

DOCTORAL THESIS

A study of optimised network flows
for prediction of force transmission
and crack propagation in bonded
granular media

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Declaration

This is to certify that

- (i) the thesis comprises only my original work towards the PhD except where indicate,
- (ii) due acknowledgement has been made in the text to all other material used,
- (iii) the thesis is less than 80,000 words in length, exclusive of tables, maps, bibliographies and appendices.

Sanath Kagahalage

Abstract

This thesis focuses on study bonded granular materials. We mainly analyse discrete element method simulation data for unconfined concrete specimens subjected to uniaxial tension and compression. In these systems, the contacts can support compressive, tensile and shear forces. Thus, under applied loads, a member grain can transmit tensile and/or compressive forces to its neighbours resulting in a highly heterogeneous contact force network.

The objective of this thesis is two-fold. The first objective of this thesis is to develop algorithms for the identification and characterisation of two classes of force transmission patterns in these systems: (a) force chains, (b) force (energy) bottlenecks. The former comprises a subgroup of grains that transmit the majority of the load through the sample, while the latter comprises a subgroup of contacts that are prone to force congestion and damage. These two classes are related and coevolve as loading history proceeds. Here this coevolution is characterised quantitatively to gain new insights into the interdependence between force transmission and failure in bonded grain assemblies.

The second objective of this thesis is to establish the extent to which the ultimate (dominant) crack location can be predicted early in the prefailure regime for disordered and heterogeneous bonded granular media based on known microstructural features. To achieve this, a new data-driven model is developed within the framework of Network Flow Theory which takes as input data on contact network and contact strengths. We tested this model for a range of samples undergoing quasibrittle failure subject to various loading conditions (i.e., uniaxial tension, uniaxial compression) as well as field-scale data for an open-pit mine. In all cases, the location of the ultimate (primary) macrocrack/failure zone is predicted early in the prefailure regime as well as those of other secondary cracks.

We uncovered an optimised force transmission and damage propagation in the pre-failure regime, especially by using data from uniaxial tension tests on concrete samples. Tensile force chains emerged in routes that can transmit the global transmission capacity of the contact network through the shortest transmission pathways. Macrocracks developed along with force/energy bottlenecks. We brought some of the commonly used optimisation based fracture criteria into a single framework and showed how heterogeneity and disorder in the contact network affect the prediction.

List of publications

Journal Articles

TORDESILLAS, A., KAHAGALAGE, S., RAS, C., NITKA, M. & TEJCHMAN, J. 2020 Coupled evolution of preferential paths for force and damage in the pre-failure regime in disordered and heterogeneous, quasi-brittle granular materials. *Frontiers in Materials* **7**, 79.

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TORDESILLAS, A., KAHAGALAGE, S., CAMPBELL, L., BELLETT, P., BATTERHAM, R. & LI, J. 2020 A slope stability analytics (SStaics) framework for complex granular systems: from laboratory to field scale. *Scientific Reports*. (in draft)

KAHAGALAGE, S., RAS, C., TORDESILLAS, A., NITKA, M. & TEJCHMAN, J. 2020 A source-sink independent maximum flow method for predicting crack patterns in bonded granular materials. *Engineering Fracture Mechanics* (in draft)

Conference papers

KAHAGALAGE, S., TORDESILLAS, A., NITKA, M. & TEJCHMAN, J. 2016 Emergence of cracks along force bottlenecks in a cementitious granular material. *Third SM² Meeting, the University of Melbourne, Parkville, Australia, 28–29, November*.

KAHAGALAGE, S., TORDESILLAS, A., NITKA, M. & TEJCHMAN, J. 2017 Of cuts and cracks: data analytics on constrained graphs for early prediction of failure in cementitious materials. *Powders and Grains 2017 – 8th International Conference on Micromechanics on Granular Media, Montpellier, France, 3–7 July*.

TORDESILLAS, A., KAHAGALAGE, S., NITKA, M. & TEJCHMAN, J. 2019 Inter-dependent evolution of robustness, force transmission and damage in a heterogeneous quasi-brittle granular material: from suppressed to cascading failure. *The 2019 EMI International Conference, INSA Lyon, Villeurbanne, France, 3–5, July*.

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Nomenclature

Roman symbols

Symbol	Description
a	area of the path Γ
A	a set of arcs
A_b	the bond (contact) area
B_{min}	minimum edge cut
$\mathcal{C}$	actual path of the ultimate macrocrack
$B(\mathcal{F}_E)$	the bottleneck of the energy flow network $\mathcal{F}_E$
$B(\mathcal{F}_F)$	the bottleneck of the force flow network $\mathcal{F}_F$
$B(\bar{\mathcal{F}}_E)$	the bottleneck of the residual energy flow network $\bar{\mathcal{F}}_E$
$B(\bar{\mathcal{F}}_F)$	the bottleneck of the residual force flow network $\bar{\mathcal{F}}_F$
B^*	the primary force bottleneck
$B_8(B_{32})$	the secondary force bottleneck in 1T (3T)
b	demand function
b_v	demand of v
c	cost function
c_e	cost of e
C	a cost function (objective function)
E	Young's elastic modulus
$E_{res}(\Gamma)$	residual capacity of Γ
$E_r(e)$	realised energy of edge e
$E_{strain}(\mathcal{N} \setminus \Gamma, \epsilon)$	the sum of elastic strain energies stored at all the contacts in $\mathcal{N}$ excluding those in the virtual path (cut) Γ at loading stage ϵ
$E_{tot}(\Gamma, \epsilon)$	the total energy of body Ω at loading stage ϵ

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Symbol	Description
e	a edge in E corresponding to a bond in $\mathcal{N}$
$\mathcal{F}$	a flow network
$\mathcal{F}_1$	flow network with unit capacity function
$\mathcal{F}_C$	flow network with uniform capacity function
$\mathcal{F}_E$	energy flow network
$\bar{\mathcal{F}}$	residual flow network
$\mathcal{F}_F$	force flow network
$\bar{\mathcal{F}}_E$	residual energy flow network
$\bar{\mathcal{F}}_F$	residual force flow network
$F_{min}^n(e)$	fracture strength of bond or edge e
$\vec{F}_n$	tensile normal force
G	a directed network
m	the final time stage of loading
$\mathcal{N}$	the bonded contact network
$\mathcal{P}$	optimized flow routes
P_e	the percentage error of prediction
p_{min}	pathway redundancy
q	capacity function
$q(B(\mathcal{F}))$	capacity of the bottleneck $B(\mathcal{F})$
$q(e)$	capacity of e
$q_F(e)$	force capacity (bond strength) of e
$q_E(e)$	energy capacity (fracture surface energy) of e
$\bar{q}_F(e)$	residual force capacity of e
$\bar{q}_E(e)$	residual energy capacity of e
$q(\delta^+(S))$	capacity of $\delta^+(S)$
$r = r_{min}$	the radius of the smaller of the two grains sharing the bond
r_A, r_B	the radii of the two grains sharing the bond
r_Γ	ratio of number of grains in the smallest component to the largest component corresponds to cut Γ

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Symbol	Description
$\mathbb{R}$	Real numbers
$\mathbb{R}_0^+$	non negative real numbers
R_{re}	Reroute score
$S(\Gamma)$	set of saturated edges in Γ
s	a source (supersource) node
t	a sink (supersink) node
$T_n(e)$	minimum normal tensile stress of bond or edge e
U	total strain energy
$U(e, \epsilon)$	the potential energy of bond or edge e at loading stage ϵ
V	a set of nodes
v	a node
V_{B_u}	set of grains in the upper part of the bottleneck
$V_{\mathcal{C}_u}$	set of grains in the upper part of the macrocrack
V_T	all the grains in the sample
x	feasible (s, t) -flow, feasible (S, T) -flow
$x(e)$	flow of edge e
$x_E(e)$	realised energy flow of edge e
$x_F(e)$	realised force flow of edge e
$x(\Gamma)$	total flow across Γ

Greek symbols

Symbol	Description
α	number of replacement links to which flow is diverted
ϵ	time stage
β	number of links that cease to be part of $\mathcal{P}$
Γ	an arbitrary, feasible crack path (cut) in $\mathcal{N}$
Γ_{min}	a minimum cut in $\mathcal{N}$
Γ_{max}	a maximum cut in $\mathcal{N}$
$\gamma(e)$	Griffith fracture surface energy of edge e
$\gamma(\Gamma)$	the Griffith fracture surface energy for path (cut) Γ
$\hat{\gamma}(\Gamma)$	the Griffith fracture surface energy density for path Γ

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Symbol	Description
$ \Delta u $	magnitude of relative displacement corresponds to two grains (pixels) in contact
$\delta^-(v)$	arcs entering node v
$\delta^+(v)$	arcs leaving node v
$\delta^-(s)$	arcs entering the source or supersource s
$\delta^+(s)$	arcs leaving the source or supersource s
$\delta^+(S)$	cut of G induced by S
σ_Γ	the normal stress for a path Γ
ρ	ratio of the number of links in $\mathcal{P}$ relative to its value prior to damage
$\Theta(\Gamma)$	the energy release rate at Γ

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1. Introduction

1.1. Complex bonded granular materials and failure

Granular materials are common in everyday life. They are collections of distinct particles or grains which interact with each other and give rise to complex and often unpredictable mechanical behaviour. This thesis focuses on the characterisation and modelling of failure for a specific class of these materials, namely, *granular composite materials* (Figure 1.1). These comprise grains which individually exhibit different constitutive and/or geometric properties as well as being bonded together at their contacts. Many important everyday examples of these include rocks, ceramics, concrete, asphalt, as well as various food products like sugar cubes, granola bars, rocky road, etc.

This thesis focuses on a subclass of granular composite materials which are known for their strength, namely, concrete and rocks (Wriggers & Moftah 2006; Hilal 2016; Prayogo *et al.* 2017). Concrete is the most widely used man-made composite material and is composed of coarse aggregates bonded together with cement. Cement is a granular material consisting of small particles (Ok *et al.* 2007). Rocks, being a natural material, consists of several minerals bonded together with chemical bonds (Fairchild & Baker 2012). In general, concrete and rocks share two things in common: both are disordered and heterogeneous (Figure 1.1 (a)). The former means microstructure deviates from the crystal structure, i.e., the connectivity is not regular (Potyondy & Cundall 2004). This is mainly due to the aggregate particles in concrete is larger in size compared to the cement matrix grains. This results in more cement matrix grains attached to aggregate particles while less connection between cement matrix grains (Figure 1.2). The latter means the material properties vary from point to point (Van Mier 2012). This is mainly due to the different properties of concrete mixture and the connectivity. In particular cement-cement contacts are more stronger than other contacts (Van Mier 1996).

A beneficial consequence of disorder and heterogeneity in concrete and rocks is their robustness to damage (Daniel *et al.* 2019). That is, they can withstand certain levels of internal damage (cracks, fissures etc.) before they fail globally (Vu *et al.* 2019). As can be seen from Figure 1.3, many buildings, roads, bridges, and other supporting structures, including those found in nature like rocks, contain cracks and fractures and yet are still in everyday use. Due to their robustness to damage, these materials are essential to the building and construction of cities and associated infrastructure. They are heavily used in building and construction of footings, foundations, columns, beams,

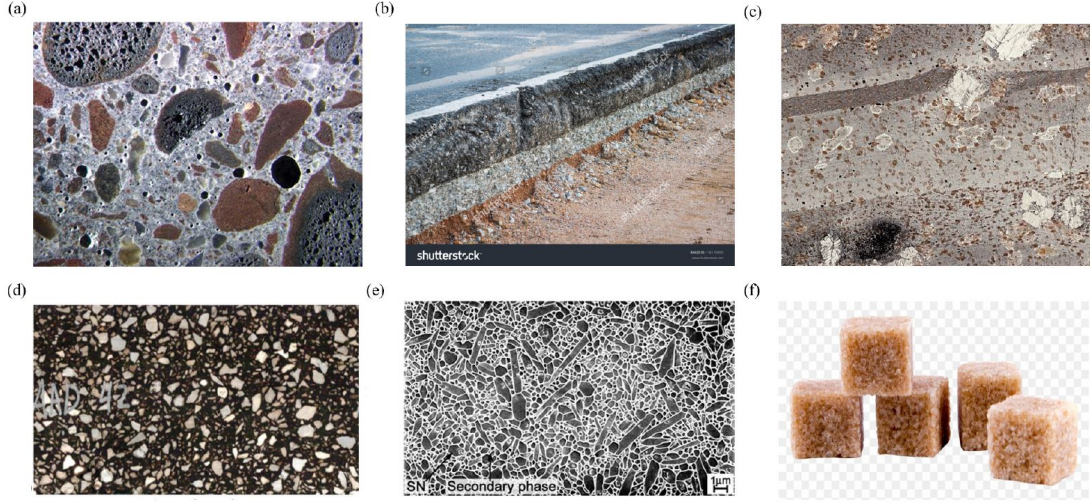


Figure 1.1.: *Disordered and heterogeneous bonded granular materials.* (a) A microstructure of concrete ^a. (b) A cross-section of a road ^b. (c) A microstructure of a rock ^c. (d) A microstructure of asphalt (Zhang et al. 2011). (e) A microstructure of ceramic ^d. (f) Sugar cubes ^e.

^a<https://www.structuremag.org/?p=1163>

^b<https://avopix.com/premium-photo/116119399-shutterstock-layer-of-aspha>

^chttps://www.earth.ox.ac.uk/~davewa/research/kinetics/ispet/ispet_case2.html

^dhttp://www.keramverband.de/brevier_engl/3/4/3/3_4_3_2.html

^ehttps://favpng.com/png_view/sugar-chocolate-brownie-brown-sugar-sugar-cubes-png/ig1cfntA

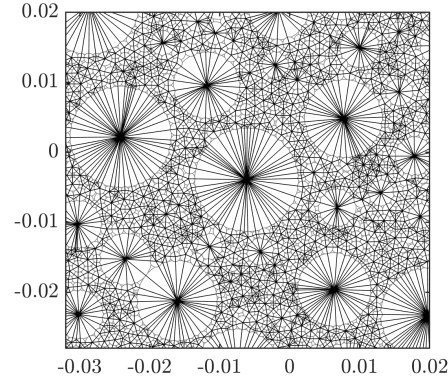


Figure 1.2.: Grain size distribution causes disordered and heterogeneous contact network. Zoomed in image of the contact network (black links) with actual size distribution of grains (grey outlined circle) for 3-phase tension sample at stage 1. The data set was provided to our group by Dr Michał Nitka and Prof Jacek Tejchman.

slabs, roads and bridges, tunnels etc. In some applications, like in the mining, energy, oil and gas industries, rocks are what support buildings, heavy equipment and vehicles. Consequently, the failure of these materials can lead to significant damage to property, human life, economy, environment, and social stability (Chen & Cao 2014) (Figure 1.4). It is therefore important to understand the conditions under which these materials fail,

how they fail, and whether or not their failure can be predicted sufficiently early for mitigative and preventative action to be taken (Gu *et al.* 2013; Yin *et al.* 2015). To this end, this research is focused on developing methods for characterisation and modelling that can help answer these questions.

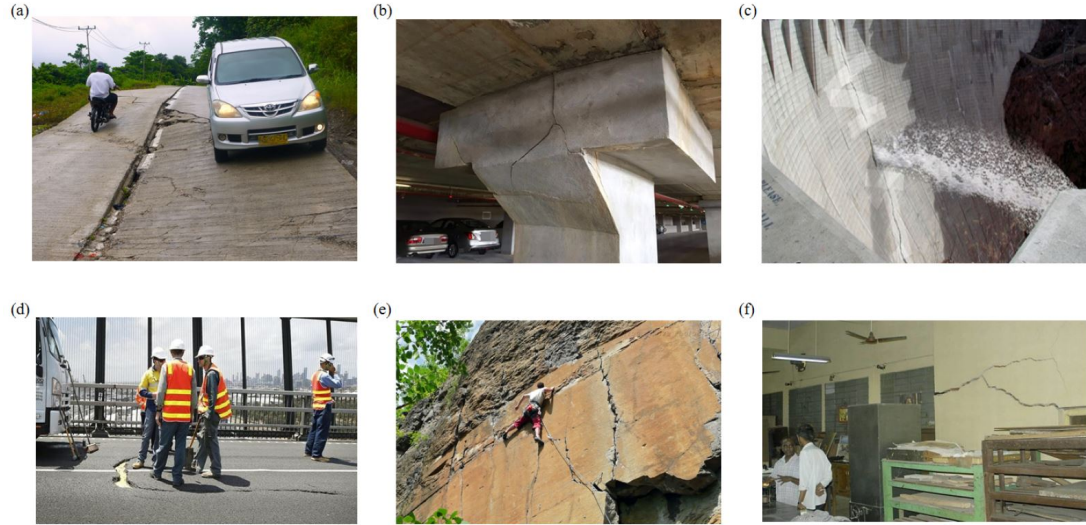


Figure 1.3.: *Complex bonded granular materials are robust and can withstand certain amount of damage before catastrophic failure. Figures show that some structures contain cracks, yet are still in use. (a) Cracks on a road ^a. (b) Cracks in a supporting structure ^b. (c) A crack on a dam ^c. (d) A large crack found on West Gate Bridge, Melbourne ^d. (e) Crack climbing ^e. (f) Cracks in a building ^f.*

^a<https://www.jcu.edu.au/news/releases/2017/october/many-planned-tropical-roads-shouldnt-be-built,-concludes-major-study>

^b<https://images.app.goo.gl/1TbzyShaR2jmqdGCA>

^c<https://treevalley.files.wordpress.com/2012/12/crack-in-dam.jpeg>

^d<https://cdn.newsapi.com.au/image/v1/f70b942806624b11f25b28eed19c93df?width=650>

^e<http://fromaboveblog.com/crack-climbing-slovakia/>

^f<https://gosmartbricks.com/reasons-cracks-in-buildings/>

Another reason why it is important to understand the failure of these materials is that it can teach us how to design more sustainable building materials with potentially improved robustness and resistance to failure, especially under hazardous conditions such as an earthquake (Wang & Adeli 2014; Arya *et al.* 2014). Sustainable structures are not only environmentally friendly but they may also lead to lower costs of construction. The classical engineering designs are conservative in nature and incorporates a high safety factor to compensate for various uncertainties in design and operational conditions (Rao 2017). Generally, this means that more raw materials are used than required and/or wasted. Ultimately, this means more harm to the environment (Yeo & Gabbai 2011; Foraboschi *et al.* 2014) not to mention cost to society.

The potential benefits of a better understanding of failure in concrete and rocks are significant. In the state of Victoria alone, the cost of maintaining roads and bridges

is significant. According to VicRoads ¹ “The West Gate Bridge maintenance is part of more than \$870 million invested in road maintenance over the next two years and is part of a record amount of work being carried out on Victoria’s Big Build over the summer months.” Mathematical models are important in achieving this, especially those that can deliver an early prediction of the initiation and propagation of cracks on road pavements (Wiyono 2012). As discussed in Ko & Ni 2005, early detection of cracks is essential in prioritising road maintenance and repair. Cracks are the most common manifestation of damage in infrastructure systems like roadways and bridges (Gavilán *et al.* 2011). However, cracks often initiate and develop internally before they reach the surface where they become visible. Once they become visible, it may be too late to take any preventive action. Hence methods to detect internal cracks are employed: the feature from the embedded ultrasonic signals is used to determine the changes in the whole structure of reinforced concrete (Chakraborty *et al.* 2019); a computer simulation model to predict expected changes of road pavement in future (Wiyono 2012); visual inspection of sequence of infrared images (Wang *et al.* 2018). However, if we have a way to predict the location of the crack before they manifest, then we can even minimise the maintenance cost.

There is also the immeasurable cost to human life and livelihoods when a catastrophic failure occurs in the structures built with these materials. In Australia, we pride ourselves in our mineral resources. The mining industry contributes around 9% to Australia’s economy and employs nearly 140,000 workers annually ². Australia currently has around 14 open-pit mines ³, producing coal, gold, copper, uranium, zinc, lead, silver and other precious minerals. A major hazard encountered in open-pit mining are rockfalls and landslides. Mitigating and managing these events are very important since these collapses can lead to fatalities, mine closure and hence loss of livelihood for not just the staff and their families but also the many communities and townships that depend on this industry (Kitula 2006; Kossoff *et al.* 2014; Pankow *et al.* 2014).

