, one can, in principle, predict the macroscopic properties of the system with the given configuration, such as the diffusion coefficient and the thermal conductivity. Although this is a well-defined boundary value problem, it is non-trivial, as one has to deal with a many-body problem. To tackle this problem, various schemes have been developed in the past [57]. The problem is particularly difficult when the particles or aggregates have a complex shape. Colloidal aggregates [58, 59, 60] are fractal objects with very complex structures, and moreover their properties scale with their linear size or mass, so that their true fractal behaviour does not manifest itself, unless the size of the aggregate becomes large. For these reasons, calculating various properties of aggregates that are suspended in a flowing fluid, such as the distribution of the hydrodynamic forces
5.2 Flow in a Single Fracture with Fractal Surfaces

that act on the aggregates, and the dependence of the friction factor on the Reynolds number, is a computationally difficult problem. Even sophisticated approaches that have been developed in the past [57] cannot be used with aggregates of more than a few hundred particles, unless one is willing to use a prohibitive amount of computer time. Moreover, the distribution of hydrodynamic forces exerted by the fluid on the particles of the aggregate becomes very broad, since (relatively) large forces will be exerted on the most exposed parts of the aggregate, whereas the particles deep inside the aggregate will feel small forces. These measures require the consideration of large aggregates.

In this chapter, we use the lattice gas simulation to study flow in a three-dimensional fracture with self-affine fractal surfaces, and to evaluate the distribution of the hydrodynamic forces that are exerted on a colloidal fractal aggregate that is suspended in a slowly moving fluid.

The plan of this chapter is as follows. In next section, I shall concentrate on the results of simulation for flow in fractures with rough surfaces and in the following section, the results for the hydrodynamics of flow over DLA aggregates are presented. The chapter is summarized in last section, where a few points concerning the future directions in this research field are made.

5.2 Flow in a Single Fracture with Fractal Surfaces

The morphology of fracture surfaces is strongly dependent on the material, its fracture mechanism and the scale of observation. There has been much progress recently in the statistical characterization of the topography of fracture surfaces. In particular, the observation of scale invariance has been made in many experimental cases leading to a more reliable description of the statistics of fracture roughness. It has been shown in many instances that fracture surfaces exhibit statistically self-affine scaling properties. A self-affine surface \( z(x, y) \), isotropic in the \( (x, y) \) plane, in invariant under the scale transformation \( (\lambda x, \lambda y, \lambda^H z) \) where \( H \) is the roughness exponent. For simulating
flow in a single fracture, the fracture is modelled by a three-dimensional channel whose surface is rough and obeys fractal statistics. The roughness of the surface was generated by a fractional Brownian motion (fBm)\cite{61}, which is a stationary stochastic process $B_H(r)$ with the following properties

\begin{equation}
\langle B_H(r) - B_H(r_0) \rangle = 0 ,
\end{equation}

\begin{equation}
\langle [B_H(r) - B_H(r_0)]^2 \rangle \sim |r - r_0|^{2H} ,
\end{equation}

where $r=(x, y, z)$ and $r_0=(x_0, y_0, z_0)$ are two arbitrary points, and $H$ is the roughness or Hurst exponent. A remarkable property of fBm is that it generates correlations whose extent is infinite. For example, if we define a one-dimensional correlation function $C(r)$ by

\begin{equation}
C(r) = \frac{\langle -B_H(-r)B_H(r) \rangle}{\langle B_H(r)^2 \rangle} ,
\end{equation}

then one finds that $C(r) = 2^{2H-1} - 1$, independent of $r$. Moreover, the type of correlations can be tuned by varying $H$. If $H > 1/2$, then $C(r) > 0$ and fBm displays persistence, i.e., a trend (for example, a high or low value) at $r$ is likely to be followed by a similar trend at $r + \Delta r$. If $H < 1/2$, then $C(r) < 0$ and fBm generates antipersistence, i.e., a trend at $r$ is not likely to be followed by a similar trend at $r + \Delta r$. For $H = 1/2$ the trace of $B_H(r)$ is similar to that of a random walk, while $H = -1/2$ represents the white noise limit. It has been shown by Schmittbuhl et al. \cite{62} that, if we consider a two-dimensional roughness profile on a fracture surface, then the average height $h$ of the profile is related to its length $L$ by

\begin{equation}
h \sim L^H ,
\end{equation}

where $H$ is the roughness or Hurst exponent defined above. A value $H \approx 0.85$ was found by Schmittbuhl et al. for granitic faults, indicating strong positive and long-range correlations. In the present chapter, we use a range of values for $H$ in order to assess its effect on the permeability of the fracture and its relation with the fracture aperture. Fig. 5.1 shows an example of a two-dimensional rough surface generated
5.2 Flow in a Single Fracture with Fractal Surfaces

Figure 5.1: Two self-affine surfaces generated using fBm. The two surfaces are aligned on top of each other to model a crack or rock joint.

by the fBm. Fig. 5.2 illustrates the slices of the crack when separation between the upper and lower surfaces is adjusted.

Once the roughness of the surface is generated, simulation of the flow problem is started. We used an $L_x \times L_y \times L_z$ system, where $z$ denotes the direction of flow, and in our simulations $L_x = L_y = 64$ and $L_z = 128$ (all distances are measured in units of lattice gas bonds). The simulations start by introducing a flat velocity profile (piston flow) at the entrance to the fracture. We then allow the system to relax and reach a steady state. Typically, this is achieved after about 8,000 time steps, after which we measure the desired quantities for another 2,000 time steps. The pressure gradient $\Delta P/L_z$ in the system is measured by calculating the momentum transfer across imaginary planes perpendicular to the flow direction. A fit to the permeability
Figure 5.2: To illustrate how we vary the average aperture of the crack, two fracture surfaces generated from the simulation of fracture are imposed on top of each other to model the crack. From top: (a) the two surfaces are initially at large separation; (b) the two surfaces are then pushed together and (c) at very small separation the porous medium-like structure appears.
5.2 Flow in a Single Fracture with Fractal Surfaces

$k$ of the fracture is then calculated by using Darcy's law:

$$v = \frac{-k \Delta P}{\mu L_z},$$  \hspace{1cm} (5.5)

where $v$ is the average fluid speed and $\mu$ is the fluid viscosity. The simulations are carried out at low enough Reynolds number to ensure that Darcy's law is applicable. The results are then averaged over a minimum of 20 different realizations of the fracture for a given $H$, the Hurst exponent.

5.2.1 A comparison between hydrodynamic properties of flat surface and fractal surface

Rock fractures are commonly modelled as a pair of parallel plates, where the fracture surfaces are smooth and parallel with a constant separation or aperture. For this geometry, the steady state solution of the Navier-Stokes equations for laminar flow yields a cubic law; the volumetric flow rate is proportional to the cube of the aperture. We first compare the fluid flow properties in this model flat crack geometry with that of realistic rough cracks.

We show in Fig. 5.3(a) a parabolic velocity profile rendered from flow between parallel smooth surfaces in LGA. This profile is well developed after less than 3,000 automaton step at cross-sections along the channel—the one shown in the figure is taken from the mid-plane along the channel. A detailed plot of the streamlines of the flow in this channel shows the streamlines to be straight through all the regions of the channel.

Shown in Fig. 5.3(b) is a plot of streamlines of steady fluid flow in a crack with self-affine roughness. The crack axis is shown vertically in the plot. The pressure bias is applied along the crack from bottom to top of the plot. The streamlines are generated by tracking and following the local fluid flow starting from the nodes at central lateral position and same vertical position but different positions into the paper (in the third dimension). We define local aperture as the distance between upper and lower surfaces of the crack along the third dimension (into the paper).
Figure 5.3: (a) Fluid speed profile after 3,000 automaton step at \( Z = 64, Y = 31 \) in a square channel. Pressure bias is applied along the elongated direction. The dashed line is the fit to the parabolic curve. (b) The background greyscale shows the aperture size of the crack at the point. The darker the regions signify smaller local openings between the upper and lower surfaces. Lines are streamlines starting from same position along the lateral direction and dispersed in the course of flowing downstream along the crack.
5.2 Flow in a Single Fracture with Fractal Surfaces

The grayscale background in Fig. 5.3(b) illustrates local aperture; excluding the solid regions to the left and right in the plot, the lighter shades signify a larger local aperture. All the chosen streamlines are projected onto the grayscale aperture map. As we can see, the streamlines are distorted and dispersed considerably. Assuming a simple parabolic fluid velocity profile clearly leads to significant errors.

5.2.2 Permeability of single cracks

We now consider the dependence of the permeability of the fracture on the fracture aperture. For this purpose, we generate self-affine surfaces of the thickness $\ell$. The aperture $\delta$ is then defined as the distance between the two mean surfaces perpendicular to the flow direction; $\delta = L_y - 2\ell$. Aperture is varied by pushing the two surfaces of

![Graph](image)

Figure 5.4: The upper and lower surfaces are of $H=0.8$: (△) for $\ell = 10$, which gives $\beta = 2.64$; (⋆) for $\ell = 18$, which shows a transition at medium aperture range, it gives $\beta = 2.71$ for bigger separation of upper-lower surfaces and $\beta = 1.99$ for smaller separations.
5.2 Flow in a Single Fracture with Fractal Surfaces

Figure 5.5: The upper and lower surfaces are of $H=0.8$. The plot are now scale to the dimensionless aperture which correlates the thickness of the surfaces and the separation of the upper and lower surfaces: $(\triangle)$ for $l=10$, which gives $\beta = 2.64$; $(\times)$ for $l=18$, which shows a transition at medium aperture range, it gives $\beta = 2.71$ for bigger separation of upper-lower surfaces and $\beta = 1.99$ for smaller separations.

constant $\ell$ together.

To probe large separation $\delta$ requires large grids. Due to the limitation of the CM2 machine, it is not practical for us to vary the $\delta$ and $\ell$ seperately on a large range. We instead choose to reduce $\ell$ and to probe the region where $\delta > \ell$. We introduce a dimensionless aperture $A_s$ which allows us to investigate a wide range for $\delta > \ell$; this takes the form:

$$A_s = \frac{\delta}{\ell}. \quad (5.6)$$

Companying the definition of dimensionless aperture $A_s$, a representative permeability
5.2 Flow in a Single Fracture with Fractal Surfaces

Figure 5.6: The upper and lower surfaces are of \( H = 0.3 \): (\( \triangle \)) for \( \ell = 10 \), which gives \( \beta = 3.09 \); (\( \times \)) for \( \ell = 18 \), it gives \( \beta = 3.30 \).

\( K_s \) of the system is defined as,

\[
K_s = \frac{k}{\mu \ell^2},
\]

where \( \mu \) is the viscosity of the fluid and \( k \) is the permeability.

The Fig. 5.4 shows the dependence of \( k \) on the aperture for \( H = 0.8 \) for the two values of \( \ell \). \( H = 0.8 \) is a value close to what Schmittbuhl et al. [62] measured for fracture surfaces of rock. As can be seen in both cases, one has

\[
k \sim \delta^\beta,
\]

with \( \beta \approx 2.64 \), except that for \( \ell = 18 \) one has an apparent crossover to \( \beta \approx 2 \). This crossover is associated with the significant overlap of the rough fracture surfaces. In this case, the system reverts to behaving like a simple porous medium. From Darcy’s law we would expect \( \beta = 2.0 \) in a porous medium. The results for \( \ell = 10 \) and \( \ell = 18 \) at large separations differ however from the classical result for fracture with smooth surfaces (\( \beta = 2 \)).
Figure 5.7: The upper and lower surfaces are of $H = 0.3$: (△) for thickness of surface $\ell = 10$, which gives $\beta = 3.09$; (×) for $\ell = 18$, which gives $\beta = 3.30$.

The effect of a range of dimensionless aperture on permeability is shown in the Fig. 5.5. The permeability curves for different $\ell$ overlap. This indicates that the dimensionless parameters chosen capture the major geometric characteristics of the system discussed here.

We now consider the effect of varying $H$. Fig. 5.6 shows the results for $H = 0.3$. No obvious crossover is noted for either value of $\ell$. In both cases we find $\beta \simeq 3.20$, significantly different from the classical results. Fig. 5.7 shows the plot for dimensionless aperture. This illustrates the range of separation distance $\delta$ we are probing. In this case, it is perhaps surprising that no crossover at small $\delta$ to Darcy's behaviour nor at large $\delta$ to channel-like flow is observed.

We observe that as the Hurst exponents of the self-affine surfaces decreases, the exponents $\beta$ increases. To observe how strong the deviation from classical ($\beta = 2$) behaviour can become, we performed simulations on crack with very rough surfaces;
5.2 Flow in a Single Fracture with Fractal Surfaces

Figure 5.8: The upper and lower surfaces are of $H = -0.5$ and of $l = 14$: upper slope $\beta$ was found to be 4.15 and the lower found 5.18.

$H = -0.5$. The result is summarized in Fig. 5.8. We find the exponent of the permeability curve to be 4.15 in the range of bigger apertures and 5.18 for very small apertures.

