Multiscale Modeling of Fracture Processes in Cementitious Materials
Multiscale Modeling of Fracture Processes in Cementitious Materials

Proefschrift

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Keywords: Lattice fracture model, Anm material model, Parameter-passing upscaling, Cement paste, Mortar, Concrete

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To my beloved mother and father
Concrete is a composite construction material, which is composed primarily of coarse aggregates, sands and cement paste. The fracture processes in concrete are complicated, because of the multiscale and multiphase nature of the material. In the past decades, comprehensive effort has been put to study the cracks evolution in concrete, both experimentally and numerically.

Among all the computational models dealing with concrete fracture, the lattice fracture model wins at several aspects, such as being able to capture detailed crack information, high computational efficiency and stability. The lattice fracture model also enables to investigate how the fracture properties of concrete depend on its material structure. This can be achieved by projecting the lattice network on top of the original material structure of concrete. In this thesis a parallel computing code is described, which is implemented for the lattice fracture model, in order to reduce the computational time and to enable the analysis on even larger lattice system.

The fracture properties of cement paste, mortar and concrete are highly related in nature. In this thesis the lattice fracture model is coupled with the parameter-passing multiscale modeling scheme to study the relationship of the fracture processes in cement paste, mortar and concrete. A multiscale fracture modeling procedure is proposed and demonstrated. Three levels are defined, including micrometer scale for cement paste, millimeter scale for mortar and centimeter scale for concrete. The lattice fracture model is applied at each scale respectively. The inputs required at a certain scale are obtained by
the simulation at a lower scale. At the lowest scale in question, the mi-
crometer scale for cement paste, inputs are determined by laboratory
experiments and/or nanoscale modeling from literature.

Besides the multiscale lattice fracture model, another highlight in this
thesis is the development of the Anm material model, which can sim-
ulate a material structure of concrete with realistic shape aggregates.
Compared with classic concrete material models, the shape of aggre-
gates is changed from spheres to irregular ones, which is closer to
reality. The aggregate particle shape is represented by spherical har-
monic expansion, where a set of spherical harmonic coefficients is used
to describe the irregular shape. The take-and-place parking method
is employed to put multiple particles together within a pre-defined
empty container, which can be interpreted as the material structure
of concrete. The key element in this parking algorithm is to check
whether two particles overlap, as no overlap is allowed in the result-
ing simulated material structure.

The multiscale lattice fracture model and the Anm material model,
proposed and established in this thesis, can be used by researchers in
concrete community, to study the various factors which influence the
mechanical performance of cementitious materials. They can also be
adapted with other computational models to form a complete fully
multiscale modeling framework, from nanoscale to macroscale.
Samenvatting

Beton is een composiet constructiemateriaal dat is samengesteld uit grind, zand en cementsteen. Breukprocessen in beton zijn gecompliceerd omdat het materiaal van nature verschillende schalen en componenten bevat. In de laatste decennia was er veel aandacht voor het besturen van scheurgroei in beton, zowel op experimenteel vlak als ook numeriek.

Kijkend naar al de numerieke modellen voor scheurvorming in beton kan gesteld worden dat het lattice fracture model op enkele aspecten duidelijk als winnaar uit de bus komt. Deze zijn het vermogen om gedetailleerde scheurinformatie te produceren en de hoge numerieke efficiëntie en stabiliteit. Het lattice fracture model maakt het ook mogelijk om breukeigenschappen van beton te onderzoeken als functie van de materiaalstructuur. Hiervoor kan het lattice netwerk worden geprojecteerd bovenop de materiaalstructuur van beton. In dit proefschrift is een parallelle computer code beschreven, die is geïmplementeerd in het lattice fracture model, om de benodigde rekentijd te reduceren en het berekenen van grotere lattice systemen mogelijk te maken.

De breukeigenschappen van cementsteen, mortel en beton zijn sterk aan elkaar gerelateerd. In dit proefschrift is het lattice fracture model gekoppeld met het parameter-passing multi-schaal modelleren schema om de relatie te besturen tussen de breuk processen in cementsteen, mortel en beton. Een multi-schaal scheurmodeller procedure is uitgewerkt en gedemonstreerd. Drie niveaus zijn gedefinieerd: de micrometerschaal voor cementsteen, de millimeterschaal voor mortel en de centimeterschaal voor beton. Het lattice fracture model is
toegepast op elke afzonderlijke schaal. De benodigde invoerparameters voor een bepaalde schaal volgen uit de simulatie van een lagere schaal. Bij de laagste schaal, de micrometerschaal voor cementsteen, zijn de invoerparameters bepaald op basis van laboratoriumexperiments en/of nanoschaal modellering uit de literatuur.

Een ander belangrijk onderwerp in dit proefschrift, naast het ontwikkelen van het multi-schaal lattice fracture model, is de ontwikkeling van het Anm materiaal model. Dit model kan een materiaalstructuur van beton simuleren, waarbij de toeslagkorrels realistische vormen hebben. Vergeleken met klassieke materiaalmodellen voor beton kunnen in het Anm model naast bolvormige ook onregelmatige vormen worden gebruikt voor de toeslagkorrels, hetgeen realistischer is. De vorm van de toeslagkorrels wordt weergegeven met spherical harmonic expansion, waarbij een set van sperical harmonic coëfficiënten wordt gebruikt om de onregelmatige vorm te beschrijven. De take-and-place parkeer methode is toegepast om korrels in een gedefinieerde container te positioneren. Het resultaat levert vervolgens de materiaalstructuur van beton op. Het belangrijkste element in dit parkeeralgoritme is om te controleren of twee korrels elkaar niet overlappen. Overlappende korrels zijn niet toegestaan in de gesimuleerde materiaalstructuur.

Het multi-schaal lattice fracture model en het Anm materiaal model die beide zijn voorgesteld en uitgewerkt in dit proefschrift kunnen worden gebruikt door onderzoekers in de betonwereld. Met de modellen kunnen de verschillende factoren worden bestudeerd die het mechanisch gedrag van cementgebonden materialen beïnvloeden. Ze kunnen ook worden verweven met andere numerieke modellen om zo een compleet multi-schaal modellere kader te vormen van nano- naar macroschaal.
Acknowledgements

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It would not have been possible to complete this PhD research work and to write this thesis without the help and support of the kind people around me, to only some of whom it is possible to give particular mention hereby.

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Zhiwei Qian
Delft, the Netherlands
May 2012
# Contents

List of Figures ................................................. 15
List of Tables .................................................. 21
Symbols .......................................................... 23

1 Introduction .................................................... 25
   1.1 Background ................................................. 25
   1.2 State of the art .............................................. 26
   1.3 Objectives and methodology of this research .................. 27
   1.4 Outline of the thesis ......................................... 27

2 Three-dimensional Lattice Fracture Model ....................... 31
   2.1 Background ................................................. 31
   2.2 Modeling procedures ........................................ 33
      2.2.1 Lattice network construction ......................... 34
      2.2.2 Test setup ............................................. 44
      2.2.3 Fracture processes simulation ....................... 48
      2.2.4 Load-displacement response and cracks propagation .... 66
   2.3 Summary .................................................... 67

3 Cement Paste at Microscale ................................... 69
   3.1 Micromechanical modeling of cement paste .................... 70
      3.1.1 Simulated microstructures of cement paste ............. 71
      3.1.2 Mechanical performance evaluation of the microstructures 74
### CONTENTS

3.1.3 CT-scanned microstructures and its micromechanical properties ........................................... 83
3.2 Influences of various factors ................................................................. 86
  3.2.1 Degree of hydration ................................................................. 88
  3.2.2 Cement fineness ................................................................. 93
  3.2.3 Water/cement ratio ............................................................... 96
  3.2.4 Mineral composition of cement ..................................................... 98
3.3 Summary ......................................................................................... 105

4 Mortar and Concrete at Mesoscale .............................................. 109
  4.1 Ann material model ................................................................. 110
    4.1.1 Irregular shape description ......................................................... 111
    4.1.2 Individual particle properties and operations .................................... 115
    4.1.3 Parking procedures and algorithms ................................................ 116
    4.1.4 Periodic and non-periodic material boundaries .................................... 122
  4.2 Material mesostructures for mortar and concrete ......................... 123
    4.2.1 Mortar mesostructure ........................................................... 123
    4.2.2 Concrete mesostructure ........................................................... 124
  4.3 Summary ......................................................................................... 126

5 Multiscale Modeling ................................................................. 129
  5.1 Parameter-passing scheme and size effect of cement paste ............. 129
  5.2 Bridging scales among cement paste, mortar and concrete ............. 134
    5.2.1 Connecting cement paste to mortar .............................................. 135
    5.2.2 Upscaling mortar to concrete ...................................................... 137
  5.3 Summary ......................................................................................... 140

6 Conclusions and Outlook .......................................................... 143
  6.1 Conclusions ...................................................................................... 143
  6.2 Outlook ........................................................................................... 145

References ...................................................................................... 147
List of Figures

1.1 Layout of the thesis main body ........................................... 27
2.1 An overview of the lattice fracture analysis .......................... 34
2.2 Lattice network construction for general material and scale ....... 35
2.3 Prism of the size 40 mm × 40 mm × 60 mm subject to uniaxial tensile load ................................................................. 36
2.4 Linear-brittle constitutive law of lattice elements .................... 37
2.5 Microcracks pattern of perfect homogeneous material subject to uniaxial tension ......................................................... 40
2.6 Simulated global mechanical properties reduction against randomness ................................................................. 41
2.7 Lattice element type determination and its constitutive relation .... 42
2.8 Microstructure of cement paste simulated by the HYMOSTRUC3D model ................................................................. 43
2.9 3D contact particles, lattice element and network .................... 43
2.10 Determination of particle modulus (first step averaging) ............ 45
2.11 Determination of lattice element modulus (second step averaging) .... 46
2.12 Uniaxial tensile test setup .................................................... 47
2.13 Flowchart of lattice fracture analysis kernel solver .................... 49
2.14 3D lattice beam element in local domain ............................... 50
2.15 Local and global domains .................................................... 63
2.16 Multi-linear constitutive law of lattice elements ....................... 66
3.1 Combined application of the HYMOSTRUC3D model and the 3D lattice fracture model ......................................................... 70
LIST OF FIGURES

3.2 Hydration of a single cement particle ........................................ 72
3.3 Contact of hydrating cement particles ....................................... 72
3.4 Microstructures of cement paste at different degrees of hydration with the specification in Table 3.1 ........................................ 73
3.5 Simulated degree of hydration diagram against hydration time ...... 74
3.6 Voxel-based image of the microstructure of cement paste in Figure 3.4(b) (100 µm × 100 µm × 100 µm) .......................................... 75
3.7 Individual phases of the microstructure of cement paste in Figure 3.6 76
3.8 Uniaxial tensile test on lattice system of cement paste at microscale 78
3.9 Simulated stress-strain diagram of cement paste at microscale ....... 80
3.10 3D microcracks propagation of cement paste due to tension at microscale, corresponding with Figure 3.9 .......................... 80
3.11 Deformed specimen due to vertical tension in the final failure state, corresponding with Figure 3.9 .......................... 81
3.12 Simulated stress-strain diagrams of cement paste at microscale, loaded horizontally along x-direction or y-direction, and vertically along z-direction ........................................ 82
3.13 Cracks patterns in the final failure state, loaded horizontally along x-direction or y-direction, and vertically along z-direction ......... 82
3.14 Simulated stress-strain diagrams of cement paste with regular lattice mesh, and irregular lattice mesh at the randomness of 0.5 .... 83
3.15 Pre-peak and post-peak microcracks for the regular meshed lattice system, and the irregular meshed lattice system at the randomness of 0.5 ........................................ 83
3.16 Microstructure of cement paste of size 75 µm × 75 µm × 75 µm at the curing age 28 days with water/cement ratio 0.5 from CT scan (provided by UIUC) ........................................ 84
3.17 Phase segmentation of the microstructure of cement paste in Figure 3.16 ........................................ 85
3.18 Simulated stress-strain diagram of the experimental cement paste at microscale ........................................ 87
3.19 Simulated cracks pattern in the final failure state for the experimental cement paste at microscale, corresponding with Figure 3.18 88
<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.20</td>
<td>Porosity of the hydrating cement paste system against degree of hydration</td>
</tr>
<tr>
<td>3.21</td>
<td>Development of the Young’s modulus and the tensile strength against the degree of hydration</td>
</tr>
<tr>
<td>3.22</td>
<td>Trendlines of the Young’s modulus and the tensile strength against the porosity of the cement paste system</td>
</tr>
<tr>
<td>3.23</td>
<td>Relationship between the strain at peak load and the degree of hydration</td>
</tr>
<tr>
<td>3.24</td>
<td>Relationship between the fracture energy and the degree of hydration</td>
</tr>
<tr>
<td>3.25</td>
<td>Relationship between the fracture energy and the porosity</td>
</tr>
<tr>
<td>3.26</td>
<td>Influences of degree of hydration on the tensile stress-strain response</td>
</tr>
<tr>
<td>3.27</td>
<td>Influences of degree of hydration on the cracks pattern in the final failure state, corresponding with Figure 3.26</td>
</tr>
<tr>
<td>3.28</td>
<td>Influences of cement fineness on the cracks pattern in the final failure state, compared at the same curing age of 28 days, corresponding with Table 3.12</td>
</tr>
<tr>
<td>3.29</td>
<td>Influences of cement fineness on the tensile stress-strain response, compared at the same degree of hydration 69%</td>
</tr>
<tr>
<td>3.30</td>
<td>Influences of cement fineness on the cracks pattern in the final failure state, compared at the same degree of hydration 69%, corresponding with Figure 3.29</td>
</tr>
<tr>
<td>3.31</td>
<td>Influences of water/cement ratio on the cracks pattern in the final failure state, compared at the same curing age of 28 days, corresponding with Table 3.13</td>
</tr>
<tr>
<td>3.32</td>
<td>Influences of water/cement ratio on the tensile stress-strain response, compared at the same degree of hydration 69%, corresponding with Table 3.14</td>
</tr>
<tr>
<td>3.33</td>
<td>Influences of water/cement ratio on the cracks pattern in the final failure state, compared at the same degree of hydration 69%, corresponding with Figure 3.32</td>
</tr>
<tr>
<td>3.34</td>
<td>Particle size distribution of the special cements</td>
</tr>
<tr>
<td>3.35</td>
<td>Initial microstructure of the special cement paste (porosity=56%)</td>
</tr>
<tr>
<td>3.36</td>
<td>Degree of hydration diagrams for the special cement pastes</td>
</tr>
</tbody>
</table>
## LIST OF FIGURES

3.37 Microstructures of the special cement pastes at the curing age of 28 days ........................................... 104
3.38 Stress-strain response diagrams for the special cement pastes at the curing age of 28 days .......................... 105
3.39 Cracks patterns in the final failure state for the special cement pastes at the curing age of 28 days, corresponding with Figure 3.38 106

4.1 Cement paste, mortar and concrete ........................................... 109
4.2 Particles embedded matrix material model ................................. 110
4.3 Spheres, ellipsoids and multi-faceted polyhedrons [http://wikipedia.org] ..................................................... 111
4.4 Spherical coordinate system [http://wikipedia.org] ....................... 112
4.5 Spherical harmonic coefficients data structure .............................. 113
4.6 An irregular shape particle described by spherical harmonics .... 114
4.7 Flowchart of parking procedures ............................................. 118
4.8 Two particles overlap ............................................................. 119
4.9 Newton-Raphson iteration scheme ........................................... 121
4.10 Periodic and non-periodic material boundaries ............................. 123
4.11 Particle size distribution for the sands in mortar ......................... 125
4.12 The mesostructure of the mortar specimen with irregular shape sand particles ........................................... 125
4.13 Particle size distribution for the coarse aggregates in concrete ...... 126
4.14 The mesostructure of the concrete specimen with irregular shape crushed stones ............................................ 127

5.1 Parameter-passing multiscale modeling scheme .............................. 130
5.2 Approximation of non-linear stress-strain response by multi-linear curve ....................................................... 131
5.3 Simulated stress-strain response for the $7 \text{ mm} \times 7 \text{ mm} \times 7 \text{ mm}$ specimen of cement paste at mesoscale ........ 132
5.4 Simulated stress crack opening diagram for the $7 \text{ mm} \times 7 \text{ mm} \times 7 \text{ mm}$ specimen of cement paste at mesoscale . 133
5.5 Affected lattice elements during the fracture processes in the cement paste specimen of the size $7 \text{ mm} \times 7 \text{ mm} \times 7 \text{ mm}$ at mesoscale 134
5.6  Lattice mesh for the 10 mm × 10 mm × 10 mm mortar at mesoscale 136
5.7  Simulated Young’s modulus and tensile strength of every block in
     the 10 mm × 10 mm × 10 mm mortar at mesoscale . . . . . . . . 137
5.8  40 mm × 40 mm × 40 mm out of 150 mm × 150 mm × 150 mm con-
     crete specimen . . . . . . . . . . . . . . . . . . . . . . . . . . . . 138
5.9  Lattice mesh for the 40 mm × 40 mm × 40 mm concrete at mesoscale139
5.10 Simulated stress-strain response for the 40 mm × 40 mm × 40 mm
     concrete at mesoscale . . . . . . . . . . . . . . . . . . . . . . . . 140
5.11 Simulated stress crack opening diagram for the 40 mm × 40 mm × 40 mm
     concrete at mesoscale . . . . . . . . . . . . . . . . . . . . . . . . 141
## List of Tables

<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>System size of the prism in Figure 2.3</td>
<td>37</td>
</tr>
<tr>
<td>2.2</td>
<td>Local mechanical properties of lattice elements in Figure 2.4</td>
<td>37</td>
</tr>
<tr>
<td>2.3</td>
<td>Simulation configurations with regard to lattice network construction</td>
<td>38</td>
</tr>
<tr>
<td>2.4</td>
<td>Influence of randomness on the simulated global Young’s modulus $E$, tensile strength $f_t$ and fracture energy $G_F$</td>
<td>39</td>
</tr>
<tr>
<td>2.5</td>
<td>Influence of boundary settings on the simulated global Young’s modulus $E$, tensile strength $f_t$ and fracture energy $G_F$</td>
<td>48</td>
</tr>
<tr>
<td>3.1</td>
<td>Specification of the cement mix used in the simulation</td>
<td>73</td>
</tr>
<tr>
<td>3.2</td>
<td>Assumed local mechanical properties of solid phases of cement paste</td>
<td>76</td>
</tr>
<tr>
<td>3.3</td>
<td>Classification of lattice element types</td>
<td>77</td>
</tr>
<tr>
<td>3.4</td>
<td>Local mechanical properties of lattice elements</td>
<td>77</td>
</tr>
<tr>
<td>3.5</td>
<td>Simulated mechanical properties of cement paste at microscale, corresponding with Figure 3.9</td>
<td>79</td>
</tr>
<tr>
<td>3.6</td>
<td>Simulated mechanical properties of cement paste at microscale, loaded horizontally along $x$-direction or $y$-direction, and vertically along $z$-direction</td>
<td>81</td>
</tr>
<tr>
<td>3.7</td>
<td>Simulated mechanical properties of cement paste with regular lattice mesh at the randomness of 0, and with irregular lattice mesh at the randomness of 0.5</td>
<td>84</td>
</tr>
<tr>
<td>3.8</td>
<td>Local mechanical properties of solid phases of experimental cement paste</td>
<td>86</td>
</tr>
<tr>
<td>3.9</td>
<td>Local mechanical properties of lattice elements for experimental cement paste</td>
<td>87</td>
</tr>
</tbody>
</table>
### LIST OF TABLES

3.10 Simulated mechanical properties of the experimental cement paste at microscale, corresponding with Figure 3.18 .......................... 87
3.11 Influences of degree of hydration on the tensile mechanical properties of cement paste at microscale ............................... 89
3.12 Influences of cement fineness, compared at the same curing age of 28 days, all values are resulted from simulations .................... 95
3.13 Influences of water/cement ratio, compared at the same curing age of 28 days ................................................................. 97
3.14 Influences of water/cement ratio, compared at the same degree of hydration 69% ............................................................... 99
3.15 Mineral compositions of the special cements ............................ 100
3.16 Degree of hydration and phase segmentation for the special cement pastes at the curing age of 28 days, corresponding with Figure 3.37 102
3.17 Global mechanical properties of the special cement pastes at the curing age of 28 days, corresponding with Figure 3.38 ............ 107
4.1 A normal concrete mix ................................................................. 124
4.2 Particle size sieve ranges for the sands in mortar ........................ 124
5.1 Mechanical properties of the cement paste specimen of the size 100µm × 100µm × 100µm, corresponding with Figure 5.2 .............. 132
5.2 Simulated mechanical properties for cement paste at microscale and mesoscale respectively ............................................... 133
5.3 Scale division and specifications of the specimens .................... 135
5.4 Local mechanical properties of sand, cement paste and interface elements in mortar at mesoscale ................................. 136
5.5 Local mechanical properties of stone, mortar and interface elements in concrete at mesoscale ........................................... 139
5.6 Simulated mechanical properties of concrete at mesoscale, corresponding with Figure 5.10 ................................................. 140
Symbols

\( \alpha_M \) bending influence factor
\( \alpha_N \) normal force influence factor
\( \epsilon \) strain
\( \kappa \) shear correction factor
\( \nu \) Poisson’s ratio
\( \sigma \) stress
\( A \) cross-sectional area of lattice element
\( a_{nm} \) spherical harmonic coefficients which are complex numbers
\( E \) Young’s modulus
\( f_t \) tensile strength
\( G \) shear modulus
\( G_F \) fracture energy
\( I \) moment of inertia
\( J \) polar moment of inertia
\( l \) length of lattice element
\( M \) bending moment
\( N \) normal force
\( P_n^m(\cos \theta) \) associated Legendre polynomials
# SYMBOLS

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R$</td>
<td>radius of particle</td>
</tr>
<tr>
<td>$r$</td>
<td>radius of lattice element cross-section</td>
</tr>
<tr>
<td>$r(\theta, \phi)$</td>
<td>a function defined in spherical coordinate system which represents the shape of a particle</td>
</tr>
<tr>
<td>$W$</td>
<td>cross-sectional factor for bending resistance</td>
</tr>
<tr>
<td>$Y^m_\pi(\theta, \phi)$</td>
<td>spherical harmonic functions</td>
</tr>
</tbody>
</table>
Chapter 1

Introduction

1.1 Background

Cement-based materials, such as cement paste, mortar and concrete, have a multiphase heterogeneous structure at microscale/mesoscale. In cement paste the size of cement grain particles is in the range of 0.5 ∼ 50 µm, the sands in mortar have the sizes of 0.1 ∼ 4 mm, and the coarse aggregates in concrete are sized 4 ∼ 32 mm. Cement paste is classified as heterogeneous material at microscale, but it can be homogenized at a higher scale. This principle also applies to mortar and concrete, which are deemed as heterogeneous materials at mesoscale and can be regarded as homogeneous materials at macroscale.

The global mechanical performance of materials is determined by the material structures and the local properties of constituents. The constituents also have their own material structures at a lower scale, which determine their mechanical properties. Take cement-based materials as an example. Concrete is a composite material consisting of coarse aggregates and mortar. The global mechanical behavior of concrete is determined by the material structure of concrete and the mechanical properties of coarse aggregates and mortar. At a lower scale mortar is made up with sands in cement paste. The properties of mortar are related to the material structure of mortar, as well as the local properties of sands and cement paste.

The fracture processes in concrete, mortar and cement paste must be relevant from a multiscale study point of view. The research about multiscale failure
modeling has received comprehensive investment during the last decades, as researchers keep looking for the origin of the load bearing capacity of materials. The macroscopic mechanical properties of concrete, such as Young’s modulus and compressive strength, are often of interest to the structural engineers. But to answer the question why concrete has these properties, it is necessary to turn attention to what is happening at a lower scale during the failure of concrete. The research work in this area helps to explain the damage mechanisms, to improve the mechanical properties and to design better cement-based materials.

1.2 State of the art

Homogenization method [1] and concurrent method [2] are usually employed to address the failure modeling problem of heterogeneous materials. The homogenization method applies when the scales can be ideally divided and separated, while the concurrent method is used when the scales are somehow coupled. Generally speaking the homogenization method consumes less computational resources, and the concurrent method provides more accurate simulation results.

Suppose that there is a piece of heterogeneous material, and it is meshed into a network of blocks. The homogenization method requires that each block of heterogeneous material is taken out and isolated to evaluate its mechanical properties, and then these properties are used as the homogenized properties of the blocks and are put back to the network to simulate the global performance of the original piece of material. The concurrent method demands that the connection between neighboring blocks is preserved and the boundaries of blocks remain compatible with each other during the simulation, the stress and strain fields also remain the same as if the domain was not decomposed.