1.2. Challenges of understanding and predicting failure of disordered and heterogeneous quasibrittle granular composites

Although concrete and rocks are commonly used materials, our understanding of their failure remains limited even to this day (Baker & Karihaloo 1994; Qu *et al.* 2016). Fundamentally, these materials belong to the broad class of so-called quasibrittle materials which fail by fracture (cracks) as opposed to plastic deformation as seen in ductile gran-

¹<https://transport.vic.gov.au/about/transport-news/news-archive/post-christmas-closures-on-west-gate-bridge>

²https://en.wikipedia.org/wiki/Economy_of_Australia

³https://en.wikipedia.org/wiki/List_of_open-pit_mines#Australia

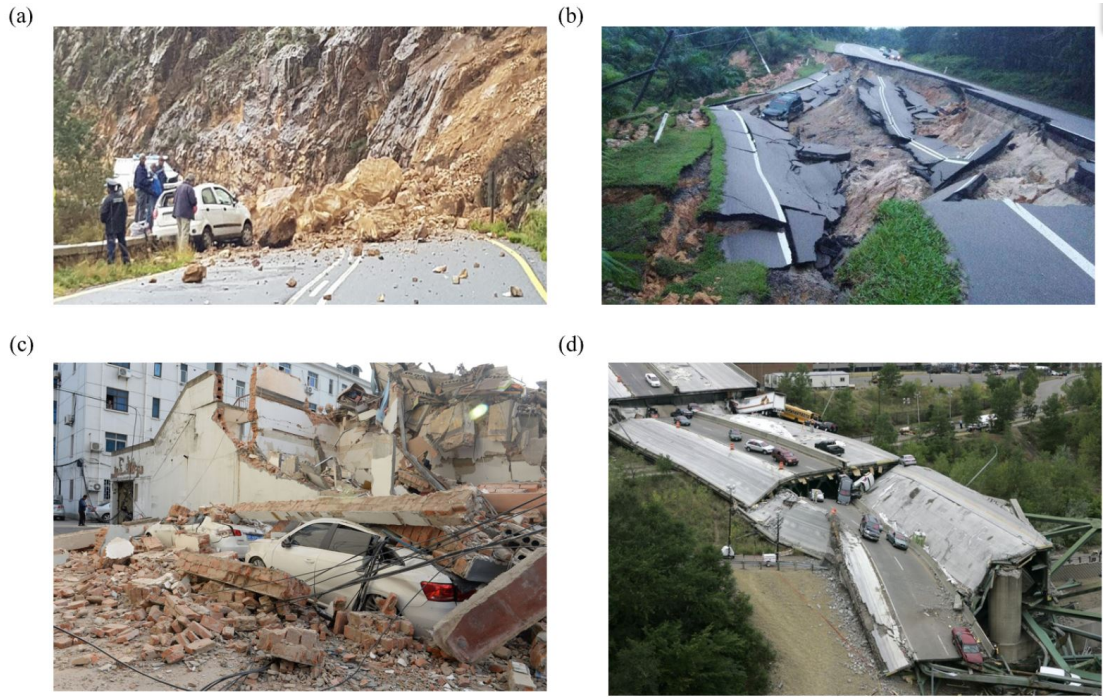


Figure 1.4.: Failures in bonded granular materials, which can lead to property losses and even fatality. (a) Rockfalls on a road ^a. (b) A road Collapse ^b. (c) A building collapse ^c. (d) A bridge collapse ^d.

^a<https://cdn.24.co.za/files/Cms/General/d/8535/12c996b5bae5406287755126cf11be88.jpeg>

^b<https://forum.fishingkaki.com/discussion/288534/road-collapse-along-highway-to-mersing-rompin/>

^c<https://www.nbcnews.com/news/photo/rescuers-rush-scene-building-collapse-china-n554716>

^d<https://www.fox21online.com/2017/07/31/35-bridge-collapse-still-reverberates-10-years-later/>

ular materials (e.g., unbonded grain assemblies like dry sand). Their basic properties for simple loading tests are depicted in Figure 1.5. In the failure of quasibrittle materials, initially, we do not see much movement as there are not many microcracks (broken bonds in the sense of discrete element models). But, when the external load reaches the critical value (i.e., peak load), a cascade of broken bonds occurs. This leads to a sudden drop in the external load in the failure regime (softening). This thesis focuses on the prediction of the failure location in the stages prior to the critical peak load.

A distinctive property of disordered and heterogeneous granular materials, known to govern failure, manifests at the mesoscopic scale. These comprise the preferred paths for force transmission and preferred paths for damage (Figure 3.1 (a)). The former are force chains. The latter are the ultimate macrocrack paths (Figure 3.1 (b,c)).

These two pathways do not evolve independently. Instead, they are coupled together. According to Aggelis *et al.* 2013 “The monitoring is complemented by Digital Image Correlation (DIC) which gives a clear depiction of the surface strain field and its transient changes according to stress redistribution which occurs after fracture moments.” This shows that stress redistributes to cope with the damage. This process of coevolution

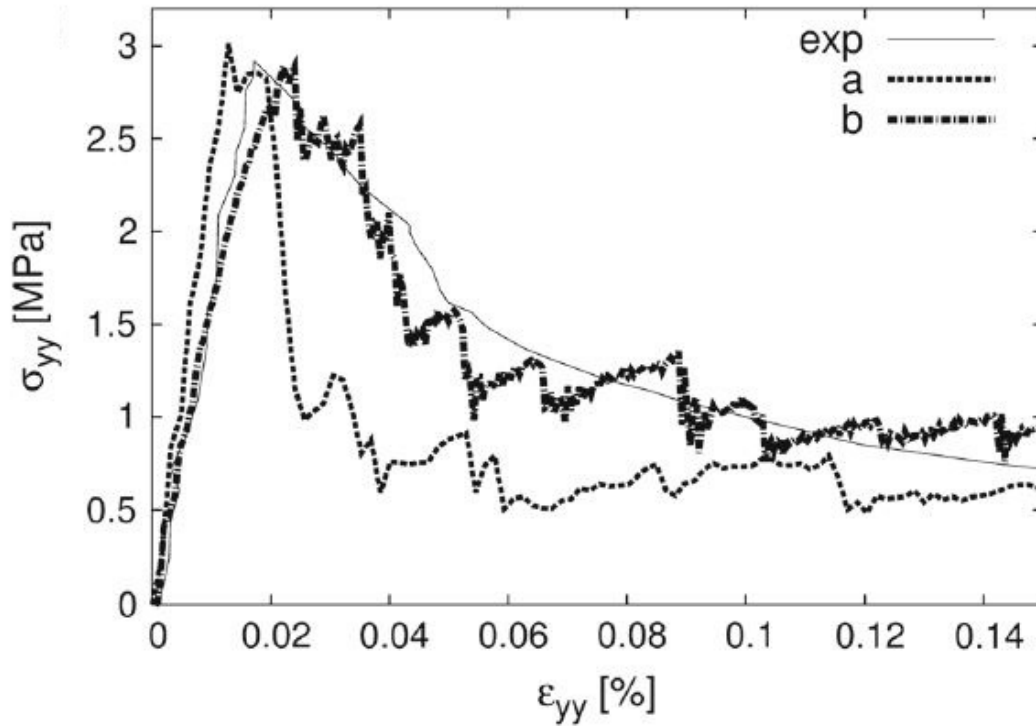


Figure 1.5.: Stress strain response of quasibrittle material highlighting the stress-strain response of the sample under uniaxial tension test: a – DEM simulation for 1-phase tension, b – DEM simulation for 3-phase tension and ‘exp’ – experiments by [Van Vliet & Van Mier 1999](#) ([Nitka & Tejchman 2015](#)).

remains poorly understood. What is, however, widely recognised are twofold:

- the coupled evolution of force and damage pathways holds the key to early prediction of failure in these materials and related systems and structures;
- this coupled process is strongly influenced by the properties at the microscopic level – the level of individual grains and their contacts.

Accordingly, this thesis focuses firstly on the characterization and modelling of this coupled evolution from microstructural data. Next, we build on this knowledge to predict the failure location (i.e., the ultimate location of the macrocrack) for two classes of systems: small scale and idealised laboratory test systems, and field-scale data on a developing landslide. This thesis is mostly devoted to the study of the former. The latter study is preliminary and is aimed at testing a new technique ([Tordesillas *et al.* 2018](#); [Tordesillas & Batterham 2020](#)) on radar monitoring data from an open-pit mine as part of an industry partnership between the University of Melbourne and GroundProbe-Orica.

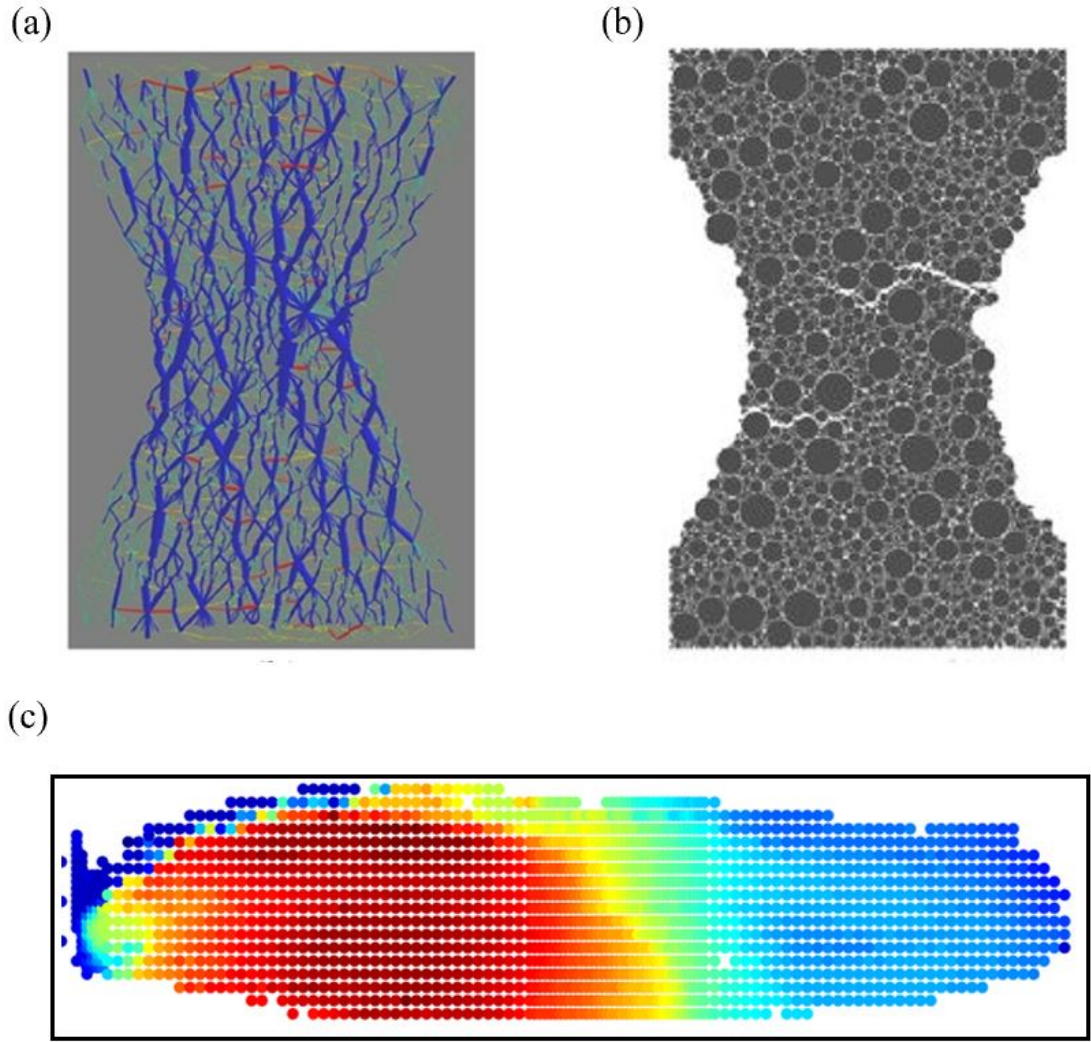


Figure 1.6.: (a, b) for 1-phase tension (Nitka & Tejchman 2015). (c) for large scale rock slope in the field (Tordesillas *et al.* 2018). This shows spatial distribution of the displacement field at failure with red-blue colour map (the highest to lowest) which highlights the failure zone. (a) Visuals of the preferred paths for force transmission in the prepeak regime. Line thickness is proportional to the normal contact force magnitude: blue for tensile and red for compression. (b, c) The preferred path for damage propagation.

1.2.1. Microstructural data from laboratory tests

Reliable microstructural data on concrete and rock samples are rare. It is extremely difficult to measure the internal properties of samples under load in a noninvasive manner, even under the simplest and idealised laboratory conditions. One promising way forward that has been employed with great success is to construct a simulation using the discrete element method (DEM) of a simple laboratory test, such that (a) the parameters of the numerical DEM test are carefully calibrated to the physical laboratory

test and (b) the properties of the real concrete composite sample are reproduced in the DEM sample with the aid of X-ray CT images. For this thesis, we are fortunate to have such data. These data sets have been the product of almost two decades of work in the laboratory of Professor Jacek Tejchman from Gdańsk University of Technology, Poland, specialising on high fidelity concrete modelling. Here we analyse their data from concrete samples under uniaxial tension and compression. Details of these tests are described in Chapter 3.

1.2.2. Microstructural data from field tests

We also have data from ground-based radar on a developing rockfall from an open-pit mine, from an undisclosed industry partner (Tordesillas *et al.* 2018). While these do not provide information at the level of individual grains, they are special in that they possess very high spatial and temporal resolution and cover the whole slope. Published details of this data set are described in section 9.1 of Chapter 9.

1.3. Focus of this thesis

This thesis aims to develop methods that can help improve understanding and prediction of failure in bonded granular composite materials. Its key focus is to characterise and model the coupled evolution of force, energy and damage pathways in systems driven to failure in the framework of Network Flow Theory (Figure 1.7). The models developed are data-driven and depend on microstructural data for input.

The questions we specifically address are:

1. What are the rules that govern the coupled evolution of force and damage pathways and how do these relate to the connectivity and strengths of the bonds in the contact network?
2. Can the ultimate pattern of failure be predicted from microstructural data, early in the prefailure regime?
3. Can similar principles be employed to analyse kinematic data for early prediction of the failure location at the field-scale?

1.4. Structure of the thesis

Other than the Introduction, there are 9 chapters in this thesis. Each chapter begins with a brief introduction of the content and ends with a summary highlighting the key findings. Note that the main body of the thesis includes only the analysis relevant to the network flow. All other additional work undertaken in support of the main theme

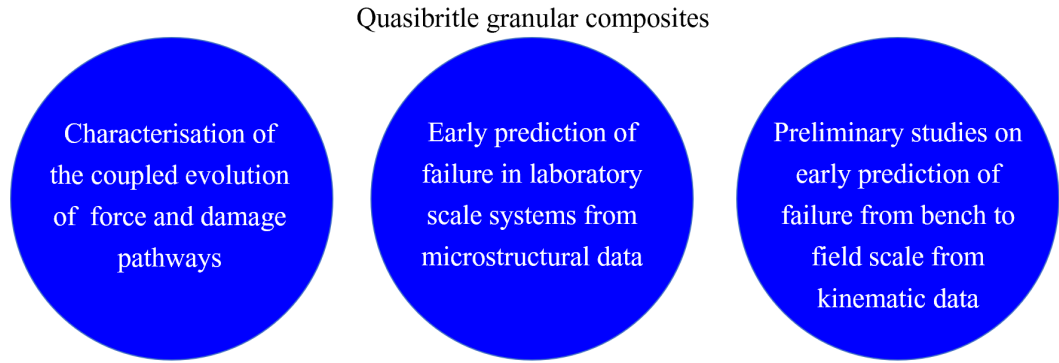


Figure 1.7.: A depiction of the key themes of this thesis.

of this thesis is presented in the appendixes and referred to in the main text. The thesis is structured as follows and summarised in Figure 1.8.

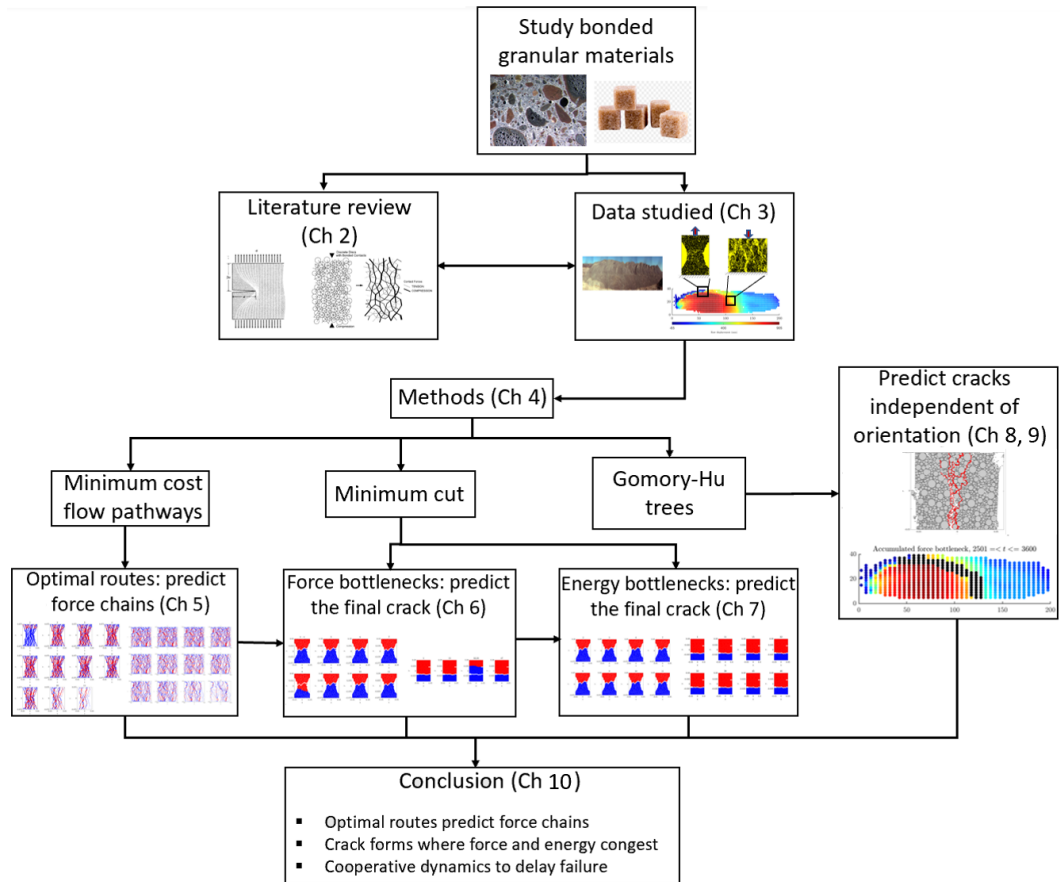


Figure 1.8.: A flow chart summarising the structure of the thesis.

Chapter 2: The current state of knowledge on force transmission and crack propagation in quasibrittle materials is presented. Models that predict force chains and the

location of the ultimate macrocrack are also discussed.

Chapter 3: Discrete element method simulation data studied in this research are described. These data sets were provided to our group by Dr Michał Nitka and Prof Jacek Tejchman.

Chapter 4: The method used for characterisation and modelling of the coupled evolution of preferential paths for force and energy transmission and damage is formulated. This arose from a collaboration between myself, my principal supervisor Prof Antoinette Tordesillas, Dr Michał Nitka, Prof Jacek Tejchman and my co-supervisor Dr Charl Ras.

Chapter 5: Results on the preferred force transmission pathways derived using the method described in Chapter 4 are discussed for samples under uniaxial tension. Part of the results is published in [Tordesillas *et al.* 2020](#).

Chapter 6: Results on the preferred damage pathway from *force transmission analysis* are discussed for samples under uniaxial tension. Part of the results is published in [Tordesillas *et al.* 2020](#).

Chapter 7: Results on the preferred damage pathway from *energy transmission analysis* are discussed for samples under uniaxial tension. Results are submitted to Nature Scientific Report.

Chapter 8: Preliminary results on the prediction of crack patterns in compression samples are discussed. This arose from a collaboration between myself, my principal supervisor Prof Antoinette Tordesillas, my co-supervisor Dr Charl Ras, Dr Michał Nitka, and Prof Jacek Tejchman.

Chapter 9: Preliminary results for field-scale predictions of a landslide from radar data are presented. These results arose from a collaboration between myself, my principal supervisor Prof Antoinette Tordesillas and my co-supervisor Dr Charl Ras.

Chapter 10: The main findings, limitations and future work are discussed to conclude the thesis.

2. Literature review

In this chapter, we give a critical review of the current state-of-knowledge on the prediction of failure in disordered and heterogeneous quasibrittle granular materials. Attention is paid to three key elements: (1) preferential pathways for force transmission, (2) preferential pathways for damage and (3) models to predict these two pathways.