The significant difference between these simulation results discussed here and the classical results clearly suggest the important role roughness of the fracture surface plays on flow properties. Our simulations show quantitatively that experimentally observed deviations from the cubic law can be attributed to surface roughness.
The next problem considered is for fluid flow over a fractal aggregate. This study represents the first step towards one of the ultimate goal of this group, studying suspensions of colloidal aggregates and their dynamical properties, such as the vis-

Figure 5.9: Simulation of hydrodynamic screening force on a DLA cluster. The DLA cluster shown is of mass 349 and immersed in quiescent fluid field. The cone on each sphere (particle) represents the direction (orientation) and magnitude (length) of the force exerted by fluid flowing around sphere. Bounding box shows the extent of the cluster.
cocity of the suspension. It is now well established that many colloidal aggregates have a fractal structure. The fractal object studied here is the three-dimensional DLA aggregate which has been extensively invoked as a model structure for colloidal aggregates[60]. The three-dimensional DLA cluster has a fractal dimension $D_f \approx 2.5$. A similar problem has already been studied by Meakin[63, 64], who used the Kirkwood-Riseman theory to investigate hydrodynamics of a fractal aggregate moving with a constant velocity in a quiescent fluid. However, due to computational difficulties, Meakin’s study was limited to the consideration of only very small aggregates with at most 400 elementary particles in them (Meakin used diffusion-limited cluster-cluster aggregates which have a fractal dimension $D_f \approx 1.8$ in three dimensions).

Using the LGA method, we have studied the problem with aggregates whose masses $M$ varied between 427 and 4507 particles. The size of aggregates is limited by the configuration of the local CM2. The DLA cluster was first generated and then placed on the lattice system. For clusters with $M < 800$, $32 \times 32 \times 64$ lattices was used, while for the larger aggregates, $64 \times 64 \times 128$ lattices was used. Periodic boundary conditions were used in the lateral directions to minimize the effect of the finite lattice size. No-slip boundary conditions are used at the interface between the fluid and solid phases. The simulation details are similar to those described previously. At the entrance to the system, a velocity profile is introduced, and the system (fluid plus the solid phase) is allowed to relax. In this problem, the system reached equilibrium after about 5,000-6,000 time steps. In practice, the measurement of various quantities of interest after 7,000 automaton steps and are averaged over the next 3,000 steps. The results were then averaged over more than 100 realizations of the system. Fig. 5.9 shows a simulation result: a cluster immersed in the fluid with local forces associated with fluid flow illustrated for each particle.

The hydrodynamic force distribution on the surface of a fractal aggregate reflects the flow rate near the aggregate and the multifractal distribution of force components associated with the fractal aggregates may have important implications for
We choose to focus on the distribution of hydrodynamic force component parallel to the macroscopic flow direction. The logarithmic distribution of the parallel force component $F_\parallel$ is defined as,

$$N(ln(F_\parallel), \Delta F_\parallel) = N(ln(F_\parallel)) \Delta F_\parallel,$$

where $N(ln(F_\parallel), \Delta F_\parallel)$ is the number of particles the force components of which lie in the interval $(ln(F_\parallel), ln(F_\parallel) + \Delta F_\parallel)$ and $\Delta F_\parallel$ is given constant small value in practice. The distribution of force component can also be presented in terms of the distribution
of normalized force components. A normalized parallel force component \( F_{||}^n \) is given by,

\[
(F_{||}^n)_i = \frac{(F_{||})_i}{\sum_{j=1}^{M}(F_{||})_j},
\]

where \((F_{||})_i\) is the corresponding unnormalized force component parallel to the flow direction and \(M\) is the total number of particles in the cluster. The distributions of the normalized force are shown in Fig. 5.10 for various aggregate sizes. These distributions are skewed and similar to a log-normal distribution.

It has been shown that the distribution of the force components on the particles exerted by the fluid flowing across a diffusion-limited cluster-cluster aggregate and the scaling of this distribution with the cluster size can be described in terms of a fractal measure or a multifractal distribution [60]. Such distributions can be described in terms of an infinite family of moments and associated fractal dimensionalities [65, 66, 67, 68].

It has also been shown that construction of a spectrum \(f(\alpha)\) of singularities can be an useful measure of multifractal properties [69]. The \(f(\alpha)\) is the fractal dimensionality of the subset on which the singularities of \(\alpha\) lie. This picture is a useful description for a variety of dynamics. It has been found to be applicable to a variety of other processes such as the growth of fractal aggregates, voltage distributions on conducting percolation clusters, the force distribution on a fractal embedded in an elastic medium, and the harmonic field near to an absorbing polymer.

In following sections, we will discuss the scaling properties that the force distributions exhibit and the multifractal scaling of these force component distributions.

### 5.3.1 Scaling properties of DLA hydrodynamics force spectrum

The force distributions shown in Fig. 5.10 suggest that they are from an infinite multifractal family, \textit{i.e.}, each of the moments scales with a different power of \(M\).
If this is true, there may be a universal scaling curve for these distributions of the hydrodynamic forces in the limit \( M \rightarrow \infty \).

The force distribution can be displayed in the form of plots of \( \ln(N[\ln(F_{||})]) \) on \( \ln(F_{||}) \). An estimation of the spectrum singularity can be obtained by plotting \( \ln(N[\ln(F_{||})])/\ln(M) \) against \( \ln(F_{||})/\ln(M) \) [70]. If multifractality exists in these distributions, which is typical in fractal aggregates, these distributions should collapse onto a single universal scaling curve in the limit \( M \rightarrow \infty \). If this is true, one may suggest a scaling form:

\[
\ln(N[\ln(F_{||}^{n})]) = \ln(M)g[\ln(F_{||}^{n})/\ln(M)],
\]

(5.11)

where \( g(x) \) is the scaling function describing the curve onto which the logarithmic force distributions shown in Fig. 5.10 should collapse. From the knowledge of \( g(x) \) one can construct a spectrum of singularities \( f(\alpha) \) [70], describing the multifractal properties of the distribution, given by

\[
f(\alpha) = D_1g(-D_1^{-1}\alpha).
\]

(5.12)

The \( f(\alpha) \) is interpreted as the fractal dimensionality of the \textit{subset} supporting singularities with a scaling index of \( \alpha \). This \( f(\alpha) \) suggests a scaling form for the force distribution [70, 71]:

\[
\ln(N[\ln(F_{||}^{n})]\ln(M)) = \ln(M)g'[\ln(F_{||}^{n})/\ln(M)],
\]

(5.13)

where \( g'(x) \) is the scaling function giving the universal scaling curve. The scaling forms given by equations (5.11) and (5.13) should result in the same scaling function \( g(x) = g'(x) \) in the limit \( M \rightarrow \infty \) [60].

Shown in Fig. 5.11(a,b) are spectrums \( g(x) \) and \( g'(x) \) in equations (5.11) and (5.13) correspondingly. For all the clusters with various mass, the spectrums are convex function with a maximum value less than or equal to unity. All spectrums resulting from Eqn. (5.13) (Fig. 5.11(b)) are of a maximum value of 1.0. This confirms the observation by Halsey \textit{et al.} [70]. Compared to the Meakin's result [60], the

\[1\text{The subset means the finite set of DLA cluster samples of limited mass.}\]
Figure 5.11: In this figure, (a) and (b) are the logarithmic distributions in Fig. 5.10 scaled by using the scaling form given by Eqn. (5.11) and Eqn. (5.13) respectively.
scaling collapse behaviour shown here is incomplete although we have used much larger aggregates. Reasons for the incomplete scaling collapse by using the analysis method outlined in this sub-section are two-fold: the DLA clusters used for this study are not large enough and the number of realizations for each mass is not sufficiently large to insure good statistics\(^2\).

### 5.3.2 Determining the spectrum of singularities \(f(\alpha)\)

Another common approach to estimate the spectrum of singularities \(f(\alpha)\) from data has been using the moment \(Z_q\) of the distribution which define a fractal measure on the system of interest. In this case,

\[
Z_q = \sum_i f_i^q
\]

where \(f_i^q\) is the force component. In this case, \(f_i\) is the normalized parallel force components. For a fractal measure, one assume that,

\[
Z_q \sim L^{-\tau(q)},
\]

where \(\tau(q) = (q - 1)D_q\), \(L\) is the characteristic system size and \(D_q\) is, in the study of this section, the fractal dimension of the three-dimension DLA \((D_q = 2.53)\). The \(\alpha\) is determined using relation,

\[
\alpha(q) = \frac{d\tau(q)}{dq},
\]

and then one can obtain that,

\[
f[\alpha(q)] = q\alpha(q) - \tau(q) = q\alpha(q) - \lim_{L \to \infty} \frac{\log(Z_q)}{\log(L)}.
\]

Fig. 5.12 shows the resulting spectrums. Fig. 5.12(a) shows the \(f(\alpha)\) obtained. That the curves do not collapse indicates that the mass of the clusters are far from the

\(^2\)The machine CM2 of SIMD structure for LGA simulation was decommissioned at the time these simulations were made due to a scheduled update to CM5. The latter of a MIMD structure is much less efficient for LGA applications specifically. The analysis on these distributions have been limited to 6 realizations for each mass studied.
5.3 Hydrodynamics of Flow over a Fractal Aggregate

Figure 5.12: Three scaling of the spectral methods: (a) $f(\alpha)$ for clusters of 3 different sizes using method outlined in this section. The system size is taken from the hydraulic radius of the individual cluster. This plot indicates that the Mass of the cluster are far from the asymptotic limit $M \rightarrow \infty$. (b) A different but convergence obtained by using the different Length $L = 2R_h$ in comparison to Fig. 5.12(a). (c) Plot made to compare with the Fig. 5.11 using $f(\alpha)/D_q$ versus $\alpha/D_q$, here $D_q = 2.53$ for 3D DLA cluster.
asymptotic limit $M \to \infty$. In Fig. 5.12(b), twice the hydraulic radius$^3$ of the clusters are used as the length $L$. In this case, the scaling collapse is obvious. Fig. 5.12(c) facilitates the comparison between $f(\alpha)$ and the results shown in Fig. 5.11. Comparing Fig. 5.12(c) and Fig. 5.11(a,b), we see that all the curves exhibit the similar behaviour; however, the spectral method used here reveals more clearly the scaling collapse associated with a multifractal distribution of parallel force components.

5.3.3 Relationship between the frictional coefficient and Reynolds number

Another important quantity is the friction factor $C_f$ and its dependence on the Reynolds number $Re$. $C_f$ is defined by

$$C_f = \frac{\tau_s}{\frac{1}{2} \rho \langle v \rangle^2},$$

where $\rho$ is the density of the fluid particles, $\tau_s$ is the shear stress on the solid surface, and $\langle v \rangle$ is the mean flow velocity. For a spherical particle in low Reynolds number fluid flow, one has the classical result[72].

$$C_f = \frac{24}{Re},$$

LGA simulations are first used to measure $C_f$ across spherical particles. The simulation result fully confirms this equation (see Fig. 5.13). Fig. 5.13 also shows the results for the DLA aggregates with three different masses. For over two orders of magnitude variations in $Re$ in the range $0.1 < Re < 10$ we have

$$C_f = \frac{a}{Re \zeta},$$

For all the studied clusters, $\zeta$ were found to be $\simeq 0.85$. No simple theoretical explanation for this value of $\zeta$ is evident.

$^3$The hydraulic radius in the current context is the root mean square radius to the center of mass of the DLA clusters. The latter confirms Meakin's observation [60] that the factor 2 gives the best collapse.
5.4 Conclusion

The study of flow in systems with rough surfaces involves complex phenomenon. While several models have been developed for studying these systems, they were not completely satisfactory and could not provide quantitative, and in some cases even qualitative, predictions for the quantities of interest. In many cases the structure of the surface of these systems obeys fractal statistics. We show quantitatively that fracture roughness accounts for strong deviations from the simple fracture flow model.
5.4 Conclusion

based on a parallel plate geometry. We also find that the friction factor across fractal aggregates has an anomalous Reynolds number dependence. In our opinion, the systems that we studied in this chapter represent definitive examples of the problems for which lattice-gas models are more appropriate than the continuum, or other discrete models. This method is the ideal tools for vector computers and parallel computations, which are the way the present massive computations are carried out. As such models become more sophisticated and realistic, more traditional numerical methods of simulating fluid flow in complex systems, such as the finite-difference methods, lose their competitive edge, and may be phased out in the future.
Part II

Fracture in Heterogeneous Media
Chapter 6

Modelling Fracture Phenomena in Heterogeneous Media

Wheat breaks in a mill and yields flour, a pair of glasses drops onto floor and shatters, a segment of highway in Los Angelas collapses in the middle of an earthquake and a pressurized nuclear reactor in Cheynobyl develops cracks in its structure and causes severe problems. Fracturing is an everyday occurrence observable in many contexts. The earliest studies date back to Galileo [73]. Recently the technological desire to understand the fracture of metals, concrete or polymers has led to much research and a large volume of literature. Little work has however considered the effect of disorder on fracture properties. We investigate in the next three chapters of the thesis the fracture properties of materials with realistic disorder.

6.1 Introduction

Every solid breaks if a sufficiently large load is applied on it. The value of this load as well as the shape and other characteristics of the resulting crack strongly depend on the material and on the way the load has been applied.

Fracture phenomena are often categorized as either brittle or ductile. As a simple
example, fresh potato chips break in a brittle manner and chewing gum in a ductile manner. The difference is best explained by a thought experiment. A rod is placed on a frame with two ends fixed to a pulling mechanism. The elongation $\delta$ is imposed on the rod and force $F$ exerted on the rod is observed. With static increase of elongation, $F$ can be plotted as a function of $\delta$. On the plot, one observes that $F$ increases with $\delta$ initially, but starts to decrease when a certain value of $\delta$, $\delta_c$ is reached. The $\delta_c$ depends on the properties of the sample material and also the temperature and pressure. If the $\delta_c$ is small, the fracture is called brittle; otherwise it is ductile. The fracture phenomena on which we are focused is in the brittle regime.