In this thesis the concept of homogenization is adapted and combined with 3D lattice fracture analysis [3] to develop a parameter-passing multiscale modeling scheme. In addition the HYMOSTRUC3D model [4] is used to simulate the cement hydration and microstructure formation process at microscale, and the Anm material model (see Chapter 4 for details) is proposed and implemented to simulate the material structures of mortar and concrete with irregular shape particles at mesoscale.
1.3 Objectives and methodology of this research

The work in this research aims at developing a set of algorithms and procedures, which enable the multiscale modeling of fracture processes in cementitious materials, such as cement paste, mortar and concrete.

In this thesis there are two types of models serving as the fundamental tools, which include a material model to simulate the material structures, and a mechanical model to evaluate the mechanical performance of material structures. These two types of models can be combined to study the fracture processes at a single scale, while the multiscale modeling scheme makes it possible that the data exchange between different scales can be done by passing parameters. Examples are given to illustrate how these models can be used in a coupled way to solve practical problems.

1.4 Outline of the thesis

The thesis discusses the multiscale modeling of fracture processes in cementitious materials. It is divided into six chapters, including an introduction (Chapter 1) and conclusions (Chapter 6). The layout of the main body is given in Figure 1.1.

Figure 1.1: Layout of the thesis main body
1. INTRODUCTION

Chapter 1 introduces the multiscale problems to be addressed in this thesis. Cement paste, mortar and concrete are studied numerically for their mechanical performance. The relations between these three cementitious materials are emphasized in the parameter-passing multiscale modeling scheme developed in this thesis.

Chapter 2 deals with the 3D lattice fracture model. The mechanical performance of cement paste, mortar and concrete can be evaluated by the 3D lattice fracture analysis. Quadrangular lattice mesh, uniaxial tensile test setup, fracture processes simulation, stress-strain response, microcracks propagation and cracks pattern in final failure state are discussed in detail.

Chapter 3 focuses on the cement paste at microscale. The microstructures of cement paste can be obtained through the computer modeling program HYMOSTRUC3D model, as well as the experimental method of micro computed tomography. The lattice fracture model is employed to predict the uniaxial tensile properties based on the microstructures. Various factors are examined to evaluate their influences on the mechanical performance of cement paste, including the degree of hydration, cement fineness, water/cement ratio and mineral composition of cement.

Chapter 4 proposes an innovative model to simulate the material mesostructures of mortar and concrete: the Anm material model. From modeling point of view the material structures of mortar and concrete can be represented by particles embedded in matrix. The particle shapes are irregular in reality and the spherical harmonics provides a good mathematical representation of irregular shapes. The Anm material model parks multiple irregular shape particles together into an empty container to stand for the mesostructures of mortar and concrete. The parking algorithm is illustrated in detail, and examples are given to show how the mesostructures of mortar and concrete can be simulated respectively.

Chapter 5 makes use of all the tools discussed in previous chapters to address two types of multiscale modeling problems: for cement paste only but at different sizes, and for the integrated system of cement paste, mortar and concrete at microscale/mesoscale. The scale division and parameter-passing scheme are
discussed, and the domain decomposition modeling technique is also employed to solve the length scale overlap.

Chapter 6 summarizes the work and achievements in this thesis and presents all the findings in a brief way. An outlook is also given for the further development and potential future use of the algorithms and numerical models proposed in this thesis.
1. INTRODUCTION
Chapter 2

Three-dimensional Lattice Fracture Model

2.1 Background

Numerical modeling of fracture processes in brittle materials, such as cement paste, mortar, concrete and rocks, started in the late 1960s with the landmark papers of Ngo and Scordelis [5] and Rashid [6], in which the discrete and smeared crack models were introduced. Especially the latter approach gained much popularity, and in the 1970s comprehensive efforts were invested in developing constitutive models in a smeared setting which could reproduce the experimentally observed stress-strain characteristics of concrete. However, neither of them could tell the fracture processes in detail. In the 1990s, Schlangen and van Mier proposed another model to compensate the drawbacks of discrete and smeared crack models, which is called lattice fracture model [7].

The concept of lattice was proposed by Hrennikoff in the 1940s to solve elasticity problems using the framework method [8]. In the 1970s and 1980s the lattice model was introduced in theoretical physics to study the fracture behavior of disordered media [9] [10]. In the field of material sciences, a model was proposed by Burt and Dougill to simulate uniaxial extension tests, which consists of a plane pin-jointed random network structure of linear elastic brittle members having a range of different strengths and stiffnesses [11].
2. THREE-DIMENSIONAL LATTICE FRACTURE MODEL

In the last two decades, plenty of efforts have been made to develop the lattice fracture model in a variety of different settings: regular/irregular network, triangular/quadrangular mesh, truss/beam element, the way to implement heterogeneity (random distribution of local properties/microstructure mapping) and whether to introduce the softening at the element level. A lattice system of truss elements was constructed based on a random particle model to study the fracture of aggregate or fiber composites by Bazant et al. [12]. The tension softening response of the matrix phase was implemented in the lattice fracture analysis for concrete by Arslan et al. [13]. The fracture of particle composites due to large deformation was investigated by Karihaloo et al. using lattice fracture model [14]. Vervuurt made use of lattice fracture analysis to study the interface fracture in concrete [15], and van Vliet investigated the size effect in tensile fracture of concrete and rock [16]. The size effect on strength in numerical concrete was also studied by Man, where the influences of aggregate density and shape were discussed [17]. An irregular lattice model was proposed by Bolander and Sukumar for simulating quasistatic fracture in softening materials, in which accurate modeling of heterogeneity is enabled by constructing the lattice geometry on the basis of a Voronoi discretization of the material domain [18]. Lattice modeling of uniaxial compression was studied and applied to normal concrete, high strength concrete and foamed cement by Caduff and van Mier [19]. Grassl and Davies modeled corrosion induced cracking and bond in reinforced concrete using lattice approach [20]. Fracture laws for simulating compressive fracture in lattice-type models were explored and discussed by van Mier [21]. The possibility of modeling self-healing of cementitious materials using lattice approach was investigated by Joseph [22].

In the lattice fracture model, the continuum is replaced by a lattice of beam elements. Subsequently, the microstructure of the material can be mapped onto these beam elements by assigning them different properties, depending on whether the beam element represents a grain or matrix. Detailed modeling procedures are given in Section 2.2. Various conventional laboratory experiments like uniaxial tensile test, compressive test, shear test, bending test and torsional test can be simulated by the lattice fracture model and the model can be applied towards
2.2 Modeling procedures

The lattice fracture model can simulate the stress-strain response, cracks pattern and microcracks propagation, based on the microstructure or mesostructure of the material in question. Three stages are defined to make the modeling procedures clear: pre-processing, fracture processes simulation and post-processing. In the pre-processing stage, a lattice network is constructed and the local mechanical properties are assigned to every lattice element, and then appropriate boundary conditions are imposed, depending on the type of the test to be simulated (e.g. uniaxial tensile test, bending test, shear test). The fracture processes are simulated by removing the critical element from the system one after one, representing the microcrack occurrence. The critical lattice element is the element with the highest stress/strength ratio. In the post-processing stage, the stress-strain response diagram and the cracks pattern can be obtained, and the microcracks propagation can be animated as well. An overview of the lattice fracture analysis is given in Figure 2.1.
2. THREE-DIMENSIONAL LATTICE FRACTURE MODEL

2.2.1 Lattice network construction

A lattice network can be constructed based on the microstructure of materials. Two construction methods are presented in this subsection, which are ImgLat (Image to Lattice) and HymLat (Hymostruc3D to Lattice). The first method, ImgLat, is good for any microstructure in terms of voxels, and the second one, HymLat, can only be applied to a spherical particles embedded microstructure. The construction method ImgLat is more general and has a wider range of applications, as a spherical particles embedded microstructure can always be converted into a voxel-based digital image. However, the lattice network resulting from the second construction method HymLat usually has less nodes and elements, and thus costs less computational resources for the fracture processes simulation. During the lattice network construction, the following parameters need to be determined: location of lattice node, and length, radius, Young’s modulus, shear modulus and tensile strength of lattice element (the cross-section is assumed to be circular for simplicity).
2.2 Modeling procedures

General construction method ImgLat: applicable to voxel-based digital image

The lattice network construction is illustrated in Figure 2.2. The sketch at left side is shown in 2D for a more clear illustration, and the mesh method also works for 3D case. A digital image consisting of multiple phases can be taken as the basis for the lattice mesh. A network of cells is generated first, and a sub-cell can be defined within each cell. A lattice node is randomly chosen within each sub-cell which represents solid phase. The pore phase cells do not generate any lattice node. Then the lattice nodes in the neighboring cells are connected by lattice beam elements, which eventually form a lattice network system. The lattice system is able to carry loads and thus replaces the original continuum materials in terms of mechanical performance. The lattice network shown in Figure 2.2 is quadrangular. Alternatively it can also be meshed to a triangular system. If a perfect regular lattice network is generated, then the quadrangular option leads to the Poisson’s ratio 0, while the triangular one not. The above construction method implements the heterogeneity of the materials through the network geometry irregularities. It is also possible to achieve this by assigning random local mechanical properties to different lattice beam elements. See [3, 25, 27, 28] for more information about the construction of random lattice network.

The length ratio of the sub-cell to the cell is defined as the randomness of the lattice system, which represents the disorder of the materials. The value of the randomness is in the range of [0, 1]. When it takes 0, the lattice node is always

Figure 2.2: Lattice network construction for general material and scale
2. THREE-DIMENSIONAL LATTICE FRACTURE MODEL

Figure 2.3: Prism of the size 40 mm × 40 mm × 60 mm subject to uniaxial tensile load

located at the center of the cell, and a perfect quadrangular lattice system is generated, but the Poisson’s ratio of the materials represented is restricted to 0. When the randomness is equal to 1, the sub-cell becomes identical to the cell, and the materials have the maximum degree of disorder. The choice of randomness affects the simulated fracture behavior of the materials, and the following numerical experiment is carried out to show the influence of randomness on the simulated mechanical properties of single phase perfect homogeneous materials.

A specimen in the shape of a prism at the size 40 mm × 40 mm × 60 mm is analyzed for its global mechanical properties through a uniaxial tensile test by lattice fracture model. It is modeled as a single phase homogeneous material and represented in terms of voxels at the resolution 1 mm/voxel, as shown in Figure 2.3.

A lattice network is constructed based on the voxel image. In each voxel, a sub-cell is created, and the length ratio of the sub-cell to the voxel is the randomness. A lattice node is positioned randomly within the sub-cell, and then the neighboring lattice nodes are connected to form lattice elements as shown in
2.2 Modeling procedures

Table 2.1: System size of the prism in Figure 2.3

<table>
<thead>
<tr>
<th>Number of voxels:</th>
<th>$40 \times 40 \times 60 = 96000$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of lattice nodes:</td>
<td>96000</td>
</tr>
<tr>
<td>Number of lattice elements:</td>
<td>$39 \times 40 \times 60 \times 2 + 59 \times 40 \times 40 = 281600$</td>
</tr>
</tbody>
</table>

Figure 2.4: Linear-brittle constitutive law of lattice elements

Figure 2.2: The system size of the resulting lattice network is listed in Table 2.1. The lattice elements follow linear-brittle constitutive law as shown in Figure 2.4 and the corresponding local mechanical properties are given in Table 2.2.

During the lattice network construction, the randomness is varied at 0, 0.25, 0.5, 0.75 and 1 respectively in the computational model to study its influence on the simulated global mechanical properties. At each randomness, three instances are taken using different random seed 1, 2 and 3 respectively. The random seed controls the pseudo random number sequence in the C++ programming language, thus the resulting lattice networks would be different using different random seeds.

Table 2.2: Local mechanical properties of lattice elements in Figure 2.4

<table>
<thead>
<tr>
<th>Young’s modulus $E$ (GPa)</th>
<th>Shear modulus $G$ (GPa)</th>
<th>Poisson’s ratio $\nu$</th>
<th>Tensile strength $f_t$ (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>35</td>
<td>14</td>
<td>0.25</td>
<td>3.5</td>
</tr>
</tbody>
</table>
2. THREE-DIMENSIONAL LATTICE FRACTURE MODEL

Table 2.3: Simulation configurations with regard to lattice network construction

<table>
<thead>
<tr>
<th>Randomness</th>
<th>0</th>
<th>0.25</th>
<th>0.5</th>
<th>0.75</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Random seed</td>
<td>1/2/3</td>
<td>1/2/3</td>
<td>1/2/3</td>
<td>1/2/3</td>
<td>1/2/3</td>
</tr>
</tbody>
</table>

even though at the same randomness, but the global properties should be more or less the same. The simulation configurations with regard to lattice network construction are summarized in Table 2.3, and in total 15 simulations are executed.

The specimen is loaded in vertical direction as shown in Figure 2.3. The external surface load is imposed on the top and the bottom surface is fixed. All the other four side surfaces are free to expand/shrink. The lattice elements on the top and bottom boundaries are not allowed to be broken during the fracture processes as the external load requires a path into the specimen.

The fracture processes of the prisms are simulated using lattice fracture model, and the simulated global Young’s modulus $E$, tensile strength $f_t$ and fracture energy $G_F$ are presented in Table 2.4.

From the Table 2.4 it is concluded that the influences of using different random seeds to generate the pseudo random number sequences can be neglected, but the choice of randomness really matters the simulation results. When the randomness is taken as 0, the simulated global Young’s modulus and tensile strength are the same as the local mechanical properties inputs, and all the microcracks are located on one plane as shown in Figure 2.5, which is due to the fact that a piece of perfect homogeneous material is modeled. The increase of the randomness results in a decrease of the simulated global Young’s modulus and tensile strength, as artificial disorder of the materials is introduced gradually by increasing the randomness in the model. The change of fracture energy is somehow more complicated, as it decreases first and then increases again. The decrease of the fracture energy is because of the decrease of the strength, and the increase is due to the fact that more microcracks are generated with more heterogeneous materials. These two forces push the change of fracture energy in opposite directions, and the decrease of strength wins when the randomness is still small, but the more microcracks become dominant when the randomness is
### Table 2.4: Influence of randomness on the simulated global Young’s modulus $E$, tensile strength $f_t$ and fracture energy $G_F$

<table>
<thead>
<tr>
<th>Randomness</th>
<th>Random seed</th>
<th>Young’s modulus $E$ (GPa)</th>
<th>Tensile strength $f_t$ (MPa)</th>
<th>Fracture energy $G_F$ (J/m$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>35.0</td>
<td>3.50</td>
<td>0.753</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>35.0</td>
<td>3.50</td>
<td>0.753</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>35.0</td>
<td>3.50</td>
<td>0.753</td>
</tr>
<tr>
<td>Average properties:</td>
<td></td>
<td>35.0</td>
<td>3.50</td>
<td>0.753</td>
</tr>
<tr>
<td>0.25</td>
<td>1</td>
<td>33.8</td>
<td>3.08</td>
<td>0.589</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>33.8</td>
<td>3.03</td>
<td>0.661</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>33.8</td>
<td>3.06</td>
<td>0.591</td>
</tr>
<tr>
<td>Average properties:</td>
<td></td>
<td>33.8</td>
<td>3.06</td>
<td>0.614</td>
</tr>
<tr>
<td>0.5</td>
<td>1</td>
<td>30.8</td>
<td>2.64</td>
<td>0.644</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>30.8</td>
<td>2.66</td>
<td>0.637</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>30.8</td>
<td>2.66</td>
<td>0.644</td>
</tr>
<tr>
<td>Average properties:</td>
<td></td>
<td>30.8</td>
<td>2.65</td>
<td>0.642</td>
</tr>
<tr>
<td>0.75</td>
<td>1</td>
<td>26.8</td>
<td>2.28</td>
<td>0.717</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>26.8</td>
<td>2.22</td>
<td>0.722</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>26.8</td>
<td>2.29</td>
<td>0.698</td>
</tr>
<tr>
<td>Average properties:</td>
<td></td>
<td>26.8</td>
<td>2.26</td>
<td>0.712</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>22.8</td>
<td>1.95</td>
<td>0.981</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>22.8</td>
<td>1.94</td>
<td>1.009</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>22.8</td>
<td>1.91</td>
<td>0.911</td>
</tr>
<tr>
<td>Average properties:</td>
<td></td>
<td>22.8</td>
<td>1.93</td>
<td>0.967</td>
</tr>
</tbody>
</table>
large enough. The diagram of simulated global mechanical properties reduction against the randomness is shown in Figure 2.6.

The randomness defined in the lattice mesh represents the heterogeneity of the materials in reality. The following procedures may be employed to determine the value of randomness. The first step is to obtain the material structure of the specimen through CT scan (see Subsection 3.1.3 for more information), and then construct a lattice network based on the material structure with different values of randomness. Afterwards the lattice systems with different randomness values are evaluated by the lattice fracture analysis for their mechanical properties such as Young’s modulus and tensile strength. The simulated mechanical properties are compared with the measured value to find out the best simulation, and it is concluded that the randomness used in the best simulation is the correct one.

The next step after creating the lattice network is to assign local mechanical properties to all lattice elements. Either truss element or beam element may be employed in lattice fracture analysis, and the choice is dependent on the application. Generally speaking beam elements are preferred as a beam network can
simulate a wider range of Poisson’s ratios and more complicated crack patterns [25, 29].

The local mechanical properties of a lattice element is determined by the location of the element, whether it is within a grain or in the matrix, or it connects a grain to the matrix, as shown in Figure 2.7. If both ends of an element are located in the same phase, then this element is assigned the same mechanical properties as the phase in question, otherwise it is classified as an interface element. The mechanical properties of an interface element are preferred to be measured in laboratory test, but in case of lack of experimental data, the following guidelines may be applied. The Young’s modulus of an interface element is the harmonic average of the Young’s moduli of the grain and the matrix, and its tensile strength takes the lower value of the two phases, as determined by the equation (2.1) and the equation (2.2). Shear modulus of an interface element is determined in a similar way to the determination of its Young’s modulus.

\[
\frac{2}{E_I} = \frac{1}{E_A} + \frac{1}{E_B} \tag{2.1}
\]

in which \(E_I, E_A\) and \(E_B\) are the Young’s modulus for interface element, phase A and phase B respectively.

\[
f_{t_I} = \min(f_{t_A}, f_{t_B}) \tag{2.2}
\]
2. THREE-DIMENSIONAL LATTICE FRACTURE MODEL

Figure 2.7: Lattice element type determination and its constitutive relation

where \( f_{tI} \), \( f_{tA} \) and \( f_{tB} \) are the tensile strength for the interface element, phase A and phase B respectively.

Special construction method HymLat: only applicable to spherical particles embedded microstructure

Having introduced the general lattice network construction method for voxel-based microstructure of materials, a special construction method is also developed for the spherical particles embedded microstructure of cement paste from the HYMOSTRUC3D model. A sample of the microstructure simulated by the HYMOSTRUC3D model is given in Figure 2.8. Details about the simulation of microstructures of cement paste can be found in Chapter 3. In total four phases are presented in the microstructure, including one pore (P) phase and three solid phases which are unhydrated cement (U), inner product (I) and outer product (O).

During the lattice network construction, a lattice element is generated if the two particles have overlap, as shown in the Figure 2.9(a). The lattice element goes from the center of the first particle to the center of the other one. The cross-section of the lattice element is assumed to be circular and its area is equal to the contact area of the two particles in question. This construction principle applies to all the pairs of overlapped particles, thus a lattice network can be created, as shown in Figure 2.9(b) for the case of three pairs.
2.2 Modeling procedures

Figure 2.8: Microstructure of cement paste simulated by the HYMOSTRUC3D model

Figure 2.9: 3D contact particles, lattice element and network
2. THREE-DIMENSIONAL LATTICE FRACTURE MODEL

The determination of Young’s modulus of a lattice element is through a two-step averaging. The particle modulus is computed as a result of the length-weighted harmonic average modulus of unhydrated cement, inner product and outer product, as determined by the equation (2.3) and illustrated in Figure 2.10,

\[
\frac{R_O}{E_p} = \frac{R_U}{E_U} + \frac{R_I - R_U}{E_I} + \frac{R_O - R_I}{E_O}
\]  

(2.3)

where \( R_U, R_I \) and \( R_O \) are the radius for unhydrated cement, inner product and outer product respectively, \( E_U, E_I \) and \( E_O \) are the corresponding Young’s modulus, \( E_p \) is the computed particle modulus. The lattice element modulus is the length-weighted harmonic average of the particle moduli of the two particles which it links. The formula depends on the two particles’ relative locations, as given in the equation (2.4) and shown in Figure 2.11

\[
E = \begin{cases} 
\frac{1E_{p1}E_{p2}(E_{p1} + E_{p2})}{(l - R_1)E_{p1}^2 + (R_1 + R_2)E_{p1}E_{p2} + (l - R_2)E_{p2}^2} & \text{if case 1} \\
\frac{1E_{p1}(E_{p1} + E_{p2})}{E_{p1}^2 + (l - R_2)E_{p2}} & \text{if case 2} \\
\frac{E_{p1} + E_{p2}}{2} & \text{if case 3}
\end{cases}
\]  

(2.4)

where \( R_1 \) and \( R_2 \) are the radius of the first and the second particle, \( E_{p1} \) and \( E_{p2} \) are the corresponding particle moduli, \( l \) is the lattice element length, and \( E \) is the computed element modulus. Shear modulus of a lattice element can be determined through the same procedures, and its tensile strength takes the lowest tensile strength among unhydrated cement, inner product and outer product, as given in the equation (2.5),

\[
f_t = \min (f_{tU}, f_{tI}, f_{tO})
\]  

(2.5)

where \( f_{tU}, f_{tI} \) and \( f_{tO} \) are the tensile strength for unhydrated cement, inner product and outer product respectively, and \( f_t \) is the tensile strength of the lattice element.

2.2.2 Test setup

Similarly to various laboratory experiments, many types of tests can be simulated on a lattice network, including but not limited to tensile test, three-point (four-
2.2 Modeling procedures

![Diagram](image)

**Figure 2.10:** Determination of particle modulus (first step averaging)

point) bending test, shear test and more. They are implemented by setting up proper boundary conditions of the sample. For example a uniaxial tensile test can be configured by fixing all the nodes on the bottom surface of the specimen and imposing a uniform surface load on the top surface, as shown in Figure 2.12. During the lattice network construction, all the layers close to the surfaces are forced to be regularly meshed, irrespective of the material randomness setting, as irregular geometry on the boundaries might create some extra stresses which may have negative influence on the fracture processes simulation. In addition all the lattice elements involved in the bottom and top layers are not allowed to be broken, even if the stress in such an element has already exceeded its strength, as the external loads need a path to be transferred into the specimen. In other words, it is assumed that all the restraint elements have infinite strength.

In the laboratory tensile test, there are two possible methods to connect the specimen to the testing device: glued and clamped. In the numerical model, these are implemented through whether or not to fix the degrees of freedom of the nodes at the bottom and top surfaces. In both cases for a tensile test, the vertical displacements of all the nodes at the bottom surface are prescribed to be 0, and the top surface to be unit deformation. In the case of a glued specimen, all the other degrees of freedom of the nodes in question are restricted to be 0. But only one node is chosen to be fixed completely in the case of a clamped specimen, as this is required to prevent possible rigid body movement. The clamped setting is suitable for the study about Poisson’s ratio. The following example demonstrates
2. THREE-DIMENSIONAL LATTICE FRACTURE MODEL

![Diagram](image)

(a) Case 1

(b) Case 2

(c) Case 3

Figure 2.11: Determination of lattice element modulus (second step averaging)
2.2 Modeling procedures

Figure 2.12: Uniaxial tensile test setup

the influences of these two different settings on the simulated global mechanical properties.