2.1. Preferential paths for force transmission

Preferential paths for force transmission manifest as so-called “force chains” (Figure 2.1). Force chains are quasi-linear chains of at least three grains, which carry the majority of the applied load (Muthuswamy & Tordesillas 2006). In analogy to road networks, we can think of these as the highways for force transmission. The spatial and temporal evolution of these mesoscale force structures governs macroscopic behaviour. Therefore, a proper understanding of the evolution of such preferential force transmission paths is essential for prediction and control of failure in granular materials. Studies of force chains have received significant attention (Majmudar & Behringer 2005; Oda & Kazama 1998; Oda *et al.* 1982; Radjai *et al.* 1998). Among the earliest observations of these were in experiments involving photoelastic disks (Wakabayashi 1950). Even Clear evidence of the existence of force chains was observed for the same material later in (Drescher & De Jong 1972). Similarly, the first experimental measurements of contact forces over many stages of a test were achieved using the same material (Majmudar & Behringer 2005).

In this thesis, we only focus on force chains in bonded granular materials (Figure 2.2). The major difference between bonded and unbonded granular materials is that bonded contacts can support both compressive and tensile forces, whereas unbonded frictional contacts can only support compressive forces. As a consequence, both tensile and compressive force chains can form (Buttler & You 2001; Diederichs 2003; Potyondy & Cundall 2004; Khanal *et al.* 2005; Liu *et al.* 2017; Sinaie *et al.* 2018). Experimental evidence for the existence of force chains in bonded grains can be found in (Baig *et al.* 2015; Li *et al.* 2019; Bigoni & Noselli 2010*a,b*). Baig *et al.* observed the force chains using DEM models also. They pointed out that force chains are the optimised paths to transmit the externally applied load. This suggests preferential paths for force transmission exist in bonded granular materials. Li *et al.* observed tree-like force transmission patterns due to the discreteness of the contact network. If the contact network is discrete, then

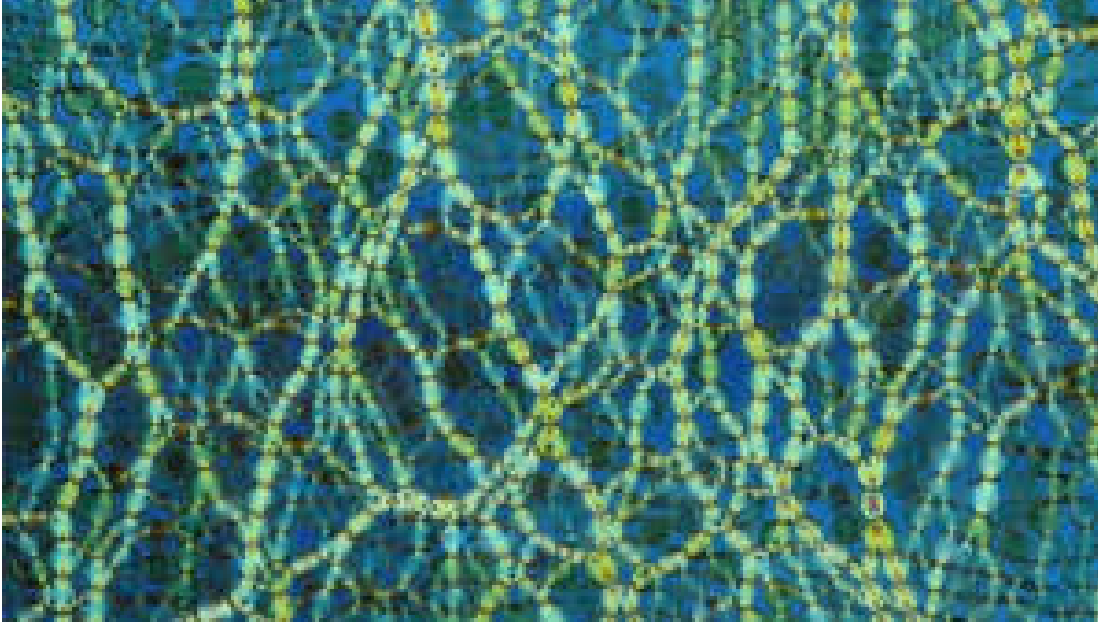


Figure 2.1.: Existence of force chains in unbonded granular materials. Bright color chains are major force transmission pathways observed in photo-elastic disc experiment conducted by Jie Zhang, Trushant Majmudar, and Bob Behringer, Duke University (<https://www.aps.org/about/physics-images/archive/chains.cfm>).

there might not be direct percolation path for high-stress transfer which results in tree-like patterns. Therefore, they could see some stress-free regimes due to highly localised stress percolation. Similar stress-free regimes were observed in Bigoni & Noselli 2010a,b (Figure 2.2).

Although there are many more studies of force chains in unbonded grains, there is growing recognition in the literature that they are important to the mechanical behaviour of bonded granular materials (Nicksiar & Martin 2013; Potyondy & Cundall 2004), in particular their strength and failure. Still, the majority of studies are qualitative and confined to visualisations of force chains from discrete simulations (Khanal *et al.* 2005; Sinaie *et al.* 2018). There has been some quantitative characterisation of force chains in Tordesillas *et al.* 2015b but only for compressive loading conditions. Therefore, quantitative analysis of force chains in samples under tension and compression is needed to improve understanding of the mechanical behaviour of bonded granular materials. Here, we seek to fill this knowledge gap by first extending the existing force chain detection algorithm presented in Muthuswamy & Tordesillas 2006 to identify both compressive and tensile force chains in bonded grain assemblies. This is presented in Appendix B.

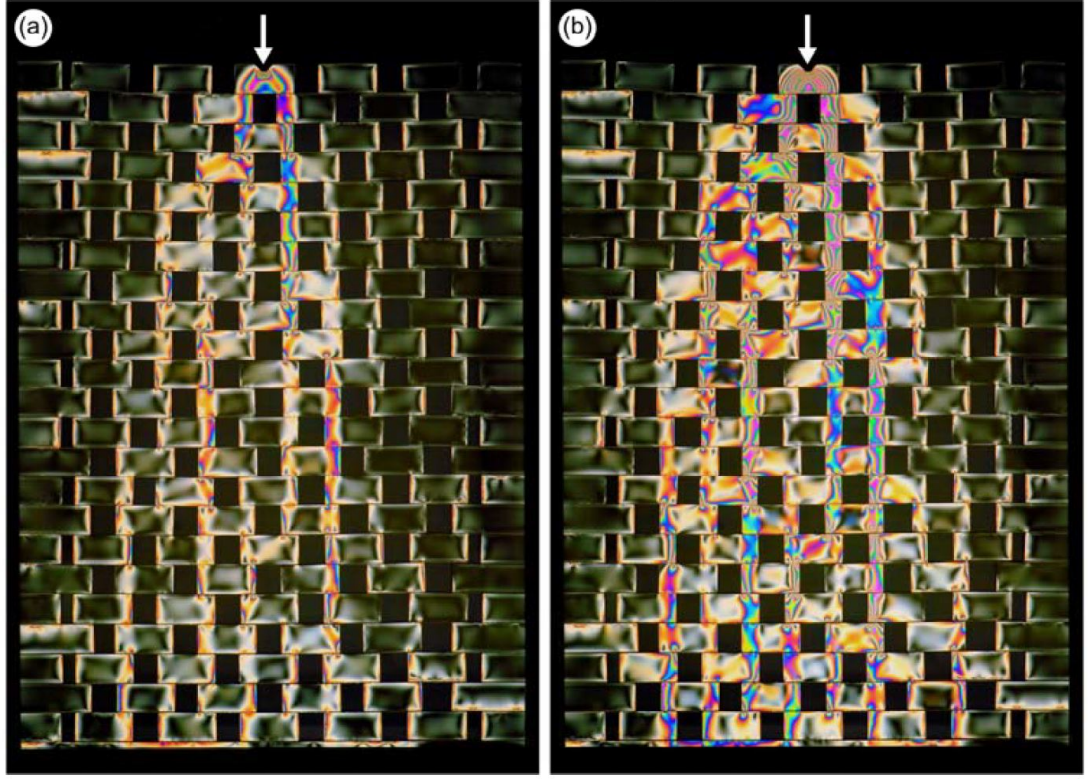


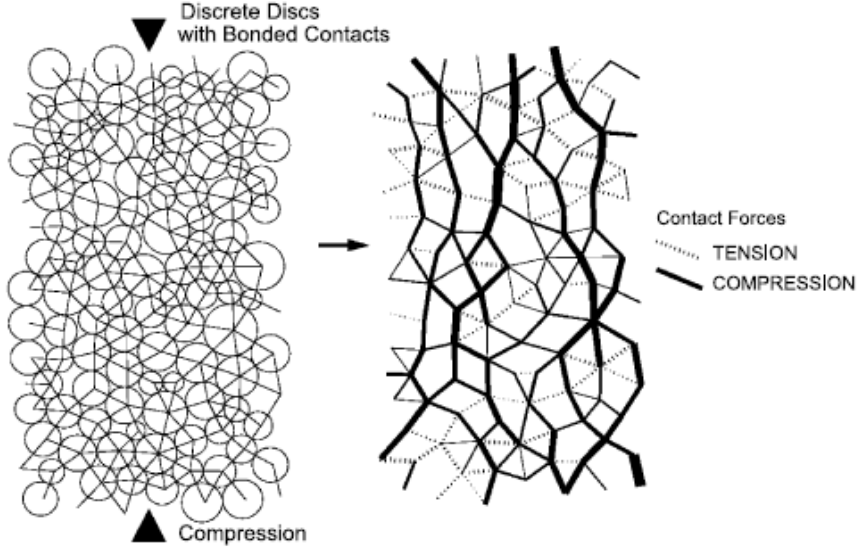
Figure 2.2.: Existence of force chains in bonded granular materials. This shows stress percolation paths in dry masonry walls by using photoelasticity (Bigoni & Noselli 2010a).

2.1.1. Force chains in samples under uniaxial tension and compression

In a discrete element method simulation study of fracture in tension test, Nguyen *et al.* 2017 observed that tensile force chains are aligned with the direction of applied loading. Before the development macrocrack along the two notches in the middle, they observed that uniform and dense distribution of tensile force chains. But, when the macrocrack appeared, tensile force chain distribution becomes nonuniform and sparse. This is mainly due to the macrocrack disconnects some available paths for force transfer. In this instance, compressive force chains were mainly appeared along the macrocrack path and also below the two notches in the sides.

Potyondy & Cundall 2004 revealed that cement-filled contacts experience a combination of compressive, tension and shear loading. As a result, applied loading produced heterogeneous force transmission and induces many sites of tension and compression (see Figure 2.4 (a)). Khanal *et al.* 2005 also observed that the boundaries of major fragments experienced compressive stress. Moreover, tensile forces were also developed in the fragments. This suggests that there exist different stress states in the specimen during the fracture, which governs the crack propagation (see Figure 2.4 (b)). This

(a)



(b)

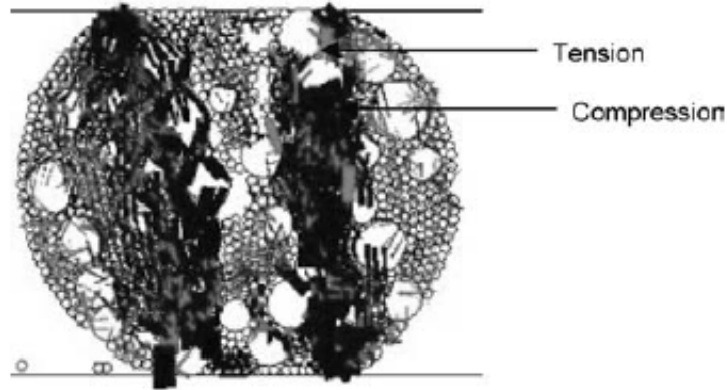


Figure 2.3.: Compressive force chains are dominant and aligned with applied load. Compressive and tensile force chains coexist. Images are taken from (a) [Diederichs 2003](#) and (b) [Khanal *et al.* 2005](#).

may result in a formation of both compressive and tensile force chains. But, better qualitative and quantitative explanations are still lacking. We will discover and explain two mechanisms which are responsible for the formation of tensile force chains in compression tests. Results are reported in [Appendix C](#).

[Potyondy & Cundall 2004](#) found out that force chains are nonuniform with a few chains carried a higher load, while the others carried a lower load. These high loaded contacts in these force chains cause lateral contacts to break in tension, as shown in [Figure 2.5](#). The mechanism of compression-induced tensile cracking is called *force-chain crack*. This results in force redistribution that reroute forces to lightly loaded force

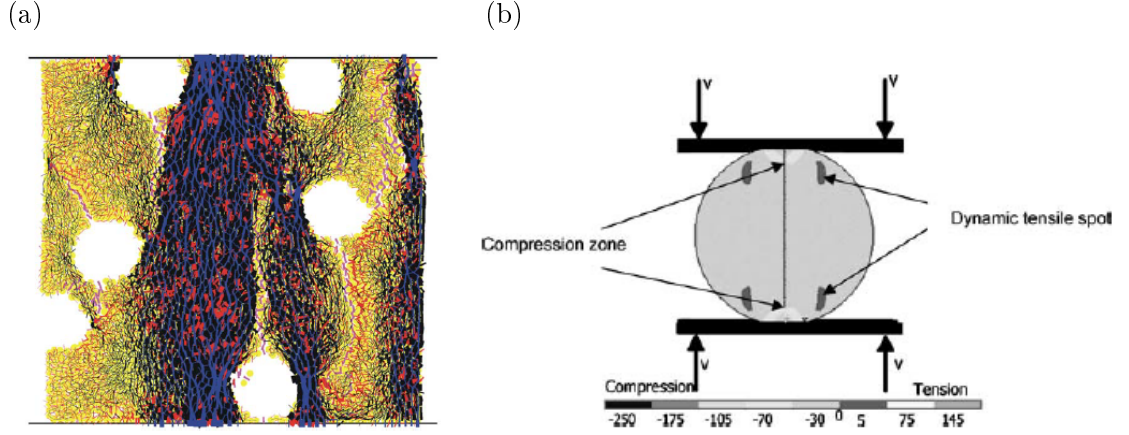


Figure 2.4.: Specimens are subjected to combination of compressive and tensile forces. Visualisation of compressive and tensile sites from (a) Potyondy & Cundall 2004: black – compression, red – tension and (b) Khanal *et al.* 2005.

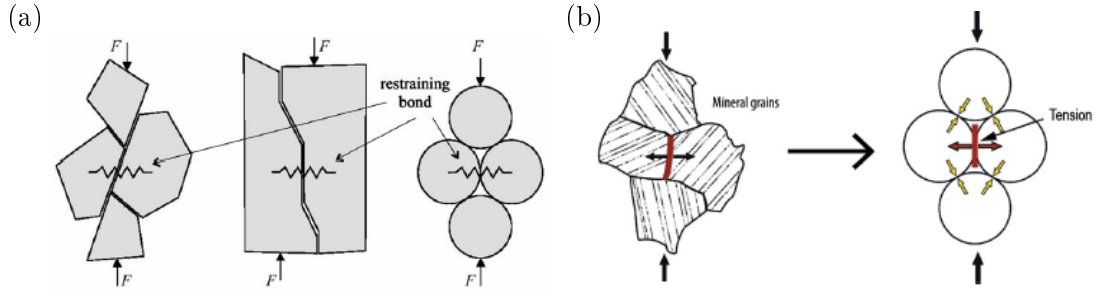


Figure 2.5.: Illustration of mechanism of compression-induced tensile cracking called *force-chain crack model* from (a) Potyondy & Cundall 2004 and (b) Hoek & Martin 2014. High compressive forces in force chains cause lateral contacts to break in tension. The main bond failure model is tension even though the specimen is subjected to uniaxial compression.

chains to prevent overloading the bonds in force chains that are close to their breaking point. This process continues and eventually leads to the formation of a macrocrack that leads to global failure. Furthermore, the breakage of bonds in force chain contacts induces micro-moments, which may lead to another form of force chain failure which is by buckling.

In a numerical study of a fracture process of uniaxial compression test for concrete, Su *et al.* 2017 noticed that uniform, fine and dense force chain distribution at the beginning of the test. Su *et al.* also observed few internal microcracks on the coarse aggregate surface, but there were no externally visible macroscopic cracks on the specimen (see Figure 2.6). When the applied load was increased, the microcracks expanded and connected with each other to form macroscopic cracks. In this instance, they noticed that force chains disappeared in the cracked location and the rest of the area became stronger. Furthermore, they observed non-uniform distribution of force chains which are concentrated in some places. As the applied load increased beyond the peak load,

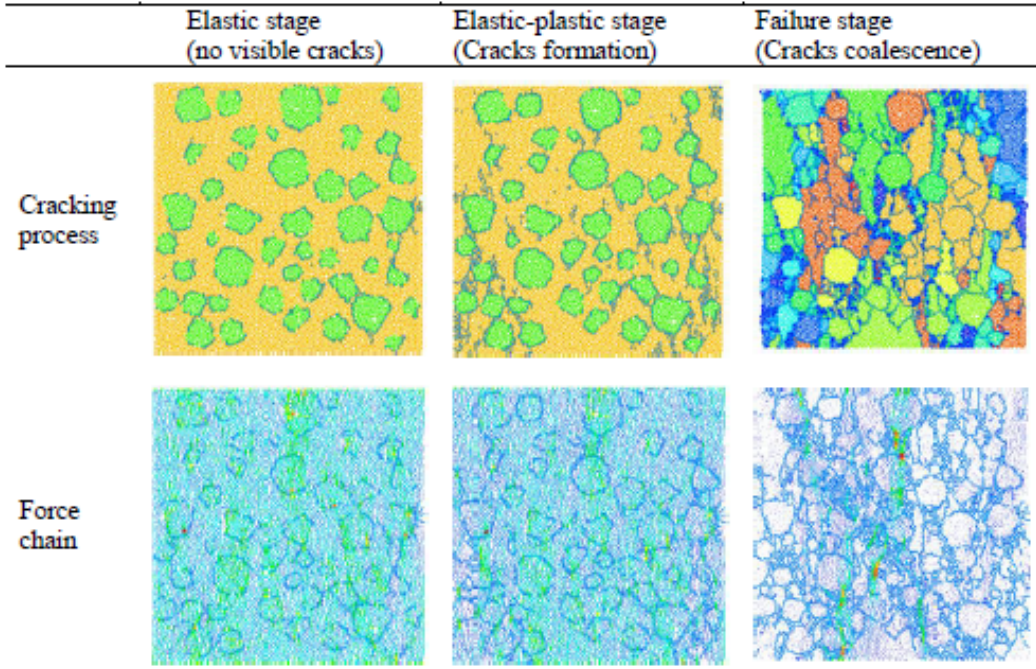


Figure 2.6.: Force chains distribution is uniform at the beginning and degrades towards the failure. Visualisation of fracture process and corresponding evolution of force chains (Su *et al.* 2017).

cracks developed rapidly leading to the specimen breaking up into multiple pieces. In this instance, only a few strong force chains remained in the sample. Similar behaviour has been observed in (Sinaie *et al.* 2018). Force chains may disappear due to the paths through the cracked locations have become disconnected. Therefore, these no longer percolate and in turn, these cannot transmit forces. This means that the few remaining percolating paths must now carry ‘most of the force’ meaning to say only a few strong force chains remained in the sample. The authors visualised force chains by using the magnitude of contact forces. They did not have a method to identify individual force chains. They simply observed the disappearance of force chains in cracked locations visually.

2.2. Preferential pathways for damage propagation

Preferential pathways for damage manifest as macrocracks. For disordered and heterogeneous material like concrete, macrocrack happens with a sequence of events of microcracking (bond breakages). According to Diederichs 2003, most bonds fail in tension even in the specimens subjected to compression. Hence tensile microcracks are more common than bonds that break under shear. At the beginning of loading history, there are a few numbers of microcracks which spread in the sample. As loading progress, microcracks accumulate and concentrate in some region later causing catastrophic failure.

Microcracks initiate, propagate and finally interconnect to form a macrocrack (Xiao *et al.* 2012). In simple loading conditions like uniaxial tension test, there is often just one macrocrack – the so-called ‘ultimate macrocrack’. This forms perpendicular to the applied tensile load (Topin *et al.* 2007; Stamati *et al.* 2019). However, samples subjected to compression give rise to complex crack patterns (Qin & Zhang 2011; Meguro & Hakuno 1989; Xiao *et al.* 2012; Cho *et al.* 2007) (see Figure 2.7).