![Figure 6.1: Inter-granular fracture of steel in micron scale.](image)

The fracture characteristics of a material depends on many factors: the geometry of the material; the way the external drive is applied; the physical conditions under which the rupture or fracture occurs; material properties of the sample, etc. Disorder of material properties, which are exhibited on all scales in real materials, plays a decisive role in the process of rupture and fracture. There is ample evidence from both the engineering literature and everyday observation illustrating the effect of intrinsic disorder of materials on the resultant rupture and fracture at all length scales. Shown in Fig. 6.1 is an inter-granular fracture surface in metal on a micron scale [74]. In Fig. 6.2 the pattern of the interconnected cracks on a dried clay-rich
Figure 6.2: Cracking pattern of a clay-rich mud after drying.

Figure 6.3: Fracture (fault) map of an earthquake — prone region in Japan.

mud on a meter scale is shown [75] and Fig. 6.3 illustrates a fault map; a disordered fracture pattern on a geological scale (kilometre scale).

The traditional approaches of fracture mechanics to failure phenomena have pro-
vided the framework for analyzing a wide variety of problems *without* considering the effect of disorder. The basis for most of these traditional approaches is the criterion developed by Griffiths [76] who proposed that a *single* crack becomes unstable to extension when the elastic energy released in the crack extension by a small length $\Delta l$ becomes equal to the surface energy required to create a length $\Delta l$ of crack surface. However, this criterion is valid for solids that are essentially homogeneous; microscopic or macroscopic disorder plays no important role.

In natural rocks, and also in most engineering materials, one observes the presence of a large number of flaws with various sizes, shapes and orientations. The problem is far more complex than the one treated by Griffiths. Fracture is a collective phenomenon in which disorder plays a fundamental role. In fact, due to disorder brittle materials generally exhibit large statistical fluctuations in fracture strengths, when nominally identical samples are tested under identical loading. Because of these statistical fluctuations, it is insufficient, and indeed inappropriate, to represent the fracture behaviour of a disordered medium by only its *average* properties, an idea which is used in mean-field approaches: fluctuations are important and must not be neglected.

Accompanying such phenomenological theories has been direct numerical modelling using the finite element method (FEM). The stress field for arbitrary configurations of grains, fibers or cracks may be calculated by the FEM. The mesh size of the FEM must be smaller than the scale on which the stress field is expected to vary, which is much smaller that the relevant length scale of the disorder. Therefore, only limited regions of a disordered material can be analyzed using the FEM. To connect small-scale FEM studies to larger-scale behaviour and consider nucleation, crack interactions, and actual crack growth at a larger scale is a rather formidable, if not impossible, computational problem.

An alternative approach to FEM computations is based on identifying the key microstructural features associated with the disorder relevant to the failure process. One then subsumes all the details of the mechanical behaviour of that material region
or *element*, including the failure of the region by the nucleation of a stable crack of the same size, into a local constitutive law. Disorder is included by allowing the constitutive law to vary, according to some probability distribution, from element to element. A network of such elements, analogous to a uniform mesh in FEM, is then used to numerically calculate local stresses on, and interactions between, the elements under the application of a macroscopic stress or strain. By allowing for failure of such elements under their local stress conditions, cracks are formed which may interact, generate new cracks via load transfer, and propagate to macroscopic size, leading to material failure. Thus, one is able to account for the nucleation of cracks on the key length scales and also the effects of disorder on such phenomena. This is the essence of the approach [77] for mechanical failure of disordered media. Various versions of this idea have been developed which are now briefly described.

Generally speaking, three variations of such ideas have been developed for studying mechanical and electrical breakdown in disordered solids. These approach are based on discrete or lattice models and have provided new insight into these processes. The first and second approaches are probabilistic. One of them [78, 79] makes an analogy between mechanical breakdown and the dielectric breakdown model of Niemeyer *et al.* [80] which is closely related to the diffusion-limited aggregation models [81]. At each stage of simulations, a bond is broken with a probability proportional to a power of strain in that bond. These models give rise to fractal crack patterns, and may be appropriate for systems in which disorder is *annealed*. The second class of probabilistic models was developed by Termonia, Smith and Meakin [82] and was intended for fracture of polymeric materials. In this model, an elastic element breaks with a probability proportional to a Boltzmann’s factor, taking into account the effect of temperature, the activation and the elastic energies stored in an elastic element. These two classes of models have been discussed extensively by Meakin [83].

In the third approach which is totally deterministic, one uses a random network, each bond of which describes the system on a microscopic level, with failure characteristic described by a few control parameters. One applies an external potential,
strain or stress to the network and gradually increases it, as a result of which the individual bonds break irreversibly according to a given criterion. In one example, at each stage of simulation the bond that has suffered the largest stress or strain, or potential drop, breaks down irreversibly. In a second example, all bonds that have suffered a stress, strain or potential drop larger than a threshold value break down. Various properties of such failure process have recently been investigated and several interesting results have emerged [84, 85, 86, 87, 88, 89, 90, 91, 92, 86, 93, 94]. This class of models are appropriate for systems in which the disorder is quenched.

In this thesis, we concentrate on the application of the last class of models; the study of random network models for the two- and three-dimensional fracture in heterogeneous media. To date computational studies of fracture have been almost exclusively limited to two spatial dimensions. Three dimensional studies have been limited to small grid sizes. One aspect of our work is the study of large-scale 3D fracture in heterogeneous fields. This allows one to compare the results in two dimensions with those in three dimensions. We consider two other aspects of fracture problem. One is the question of the extent of universal properties, i.e., those that are independent of microscopic features and disorder, and depend only on the dimensionality of the system. The existence of such universal properties is particularly important since, if these models do possess properties that obey universal laws, then, one may employ the simplest of such models and study failure phenomena in microscopically and/or macroscopically disordered media. The second aspect of these models that we emphasize is their ability in predicting quantitatively some of the available experimental data.

6.2 Resistor network model for study of fracture phenomena

In this section, I shall discuss a few aspects on the resistor network model and the model of material properties, on which the simulations for fracturing phenomena
6.2 Resistor network model for study of fracture phenomena

on two- and three-dimensional lattices are based. The result associated with these simulations will be discussed in the following chapters.

6.2.1 The Resistor Network Model

Let us start with a description of the resistor network model and its relationship to fracture problem. A network of Hookean springs with natural length zero is stretched onto a frame. Each spring is assigned a value of maximum elongation $\delta_c$ it can suffer and the spring will break when the actual elongation $\delta > \delta_c$. There is an exact mapping of this frame of Hookean springs onto the random resistor network problem [95] where the $\delta_c$ is represented by the maximum current a specific resistor could carry without being fused and the $\delta$ on the spring is represented by the current across the corresponding resistor. Assuming a network on square lattice where all resistors are of unit conductances, the response of the whole resistor network, such as the sequence of resistor fusing in presence of uniform voltage gradient, will be an analogue to what happens to the frame of Hookean springs of identical Hookean coefficients in presence of the uniform stretch – given that the $\delta_c$ of the spring is proportional to the fuse criterion of the corresponding resistor by a common constant throughout the whole network.

The resistor network model for studies of fracture phenomena is phrased in terms of the failure of a network of the electrical resistors which acts as fuses (divisions of bulk material of certain local mechanical properties, such as breaking criterion under given i.e. local stress), burning out (breaking) when an appropriately defined criterion (such as critical elongation $\delta_c$) is met. The advantage of studying fracture phenomena using resistor networks is that, because only scalar quantities are involved, the network models are less expensive to simulate. Furthermore, the use of such networks helps to unveil the essential physics without the need to introduce a large number of variables and parameters that a full tensor formalism would require. Studies of resistor networks have concentrated on several types of models in which resistors are burnt out one at a time during the breakdown process. The models differ in the
6.2 Resistor network model for study of fracture phenomena

criterion for burning of a resistor.

• **Type-1:**

One begins with a regular network of identical resistors, say a two-dimensional (2D) square lattice confined between a pair of parallel bus bars [94, 96, 86, 97]. Before the simulation commences, each resistor is inspected and declared to be burnt out already, (i.e., to have infinite resistance) with probability $1 - p$. A potential difference is now applied across the bus bars. The resistors are now burnt out one at a time, the resistor selected being that with the greatest voltage across it. The process continues until a sufficient number of fuses burn out to disconnect the system and preclude further current flow.

• **Type-2:**

The previous model may be generalized by assigning a general probability density function $f(g)$ to the bond conductances $g$ [93]. The type-1 corresponds to the special case where, $f(g) = (1 - p)\delta_{+}(g) + p\delta(g - g_0)$, the resistors are now burnt out one at a time, with one of the following three failure criteria being selected: (1) the resistor that carries the greatest current is broken at each step; (2) the resistor with the greatest voltage drop across it is broken at each step; (3) the resistor with the greatest power dissipation is broken at each step. A converse of this model, in which the fuses turn into near short circuits when they blow, has also been proposed [84].

• **Type-3:**

In the third model the resistors in a regular network are all assigned the same resistance and the stochastic element is introduced by assigning random breakdown voltages to the components. At each stage in the simulation, the applied voltage is raised until one resistor suffers a voltage drop that exceeds its breakdown voltage and this resistor is immediately burnt out. As response of the network is linear, this is equivalent to burning out the resistor which has the largest value for the ratio of the voltage drop to the breakdown voltage [92].
In all three of these models, there is usually a zero probability that the need to break two fuses simultaneously will arise. Comparisons between these three models have been made by Chan, *et al.* [91] with their simulations for brittle fractures on a 2D square lattices.

We have chosen to concentrate on the *type*-3 model and to extend this model to three-dimensional systems. The reason for choosing the *type*-3 resistor network model is that we wish to examine, in particular in 3D, the importance of disorder in the material breakdown strength properties, *i.e.* the distributions of fusing criteria for the resistors which governs the forming, branching and amalgamation of the local fractures under given local conditions (*e.g.* stress) at each stage. This model decouples the influence of the fluctuation in the local intrinsic strength of the system from the influence of the fluctuation of resistance. In another context, the presence of two radically different forms of fluctuation, resistance and breakdown voltage, may result in the effects of one field dominating over the other\(^1\).

### 6.3 Implementation of Network Model on CM5

The simulations for two- and three-dimensional fracture on random media have been carried out on Thinking Machine Co. Connection Machine 5 (CM5) parallel computer which has been available in ANU since 1993. The CM5, consisting of 32 processors and 4 vector units in each of the processors is a MIMD (Multiple Instruction Multiple Data) machine.

The general algorithm for fracture is outlined below:

- Initialization: All the bonds are declared to have unit conductance. The breakdown criteria field generated from a distribution is read in and sets the local breakdown criteria for each bond.

\(^{1}\)In a parallel study of fluid displacement in porous media, Chan *et al.* found that the fluctuation in the local fluid capacity (analogous to the breakdown voltage) dominate over fluctuations in the local permeability (resistance) [98, 99].
6.4 Simulation

- 1 - Solve the potential field: Potential on each node \( V(r) \) on the lattice are solved on the lattice by using Laplacian solver (see Appendix A) with the declared boundary values.

- 2 - Check if catastrophic fracture has occurred by monitoring the maximum local current on all the conducting bonds, when the maximum local current drops at least an order of magnitude, the simulation is finished.

- 3 - If system failure has not occurred, find the weakest bond and break it. Scan through whole lattice and locate the conducting bond which gives the maximum ratio of the voltage drop against the fusing criteria. This bond is now declared insulative;

- 4 - go to step 1.

As one can see, the simulation based on the resistor network model is computationally expensive. Particular, when the simulation is performed on a three dimensional lattice on a large scale with a wide range of disorder. The most computation extensive part is the repetitive use of the solver for Laplacian equations, which consumes, typically, more than 97% of the cpu time for the duration of simulation. The implementation of fast algorithm for the Laplacian solver itself is therefore crucial to the success of the simulation, in particular, for the three-dimensional simulation. We discuss in detail the implementation of the solver for Laplacian equations in Appendix A.

6.4 Simulation

In this section, we shall discuss a few general aspects about the simulation studies of fracture problem using the resistor network model.
6.4 Simulation

6.4.1 Lattice geometry and boundary conditions

Normally, the square lattice $L \times L$ for two-dimensional simulations and $L \times L \times 2L$ cubic lattice for the three-dimensional problem are used for all simulations for three reasons:

1. For this geometry of the lattice, the pattern for the communication between the nearest neighbours on the lattice - a crucial part for the efficient solver - is well-defined:

2. Boundary conditions, periodic or non-periodic, are easy to implement:

3. A direct comparison between two- and three-dimensional simulation can be made.

![Figure 6.4: Illustration of simulation set-up: the total macroscopic and as well as the maximum local current the conducting bond carries within the system are monitored throughout the simulation.](image)

For simplicity, I will first describe simulation details for the two-dimensional case. Fig. 6.4 shows how the simulation is set up. The uniform voltage $\phi$ is applied on the entrance ($Y = 1$) and the exit ($Y = L$). At $Y = 1$, the system is attached to a conducting plate on which the voltage is uniformly unit. At $Y = L$, the sample is
attached to the plate with zero voltage. Conductance on all the bonds is unity. The lateral boundaries are declared to be zero-current boundaries – the current can flow along but can not flow across. For three-dimensional simulation the voltage drop is applied along the $Z$ direction which is of length $2L$.