A cubic specimen of the size 20 mm at the resolution 1 mm/voxel is configured for a uniaxial tensile test using two different aforementioned boundary conditions, as shown in Figure 2.12. The input local mechanical properties are given in Table 2.2 and it behaves linear-brittle locally as shown in Figure 2.4. The randomness of the material is taken as 0.5 in the numerical experiments. The simulated global Young’s modulus, tensile strength and fracture energy are presented in Table 2.5. The comparisons show that the differences are so small that they can be neglected for the glued and the clamped boundary settings, at least this is true for specimens with Poisson’s ratio close to 0. If the Poisson’s ratio of the specimen is far from 0, then the restriction on the boundaries will affect the deformation of side surfaces, thus the mechanical responses will be different for different boundary settings.
2. THREE-DIMENSIONAL LATTICE FRACTURE MODEL

Table 2.5: Influence of boundary settings on the simulated global Young’s modulus $E$, tensile strength $f_t$ and fracture energy $G_F$

<table>
<thead>
<tr>
<th>Boundary settings</th>
<th>Young’s modulus $E$ (GPa)</th>
<th>Tensile strength $f_t$ (MPa)</th>
<th>Fracture energy $G_F$ (J/m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Glued</td>
<td>31.4</td>
<td>2.74</td>
<td>0.638</td>
</tr>
<tr>
<td>Clamped</td>
<td>31.3</td>
<td>2.74</td>
<td>0.643</td>
</tr>
</tbody>
</table>

2.2.3 Fracture processes simulation

After the lattice network is constructed and boundary conditions are imposed, it is ready to proceed with the fracture processes simulation which is the kernel part in the entire lattice fracture analysis. The flowchart of lattice fracture analysis kernel solver is given in Figure 2.13. It seems similar to the traditional finite element analysis, but two major differences exist. One is about the removal of broken lattice elements from the system and the other is the absence of the explicit assembly of global stiffness matrix.

In lattice fracture analysis, a unit prescribed displacement is imposed on the system. At every analysis step it is required to determine the critical element and the corresponding system scaling factor after the calculation of comparative stress in every lattice element. The critical element is the one with highest stress/strength ratio when the system is loaded by a unit prescribed displacement. The inverse of the ratio is defined as system scaling factor. The system scaling factor, together with the reactions on the restraint boundaries, determines one scenario of critical load-displacement pairs. The critical element is removed from the system and if the system does not fail completely yet, it is recomputed as the system is updated due to the element removal. Multiple analysis steps are carried out until the system fails. Hence a set of load-displacement pairs can be obtained and used to plot the load-displacement diagram, which can be converted to a stress-strain diagram later to represent the constitutive relation of the material. The step-by-step removal of critical lattice elements indicates the microcracks evolution in the specimen. Thus the microcracks propagation and the cracks pattern in the final failure state can be simulated.
2.2 Modeling procedures

- **Element stiffness matrix in local domain**
- **Transformation matrix**
- **Element stiffness matrix in global domain**
- **Link local degrees of freedom to global degrees of freedom**
- **Calculate total reaction force(s)**
- **Calculate element internal force vector in local domain**
- **Calculate element comparative stress**
- **Determine critical element(s) and system scaling factor(s)**
- **Impose boundary conditions**
- **Solve linear algebraic equations to get node displacement vector**
- **Update system due to damage**
- **Assemble load vector**
- **Calculate element internal force vector in local domain**
- **System failed?**
  - No
  - Yes
  - **End**

**Figure 2.13:** Flowchart of lattice fracture analysis kernel solver
Another highlight in the lattice fracture analysis is the adoption of the matrix free technique in the linear algebraic equation solver to reduce the computer memory demand. The global stiffness matrix is not assembled or stored explicitly, rather than that the element stiffness matrices in global domain and the connectivity array, which links local degrees of freedom to global degrees of freedom, are sent to the equation solver directly to get the node displacement vector. Jacobi pre-conditioned conjugate gradient iterative method is employed to solve the set of linear equations. More details about the algorithm can be found later in this subsection on Page 64.

3D lattice beam element stiffness matrix in local domain and in global domain

In lattice fracture analysis, continuum materials are discretized into a network of lattice elements. The lattice beam element is a straight bar of uniform cross-section and can transmit axial forces, shear forces, bending moments and torsional moments as shown in Figure 2.14. The formulation of a 3D lattice beam element stiffness matrix is based on the Timoshenko beam theory, which can be found in many textbooks about Finite Element Analysis.

The 3D lattice beam element has two nodes and each node has six degrees
2.2 Modeling procedures

of freedom including three translational and three rotational degrees of freedom. The element stiffness matrix in local domain is of the size $12 \times 12$ and can be formulated by assembling axial component, torsional component, bending and shear components in the planes $xOy$ and $xOz$. The element cross-sectional bending and shear centers are assumed to be coincident.

Along the axial direction as shown in Figure 2.14 the kinematics, equilibrium and constitutive equations are,

\[
\begin{align*}
\epsilon_x(x) &= \frac{du(x)}{dx} \\
A \frac{d\sigma_x(x)}{dx} + f(x) &= 0 \\
\sigma_x(x) &= E\epsilon_x(x)
\end{align*}
\]

where $E$ is the axial elastic modulus, $A$ is the cross-sectional area of the element, $f(x)$ is the external body force along the axial direction, $\sigma_x(x)$, $\epsilon_x(x)$ and $u(x)$ are the stress, strain and displacement respectively.

The strong form of the axial governing equation can be derived from the equations (2.6) and it is

\[
EA \frac{d^2u(x)}{dx^2} + f(x) = 0
\]

The corresponding Dirichlet and Neumann boundary conditions are

\[
\begin{align*}
\begin{cases}
u(x) &= u_0 & \text{on } \Gamma_u \\
EA \frac{du(x)}{dx} n &= P_0 & \text{on } \Gamma_F
\end{cases}
\end{align*}
\]

where $u_0$ and $P_0$ are the given displacement and force at the boundaries respectively, $n$ is the outward unit normal vector, $\Gamma$ represents the boundaries of the element and it satisfies

\[
\Gamma_u \cup \Gamma_F = \Gamma, \Gamma_u \cap \Gamma_F = \emptyset
\]

To develop the weak form of the governing equation, the strong form equation (2.7) needs to be multiplied by a scalar weight function $w(x)$, which comes from an appropriately defined space $V$. An important requirement on the space $V$ is that weight functions $w(x)$ be zero where Dirichlet boundary conditions
2. THREE-DIMENSIONAL LATTICE FRACTURE MODEL

are applied. Multiplying the equation \((2.7)\) by the weight function \(w(x)\) and integrating over the element \(\Omega\) yields

\[
\int_\Omega w(x)EA \frac{d^2u(x)}{dx^2} d\Omega + \int_\Omega w(x)f(x)d\Omega = 0 \tag{2.10}
\]

Applying integration by parts once yields

\[
- \int_\Omega \frac{dw(x)}{dx} EA \frac{du(x)}{dx} d\Omega + \int_\Gamma w(x) E A \frac{du(x)}{dx} n d\Gamma + \int_\Omega w(x)f(x)d\Omega = 0 \tag{2.11}
\]

As the boundary \(\Gamma\) can be decomposed into two parts \(\Gamma_u\) and \(\Gamma_F\), the above equation can be re-written as

\[
- \int_\Omega \frac{dw(x)}{dx} EA \frac{du(x)}{dx} d\Omega + \int_{\Gamma_u} w(x) E A \frac{du(x)}{dx} n d\Gamma + \int_{\Gamma_F} w(x) E A \frac{du(x)}{dx} n d\Gamma + \int_\Omega w(x)f(x)d\Omega = 0 \tag{2.12}
\]

The term \(\int_{\Gamma_u} w(x) E A \frac{du(x)}{dx} n d\Gamma\) is always equal to zero as by definition the weight function \(w(x)\) is equal to zero at Dirichlet boundary. The weak form of the governing equation can be obtained by inserting the Neumann boundary condition \((2.8)\) into the above equation. Solving it involves to find a trial function \(u(x) \in S\) such that

\[
- \int_\Omega \frac{dw(x)}{dx} EA \frac{du(x)}{dx} d\Omega + \int_{\Gamma_F} w(x) P_0 n d\Gamma + \int_\Omega w(x)f(x)d\Omega = 0 \quad \forall w(x) \in V \tag{2.13}
\]

where \(S\) is an appropriately defined space of functions which satisfies the Dirichlet boundary condition \((2.8)\). The mathematical description for the spaces \(S\) and \(V\) is that

\[
\begin{align*}
S &= \{ u(x) \mid u(x) \in \mathcal{L}(\Omega), u(x) = u_0 \text{ on } \Gamma_u \} \\
V &= \{ w(x) \mid w(x) \in \mathcal{L}(\Omega), w(x) = 0 \text{ on } \Gamma_u \} 
\end{align*}
\tag{2.14}
\]

Based on the weak form of the governing equation \((2.13)\), a Galerkin problem can be formulated which involves to find \(u^h(x) \in S^h\) such that

\[
\int_\Omega \frac{dw^h(x)}{dx} EA \frac{du^h(x)}{dx} d\Omega = \int_{\Gamma_F} w^h(x) P_0 n d\Gamma + \int_\Omega w^h(x)f(x)d\Omega \quad \forall w^h(x) \in V^h \tag{2.15}
\]

where \(S^h \subset S\) and \(V^h \subset V\) are finite-dimensional spaces.
2.2 Modeling procedures

The Galerkin method (more specifically, the Bubnov-Galerkin method) requires that the trial function and the weight function come from the same finite-dimensional space, taking into account the requirements on the trial and weight functions where Dirichlet boundary conditions are applied.

To find the solution to the Galerkin problem (2.15), Lagrange polynomials can be used to construct the shape functions, which results in a linear interpolation of the displacement field in the element,

\[ u^h(x) = N_i(x)u_i + N_j(x)u_j \]  

(2.16)

where \( u_i \) and \( u_j \) are the axial displacements at node \( i \) and \( j \) respectively, and the shape functions are

\[
\begin{align*}
N_i(x) &= 1 - \frac{x}{l} \\
N_j(x) &= \frac{x}{l}
\end{align*}
\] 

(2.17)

Denoting that

\[ N(x) = \begin{bmatrix} N_i(x) & N_j(x) \end{bmatrix} \] 

(2.18)

and

\[ a_e = \begin{bmatrix} u_i \\ u_j \end{bmatrix} \] 

(2.19)

Thus the displacement field (2.16) can be re-written as

\[ u^h(x) = N(x)a_e \] 

(2.20)

The first derivative of the trial function \( u^h(x) \) is given by

\[ \frac{du^h(x)}{dx} = \frac{dN(x)}{dx}a_e \] 

(2.21)

Similarly the weight function and its first derivative are given by

\[ w^h(x) = N(x)b_e \] 

(2.22)

and

\[ \frac{dw^h(x)}{dx} = \frac{dN(x)}{dx}b_e \] 

(2.23)
Inserting the equations (2.21), (2.22) and (2.23) into the Galerkin problem (2.15) yields

\[
\int_{\Omega} \left[ \frac{dN(x)}{dx} b_x \right]^T E A \left[ \frac{dN(x)}{dx} a_x \right] d\Omega = \int_{\Gamma} [N(x)]^T P_0 d\Gamma + \int_{\Omega} [N(x)]^T f(x) d\Omega \quad (2.24)
\]

Rearranging the above equation yields

\[
\int_{\Omega} \left[ \frac{dN(x)}{dx} \right]^T E A \left[ \frac{dN(x)}{dx} \right] d\Omega a_x = \int_{\Gamma} [N(x)]^T P_0 d\Gamma + \int_{\Omega} [N(x)]^T f(x) d\Omega \quad (2.25)
\]

Hence the element stiffness matrix for the axial deformation is given by

\[
K^a = \int_{\Omega} \left[ \frac{dN(x)}{dx} \right]^T E A \left[ \frac{dN(x)}{dx} \right] d\Omega = \int_0^l \begin{bmatrix} -\frac{1}{l} & \frac{1}{l} \end{bmatrix} E A \begin{bmatrix} -\frac{1}{l} & \frac{1}{l} \end{bmatrix} dx = \begin{bmatrix} \frac{E A}{l} & -\frac{E A}{l} \\ -\frac{E A}{l} & \frac{E A}{l} \end{bmatrix} \quad (2.26)
\]

where \( E \) is the axial elastic modulus, \( A \) and \( l \) are the cross-sectional area and the length of the element respectively.

The element stiffness matrix for the torsional deformation can be formulated in a similar way and is given by

\[
K^t = \begin{bmatrix} G J & -G J \\ \text{sym.} & G J \end{bmatrix} \quad (2.27)
\]

where \( G \) is the shear modulus, \( J \) is the polar moment of inertia about the axial direction, and \( l \) is the length of the element.

The element stiffness matrix for the bending and shear deformation in the plane \( xOy \) is formulated through two steps. The first step derives the stiffness matrix for Euler-Bernoulli beam element, and then the shear effect is taken into account at the second step, thus the Timoshenko beam element is developed.

In the plane \( xOy \) as shown in Figure 2.14 the translational equilibrium requires that

\[
\int_{\Gamma} q(x) n d\Gamma + \int_{\Omega} f_y(x) d\Omega = 0 \quad (2.28)
\]
where \( f_y(x) \) is the body force, \( q(x) \) is the distributed load, \( n \) is the outward unit normal vector, \( \Omega \) and \( \Gamma \) are the body and the boundaries of the element respectively.

Noting that \( \int_{\Gamma} q(x)nd\Gamma = \int_{\Omega} \frac{dq(x)}{dx}d\Omega \), the above equation can be re-arranged as

\[
\int_{\Omega} \frac{dq(x)}{dx}d\Omega + \int_{\Omega} f_y(x)d\Omega = 0 \tag{2.29}
\]

Since equilibrium must hold for an infinitely small segment of a beam, it requires that

\[
\frac{dq(x)}{dx} + f_y(x) = 0 \tag{2.30}
\]

For rotational equilibrium, it is required that

\[
\int_{\Gamma} m(x)nd\Gamma - \int_{\Gamma} q(x)nxd\Gamma - \int_{\Omega} f_y(x)xd\Omega = 0 \tag{2.31}
\]

where \( m(x) \) is the distributed moment.

Noting that \( \int_{\Gamma} m(x)nd\Gamma = \int_{\Omega} \frac{dm(x)}{dx}d\Omega \) and integration by parts \( \int_{\Omega} x\frac{dq(x)}{dx}d\Omega = -\int_{\Omega} q(x)d\Omega + \int_{\Gamma} xq(x)nd\Gamma \), the above equation can be re-written as

\[
\int_{\Omega} \frac{dm(x)}{dx}d\Omega - \left[ \int_{\Omega} x\frac{dq(x)}{dx}d\Omega + \int_{\Omega} q(x)d\Omega \right] - \int_{\Omega} f_y(x)xd\Omega = 0 \tag{2.32}
\]

Rearranging the above equation yields

\[
\int_{\Omega} \left[ \frac{dm(x)}{dx} - q(x) \right] d\Omega - \int_{\Omega} \left[ \frac{dq(x)}{dx} + f_y(x) \right] xd\Omega = 0 \tag{2.33}
\]

The term \( \int_{\Omega} \left[ \frac{dq(x)}{dx} + f_y(x) \right] xd\Omega \) must be zero due to the satisfaction of the translational equilibrium \( (2.30) \), and equilibrium must hold for an infinitely small segment of a beam, hence,

\[
\frac{dm(x)}{dx} - q(x) = 0 \tag{2.34}
\]

The kinematics equation is based on the Euler-Bernoulli hypothesis, which is plane cross-sections remain plane and normal to the longitudinal axis after deformation. This assumption implies that the shear rotation is equal to zero, hence, the rotation can be directly related to the translational displacement,

\[
\theta(x) = \frac{dv(x)}{dx} \tag{2.35}
\]
2. THREE-DIMENSIONAL LATTICE FRACTURE MODEL

which also implies that

\[ \kappa(x) = \frac{d\theta(x)}{dx} = \frac{d^2v(x)}{dx^2} \]  \hspace{1cm} (2.36)

where \( \kappa(x) \) is the bending curvature, \( \theta(x) \) and \( v(x) \) are the rotational and translational displacement respectively.

The constitutive equation relates the bending moment in the beam to the curvature by

\[ m(x) = -EI_z \kappa(x) \]  \hspace{1cm} (2.37)

where \( I_z \) is the moment of inertia of the cross-section about the \( z \)-axis.

On the basis of the equations (2.30), (2.34), (2.36) and (2.37), the strong form of the governing equation can be obtained,

\[ EI_z \frac{d^4v(x)}{dx^4} - f_y(x) = 0 \]  \hspace{1cm} (2.38)

The corresponding Dirichlet and Neumann boundary conditions are

\[
\begin{cases}
  v(x) = v_0 & \text{on } \Gamma_v \\
  \theta(x) = \theta_0 & \text{on } \Gamma_\theta \\
  m(x)n = M_0 & \text{on } \Gamma_M \\
  q(x)n = Q_0 & \text{on } \Gamma_Q
\end{cases}
\]  \hspace{1cm} (2.39)

The Neumann boundary conditions can also be expressed in terms of translational displacement \( v(x) \), which are

\[
\begin{cases}
  -EI_z \frac{d^2v(x)}{dx^2} n = M_0 & \text{on } \Gamma_M \\
  -EI_z \frac{d^3v(x)}{dx^3} n = Q_0 & \text{on } \Gamma_Q
\end{cases}
\]  \hspace{1cm} (2.40)

where \( v_0 \) and \( \theta_0 \) are the given translational and rotational displacement at the boundaries respectively, \( M_0 \) and \( Q_0 \) are the given moment and shear force at the boundaries respectively.

The boundary \( \Gamma \) of the element is partitioned such that

\[
\begin{cases}
  \Gamma_v \cup \Gamma_Q = \Gamma, \Gamma_v \cap \Gamma_Q = \emptyset \\
  \Gamma_\theta \cup \Gamma_M = \Gamma, \Gamma_\theta \cap \Gamma_M = \emptyset
\end{cases}
\]  \hspace{1cm} (2.41)
To develop the weak form of the governing equation, multiplying both sides of the equation (2.38) by a weight function \( w(x) \) and integrating over the beam \( \Omega \) yields

\[
\int_{\Omega} w(x)EI_z \frac{d^4v(x)}{dx^4} d\Omega - \int_{\Omega} w(x)f_y(x) d\Omega = 0 \tag{2.42}
\]

Integrating by parts once yields

\[
- \int_{\Omega} \frac{dw(x)}{dx} EI_z \frac{d^3v(x)}{dx^3} d\Omega + \int_{\Gamma} w(x)EI_z \frac{d^3v(x)}{dx^3} nd\Gamma - \int_{\Omega} w(x)f_y(x) d\Omega = 0 \tag{2.43}
\]

Applying integration by parts again yields

\[
- \left[ - \int_{\Omega} \frac{d^2w(x)}{dx^2} EI_z \frac{d^2v(x)}{dx^2} d\Omega + \int_{\Gamma} \frac{dw(x)}{dx} EI_z \frac{d^2v(x)}{dx^2} nd\Gamma \right] \\
\quad + \int_{\Gamma} w(x)EI_z \frac{d^3v(x)}{dx^3} nd\Gamma - \int_{\Omega} w(x)f_y(x) d\Omega = 0 \tag{2.44}
\]

The above equation can be simplified as

\[
\int_{\Omega} \frac{d^2w(x)}{dx^2} EI_z \frac{d^2v(x)}{dx^2} d\Omega - \int_{\Gamma} \frac{dw(x)}{dx} EI_z \frac{d^3v(x)}{dx^3} nd\Gamma \\
\quad + \int_{\Gamma} w(x)EI_z \frac{d^3v(x)}{dx^3} nd\Gamma - \int_{\Omega} w(x)f_y(x) d\Omega = 0 \tag{2.45}
\]

Inserting the moment part of the Neumann boundary conditions (2.40) into the term \( \int_{\Gamma} \frac{d^2w(x)}{dx^2} EI_z \frac{d^2v(x)}{dx^2} nd\Gamma \) and noting that the first derivative of the weight function is equal to zero on \( \Gamma_\theta \) yields

\[
\int_{\Gamma} \frac{dw(x)}{dx} EI_z \frac{d^2v(x)}{dx^2} nd\Gamma = \int_{\Gamma_M} \frac{dw(x)}{dx} EI_z \frac{d^2v(x)}{dx^2} nd\Gamma + \int_{\Gamma_\theta} \frac{dw(x)}{dx} EI_z \frac{d^2v(x)}{dx^2} nd\Gamma \\
\quad = - \int_{\Gamma_M} \frac{dw(x)}{dx} M_0 d\Gamma \tag{2.46}
\]

Inserting the shear force part of the Neumann boundary conditions (2.40) into the term \( \int_{\Gamma} w(x)EI_z \frac{d^3v(x)}{dx^3} nd\Gamma \) and noting that the weight function is equal to zero on \( \Gamma_v \) yields

\[
\int_{\Gamma} w(x)EI_z \frac{d^3v(x)}{dx^3} nd\Gamma = \int_{\Gamma_Q} w(x)EI_z \frac{d^3v(x)}{dx^3} nd\Gamma + \int_{\Gamma_v} w(x)EI_z \frac{d^3v(x)}{dx^3} nd\Gamma \\
\quad = - \int_{\Gamma_Q} w(x)Q_0 d\Gamma \tag{2.47}
\]
The weak form of the governing equation can be obtained by substituting the equations (2.46) and (2.47) into the equation (2.45). Solving it involves to find a trial function \( v(x) \in S \) such that

\[
\int_{\Omega} \frac{d^2 w(x)}{dx^2} EI_z \frac{d^2 v(x)}{dx^2} d\Omega + \int_{\Gamma_M} \frac{dw(x)}{dx} M_0 d\Gamma \\
- \int_{\Gamma_Q} w(x)Q_0 d\Gamma - \int_{\Omega} w(x)f_y(x) d\Omega = 0 \quad \forall w(x) \in V
\]

where \( S \) and \( V \) are appropriately defined spaces satisfying the following conditions

\[
\begin{align*}
S &= \{ v(x) \mid v(x) \in \mathcal{H}^2(\Omega), v(x) = v_0 \text{ on } \Gamma_v, \frac{dv(x)}{dx} = \theta_0 \text{ on } \Gamma_\theta \} \\
V &= \{ w(x) \mid w(x) \in \mathcal{H}^2(\Omega), w(x) = 0 \text{ on } \Gamma_v, \frac{dw(x)}{dx} = 0 \text{ on } \Gamma_\theta \}
\end{align*}
\]

Both \( S \) and \( V \) must be sub-spaces of the Sobolev space \( \mathcal{H}^2(\Omega) \), which requires that

\[
\begin{align*}
\int_{\Omega} \left\{ v^2(x) + \left[ \frac{dv(x)}{dx} \right]^2 + \left[ \frac{d^2 v(x)}{dx^2} \right]^2 \right\} dx < \infty \\
\int_{\Omega} \left\{ w^2(x) + \left[ \frac{dw(x)}{dx} \right]^2 + \left[ \frac{d^2 w(x)}{dx^2} \right]^2 \right\} dx < \infty
\end{align*}
\]

Based on the weak form of the governing equation (2.48), a Galerkin problem for the beam can be formulated, which involves to find \( v^h(x) \in S^h \) such that

\[
\int_{\Omega} \frac{d^2 w^h(x)}{dx^2} EI_z \frac{d^2 v^h(x)}{dx^2} d\Omega = -\int_{\Gamma_M} \frac{dw^h(x)}{dx} M_0 d\Gamma \\
+ \int_{\Gamma_Q} w^h(x)Q_0 d\Gamma + \int_{\Omega} w^h(x)f_y(x) d\Omega \quad \forall w^h(x) \in V^h
\]

where \( S^h \subset S \) and \( V^h \subset V \) are finite-dimensional spaces.

The Galerkin method (more specifically, the Bubnov-Galerkin method) requires that the trial function and the weight function come from the same finite-dimensional space, taking into account the requirements on the trial and weight functions where Dirichlet boundary conditions are applied.