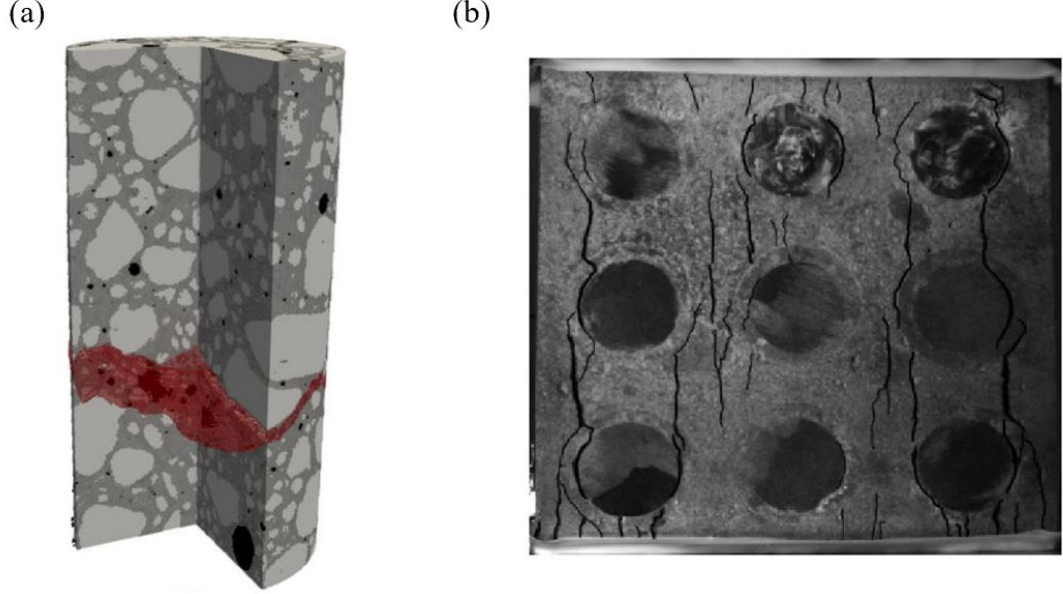


Figure 2.7.: Crack pattern in (a) uniaxial tension by using X-ray image (Stamati *et al.* 2019) and uniaxial compression (Xiao *et al.* 2012).

In direct observations of fracture in ceramics at the atomic scale, Kondo *et al.* 2019 observed that grain packing has a strong influence on the macrocrack path. In general, grain packing determines the connectivity of the bonded contact network. They found that the actual crack path preferred a zigzag pattern over a straight path which is assumed in classical fracture mechanics. Kondo *et al.* 2019 explained this phenomenon with the aid of cleavage energy, i.e., the energy needed to break apart the specimen along a path or surface. This is equivalent to the Griffith fracture surface energy (Wittmann *et al.* 2010). They quantified the energy required to produce experimentally observed zigzag path versus those from straight crack paths (the possible crack paths are the paths with the same number of atomic bonds as in the zigzag path). Results revealed that the zigzag path has the least fracture surface energy. Similar zigzag (tortuous) patterns were observed in studies of concrete specimens (Pease *et al.* 2006; Schlangen 2008; Mindess & Diamond 1982; Bentur & Mindess 1986). In these cases, cracks formed around the aggregate grain boundaries, since these are the weakest sites in the sample. Aggregate grains are the biggest grains in concrete (recall Figures 1.1 (a) and 1.2). Since these are randomly distributed in concrete, a tortuous crack path may form.

In [Qu *et al.* 2016](#), they proposed a generalized energy failure criterion to predict fracture in metallic glasses. They conducted a series of fracture-controlled tensile tests and observed that fracture always happens along a plane with the minimum input energy. Here input energy is defined as the minimum energy needed to break the specimen which they described as “the most dangerous plane where the failure will happen”. Hence, their proposal is in line with the macrocrack path being that path with the minimum Griffith fracture surface energy.

Studies of fracture toughness in nanostructured ceramics have revealed that fracture toughness depends on the individual components (bonds), their strength and/or connectivity ([Daniel *et al.* 2019](#)). Fracture toughness is the critical stress where crack propagation becomes catastrophic ([Ritchie *et al.* 1973](#)). Hence, fracture toughness determines when macrocrack occurs. This means that fracture strength depends on the topology and strength of individual bonds. They also observed that the crack path prefers to form along the weak grain-grain boundaries as opposed to forming through grains which would entail grain breakage. This implies that bond strength matters and that the macrocrack forms the path of least resistance (total minimum strength).

In what follows, we describe the most commonly used fracture mechanics criteria which are based on an energy or stress extremal: minimisation or maximisation of some functional based on energy or stress.

2.2.1. Existing fracture mechanics criteria

Here we discuss some of the most commonly used fracture mechanics criteria starting with Griffith theory. Currently, there exists an extensive number of fracture mechanics criteria to predict crack growth in bonded granular materials ([Miarka *et al.* 2018](#)). The development of fracture mechanics goes back to the early 20th century with the pioneering work done by the English Aeronautical Engineer A. A. Griffith ([Qu *et al.* 2016](#)). Griffith observed that, after surface treatment in brittle materials, the strength of the material could not be explained by the classical theory of failure ([Griffith 1921](#)). Therefore, he attacked this problem with the concept of total minimum energy.

Since then, researchers have been interested in the location of cracks, crack growth direction and competing cracks in the specimens ([Sutula *et al.* 2018a](#)). Different approaches such as continuum theory ([Talebi *et al.* 2014](#)) and discrete models ([Munjiza *et al.* 1999, 1995; Munjiza 2004](#)) have been used to describe bonded systems. They used different criteria to determine the location of the crack, crack growth direction and competing cracks. Some of the commonly used criteria are total minimum energy ([Francfort & Marigo 1998](#)), the maximum energy release rate ([Palaniswamy & Knauss 1972](#)), the minimum strain energy density ([Sih 1973](#)), and the Rankine stress criterion (maximum normal stress criterion ([Rankine 1857](#))). Among them, the most commonly used crite-

tion is the minimum total energy criterion which stems directly from famous Griffith's theory. We will discuss these fracture mechanics criteria in detail next.

2.2.1.1. Griffith's theory

Stress analysis of glass revealed that there is a significant difference between the stress required to fracture bulk glass and breaking atomic bonds of glass. Stress needed to break atomic bonds of glass is much higher than stress required to fracture bulk glass. As mentioned above, after surface treatment in brittle materials, the strength of the material could not be explained by the classical theory of failure. These suggested that a new theory is needed to resolve these conflicting observations. This was a motivation for Griffith's work. Griffith, also himself observed that the fracture stress of glass increases as the diameter of the specimen decreases ([Griffith 1921](#)). Thus, he concluded that the uniaxial tensile strength is not a specimen-independent material property. The tensile strength was heavily used to predict material failure before Griffith's work. Griffith proposed a criterion for critical stress. Griffith derived and validated his theory using brittle materials like glass. On average, experimental results were 10% below the theoretical value. Note that, when Griffith derived the critical stress, he assumed material has an infinite length as will discuss below. But, in his experimental setup, this was not the case.

Griffith criterion gives critical stress of materials. When this critical stress reached, the material fails, i.e., all bonds break at the same time along the macrocrack path. He derived this theory for homogeneous and isotropic materials like glass. But, today Griffith theory is used to predict cracks in various disordered and heterogeneous materials like concrete, rock, graphene, etc. However, the validity of the usage of Griffith's theory is debatable as theory built for a particular class of materials ([Vu *et al.* 2019](#)). In the following, we are going to derive the Griffith energy balance criterion. We also show how assumptions in Griffith theory deviate for disordered and heterogeneous materials, which we interest in this research. We also present the relation of this continuum approach to the discrete system.

Derivation of Griffith criterion

Here we are going to derive the equation for critical stress proposed by Griffith which used the energy approach. In the derivation, the followings were assumed.

1. Material is homogeneous and isotropic. Therefore, fracture surface energy γ_s (energy per unit area that is required to form a surface) is a constant.
2. Material is linear elastic. Thus, it obeys Hook's law.

3. Crack is straight and passes normally through (perpendicular to the applied stress) the material.
4. To form a crack, atomic bonds must be broken. The energy required to break atomic bonds (this energy release as bonds break) is assumed to be absorbed by the two surfaces form upon the creation of crack.
5. The material is an infinite plate and has a unit thickness which is subjected to uniaxial tension. This assumption enables him to use Inglis's solution ([Inglis 1913](#)) for energy release due to crack form.

Griffith derived the formula for the critical stress in the presence of elliptical crack with a length of $2a$ (along the major axis) in the centre of the material as shown in Figure 2.8.

Since the material is homogeneous and isotropic, we can consider the right half-plane for the simplicity when deriving the formula for the critical stress. This is due to the symmetry about the y-axis. Without loss of generality, we can assume the case of infinite length ($L \rightarrow \infty$) as shown in Figure 2.9.

Let U^* be the strain energy density (energy per unit volume) of stressed material with length L and cross sectional area A . Let's assume material is elongated by dy due to applied load f . Then the external work done is $\int f dy$. This is equal to the strain energy of the system. Therefore, U^* is given by;

$$U^* = \frac{1}{V} \int f dy = \int \frac{f}{A} \frac{dy}{L} = \int \sigma d\epsilon, \quad (2.1)$$

where $V = AL$ is the volume of the material, $\sigma = f/A$ is the stress and ϵ is the strain. As material is linear elastic, we have $\sigma = E\epsilon$, where E is the Young's modulus or Elasticity modulus. Thus, Equation (2.1) can be rewritten as follows;

$$U^* = \int E\epsilon d\epsilon = \frac{E\epsilon^2}{2} = \frac{\sigma^2}{2E}. \quad (2.2)$$

The strain energy density is a constant since the material is homogeneous and isotropic. Thus, we can write the total strain energy U for the uncracked material as

$$U = U^*V = \frac{\sigma^2}{2E}V. \quad (2.3)$$

Due to crack growth, the strain energy releases. When a crack has grown to a depth a as shown in Figure 2.8, the top and bottom surfaces of crack become stress-free (free surfaces) and a region adjacent to it is unloaded. From the work done by Inglis ([Inglis 1913](#)), this release energy for a crack with length a was found to be $\frac{\sigma^2}{2E}\pi a^2$. Therefore, the total strain energy after the crack form can be expressed as a function of crack length a as follows;

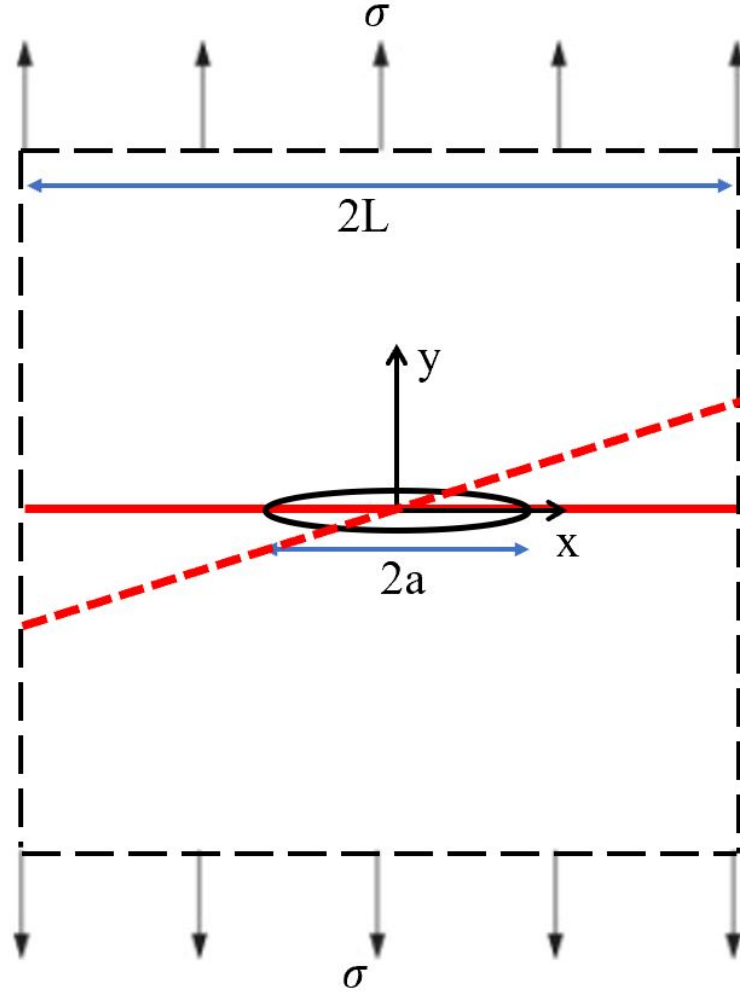


Figure 2.8.: Illustration of an elliptical crack with a length of $2a$ in the middle of a plate with unit thickness subjected to uniform stress σ . The length of the plate is $2L$. The solid red line shows a horizontal crack path with minimum length while the dashed red line represents an arbitrary cut which does not pass through the top and/or the bottom walls.

$$U = \frac{\sigma^2}{2E}V - \frac{\sigma^2}{2E}\pi a^2. \quad (2.4)$$

To form a crack, bonds must be broken along the crack path. This requires a certain amount of work to overcome the atomic bond energy. When atomic bonds break, a certain amount of energy releases. Due to the energy balance, this energy is absorbed by two free surfaces (one above and the other below the crack) created by the crack in the material. The total energy required to break the atomic bonds is therefore expressed as

$$E_{bond} = 2\gamma_s a, \quad (2.5)$$

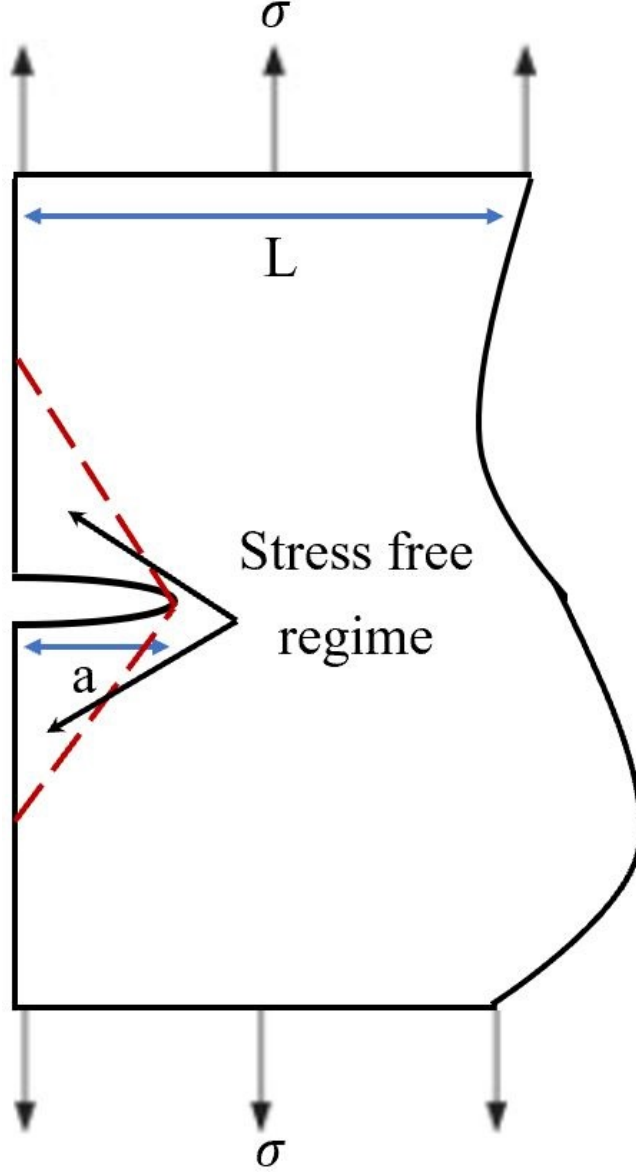


Figure 2.9.: Visuals of a crack in continuum model. Illustration of an elliptical crack in the middle of infinite plate with unit thickness. For the simplicity and symmetry about the vertical axis (y-axis), here we only consider the right-half plane only. This highlights the unloaded region near crack with half-length a for infinite plate subjected to uniform stress σ .

where γ_s is the surface energy and is equal to the fracture energy of the bonds in the nano scale (Wittmann *et al.* 2010). Factor 2 is needed in the above equation as there are two free surfaces. Here the assumptions that crack is straight and surface energy is constant have been used. Note here that E_{bond} is equal to the fracture energy of the material, i.e., the sum of the energy required to break the individual bonds along the fracture path (Wittmann *et al.* 2010). For our data, this is equal to the sum of the

maximum elastic energy for bonded contact along the macrocrack.

The total energy of the system is the sum of the strain energy, U and the energy required to break the atomic bonds, E_{bond} and given by;

$$E_{tot} = \frac{\sigma^2}{2E}V - \frac{\sigma^2}{2E}\pi a^2 + 2\gamma_s a. \quad (2.6)$$

Now to find the critical crack length, we differentiate E_{tot} with respect to crack length a and equate to zero.

$$\frac{dE_{tot}}{da} = 2\gamma_s - \frac{\sigma^2}{E}\pi a = 0. \quad (2.7)$$

Rearranging terms in Equation (2.7), we get Griffith's equation for critical stress as

$$\sigma = \sqrt{\frac{2\gamma_s E}{\pi a}} = \sqrt{\frac{G_c E}{\pi a}}, \quad (2.8)$$

where $G_c = 2\gamma_s$ is the *Griffith Critical Energy Release Rate*.

When the stress of a sample reaches the critical stress, the sample fails. Therefore, we can see that after the critical crack length, the failure is catastrophic. Thus, we can conclude that the fracture path minimises the total energy.

The effect of assumptions and relationship of Griffith theory to discrete models

Here we compare the assumptions used in deriving Griffith's equation for critical stress to disordered and heterogeneous granular materials such as concrete. We consider two cases. (1) Bonds break along the crack path only (toy illustration) and (2) bond breakages can happen anywhere (generic case). Discrete element models have been proposed to study the fracture process in concrete.

Case I: Bonds break along the crack path only

A crack in continuum models (Figure 2.8) can be mapped into a group of interconnected broken contacts along the path for a discrete model (Figure 2.10). For this toy illustration, assume that bonds break along the crack path only (contains a single crack). Now let's assume that this system has n number of bonded contacts which are not shown in the figure. The crack path contains six broken contacts. Assume that bond strength (=maximum elastic energy. When elastic strain energy reaches Griffith surface energy, bonds break.) and strain energy for contact e is E_{max} and E_r respectively.

The assumption that fracture surface energy is constant is valid only for homogeneous materials. As Griffith developed his theory for brittle material like glass, this assumption is valid as the material is homogeneous. But, the systems we studied (data from DEM simulation for concrete samples) are heterogeneous as discussed in the previous chapter and this chapter. Moreover, the structure of concrete deviates from the perfect crystal

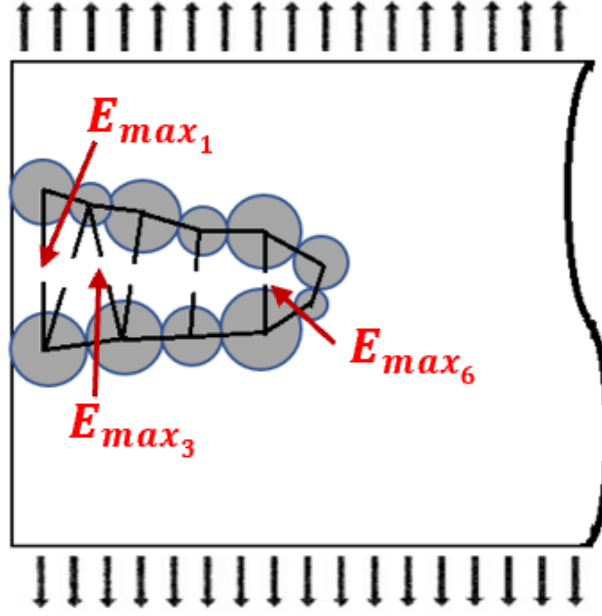


Figure 2.10.: An equivalent discrete model illustration for a crack shown in Figure 2.8. Six bonds must be broken to form the crack. When actual energy E_r reaches the maximum energy E_{max} , bonds break. $E_{max_1}, \dots, E_{max_6}$ corresponds to the fracture energy for six broken contacts.

structure [Egami & Billinge \(2003\)](#). Therefore, this assumption is not valid for the systems that we studied.