For two-dimensional simulation, the size of the lattice is a multitude of $L = 128$. For three-dimensional simulation $L$ is generally 32 and the largest we ever simulated is for $L = 128$. To use the Laplacian solver for solving the potential field, the tolerance of value $10^{-6}$ is generally used. The constant voltage is applied across the system and remains constant throughout the simulation. For 3D, the voltage is applied along the direction of $2 \times L$. The theoretical maximum speed for the 128 (32 Sun Spark processors and 4 vector units in each of the processor) node CM5 is 4.0 G-Flops. With the same physical configuration, the simulation program runs at about 2.0 GFlops for the simulation on lattices of $L = 256$ for 2D and 1.93 GFlops when $L = 32$ for 3D.

### 6.4.2 Criterion for detection of catastrophic point

With the unit voltage drop applied through the system, the macroscopic current across the system drops as the number of fused bonds increases. When system fails, the macroscopic current should be zero. Due to numerical noise, zero macroscopic current across the system at the point of system failure can not be achieved in numerical simulations. However, by monitoring the macroscopic current, one can detect the point of system failure by finding the sharp drop of the current. Shown in Fig. 6.5 is a plot of macroscopic current versus the number of fused resistors near the point of system failure for a 3D simulation. We can see in the figure that when the system approaches the point of system failure, the macroscopic current experiences frequent large drops.

In two-dimensional cases, a drop of the macroscopic current by an order of magnitude or so suffices to detect the catastrophic point of the system. This criterion has
6.4 Simulation

Figure 6.5: The macroscopic current versus the number of fused resistors near the point of system failure for 3D system of power law distribution with $n = 2$.

Figure 6.6: Maximum local current (a) and macroscopic current (b) vs number of broken bonds for system of power law ($n = 8$) breakdown strength distribution for 3D lattice of $32 \times 32 \times 64$.

been applied with success to two-dimensional fracture simulations using the resistor network model [91]. However, in the case of three-dimensional simulation and also
Figure 6.7: Three stages in resistor network simulation on a 2D anisotropic field (Levy distribution).
for large disorder this criterion can lead to errors. For example, when the system is near the critical point, in some cases the fusing of one of the few remaining critical bonds may cause a drop of macroscopic current by an order of magnitude or more (see Fig. 6.5). This is especially noted on three-dimensional systems of very large disorder, i.e. with power law distribution for large $n$. Near the catastrophic point, the system macroscopic current undergoes relatively large drops whenever it fuses one of a few remaining critical bonds. These bonds are not necessarily the last bond which leads to complete disconnection. This makes the detection of the point of system failure by monitoring the drop in macroscopic current problematic.

To solve this problem, another criterion has been tested and applied to the simulations in this thesis. We instead monitor the maximum local current during a fracture process. The Fig. 6.6 shows that in the process of local crack forming, the maximum local current increases in spite of the decrease in macroscopic conductivity. At breakdown the maximum microscopic current drops by orders of magnitude. A direct comparison of Fig. 6.5 and Fig. 6.6(a) clearly indicates the maximum local current serves better as a criterion than macroscopic current for detection of the catastrophic point for the three-dimensional simulation.

In Fig. 6.7 we show an illustration of one complete simulation in two-dimensions. Three snapshots of the resistor network simulation on a $128 \times 128$ square lattice with an anisotropic Levy distribution as the breakdown criteria field [100]. In the figure we show from left to right: the left column shows in the background the breakdown criteria field - the darker the region is, the lower the breakdown criteria in that region. The white lines highlight the already fused bonds: The central column shows the potential field, the potential is linearly interpolated to a colour table in which red in full intensity corresponds to unit voltage and navy blue zero voltage, the region of large local contrast shows the extent of the large existing cracks: The right column shows the distribution of local current density. The system with 1592, 1738 and 1803 resistors fused is shown. The last stage shown in Fig. 6.7(g,h,i) is very close to the point of system failure. The evolution of the fracture in two-dimensions can be
6.4 Simulation

simulated and visualized in real time. This allows one to observe important fracture events like crack development, healing and crack interactions interactively.
Chapter 7

Simulation of Fracture in Heterogeneous Media

In this chapter, we shall present and discuss the results of simulation studies on fracture phenomena in heterogeneous media. We wish to study the influence of disorder of material properties on the resultant structure of the fracture network and on the morphology of the critical fracture surfaces. We will focus in particular on differences between the 2D simulations and 3D simulations throughout this chapter.

7.1 The statistical description for disorder of material properties

Efforts to correlate material properties to fracture patterns have led to the statistical models for studies of fracture of the disordered systems. Statistical descriptions of the disordered material properties have been previously established and Alex Hansen has written a comprehensive review [101] on this subject.

The earliest study was due to Kahng et al. [92] of the breakdown of resistor networks, based on a type-3 model. Their results suggested that the pattern of burnt-out resistors as well as the fraction of resistors burnt at the limit where the entire
network becomes disconnected, depends on the form of the distribution function of break down voltages as well as the network size. They considered $N$ resistors in a $2D$ square lattice network in which the breakdown voltage $\phi$ of each element is given by the normalized distribution function,

$$f(\phi) = 1/w \quad \text{where} \quad 1 - w/2 < \phi < 1 + w/2 \quad \text{and} \quad 0 < w \leq 2. \quad (7.1)$$

For small values of $w$, they observed that when the network breaks down, the pattern of burnt resistors forms a linear chain with the mean number of burnt-out resistors $< N_b >$ being proportional to $N^{1/2}$. They called this the brittle regime. As $w$ becomes larger, say $> 1.5$, the mean number of burnt-out resistors $< N_b >$ increases faster than $N^{1/2}$. In addition to the pattern of burnt resistors that caused the network to become disconnected, there are also many clusters of burnt resistors which are not attached to the main critical cluster – this was termed the ductile regime. Kahng et al. conjectured that in the limit $w = 2$, the mean number of burnt-out resistors $< N_b >$ will increase with the lattice size as $N$ does.

In this chapter we consider the breakdown characteristics of a resistor network as a function of the distribution of the breakdown voltages of the elements. In particular, we consider in three dimensions the distributions studied by Chan et al. [91]. This complements their previous study which was limited to two-dimensions. In particular, we examine whether the characteristics of fracture patterns in three-dimensions can be related to the previous work in two-dimensions.

In a simple random bond percolation model, bonds in a network are selected at random and then broken. The network breaks down when one particular cluster of broken bonds separates the network into two disconnected portions. In a type-3 resistor network discussed in Chapter 6, the criterion for breaking a particular bond or resistor is not random, but is controlled by the ratio of the voltage drop across the resistor to the breakdown voltage of the resistor. The magnitude of the breakdown voltage $\phi$ depends on the choice of the normalized distribution function $f(\phi)$, while the
Figure 7.1: The Probability $P_L$ (courtesy of D. Y. C. Chan [91]) that, in a pair of resistors, the resistor with larger voltage drop will be burnt, as a function of the ratio $\rho$ of the voltage drops across the two resistors, $0 < \rho < 1$, for the distribution functions: uniform (Eqn. (7.3)); Kahng uniform (Eqn. (7.1)) with $w = 0.5$; exponential (Eqn. (7.4)) with $\alpha = 1$; power law distribution (Eqn. (7.5)) with $n = 2, 4, 16$ respectively.

Voltage drop is found using the Kirchoff equations for the local current configuration of intact resistors. To gain insight in the role of the breakdown voltage distribution function, Chan et al. [91] analyzed a simple case of two resistors with breakdown voltages $\phi_1$ and $\phi_2$ chosen according to some normalized distribution $f(\phi)$ where the voltage drops across the two resistors are $V_1$ and $V_2$, respectively and the ratio of the voltage drops across the two resistors is defined as $\rho = V_2/V_1$ and $\rho < 1$. They defined the probability $P_L$ that the resistor with the larger voltage drop across it will be burnt [91], where $P_L$ is given by,

$$P_L = \int_{\phi_1}^{\infty} d\phi_1 f(\phi_1) \int_{\phi_1 \rho}^{\infty} d\phi_2 f(\phi_2).$$  \hspace{1cm} (7.2)

They considered in particular following distribution functions $f(\phi)$. 

7.1 The statistical description for disorder of material properties

- Uniform distribution:
  
  \[ f(\phi) = 1 \quad \text{where} \quad 0 < \phi < 1, \quad P_L = 1 - \frac{\rho}{2} \]  \hspace{1cm} (7.3)

- Exponential distribution:
  
  \[ f(\phi) = \alpha e^{-\alpha \phi} \quad \text{where} \quad 0 < \phi < \infty, \quad P_L = \frac{1}{1 + \rho} \]  \hspace{1cm} (7.4)

- Power law distribution:
  
  \[ f(\phi) = (1-q)^{n-q} \quad \text{where} \quad 0 < \phi < 1, \quad P_L = 1 - \frac{\rho^{n-1-q}}{2}, \]  
  
  \[ q = \frac{n-1}{n} \quad \text{for} \quad n > 0. \]  \hspace{1cm} (7.5)

- The \( P_L \) for Kahng distribution (Eqn. (7.1)) is: for \( 0 < \rho < \rho_1, \) \( P_L = 1 \) and for \( \rho_1 < \rho < 1, \)
  
  \[ P_L = \frac{3}{4} + \frac{1}{8w^2}[8 - \rho(w + 2)^2 - \frac{1}{\rho}(w - 2)^2]. \]  \hspace{1cm} (7.6)

The probability \( P_L \) for these four distributions is summarized in Fig. 7.1. Since \( f(\phi) \) is assumed to be normalized over some interval, the probability \( P_L \to 0.5 \) in the limit \( \rho \to 1 \) for all models. A value of \( P_L = 0.5 \) is equivalent to the simple random percolation model in which one of the two resistors is chosen at random to be burnt irrespective of their breakdown voltages. Thus at a given \( \rho \) value, the model that has the lowest \( P_L \) will yield the most "random" cluster of burnt resistors. From Fig. 7.1 we see that the power law distribution (Eqn. (7.5)) with large \( n \) is expected to yield the most random distribution of burnt resistor clusters at breakdown.

We consider these same distributions of breakdown criteria in 3D to complement the previous study. In particular, it allows us to compare the three-dimensional simulations with their two-dimensional counterparts. Three-dimensional simulation is important, as it can be directly compared to experiment. Moreover, this will clarify whether 3D fracture processes can be effectively modelled by 2D simulations.
7.2 Simulations

We have performed simulations on fracture problems using three-dimensional cubic lattice, along with the simulations on two-dimensional square lattice. The typical geometry used for 3D simulations is $32 \times 32 \times 64$ while $128 \times 128$ for 2D. For samples of same kind of disorder, e.g. power law $n = 2, 4, \ldots$, etc. in their breakdown criteria, we normally run for more than 100 realizations for two-dimensional systems, whilst 40 or more for the three-dimensional systems. It has been observed from the analysis of simulations that the larger the disorder in the distribution of breakdown criteria, the more realizations are needed to achieve the satisfactory statistics for the quantities we are interested in; while less realizations needed for that of smaller disorder. It has also been observed that statistical properties for the three-dimensional simulations behave, generally, better than their two-dimensional counterparts given the same number of realizations.

7.3 Discussion

7.3.1 The macroscopic conductivities when system ruptures

The relationship between the system macroscopic conductivity and the extent of breakdown (number of broken bonds) is the most straightforward to measure. It reflects to some extent the dependence of the resulting fracture network on the material properties. In Fig. 7.2(a,b) we show the macroscopic current across the system during the fracture process for the various distributions of breakdown voltage on two- and three-dimensional materials. In agreement with previous work [91], the larger the "disorder" in the material property, the greater the number of bonds broken at the catastrophic point. Fig. 7.2(c,d) shows the same as Fig. 7.2(a,b) except that the number of broken bonds are now normalized to unity. Fig. 7.2(c,d) show that curves collapse onto each other in the region near the point of system failure. This indicates that the failure criteria are somewhat universal and independent of the
7.3 Discussion

Figure 7.2: Macroscopic conductivities (raw and normalized) from the onset of failure to the system failure for $2D$ (a,c) and $3D$ (b,d) simulations. In plots (a) and (b), all curves from right to left read: power law distribution $n = 8$; $n = 4$; $n = 2$; exponential distribution; Kahng distribution $w = 2$; Kahng distribution $w = 1.0$. Plots (c) and (d) show the scaled results. The curves in the upper left region of plot represent from bottom to top: power law distribution $n = 8$; $n = 4$; $n = 2$; exponential distribution; Kahng distribution $w = 2$ and $w = 1.0$, correspondingly.
7.3 Discussion

disorder exhibiting in the material properties.

By comparing the Fig. 7.2(a) and (b) and also the Fig. 7.2(c) and (d), we note that the macroscopic conductivities for 2D and 3D during fracturing process exhibit similar behaviour.

7.3.2 Fracture morphology

Another important aspect of the fracturing phenomena is the morphology of the critical fracture surface and that of the clusters on which the critical fracture surface embeds. Fig. 7.3 and 7.4 show the 3D fracture surfaces and the clusters connected to the 3D fracture surfaces respectively. The bounding boxes show the extent of the clusters and surfaces. The Fig. 7.5 shows the fracture surface and full fracture pattern for a number of 2D cases. These plots give visual evidence that the broader the breakdown criteria distribution, the rougher the resultant fracture surface.

The length of the fracture surface is a natural measure of surface roughness. We performed several measurements on the geometry of the critical fracture surfaces. For the 2D fractures, we measure the ratio of the fracture surface length over the lattice size \(L\) and for 3D, the similar measurements are performed for the length ratio for slices and for the contour of the fracture surfaces. We have also measured the ratio of the fracture surface area for 3D and lattice cross-sectional area \(L \times L\). In Table 7.1 we summarise these measurements.