To find the solution to the Galerkin problem (2.51), Hermitian polynomials can be used to construct the shape functions, which results in a cubic interpolation of the displacement field in the element,

\[
v^h(x) = N_i(x)v_i + M_i(x)\theta_i + N_j(x)v_j + M_j(x)\theta_j
\]

\[58\]
where $v_i$, $\theta_i$, $v_j$ and $\theta_j$ are the translational and rotational displacements at node $i$ and $j$ respectively, and the shape functions are

\[
\begin{align*}
N_i(x) &= 1 - 3\frac{x^2}{l^2} + 2\frac{x^3}{l^3} \\
M_i(x) &= x - 2\frac{x^2}{l} + \frac{x^3}{l^2} \\
N_j(x) &= 3\frac{x^2}{l^2} - 2\frac{x^3}{l^3} \\
M_j(x) &= -\frac{x^2}{l} + \frac{x^3}{l^2}
\end{align*}
\] (2.53)

Denoting that

\[
\overline{N}(x) = \begin{bmatrix} N_i(x) & M_i(x) & N_j(x) & M_j(x) \end{bmatrix}
\] (2.54)

and

\[
a_e = \begin{bmatrix} v_i \\ \theta_i \\ v_j \\ \theta_j \end{bmatrix}
\] (2.55)

Thus the displacement field (2.52) can be re-written as

\[
v^h(x) = \overline{N}(x)a_e
\] (2.56)

The second derivative of the trial function $v^h(x)$ is given by

\[
\frac{d^2 u^h(x)}{dx^2} = \frac{d^2 \overline{N}(x)}{dx^2} a_e
\] (2.57)

Similarly the weight function, and its first and second derivatives are given by

\[
w^h(x) = \overline{N}(x)b_e
\] (2.58)

\[
\frac{dw^h(x)}{dx} = \frac{d\overline{N}(x)}{dx} b_e
\] (2.59)

\[
\frac{d^2 w^h(x)}{dx^2} = \frac{d^2 \overline{N}(x)}{dx^2} b_e
\] (2.60)
2. THREE-DIMENSIONAL LATTICE FRACTURE MODEL

Inserting the equations (2.57), (2.58), (2.59) and (2.60) into the Galerkin problem (2.51) yields

\[
\int_{\Omega} \left[ \frac{d^2 N(x)}{dx^2} b_x \right]^T EI_z \left[ \frac{d^2 N(x)}{dx^2} a_x \right] d\Omega \\
= - \int_{\Gamma_m} \left[ \frac{dN(x)}{dx} b_x \right]^T M_0 d\Gamma + \int_{\Gamma_Q} \left[ N(x) b_x \right]^T Q_0 d\Gamma + \int_{\Omega} \left[ N(x) b_x \right]^T f_y(x) d\Omega
\]  

(2.61)

Rearranging the above equation yields

\[
\int_{\Omega} \left[ \frac{d^2 N(x)}{dx^2} \right]^T EI_z \left[ \frac{d^2 N(x)}{dx^2} \right] d\Omega a_x \\
= - \int_{\Gamma_m} \left[ \frac{dN(x)}{dx} \right]^T M_0 d\Gamma + \int_{\Gamma_Q} \left[ N(x) \right]^T Q_0 d\Gamma + \int_{\Omega} \left[ N(x) \right]^T f_y(x) d\Omega
\]  

(2.62)

Hence the element stiffness matrix (Euler-Bernoulli beam) for the bending and shear deformation in the plane \(xOy\) is given by

\[
K_{bExOy} = \int_{\Omega} \left[ \frac{d^2 N(x)}{dx^2} \right]^T EI_z \left[ \frac{d^2 N(x)}{dx^2} \right] d\Omega \\
= \int_0^l \left[ \begin{array}{ccc}
-\frac{6}{l^2} + \frac{12}{l^2} x \\
-\frac{2}{l} + \frac{6}{l^2} x \\
\frac{6}{l^2} - \frac{12}{l^2} x \\
-\frac{2}{l^2} + \frac{6}{l^2} x
\end{array} \right] EI_z \left[ \begin{array}{cccc}
-\frac{6}{l^2} + \frac{12}{l^2} x & -\frac{4}{l} + \frac{6}{l^2} x & \frac{6}{l^2} - \frac{12}{l^2} x & -\frac{2}{l^2} + \frac{6}{l^2} x
\end{array} \right] dx
\]

\[
= \begin{bmatrix}
\frac{12EI_z}{l^2} & \frac{6EI_z}{l} \\
\frac{6EI_z}{l} & \frac{2EI_z}{l^2} \\
\frac{12EI_z}{l^2} & \frac{6EI_z}{l} \\
\frac{6EI_z}{l} & \frac{4EI_z}{l^2}
\end{bmatrix}
\]

(2.63)

The shear deformation and rotational inertia effects can be taken into account (Timoshenko beam) by introducing an adjustment factor \(\Phi\) into the above element stiffness matrix (2.63), and it is given by

\[
K_{bExOy}^{\Phi} = \begin{bmatrix}
\frac{12EI_z}{l^2} & \frac{6EI_z}{l} & \frac{6EI_z}{l} & \frac{6EI_z}{l} \\
\frac{6EI_z}{l} & \frac{12EI_z}{l^2} & \frac{12EI_z}{l^2} & \frac{12EI_z}{l^2} \\
\frac{6EI_z}{l} & \frac{12EI_z}{l^2} & \frac{12EI_z}{l^2} & \frac{12EI_z}{l^2} \\
\frac{6EI_z}{l} & \frac{12EI_z}{l^2} & \frac{12EI_z}{l^2} & \frac{12EI_z}{l^2}
\end{bmatrix}
\]

(2.64)
2.2 Modeling procedures

where $E$ is the elastic modulus, $I_z$ is the moment of inertia of the cross-section about the $z$-axis, $l$ is the length of the element and $\Phi_1$ is the shear effect adjustment factor in the plane $xOy$.

The element stiffness matrix for the bending and shear deformation in the plane $xOz$ can be formulated in a similar way and is given by

$$K^e_{\text{bTxOz}} = \begin{bmatrix}
\frac{12EI_y}{l^2(1+\Phi_2)} & \frac{6EI_y}{l^2(1+\Phi_2)} & \frac{12EI_y}{6EI_y} & \frac{6EI_y}{l^2(1+\Phi_2)} \\
\frac{l^2(1+\Phi_2)}{l(1+\Phi_2)} & \frac{l^2(1+\Phi_2)}{l(1+\Phi_2)} & \frac{l^2(1+\Phi_2)}{l^2(1+\Phi_2)} & \frac{l^2(1+\Phi_2)}{l(1+\Phi_2)} \\
\frac{6EI_y}{6EI_y} & \frac{6EI_y}{6EI_y} & \frac{6EI_y}{6EI_y} & \frac{6EI_y}{6EI_y} \\
\frac{l^2(1+\Phi_2)}{l^2(1+\Phi_2)} & \frac{l^2(1+\Phi_2)}{l^2(1+\Phi_2)} & \frac{l^2(1+\Phi_2)}{l^2(1+\Phi_2)} & \frac{l^2(1+\Phi_2)}{l^2(1+\Phi_2)} \\
\end{bmatrix}$$

(2.65)

where $E$ is the elastic modulus, $I_z$ is the moment of inertia of the cross-section about the $z$-axis, $l$ is the length of the element and $\Phi_1$ is the shear effect adjustment factor in the plane $xOy$.

The element stiffness matrix in local domain for a lattice Timoshenko beam element can be obtained by assembly of the axial (2.26), torsional (2.27), bending and shear components in the plane $xOy$ (2.64) and in the plane $xOz$ (2.65), and it is given by

$$K^e_{\text{eval}} = \begin{bmatrix}
\frac{EA}{l(1+\Phi)} & 0 & 0 & 0 & 0 & \frac{EA}{l(1+\Phi)} & 0 & 0 & 0 & 0 & \frac{EA}{l(1+\Phi)} & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{12EI_y}{l^2(1+\Phi)} & 0 & 0 & 0 & 0 & \frac{12EI_y}{l^2(1+\Phi)} & 0 & 0 & 0 & 0 & \frac{12EI_y}{l^2(1+\Phi)} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{6EI_y}{l^2(1+\Phi)} & 0 & 0 & 0 & \frac{6EI_y}{l^2(1+\Phi)} & 0 & 0 & 0 & \frac{6EI_y}{l^2(1+\Phi)} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{EI_y}{l^2(1+\Phi)} & 0 & 0 & 0 & \frac{EI_y}{l^2(1+\Phi)} & 0 & 0 & 0 & \frac{EI_y}{l^2(1+\Phi)} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{12EI_y}{l^2(1+\Phi)} & 0 & 0 & 0 & \frac{12EI_y}{l^2(1+\Phi)} & 0 & 0 & 0 & \frac{12EI_y}{l^2(1+\Phi)} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \frac{12EI_y}{l^2(1+\Phi)} & 0 & 0 & 0 & \frac{12EI_y}{l^2(1+\Phi)} & 0 & 0 & 0 & \frac{12EI_y}{l^2(1+\Phi)} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \frac{12EI_y}{l^2(1+\Phi)} & 0 & 0 & 0 & \frac{12EI_y}{l^2(1+\Phi)} & 0 & 0 & 0 & \frac{12EI_y}{l^2(1+\Phi)} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{12EI_y}{l^2(1+\Phi)} & 0 & 0 & 0 & \frac{12EI_y}{l^2(1+\Phi)} & 0 & 0 & 0 & \frac{12EI_y}{l^2(1+\Phi)} & 0 & 0 & 0 & 0 & 0 \\
\end{bmatrix}$$

(2.66)

where $E$ is the elastic modulus, $G$ is the shear modulus, $A$ is the cross-sectional area of the element, $l$ is the length of the element, $I_z$ and $I_y$ are the moment of inertia about the $z$-axis and the $y$-axis respectively, $J$ is the polar moment of inertia about the $x$-axis, $\Phi_1$ and $\Phi_2$ are the shear effect adjustment factors in the plane $xOy$ and $xOz$ respectively and can be computed by

$$\begin{align*}
\Phi_1 &= \frac{12EI_z}{GA_lT^2} \\
\Phi_2 &= \frac{12EI_y}{GA_lT^2}
\end{align*}$$

(2.67)
2. THREE-DIMENSIONAL LATTICE FRACTURE MODEL

in which \( A_s \) is the shear cross-sectional area and is given by

\[
A_s = \frac{A}{\kappa}
\]  
(2.68)

where \( \kappa \) is the shear correction factor and it is equal to \( \frac{10}{9} \) for circular cross-section.

In 3D lattice network construction a circular cross-section of the element is preferred to rectangular one as it gives isotropic geometry properties about the cross-section, and the following formulas apply,

\[
\begin{align*}
A &= \pi r^2 \\
I_z &= \frac{\pi}{4} r^4 \\
I_y &= \frac{\pi}{4} r^4 \\
J &= \frac{\pi}{2} r^4
\end{align*}
\]  
(2.69)

The element stiffness matrix in global domain can be computed by the following formula,

\[
K_{\text{global}}^e = T K_{\text{local}}^e T^T
\]  
(2.70)

where \( K_{\text{local}}^e \) is the element stiffness matrix in local domain as shown in the expression (2.66), \( T \) is the transformation matrix of local and global domains, and \( T^T \) represents the transposed matrix of \( T \).

The local and global domains are illustrated in Figure 2.15 and the local domain \( O^*x^*y^*z^* \) is attached to the element. The relationship of the two domains is indicated by the transformation matrix \( T \), which is in the size of 12 × 12 and in the form of

\[
T = \begin{bmatrix}
t & t & t \\
t & t & t \\
t & t & t
\end{bmatrix}
\]  
(2.71)

where the matrix \( t \) of the size 3 × 3 is given by

\[
t = \begin{bmatrix}
l_1 = \cos(x, x^*) & l_2 = \cos(x, y^*) & l_3 = \cos(x, z^*) \\
m_1 = \cos(y, x^*) & m_2 = \cos(y, y^*) & m_3 = \cos(y, z^*) \\
n_1 = \cos(z, x^*) & n_2 = \cos(z, y^*) & n_3 = \cos(z, z^*)
\end{bmatrix}
\]  
(2.72)

in which nine direction cosines are defined.
2.2 Modeling procedures

Figure 2.15: Local and global domains

*Procedure.* The nine direction cosines can be determined based on the coordinates of the two nodes \(i(x_i, y_i, z_i)\) and \(j(x_j, y_j, z_j)\) in global domain. The procedure is

1. calculate \(a_1, a_2\) and \(a_3\) according to
   \[
   \begin{aligned}
   a_1 &= x_j - x_i \\
   a_2 &= y_j - y_i \\
   a_3 &= z_j - z_i
   \end{aligned}
   \]  
   \hspace{1cm} (2.73)

2. choose an arbitrary reference point \(B(x_b, y_b, z_b)\) on the principal plane \(x^*O^*y^*\) or \(x^*O^*z^*\), provided that the point \(B\) is not located at the \(x^*\)-axis, and then compute \(b_1, b_2\) and \(b_3\) according to
   \[
   \begin{aligned}
   b_1 &= x_b - x_i \\
   b_2 &= y_b - y_i \\
   b_3 &= z_b - z_i
   \end{aligned}
   \]  
   \hspace{1cm} (2.74)

3. calculate \(c_1, c_2\) and \(c_3\) using the following formulas,
   \[
   \begin{aligned}
   c_1 &= a_2b_3 - a_3b_2 \\
   c_2 &= a_3b_1 - a_1b_3 \\
   c_3 &= a_1b_2 - a_2b_1
   \end{aligned}
   \]  
   \hspace{1cm} (2.75)
(4) compute \( d_1, d_2 \) and \( d_3 \) according to
\[
\begin{align*}
  d_1 &= c_2 a_3 - c_3 a_2 \\ 
  d_2 &= c_3 a_1 - c_1 a_3 \\ 
  d_3 &= c_1 a_2 - c_2 a_1 
\end{align*}
\] (2.76)

(5) calculate the length of the element \( l = \sqrt{a_1^2 + a_2^2 + a_3^2} \), and then \( l_1, m_1 \) and \( n_1 \) can be obtained,
\[
\begin{align*}
  l_1 &= \frac{a_1}{l} \\ 
  m_1 &= \frac{a_2}{l} \\ 
  n_1 &= \frac{a_3}{l} 
\end{align*}
\] (2.77)

(6) compute the expression \( d = \sqrt{d_1^2 + d_2^2 + d_3^2} \), and then \( l_2, m_2 \) and \( n_2 \) can be obtained,
\[
\begin{align*}
  l_2 &= \frac{d_1}{d} \\ 
  m_2 &= \frac{d_2}{d} \\ 
  n_2 &= \frac{d_3}{d} 
\end{align*}
\] (2.78)

(7) finally \( l_3, m_3 \) and \( n_3 \) can be computed according to
\[
\begin{align*}
  l_3 &= m_1 n_2 - m_2 n_1 \\ 
  m_3 &= n_1 l_2 - n_2 l_1 \\ 
  n_3 &= l_1 m_2 - l_2 m_1 
\end{align*}
\] (2.79)

**Jacobi pre-conditioned conjugate gradient linear equations solver**

A set of linear equations are formulated and solved during the lattice fracture analysis, and the Jacobi pre-conditioned conjugate gradient method [30] is employed. The basic algorithm is presented as following.

*Algorithm.* Suppose that a system of linear equations is represented by

\[
Ax = b \tag{2.80}
\]

where \( A \) is the coefficient matrix, \( b \) is the constant vector, \( x \) is the solution vector.
2.2 Modeling procedures

Given the inputs $A$, $b$, an initial guess of $x$, absolute error tolerance $\epsilon_a < 1$, relative error tolerance $\epsilon_r < 1$, and a maximum number of iterations $i_{\text{max}}$.

$$m \leftarrow \text{diag}(A) \quad m \leftarrow m^{-1} \quad r \leftarrow b - Ax \quad d \leftarrow m \ast r \quad \delta_{\text{new}} \leftarrow r^T d \quad \delta_0 \leftarrow \delta_{\text{new}}$$

if $\delta_0 < \epsilon_a^2$, then terminate;

for (int $i = 1; i \leq i_{\text{max}}; i++$)

{}{\footnotesize

$$q \leftarrow Ad \quad \alpha \leftarrow \frac{\delta_{\text{new}}}{d^T q} \quad x \leftarrow x + \alpha d \quad r \leftarrow r - \alpha q \quad s \leftarrow m \ast r \quad \delta_{\text{old}} \leftarrow \delta_{\text{new}} \quad \delta_{\text{new}} \leftarrow r^T s$$

if $\delta_{\text{new}} < \epsilon_a^2$ or $\delta_{\text{new}} < \epsilon_r^2 \delta_0$, then terminate;

{}{\footnotesize

$$\beta \leftarrow \frac{\delta_{\text{new}}}{\delta_{\text{old}}} \quad d \leftarrow s + \beta d$$

}

Fracture law

The most frequently used fracture law in lattice fracture model is the classic Rankine failure criterion, which requires the comparative stress in the lattice beam element is smaller than its strength. Other fracture laws are also possible, and see [21] for more discussions. The comparative stress defined in this thesis is caused by the normal force and bending moments, and can be computed by

$$\sigma = \alpha_N \frac{N}{A} + \alpha_M \frac{\max(M_{xOy}, M_{xOz})}{W} \quad (2.81)$$
where $A$ is the area of the cross-section, $W$ is the cross-sectional factor for bending resistance, $\alpha_N$ and $\alpha_M$ are the normal force influence factor and the bending influence factor whose values are 1.0 and 0.05 respectively in this thesis.

**Lattice element removal mechanisms**

The basic removal procedure is to remove one element at one lattice analysis step. To speed up the analysis, it is also possible to remove multiple elements at one analysis step. Alternatively the bending resistance of an element may be removed first and then the axial resistance. In the case of local softening implemented, as shown in Figure 2.16, the element loses its stiffness and strength gradually and eventually quits from the system through several analysis steps.

**2.2.4 Load-displacement response and cracks propagation**

The major outputs of lattice fracture analysis include the load-displacement response, microcracks propagation and cracks pattern in the final failure state. The load-displacement response can be converted to stress-strain diagram, which represents the constitutive relation of the material analyzed. The cracks are represented by the broken lattice elements. As the broken lattice elements are removed step by step during the analysis, the sequence of the removal is traced, which simulates the microcracks propagation. At the end of the lattice fracture
analysis, all the broken lattice elements form the cracks pattern in the final failure state. An application of the 3D lattice fracture model is given in Section 3.1 on Page 70 which is about the micromechanical modeling of cement paste.

2.3 Summary

In this chapter the development of some fracture models (such as discrete cracking model, smeared cracking model and lattice fracture model) for brittle materials were reviewed. The 3D lattice fracture model is implemented for parallel computing on shared memory architecture computers, which enables the study on large systems within a relatively short computing time.

The modeling procedures of 3D lattice fracture model are discussed in detail. The lattice network may be constructed according to ImgLat scheme and/or HymLat scheme, depending on whether the input microstructure of materials is described in terms of voxels or spheres. The influences of mesh randomness and random seed are investigated through a uniaxial tensile test on a prism of the size $40 \text{ mm} \times 40 \text{ mm} \times 60 \text{ mm}$. The local mechanical properties determination principles for lattice elements are developed for ImgLat and HymLat schemes respectively.

The lattice fracture model can be configured to simulate various laboratory tests such as tensile test, shear test, bending test and more. The uniaxial tensile test is illustrated in detail and two types of boundary conditions are distinguished and compared: glued and clamped boundaries. It turns out that the influences of different boundaries on the tensile behavior of materials can be neglected, provided that the Poisson’s ratio of the specimen is close to 0, otherwise the influences are significant.

The fracture process simulation is the kernel part of the lattice fracture analysis. The critical lattice elements are removed from the system step by step, representing the propagation of microcracks. The lattice element fracture law and removal mechanisms are also discussed. The load-displacement response of the specimen in question can be obtained from lattice fracture analysis, and it
2. THREE-DIMENSIONAL LATTICE FRACTURE MODEL

can be converted to stress-strain diagram, based on which some mechanical properties such as Young’s modulus, strength and fracture energy can be computed. The cracks pattern and microcracks propagation can also be obtained.

The 3D lattice fracture model described in this chapter is applied to simulate the fracture processes in cement paste at microscale in Chapter 3, and the fracture processes in mortar and concrete at mesoscale in Chapter 5.
Chapter 3

Cement Paste at Microscale

The microstructure of materials determines its global performance. This funda-
mental principle of materials science is adapted in this chapter to predict the
mechanical performance of cement paste.

The microstructure of cement paste can be imaged either experimentally or
numerically. The micro X-ray computed tomography (CT) \textsuperscript{31} offers a non-
destructive experimental technique to collect microstructure information of ce-
ment paste in terms of digitized voxels. Computer modeling packages are also
available to simulate the cement hydration and microstructure formation pro-
cesses, for instance, the HYMOSTRUC3D model developed by TU Delft \textsuperscript{4, 32},
the NIST CEMHYD3D toolkit \textsuperscript{33} and the Mic model by EPFL \textsuperscript{34}. Subsec-
tion 3.1.1 talks about simulations of microstructures of cement paste using the
HYMOSTRUC3D model, and Subsection 3.1.3 introduces a microstructure of
cement paste obtained through CT scan.

After obtaining the microstructure of cement paste, the 3D lattice fracture
model can be employed to simulate the fracture behavior of the cement paste.
For example, a uniaxial tensile test can be set up and simulated on the cement
paste to predict its Young’s modulus, tensile strength and fracture energy, as well
as the microcracks propagation and cracks pattern in the final failure state. It
will be elaborated in Subsection 3.1.2.

The cement hydration and microstructure formation model, HYMOSTRUC3D
model, and the mechanical performance evaluation model, 3D lattice fracture
3. CEMENT PASTE AT MICROSCALE

![Diagram](image)

**Figure 3.1**: Combined application of the HYMOSTRUC3D model and the 3D lattice fracture model

model, can be combined to study the influences of various factors on the mechanical properties of cement paste, including but not limited to the influences of degree of hydration, cement fineness, water/cement ratio and mineral composition of cement. Details and findings can be found in Section 3.2.

### 3.1 Micromechanical modeling of cement paste

In Subsection 3.1.1 and 3.1.2, a numerical experiment is carried out to illustrate the combined application of the HYMOSTRUC3D model and the 3D lattice fracture model. A series of microstructures are simulated for the cement paste at different degrees of hydration by the HYMOSTRUC3D model, and then the mechanical performance of the microstructure at the curing age of 28 days is evaluated through the 3D lattice fracture analysis. The workflow is shown in Figure 3.1.

In Subsection 3.1.3, an alternative method to obtain the microstructure of cement paste is introduced, which is the micro X-ray computed tomography [35]. A sample microstructure at the curing age of 28 days is scanned and provided by the researchers at UIUC (University of Illinois at Urbana-Champaign, United States) [36], and then it is tested for its uniaxial tensile properties using the 3D lattice fracture model [37]. This example demonstrates that the 3D lattice
3.1 Micromechanical modeling of cement paste

fracture analysis can accept microstructures of cement paste from laboratory experiments, in addition to the computer simulated microstructures.

3.1.1 Simulated microstructures of cement paste

The clinker of Portland cement is mainly composed of calcium, silicon and oxygen. In cement chemistry it is usually represented in terms of constituents as tricalcium silicate $3\text{CaO} \cdot \text{SiO}_2$ ($C_3S$), dicalcium silicate $2\text{CaO} \cdot \text{SiO}_2$ ($C_2S$), tricalcium aluminate $3\text{CaO} \cdot \text{Al}_2\text{O}_3$ ($C_3A$) and calcium ferroaluminate $4\text{CaO} \cdot \text{Al}_2\text{O}_3 \cdot \text{Fe}_2\text{O}_3$ ($C_4AF$). A set of chemical reactions is initiated when water is mixed with cement, the process of which is called hydration. The hydration process is always accompanied by heat release as the energy state of cement mixture turns from higher one to lower one. The heat release indicates the degree of hydration and it can be used as a measurement to determine the extent of hydration. The hydration products are also generated during the hydration process, which mainly include calcium silicate hydrates (CSH) and calcium hydroxides (CH).

In the HYMOSTRUC3D model, the cement particles are modeled as spheres and these spherical particles grow during the hydration process. The inputs include the specimen size, the mineralogical composition of cement, the cement fineness in terms of Blaine value (Rosin-Rammler particle size distribution is assumed) and the water/cement ratio. The amount of hydration products is dependent on the degree of hydration. A simplification is made in the model that the amount of CH product is substituted with the same amount of CSH product. In general the hydrating cement particle contains three layers from center to outward surface, namely unhydrated cement, inner product and outer product, as shown in Figure 3.2.

The cement grain dissolves and the hydration products are generated gradually during the hydration process, which yields expansion and layer thickness change of the cement particle, as shown in Figure 3.2. The amount of unhydrated cement is decreasing, while inner product and outer product are being produced.

The interactions between neighboring particles are taken into account in the HYMOSTRUC3D model. If the outer product of one hydrating cement particle
3. CEMENT PASTE AT MICROSCALE

![Figure 3.2: Hydration of a single cement particle](image1)

![Figure 3.3: Contact of hydrating cement particles](image2)

meets the outer product of another particle, then the overlapping part is redistributed to the outer layer of the particles. As a result contact volume and area can be formed as shown in Figure 3.3. In [38] it is found that the mechanical properties (such as Young’s modulus, shear modulus and compressive strength) of cement paste can be related to the contact area.