There is experimental evidence that the ultimate crack path takes a zigzag path rather a straight path as explained above. Bond strength is what matters most when deciding a preferential path for crack propagation. Thus, the assumption, the crack is straight is not generally true. Our samples do not manifest a straight crack path either. This assumption together with the previous assumption is used to calculate E_{bond} . But, for the discrete case, the assumption of a straight crack has no effect due to the availability of bond strength data, as explained next. Note that, contact level information was limited or out of reach when Griffith developed his theory.

For this illustration, we have the individual information on elastic energy as well as the bond strength. Therefore, without assuming the energy liberated by the crack is absorbed by the surface of it, we can directly calculate the energy required to form the crack. Hence, we do not need the assumption that surface energy is constant. Moreover, the crack is not necessarily straight. As six bonds are broken along the crack, E_{bond} is given by

$$E_{bond} = \sum_{k=1}^6 E_{max_k} = E_{max_1} + \dots + E_{max_6}.$$

The crack length a can be approximated by

$$a = \sum_{k=1}^6 r_{min_k} = r_{min_1} + \dots + r_{min_6},$$

where r_{min_k} is the minimum radii of two grains in the broken contact e^* .

Since data contain individual contact level information on strain energy, we can calculate the total strain energy for the cracked state without using Inglis's solution. Therefore, the total strain energy U is given by

$$U = \sum_{k=1}^n E_{r_k}.$$

This depends on the crack length a . Now the total energy of the system E_{tot} can be expressed as

$$E_{tot} = \sum_{k=1}^n E_{r_k} + \sum_{k=1}^6 E_{max_k}. \quad (2.9)$$

Case II: Bonds can break anywhere

However, the data we studied contain multiple broken contacts. Moreover, these broken contacts are spread throughout the samples (Figure 2.11). Therefore, here we are interested to find which microcrack grows or which of them are interconnected to form the ultimate macrocrack. We want to predict the location of the ultimate macrocrack will likely form. Now let's assume, for a given time stage ϵ , there are m broken contacts and n bonded contacts. We can write the total energy for the system as

$$E_{tot} = \sum_{k=1}^n E_{r_k} + \sum_{k=1}^m E_{max_k}. \quad (2.10)$$

Since Griffith developed his theory in the presence of single microcrack, we cannot apply his concept directly to our systems as they manifest multiple microcracks. In this case, the intuitive approach to write the total energy for each microcrack separately. Then the microcrack which minimises the total energy should be the critical fracture path. We have shown such a microcrack in Figure 2.11 (c). Let's assume there is l number of broken contacts along with this. For this crack path, the total energy is given by

$$E_{tot} = \sum_{k=1}^n E_{r_k} + \sum_{k=1}^l E_{max_k}. \quad (2.11)$$

Our aim here is to predict the location of the ultimate macrocrack will likely form. Note also that these data do not contain broken contacts for some prefailure stages of

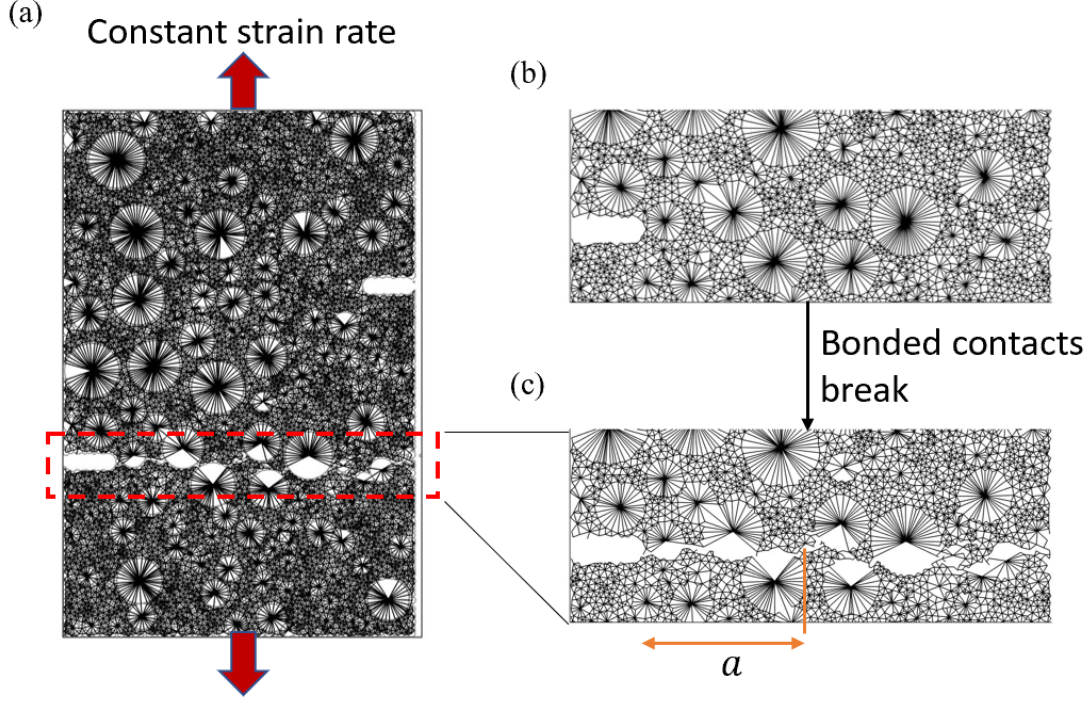


Figure 2.11.: Visuals of a crack in discrete model. (a) Analogues representation of a crack with length a in the discrete model of 3-phase tension sample, which is subjected to constant strain rate. Black lines represent the bonded contacts at stage 47 visulised as line joining the centers of two grains in bonded contacts. (b) Zoomed in image for the highlighted region in (a) with bonded contacts at stage 1 and (c) at stage 47. Interconnected broken contacts (contact not shown here i.e., the white opening) constitute a crack with length a . Number of broken contacts depend on the crack length a and vice versa.

the loading history (e.g., stages 1 – 4 of Figure 3.7). Therefore, we can consider two possible cases: (1) a virtual crack path and (2) a system spanning crack.

If we assume system spanning crack path Γ , the elastic energy of the system U should be zero. Then, the total energy of the system

$$E_{tot} = U + E_{bond} = E_{bond} = \gamma(\Gamma) = \sum_{e \in \Gamma} E_{max}.$$

In this case, E_{bond} is the fracture energy. Therefore, consistent with Griffith theory, the actual crack path should minimise the fracture energy. Hence, we can predict the location of the ultimate macrocrack by finding the path which minimises the fracture energy. This will be discussed in Chapter 4.

On the other hand, if we assume a virtual crack path, then we can formulate our problem as follows. The virtual path Γ , which minimises the total energy, should be the predicted path for the crack that will form in the failure regime. This leads to the method proposed by [Francfort & Marigo 1998](#), which we discuss next.

2.2.1.2. The minimum total energy criterion

This criterion assumes that fracture happens along the path which minimises the total energy of the system (Francfort & Marigo 1998). The total energy for a virtual cut (path) Γ for a given time state ϵ is given by

$$E_{tot}(\Gamma, \epsilon) = E(\Gamma, \epsilon) = E_d(\Gamma \setminus \mathcal{N}, \epsilon) + E_s(\Gamma), \quad (2.12)$$

where $E_d(\Gamma \setminus \mathcal{N}, \epsilon)$ is the sum of elastic strain energies stored at all the contacts in the system $\mathcal{N}$ excluding those in the virtual cut (path) Γ and $E_s(\Gamma)$ is fracture energy or energy dissipated due to crack formation) for the virtual cut Γ .

This is a variational approach that leads to an optimisation problem that minimises the total energy of the solid undergoing a fracture. Another key merit of this theory is “the crack path forms as a part of the solution to the minimisation problem”. This is considered to generalise Griffith’s theory and consistent with the discussion given above.

2.2.1.3. The maximum energy release rate criterion

This criterion assumes that crack will propagate along the path with maximum energy release rate (Palaniswamy & Knauss 1972). The maximum energy release rate criterion is one of the well-accepted criteria among the fracture mechanics community for tensile (Mode I) fracture (Nuismer 1975). The driving force for crack propagation in Mode I fracture is the energy release rate. Therefore, it is intuitive to assume *the crack will propagate in the direction, where the energy release rate is maximum*. Moreover, this criterion can be used to determine both the direction of crack propagation and the onset of crack for a single propagating crack (Sutula *et al.* 2018b; Williams & Knauss 2012). This criterion is the only criterion which is consistent with Griffith’s energy release rate concept (Sutula *et al.* 2018b; Wu 1978). Furthermore, this criterion is consistent with thermodynamical principles as well (Wu *et al.* 2006). According to this criterion, we can conclude that fracture happens along the path which minimises the energy release rate.

For the DEM data we studied, the energy release is mainly calculated from the dissipated energy of broken contacts. There exists also numerical damping and plastic dissipation and they are negligible. Thus, the energy releases rate for a path Γ for a given time stage ϵ is given by

$$E_{rr} = \sum_{e* \in \Gamma(\epsilon)} E_{max} - \sum_{e* \in \Gamma(\epsilon-1)} E_{max}, \quad (2.13)$$

where e^* denotes a broken contact.

2.2.1.4. The minimum strain energy density criterion

The minimum strain energy density criterion assumes that fracture propagates in the direction where the strain energy density is minimum (Sih 1973). According to (Sutula *et al.* 2018b), this criterion can also be used to determine both the direction of crack propagation and the onset of crack. The crack will propagate when the minimum strain energy density S reaches a critical value S_{cr} (Mirsayar & Hartl 2019; Sun & Jin 2012). This means that crack initiates (onset of crack) when $S = S_{cr}$. The critical value is related to the fracture toughness (the ability to resist fracture for a material containing a crack) and is a material property.

Therefore, it is intuitive to assume that fracture will occur along the path with the minimum strain energy density. For the DEM data we studied, we have information on strain energy and critical strain energy for individual bonded contacts. Therefore, the energy density for a path Γ for a given time stage ϵ is given by

$$S = \sum_{e \in \Gamma} E_r / (r_{min})^2, \quad (2.14)$$

where $E_r / (r_{min})^2$ is the energy density for the bonded contact e . $(r_{min})^2$ is the bond (contact) area.

According to this criterion, crack initiates when $S = S_{cr}$. Therefore, this criterion cannot be used to predict the ultimate macrocrack path. But, we can test the predictive capacity of the critical strain energy density criterion given by

$$S_{cr} = \sum_{e \in \Gamma} E_{max} / (r_{min})^2, \quad (2.15)$$

where $E_{max} = \gamma$ is the fracture energy of e .

2.2.1.5. The maximum normal stress criterion (the Rankine stress criterion)

Galileo introduced the concept of stress in the 17th century. He studied the failure of solids by using combined mathematical and experimental methods. He observed that macrocrack occurs along the plane with the maximum normal stress (Qu *et al.* 2016). This criterion is now referred as the Rankine stress criterion (Rankine 1857) or the maximum normal stress criterion. It can be used to predict a macrocrack of a brittle material that failed by crack formation. The normal stress for a virtual path Γ is given by

$$\sigma_\Gamma = |\vec{F}_n| / a, \quad (2.16)$$

where $|\vec{F}_n|$ is the magnitude of the normal force and a is the area of the path Γ .

For the DEM data we studied, the normal stress for a path Γ for a given time stage ϵ is given by

$$\sigma_{\Gamma} = M = \sum_{e \in \Gamma} \sigma_e, \quad (2.17)$$

where $\sigma_e = \sqrt{f_x^2 + f_y^2} / (r_{min})^2$ is the normal stress for the bonded contact e . f_x and f_y are the tensile normal contact forces for bonded contact e in global directions.

2.2.2. Limitations and current issues of existing fracture/failure criteria

Here we discuss the drawbacks of the above-mentioned fracture mechanics criteria. The aforementioned crack prediction criteria can be used to predict the onset of crack location and the direction of crack propagation. However, the Rankine criterion and minimum strain energy density (S-criterion) predict the failure at some critical states (Wu 1978; Qu *et al.* 2016). Critical states are characterised by critical stress. This means that these criteria may not have a predictive capability. These criteria were mainly developed for the presence of a single microcrack or interaction of few microcracks. These criteria are mainly applicable for brittle materials. In reality, bonded granular materials may contain a few hundred of microcracks such that some of them interconnect to form a macrocrack. In particular, the DEM data we studied contain many microcracks and a few interconnected to form the ultimate macrocrack. It is important to study crack interactions in order to better understand the mechanical behaviour of bonded granular materials. However, there was a handful of research carried out to study both crack initiation and crack interaction than the single crack problem (Sutula *et al.* 2018a).

As discussed in Chapter 1, concrete is complex, heterogeneous and disordered material. The classical fracture and failure criteria like Griffith theory or the Coulomb failure criterion are for homogeneous and isotropic materials (Vu *et al.* 2019). This is also clear from the assumptions given above in deriving Griffith's critical stress formula. Therefore, these criteria predict global failure without an early warning. However, a precursory phenomenon is important in hazard monitoring like earthquakes, cliff collapses, landslides or volcanic eruptions to prevent losses. Therefore, it is important to predict those failures well before it happens in order to take preventive and mitigative actions. Another limitation of Griffith's theory is that the assumption of a straight crack (Trent & Margolin 1992). But, in reality, this is not generally true, as discussed above. Moreover, Griffith's theory is developed for brittle materials like the glass where the structure is homogeneous. Therefore, a straight crack is possible. However, for heterogeneous materials like concrete, bond strength is what matters when deciding the crack path.

Today, Griffith's theory has appeared as the platform when developing a new fracture criterion (Sutula *et al.* 2018b). Many fracture criteria exist (Razavi *et al.* 2018). Yet despite this, predicting where and when a crack initiates and propagates is still debating

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(Vu *et al.* 2019; Yin *et al.* 2015). As pointed in Tanné *et al.* 2018, fracture mechanics still faces many challenges in identifying crack path and far from the settlement.

In conclusion, the validity of the aforementioned fracture mechanics and failure criteria are still debating and there is no universally accepted criterion. Those classical theories may not have a predictive capability, i.e., cannot predict the failure sufficiently early in the prefailure regime. Therefore, developing a method to predict the ultimate location of the failure path in disordered and heterogeneous granular materials is still an open question and flourishing field.

2.3. Models to predict preferential paths for force transmission and crack propagation

Here we discuss the existing network flow models to predict preferential path for force transmission and damage propagation. There are experimental and numerical evidence for the existence of preferential paths for force transmission and crack propagation as discussed above. To visualise the preferential paths for force transmission, researchers have been using the measure of contact forces or developed algorithm which uses the information on contact forces. Experimental measurements of contact forces in bonded granular materials remain limited. Thus, a method that can identify the majority of the grains in force chain structures without knowledge of contact forces is useful. Such a method is proposed in Tordesillas *et al.* 2015b. That utilises a network flow approach called the maximum flow minimum cost analysis. The idea there was to map the given contact network to a flow network and find the optimised routes. Findings suggest that the majority of compressive force chains lie along the optimised routes. However, there is no study on predicting tensile force chains in a tension test. Here we seek to fill this knowledge gap by employing a similar technique to Tordesillas *et al.* 2015b.

A network flow framework has been also used to predict the localised failure zone (shear bands) in unbonded systems for 2D and 3D Tordesillas *et al.* 2013; Lin & Tordesillas 2014; Tordesillas *et al.* 2015a. Data came from experimental or numerical simulation of different syntactic or natural granular materials under different loading conditions. In those studies, the idea was to model the force transmission in those unbonded systems and use force bottleneck to predict the localised failure zone. The force bottleneck is the location where it impedes the applied load and hence, the most vulnerable part of the system. To find the force bottleneck, the contact network was mapped to a flow network. Two artificial nodes so-called the source and the sink are selected according to the applied load. Due to a general lack of *a priori* information on the contact strengths, the contact strength was modelled using the readily available kinematic data and the contact topology (Tordesillas *et al.* 2013, 2015a). The maximum flow minimum cut analysis then carried out to identify the minimum cut which corresponds to the force

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bottleneck. Results revealed that minimum cut (force bottleneck) predicts the localised failure zone well before the peak stress and prediction persists.

[Patel *et al.* 2019](#) investigated the stress flow pattern in bio-structures using the rostrum of Paddle-fish. The strain localisation in the tensile region and buckling in the compression region plays a vital role in failure mechanisms. To study the evolution of stress in the rostrum, [Patel *et al.*](#) formulated the problem as a network flow problem. The flow network is constructed by using the extracted information on the node and the connectivity from the numerical model of the rostrum. The flow network was weighted based on the stress. Results showed that this approach identified strain localisation in tensile regions, and buckling/crushing in compressive regions.

An imaged based technique to predict the crack path in brittle materials such as ceramics, fibre composite, and metals has been proposed in [Sundararaghavan & Srivastava 2017](#). The idea was to find the path with the least resistance in the microstructure. The path of least resistance was formulated as a process of minimising a discretised cost function, based on an Ising-type energy model and solved by using the maximum flow minimum cut theorem. A good agreement has been archived with the prediction and user imposed macroscopic crack. In this case, [Sundararaghavan & Srivastava](#) does not formulate a problem as a network flow problem.

As discussed above, there are existing network flow models to predict the localised failure zone in unbounded granular materials. However, according to the best of our knowledge, there is no network flow method to predict the location of the ultimate macrocrack in disordered and heterogeneous bonded granular materials like concrete. In the literature, various aspects of force transmission and crack propagation have been studied for bonded and unbonded systems as discussed above. However, the coevolution of force transmission and damage propagation has not been explored universally. These paths coevolve and depends on each other. When damage occurs, stress redistributes to cope with the damage ([Aggelis *et al.* 2013](#); [Mazars *et al.* 1991](#)). Also, redundancy plays a major role in stress redistribution ([Fernández Ruiz & Muttoni 2018](#)). This thesis aims to fill these knowledge gaps by developing methods within a network flow framework to predict preferential paths for force transmission and damage propagation where the precise information on contact (bond) strength is available.

3. Discrete element method (DEM) simulation data studied

One of the key difficulties in analysing the development of failure in *real granular systems* is the complexity of the loading conditions to which the material is often subjected. Consequently, a common approach is to decompose real loading conditions to a set of basic and idealised loading conditions, for example, uniaxial tension and uniaxial compression, where system behaviour can be more easily interpreted. This is reasonable since these idealised loading conditions mimic conditions experienced locally in some real-world granular structures. For example, as shown in Figure 3.1, the head of a landslide develops tension cracks similar to those seen in uniaxial tension while shear cracks develop along the sides similar to those seen in uniaxial compression (Martel 2004). Thus, an understanding of the evolution of failure in idealised laboratory test systems is useful if not essential to understanding what happens in complex real-world settings. Equally important is that by analysing these basic tests, we can more readily compare the performance of our new predictive models of fracture relative to existing theories that are commonly applied to these tests.

Accordingly, in this research, we study four data sets from simulations of laboratory specimens under uniaxial loading conditions: two from uniaxial tension and two from uniaxial compression. These data were provided to our group by, and as part of a collaboration with, Dr Michał Nitka and Prof Jacek Tejchman from Gdańsk University of Technology, Poland. The data sets for uniaxial tension have been described and analysed in Tordesillas *et al.* 2020.

The rest of this chapter is organised as follows. In section 3.1, we discuss data sets for tension. In section 3.2, we discuss data sets for compression. However, detailed descriptions of data are given for tension samples unless there exists a difference as they come from the same family of DEM simulations.