We have found that all the length ratios measured for 2D and 3D fractures increase monotonically as the extent of disorder increases. The area ratio exhibits the similar tendency. We have not included the measure for the Kahng distribution with \(w = 1\) as the resultant fracture surface is trivial (see Fig. 7.3); all ratios measured are close to unity. For the 2D simulation, the length ratio increases from 1.64 at \(n = 2\) to 3.24 when \(n = 16\). For the 3D surface, the length ratios measured from the peripheral surface contour are found in very good agreement with those measured on slices of the 3D surface. The ratio of 3D surface area to sample cross-sectional area increases as
Figure 7.3: Fracture surfaces for system of, from top down, increasing order of disorder. For (a,b) Kahng distribution with $w = 1$, (c,d) for power law $n = 2$ and (e,f) $n = 4$. The colour indicates the time resistor is fused— red the latest and dark blue earliest.
Figure 7.4: Critical clusters (fracture surface plus all adjoining fractures) for breakdown criteria of power law distribution: (a) $n = 4$ and (b) $n = 2$. The colour indicates the time the crack is formed; red the latest and dark blue earliest.
Figure 7.5: Fracture surfaces (left column) and fracture network (right column) on 2D system for system of, from top down, increasing extent of disorder: (a,b) is For Kahng distribution with $w = 1$, (c,d) for power law $n = 2$ and (e,f) $n = 8$. 
Table 7.1: The measurements of geometric parameters for 2D fracture, 2D slices of 3D fracture surfaces, contour of 3D fracture surfaces and 3D surface area ratios. For power law distribution of \( n = 16 \), the measurements are made from 60 and 12 simulation for 2D and 3D fracture surfaces, correspondingly, while the measurements are made from 120 simulations for 2D and 48 for 3D fracture surfaces in all other cases.

<table>
<thead>
<tr>
<th>Distribution</th>
<th>Length ratio</th>
<th>Area ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>2D</td>
<td>3D slices</td>
</tr>
<tr>
<td>exp ( \alpha = 1 )</td>
<td>1.64±0.02</td>
<td>1.52±0.04</td>
</tr>
<tr>
<td>n=2</td>
<td>1.75±0.04</td>
<td>1.59±0.03</td>
</tr>
<tr>
<td>n=4</td>
<td>1.90±0.05</td>
<td>1.86±0.09</td>
</tr>
<tr>
<td>n=8</td>
<td>2.68±0.10</td>
<td>2.47±0.17</td>
</tr>
<tr>
<td>n=16</td>
<td>3.24±0.14</td>
<td>3.49±0.19</td>
</tr>
</tbody>
</table>

the extent of disorder increases. All the measurements are bounded within reasonably tight error bars. Table 7.1 suggests that there is a possibility of parametrizing the fracture morphology and relating this to material properties.

7.3.3 Cluster size distribution in fracture network

The fracture patterns in natural materials are often very complicated. As seen in Fig. 7.4 (a) and (b), it is often the case that the major crack is serrated with branches and coexists with many isolated clusters of cracks. In reality, these isolated cracks may play an important role. For example, the properties of the fracture pattern in a porous system will affect the measured permeability or dispersivity. In Fig. 7.4(a), we see the whole cluster in which the critical fracture surface (Fig. 7.3(e,f)) embeds. In this picture, we have only shown the fracture surface as well as dead-ends branching
off the fracture surface. There are also numerous isolated clusters of various sizes in the system which are not shown in the picture. We have considered the distribution of cluster sizes for different disorder. The cluster size distribution $N(S)$ gives the percentage of fused resistors in clusters of size ranging from $S$ to $S + \Delta S$. The cluster size $S$ may be normalized where the maximum cluster size is unity. A discussion of the algorithm developed and used to identify clusters of bonds in the resistor network simulation is given in the Appendix B.

We have measured the histograms of the cluster size distribution at time of system failure. Shown in Fig. 7.6 are the integral histograms for the cluster size distribution versus the number of total fused bonds, the latter having been normalized to unity, for a power law breakdown distribution ($n = 2$) in two- and three-dimensions. The histograms are generated from 100 realizations for the 2D system and 32 realizations for the 3D system. Differences in the histograms are evident. At system failure about 70 percent of fused bonds form clusters of very small size in 2D simulations;
in contrast, only 35 percent form small clusters in 3D. The integral histograms for the 3D system exhibits frequent jumps, in particular, in the intermediate range of the cluster sizes, indicating the existence of many isolated clusters of intermediate size. This contrasts with the 2D results, which has a very large proportion of small clusters and then a few clusters of very large size.

For identical disorder in two- and three-dimensions, the cluster size distribution exhibits important differences. For decades, efforts to model 3D fracturing phenomena by using a 2D analogue have been made. These efforts have been successful in predicting, for example, the scaling properties of the roughness of the 3D fracture surface. Our results indicate that the 2D analogue is however not sufficient in describing some properties of the true 3D system.

2D slice-wise information of the 3D system is also important. It is often impractical in engineering to measure full 3D information, and information from slices
Figure 7.8: Integral $N(S)$ vs size of clusters $S$ for 2D slices with various distribution, where (b) is the normalized plot of (a): (\(\text{---}\)) exponential distribution; (\(--\)) power law ($n = 2$); (\(\cdots\)) $n = 4$. 

(a)  

(b)
through the 3D material are made. We compare the cluster size distribution of the
2D slices of full 3D simulations with both 2D and 3D simulations. The crack size
distributions are shown in Fig. 7.7. The differences between the 2D slice-wise infor-
mation and 3D is evident. Moreover, no clear similarities can be found between the
2D simulation and the 2D slices of 3D simulation. Note that the integral histogram
of 2D slices of 3D system shows smooth behaviour in comparison to the other two.
This smoothing of the distribution is in part due to removal of the third dimension
which removes the correlations (connections) between clusters of large size in three
dimensions. The contribution to the cluster size distribution from the clusters of all
intermediate sizes therefore increases. Again, for identical disorder large differences
are evident when compare the cluster size distribution for 2D slices with the full two-
and three-dimensional counterparts.

Finally, we compare the behaviour of the histogram for different disorder. Shown
in Fig. 7.8, are the integral histograms for the 2D slices of 3D simulations on sys-
tems with disorder given by both the exponential distribution and the power law
distribution for $n = 2$ and $n = 4$. Fig. 7.8(a) gives the raw data, and Fig. 7.8(b)
the normalized data. Fig. 7.8(b) shows a clear trend at the limit of small cluster
size. A large proportion of fused resistors remain within small clusters for small dis-
order (exponential distribution); a smaller proportion is evident for larger ($n = 4$)
disorder. In the intermediate and large size regions no trends are evident.

7.4 Evolution of crack size distribution

As a general observation, no materials breaks right away when the external energy
source is applied. However, the system, assuming a perfect flawless material, first de-
velops small and often isolated cracks. If the system continues to suffer such external
load, new and isolated cracks may form and the existing ones may grow or amalga-
mate with another. The time evolution of the crack size distribution may provide
insight into the rupturing process of a system from a statistical point of view.
7.4 Evolution of crack size distribution

Figure 7.9: The evolution of histogram $N(\log_{10}(S))$ vs logarithmic size of clusters $S$ for 3D system of power law distribution $n = 4$, at different time $t_b$.

Shown in Fig. 7.9 is the time evolution of the crack size distribution for 3D 32x32x64 lattice with a breakdown criteria field of power law distribution $n = 4$. The $t_b$ is defined as the ratio of number of the fused resistor $N_b$ when the histogram is made over the total number of fused resistor at system failure $N_f$. At system failure point, $t_b$ is therefore unity. We study the histogram of fracture size on a log-scale. At very small $t_b$, the histogram is a monotonically decreasing distribution. When $t_b$ increases, the peak of the histogram curve moves to the right and the whole curve becomes skewed. At still larger $t_b$, the curve splits into two major parts. One peak moves faster to the right. The other peak flattens with a non-vanishing tail in the small crack size region. For $t_b > 0.6$, peaks at large $\log(S)$ begin to break up into a

---

1On a linear scale the histogram exhibits a series of of delta functions at larger cluster scales even after averaging over hundreds of samples. The log-scale allows trends at larger scales to become more evident.
7.4 Evolution of crack size distribution

series of δ functions, signifying the appearance of clusters of all sizes in the system. With no exception, all the distributions with different extent of disorder we have studied exhibit the similar transition of \( N(\log(S)) \) as \( t_b \) increases.

As an effort to gain insight into these transitions, here we define a measure \( \ell_m \),

\[
\ell_m = \frac{\int d(\log_{10}(S))N(\log_{10}(S))\log_{10}(S)}{\int d(\log_{10}(S))N(\log_{10}(S))}.
\]  

(7.7)

The \( \ell_m \) can be related to the mean span of the clusters within the system. In another context \( \ell_m \) is comparable to the correlation length for the crack size distribution. The rapid increase of \( \ell_m \) as \( t_b \) increases is shown in Fig. 7.10, and illustrates the tendency of \( \ell_m \) to diverge for \( t_b > 0.6 \).

![Figure 7.10: The \( \ell_m \) for various \( t_b \) used in Fig. 7.9.](image)

Fig. 7.9 and Fig. 7.10 allows us to postulate as to what happens in the system during the fracturing process. When the system starts to rupture, the fusing is a random event, the correlation between the fused resistors is short ranged: All the cracks are isolated and few cracks form clusters. When the system is near its point of system failure, the correlation length becomes comparable to the system dimension; local bonds are now fused in a collective manner. The most direct visual evidence for the transition of correlation with time (\( t_b \)) is given by the time evolution of the fusing
events shown in Fig. 7.3(a,b). In this figure, the darker (blue) spot indicate a fusing event at a very early stage, red the late stage fusing events, other colours interpolated in order of blue, green, yellow, orange and red indicating the time when the fusing event happens. From the figure we can see that the blue and the dark green spots are scattered (evidently no correlation) in the picture whilst the colours indicating the intermediate and late stage are organized in a highly correlated pattern.

Figure 7.11: The $N(S)$ vs size of clusters $S$ for clusters of size less than 10 fused resistors for system of power law distribution $n = 4$ at point of system failure.

We finally consider the non-vanishing tail of the crack size histogram in the small crack size limit at system failure. As noted in Fig. 7.8, the effect of disorder was evident in the small crack size limit. Shown in Fig. 7.11 is the contribution to the crack size distribution from the cracks of a small size (less than 9 fused resistors) for a system of power law $n = 4$ at failure. In Fig. 7.12, the results for the five distributions are presented in format of $\log(N(S))$ versus $\log(S)$. Each data point for system of small disorder ($n \leq 4$) is averaged for given $S$ over 20 realizations and 5 realizations for $n = 8$ and $n = 16$. In the figure, the $N(S)$ is shifted so that $N(S) = 1$ when $S = 1$ to facilitate the comparison. The linear regression indicates that, in the small crack size limit, the crack size histogram obeys a power law at system failure: $N(S) \sim S^{-\beta}$ whereas the $\beta$ is dependent upon the disorder of the system breakdown.
7.5 Conclusion

Figure 7.12: The scaled logarithmic plots of $N(S)$ vs size of clusters $S$ for clusters of size less than 9 fused resistors: $(- - -)$ is for power law distribution $n = 16$, $n = 8 (-----)$, $n = 4 (-)$, $n = 2 (-------)$ and exponential distribution with $\alpha = 1 (-\cdot\cdot\cdot)$.

criteria distribution. The exponent $\beta$ may be a measure of the disorder in material properties.

7.5 Conclusion

To date, the recorded computational studies of fracture in three dimensions has been limited to small (10×10×10) grid sizes. The simulation work we discussed here enables us to compare the measures of the fracture phenomena as well as breakdown criterion in three dimensions at a scale which are larger by an order of magnitude than the conventional methods.