An example is given to demonstrate the application of the HYMOSTRUC3D model. The cement CEM I 42.5N is used, and the specification of the cement mix is summarized in Table 3.1. The initial microstructure of cement paste can be created by parking multiple spherical particles into an empty container, as shown in Figure 3.4(a). The simulated degree of hydration diagram is given in Figure 3.5, on which each point corresponds to a microstructure. The microstructures at the curing ages of 28 days and 365 days are shown in Figure 3.4(b) and 3.4(c) respectively, the corresponding degrees of hydration are 69% and 88%. Periodic material boundary conditions apply.
### 3.1 Micromechanical modeling of cement paste

**Table 3.1:** Specification of the cement mix used in the simulation

<table>
<thead>
<tr>
<th>Property</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cement type</td>
<td>CEM I 42.5N</td>
</tr>
<tr>
<td>Mineralogical composition</td>
<td>$C_3S$: 64 $%$, $C_2S$: 13 $%$, $C_3A$: 8 $%$, $C_4AF$: 9 $%$</td>
</tr>
<tr>
<td>Fineness (Blaine value)</td>
<td>420 $m^2/kg$</td>
</tr>
<tr>
<td>Minimum particle diameter</td>
<td>1 $\mu m$</td>
</tr>
<tr>
<td>Maximum particle diameter</td>
<td>37 $\mu m$</td>
</tr>
<tr>
<td>Particle size distribution</td>
<td>Rosin-Rammler distribution $F(x) = 1 - e^{-bx^n}$</td>
</tr>
<tr>
<td>($n = 1.0698$, $b = 0.04408$)</td>
<td></td>
</tr>
<tr>
<td>Specimen size</td>
<td>100 $\mu m \times 100 \mu m \times 100 \mu m$</td>
</tr>
<tr>
<td>Water/cement ratio</td>
<td>0.4</td>
</tr>
<tr>
<td>Curing temperature</td>
<td>20 $^\circ C$</td>
</tr>
</tbody>
</table>

**Figure 3.4:** Microstructures of cement paste at different degrees of hydration with the specification in Table 3.1

(a) Initial  
(b) Degree of hydration 69 $\%$ (28 days)  
(c) Degree of hydration 88 $\%$ (365 days)
3. CEMENT PASTE AT MICROSCALE

![Simulated degree of hydration diagram against hydration time](image)

**Figure 3.5:** Simulated degree of hydration diagram against hydration time

The cement paste of curing age 28 days is usually of interest, as the strength at 28 days is commonly used in many structural design codes, hence the microstructure in Figure 3.4(b) is further analyzed after it is converted to a voxel-based digital image, as shown in Figure 3.6. It can be decomposed to four phases, including a pore phase shown in Figure 3.7(a) and three solid phases namely unhydrated cement shown in Figure 3.7(b), inner product in Figure 3.7(c) and outer product in Figure 3.7(d). The volume percentage of every individual phase is indicated in the subcaptions in Figure 3.7.

3.1.2 Mechanical performance evaluation of the microstructures

Having obtained the microstructure of cement paste, the next step is to evaluate its mechanical performance using the 3D lattice fracture model. It is required to convert the spherical particle embedded microstructure to a voxel-based digital image, where the ImgLat lattice construction method applies, as discussed in Subsection 2.2.1 on Page 35. The microstructure of cement paste in Figure 3.6 is taken for the mechanical performance evaluation. The water/cement ratio is 0.4, the degree of hydration is 69% and the porosity is 13%.
The specimen of the size 100 µm × 100 µm × 100 µm is meshed at the resolution 1 µm/voxel, and a quadrangular lattice network is constructed. The randomness of the lattice system is set to 0 for all the boundary cells and 0.5 for other cells. This configuration would yield a realistic crack pattern and a regular specimen shape. The influence of randomness on the simulated mechanical performance is studied in Subsection 2.2.1 and the results are summarized in Table 2.4. The cross-section of a lattice element is assumed to be circular, and its area is equal to the perpendicular voxel surface area which is 1 µm² in this example. The elastic properties of solid phases can be measured or simulated as presented in [39, 40], the values of which are scattered due to different measurement approaches used. The tensile strength ratio of each phase is considered equal to the nanoindentation hardness ratio. The assumed local mechanical properties of individual solid phases are given in Table 3.2. More discussions about the local mechanical properties can be found in [41].

The assignment of local mechanical properties to a lattice element is related to the type of the lattice element in question, which is determined by the locations
3. CEMENT PASTE AT MICROSCALE

![Figure 3.7: Individual phases of the microstructure of cement paste in Figure 3.6](image)

![Table 3.2: Assumed local mechanical properties of solid phases of cement paste](table)

### Table 3.2

<table>
<thead>
<tr>
<th>No</th>
<th>Solid phase</th>
<th>Young’s modulus $E$ (GPa)</th>
<th>Shear modulus $G$ (GPa)</th>
<th>Tensile strength $f_t$ (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Unhydrated cement</td>
<td>135</td>
<td>52</td>
<td>1.8</td>
</tr>
<tr>
<td>2</td>
<td>Inner product</td>
<td>30</td>
<td>12</td>
<td>0.24</td>
</tr>
<tr>
<td>3</td>
<td>Outer product</td>
<td>22</td>
<td>8.9</td>
<td>0.15</td>
</tr>
</tbody>
</table>
3.1 Micromechanical modeling of cement paste

Table 3.3: Classification of lattice element types

<table>
<thead>
<tr>
<th>No</th>
<th>Element type</th>
<th>Node 1 phase</th>
<th>Node 2 phase</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Unhydrated cement</td>
<td>Unhydrated cement</td>
<td>Unhydrated cement</td>
</tr>
<tr>
<td>2</td>
<td>Inner product</td>
<td>Inner product</td>
<td>Inner product</td>
</tr>
<tr>
<td>3</td>
<td>Outer product</td>
<td>Outer product</td>
<td>Outer product</td>
</tr>
<tr>
<td>4</td>
<td>Interface U-I</td>
<td>Unhydrated cement</td>
<td>Inner product</td>
</tr>
<tr>
<td>5</td>
<td>Interface I-O</td>
<td>Inner product</td>
<td>Outer product</td>
</tr>
<tr>
<td>6</td>
<td>Interface O-U</td>
<td>Outer product</td>
<td>Unhydrated cement</td>
</tr>
</tbody>
</table>

Table 3.4: Local mechanical properties of lattice elements

<table>
<thead>
<tr>
<th>No</th>
<th>Element type</th>
<th>Young’s modulus $E$ (GPa)</th>
<th>Shear modulus $G$ (GPa)</th>
<th>Tensile strength $f_t$ (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Unhydrated cement</td>
<td>135</td>
<td>52</td>
<td>1.8</td>
</tr>
<tr>
<td>2</td>
<td>Inner product</td>
<td>30</td>
<td>12</td>
<td>0.24</td>
</tr>
<tr>
<td>3</td>
<td>Outer product</td>
<td>22</td>
<td>8.9</td>
<td>0.15</td>
</tr>
<tr>
<td>4</td>
<td>Interface U-I</td>
<td>49</td>
<td>20</td>
<td>0.24</td>
</tr>
<tr>
<td>5</td>
<td>Interface I-O</td>
<td>25</td>
<td>10</td>
<td>0.15</td>
</tr>
<tr>
<td>6</td>
<td>Interface O-U</td>
<td>38</td>
<td>15</td>
<td>0.15</td>
</tr>
</tbody>
</table>

of its two nodes, as shown in Figure 2.7. Three solid phases in the microstructure result in six types of lattice elements, as listed in Table 3.3. No lattice node is generated in the voxels which represent pore phase, as it does not contribute to the global mechanical performance of the specimen.

The local mechanical properties of lattice elements are determined according to the rules laid down in Subsection 2.2.1 on Page 41. All lattice elements behave linear-brittle, and the Young’s modulus, shear modulus and tensile strength are given in Table 3.4.

A conventional uniaxial tensile test is simulated on the lattice system, the external load is imposed on the top and bottom surfaces in the $z$-direction, and all the other surfaces are free to expand and/or shrink as shown in Figure 3.8.

The fracture process is simulated by the removal of lattice elements step by
Figure 3.8: Uniaxial tensile test on lattice system of cement paste at microscale
3.1 Micromechanical modeling of cement paste

Table 3.5: Simulated mechanical properties of cement paste at microscale, corresponding with Figure 3.9

<table>
<thead>
<tr>
<th></th>
<th>$E$ (GPa)</th>
<th>$f_t$ (MPa)</th>
<th>$\epsilon_p$</th>
<th>$G_F$ (J/m$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus</td>
<td>13</td>
<td>20</td>
<td>0.18%</td>
<td>22</td>
</tr>
<tr>
<td>Tensile strength</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Strain at peak load</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fracture energy</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The basic idea of lattice fracture analysis is that imposing a prescribed displacement on the lattice structure, finding the critical element that has highest stress/strength ratio, and then removing it from the system. This procedure is repeated until the system fails. The final outcomes of the simulation include the load-displacement diagram which can be converted to a stress-strain diagram, as shown in Figure 3.9 and the microcracks propagation as shown in Figure 3.10.

The stress-strain diagram reveals the tensile behavior of cement paste at microscale, from which the elastic modulus, tensile strength, strain at peak load and fracture energy can be obtained. For the example given hereby, the simulated mechanical properties of cement paste at microscale are given in Table 3.5. The Young’s modulus is the slope of the curve at the linear stage in the stress-strain diagram in Figure 3.9, the tensile strength corresponds to the peak point, and the fracture energy can be computed as the area below the stress-strain curve. The absolute values of global tensile strength and the strain at peak load are linearly dependent on the local input strength listed in Table 3.4. If all the local strengths would be doubled, then the resulting global tensile strength and the strain at peak load would also be doubled, and the fracture energy would be four times larger as it is related to the square of the local strength values.

Figure 3.10 shows that first a few microcracks are initiated around the middle part of the specimen, and then the microcracks spread further until the final failure state. In total 38\,106 lattice analysis steps are performed, which means 38\,106 lattice elements are broken and thus removed from the system, as all elements behave linear-brittle locally. The pre-peak and post-peak microcracks are also shown in Figure 3.10. The deformed specimen in the final failure state is shown in Figure 3.11.
3. CEMENT PASTE AT MICROSCALE

Figure 3.9: Simulated stress-strain diagram of cement paste at microscale

Figure 3.10: 3D microcracks propagation of cement paste due to tension at microscale, corresponding with Figure 3.9
3.1 Micromechanical modeling of cement paste

**Figure 3.11:** Deformed specimen due to vertical tension in the final failure state, corresponding with Figure 3.9.

**Table 3.6:** Simulated mechanical properties of cement paste at microscale, loaded horizontally along \( x \)-direction or \( y \)-direction, and vertically along \( z \)-direction

<table>
<thead>
<tr>
<th>Loading direction</th>
<th>Young’s modulus ( E ) (GPa)</th>
<th>Tensile strength ( f_t ) (MPa)</th>
<th>Strain at peak load ( \epsilon_p )</th>
<th>Fracture energy ( G_F ) (J/m(^2))</th>
</tr>
</thead>
<tbody>
<tr>
<td>( x )-axis</td>
<td>13</td>
<td>21</td>
<td>0.18%</td>
<td>17</td>
</tr>
<tr>
<td>( y )-axis</td>
<td>13</td>
<td>21</td>
<td>0.21%</td>
<td>20</td>
</tr>
<tr>
<td>( z )-axis</td>
<td>13</td>
<td>20</td>
<td>0.18%</td>
<td>22</td>
</tr>
</tbody>
</table>

**Influences of loading directions**

The external tensile load is imposed along the vertical \( z \)-direction in Figure 3.8, alternatively the specimen can also be loaded horizontally along \( x \)-direction or \( y \)-direction. The simulated mechanical properties are not necessary to be exactly the same, as summarized in Table 3.6, due to the fact that the cement paste is not ideal isotropic homogeneous. The stress-strain responses are given in Figure 3.12 and the cracks patterns are shown in Figure 3.13.

Comparisons can be made based on Table 3.6 and Figure 3.12 to learn the influences of loading directions on the simulated stress-strain response. It is apparent that differences exist but not too much. The cracks patterns in the final failure state also have some differences, as shown in Figure 3.13.
3. CEMENT PASTE AT MICROSCALE

Figure 3.12: Simulated stress-strain diagrams of cement paste at microscale, loaded horizontally along $x$-direction or $y$-direction, and vertically along $z$-direction

Figure 3.13: Cracks patterns in the final failure state, loaded horizontally along $x$-direction or $y$-direction, and vertically along $z$-direction
3.1 Micromechanical modeling of cement paste

Figure 3.14: Simulated stress-strain diagrams of cement paste with regular lattice mesh, and irregular lattice mesh at the randomness of 0.5

Regular lattice mesh

During the construction of the lattice network, the randomness is set to 0 for all the boundary cells and 0.5 for other cells in the previous examples in this chapter. A regular mesh can be made by setting the randomness to 0 for all cells. The simulated tensile mechanical response is shown in Figure 3.14. Some mechanical properties can be computed based on this diagram, as listed in Table 3.7. Comparisons can be made based on Figure 3.14 and Table 3.7 to see the influences of randomness on the simulated mechanical properties. Adopting an irregular mesh introduces artificial heterogeneity and thus makes the simulated Young’s modulus lower. This finding is in accordance with the trend found in Table 2.4, which studies the influences of randomness using a homogeneous prism. The pre-peak and post-peak microcracks are shown in Figure 3.15 for the regular meshed lattice system and the irregular meshed lattice system at the randomness of 0.5.

3.1.3 CT-scanned microstructures and its micromechanical properties

A lattice network can be constructed based on a microstructure simulated by a computer modeling package, as shown in the examples in Subsection 3.1.1 and
3. CEMENT PASTE AT MICROSCALE

Table 3.7: Simulated mechanical properties of cement paste with regular lattice mesh at the randomness of 0, and with irregular lattice mesh at the randomness of 0.5

<table>
<thead>
<tr>
<th>Mesh</th>
<th>Young’s modulus $E$ (GPa)</th>
<th>Tensile strength $f_t$ (MPa)</th>
<th>Strain at peak load $\epsilon_p$</th>
<th>Fracture energy $G_F$ (J/m$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Regular</td>
<td>14</td>
<td>20</td>
<td>0.15 %</td>
<td>16</td>
</tr>
<tr>
<td>Irregular</td>
<td>13</td>
<td>20</td>
<td>0.18 %</td>
<td>22</td>
</tr>
</tbody>
</table>

Figure 3.15: Pre-peak and post-peak microcracks for the regular meshed lattice system, and the irregular meshed lattice system at the randomness of 0.5
3.1 Micromechanical modeling of cement paste

Figure 3.16: Microstructure of cement paste of size $75\mu m \times 75\mu m \times 75\mu m$ at the curing age 28 days with water/cement ratio 0.5 from CT scan (provided by UIUC)

Subsection 3.1.2 Alternatively the microstructure can also be obtained through laboratory experimental method like CT scan. A microstructure of real cement paste is given in Figure 3.16, which is taken from an X-ray tomograph of a real cement paste sample captured using a micro X-ray CT system located at UIUC (University of Illinois at Urbana-Champaign, US). The water/cement ratio of the paste is 0.5, the curing age is 28 days and the size of the specimen is $75\mu m \times 75\mu m \times 75\mu m$. The resolution of the digital image in Figure 3.16 is $0.5\mu m$/voxel, resulting in 150 voxels per direction.

In the microstructure shown in Figure 3.16, three phases are distinguished, including the pore phase and two solid phases, namely unhydrated cement and hydration products [36]. The phase segmentation is carried out on the microstructure and the result is given in Figure 3.17.

The local mechanical properties of individual solid phases are given in Table 3.8 which are derived from the properties in Table 3.2. Two solid phases result in three types of lattice elements, as listed in Table 3.9. The tensile strength
3. CEMENT PASTE AT MICROSCALE

![Figure 3.17: Phase segmentation of the microstructure of cement paste in Figure 3.16](image)

**Figure 3.17:** Phase segmentation of the microstructure of cement paste in Figure 3.16

<table>
<thead>
<tr>
<th>No</th>
<th>Solid phase</th>
<th>Young’s modulus $E$ (GPa)</th>
<th>Shear modulus $G$ (GPa)</th>
<th>Tensile strength $f_t$ (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Hydration products</td>
<td>26</td>
<td>10</td>
<td>0.2</td>
</tr>
<tr>
<td>2</td>
<td>Unhydrated cement</td>
<td>135</td>
<td>52</td>
<td>1.8</td>
</tr>
</tbody>
</table>

Table 3.8: Local mechanical properties of solid phases of experimental cement paste

The ratio of hydration products to unhydrated cement is 1:9, which is equal to the measured nanoindentation hardness ratio.

A uniaxial tensile test is simulated on the experimental microstructure, and the stress-strain response is shown in Figure 3.18. Some mechanical properties are computed and summarized in Table 3.10. The cracks pattern in the final failure state is given in Figure 3.19.

### 3.2 Influences of various factors

The combination of the HYMOSTRUC3D model and 3D lattice fracture analysis makes it possible to investigate the influences of various factors on the global mechanical performance of cement paste at microscale, including but not limited to the degree of hydration, cement fineness, water/cement ratio and mineral
3.2 Influences of various factors

Table 3.9: Local mechanical properties of lattice elements for experimental cement paste

<table>
<thead>
<tr>
<th>No</th>
<th>Element type</th>
<th>Young’s modulus $E$ (GPa)</th>
<th>Shear modulus $G$ (GPa)</th>
<th>Tensile strength $f_t$ (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Hydration products</td>
<td>26</td>
<td>10</td>
<td>0.2</td>
</tr>
<tr>
<td>2</td>
<td>Unhydrated cement</td>
<td>135</td>
<td>52</td>
<td>1.8</td>
</tr>
<tr>
<td>3</td>
<td>Interface</td>
<td>44</td>
<td>17</td>
<td>0.2</td>
</tr>
</tbody>
</table>

Figure 3.18: Simulated stress-strain diagram of the experimental cement paste at microscale

Table 3.10: Simulated mechanical properties of the experimental cement paste at microscale, corresponding with Figure 3.18

<table>
<thead>
<tr>
<th>Young’s modulus $E$ (GPa)</th>
<th>Tensile strength $f_t$ (MPa)</th>
<th>Strain at peak load $\epsilon_p$</th>
<th>Fracture energy $G_F$ (J/m$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>27</td>
<td>0.19 %</td>
<td>34</td>
</tr>
</tbody>
</table>

87
3. CEMENT PASTE AT MICROSCALE

Figure 3.19: Simulated cracks pattern in the final failure state for the experimental cement paste at microscale, corresponding with Figure 3.18

composition of cement. Numerical experiments are carried out to simulate the microstructure and the corresponding tensile properties of the cement paste samples of the size $100\mu m \times 100\mu m \times 100\mu m$. The starting point is the cement mixture and the resulting outcomes are the Young’s modulus, tensile strength, fracture energy and cracks pattern, as shown in Figure 3.1.

3.2.1 Degree of hydration

For the cement mixture given in Table 3.1, the HYMOSTRUC3D model is employed to simulate the initial microstructure and a set of microstructures at various degrees of hydration. The resulting degree of hydration curve is shown in Figure 3.5. The following curing ages and degrees of hydration are chosen for further mechanical performance evaluation, as given in Table 3.11. The corresponding microstructures are simulated and analyzed, and the results are summarized in Table 3.11. The local mechanical properties of individual phases are given in Table 3.2.
3.2 Influences of various factors

Table 3.11: Influences of degree of hydration on the tensile mechanical properties of cement paste at microscale

<table>
<thead>
<tr>
<th>Curing age (h)</th>
<th>29</th>
<th>67</th>
<th>83</th>
<th>162</th>
<th>203</th>
<th>1999</th>
<th>7947</th>
<th>12593</th>
</tr>
</thead>
<tbody>
<tr>
<td>Degree of hydration</td>
<td>31%</td>
<td>44%</td>
<td>47%</td>
<td>55%</td>
<td>58%</td>
<td>79%</td>
<td>88%</td>
<td>90%</td>
</tr>
<tr>
<td>Porosity</td>
<td>36.2%</td>
<td>27.2%</td>
<td>25.2%</td>
<td>20.0%</td>
<td>18.4%</td>
<td>8.2%</td>
<td>5.4%</td>
<td>4.8%</td>
</tr>
<tr>
<td>Young’s modulus $E$ (GPa)</td>
<td>1.9</td>
<td>4.8</td>
<td>5.6</td>
<td>8.2</td>
<td>9.1</td>
<td>15.7</td>
<td>17.5</td>
<td>17.9</td>
</tr>
<tr>
<td>Tensile strength $f_t$ (MPa)</td>
<td>2.7</td>
<td>6.9</td>
<td>8.5</td>
<td>12.4</td>
<td>14.1</td>
<td>27.1</td>
<td>31.5</td>
<td>31.6</td>
</tr>
<tr>
<td>Strain at peak load $\epsilon_p$</td>
<td>0.37%</td>
<td>0.28%</td>
<td>0.21%</td>
<td>0.22%</td>
<td>0.19%</td>
<td>0.19%</td>
<td>0.20%</td>
<td>0.20%</td>
</tr>
<tr>
<td>Fracture energy $G_F$ (J/m²)</td>
<td>6.4</td>
<td>13.1</td>
<td>14.7</td>
<td>20.8</td>
<td>24.1</td>
<td>14.9</td>
<td>14.3</td>
<td>14.4</td>
</tr>
</tbody>
</table>

Figure 3.20: Porosity of the hydrating cement paste system against degree of hydration

The porosity of the hydrating cement paste is decreasing when the hydration process continues, as shown in Figure 3.20 and strong linear relevance is found. The pores in the system are filled by hydration products gradually, resulting in a microstructure with low porosity in the end.

Both the Young’s modulus and the tensile strength increase linearly with the increase of degree of hydration, as shown in Figure 3.21, which is obtained based on the data from Table 3.11. As the porosity is linearly dependent on the degree of hydration, it can be derived that the Young’s modulus and the tensile strength also change linearly against the porosity, as shown in Figure 3.22. The
development of Young’s modulus and tensile strength is due to the continuous maturing of the microstructure of cement paste during hydration, and eventually a well developed system is obtained.

At the initial stage of hydration, the strain at peak load is relatively high, up to 0.37% at the degree of hydration 31%, then it drops to the range of [0.19%, 0.22%] when the degree of hydration reaches 47%, and then it stays in that range although the hydration process continues, as shown in Figure 3.23. This suggests that the tensile strain at peak load for well developed cement paste is about 0.2% at microscale.

The fracture energy increases first and then decreases during the hydration process, as shown in Figure 3.24. The paste system is getting stronger all the time, which would increase the fracture energy. At earlier stage the number of microcracks in the final failure state also increases as shown in Figure 3.27(a) and (b) thus the more fracture energy is required to break the system. However, a more localized cracks pattern shows up for better developed microstructure at later stage as shown in Figure 3.27(b) and (c). Thus less microcracks are required to bring the system to failure, which would decrease the fracture energy. The two forces that higher strength and less microcracks push the change of fracture
3.2 Influences of various factors

**Figure 3.22:** Trendlines of the Young’s modulus and the tensile strength against the porosity of the cement paste system

**Figure 3.23:** Relationship between the strain at peak load and the degree of hydration
3. CEMENT PASTE AT MICROSCALE

Figure 3.24: Relationship between the fracture energy and the degree of hydration

energy towards opposite directions, hence the net effect is dependent on which force wins. The curve in Figure 3.24 shows that the effect of less microcracks becomes dominant for paste at high degree of hydration.

In this particular example it is observed that the fracture energy reaches the maximum when the porosity of the system is 18.4%, as shown in Figure 3.25. It indicates that a low porosity does not correspond to a system which can absorb maximum energy during the fracture processes. If seeking capacity to absorb fracture energy is the objective when designing a material, then leaving some pores in the system may help. More investigations on this aspect could be done to find out the relationship between the fracture energy and the porosity of the system under varying conditions.

The entire stress-strain responses are compared at three different degrees of hydration, which are 44%, 58% and 90%, as shown in Figure 3.26. The cracks patterns in the final failure state are given in Figure 3.27. The two figures suggest that the paste behaves more brittle and microcracks are more localized at higher degree of hydration. The number of microcracks in the final failure state increases with the degree of hydration at early stage of hydration, and then decreases after the degree of hydration exceeds a certain level. The increase is because more and more solid phases are present in the microstructure, while the decrease is the
3.2 Influences of various factors

3.2.2 Cement fineness

The cement fineness can be indicated by the Blaine value. A higher Blaine value represents finer cement particles. The cement paste mixture in Table 3.1 is used and the cement fineness is varied at 210 m$^2$/kg, 420 m$^2$/kg and 600 m$^2$/kg respectively. The microstructures are simulated by the HYMOSTRUC3D model and then their mechanical properties are predicted by the 3D lattice fracture analysis. The local mechanical properties of individual solid phase are listed in Table 3.2.