3.1. Data sets for uniaxial tension

Here we discuss discrete element method (DEM) simulation data for concrete samples under quasistatic uniaxial tension without confining pressure. Concrete is modelled as 1-phase and 3-phase materials. We denote these two data sets 1T (1-phase tension) and 3T (3-phase tension). The DEM data sets come from a family of discrete element

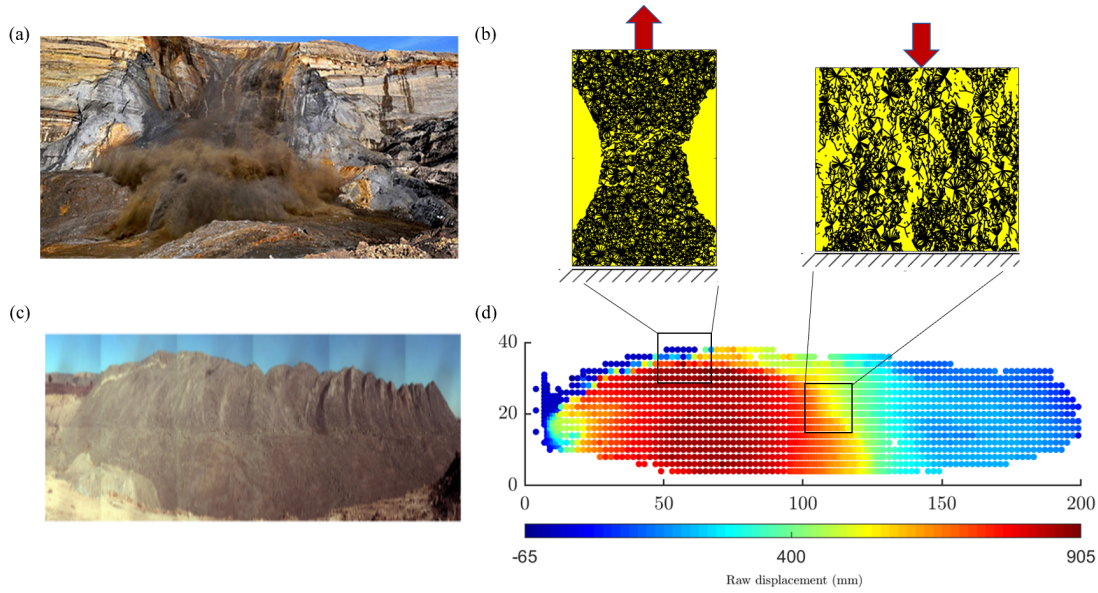


Figure 3.1.: *DEM data mimic basic loading conditions experience by small ensembles of real-world data. (a) Rockslide in an open-pit mine ^a. (b) Remaining bonded contacts in 1-phase tension and compression samples here visualised as a line joining centres of two grains in contact. This highlights the final crack pattern (space without black lines). The yellow background is only for improving contrast. (c) A visual of a monitored open-pit mine with known location and time of failure (Tordesillas et al. 2018). Failure is similar to (a). (d) The spatial distribution of accumulated displacement at failure. This highlights the failure boundary.*

^a<http://dzhnews.com.ph/philippines-coal-mine-collapses-3-dead-6-missing/>

method (DEM) simulations of fracture in concrete (Nitka & Tejchman 2015; Skarżyński et al. 2015; Suchorzewski et al. 2018a,b; Nitka & Tejchman 2018). Models in two- and three-dimensions were developed for 1-phase (contain aggregate and cement matrix, but contact properties are the same), 3-phase (aggregate, cement matrix, interfacial transitional zones (ITZs)), using the explicit 3D spherical, open-source DEM code YADE (Kozicki & Donzé 2008; Šmilauer & Chareyre 2010).

The 3D simulations provide more realistic outcomes than the 2D ones (Nitka & Tejchman 2018). The stress differences between 2D and 3D DEM simulations for concrete were found to be minimum at the peak load. Those differences increase with growing postpeak deformation when assuming the same material parameters. However, the 2D analyses may be also used for obtaining realistic results of fracture (location, shape and width) and a postpeak stress-strain response when: a) the 2D DEM model is properly calibrated for concrete with laboratory tests and b) the 2D calculations are performed for the given concrete mesostructure in a cross-section.

When preparing the DEM samples, X-ray micro-computed tomography was used to ensure a realistic representation of the aggregate sizes and shapes and other geometrical

properties of the mesostructure (Figure 3.3). We will discuss this in more detail next.

3.1.1. Mapping of mesostructure of real concrete to DEM models

The structure of concrete is heterogeneous and disordered as shown in Figure 1.1 (a) of Chapter 1. Therefore, it is important to mimic the real mesostructure of concrete when designing numerical samples to get a realistic representation. That is, we need to map the size and shape of the grains. This enables us to study the mechanical behaviour of concrete more accurately. Moreover, these factors control the trajectory of the crack path. The size distribution of grains determines the packing of the concrete sample and hence the connectivity of the specimen. In our analysis, as we will discuss in Chapter 4 bonded contact network (contact network consisting only the bonded contacts) is one of the inputs.

X-ray micro-tomography is used to render the real shape and size of the aggregate particles. Here the concrete sample is subjected to X-rays and the detector is placed directly opposite to the X-ray source. Then the 3D rendering process is used to process the X-ray image to determine the size and the shape (Figure 3.2). This information will be mapped when preparing the DEM samples for concrete to ensure a realistic representation of the aggregate sizes and shapes and/or geometry of the mesostructure (Figure 3.3). To get the real shape of aggregate, they are modelled as clusters of spheres. But, for the data we study, aggregates are modelled as single spheres with the actual size distribution for the simplicity.

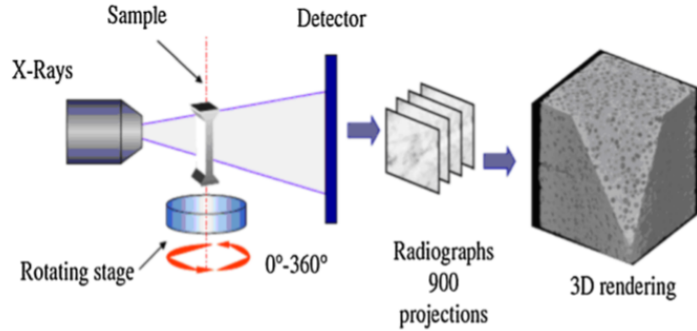


Figure 3.2.: Operation principle of X-ray micro-tomography. This figure shows the procedure used to determine the real size and shape of aggregate in concrete sample (Skarżyński & Tejchman 2016).

Not only the mapping of size and shape of the aggregate is important, but also other materials properties like contact strength. The contact strength has a major influence in deciding the macrocrack path. Therefore, it is paramount of importance to calibrate other parameters in DEM models against the experiments to get a realistic representation of actual concrete. In our analysis, the most important input is the contact strength. In the DEM data, the five main local parameters are necessary (Nitka

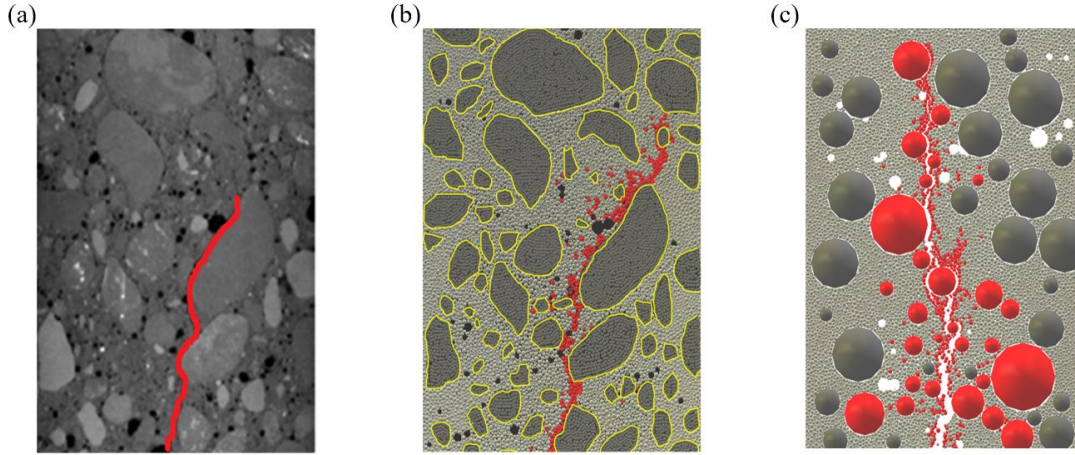


Figure 3.3.: Mapping of the experimental sample properties to the discrete element method (DEM) simulation (Skarżyński *et al.* 2015). Two-dimensional microstructure of concrete: (a) experiment (μ CT image), (b) DEM for real aggregate (clusters of spheres) and (c) DEM for real aggregate (spheres). Cracks and particles along cracks are shown in red; voids are white; aggregates are dark grey; cement matrix is light grey.

& Tejchman 2015). These parameters are calibrated against the experiments. Next, we will discuss this in more detail.

3.1.2. Laboratory tests to calibrate the DEM models

The performance of these models for describing fracture, fracture characteristics and size effect in concrete has been assessed under different loading conditions: bending (Skarżyński *et al.* 2015; Nitka & Tejchman 2018), uniaxial compression (Nitka & Tejchman 2015; Suchorzewski *et al.* 2018a) and splitting tension (Suchorzewski *et al.* 2018b; Suchorzewski & Tejchman 2018). Good agreement between numerical and experimental results on real concrete was achieved.

Numerical calculations were based on laboratory experiments on concrete performed by (Van Vliet & Van Mier 1999). The modulus of elasticity E_c , Poisson's ratio ν_c , inter-particle friction angle was μ , cohesive bond strength F_{max}^s , and tensile bond strength F_{min}^n was calibrated (Nitka & Tejchman 2015). In particular to calibrate 1-phase tension sample, concrete with the following properties was used (see Tab.1): water-cement ratio $w/c = 0.5$, Portland cement type B 375 kg, aggregates 2-8 mm in diameter - 903 kg and sand 0.125-2 mm in diameter - 905 kg). The average compressive strength of cubes was 50 MPa. The size and shape of the specimen (dog-bone shape) were shown in Fig. 1 of Van Vliet & Van Mier 1999 (specimen "B": height - 150 mm, width - 100 mm and depth - 100 mm). The experimental force - deformation curve was shown in Fig.3 of Van Vliet & Van Mier 1999. The experimental nominal tensile strength was $f_t = 2.97$ MPa. The shape of the crack in the numerical calculation was similar to that in the

experiment (Van Vliet & Van Mier 1999).

For 3-phase sample, the thickness of the concrete specimen in experiments was 100 mm. The physical model was three-dimensional. To shorten a computer effort related to a huge number of particles in 3D conditions, the numerical concrete specimen was 2D one, i.e., it solely included one layer of particles. The particles of different sizes were made of aggregate and mortar. There were 200 aggregate spherical grains (diameter range 2 - 16 mm) and 8,000 mortar spherical grains (diameter range 0.25 - 2 mm).

3.1.3. Bond strength

Albeit bonds can break by shear in both specimens, the essential microscale mechanism for damage in the prefailure regime is bond breakage in tension (Nitka & Tejchman 2015). No new bonded contacts form during the tests. Moreover, bond breakage immediately results in loss of contact until after peak load when a small fraction of slip contacts emerge: from a mere 0.06% of all contacts just after peak through to 0.18% at the residual state for both specimens. Shear forces are relatively small throughout the prepeak regime: at peak load, the sum of the magnitudes of the tangential contact forces relative to that of the total contact forces is 26% for 1-phase tension (17% for 3-phase tension). Thus the contact capacity that is relevant to our analysis of force propagation is the tensile bond strength which is defined to be the force needed to break a bonded contact. Specifically, the bond strength is given by the minimum normal force F_{min}^n :

$$F_{min}^n = T_n(r_{min})^2. \quad (3.1)$$

where T_n is the minimum tensile normal stress and r_{min} is the radius of the smaller of the two spherical grains in bonded contact. For 1-phase tension, $T_n = 25$ MPa. For 3-phase tension, $T_n = 24.5$ MPa for cement-cement contacts, while $T_n = 17.5$ MPa for cement-aggregate(ITZ) contacts. Thus, the weakest bonds are those between aggregate and cement matrix grains. Next, we will give additional information on the contact laws and material parameters.

3.1.3.1. The contact laws and material parameters

Here, we give more detail on the contact models used since the contacts and their capacities form an input to the network flow analysis. The DEM model takes advantage of the so-called soft-particle approach (i.e., the model allows for grain deformation that is modelled as an overlap of grains) (Fig.1, Eqns. 1-6 in Nitka & Tejchman 2015). The interaction force vector representing the action between two spherical discrete elements in contact was decomposed into a normal and tangential vector, respectively (Fig. 1(A) and 1(B) in Nitka & Tejchman 2015). A linear normal contact model under compression was used (Fig. 1(B) in Nitka & Tejchman 2015). The normal forces acting on spheres

were modelled by an elastic law with cohesion. The normal and tangential forces were linked to the displacements through the normal stiffness and the tangential stiffness. These stiffness values were computed as functions of the modulus of elasticity of the grain contact and the radii of the grains in contact for the normal stiffness, and the modulus of elasticity, Poisson's ratio of the grain contact, and the radii of the grains in contact for the tangential stiffness (Eqn. 3 in Nitka & Tejchman 2015). The unloading was purely elastic (Fig.1(C) in Nitka & Tejchman 2015).

The tangential and normal forces at contact were coupled together by the cohesive-frictional Mohr-Coulomb equation (Fig. 1(D), Eqn. 4 in Nitka & Tejchman 2015). The cohesive force and tensile force were assumed as a function of the cohesive stress (maximum shear stress at a pressure equal to zero), tensile normal stress and sphere radius (Eqn. 5 in Nitka & Tejchman 2015).

For 1-phase tension, the contact properties were as follows. For all grain-grain contacts, the modulus of elasticity $E_c = 15$ GPa, Poisson's ratio $\nu_c = 0.2$, cohesion $C = 140$ MPa. The grain-grain friction angle was $\mu = 30^\circ$, the mass density $\rho = 2500$ kg/m³ and the damping parameter $\alpha_d = 0.08$.

For 3-phase tension, the contact properties were as follows. For the cement-cement contacts, we assume: modulus of elasticity $E_c = 11.2$ GPa, Poisson's ratio $\nu_c = 0.2$, cohesion $C = 140$ MPa. For the cement-aggregate(ITZ) contacts, we assume: modulus of elasticity $E_c = 7.8$ GPa, Poisson's ratio $\nu_c = 0.2$, cohesion $C = 100$ MPa. The grain-grain friction angle was $\mu = 18^\circ$, the mass density $\rho = 2500$ kg/m³ and the damping parameter $\alpha_d = 0.08$.

3.1.4. Bonded contact network and the applied loading direction

As mentioned before bonded contact network is one of the inputs to our analysis. The applied direction of loading is another important input as we will discuss in Chapter 4.

For 1-phase tension, the specimen was subjected to a top boundary-driven tension while the bottom boundary was held at a fixed vertical position; both boundaries were free to move in the horizontal direction. The constant vertical strain rate of 10^{-3} per second, applied on the top boundary, was small enough to ensure the test was conducted under quasistatic conditions. The evolution of the macroscopic tensile load (vertical force on the top boundary) and the number of broken bonds (normal grain contacts) with the vertical normal strain are shown in Figure 3.4. We analyze 11 equilibrium stages of the loading program: stages 1-9 in the prepeak regime and stages 10-11 in the postpeak failure regime. The initial and final number of bonds were 12,350 and 11,984, respectively. Initially, bonds did not break (stages 1-4, Figure 3.4). From stage 5 onwards, the damage was progressive as seen in the steady increase in the population of broken bonds (reaches 240 in stage 9 just before the peak load).

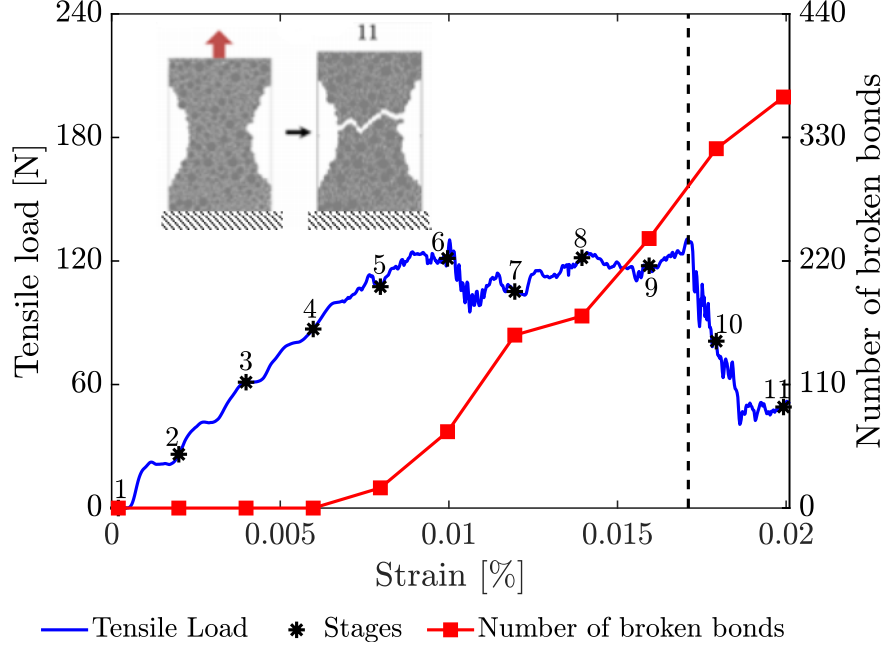


Figure 3.4.: 1T: Evolution with strain of the applied tensile load and total number of broken bonds in the sample. Dashed vertical line marks strain at peak load.

For 3-phase tension, the top and bottom boundaries of the specimen were pulled in opposite directions, at a constant vertical strain rate of 10^{-3} per second; both boundaries were free to move in the horizontal direction. We analyzed 47 equilibrium stages: stages 1-45 in the prepeak regime and stages 46-47 in the postpeak failure regime (Figure 3.5). The initial and final number of bonds were 23,492 and 23,062, respectively. Initially, bonds did not break (stages 1-14). From stage 15 onwards, progressive damage can be seen in the near-linear increase in the population of broken bonds (reaches 175 in stage 45 just before peak load).

As damage is progressive after stage 5 (15) for 1-phase tension (3-phase tension), some of the bonded contacts break (see Figure 3.6 for an example). This leads to the dynamic bonded contact network (bonded contact network will be different for each time stage of loading). But, contact strength for the bonded contacts will be the same throughout the loading history. Therefore, it is clear that we study dynamic contact network as one of the inputs being the bonded contact network in our analysis.

3.1.5. Crack pattern

One of the objectives of this research is to predict the location of the ultimate macrocrack. Note that we do not input the crack pattern to our analysis. We use only the location of the ultimate macrocrack to compare the prediction from our analysis with the actual macrocrack in Chpaters 6 and 7. In the DEM data, we have individual infor-

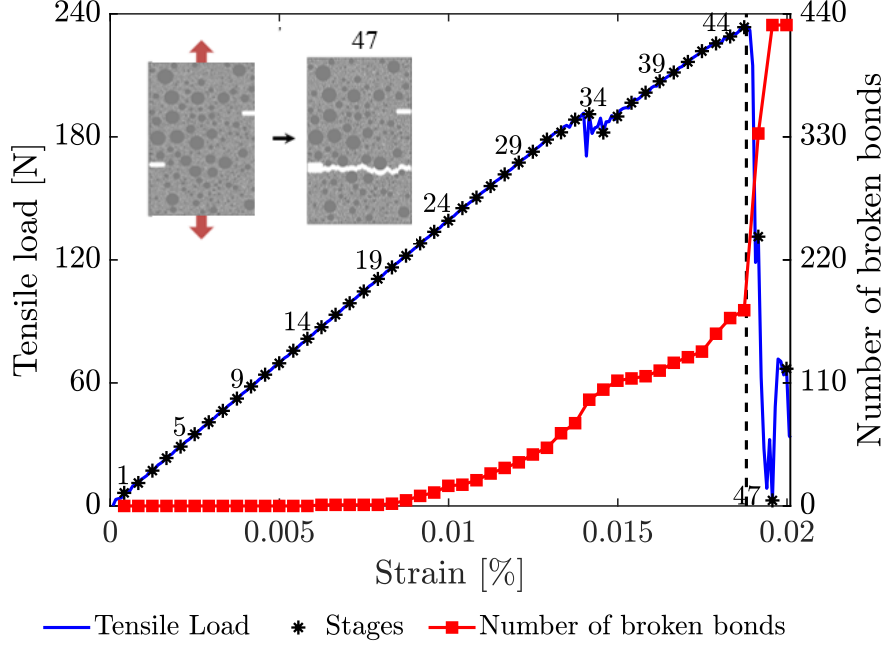


Figure 3.5.: 3T: Evolution with strain of the applied tensile load and total number of broken bonds in the sample. Dashed vertical line marks strain at peak load.

mation for each contact throughout the loading. That means, for a given time stage, we know which contact (bond) broke and what are the unbroken bonded contacts. Therefore, the location of broken bonds at the final stage gives us the final macrocrack as we discuss next.

For 1-phase tension, damage evolves as shown in Figure 3.7. The initial sites of damage were spread throughout the specimen, although fracture started almost simultaneously at the right and left corners of the specimen along the mid-region or “neck” of the specimen (stage 5); these form the ends of what will later become the primary macrocrack. At stage 6, a group of interconnected bonds on the lower-left region of the specimen collectively broke, giving way to a second macrocrack in the lower region of the specimen (stages 7-8). Just before peak load, the crack in the mid-region became dominant as damage spread rapidly across the neck of the specimen, while the second crack did not develop further (crack arrest and closed in stages 9-11). The primary macrocrack that formed in stage 11 exhibited a zigzag pattern that spanned the neck of the specimen (Figure 3.6 (c)). Similar tortuous patterns were found in other studies of concrete specimens, especially where cracks formed around the aggregate grains, i.e., ITZ zones and aggregate-cement contacts (Pease *et al.* 2006; Schlangen 2008; Mindess & Diamond 1982; Bentur & Mindess 1986).