A simple characteristic of the fracture pattern is the measure of crack sizes within the fracture pattern. We measured the normalized crack-size distribution for the two- and three- dimensional systems at the time of system failure. In engineering, it is hard to measure the three-dimensional structure of a fractured material and one is instead limited to measuring structure on two-dimensional slices of the material. We
therefore measure the crack-size distribution of slices of the three-dimensional system orthogonal to the fracture surface. The differences in this characteristic measure of the fracture pattern are clear. We also compare the breakdown characteristics of the two- and three-dimensional system with identical heterogeneity. No clear correlations between the simulations of 2D and 3D system with same disorder can be found. The result highlights the need to simulate in three-dimensions when modelling fracture in random materials.
Chapter 8

The Scaling Properties of Fracture Surface Roughness

In this chapter, we will consider in depth the measurement of the roughness of fracture surfaces generated in uniaxial tension for model materials in two and three dimensions using the resistor network model. We will also discuss the effect of disorder, of anisotropy of material properties and of scale on surface roughness. The roughness exponent is used to describe the scaling property of the surface roughness. Although the roughness exponent $\zeta$ is always found within a narrow range, its value systematically decreases as the extent of disorder is increased. For anisotropic materials the scaling properties are found to be independent of the orientation of the imposed stress despite a visible difference in the fracture surface morphology. These results indicate that the scaling properties of the fracture surface are not universal, but depend albeit weakly, on material properties. Values of the roughness exponent $\zeta$ are consistent for the same breakdown distribution in two and three dimensions.
The morphology of fracture surfaces is strongly dependent on the material, its fracture mechanism and the scale of observation. There has been much progress recently in the statistical characterization of the topography of fracture surfaces. In particular the observation of scale invariance has been made in many experimental cases leading to a more reliable description of the statistics of fracture roughness [100, 101]. It has been shown in many instances that fracture surfaces exhibit statistically self-affine scaling properties. A self-affine surface $z(x,y)$, isotropic in the $(x,y)$ plane, is invariant under the scale transformation $(\lambda x, \lambda y, \lambda^\zeta z)$ where $\zeta$ is defined as the roughness exponent. Values of $\zeta$ reported in the literature on various materials are all in the range 0.68-0.9 for measurements with resolution from the micron to the meter scale [101, 102, 103, 104, 62, 105]. This has led authors to suggest that the value of $\zeta$ could be universal or independent of the material studied. For example Maloy et al. [102] used six very different brittle materials and found a roughness exponent $\zeta = 0.87$ for all materials with a precision of 10%. Schmittbuhl et al. [62] studied the roughness of a granitic fault surface at field scale and found $\zeta$=0.84. The universality hypothesis is also believed to hold for anisotropic brittle fracture surfaces [105]. The universality hypothesis has been questioned recently. The conclusion of experimental studies of fracture at a nano-scale [106] shows correlations between the roughness exponents and material properties. It seems reasonable to assume that material properties should affect both the morphology and the scaling of the fracture surface. However no clear understanding of what limits the class of materials with the same scaling properties has been reached. An important issue remains how to best parametrize surfaces with the same $\zeta$. Computational methods, which allow one to systematically vary disorder and introduce anisotropy, can lend insight into these questions.
8.2 Simulation

The computational study of the brittle fracture surface roughness for a fuse model in two and three dimensions are discussed in this chapter. Boundary conditions are applied that correspond to uniaxial tension. We vary the distribution of breakdown strengths in the material and evaluate the scaling properties of the fracture surface for a range of different disorders. We study the effect of both correlated and uncorrelated disorder, and anisotropy of material properties on surface roughness. Although the roughness exponent $\zeta$ is always found within a narrow range for all imposed disorder, its value systematically decreases as the extent of disorder is increased. We introduce a physically-motivated anisotropic model for fracture toughness and evaluate $\zeta$ for fractures formed orthogonal to and parallel to the stretched plane. We find the scaling properties of the fracture surfaces to be dependent on the extent of disorder, but independent of the orientation of the imposed tensile stress despite a visible difference in the fracture surface morphology. This is in agreement with recent experimental work on fracture in wood [105]. These results indicate that the scaling properties of the fracture surface are not universal, but depend albeit weakly, on material properties. Values of the roughness exponent $\zeta$ are consistent for the same breakdown distribution in two and three dimensions.

The simulations have been performed on CM5 parallel computer using resistor network model. The implementation and relevant algorithms have been discussed in Chapter 6. For the two-dimensional system, we use $256 \times 256$ square lattice and for three-dimensional system $32 \times 32 \times 64$ cubic lattice is generally used. Unit constant voltage drop is applied across the system and the lateral boundaries of the lattice are declared zero-current boundaries.

We consider a number of relevant threshold distributions in the fuse model:

1. uncorrelated isotropic distributions exhibiting varying magnitudes of disorder (Eqn. (7.1), (7.4), (7.5));

2. correlated isotropic distributions — unstretched Levy distribution [98, 107];
Figure 8.1: Example of full fracture surface upon disconnection for system of exponential distribution with $\alpha = 1$. Shown in (a) and (b) are the physically observable fracture surface and in (c) is the fracture surface and all the dangling ends connected to the surface. The colour indicates the time of local bond breaking — blue for earliest, red for latest.
3. anisotropic distributions — stretch Levy distribution [98, 107].

An example of the fracture configuration is shown in Fig. 8.1. The 'visible' fracture surface shown in Fig. 8.1(a) and Fig. 8.1(b) is the 2D planar backbone of the crack that completely separates the two domains of material. In this Chapter we focus on the measurement of the roughness of the surface. Fig. 8.1(c) shows the full fracture upon disconnection including cracks connected to the fracture surface.

### 8.3 Result and Discussion

<table>
<thead>
<tr>
<th>Breakdown Distribution</th>
<th>$\zeta$ (3D)</th>
<th>$\zeta$ (2D)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exponential ($\alpha = 1$)</td>
<td>0.72 ±0.05</td>
<td>0.76 ±0.04</td>
</tr>
<tr>
<td>Power Law ($n = 2$)</td>
<td>0.72 ±0.06</td>
<td>0.74 ±0.06</td>
</tr>
<tr>
<td>Power Law ($n = 4$)</td>
<td>0.69 ±0.04</td>
<td>0.71 ±0.07</td>
</tr>
<tr>
<td>Power Law ($n = 8$)</td>
<td>0.52 ±0.07</td>
<td>0.58 ±0.04</td>
</tr>
<tr>
<td>Power Law ($n = 16$)</td>
<td>0.44 ±0.10</td>
<td>0.49 ±0.10</td>
</tr>
<tr>
<td>Levy Field (meter)</td>
<td></td>
<td>0.83 ±0.09</td>
</tr>
<tr>
<td>Levy Field (kilometer)</td>
<td></td>
<td>0.78 ±0.07</td>
</tr>
</tbody>
</table>

Table 8.1: Values of the roughness exponent derived for the various fracture samples. All results are averaged over at least 20 runs. The three dimensional results for systems of size $32\times32\times64$ are compared to two dimensional systems of size $256\times256$.

To gain insight into the role of the disorder on fracture surface roughness, we consider an exponential breakdown distribution ($f(\varphi) = \alpha \exp(-\alpha \varphi)$) and a power law distribution $f(\varphi) = (1 - q) \varphi^{-q}$, where $q = \frac{n-1}{n}$. As discussed in Chapter 7, one can show that the extent of disorder increases as one goes from exponential to a power-law distributions and for power law distributions with increasing $n$ [91]. Experimental measurements of the roughness of brittle cracks in three dimensional materials record
the height of the crack surface as a function of position along one-dimensional cuts orthogonal to the fracture surface [102]. The width of the crack is then defined by \[ w = \left( < h(x_0)^2 > - < h^2 > \right)^{\frac{1}{2}}. \] The exponent \( \zeta \) is defined by measuring the crack width \( w \) over a window size \( L \) where \( w \propto L^\zeta \). Our measurement of \( \zeta \) for various breakdown distributions is summarized in Table 8.1. All the uncertainties reported in the table are statistical standard deviations. There is a slight but systematic decrease in the value of \( \zeta \) as the extent of disorder is increased. For self-affine surfaces, one must distinguish between a local and a global dimension. The global dimension, which is measured at large length scales is simply \( d = 2 \) (the surface is asymptotically smooth). The local fractal dimension is related to \( \zeta \) by \( d_f = d - \zeta \). As one would expect intuitively, the fractal dimension increases with increasing disorder. The simulation result shown in Table 8.1 indicates that \( \zeta \) is not universal, but depends weakly on the extent of disorder. In the case of large disorder \( (n = 8, n = 16) \) the value of \( \zeta \) is significantly less. In this case overhangs in the roughness can exist at small (1-5 lattice units) scales. We therefore performed simulations in two dimensions at up to 512x512. Fig. 8.2 shows the evaluation of \( \zeta \) for a system with large disorder with \( n = 8 \). \( \zeta \) is evaluated based on data for window sizes with \( 10 \leq L \leq 128 \).

An important question is whether simulation results for roughness of the fracture surface in two-dimensional materials is relevant to studies of fracture in three-dimensional materials. To check this we studied the fuse model in two dimensions with identical breakdown characteristics. We compare the values of the surface roughness exponent for orthogonal cuts along three dimensional surfaces with the two dimensional computations in Table 8.1. Values of the roughness exponent \( \zeta \) are consistent for the same breakdown distribution in two and three dimensions. This indicates that \( \zeta \) is independent of dimension.

All previous computational studies of fracture properties of materials are for uncorrelated isotropic systems. Most natural materials are not random and exhibit correlated and anisotropic mechanical properties. Examples include fibrous materials (e.g., wood and reinforced concrete) and geological media. Sedimentary rocks
Figure 8.2: Determination of the roughness exponent $\zeta$ for a system with large (power law with $n = 8$) disorder. The $\zeta$ is evaluated based on data with window size $L$ on $[10, 128]$. The value of $\zeta$ for this system is 0.54.

are notoriously heterogeneous even at the millimeter scale, and are known to exhibit anisotropy at all scales. Recently Painter [98], introduced a fundamentally more realistic approach to modelling of spatial variability in sedimentary rock. Measurements of increments of the acoustic transit time (which is closely related to the density of rock) from various geologic settings was accurately modelled as having Levy-stable distributions. The model reproduces the statistical properties of sedimentary formations and mimics the visual features of the formations. Other material properties (e.g., porosity) have been shown to exhibit Levy scaling. Although one cannot make any direct inference about the mechanical properties of sedimentary rock from the acoustic data, density is a significant parameter characterizing material properties. We choose therefore to model successive increments in the breakdown field as having Levy-stable distributions.

Associated with the isotropic Levy field are two parameters; the Levy index, which is a useful measure of heterogeneity in the rock, and a scale parameter. The
Figure 8.3: Two dimensional fracture across anisotropic materials. (a) and (b) show the identical breakdown fields positioned orthogonally. The background colour denotes the local breakdown strength. Clearly when the tension is orthogonal to the stretched axis (b) the extent of fracture is far greater. (c) and (d) show the fracture surface for the two cases illustrated in (a) and (b) respectively. A visible difference in the fracture profile is noted.
Table 8.2: Values of the roughness exponent derived for the anisotropic breakdown criteria fields — averaged over 30 runs.

<table>
<thead>
<tr>
<th>Stretch Factor</th>
<th>$\zeta_{Par}$</th>
<th>$\zeta_{Orth}$</th>
<th>$L_{Par}$</th>
<th>$L_{Orth}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>.69 ± .05</td>
<td>.70 ± .08</td>
<td>1.35</td>
<td>2.24</td>
</tr>
<tr>
<td>7</td>
<td>.72 ± .05</td>
<td>.71 ± .06</td>
<td>1.31</td>
<td>2.47</td>
</tr>
</tbody>
</table>

scale parameter in the Levy model can be varied to model increments in sedimentary rock properties from the meter to the kilometer scale [108]. We first consider the effect of scale on fracture surface properties. Varying the scale parameter changes the magnitude of the variance in the breakdown distribution. At small scales the magnitude of jumps in material properties are clearly reduced. In the Levy model, at the smallest scale the breakdown path is relatively straight. As the extent of disorder is increased the breakdown path becomes more random. Consistent with our earlier observation the roughness exponent $\zeta$ decreases as the extent of disorder increases (see Table 8.1). The value of $\zeta$ is slightly higher than the value obtained for uncorrelated disorder and consistent with the results of Schmittbuhl et al. [62] for granitic surfaces.

Rocks are notoriously anisotropic. We consider the effect of anisotropic breakdown fields on the scaling properties of the fracture surface. Anisotropic Levy fields that mimic geological stratification are generated by stretching along one of the axes [98]. Fig. 8.3(a) and (b) illustrates local breakdown fields in the anisotropic Levy model. We consider fracture where the uniaxial tension is imposed both orthogonal to and parallel to the stretched axes. Fig. 8.3(c) and (d) illustrates a representative fracture surface in both cases. Surprisingly when we compare the measured roughness exponent for both cases $\zeta$ is independent of the orientation of the imposed stress. This is despite a clear visible difference in the fracture profile (compare Fig. 8.3(c) and (d)). This is further illustrated in Table 8.2 where the average contour length of the fracture is compared to the system size. Despite a large difference in the contour length, the exponent is invariant. This remarkable result is consistent with the recent experimental study of
Engoy et al. [105] who measured the roughness profiles of fracture surfaces in wood. In their study tangential and radial surfaces which exhibit very different morphologies gave identical scaling properties.

8.4 Conclusion

It is reasonable to assume that material properties should affect both the morphology and the scaling of the fracture surface. However no clear understanding of what limits the class of materials with the same scaling properties has been reached. We have employed computational methods and systematically studied the effect of disorder, anisotropy and dimensionality on the scaling properties of the fracture surface. We find the scaling properties of the fracture surfaces to be weakly dependent on the extent of disorder. Anisotropic materials exhibit scaling properties independent of the orientation of the imposed tensile stress for the same disorder despite a clear visible difference in the fracture surface morphology, and independent of dimensionality. While values of the roughness exponent $\zeta$ are independent of dimension, differences in the fracture pattern are noted. To conclude we have shown that correlations between $\zeta$ and the material properties can be observed. The question of how to best characterize the distribution of breakdown strengths in real materials remains.
Chapter 9

Percolation in Geological Material

In this chapter, we will study percolation in media with a statistical character of common sedimentary rocks. The latter was made possible by a recent study [98, 107] which demonstrated that the spatial variations of rock properties are accurately and consistently reproduced by a random scaling model based on fractional Levy motion (fLm). Most studies of percolation relevant to flow in porous media ignore these long range correlations and only consider microscopic homogeneous media. We determine the scaling exponents associated with both structural and dynamic properties of percolating system with a Levy-based disorder. Scaling exponents associated with the Levy percolation model are very different to exponents of ordinary percolation.

9.1 Model of geological media

Relating the characteristics of a naturally occurring porous medium to its transport properties is one of the key challenges in understanding the physics of flow, dispersion and displacement in porous soils, groundwater aquifers, and petroleum reservoirs. The ability to accurately simulate flow phenomena in reservoirs is severely limited by the ability to numerically model reservoir scale geology. Only a relatively small volume of any subterranean reservoir is actually sampled by cored or lagged wells. Due to the incompleteness of the available data, a description based on these data
must have a probabilistic nature. Percolation networks are natural tools for studying such issues, as they provide one of the simplest prototypes of a disordered medium, and the large literature on transport in porous media has relied heavily on percolation concepts [52, 109]. For example, capillary controlled two-phase flow and displacement studies in sedimentary rocks have been modelled as a percolation process in a random medium [110].