The fineness of cement affects the hydration rate, i.e. finer cement hydrates faster, as shown in Table 3.12. Higher degree of hydration corresponds with lower porosity, higher Young’s modulus and higher tensile strength. The strains at peak load for these three microstructures are almost the same, around 0.2 %, which supports the findings from Figure 3.23. The fracture energy goes with cement fineness due to the fact that higher strength is reached at a higher degree of hydration at 28 days and the crack localization is not dominant yet, as shown in Figure 3.28.

It is also possible to compare the mechanical behavior of paste at the same degree of hydration instead of at the same curing age. The stress-strain response

![Figure 3.25: Relationship between the fracture energy and the porosity](image)

result of cracks localization.
3. CEMENT PASTE AT MICROSCALE

Figure 3.26: Influences of degree of hydration on the tensile stress-strain response

Figure 3.27: Influences of degree of hydration on the cracks pattern in the final failure state, corresponding with Figure 3.26
3.2 Influences of various factors

Table 3.12: Influences of cement fineness, compared at the same curing age of 28 days, all values are resulted from simulations

<table>
<thead>
<tr>
<th>Cement fineness (m²/kg)</th>
<th>210</th>
<th>420</th>
<th>600</th>
</tr>
</thead>
<tbody>
<tr>
<td>Degree of hydration</td>
<td>62 %</td>
<td>69 %</td>
<td>73 %</td>
</tr>
<tr>
<td>Porosity</td>
<td>15.0%</td>
<td>12.5%</td>
<td>11.1%</td>
</tr>
<tr>
<td>Young’s modulus $E$ (GPa)</td>
<td>11.0</td>
<td>12.9</td>
<td>14.3</td>
</tr>
<tr>
<td>Tensile strength $f_t$ (MPa)</td>
<td>14.9</td>
<td>20.3</td>
<td>28.2</td>
</tr>
<tr>
<td>Strain at peak load $\epsilon_p$</td>
<td>0.18%</td>
<td>0.18%</td>
<td>0.21%</td>
</tr>
<tr>
<td>Fracture energy $G_F$ (J/m²)</td>
<td>18.9</td>
<td>21.6</td>
<td>23.2</td>
</tr>
</tbody>
</table>

![Figure 3.28: Influences of cement fineness on the cracks pattern in the final failure state, compared at the same curing age of 28 days, corresponding with Table 3.12](image)

(a) Blaine=210 m²/kg (27847 microcracks)  
(b) Blaine=420 m²/kg (38106 microcracks)  
(c) Blaine=600 m²/kg (36810 microcracks)
3. CEMENT PASTE AT MICROSCALE

![Graph showing stress-strain response for different Blaine values](image)

**Figure 3.29:** Influences of cement fineness on the tensile stress-strain response, compared at the same degree of hydration 69%

Diagrams are given in Figure 3.29 for cement paste specimens with different cement fineness. The computed Young’s modulus is independent of the Blaine value. The tensile strength and fracture energy are higher for finer cement paste system, as it contains smaller but more particles to fill the gap between big particles. The cracks patterns in the final failure state are shown in Figure 3.30.

### 3.2.3 Water/cement ratio

The water/cement ratio of the cement paste mixture in Table 3.1 is varied at 0.3, 0.4 and 0.5 to study its influences on the mechanical properties of paste. The HYMOSTRUC3D model gives the microstructures, and then the 3D lattice fracture model evaluates the mechanical performance by simulating a uniaxial tensile test on the 100\(\mu\text{m}\) × 100\(\mu\text{m}\) × 100\(\mu\text{m}\) specimen, using the local mechanical properties of individual solid phases given in Table 3.2.

The water/cement ratio influences the hydration rate. A higher water/cement ratio speeds up the hydration process, as shown in Table 3.13. However, a higher degree of hydration does not result in lower porosity, because of the higher initial water/cement ratio. The change trend of Young’s modulus and tensile strength can be linked to the porosity. The strain at peak load is about 0.2%, which
3.2 Influences of various factors

(a) Blaine=210 m$^2$/kg (35932 microcracks)
(b) Blaine=420 m$^2$/kg (38106 microcracks)
(c) Blaine=600 m$^2$/kg (36579 microcracks)

Figure 3.30: Influences of cement fineness on the cracks pattern in the final failure state, compared at the same degree of hydration 69%, corresponding with Figure 3.29

supports the findings from Figure 3.23. The fracture energy decreases when the water/cement ratio increases, which is dominated by the decrease of the tensile strength. The cracks patterns at the same curing age of 28 days are shown in Figure 3.31. It is apparent that a more localized microcracks pattern is observed in the cement paste with lower water/cement ratio.

It is also possible to compare the mechanical performance of paste at the same degree of hydration, as given in Table 3.14. Higher water/cement ratio takes less time to reach the target degree of hydration 69%, and is accompanied by higher

Table 3.13: Influences of water/cement ratio, compared at the same curing age of 28 days

<table>
<thead>
<tr>
<th>Water/cement ratio</th>
<th>0.3</th>
<th>0.4</th>
<th>0.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Degree of hydration</td>
<td>65%</td>
<td>69%</td>
<td>75%</td>
</tr>
<tr>
<td>Porosity</td>
<td>3.2%</td>
<td>12.5%</td>
<td>20.1%</td>
</tr>
<tr>
<td>Young’s modulus $E$ (GPa)</td>
<td>23.4</td>
<td>12.9</td>
<td>7.0</td>
</tr>
<tr>
<td>Tensile strength $f_t$ (MPa)</td>
<td>42.1</td>
<td>20.3</td>
<td>10.6</td>
</tr>
<tr>
<td>Strain at peak load $\epsilon_p$</td>
<td>0.19%</td>
<td>0.18%</td>
<td>0.18%</td>
</tr>
<tr>
<td>Fracture energy $G_F$ (J/m$^2$)</td>
<td>23.1</td>
<td>21.6</td>
<td>12.3</td>
</tr>
</tbody>
</table>
3. CEMENT PASTE AT MICROSCALE

Figure 3.31: Influences of water/cement ratio on the cracks pattern in the final failure state, compared at the same curing age of 28 days, corresponding with Table 3.13.

porosity, lower Young’s modulus and tensile strength. The strains at peak load for the three cases are about the same, around 0.2 %, which supports the findings from Figure 3.23. The fracture energy is dependent on the strength and the number of microcracks in the final failure state. The water/cement ratio 0.4 produces more microcracks and thus requires the highest fracture energy among the three cases, although the strength is not the highest one. The stress-strain response diagrams are given in Figure 3.32. More brittle softening behavior is observed for the lower water/cement ratio system. The cracks patterns in the final failure state are given in Figure 3.33. It is observed that microcracks are more localized in the paste with lower water/cement ratio.

3.2.4 Mineral composition of cement

The hydration processes and products are dependent on the mineral composition of cement. Hence the mechanical performance of cement paste can be altered by changing the cement mineral composition. The ordinary Portland cement usually consists of $C_3S$, $C_2S$, $C_3A$ and $C_4AF$. Four special combinations are made to study the effect of $C_3S$ and $C_2S$ on the mechanical properties of cement paste, as given in Table 3.15. These special cements are produced in laboratory by Italcementi in Italy [42]. The particle size distributions are measured and then
3.2 Influences of various factors

Table 3.14: Influences of water/cement ratio, compared at the same degree of hydration 69%

<table>
<thead>
<tr>
<th>Water/cement ratio</th>
<th>0.3</th>
<th>0.4</th>
<th>0.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Curing age (h)</td>
<td>1262</td>
<td>635</td>
<td>402</td>
</tr>
<tr>
<td>Porosity</td>
<td>2.0%</td>
<td>12.5%</td>
<td>22.5%</td>
</tr>
<tr>
<td>Young’s modulus $E$ (GPa)</td>
<td>24.2</td>
<td>12.9</td>
<td>6.0</td>
</tr>
<tr>
<td>Tensile strength $f_t$ (MPa)</td>
<td>41.7</td>
<td>20.3</td>
<td>9.0</td>
</tr>
<tr>
<td>Strain at peak load $\epsilon_p$</td>
<td>0.19%</td>
<td>0.18%</td>
<td>0.18%</td>
</tr>
<tr>
<td>Fracture energy $G_F$ (J/m$^2$)</td>
<td>17.7</td>
<td>21.6</td>
<td>12.0</td>
</tr>
</tbody>
</table>

Figure 3.32: Influences of water/cement ratio on the tensile stress-strain response, compared at the same degree of hydration 69%, corresponding with Table 3.14
3. CEMENT PASTE AT MICROSCALE

(a) w/c=0.3 (30668 microcracks)
(b) w/c=0.4 (38106 microcracks)
(c) w/c=0.5 (15225 microcracks)

Figure 3.33: Influences of water/cement ratio on the cracks pattern in the final failure state, compared at the same degree of hydration 69%, corresponding with Figure 3.32

Table 3.15: Mineral compositions of the special cements

<table>
<thead>
<tr>
<th>Combination</th>
<th>$C_3S$</th>
<th>$C_2S$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a)</td>
<td>100%</td>
<td>0</td>
</tr>
<tr>
<td>(b)</td>
<td>70%</td>
<td>30%</td>
</tr>
<tr>
<td>(c)</td>
<td>30%</td>
<td>70%</td>
</tr>
<tr>
<td>(d)</td>
<td>0</td>
<td>100%</td>
</tr>
</tbody>
</table>

hydration tests are carried out by CSIC (Spanish National Research Council) in Spain \[43\]. Several batches of the special cements are measured and a Rosin-Rammler distribution $F(x) = 1 - e^{-bx^n}$ with $n = 1.014$ and $b = 0.0754$ is fitted, as shown in Figure 3.34. The corresponding Blaine value is 600 m$^2$/kg. The fitted curve will be used in the HYMOISTRUC3D model to simulate the microstructures of cement paste.

In the numerical experiment the water/cement ratio is 0.4 and the specimen size is 100\(\mu\)m $\times$ 100\(\mu\)m $\times$ 100\(\mu\)m. The initial microstructures of cement paste for the four combinations of mineral compositions are the same, because the same particle size distribution and water/cement ratio are applied, as shown in Figure 3.35.

The degrees of hydration are measured and simulated for the four combina-
3.2 Influences of various factors

Figure 3.34: Particle size distribution of the special cements

Figure 3.35: Initial microstructure of the special cement paste (porosity=56%)
3. CEMENT PASTE AT MICROSCALE

Table 3.16: Degree of hydration and phase segmentation for the special cement pastes at the curing age of 28 days, corresponding with Figure 3.37

<table>
<thead>
<tr>
<th>Combination</th>
<th>Degree of hydration</th>
<th>Pore</th>
<th>Unhydrated cement</th>
<th>Inner product</th>
<th>Outer product</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a)</td>
<td>79%</td>
<td>8%</td>
<td>9%</td>
<td>35%</td>
<td>48%</td>
</tr>
<tr>
<td>(b)</td>
<td>84%</td>
<td>6%</td>
<td>7%</td>
<td>37%</td>
<td>50%</td>
</tr>
<tr>
<td>(c)</td>
<td>68%</td>
<td>12%</td>
<td>14%</td>
<td>30%</td>
<td>44%</td>
</tr>
<tr>
<td>(d)</td>
<td>38%</td>
<td>30%</td>
<td>27%</td>
<td>17%</td>
<td>26%</td>
</tr>
</tbody>
</table>

The microstructures at the curing age of 28 days are taken for further analysis, as shown in Figure 3.37. The corresponding degree of hydration and phase segmentation are given in Table 3.16. It is observed that $C_3S$ hydrates faster than $C_2S$ by comparing the combination (a) and (d). However, the combination (b) hydrates faster than pure $C_3S$, even though it consists of some $C_2S$. This phenomenon can be explained by separating the hydrations of $C_3S$ and $C_2S$. The combination (b) can be obtained by replacing 30% $C_3S$ with $C_2S$ based on the combination (a). At 28 days the 30% $C_2S$ consumes less water than $C_3S$ as $C_2S$ hydrates slower, the effect is the 70% $C_3S$ could attract more water, thus its hydration process speeds up. The 30% $C_2S$ hydrates slower while the 70% $C_3S$ hydrates faster, the net effect is determined by the amount portions of $C_3S$ and $C_2S$. When the weight of $C_2S$ is increased to 70%, as shown in the combination (c), the hydration rate is decreased.

The 3D lattice fracture model is employed to evaluate the mechanical performance of the microstructures in Figure 3.37 through simulating a uniaxial tensile test. The local mechanical properties for individual solid phases are taken from Table 3.2. The resulting stress-strain response diagrams are shown in Figure 3.38. Some global mechanical properties are computed and summarized in Table 3.17 based on Figure 3.38. The microcracks in the final failure state are shown in Figure 3.39. The combination (b) has the best mechanical performance in terms of Young’s modulus and tensile strength, and the most localized cracks pattern, as its degree of hydration is the highest one among the four combinations. This suggests that the mineral composition of the ordinary Portland cement is already
3.2 Influences of various factors

Figure 3.36: Degree of hydration diagrams for the special cement pastes
3. CEMENT PASTE AT MICROSCALE

Figure 3.37: Microstructures of the special cement pastes at the curing age of 28 days
3.3 Summary

The microstructure of cement paste and its mechanical performance are studied numerically in detail in this chapter. The microstructure of cement paste can be obtained by the HYMOSTRUC3D computer modeling program, and/or by the experimental method of CT scan. The 3D lattice fracture model developed in Chapter 2 is employed to predict the mechanical properties and cracks propag-
3. CEMENT PASTE AT MICROSCALE

Figure 3.39: Cracks patterns in the final failure state for the special cement pastes at the curing age of 28 days, corresponding with Figure 3.38.
3.3 Summary

Table 3.17: Global mechanical properties of the special cement pastes at the curing age of 28 days, corresponding with Figure 3.38

<table>
<thead>
<tr>
<th>Combination</th>
<th>Young’s modulus $E$ (GPa)</th>
<th>Tensile strength $f_t$ (MPa)</th>
<th>Strain at peak load $\epsilon_p$</th>
<th>Fracture energy $G_F$ (J/m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a)</td>
<td>17</td>
<td>33</td>
<td>0.22%</td>
<td>22</td>
</tr>
<tr>
<td>(b)</td>
<td>18</td>
<td>37</td>
<td>0.22%</td>
<td>23</td>
</tr>
<tr>
<td>(c)</td>
<td>14</td>
<td>26</td>
<td>0.21%</td>
<td>26</td>
</tr>
<tr>
<td>(d)</td>
<td>4.2</td>
<td>7.9</td>
<td>0.33%</td>
<td>14</td>
</tr>
</tbody>
</table>

Simulation by simulating a uniaxial tensile test on the microstructure of cement paste at microscale. The influences of loading directions and mesh randomness are examined. The simulated mechanical properties of $100\mu m \times 100\mu m \times 100\mu m$ cement paste specimen are used as input properties for mesoscale modeling in Chapter 5.

Some factors, such as degree of hydration, cement fineness, water/cement ratio and mineral composition of cement were investigated to see their influences on the mechanical performance of cement paste at microscale. It turns out that better mechanical properties can be achieved with higher degree of hydration, finer cement and lower water/cement ratio, and the mineral composition of ordinary Portland cement is already an optimal combination. Both the Young’s modulus and the tensile strength increases linearly against the increase of degree of hydration, while the fracture energy increases first and then decreases during the hydration process. At the same degree of hydration the Young’s modulus is independent of the Blaine value, but the tensile strength and fracture energy are higher for finer cement paste system. The increase of water/cement ratio results in a decrease of Young’s modulus and tensile strength, while the fracture energy goes up first and then down if compared at the same degree of hydration. It is observed that the tensile strain at peak load for well developed cement paste is about 0.2% at microscale in the numerical experiments. It is also interesting to notice that the system with lowest porosity does not have the maximum capacity to absorb the energy during the fracture processes, thus planting some pores in the system may help to improve the fracture energy dissipation.
3. CEMENT PASTE AT MICROSCALE
Chapter 4

Mortar and Concrete at Mesoscale

Concrete is a kind of multiscale and multiphase heterogeneous construction material. Normal concrete is made from coarse aggregates (e.g. crushed stones, river gravels), fine aggregates (e.g. sands), cement and water. A chemical reaction starts immediately when water is mixed with cement, and reaction products are produced. The resulting cement paste keeps aggregates together and forms a system which is able to carry loads. Mortar consists of cement paste and sand, and concrete is composed of mortar and coarse aggregates. The relationship between cement paste, mortar and concrete is illustrated in Figure 4.1.

From the modeling point of view, the material mesostructures of both mortar and concrete can be represented by particles embedded in matrix material model, as shown in Figure 4.2. The particles are interpreted as sands, and the matrix

![Figure 4.1: Cement paste, mortar and concrete](image)
4. MORTAR AND CONCRETE AT MESOSCALE

Figure 4.2: Particles embedded matrix material model

as cement paste for mortar model, while the particles are coarse aggregates, and
the matrix is mortar in the concrete model. Hence it is achievable to make a
universal material mesostructure model for mortar and concrete. However, the
particle shape characterizations can be different for sands and coarse aggregates,
and furthermore they can even be different for different classes of sands or coarse
aggregates. This requires the universal material model to be able to recognize
various particle shape characterizations. It is pointed out by Garboczi that spher-
ical harmonics is a good mathematical tool to characterize the shape of particles
numerically, and the procedures to retrieve particle shape characterizations for a
given class of aggregates from CT (computed tomography) scanned digital im-
ages are also established [44]. The next step is to place multiple irregular shape
particles into a pre-defined empty container to build up a complete particles
embedded in matrix material model, which is elaborated in Section 4.1. An ap-
plication of the proposed material model is given in Section 4.2 for simulating
the mesostructures of mortar and concrete respectively.

4.1 Anm material model

There are many existing particles embedded in matrix material models [45 46,
47 48], most of which employ regular shape particles like spheres, ellipsoids, or
multi-faceted polyhedrons, as shown in Figure 4.3. However, the real particle
shapes are more complex and sometimes play an essential role. In this section
a material model with irregular shape particles is proposed, the Anm material
4.1 Anm material model

Figure 4.3: Spheres, ellipsoids and multi-faceted polyhedrons [http://wikipedia.org]

model, which is named after the fact that the particle shapes are described in terms of spherical harmonic expansion coefficients $a_{nm}$.

4.1.1 Irregular shape description

In mathematics an arbitrary 2D surface can be represented by a function $r(\theta, \phi)$ in the 3D spherical coordinate system as shown in Figure 4.4. The particle mass center is placed at the origin in the local coordinate system.

The function $r(\theta, \phi)$ might be difficult or even impossible to be expressed explicitly for complex shapes, but it can always be approximated by a summation of spherical harmonic functions for star-like shapes [49, 50, 51]. The spherical harmonic expansion is given in the equation (4.1),

$$r(\theta, \phi) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} a_{nm} Y_n^m(\theta, \phi)$$  \hspace{1cm} (4.1)

where $r(\theta, \phi)$ is any smooth function defined on the unit sphere ($0 \leq \theta \leq \pi, 0 \leq \phi < 2\pi$), $Y_n^m(\theta, \phi)$ is the spherical harmonic function and is given in the equation (4.2),

$$Y_n^m(\theta, \phi) = \sqrt{\frac{(2n+1)(n-m)!}{4\pi(n+m)!}} P_n^m(\cos \theta)e^{im\phi}$$  \hspace{1cm} (4.2)

in which $P_n^m(\cos \theta)$ is the associated Legendre polynomial, $i$ is the imaginary unit.
The first derivatives of the function $r(\theta, \phi)$ are involved in the expressions (4.25) and can be computed as follows,

$$
\begin{align*}
\frac{\partial r(\theta, \phi)}{\partial \theta} &= \sum_{n=0}^{\infty} \sum_{m=-n}^{n} a_{nm} \frac{\partial Y_m^n(\theta, \phi)}{\partial \theta} \\
\frac{\partial r(\theta, \phi)}{\partial \phi} &= \sum_{n=0}^{\infty} \sum_{m=-n}^{n} a_{nm} \frac{\partial Y_m^n(\theta, \phi)}{\partial \phi}
\end{align*}
$$

(4.3)

where the two derivatives of the spherical harmonic function $Y_m^n(\theta, \phi)$ can be computed as below,

$$
\begin{align*}
\frac{\partial Y_m^n(\theta, \phi)}{\partial \theta} &= \frac{1}{s} \left( n x Y_n^m(\theta, \phi) - \sqrt{(2n+1)(n^2-m^2)} Y_{n-1}^m(\theta, \phi) \right) \\
\frac{\partial Y_m^n(\theta, \phi)}{\partial \phi} &= im Y_n^m(\theta, \phi)
\end{align*}
$$

(4.4)

in which $x = \cos \theta$ and $s = \sqrt{1-x^2}$.

**Proof.** Here is the derivation about $\frac{\partial Y_m^n(\theta, \phi)}{\partial \theta}$ in the equation (4.4).

$$
(x^2 - 1) \frac{dP_n^m(x)}{dx} = nxP_n^m(x) - (n + m) P_{n-1}^m(x)
$$

(4.5)
let $x = \cos \theta$, $s = \sqrt{1 - x^2}$,

\[
\frac{dP_n^m(\cos \theta)}{d\theta} = \frac{dP_n^m(x)}{dx} \frac{dx}{d\theta} = -\sin \theta \frac{dP_n^m(x)}{dx}
\]

\[
= -\sin \theta \frac{nx P_n^m(x) - (n + m)P_{n-1}^m(x)}{x^2 - 1}
\]

\[
= -\sin \theta \frac{nx P_n^m(x) - (n + m)P_{n-1}^m(x)}{-s^2}
\]

\[
= \frac{nx}{s} P_n^m(x) - \frac{n + m}{s} P_{n-1}^m(x) \tag{4.6}
\]

\[
\therefore \quad \frac{\partial Y_n^m(\theta, \phi)}{\partial \theta} = \sqrt{\frac{(2n + 1)(n - m)!}{4\pi(n + m)!}} e^{im\phi} \frac{dP_n^m(\cos \theta)}{d\theta}
\]

\[
= \sqrt{\frac{(2n + 1)(n - m)!}{4\pi(n + m)!}} e^{im\phi} \left( \frac{nx}{s} P_n^m(x) - \frac{n + m}{s} P_{n-1}^m(x) \right)
\]

\[
= \frac{nx}{s} \sqrt{\frac{(2n + 1)(n - m)!}{4\pi(n + m)!}} P_n^m(x)e^{im\phi} - \frac{n + m}{s} \sqrt{\frac{(2n + 1)(n - m)}{(2n - 1)(n + m)}} P_{n-1}^m(x)e^{im\phi}
\]

\[
= \frac{nx}{s} Y_n^m(\theta, \phi) - \frac{1}{s} \sqrt{\frac{(2n + 1)(n^2 - m^2)}{2n - 1}} Y_{n-1}^m(\theta, \phi)
\]

\[
= \frac{1}{s} \left( nx Y_n^m(\theta, \phi) - \sqrt{\frac{(2n + 1)(n^2 - m^2)}{2n - 1}} Y_{n-1}^m(\theta, \phi) \right) \tag{4.7}
\]

Proof. Here is the derivation about $\frac{\partial Y_n^m(\theta, \phi)}{\partial \phi}$ in the equation 4.4.

\[
\frac{\partial Y_n^m(\theta, \phi)}{\partial \phi} = \sqrt{\frac{(2n + 1)(n - m)!}{4\pi(n + m)!}} P_n^m(\cos \theta)e^{im\phi}im
\]

\[
= imY_n^m(\theta, \phi) \tag{4.8}
\]

The particle shape is uniquely defined by a set of spherical harmonic coefficients $a_n^m$, which is a complex number. The data structure of the coefficients $a_n^m$ is shown in Figure 4.5 where $n$ is the degree and $m$ is the order.
4. MORTAR AND CONCRETE AT MESOSCALE

\[ n = 0 \quad a_{0,0} \]
\[ n = 1 \quad a_{1,-1} \quad a_{1,0} \quad a_{1,1} \]
\[ n = 2 \quad a_{2,-2} \quad a_{2,-1} \quad a_{2,0} \quad a_{2,1} \quad a_{2,2} \]
\[ \ldots \]
\[ m = -2 \quad m = -1 \quad m = 0 \quad m = 1 \quad m = 2 \]

**Figure 4.5:** Spherical harmonic coefficients data structure

**Figure 4.6:** An irregular shape particle described by spherical harmonics

The number of the coefficients up to the degree \( n \) is \((n + 1)^2\), and the index of the coefficient is \( n(n + 1) + m \). There should be sufficient coefficients involved in the spherical harmonic expansion to describe a shape accurately. The number of the coefficients required is dependent on the shape characterizations. As a general guideline, the degree \( n \) should be about 26 for common aggregates in mortar and concrete, thus the corresponding number of coefficients is about \((26 + 1)^2 = 729\). See [44] for more discussions on this aspect. An example irregular shape particle described in terms of spherical harmonic coefficients is shown in Figure 4.6.
4.1 Anm material model

4.1.2 Individual particle properties and operations

Many geometric properties of the particle shape can be computed once the spherical harmonic coefficients are known, including the particle volume, length, width and thickness. Length is the longest surface-surface distance in the particle, width is the longest surface-surface distance in the particle such that width is perpendicular to length, and thickness is the longest surface-surface distance in the particle such that thickness is perpendicular to both length and width [44]. A particle can be scaled by multiplying each coefficient with a scaling factor. The scaling factor $s$ is determined by the equation (4.9),

$$s = \frac{W_a}{W_b} \tag{4.9}$$

where $W_a$ is the particle width after scaling, and $W_b$ is the width before scaling. The particle volume will be also be scaled according to the equation (4.10),

$$V_a = s^3 V_b \tag{4.10}$$

where $V_a$ is the particle volume after scaling, and $V_b$ is the volume before scaling.