For 3-phase tension, damage evolves as shown in Figure 3.8. The sites of damage were initially spread throughout the specimen but began to concentrate in two regions

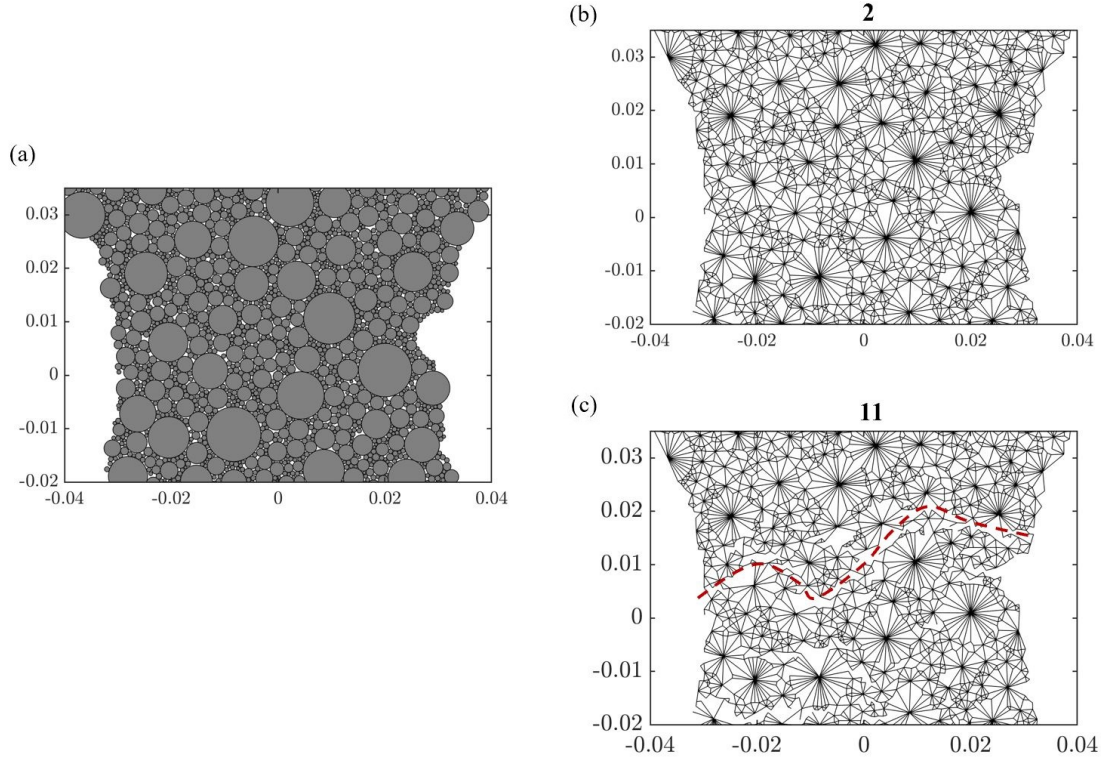


Figure 3.6.: 1T: (a) Visual of sample around the neck region. Corresponding bonded contact network for the sample in (a) at (b) initial stage and (c) the final stage. This highlights the degradation of contact network and the macrocrack path. Dashed line highlight the ultimate macrocrack.

in stages 24-33. The first site was near the lower-left notch (stage 24): just before and around peak load, damage here spread rapidly across to the right of the specimen, leading to the primary macrocrack at stage 47. The second site, located in the weak ITZ zones in the upper region of the specimen just above and near the second notch (≈ 0.035 above the specimen midline), gave way to a second macrocrack at stages 32-33. Here we also observed a zigzag crack pattern and the macrocrack path is perpendicular to the direction of applied loading. This is the typical fracture pattern observed for specimen under tension as discussed in section 2.2 of Chapter 2. Thus, we see can that the DEM model is a good representation of the mechanical behaviour of actual concrete.

3.1. DATA SETS FOR UNIAXIAL TENSION

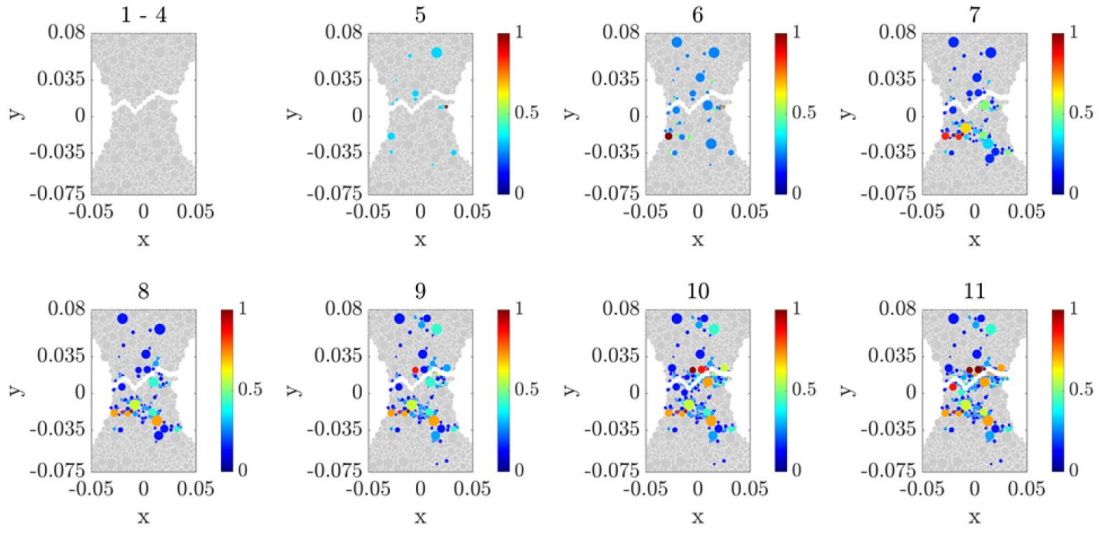


Figure 3.7.: 1T: Spatial distribution of grain damage d_p (the number of broken bonded contacts). Undamaged grains, $d_p = 0$, are colored gray. Damaged grains, $d_p > 0$, are colored according to $\hat{d}_p$ (d_p normalized to its maximum value for the given stage) using a blue-red colormap to highlight the variability of damage. An artificial separation between the grains on either side of the macrocrack that develops after peak load is introduced to aid a visual comparison with the grains that sustained damage. Damage in the lower portion of the specimen momentarily dominates over stages 7 – 8.

3.1. DATA SETS FOR UNIAXIAL TENSION

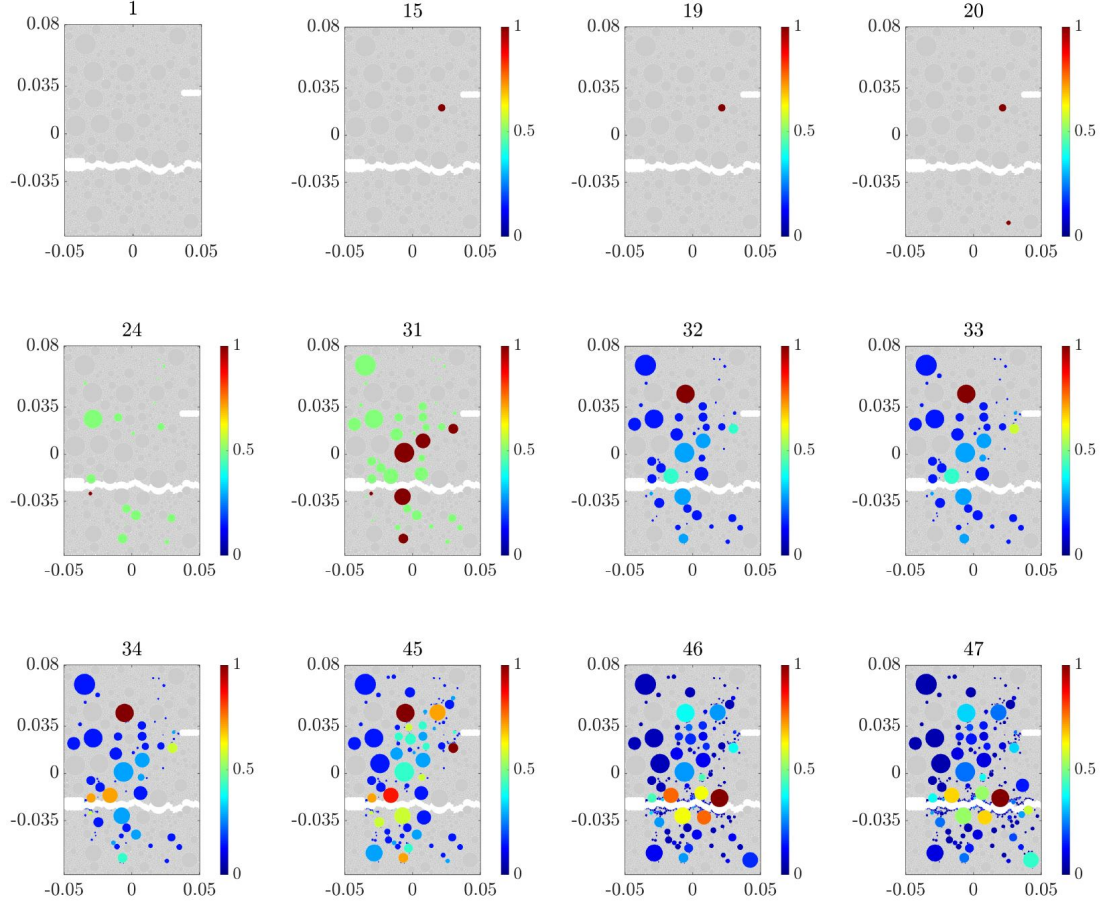


Figure 3.8.: 3T: Spatial distribution of grain damage d_p (the number of broken bonded contacts) at key stages of loading. Undamaged grains, $d_p = 0$, are colored gray. Damaged grains, $d_p > 0$, are colored according to $\hat{d}_p$ (d_p normalized to its maximum value for the given stage) using a blue-red colormap to highlight the variability of damage. An artificial separation between the grains on either side of the macrocrack that develops after peak load is introduced to aid a visual comparison with the grains that sustained damage.

3.2. Data sets for uniaxial compression

Here we discuss discrete element method (DEM) simulation data for concrete samples under quasistatic uniaxial compression without confining pressure. Concrete is modelled as 1-phase and 3-phase materials. We denote these two data sets 1C (1-phase compression) and 3C (3-phase compression). These samples also come from the same DEM family as uniaxial tension discussed above.

3.2.1. Mapping of mesostructure

When preparing a concrete sample for DEM simulations, the real mesostructure of concrete is mapped as in the case of uniaxial tension as discussed in section 3.1.1.

3.2.2. Laboratory tests to calibrate the DEM models

DEM models were calibrated as discussed in section 3.1.2. 1-phase sample contains 5016 grains having a wide distribution of radii with a minimum of 0.28 mm and a maximum of 5.3 mm. 3-phase sample contains 717 aggregate spherical grains and (diameter range 1.4 – 15 mm) and 17,959 mortar spherical grains (diameter range 0.17 – 1.6 mm).

3.2.3. Bond strength

For the compression samples, bonds can break due to both shear failure and tensile failure. However, shear failure is negligible in the prefailure regime (Nitka & Tejchman 2015). The main bond failure mode is tension even though the specimen is subjected to uniaxial compression. Therefore, bond (contact) strength relevant to force transmission is given by Equation (3.1).

3.2.3.1. The contact laws and material parameters

As these two samples come from the same family of DEM simulations, contact laws are essentially the same as those discussed for tension samples in section 3.1.3.1.

For 1-phase compression, the contact properties are similar to those for 1-phase tension. For 3-phase compression, the contact properties were as follows. For the cement-cement contacts, we assume: tensile normal stress $T_n = 25$ MPa, modulus of elasticity $E_c = 11.2$ GPa, Poisson's ratio $\nu_c = 0.2$, and cohesion $C = 140$ MPa. For the cement-aggregate(ITZ) contacts, we assume: tensile normal stress $T_n = 12.5$ MPa, modulus of elasticity $E_c = 4.48$ GPa, Poisson's ratio $\nu_c = 0.2$, and cohesion $C = 70$ MPa. The grain-grain friction angle was $\mu = 18^\circ$, the mass density $\rho = 2,500$ kg/m³ and the damping parameter $\alpha_d = 0.08$.

3.2.4. Bonded contact network and the applied loading direction

For 1-phase compression, the specimen was subjected to a top boundary-driven compression while the bottom boundary was held at a fixed vertical position; both boundaries were free to move in the horizontal direction. The constant vertical downward velocity of 10^{-3} per second, applied on the top boundary, was small enough to ensure the test was conducted under quasistatic conditions. The evolution of the macroscopic tensile load (vertical force on the top boundary) and the number of broken bonds (normal grain contacts) with the vertical normal strain are shown in Figure 3.9. We analyse 21 equilibrium stages of the loading program: stages 1-9 in the prepeak regime and stages 10-21 in the postpeak failure regime. The initial and final number of bonds was 13,757 and 7,202, respectively. Unlike the 1-phase tension sample, from stage 2 onwards, the damage was progressive as seen in the steady increase in the population of broken bonds (reaches 3,673 in stage 9 just before the peak load).

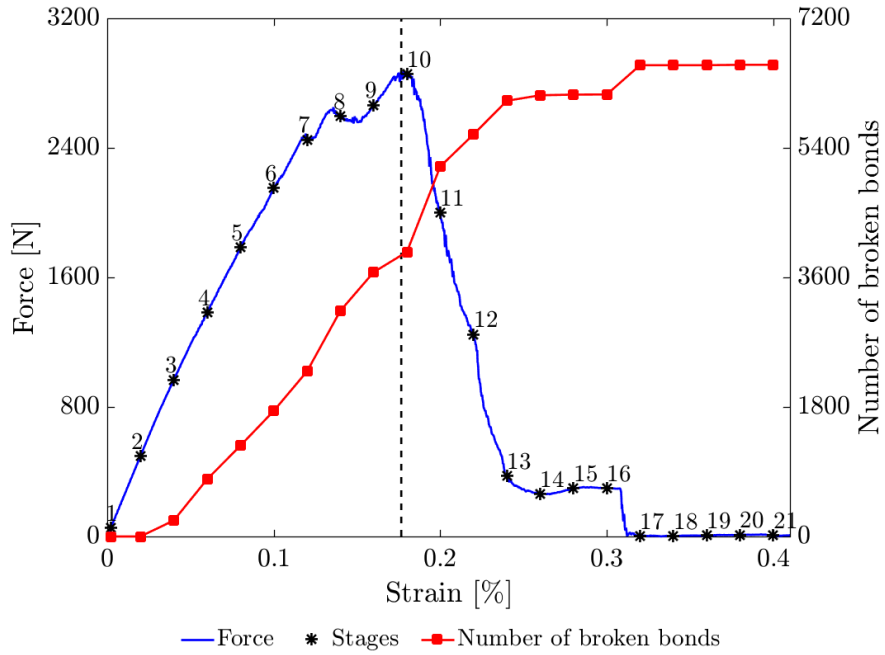


Figure 3.9.: 1C: Evolution of vertical force and number of broken bonds versus strain. Vertical dashed line indicates the strain state of the peak vertical force.

For 3-phase compression, the top and bottom boundaries of the specimen were pushed in opposite directions, at a constant vertical velocity of 10^{-3} per second; both boundaries were free to move in the horizontal direction. We analyzed 46 equilibrium stages: stages 1-15 in the prepeak regime and stages 16-46 in the postpeak failure regime (Figure 3.10). The initial and final number of bonds were 46,494 and 28,439, respectively. Unlike the 3-phase tension sample, from stage s onwards, progressive damage can be seen in the near-linear increase in the population of broken bonds (reaches 10,976 in stage 15 just

before peak load).

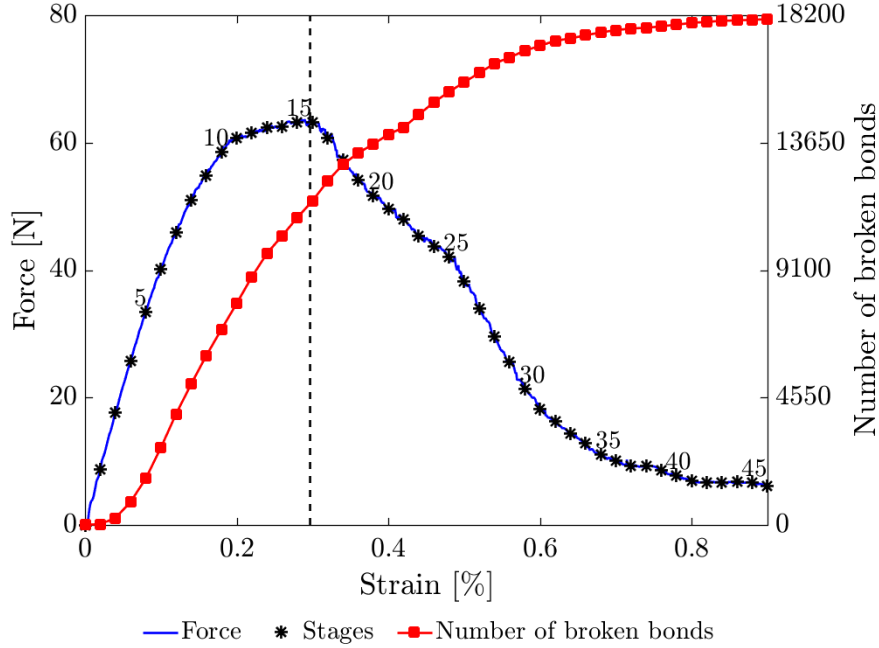


Figure 3.10.: 3C: Evolution with strain of the vertical force and total number of broken bonds in the 3-phase sample. Dashed vertical line marks strain at peak force.

These compression samples have more broken contacts compared to the tension samples even prior to the peak stress. That means the contact network of these samples degrades progressively. Moreover, these samples exhibit complicated crack patterns and pass through the top and bottom walls as we will discuss next.

3.2.5. Crack pattern

As we already pointed out, we do not input the crack pattern to our analysis. We use only the location of the ultimate macrocrack to compare the prediction from our analysis with the actual macrocrack in Chapter 8. For 1-phase compression, initially broken bonds are spread throughout. As loading progress and toward failure, broken bonds are concentrated to the final crack pattern which takes the shape of letter $\mathcal{M}$ with a tail (Figure 3.11 and Figure 3.12). The final major crack runs from the left top boundary to the middle bottom boundary. That means the final macrocrack is aligned with the direction of applied loading. There are some inclined minor cracks. This is consistent with the fracture pattern reported in the literature as discussed in Chapter 2.

The final fracture pattern ultimately splits the sample into 5 *partially connected* fragments. Three at the upper half region: left corner, middle and right corner and two at the lower half region: left and right corner of the sample. This final fracture pattern is evident from the displacement field shown in Figure 3.12 (a), as well as the spatial distribution of the remaining bonds shown in Figure 3.12 (b). The crack pattern is

3.2. DATA SETS FOR UNIAXIAL COMPRESSION

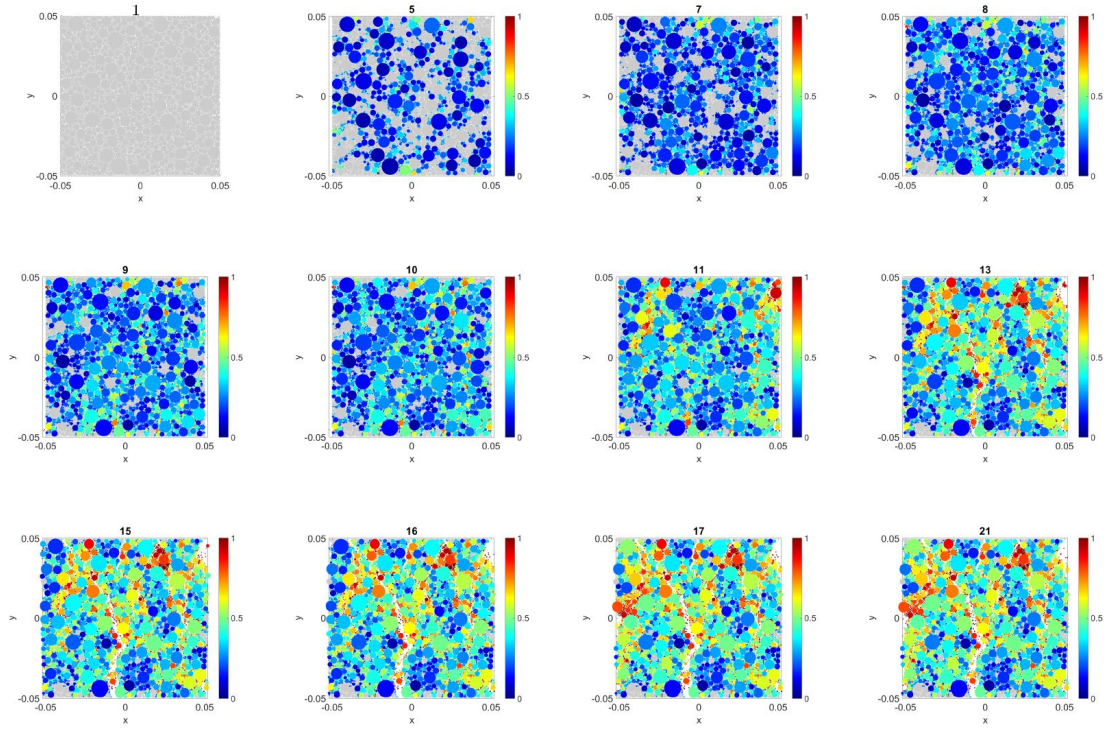


Figure 3.11.: 1C: Spatial distribution of grain damage d_p (the number of broken bonded contacts) at key stages of loading. Undamaged grains, $d_p = 0$, are colored gray. Damaged grains, $d_p > 0$, are colored according to $\hat{d}_p$ (d_p normalized to its maximum value for the given stage) using a blue-red colormap to highlight the variability of damage.

visible on the specimen after stage 11.