In most studies of the percolation model and in its application to physics of sedimentary rock, spatial disorder has been assumed to be uncorrelated, i.e., the probability for any bond to be occupied is independent of the occupancy of any other bond. This is appropriate for a medium that is microscopically disordered but macroscopically homogeneous, such as a random packing of glass beads, but it is fundamentally inconsistent with the nature of geological media. The physical properties of sedimentary rock are, for example, macroscopically heterogeneous with strong correlations over extended regions of space [111, 112, 98]. If percolation studies are to have any relevance to flow and transport in natural media, then these heterogeneities need to be considered. A quantitative understanding of heterogeneity is the critical step towards understanding flow phenomena in geological formations. It is widely recognized that internal heterogeneity plays a crucial role in determining the movement of fluids through petroleum reservoirs and groundwater aquifers.

Although it has been noted [113] that an uncorrelated distribution of bond occupancy variables is a poor assumption for modelling sedimentary rock, the lack of a geologically plausible model for the correlations has prevented the consequences from being explored. Classical methods for dealing with reservoir/aquifer heterogeneity utilize Gaussian random fields with short-range correlations. From a statistical physics perspective, this offers no new understanding, as percolation with short-range correlations belongs to the same universality class as uncorrelated percolation [114]. In an effort to introduce more realism, models based on Gaussian fractals were introduced [111, 112]. These models treat the variations in rock properties as fractional Brownian motion (fBm) or as fractional Gaussian noise (fGn). The fGn model has
two-point correlations that fall off with separation distance $x$ as $x^{-\alpha}$; percolation on these types of random fields has been studied previously [113, 115]. Spatial heterogeneity in the fBm model is even stronger; correlations enter through the incremental values. Percolation using this model has been studied by Sahimi [109]. These previous studies on long-range correlated percolation showed different behaviour from ordinary percolation. However, these studies all utilized models based on the Gaussian distribution. Gaussian-based models have been shown [98, 107] to be inappropriate models for sedimentary formations; they underestimate the extreme degree of spatial variability inherent in sedimentary formations and fail to capture the sharp property contrasts associated with the most basic geological feature: stratification.

Fractional Levy motion (fLm) [61, 116] is a generalization of fractional Brownian motion [61] in which the Gaussian distribution of incremental values is replaced by symmetric Levy-stable distribution [117, 118]. These distributions have probability density given by

$$P(x) = \pi^{-1} \int_0^\infty \exp[-(Ck)^\alpha] \cos(kx) dk, \quad (9.1)$$
9.1 Model of geological media

where $0 < \alpha \leq 2$ is the Levy index and $C$ controls the width of the distribution. This family of distributions includes the Gaussian as a special case ($\alpha = 2$). The non-Gaussian Levy distributions are useful for modelling systems with a high degree of variability because of their slowly decaying tails ($Pr(|x| \geq s) \propto s^{-\alpha}$ for large $s$). In the fLM model, the Levy scale parameter $C$ varies with separation distance $l$ via a power law relationship $C \propto l^H$ with $0 < H < 1$ over the range 0.025 to 1000 meters. The scaling parameter is $H = 1/\alpha$ for independent increments. Values greater (less) than $1/\alpha$ indicate positive (negative) dependence in the incremental values, i.e. persistence or anti-persistence. Values of the Levy indices vary for differing geology suggesting that the indices are a useful measure of heterogeneity. Shown in Fig. 9.1 is a realization based on the three-dimensional fLM model for property variations in a stratified rock. This combination of parameters is typical of that found for permeability measurement. Realizations similar to Fig. 9.1 can be regarded as permeability maps for hypothetical petroleum reservoirs or groundwater aquifers.

In a previous analysis [98, 119] of sedimentary outcrops and borehole measurements Painter demonstrated that variations in permeability and other rock properties are
consistent with the fLm model. In all the cases tested a Levy density function with \( \alpha < 2 \) was found to provide an accurate fit to the histogram of incremental values. An example is shown in Fig. 9.2. Here we are only considering two-dimensional isotropic maps, which is consistent with thin, laterally extensive formations. A two-dimensional simulation based on the fLm model with \( \alpha = 1.2 \) and \( H = 0.25 \) is shown in Fig. 9.3.

9.2 Percolation simulation and discussion

We now use the fLm to propose a percolation model relevant to geological materials. Our first step is to replace the uncorrelated occupancy variables of ordinary percolation by variables from a stochastic simulation of fLm with a given \( \alpha \) and \( H \). A cell-centered map of permeability \( k \) having fLm properties is first generated by

![Figure 9.3: Two dimensional simulation of reservoir properties based on the Levy model with \( \alpha = 1.2 \) and \( H = 0.25 \).](image_url)
Figure 9.4: The correlated and random percolation clusters. Everywhere other than the regions in navy blue is the accessible cluster. In the Levy system (a) self-similarity is evident — holes at all length scales can be identified. Compactness of the correlated percolative cluster compared to the ordinary percolative system (b) is clear.
Figure 9.5: The Levy correlated and random percolation backbone clusters. Red indicates the high local fluid flux. In the Levy system (a) nearly all of the sample spanning cluster is made up of backbone bonds. In ordinary percolation system (b) the backbone is a small subset of the spanning cluster.
substituting Levy displacements for the Gaussian ones in the midpoint displacement algorithm [120]. The bond connecting two cells is then assigned a value \( K_{ij} = \frac{k_i k_j}{k_i + k_j} \), since permeabilities in series combine like electrical conductances. To construct a percolation network we activate those bonds that have the largest property values until a sample spanning cluster is formed. Fig. 9.4 illustrates a percolation cluster generated by this model and a comparison with an ordinary percolation cluster. The differences are striking. Qualitatively one observes the connected cluster in the Levy system is clustered together with a larger proportion of the filled sites connected to the spanning clusters compared to the random percolation case. Self-similarity is still evident in the Levy case; holes at all scales can be identified. A more striking difference is noted when comparing the backbone morphology in the two cases (see Fig. 9.5). The backbone is that fraction of the occupied bonds in the infinite (spanning) cluster which actually carry current or flow; the backbone of a percolating system therefore plays a fundamental role in determining transport properties. For example, the tortuosity of transport paths is controlled by the structure of the backbone. In the Levy system nearly all of the spanning cluster is made up of backbone (fluid-carrying) bonds. This is in direct contrast to the backbone of a random percolating system where the backbone is a small subset of the spanning cluster. We next study the dependence on the correlation of various percolation quantities. We generate percolation clusters using a lattice size of \( L = 256 \) with over 100 realizations for a range of \( \alpha \) and \( H \) relevant to geological materials [98]. The percolation threshold \( p_c \) of the systems is invariant \((p_c = \frac{1}{2})\) in all cases. To study the effect of the long-range spatial correlations on the cluster structure we calculate the fractal dimension \( d_f \) of the infinite incipient cluster and of the backbone \( d_{bb} \). For random percolation, these structural exponents are universal, and in particular, \( d_f = 91/48 \) and \( d_{bb} \approx 1.64 \) for \( d = 2 \). In all cases of percolation in Levy fields the exponents \( d_f \) and \( d_{bb} \) are essentially identical and are very close to 2.0. The value of \( d_f \) and \( d_{bb} \) illustrate quantitatively the relative compactness of the clusters generated from the Levy correlated field. The results are summarized in Table 9.1.

While the morphology of ordinary and Levy percolation is different, of practical
Table 9.1: Properties associated with the heterogeneous percolation model.
The results are given for a sample of $\alpha$ and $H$ relevant to geologic media.

<table>
<thead>
<tr>
<th>$\alpha, H$</th>
<th>$p_c(\infty)$</th>
<th>$d_f$</th>
<th>$d_{bb}$</th>
<th>$\beta$</th>
<th>$\sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.2, 0.25</td>
<td>.497</td>
<td>1.98 ± 0.05</td>
<td>1.97 ± 0.05</td>
<td>0.03 ± 0.05</td>
<td>0.57 ± 0.12</td>
</tr>
<tr>
<td>1.4, 0.25</td>
<td>.492</td>
<td>2.00 ± 0.05</td>
<td>1.99 ± 0.05</td>
<td>0.07 ± 0.05</td>
<td>0.61 ± 0.11</td>
</tr>
<tr>
<td>1.6, 0.25</td>
<td>.508</td>
<td>1.99 ± 0.05</td>
<td>1.97 ± 0.05</td>
<td>0.03 ± 0.05</td>
<td>0.71 ± 0.13</td>
</tr>
</tbody>
</table>

importance is how the heterogeneity will effect transport in geological formations; for example, knowing the effect different heterogeneity will have on oil recovery. Percolation has been used previously to describe the statistical nature of capillary-controlled immiscible displacement. Although percolation is not a true indicator of oil recovery it will give insight into the likely effect on recovery that various forms of heterogeneity give. The residual oil saturation $S_{or}$ is related to the percolation order parameter $P(p)$ (the fraction of occupied sites which are in the infinite cluster) by $S_{or} = 1 - \int_0^1 P(p) dp$ [121]. $P(p)$ for the Levy system differs appreciably from ordinary percolation. Close to the critical point $P(p)$ has the behaviour $P(p) \sim (p - p_c)^\beta$. We have evaluated $\beta$ for the Levy system – the value is close to zero (see Table 9.1), in contrast to $\beta = \frac{5}{36}$ for ordinary percolation. Thus residual oil saturation is thus strongly effected by Levy heterogeneity.

Knowledge of dynamic properties like conductance is also essential if one is to understand transport in sedimentary formations; e.g., the diffusivity in and permeability of natural rock. Transport properties are known to obey scaling laws near the percolation threshold as well. Dynamic exponents associated with transport properties are largely universal. Long-range spatial correlation have been shown to have a substantial effect on the dynamic exponents [113]. We measure the conductance exponent $\mu$ defined by $g \sim (p - p_c)^\mu \sim \xi^{-\mu/\nu}$. The conductance exponent varies strongly from the ordinary percolation result (see Table 9.1) and is consistent with
9.3 Conclusion

The percolation model has proven relevant in studies of two-phase flow and displacement in porous media\(^1\). Experimental evidence on small scale \textit{homogeneous} media support this view [123]. In practical applications, such as field scale displacement of oil large-scale spatial variations of the reservoir must be considered. It has been argued [109] that field-scale displacement problems are essentially two-dimensional\(^2\). We propose that this two-dimensional Levy percolation model is directly relevant to field-scale studies of flow phenomenon in porous media.

\(^1\)\textit{Invasion} percolation is in fact relevant to two-phase immiscible displacement processes. In this model the network is initially filled with a defender. To each site of the network a random number is assigned. A displacing fluid then displaces the defender at each time step by choosing the site with the smallest assigned number. There is a close connection between invasion percolation and random percolation[122]. We have considered the invasion percolation process for a network with values selected from an fLm distribution. There is little difference noted between the fLm invasion percolation model and the current result.

\(^2\)It was noted[109] that in studies relevant to field-scale data one considers lateral distances of tens of kilometres, whereas thicknesses of < 100 metres. The media can therefore be considered essentially two-dimensional.
Chapter 10

Conclusion

In this thesis we have made contributions to two research areas of scientific and technological interest: modelling transport of steady flow in three-dimensional porous media by lattice gas simulation and modelling the two- and three-dimensional fracture phenomena in heterogeneous media by simulation using a resistor network analogue. Each of the chapters is self-contained in that the results have been discussed at the conclusion of each chapter. It is useful however to summarize and discuss the central results of the thesis in a wider context and consider areas of future research.

10.1 Part I: Simulational studies on flow in porous media

In the first part of the thesis we have utilized the lattice gas automata (LGA) method, a discrete solution of the Navier-Stokes equations, to study fluid flow in complex geometries on a large scale. We discussed in depth an implementation of LGA on parallel computer. The lattice gas method allows one to describe macroscopic flow phenomena using large-scale averaging and it also provides detail crucial to the understanding of relationships between the volume-averaged parameters used in the study of flow in porous media.
Using the LGA simulation, we have investigated the permeability of porous materials with physically realistic randomness and quantified the effect of porosity and pore size distribution on the permeability of a model porous solid. We have considered the validity of different phenomenological models used in practice to relate flow properties of porous media. The Kozeny-Carman equation is in good agreement with the data for flow in periodic media\cite{39}. The Blake-Kozeny and Rumpf-Gumpte models give excellent fits to the simulational results for monodisperse random media. The quantitative agreement between the lattice gas solution and the empirical equations for both random and periodic media indicates the strength of the method in the study of porous media flows. For media of more complicated geometries such as the bidisperse media, the empirically based models lead to errors in the permeability prediction. This indicates that the parametrization of the empirically based equations are not adequate. We believe that more extensive studies by means of simulation on this problem by taking into consideration of various microscopic structural factors of porous media such as anisotropicity should shed a light on this problem (Chapter 2 and 3).

We have researched on a long standing and unsolved problem concerning the relationship between the electrical conductivity of a fluid saturated porous medium and the permeability of the same system. Although various empirical relationships between the two properties have been suggested, none is successful over the entire range of the porosities or range of pore size distributions. We have computationally determined the permeability and conductivity for various pore size distributions and porosities, compared the fluid flow path and electrical current path for the same medium and revealed the important difference at intermediate and low porosities between, in specific, the tortuosities derived by the hydrodynamic method and electrical conductivity calculation (Chapter 4).