The operation of a rotation on the particle in the local coordinate system can be done by transforming the spherical harmonic expansion coefficients [50]. Denote the rotation Euler angles as $\alpha, \beta, \gamma$, then the new spherical harmonic coefficients after rotation can be determined by the equation (4.11),

$$a_{nm}^{new} = \sum_{m'=-n}^{n} a_{nm'} D_{m'm}^{(n)}(\alpha, \beta, \gamma) \tag{4.11}$$

where the complex number $D_{m'm}^{(n)}(\alpha, \beta, \gamma)$ is one element in the $(2n + 1) \times (2n + 1)$ square rotation matrix $D^{(n)}(\alpha, \beta, \gamma)$. The complex number $D_{m'm}^{(n)}(\alpha, \beta, \gamma)$ is computed according to the equation (4.12),

$$D_{m'm}^{(n)}(\alpha, \beta, \gamma) = e^{-im'\alpha} R_{m'm}^{(n)}(\beta) e^{-im\gamma} \tag{4.12}$$
4. MORTAR AND CONCRETE AT MESOSCALE

in which the $\beta$ dependant real number $d_{m'm'}^{(n)}(\beta)$ is calculated by the equation (4.13),

$$d_{m'm'}^{(n)}(\beta) = \sqrt{\frac{(n + m')!(n - m')!}{(n + m)!(n - m)!}} \min(n - m', n + m) \sum_{k = \max(0, m - m')} \left[ (-1)^{k + m' - m} \binom{n + m}{k} \binom{n - m}{n - m' - k} \right] \left( \frac{\cos \beta}{2} \right)^{2n + m - m' - 2k} \left( \frac{\sin \beta}{2} \right)^{2k + m' - m}$$ (4.13)

where the binomial notation $\binom{M}{N} = \frac{M!}{N!(M - N)!}$ applies.

4.1.3 Parking procedures and algorithms

In the Anm material model, the concept of particles embedded in matrix applies. An empty container is created to represent a specimen at the beginning, and then all the particles are placed one after another into this container, from the larger ones to smaller ones. It is good to start with the largest particles as it would be more difficult to place them if they were processed at a later stage. All the particles are separated into several sieve ranges according to the particle sizes indicated by the particle widths. The largest sieve range is processed first, a width within this sieve range is picked randomly and assigned to a particle which is chosen from the appropriate particle shape database. The particle shape database can be created for varying classes of powders and aggregates with the procedures proposed in [44]. An arbitrary rotation is performed on the particle to get rid of possible orientation bias, which might be introduced during the production of the particle shape database. After the rotation the particle is placed at a randomly chosen primary location in the specimen, and then the ghost locations are determined if any, depending on the type of the specimen boundary conditions and the position of the particle. See Subsection 4.1.4 for the details about periodic and non-periodic material boundaries. The primary particle and its ghost particles are checked against all the previously placed particles for overlap. If no overlap is detected, then the particle enters the simulation box successfully, otherwise it will be moved to a new randomly chosen location. The reassignment of the location is subject to a pre-defined maximum number of attempts. After the consecutive
4.1 Anm material model

failures reach the limit, the particle will be resized to another randomly selected width within the current sieve range, and then be thrown into the specimen following the same trial-and-error procedure. The particle size rescale is also subject to a pre-defined maximum number of attempts. If the rescales do not help, then the particle will be rotated again to have another orientation. If the problem still exits, then a new shape will be chosen from the particle shape database. In case the particle cannot find its position eventually, it may suggest there is no space available for new particles within the current sieve range. The next sieve range will be processed if no availability for the current sieve range is found, or all the particles within the current sieve range have already been placed. The above trial-and-error procedures are called parking procedures and are illustrated in Figure 4.7.

The key algorithm required in the parking procedures is to determine whether two particles overlap. This can be examined by formulating and solving contact equations. As shown in Figure 4.8, the mass center of the two particles are \( O_1(x_1, y_1, z_1) \) and \( O_2(x_2, y_2, z_2) \) respectively in a global coordinate system \( O(x, y, z) \). Two local coordinate systems are also defined and their origins are placed at \( O_1 \) and \( O_2 \) respectively. It is assumed that there is a contact point \( C(x_c, y_c, z_c) \), and its local coordinates are \( (\theta_{c1}, \phi_{c1}) \) and \( (\theta_{c2}, \phi_{c2}) \) respectively in the corresponding local coordinate system.

The contact point \( C \) is located on the surface of particle \( O_1 \), thus the following equations (4.14) should be satisfied,

\[
\begin{aligned}
x_c &= x_1 + r_1(\theta_{c1}, \phi_{c1}) \sin \theta_{c1} \cos \phi_{c1} \\
y_c &= y_1 + r_1(\theta_{c1}, \phi_{c1}) \sin \theta_{c1} \sin \phi_{c1} \\
z_c &= z_1 + r_1(\theta_{c1}, \phi_{c1}) \cos \theta_{c1}
\end{aligned}
\]

(4.14)

The contact point \( C \) is also located on the surface of particle \( O_2 \), thus the equations (4.15) should also be valid,

\[
\begin{aligned}
x_c &= x_2 + r_2(\theta_{c2}, \phi_{c2}) \sin \theta_{c2} \cos \phi_{c2} \\
y_c &= y_2 + r_2(\theta_{c2}, \phi_{c2}) \sin \theta_{c2} \sin \phi_{c2} \\
z_c &= z_2 + r_2(\theta_{c2}, \phi_{c2}) \cos \theta_{c2}
\end{aligned}
\]

(4.15)

The contact equations can be formulated by combining the equations (4.14) and


Figure 4.7: Flowchart of parking procedures

4. MORTAR AND CONCRETE AT MESOSCALE
4.1 Anm material model

Figure 4.8: Two particles overlap

\begin{align}
    x_1 + r_1(\theta_{c1}, \phi_{c1}) \sin \theta_{c1} \cos \phi_{c1} &= x_2 + r_2(\theta_{c2}, \phi_{c2}) \sin \theta_{c2} \cos \phi_{c2} \\
    y_1 + r_1(\theta_{c1}, \phi_{c1}) \sin \theta_{c1} \sin \phi_{c1} &= y_2 + r_2(\theta_{c2}, \phi_{c2}) \sin \theta_{c2} \sin \phi_{c2} \\
    z_1 + r_1(\theta_{c1}, \phi_{c1}) \cos \theta_{c1} &= z_2 + r_2(\theta_{c2}, \phi_{c2}) \cos \theta_{c2}
\end{align}

(4.16)

However, the equations (4.16) have four unknowns \( \theta_{c1}, \phi_{c1}, \theta_{c2}, \phi_{c2} \) but only three equations, which makes it unsolvable. The strategy to overcome this difficulty is to fix one of the four unknowns (e.g. \( \phi_{c2} \)) at pre-select values in the range of \([0, 2\pi]\), and then try to solve the three equations with the three unknowns \( \theta_{c1}, \phi_{c1}, \theta_{c2} \). If a solution is found, then it demonstrates that the contact point exits, and the two particles overlap. If no solution can be obtained for every selected value of \( \phi_{c2} \), then it may suggest that the contact point does not exist, thus there is no overlap between the two particles.

The number of select \( \phi_{c2} \) values should be sufficient, and it is recommend to take at least 20 different values evenly distributed in the range \([0, 2\pi]\) according to the following sequence (4.17),

\[ \phi_{c2} = \phi_{2d}, \phi_{2d} \pm \text{incremental(} \phi_{c2} \text{)}, \phi_{2d} \pm 2 \times \text{incremental(} \phi_{c2} \text{)} \ldots \]

(4.17)

where \( \phi_{2d} \) is the second entry in the direction vector \((\theta_{2d}, \phi_{2d})\) from particle \( O_2 \) to particle \( O_1 \) and can be determined by the equations (4.19) or (4.20).
4. MORTAR AND CONCRETE AT MESOSCALE

The direction vector \((\theta_{1d}, \phi_{1d})\) from particle \(O_1\) to particle \(O_2\) can be determined by solving the following equations (4.18),

\[
\begin{align*}
  x_2 - x_1 &= d \sin \theta_{1d} \cos \phi_{1d} \\
  y_2 - y_1 &= d \sin \theta_{1d} \sin \phi_{1d} \\
  z_2 - z_1 &= d \cos \theta_{1d}
\end{align*}
\]  

Similarly the direction vector \((\theta_{2d}, \phi_{2d})\) from particle \(O_2\) to particle \(O_1\) can be determined by solving the following equations (4.19),

\[
\begin{align*}
  x_1 - x_2 &= d \sin \theta_{2d} \cos \phi_{2d} \\
  y_1 - y_2 &= d \sin \theta_{2d} \sin \phi_{2d} \\
  z_1 - z_2 &= d \cos \theta_{2d}
\end{align*}
\]

where \(d = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2}\)

Alternatively the direction vector \((\theta_{2d}, \phi_{2d})\) can also be determined by the equations (4.20),

\[
\begin{align*}
  \theta_{2d} &= \pi - \theta_{1d} \\
  \phi_{2d} &= \phi_{1d} \pm \pi \ 	ext{(take the sign which makes \(\phi_{2d}\) in the range of \([0, 2\pi]\))} \tag{4.20}
\end{align*}
\]

The contact equations (4.16) can be re-arranged as

\[
\begin{align*}
  F(\theta_{c1}, \phi_{c1}, \theta_{c2}) &= 0 \\
  G(\theta_{c1}, \phi_{c1}, \theta_{c2}) &= 0 \\
  H(\theta_{c1}, \phi_{c1}, \theta_{c2}) &= 0 \tag{4.21}
\end{align*}
\]

in which

\[
\begin{align*}
  F(\theta_{c1}, \phi_{c1}, \theta_{c2}) &= r_1(\theta_{c1}, \phi_{c1}) \sin \theta_{c1} \cos \phi_{c1} - r_2(\theta_{c2}, \phi_{c2}) \sin \theta_{c2} \cos \phi_{c2} + x_1 - x_2 \\
  G(\theta_{c1}, \phi_{c1}, \theta_{c2}) &= r_1(\theta_{c1}, \phi_{c1}) \sin \theta_{c1} \sin \phi_{c1} - r_2(\theta_{c2}, \phi_{c2}) \sin \theta_{c2} \sin \phi_{c2} + y_1 - y_2 \\
  H(\theta_{c1}, \phi_{c1}, \theta_{c2}) &= r_1(\theta_{c1}, \phi_{c1}) \cos \theta_{c1} - r_2(\theta_{c2}, \phi_{c2}) \cos \theta_{c2} + z_1 - z_2
\end{align*}
\]

The contact equations (4.21) are non-linear equations and can be solved by Newton-Raphson iteration method. In the Newton-Raphson iteration scheme, an initial guess of the solution \((\theta_{c1}, \phi_{c1}, \theta_{c2})\) should be given and then it gets updated after every iteration step until it is close enough to the real solution, as shown in Figure 4.9.

A good initial guess can speed up the convergence. It is suggested that the direction vectors \((\theta_{1d}, \phi_{1d})\) and \((\theta_{2d}, \phi_{2d})\), which connect the two particle centers,
4.1 Anm material model

Initial guess

\[ \theta_1^{(0)}, \phi_1^{(0)}, \theta_2^{(0)} \]

Newton-Raphson iteration step 1

\[ \theta_1^{(1)}, \phi_1^{(1)}, \theta_2^{(1)} \]

Newton-Raphson iteration step 2

\[ \theta_1^{(2)}, \phi_1^{(2)}, \theta_2^{(2)} \]

Newton-Raphson iteration step 3

\[ \theta_1^{(3)}, \phi_1^{(3)}, \theta_2^{(3)} \]

... ... ... ...

Figure 4.9: Newton-Raphson iteration scheme

can be taken as the initial guess of the solution, that is,

\[
\begin{align*}
\theta_1^{(0)} &= \theta_{1d} \\
\phi_1^{(0)} &= \phi_{1d} \\
\theta_2^{(0)} &= \theta_{2d}
\end{align*}
\]

(4.22)

The iteration formulas are

\[
\begin{align*}
\theta_1^{(i)} &= \theta_1^{(i-1)} + h^{(i)} \\
\phi_1^{(i)} &= \phi_1^{(i-1)} + k^{(i)} \\
\theta_2^{(i)} &= \theta_2^{(i-1)} + l^{(i)}
\end{align*}
\]

(4.23)

where \( h^{(i)}, k^{(i)}, l^{(i)} \) are the corrections at the \( i \)th iteration step and must satisfy the following three linear equations,

\[
\begin{bmatrix}
\frac{\partial F}{\partial \theta_1^{(i-1)}} & \frac{\partial F}{\partial \phi_1^{(i-1)}} & \frac{\partial F}{\partial \theta_2^{(i-1)}} \\
\frac{\partial G}{\partial \theta_1^{(i-1)}} & \frac{\partial G}{\partial \phi_1^{(i-1)}} & \frac{\partial G}{\partial \theta_2^{(i-1)}} \\
\frac{\partial H}{\partial \theta_1^{(i-1)}} & \frac{\partial H}{\partial \phi_1^{(i-1)}} & \frac{\partial H}{\partial \theta_2^{(i-1)}} \\
\end{bmatrix}^{(i-1)} \begin{bmatrix} h^{(i)} \\ k^{(i)} \\ l^{(i)} \end{bmatrix} = \begin{bmatrix} -F(\theta_1^{(i-1)}, \phi_1^{(i-1)}, \theta_2^{(i-1)}) \\ -G(\theta_1^{(i-1)}, \phi_1^{(i-1)}, \theta_2^{(i-1)}) \\ -H(\theta_1^{(i-1)}, \phi_1^{(i-1)}, \theta_2^{(i-1)}) \end{bmatrix}^{(i-1)}
\]

(4.24)

where the derivatives of the functions \( F(\theta_1, \phi_1, \theta_2), G(\theta_1, \phi_1, \theta_2), H(\theta_1, \phi_1, \theta_2) \)
with respect to the variables $\theta_{c1}, \phi_{c1}, \theta_{c2}$ can be computed as following,

\[
\begin{align*}
\frac{\partial F(\theta_{c1}, \phi_{c1}, \theta_{c2})}{\partial \theta_{c1}} &= \cos \phi_{c1} \left( \sin \theta_{c1} \frac{\partial r_1(\theta_{c1}, \phi_{c1})}{\partial \theta_{c1}} + r_1(\theta_{c1}, \phi_{c1}) \cos \theta_{c1} \right) \\
\frac{\partial F(\theta_{c1}, \phi_{c1}, \theta_{c2})}{\partial \phi_{c1}} &= \sin \theta_{c1} \left( \cos \phi_{c1} \frac{\partial r_1(\theta_{c1}, \phi_{c1})}{\partial \phi_{c1}} - r_1(\theta_{c1}, \phi_{c1}) \sin \phi_{c1} \right) \\
\frac{\partial F(\theta_{c1}, \phi_{c1}, \theta_{c2})}{\partial \theta_{c2}} &= -\cos \phi_{c2} \left( \sin \theta_{c2} \frac{\partial r_2(\theta_{c2}, \phi_{c2})}{\partial \theta_{c2}} + r_2(\theta_{c2}, \phi_{c2}) \cos \theta_{c2} \right) \\
\frac{\partial G(\theta_{c1}, \phi_{c1}, \theta_{c2})}{\partial \theta_{c1}} &= \sin \phi_{c1} \left( \sin \theta_{c1} \frac{\partial r_1(\theta_{c1}, \phi_{c1})}{\partial \theta_{c1}} + r_1(\theta_{c1}, \phi_{c1}) \cos \theta_{c1} \right) \\
\frac{\partial G(\theta_{c1}, \phi_{c1}, \theta_{c2})}{\partial \phi_{c1}} &= \sin \theta_{c1} \left( \cos \phi_{c1} \frac{\partial r_1(\theta_{c1}, \phi_{c1})}{\partial \phi_{c1}} + r_1(\theta_{c1}, \phi_{c1}) \sin \phi_{c1} \right) \\
\frac{\partial G(\theta_{c1}, \phi_{c1}, \theta_{c2})}{\partial \theta_{c2}} &= -\sin \phi_{c2} \left( \sin \theta_{c2} \frac{\partial r_2(\theta_{c2}, \phi_{c2})}{\partial \theta_{c2}} + r_2(\theta_{c2}, \phi_{c2}) \cos \theta_{c2} \right) \\
\frac{\partial H(\theta_{c1}, \phi_{c1}, \theta_{c2})}{\partial \theta_{c1}} &= \cos \theta_{c1} \left( \cos \phi_{c1} \frac{\partial r_1(\theta_{c1}, \phi_{c1})}{\partial \theta_{c1}} - r_1(\theta_{c1}, \phi_{c1}) \sin \theta_{c1} \right) \\
\frac{\partial H(\theta_{c1}, \phi_{c1}, \theta_{c2})}{\partial \phi_{c1}} &= \cos \theta_{c1} \left( \sin \phi_{c1} \frac{\partial r_1(\theta_{c1}, \phi_{c1})}{\partial \phi_{c1}} \right) \\
\frac{\partial H(\theta_{c1}, \phi_{c1}, \theta_{c2})}{\partial \theta_{c2}} &= -\cos \theta_{c2} \left( \cos \phi_{c2} \frac{\partial r_2(\theta_{c2}, \phi_{c2})}{\partial \theta_{c2}} + r_2(\theta_{c2}, \phi_{c2}) \cos \theta_{c2} \right)
\end{align*}
\]

in which the functions $r_1(\theta_{c1}, \phi_{c1})$ and $r_2(\theta_{c2}, \phi_{c2})$, that represent the shapes of particle $O_1$ and particle $O_2$ respectively, can be computed by the equation (4.1), and the first derivatives by the formulas (4.3).

### 4.1.4 Periodic and non-periodic material boundaries

In mathematical models and computer simulations, periodic boundary conditions are a set of boundary conditions that are often used to simulate a large system by modeling a small part that is far from its edge [http://en.wikipedia.org/wiki/Periodic_boundary_conditions](http://en.wikipedia.org/wiki/Periodic_boundary_conditions). In the Anm material model, both periodic and non-periodic boundary conditions are implemented. The periodic boundary permits a particle to pass through the surface of the simulation box and the part outside the simulation box is put on the opposite surface, while the non-periodic boundary does not allow a particle to pass through the surface of the simulation box, as shown in Figure 4.10. In the specimen with periodic boundary conditions, if a particle passes through a surface, then it generates one mirroring
4.2 Material mesostructures for mortar and concrete

Concrete is a kind of heterogeneous materials with multiple phases at multiple scales. Normal concrete usually consists of hardened cement paste and aggregates like sands and stones. A normal concrete mix is given in Table 4.1 and it will be used to simulate the material mesostructures for mortar and concrete by the Anm material model.

In the simulations, the concrete specimen is a cube of the dimension 150 mm, consisting of two phases: mortar and crushed stones. The mortar specimen is in the shape of a cube at the size 10 mm and consists of two phases: cement paste and uncrushed sands. The sizes of the specimens are taken at least 2.5 times larger than the largest aggregate [52].

4.2.1 Mortar mesostructure

The mesostructure of mortar is simulated for a cubic specimen of the size 10 mm and it is represented by sand particles embedded in cement paste matrix. Periodic
4. MORTAR AND CONCRETE AT MESOSCALE

**Table 4.1: A normal concrete mix**

<table>
<thead>
<tr>
<th>Material</th>
<th>Mass Density (kg/m³)</th>
<th>Grading:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crushed stones (≥ 4 mm)</td>
<td>786</td>
<td></td>
</tr>
<tr>
<td>Uncrushed sands (&lt; 4 mm)</td>
<td>983</td>
<td></td>
</tr>
<tr>
<td>Cement</td>
<td>463</td>
<td>[8, 16] mm</td>
</tr>
<tr>
<td>Water</td>
<td>185</td>
<td>[4, 8] mm</td>
</tr>
<tr>
<td>Concrete mass density</td>
<td>2417</td>
<td>[2, 4] mm</td>
</tr>
<tr>
<td>Water/cement ratio</td>
<td>0.4</td>
<td>[1, 2] mm</td>
</tr>
<tr>
<td>Stone and sand mass density</td>
<td>2650</td>
<td>[0.25, 0.5] mm</td>
</tr>
<tr>
<td>Cement mass density</td>
<td>3150</td>
<td>[0.125, 0.25] mm</td>
</tr>
</tbody>
</table>

**Table 4.2: Particle size sieve ranges for the sands in mortar**

<table>
<thead>
<tr>
<th>Sieve ranges</th>
<th>Mass percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>[2, 4] mm</td>
<td>27%</td>
</tr>
<tr>
<td>[1, 2] mm</td>
<td>26%</td>
</tr>
<tr>
<td>[0.5, 1] mm</td>
<td>19%</td>
</tr>
<tr>
<td>[0.25, 0.5] mm</td>
<td>16%</td>
</tr>
<tr>
<td>[0.125, 0.25] mm</td>
<td>12%</td>
</tr>
</tbody>
</table>

material boundary condition is employed, which mirrors the sticking out particles onto the opposite surfaces. The total mass of the sands used in the mortar specimen is 1.397 g, the corresponding volume of which is 527 mm³ and takes up 52.7% space of the specimen. The size of the sand particles are indicated by the width and varies from 0.125 mm to 4 mm. The particle size distribution is given in Figure 4.11 and summarized in Table 4.2 in terms of sieve ranges.

The Anm material model parks all the sand particles into the empty simulation box with periodic material boundaries one after one, making sure that there is no overlap between any of the two particles. The resulting mesostructure of the 10 mm cubic mortar specimen with irregular shape sand particles is sketched in Figure 4.12.

### 4.2.2 Concrete mesostructure

Concrete specimen of the size 150 mm in the cubic shape is simulated. The specimen has two phases, the mortar matrix and crushed stone aggregates. Non-periodic material boundary applies, which requires all the particles are inside the
4.2 Material mesostructures for mortar and concrete

![Figure 4.11: Particle size distribution for the sands in mortar](image1)

**Figure 4.11:** Particle size distribution for the sands in mortar

![Figure 4.12: The mesostructure of the mortar specimen with irregular shape sand particles](image2)

**Figure 4.12:** The mesostructure of the mortar specimen with irregular shape sand particles
4. MORTAR AND CONCRETE AT MESOSCALE

Figure 4.13: Particle size distribution for the coarse aggregates in concrete

specimen and no part of a particle can pass through a surface. The total mass of the crushed stones is 2653 g, and 64% of which are in the sieve [8, 16)mm, the rest 36% are in the sieve [4, 8)mm. The particle size is taken as the particle width and its distribution for the coarse aggregates is given in Figure 4.13. The volume percentage of the crushed stones in the concrete specimen is 30%. The simulated mesostructure of the concrete specimen with irregular shape crushed stones is sketched in Figure 4.14.