In Chapter 5, we have studied the hydrodynamic screening force distribution of the DLA cluster. As colloidal particles flocculate irreversibly, they form aggregates which exhibit fractal structure. The aggregates have a very low density when com-
pared with bulk matter, yet they are very effective at screening hydrodynamic forces. These aggregates are known to exhibit a large spread of drag forces on the flowing fluid, leading to unique mass transport properties onto and off the aggregate. The quantitative nature of the force depletion around a fractal structure is important since these materials are often used for their screening properties. Previous hydrodynamic studies of flow about the fractal aggregates were limited to very small aggregates (<500 particles) and to approximate solutions of the hydrodynamics equations [64]. We have performed lattice gas simulations to measure the drag force on the Diffusion Limited Aggregate (DLA) clusters on a much larger scale of the DLA mass (up to 5,000 particles). Our result reveals the universal characteristics of the drag force distribution on a broader range of DLA mass.

Also in Chapter 5, we have studied the effect of surface roughness on the transport properties of the media. Conventionally in studies of underground reservoirs, the fracture surfaces are modelled as perfectly smooth. Flow in a single fracture is modelled as flow between parallel flat plates. Our simulation studies on this problem suggest that the incorporation of a realistic description of the fracture surfaces roughness leads to drastic and important differences in fluid flow properties.

10.2 Part II: Fracture in heterogeneous media

In the second part of this thesis, we have made simulational studies on two- and three-dimensional fracturing phenomena in presence of the material heterogeneity. The simulations are based on a resistor network analogue. We have also proposed a new percolation method for studies of transport properties in geological media.

In Chapter 7, we show that the heterogeneity existing in material properties play dominating role at given external physical conditions. The statistics has shown dependence of the resultant fracture network and fracture surface on the heterogeneity of the material. The comparison between the two- and three-dimensional simulations have been made. We have shown that the two-dimensional model may be used to
Figure 10.1: Comparison between a CT scan image of fracture network in coal sample (a, courtesy of Dr. Lincoln Paterson, CSIRO, Australia) and a simulation result of coal fracture network (b).
estimate the fracture surface properties such as the surface roughness, but it fails to capture practically more important characteristics of the fracture system, such as the crack size distribution. In Chapter 8, we have studied the universality of the scaling properties of the fracture surface roughness. The fracture surfaces are produced from the simulations using resistor network model with breakdown criteria fields of various level of disorders. Although the roughness exponent $\zeta$ is always found within a narrow range, its value systematically decreases as the extent of disorder is increased. For anisotropic materials the scaling properties are found to be independent of the orientation of the imposed stress despite a visible difference in the fracture surface morphology. These results indicate that the scaling properties of the fracture surface are not universal, but depend albeit weakly, on material properties. Values of the roughness exponent $\zeta$ are consistent for the same breakdown distribution in two and three dimensions.

We have considered the effect of isotropic breakdown criteria fields on the resultant fracture network. As a current and future direction of this research, we will consider incorporating the large scale anisotropicity in the description of material properties and extend our simulation method to study the fracture mechanism of material in presence of both heterogeneity and anisotropicity in three-dimensions on a large scale. For the latter, there are a number of immediate applications. For example, a study of the fracture properties of coal seams. Due to the global attention over the naturally occurring methane in coal seams as an unconventional source of natural gas, knowledge of the morphology of coal seam fractures, which govern the gas transport properties of a coal bed, is vital to economic success when exploiting coalbed methane. The simulation method studied here has been applied to study of fracture network in coal beds and will be applied to the studies of transport properties within those fracture networks. In Fig. 10.1(a), we show a CT scan image of coal sample. In Fig. 10.1(b), we show a preliminary result from two-dimensional simulation using resistor network model on a model media with a similar anisotropicity to material properties of the coal sample. The morphological similarity between the two fracture networks is evident.
Fluid displacement patterns have previously been studied extensively on media with uncorrelated random properties. Relating the characteristics of a naturally occurring porous medium to its transport properties is one of the key challenges in understanding the physics of flow, dispersion and displacement in porous soils, groundwater aquifers, and petroleum reservoirs. We have made preliminary investigations of the effect of heterogeneity of the geological media on the transport properties (Chapter 9). Our studies using percolation method on Levy heterogeneous field suggest that the long range spatial correlation has a substantial effect on the dynamic exponents. The conductance exponent of the system of long range spatial correlation is found to vary strongly from the ordinary system. This result hints at the drastic effect of incorporation of realistic heterogeneity on the properties of fluid flows in natural porous media.

The future research concerned on this aspect is divided into two parallel parts:

- To extend and apply invasion percolation with and without trapping to model the immiscible two-phase fluid flow on reservoir scale with realistic heterogeneity in two- and three-dimensional systems.

- In parallel, to generalise to three-dimensions an elaborate network model based on pore-scale physics for multi-phase fluid flow. Recent experimental and simulation studies by W. V. Pinczewski et. al. [124, 125, 126, 127] and the recent advances in supercomputer technology have demonstrated the possibility for accurately modelling three phase (gas, oil and water) flow in porous media.
Appendix A

Implementation of Laplacian solver

In this section, we shall discuss the implementation of the Laplacian solver on the CM5. The code discussed here is used for resistor-network simulations related to this thesis: i.e. for the simulation of electrical tortuosity in porous media (in chapter 4); for the simulation of fractures in heterogeneous media using network resistor model (in chapter 7); for the percolation studies on the transport properties in geological media (in chapter 9). The implementation of a fast solver for the repetitive use is crucial for the accomplishment of these simulations at the large scale.

To derive the electrical potential field on a source-free field with given boundary values on the lattice i.e. the square lattice for the system shown in Fig. 6.4 (or cubic lattice in case of 3D) where only the links between the nearest neighbours are considered, we need to solve the discretized elliptic equation of Laplacian type, which, in case of 3D and also assuming unit distances between all the nearest neighbouring lattice sites without losing generality, writes,

\[
\begin{align*}
\sigma_{i,j,k;i+1,j,k}(\phi_{i+1,j,k} - \phi_{i,j,k}) - \sigma_{i,j,k;i-1,j,k}(\phi_{i,j,k} - \phi_{i-1,j,k}) + \\
\sigma_{i,j,k;i,j+1,k}(\phi_{i,j+1,k} - \phi_{i,j,k}) - \sigma_{i,j,k;i,j-1,k}(\phi_{i,j,k} - \phi_{i,j-1,k}) + \\
\sigma_{i,j,k;i,j,k+1}(\phi_{i,j,k+1} - \phi_{i,j,k}) - \sigma_{i,j,k;i,j,k-1}(\phi_{i,j,k} - \phi_{i,j,k-1}) = 0
\end{align*}
\]
Implementation of Laplacian solver

and can be re-written as,

\[
\left( \sigma_{i,j,k;i+1,j,k} + \sigma_{i,j,k;i,j+1,k} + \sigma_{i,j,k;i,j-1,k} + \sigma_{i,j,k;i,j,k+1} + \sigma_{i,j,k;i,j,k-1} \right) \phi_{i,j,k} \\
- \sigma_{i,j,k;i+1,j,k} \phi_{i+1,j,k} - \sigma_{i,j,k;i,j-1,k} \phi_{i,j-1,k} \\
- \sigma_{i,j,k;i,j+1,k} \phi_{i,j+1,k} - \sigma_{i,j,k;i,j-1,k} \phi_{i,j-1,k} \\
- \sigma_{i,j,k;i,j,k+1} \phi_{i,j,k+1} - \sigma_{i,j,k;i,j,k-1} \phi_{i,j,k-1} = 0, \\
\]

(A.2)

where \( \sigma_{i,j,k,i',j',k'} \) denotes the bond conductance from node \([i, j, k]\) to \([i', j', k']\) and \( \phi_{i,j,k} \) is the potential on the node \([i, j, k]\). For example, to use this equation with network resistor model for simulation of fracture phenomena, the bond conductance is declared to be void if the bond (resistor) is fused, otherwise remains unity (see chapter 7).

The equation A.2 is written for node \([i, j, k]\) on a 3D lattice. For the whole lattice, we have a set of nodes on which the conductances for the bonds between the nearest neighbours and the node are defined, thus the set of linear equations can be summarized as,

\[
A \cdot x = b \\
\]

(A.3)

where \( x \) is the potential field to solve and \( b \) the vector holding the boundary value on the positions where the boundary nodes and zeros otherwise (source-free field). The matrix \( A \) is tridiagonal, sparse, symmetric and positive definite. There are many ways [128] to solve this equation A.3. However, when the lattice size is large, it is most practical to use the relaxation or conjugate gradient method as this requires less memory. We choose to use the CM5/CMSSL conjugate gradient iterative algorithm, which minimized \( \| A \cdot x - b \|^2 \). In particular, to use the conjugate gradient method, one has to do the multiplication of matrix and vectors for many times. For the conventional serial algorithm, the most of the computing time for solving the large set of linear equations is spent on doing these multiplications. Thanks to the simplicity of the lattice geometry we choose to use and also the rich functionalities provided by CMSSL libraries for data communication between parallel nodes, we performed the
Matrix · Vector in a way that the matrix-vector product is reduced to the sum of the products of six vector-vector inner-products. This speeds up the convergence of the iterative procedure drastically. The sum is written as:

\[
y = A_{0,0,0} \times x + A_{1,0,0} \times cshift(x, 1, 1) \\
+ A_{-1,0,0} \times cshift(x, 1, -1) \\
+ A_{0,1,0} \times cshift(x, 2, 1) \\
+ A_{0,-1,0} \times cshift(x, 2, -1) \\
+ A_{0,0,1} \times cshift(x, 3, 1) \\
+ A_{0,0,-1} \times cshift(x, 3, -1),
\]

(A.4)

where \( A_{0,0,0} \) is a vector containing the diagonal elements of the matrix \( A \) while \( A_{i,j,k} \) holding the corresponding off-diagonal matrix elements.
Appendix B

Parallel algorithm for identifying bond clusters

In this section, we shall discuss a parallel algorithm for identifying bond clusters on cubic lattice. Shown in Fig. 7.4 are the fracture surfaces serrated with branches, the clusters. The fracture surfaces are important in understanding the fracture phenomena. To identify these clusters also has important implications in, i.e. crack interaction. In geology, the branches of the critical crack play often paramount role in determining the transport properties related to the major crack. In practice, for large network and particularly for 3D, serial algorithms which systematically step through the whole lattice are often computationally expensive. To introduce the algorithms used to identifying the bond clusters in large 3D lattice, we shall first start a 2D square lattice.

![Diagram of 2D and 3D cracks](image)

Figure B.1: Relation between a fused resistor and an associated crack.
Parallel algorithm for identifying bond clusters

In the resistor network analogue for fracture simulation, the single bond crack is formed when one resistor is fused. Let us assume that the crack associated with a fused resistor (bond) is a segment of a line of the same length as that of the bond and perpendicular to the orientation of the bond. Both the crack and the bond cut each other into equally halves (see Fig. B.1). In 3D, on a cubic lattice, the crack is a square. Two single-bond cracks join each other as a cluster if one end of each single bond joins with one of end of another bond crack. Similarly in 3D, two cracks join each as a cluster if they share a common edge.

We define a super lattice which is twice the size of the original lattice. Fig. B.2 is an illustration of this super lattice. The black squares, named nodes are the nodes on the original lattice. The circles, now named bonds on the super lattice represent the bonds between the nodes on the original lattice; the black colour indicates that the bond is broken (fused) and the white colour indicates that the bond is intact (not fused). The program can be written in such a way that: (1) at the beginning, on the super lattice each black bond is assigned a unique positive integer index and each white one assigned zero; (2) all joints fetch the positive index from each neighbouring bond, the maximum integer among all fetched by the joint is preserved on that joint.

Figure B.2: Scheme for identifying bond clusters.
Parallel algorithm for identifying bond clusters

and sent back to the bond where a positive integer has been fetched from; (3) repeat (2) until there are no more updates in the bonds index. After the whole process finishes, all bonds with the same index belong to one cluster. In case of 3D cubic lattice, the algorithm is the same, except that for each single bond there are 4 joints. This algorithm in its parallel format, reduces considerably the computational need for the identification of bond clusters in 2D and 3D. By using the parallel format of this algorithm, the computational need for identifying the 2D or 3D bond clusters is proportional the maximum dimension of the cluster itself instead of the size of the system. This algorithm can also be generalized for application on lattice of other geometries. For identifying site clusters, the conventional algorithms are equally good.
Bibliography


[41] As in our simulation, in the case of non-spherical particles the surface average equivalent diameter is defined by $D_{p}^{equiv} = \frac{6V_{p}}{S_{p}}$ where $\frac{6V_{p}}{S_{p}}$ is the volume to surface ratio of the particulate matter.


[45] It is noted however, that in an experimental study the average grain size was shown to correlate well with the length scale characteristic of the transport. See E. Guyon, L. Oger, and T.J. Plona, J. Phys. D: Appl. Phys. 20:1637, 1987.
[46] The factor \( \frac{L_x}{L} \) in the equation \( v_p = \frac{U}{\phi \frac{L_x}{L}} \) is an overestimate of the correction for the tortuous flow paths. It assumes that the seepage velocity \( v_p \) is identical along all flow paths - this correction should therefore have a smaller value than \( \frac{L_x}{L} \).


[76] A. A. Griffiths, Phil. Trans. R. Soc. Lond. 221, 163 (1921).