4.3 Summary

In this chapter an innovative material model is proposed to simulate the material structures of cementitious materials: the Anm material model. In mathematics any arbitrary shape can be represented in terms of spherical harmonic coefficients $a_{nm}$. Sands in mortar or stones in concrete can be regarded as irregular shape particles in a matrix. The shapes of a class of aggregate can be captured by CT scan, and then discretized by spherical harmonic expansion. The characteristics of shapes represented by $a_{nm}$ are stored in a shape database. The material structure can be reproduced by parking multiple particles with the appropriate shape characteristics into an empty container, and the parking algorithm is the key to
Figure 4.14: The mesostructure of the concrete specimen with irregular shape crushed stones

work it out. Both periodic and non-periodic material boundaries are implemented in the Ann material model. The mesostructures of mortar and concrete are simulated in this chapter and further analyzed for the mechanical performance in Chapter 5.
4. MORTAR AND CONCRETE AT MESOSCALE
Chapter 5

Multiscale Modeling

Cement-based materials, such as cement paste, mortar and concrete, are multiscale heterogeneous construction materials. Two types of multiscale modeling problems are addressed in this chapter, for the cement paste only but at different sizes, and for the integrated system of cement paste, mortar and concrete at different scales. Section 5.1 discusses the parameter-passing scheme, and then it is applied to link the micromechanical model to the mesomechanical model of cement paste. Section 5.2 bridges the scales among cement paste, mortar and concrete by employing the parameter-passing scheme and the domain decomposition technique.

5.1 Parameter-passing scheme and size effect of cement paste

Crack localization occurs during the fracture processes of hardened cement paste and influences its mechanical behaviors. The phenomenon is observed in laboratory and must be reproduced in numerical experiments. This section attempts to answer some questions arising from the fracture processes of hardened cement paste and to study its mechanical performance using multiscale modeling approach. Uniaxial tensile tests are simulated at microscale and mesoscale respectively, by employing the 3D lattice fracture model. The two scales are seamlessly connected, and the simulated output properties of cement paste from microscale
5. MULTISCALE MODELING

modeling are used as the input properties for the mesoscale modeling, thus the parameter-passing multiscale modeling scheme is established, as illustrated in Figure 5.1.

The cement paste specimens are in the shape of a cube, and the side length is 100$\mu$m with mesh size 1$\mu$m at microscale and 7 mm with mesh size 0.1 mm at mesoscale. Hence, the length 100$\mu$m is the point which connects the microscale model to the mesoscale model. At microscale the sphere-based model is employed to represent the microstructure of cement paste, but at mesoscale the cement paste is modeled as continuum material with some heterogeneity, which is implemented during the lattice network construction by introducing some geometry randomness. The method to determine the randomness is suggested in Subsection 2.2.1 on Page 110. It is assumed that the material behaves linear-brittle locally at microscale, while some softening is allowed locally at mesoscale and is determined by the output of the microscale model.

---

**Figure 5.1:** Parameter-passing multiscale modeling scheme
At microscale the microstructure of cement paste is simulated by the hydration and microstructure formation model HYMOSTRUC3D with the specifications in Table 3.1. The microstructure at the curing age of 28 days is taken to evaluate its global mechanical properties, using the linear-brittle local mechanical properties given in Table 3.2 as input. The simulated tensile stress-strain response of the 100µm × 100µm × 100µm specimen is shown in Figure 3.9, from which the softening behavior is observed. Seven points are picked up from this stress-strain diagram to form a multi-linear curve to approximate the original non-linear one, as shown in Figure 5.2. The multi-linear curve is served as the input local mechanical properties for mesoscale modeling. The points should be chosen in such a way that makes the change of input properties gradual in terms of Young’s modulus and tensile strength, as listed in Table 5.1.

At mesoscale a uniaxial tensile test is simulated on the specimen of the size 7 mm × 7 mm × 7 mm, with a mesh size 0.1 mm. The randomness of the quadrangular lattice network is 0.5 for all the non-boundary cells, and it is 0 for all the cells located at the surfaces. The irregular geometry of the mesh introduces some numerical heterogeneity into the system. All the lattice elements share the same local mechanical properties, which originate from the microscale simulation, as given in Table 5.1. The simulated stress-strain response for the
5. MULTISCALE MODELING

Table 5.1: Mechanical properties of the cement paste specimen of the size 100\(\mu\)m \(\times\) 100\(\mu\)m \(\times\) 100\(\mu\)m, corresponding with Figure 5.2

<table>
<thead>
<tr>
<th>Point</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus (E) (MPa)</td>
<td>12846</td>
<td>11096</td>
<td>7601</td>
<td>3627</td>
<td>1590</td>
<td>611</td>
<td>87</td>
</tr>
<tr>
<td>Shear modulus (G) (MPa)</td>
<td>5265</td>
<td>4548</td>
<td>3115</td>
<td>1486</td>
<td>652</td>
<td>250</td>
<td>36</td>
</tr>
<tr>
<td>Tensile strength (f_t) (MPa)</td>
<td>10</td>
<td>20</td>
<td>18.6</td>
<td>15.1</td>
<td>10.3</td>
<td>5.4</td>
<td>2.7</td>
</tr>
</tbody>
</table>

Figure 5.3: Simulated stress-strain response for the 7 mm \(\times\) 7 mm \(\times\) 7 mm specimen of cement paste at mesoscale

7 mm \(\times\) 7 mm \(\times\) 7 mm specimen is shown in Figure 5.3. Some mechanical properties are computed based on the stress-strain diagram and given in Table 5.2. Table 5.2 shows the size effect of cement paste that the Young’s modulus and tensile strength are dependent on the specimen size, the larger the specimen is, the smaller Young’s modulus and tensile strength are. The snap back behavior is observed for the 7 mm \(\times\) 7 mm \(\times\) 7 mm specimen as shown in Figure 5.3, while post-peak softening occurs for the 100\(\mu\)m \(\times\) 100\(\mu\)m \(\times\) 100\(\mu\)m specimen as shown in Figure 3.9. One should be aware that the setting of the randomness affects the simulated global mechanical performance. For more details reference is made to Table 2.4. It is also possible to eliminate the elastic deformation from Figure 5.3 to get the stress crack opening diagram, as shown in Figure 5.4.
5.1 Parameter-passing scheme and size effect of cement paste

Table 5.2: Simulated mechanical properties for cement paste at microscale and mesoscale respectively

<table>
<thead>
<tr>
<th>Specimen size</th>
<th>Young's modulus $E$ (GPa)</th>
<th>Tensile strength $f_t$ (MPa)</th>
<th>Strain at peak load $\epsilon_p$</th>
<th>Fracture energy $G_F$ (J/m$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>100µm $\times$ 100µm $\times$ 100µm</td>
<td>13</td>
<td>20</td>
<td>0.18%</td>
<td>22</td>
</tr>
<tr>
<td>7 mm $\times$ 7 mm $\times$ 7 mm</td>
<td>11</td>
<td>16</td>
<td>0.17%</td>
<td>24</td>
</tr>
</tbody>
</table>

Figure 5.4: Simulated stress crack opening diagram for the 7 mm $\times$ 7 mm $\times$ 7 mm specimen of cement paste at mesoscale
5. MULTISCALE MODELING

Figure 5.5: Affected lattice elements during the fracture processes in the cement paste specimen of the size $7 \text{ mm} \times 7 \text{ mm} \times 7 \text{ mm}$ at mesoscale

The fracture processes can be identified as three stages marked as stage A, B and C in Figure 5.4. In stage A almost all the lattice elements along the loading direction are strengthened, as shown in Figure 5.5(a), the local tensile strength of which jumps from 10 MPa to 20 MPa while the local Young’s modulus decreases a little bit from 12 846 MPa to 11 096 MPa, following the path defined in Table 5.1. During stage B some of the strengthened lattice elements are weakened, as shown in Figure 5.5(b), the local tensile strength and Young’s modulus of which turn smaller. In stage C cracks start to localize after the peak and eventually make the specimen fail, as shown in Figure 5.5(c).

5.2 Bridging scales among cement paste, mortar and concrete

Concrete is a type of widely used multiphase heterogeneous construction materials, and it usually consists of hardened cement paste and aggregates such as sands and stones. A normal concrete mix is given in Table 4.1 and it is used to simulate the microstructure of cement paste by the HYMOSTRUC3D model and the material mesostructures of mortar and concrete by the Anm material model respectively. The specimens at the curing age of 28 days are taken for the mechanical performance evaluation through the parameter-passing scheme. The scale division is given in Table 5.3. Some conditions need to be satisfied when
5.2 Bridging scales among cement paste, mortar and concrete

<table>
<thead>
<tr>
<th>Table 5.3: Scale division and specifications of the specimens</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
</tr>
<tr>
<td>Specimen size</td>
</tr>
<tr>
<td>Mesh size</td>
</tr>
<tr>
<td>Minimum particle size</td>
</tr>
<tr>
<td>Maximum particle size</td>
</tr>
</tbody>
</table>

determining the scale division. It is suggested that the specimen size should be at least 2.5 times larger than the largest particle [52], and the mesh size should be smaller than the smallest particle. The connecting length between cement paste and mortar is 100 µm, thus the upscaling can be done seamlessly as demonstrated in Subsection [5.2.1]. However, there is some length scale overlap between mortar and concrete, and domain decomposition technique is employed to solve this problem, which will be elaborated in Subsection [5.2.1] and [5.2.2].

5.2.1 Connecting cement paste to mortar

The microstructure of a 100 µm × 100 µm × 100 µm cement paste specimen at the curing age of 28 days is simulated by the HYMOSTRUC3D model, as shown in Subsection [3.1.1] and then its tensile mechanical performance is evaluated by the 3D lattice fracture analysis, as demonstrated in Subsection [3.1.2]. The resulting stress-strain curve is approximated by a multi-linear curve as shown in Figure [5.2]. The multi-linear curve is used as the input mechanical properties of cement paste for the mortar properties prediction at mesoscale, as given in Table [5.1].

The mesostructure of mortar of the size 10 mm × 10 mm × 10 mm is simulated by the Anm material model as shown in Subsection [4.2.1]. The resulting mesostructure in Figure [4.12] is then digitized to facilitate the subsequent lattice network construction. In the mesostructure of mortar, two solid phases are presented, namely cement paste and sand. The lattice mesh size is 0.1 mm as shown in Figure [5.6], making sure that the properties of cement paste can be passed to mesoscale modeling seamlessly from microscale modeling. Three types of lattice elements are defined during the lattice network mesh, which represent sand (uncrushed US sand C109), cement paste and interface respectively. The local mechanical properties are given in Table [5.4].
5. MULTISCALE MODELING

**Figure 5.6**: Lattice mesh for the $10\text{ mm} \times 10\text{ mm} \times 10\text{ mm}$ mortar at mesoscale

<table>
<thead>
<tr>
<th>No</th>
<th>Element type</th>
<th>Young’s modulus $E$ (GPa)</th>
<th>Shear modulus $G$ (GPa)</th>
<th>Tensile strength $f_t$ (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Sand (uncrushed)</td>
<td>70</td>
<td>29</td>
<td>24</td>
</tr>
<tr>
<td>2</td>
<td>Cement paste</td>
<td>multi-linear, see Table 5.1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>Interface</td>
<td>22</td>
<td>8.9</td>
<td>0.75</td>
</tr>
</tbody>
</table>
5.2 Bridging scales among cement paste, mortar and concrete

Figure 5.7: Simulated Young’s modulus and tensile strength of every block in the 10 mm × 10 mm × 10 mm mortar at mesoscale

The lattice system in Figure 5.6 is decomposed to a network of blocks. The size of a single block is 1 mm × 1 mm × 1 mm, thus there are 10 blocks per direction in the original lattice system and in total 1000 blocks. Uniaxial tensile tests are simulated on these blocks one after one, using the local mechanical properties in Table 5.4. The resulting mechanical responses are scattered as the material structures of blocks may differ a lot. The simulated Young’s modulus and tensile strength of every block are shown in Figure 5.7.

The simulated Young’s modulus of a 1 mm × 1 mm × 1 mm block is in the range of 17 ∼ 65 GPa and averaged at 29 GPa. The tensile strength is in the range of 1.1 ∼ 19.5 MPa and averaged at 5.8 MPa. The stress-strain responses of these blocks are randomly passed onto concrete mesomechanical modeling and served as inputs there, as elaborated in Subsection 5.2.2.

5.2.2 Upscaling mortar to concrete

Domain decomposition technique is employed for the upscaling from mortar to concrete, due to the length scale overlap between them, as indicated in Table 5.3. The mortar specimen of 10 mm × 10 mm × 10 mm is decomposed into a network of 1 mm × 1 mm × 1 mm blocks, and then these blocks are evaluated by the 3D lattice fracture model one after one to get stress-strain responses, as demonstrated in Subsection 5.2.1.
Having obtained the mechanical properties of the 1 mm × 1 mm × 1 mm mortar blocks, it is ready to proceed with the concrete mesomechanical modeling. The mesostructure of concrete is simulated by the Anm material model, as presented in Subsection 4.2.2. A small piece of concrete of the size 40 mm × 40 mm × 40 mm is cut out from the original simulated 150 mm × 150 mm × 150 mm concrete specimen at its center, as shown in Figure 5.8. The 40 mm × 40 mm × 40 mm concrete specimen is then digitized at the resolution of 1 mm, and consists of two solid phases namely stone and mortar. A lattice network is constructed based on the digital concrete specimen, and three types of lattice elements are identified, which represent crushed stone, mortar and interface respectively, as shown in Figure 5.9. The local mechanical properties are given in Table 5.5. The properties of the lattice elements representing mortar are varied according to the simulation results of 1 mm × 1 mm × 1 mm mortar blocks.

A uniaxial tensile test is simulated on the lattice system meshed from the 40 mm × 40 mm × 40 mm concrete specimen as shown in Figure 5.9, using the local mechanical properties listed in Table 5.5. The resulting stress-strain response
5.2 Bridging scales among cement paste, mortar and concrete

Figure 5.9: Lattice mesh for the 40 mm $\times$ 40 mm $\times$ 40 mm concrete at mesoscale

Table 5.5: Local mechanical properties of stone, mortar and interface elements in concrete at mesoscale

<table>
<thead>
<tr>
<th>No</th>
<th>Element type</th>
<th>Young’s modulus $E$ (GPa)</th>
<th>Shear modulus $G$ (GPa)</th>
<th>Tensile strength $f_t$ (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Stone (crushed)</td>
<td>70</td>
<td>29</td>
<td>24</td>
</tr>
<tr>
<td>2</td>
<td>Mortar</td>
<td>multi-linear and varied based on the 1 mm $\times$ 1 mm $\times$ 1 mm mortar blocks</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>Interface</td>
<td>41</td>
<td>17</td>
<td>1</td>
</tr>
</tbody>
</table>
Figure 5.10: Simulated stress-strain response for the 40 mm $\times$ 40 mm $\times$ 40 mm concrete at mesoscale

Table 5.6: Simulated mechanical properties of concrete at mesoscale, corresponding with Figure 5.10

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus ($E$) (GPa)</td>
<td>31</td>
</tr>
<tr>
<td>Tensile strength ($f_t$) (MPa)</td>
<td>1.8</td>
</tr>
<tr>
<td>Strain at peak load ($\epsilon_p$)</td>
<td>0.04%</td>
</tr>
<tr>
<td>Fracture energy ($G_F$) (J/m$^2$)</td>
<td>127</td>
</tr>
</tbody>
</table>

is presented in Figure 5.10 and some mechanical properties can be computed as given in Table 5.6. The simulated stress crack opening diagram is shown in Figure 5.11.

The pattern of the simulated stress-strain response of 40 mm $\times$ 40 mm $\times$ 40 mm concrete is similar to the one observed in laboratory, and the mechanical properties computed from the stress-strain diagram are also located within the reasonable range.

5.3 Summary

In this chapter, the parameter-passing multiscale modeling scheme is established and applied to address two types of multiscale modeling problems respectively: for the cement paste only but at different sizes, and for the integrated system of cement paste, mortar and concrete at different scales. Domain decomposi-
Figure 5.11: Simulated stress crack opening diagram for the 40 mm × 40 mm × 40 mm concrete at mesoscale

tion technique is employed to solve the length scale overlap between mortar and concrete. The material structures of cement paste, mortar and concrete are simulated by the HYMOSTRUC3D model and the Anm material model respectively, in Chapter 3 and Chapter 4. The 3D lattice fracture model is used to evaluate their mechanical performance by simulating a uniaxial tensile test. The simulated output properties at lower scale are passed onto higher scale to serve as input local properties. Thus a fully multiscale lattice fracture analysis is performed. The final simulation results at mesoscale seem to be reasonable and realistic, and must be further verified by experiments in laboratory in future. The combination of the 3D lattice fracture model and the parameter-passing scheme enables the study on cement-based materials through a fully multiscale approach, which is proved to be a successful initiative in this chapter.
5. MULTISCALE MODELING
Chapter 6

Conclusions and Outlook

6.1 Conclusions

A parameter-passing multiscale modeling scheme is established in this thesis to study the fracture processes in cementitious materials, and to predict the mechanical performance, cracks pattern and propagation. The cement paste is investigated at the length scale $1 \sim 100 \mu m$, mortar at $0.1 \sim 10 \text{ mm}$ and concrete at $1 \sim 40 \text{ mm}$. Microstructure of cement paste is simulated by the HYMOSTRUC3D model, and mesostructures of mortar and concrete are simulated by the Anm material model respectively, and then they are evaluated for the mechanical properties by the 3D lattice fracture model. The upscaling between cement paste and mortar is done seamlessly at $100 \mu m$, while the domain decomposition technique is employed to solve the length scale overlap $1 \sim 10 \text{ mm}$ between mortar and concrete.

The 3D lattice fracture model is discussed in detail. The lattice network may be constructed according to the ImgLat scheme or the HymLat scheme, depending on whether the material structure is given in terms of voxels or spheres. Irregular random mesh can be applied, and the extra randomness reduces the simulated mechanical performance as artificial heterogeneity is introduced by making the geometry of lattice network irregular. The random seed does not have too much influence on the computed output properties. The influence of boundary conditions (glued or clamped) on the uniaxial tensile behavior can be
neglected, provided that the Poisson’s ratio of the specimen is close to 0, otherwise the influences are considerable.

The combined application of the HYMOSTRUC3D model and the 3D lattice fracture analysis makes it possible to study the individual influences of several factors on the mechanical performance of cement paste, such as the degree of hydration, cement fineness, water/cement ratio and mineral composition of cement. The cement paste is stronger at higher degree of hydration with finer cement and lower water/cement ratio. The study reveals that the mineral composition of ordinary Portland cement is already optimal. The 3D lattice fracture model also works with experimental microstructures of cement paste obtained by CT scan.

The mesostructures of mortar and concrete can be represented by particles embedded in matrix model. The Anm material model is proposed and implemented to park multiple irregular particles together into an empty container, thus it is possible to simulate a realistic mesostructure of mortar or concrete when the aggregate shape characteristics are available. Both periodic and non-periodic material boundaries can be used.

The size effect of cement paste is investigated using the parameter-passing multiscale modeling approach. It is found that the Young’s modulus and tensile strength decrease when the size of the specimen increases.

A complete example is given to demonstrate the multiscale modeling of fracture processes in cementitious materials, starting from 1 µm cement paste at microscale and ending with 40 mm concrete at mesoscale. The pattern of the simulated stress-strain response of the 40 mm × 40 mm × 40 mm numerical concrete is similar to the one observed in laboratory, and the mechanical properties computed from the stress-strain diagram are also within the reasonable range. This is a positive support for the multiscale modeling procedures used in this thesis, and the validity of the material parameters employed in this example.

The highlights in this thesis include the parallel implementation of 3D lattice fracture model, the development of the Anm material model and the application of parameter-passing multiscale modeling scheme for cementitious materials. The parallel computation of 3D lattice fracture analysis improves the computing efficiency and makes the modeling of very large lattice system practical. The Anm material model can generate a virtual material structure with realistic aggregate
shapes, which provides a more accurate microstructure for the further mechanical performance evaluation. Permeability analysis may also benefit from this improved material model. The successful application of parameter-passing multiscale modeling scheme for cementitious materials enables the communication among cement paste, mortar and concrete.

6.2 Outlook

The starting point of the multiscale fracture simulations is the microstructure of hardened cement paste at the microscale. It is assumed that the local mechanical properties are brittle at this scale. This is an arbitrary assumption. The properties at this scale are difficult to measure experimentally and therefore there is no proof yet for this assumption of brittle behavior at microscale. Perhaps it is necessary to go to nanoscale or even to atomistic scale to have real local brittle behavior. But at least it seems reasonable to assume that the behavior becomes more brittle at lower scale.

At microscale the local mechanical properties can be determined with the help of nanoindentation test. The test gives local stiffness and hardness, which is related to tensile strength of the components. No absolute values of the tensile strength can be measured directly by the test, but the tensile strength ratios of the components can be obtained. Therefore the tensile strength values of the components at the microscale used in this paper are based on assumptions, only the tensile strength ratio comes from the nanoindentation hardness values.

The real tensile strength values can be corrected after simulations on a level (mesoscale or macroscale) where mechanical tests can be performed easily. At microscale some attempts are done to do mechanical tests on the composite. However, the sample preparation and the boundary conditions in the tests may cause many problems which prevent obtaining reliable results.

The multiscale model will be adopted in the future to simulate fracture at multiple scales in different geometries. An experimental campaign is started at Delft University of Technology to perform tests on different levels, starting from different original materials to be able to validate the procedure further and to obtain more proof for the assumed local material properties.
References


REFERENCES


REFERENCES


REFERENCES


Propositions

1. Upscaling is a man-made challenge, hence, a good solution is to reduce the number of scales.

2. No two particles have exactly the same shape in the real world, thus neither do in the Anm material model (irregular shape particle parking model).

3. Since lattice approach is a bridge between continuum and discretization, it is (potentially) applicable to model fracture, repair and self-healing processes.

4. The purpose of computing is insight, not numbers. (R.W. Hamming)

5. ... but for the student, numbers are often the best road to insight. (A. Ralston)

6. We can’t solve problems by using the same kind of thinking we used when we created them. (A. Einstein)

7. Some problems are solved, but more problems are created, by a PhD research.

8. The future is unpredictable, but can be shaped.

9. Failing to plan is planning to fail. (A. Lakein)

10. If the human brain were so simple that we could understand it, we would be so simple that we couldn’t. (E.M. Pugh)

These propositions are regarded as opposable and defendable, and have been approved as such by the promotors Prof.dr.ir. K. van Breugel and Prof.dr.ir. E. Schlangen.
Stellingen

1. Opschalen is een door de mens verzonden uitdaging, derhalve zou het goed zijn om het aantal schalen te verminderen.

2. Geen enkele twee korrels hebben een identieke vorm in de echte wereld, dus ook in het Anm materiaal model (model voor parkeren van korrels met onregelmatige vorm) zijn alle korrels verschillend.

3. Omdat de lattice aanpak een brug is tussen continuüm en discretisatie, is deze (mogelijk) toepasbaar om breuk-, reparatie- en zelfherstellingsprocessen te modelleren.

4. Het doel van berekenen is het verkrijgen van inzicht, niet getallen. (R.W. Hamming)

5. ... maar voor de student zijn getallen vaak de beste weg voor het verkrijgen van inzicht. (A. Ralston)

6. We kunnen problemen niet oplossen door het volgen van dezelfde denkwijze als bij het creëren van de problemen. (A. Einstein)

7. Sommige problemen zijn opgelost, maar meer problemen ontstaan bij een promotieonderzoek.

8. De toekomst is onvoorspelbaar maar kan worden vormgegeven.

9. Falen om het plannen is plannen om te falen. (A. Lakein)

10. Als het menselijk brein eenvoudig genoeg was om te begrijpen, waren wij te eenvoudig om het te kunnen begrijpen. (E.M. Pugh)

   *Deze stellingen worden opponeerbaar en verdedigbaar geacht en zijn als zodanig goedgekeurd door de promotoren Prof.dr.ir. K. van Breugel en Prof.dr.ir. E. Schlangen.*
Declaration

I herewith declare that I have produced this thesis without the prohibited assistance of third parties and without making use of aids other than those specified; notions taken over directly or indirectly from other sources have been identified as such. This thesis has not previously been presented in identical or similar form to any other Dutch or foreign examination board.

The thesis work was conducted from May 2008 to May 2012 under the supervision of Prof.dr.ir. Klaas van Breugel and Prof.dr.ir. Erik Schlangen at Delft University of Technology.

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Delft, the Netherlands

May 2012
Publications


[16] Zhiwei Qian, Erik Schlangen, Guang Ye, and Klaas van Breugel. Parallel implementation of three-dimensional lattice fracture analysis on a distributed


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