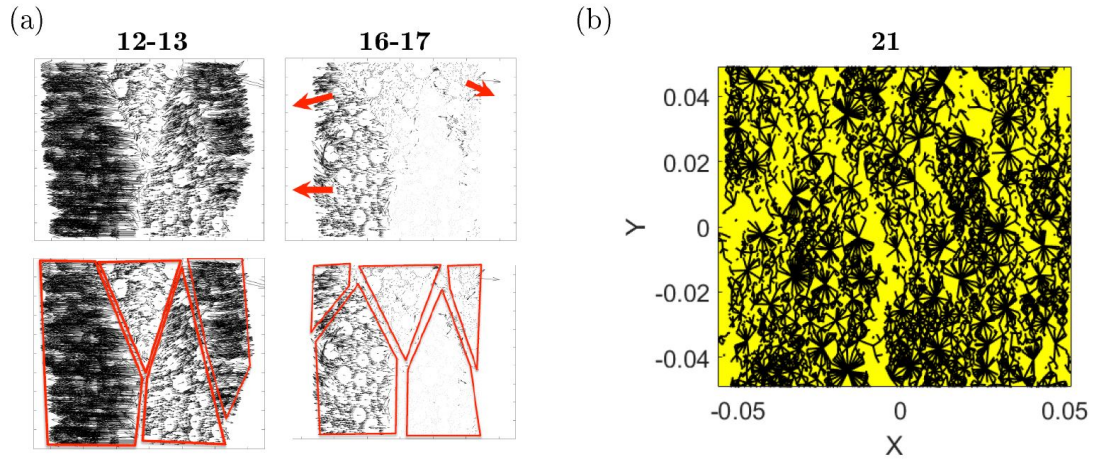


Figure 3.12.: 1C: (a) Displacement fields at two critical strain intervals, i.e., lower half of first drop and entire second drop from peak (top row), and corresponding fracture pattern highlighted (bottom row). (b) Spatial distribution of the remaining bonds (black lines) at final stage where yellow background is only to improve visual. This crack pattern is evident in Figure 3.11.

For 3-phase compression, initially broken bonds are spread throughout. As loading progress and toward failure, broken bonds are concentrated to the final crack pattern (Figure 3.13). As can be seen from Figure 3.14 (a), this specimen has different dominant cracks throughout the loading. This is evident in the displacement field (Figure 3.14 (b)). Note that crack patterns pass through the top and bottom wall as in the case of 1-phase compression, i.e., major crack is aligned with the direction of the applied load. This is the typical fracture pattern observed for specimen under compression as discussed in section 2.2 of Chapter 2. This further consolidates that the DEM model is properly calibrated with experiments. Thus, this further emphasises the DEM model is a good representation of the mechanical behaviour of actual concrete.

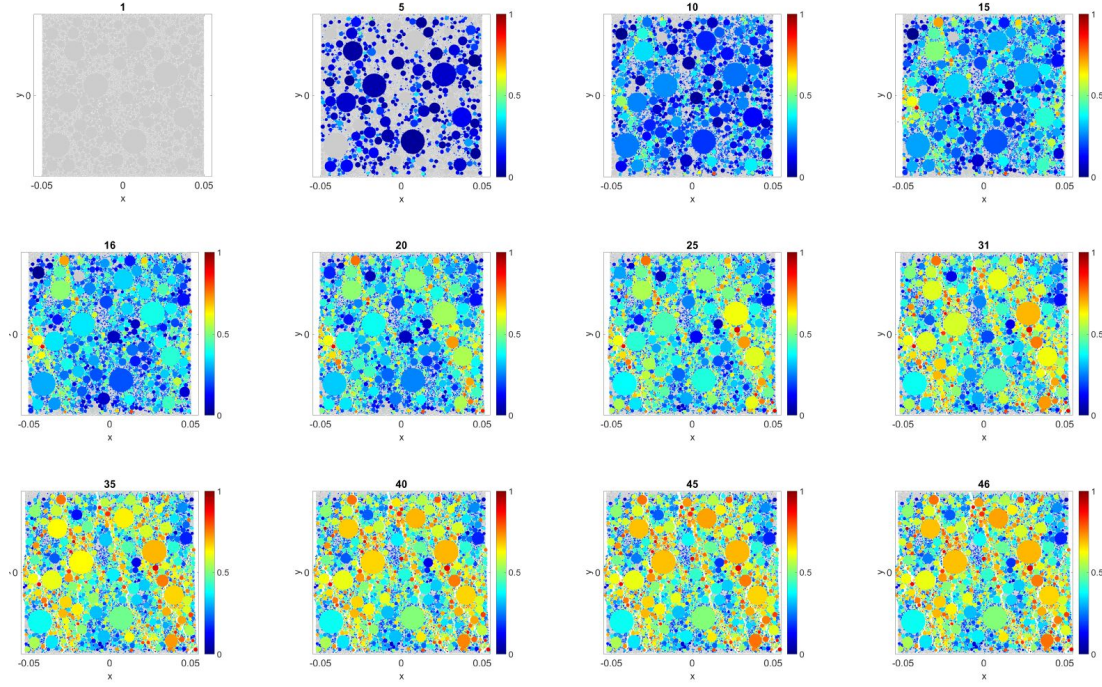


Figure 3.13.: 3C: Spatial distribution of grain damage d_p (the number of broken bonded contacts) at key stages of loading. Undamaged grains, $d_p = 0$, are colored gray. Damaged grains, $d_p > 0$, are colored according to $\hat{d}_p$ (d_p normalized to its maximum value for the given stage) using a blue-red colormap to highlight the variability of damage.

3.2. DATA SETS FOR UNIAXIAL COMPRESSION

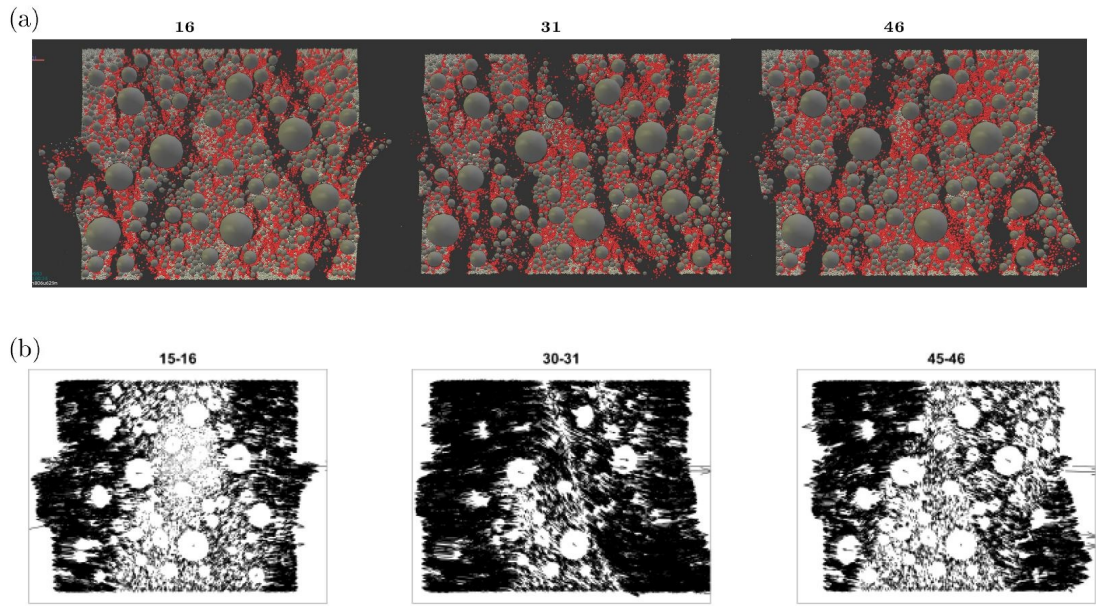


Figure 3.14.: 3C: (a) Crack patterns in 3C at different stages in the loading history. It shows that there is different dominant *major* crack through out the loading. Images are from DEM simulation data. (b) Displacement field at corresponding stages plotted for every other grains to enhance the visual. This is evident in Figure 3.13.

4. Methods

This chapter is dedicated to describing the network flow approach that is adopted in this research. In section 4.1, the model for the coupled evolution of force transmission and damage are presented along with how this model is applied to predict the preferential paths for force transmission and crack propagation. These methods are next extended to the analysis of energy transmission and the prediction of preferential paths for energy transmission and crack propagation in section 4.2. In both cases, we focus on uniaxial tension tests. More details are given for the force transmission analysis to avoid repetition of the many common steps with the study of energy transmission. In section 4.3, we address a key limitation of the approaches in sections 4.1-4.2 and propose a new method that can deal with the more complex crack patterns found in the compressions tests.

4.1. Methods for modelling force propagation

Here we develop a framework for modelling the transmission of tensile forces in the specimen (Figure 4.1). In particular, we present our network flow approach which used to predict preferential pathways for force transmission and crack propagation in tension samples. This is a data-driven approach. The key idea is to represent the transmission of tensile forces in the specimen as ‘flows’ through the contact network to extract nontrivial patterns in the data. This representation is valid and fit for purpose since the physical laws that govern the transmission of vector forces in the specimen satisfy the constraints of the underlying optimisation problem for the scalar flows in the flow network. We solve a set of optimisation problems on this network at each time stage ϵ . For each time stage, the *inputs* comprise data on the contact bond strengths and the contact network topology, and the *outputs* are the maximum flow, the preferential paths for force and damage.

This section is arranged as follows. In section 4.1.1, we discuss the creation of the flow network and how to determine the direction of flow. In sections 4.1.2 and 4.1.3, we show that the data obey the underlying constraints of the optimisation problem. In section 4.1.4, we discuss the maximum amount of flow that can be transmitted through the system (global transmission capacity) with given topology and the contact capacities. In section 4.1.5, we present a method to find optimal routes for force transmission. In section 4.1.6, we discuss a method to find force flow bottlenecks. In section 4.1.7,

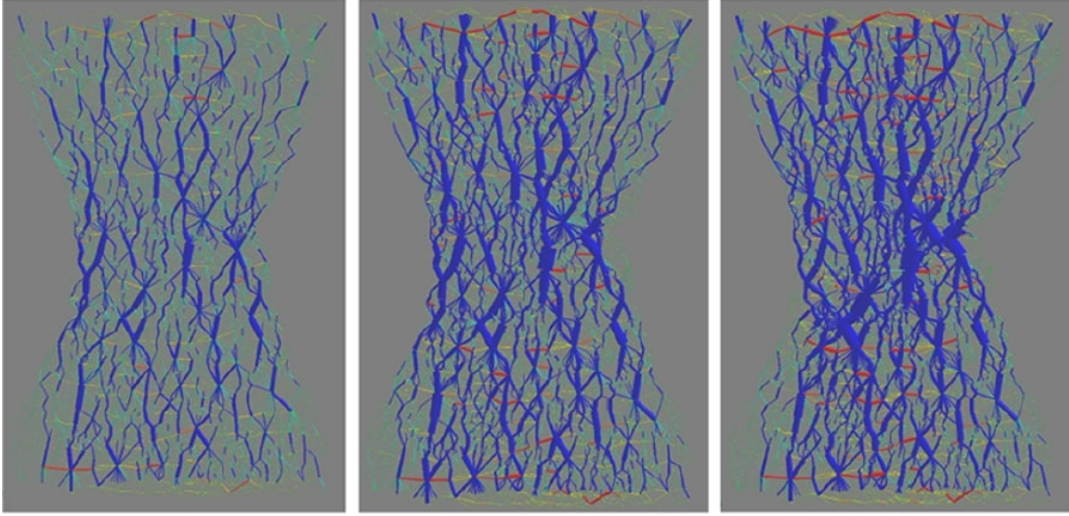


Figure 4.1.: *Tensile force propagation in bonded granular materials show tensile force chains are aligned in the direction of the applied tensile load.* Visualization of force chains in 1-phase tension at three different stages of loading (Nitka & Tejchman 2015). Force chains are visualized as a line joining the centre of two particles in contact. Line thickness is proportional to the magnitude of the normal contact force. Tensile forces are shown in blue; compressive forces are in red.

we present a method to find a cut with the minimum number of member contacts.

The network flow analysis has three key components. They are (a) the flow network and principal direction of flow, (b) the conservation of flow, and (c) the capacity rule. We will discuss these in more detail next.

4.1.1. Flow network and principal direction of flow

The flow network is represented by the bonded contact network $\mathcal{N}$ (Figures 4.2 and 3.6). Consider the bonded contact network $\mathcal{N}$ of the granular specimen for time stage ϵ . We map each grain with at least one bonded contact to a node and each bonded contact that can transmit tensile force to a link (Rattler grains with no contacts or grains with only unbonded contacts are excluded from $\mathcal{N}$). Thus, both the number of nodes and the number of links in $\mathcal{N}$ vary as loading proceeds. Next, we model $\mathcal{N}$ as a directed network G where all links are directed. Note that a directed link is usually called an arc. In G , a directed arc exists from a node w (representing a grain w) to a node v if grain w is in bonded contact with grain v . Since we model the force transmission and contact force obey Newton's third law, this is a symmetric relationship, i.e., arc (w, v) is in G if and only if arc (v, w) is in G . The set of nodes (grains) of G is denoted by V , and the set of arcs (bonded contacts) is denoted by A . Every arc e is associated with a non-negative capacity $q(e)$ which corresponds to the tensile bond strength, as

governed by the capacity function in Equation (3.1). The capacity function for all of A is therefore written as

$$q : A \rightarrow \mathbb{R}_+.$$

We designate one of the nodes of G as the *source* s , and another as the *sink* t . The quadruple $\mathcal{F} = (G, q, s, t)$ is called a *flow network*.

The principal direction of flow from source to sink is given by the direction of the applied loading. In grain contact networks, it is not immediately clear how to designate the source and sink nodes (s and t). Since the applied tensile load is in the vertical direction, an intuitive approach is to select all nodes in contact with the top wall as sources and all nodes in contact with the bottom wall as sinks. This results in a multiple source and sink flow problem. To reduce this to a single source and sink problem, we simply make the top and bottom walls as two new nodes of G , i.e., the supersource and supersink, respectively.

4.1.2. Conservation of flow

The conservation of flow requires that for any node in $\mathcal{F}$ except the source s and the sink t , the sum of the flows entering the node must equal the sum of the flows leaving the node. The vector forces that develop in the sample approximately satisfy the conservation rule due to Newton's third law, as illustrated for a representative tensile force chain grain **i** from 1-phase tension (Figure 4.2 (a)). The force flow entering grain **i** is the sum of the magnitudes of the forces from grain **i** on its neighbours (grey vectors), while the force flow leaving grain **i** is the sum of the magnitudes of the forces acting on grain **i** from its neighbours (blue vectors). Since grain **i** is in equilibrium, the force flow entering grain **i** is equal to the force flow leaving grain **i** (Figure 4.2 (b)). Figure 4.2 (c) shows the nodes and arcs between grain **i** and grains **1** and **2**: note that there are two oppositely directed arcs for each contact to take account of the symmetry of grain-grain links. Further evidence of a near-conserved flow for the entire specimen is evident in the symmetry of the polar plots for the normal tensile contact forces above and below the centroid of each grain, with a mean percentage error being less than 16% for 1-phase tension (11% for 3-phase tension) across all of loading history (Figure 4.2 (d)).

4.1.3. Capacity rule

The capacity rule dictates that the amount of flow $x(e)$ transmitted through any arc e in $\mathcal{F}$ is limited by the corresponding link capacity $q(e)$, i.e., $x(e) \leq q(e)$. In the network flow analysis, the contact capacity function plays a major role. Next, we discuss implication of the capacity function for 3 cases.

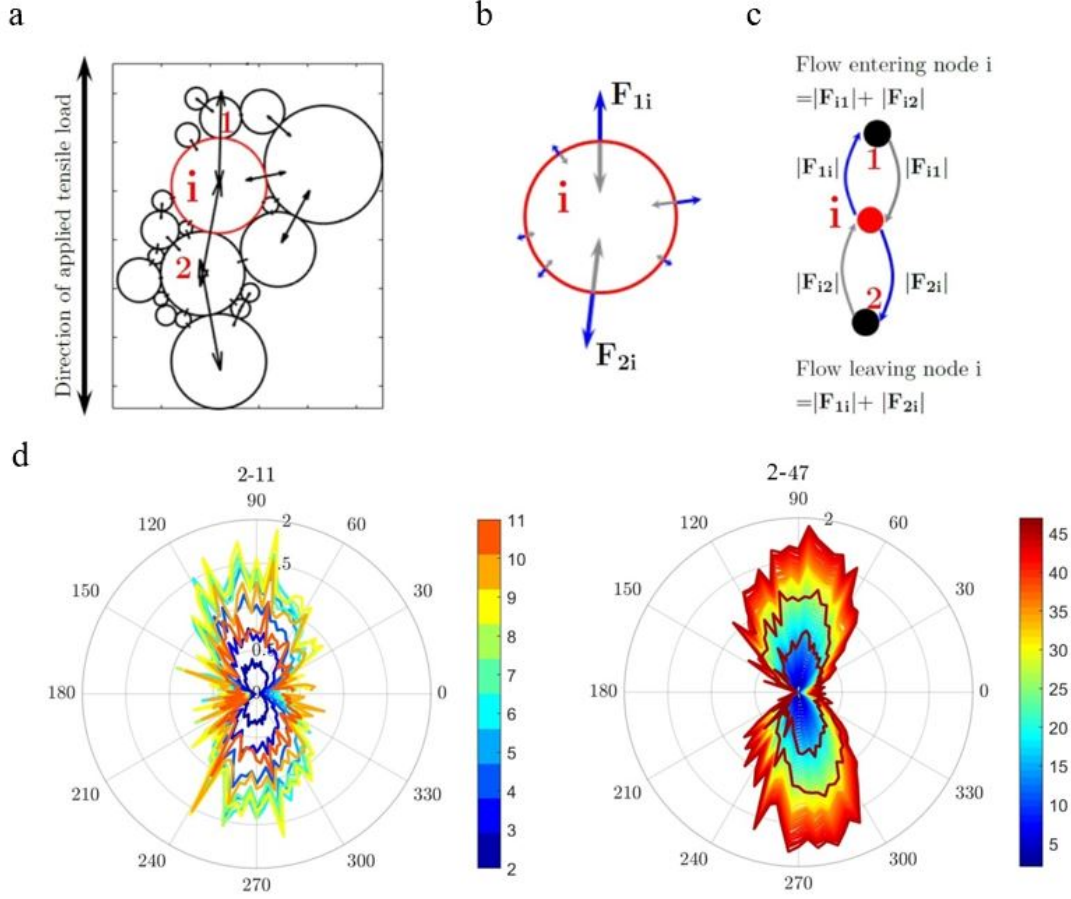


Figure 4.2.: Mapping the bonded contact network to the flow network. (a) Representative grain cluster embodying a tensile force chain with member grains $\{1, i, 2\}$, taken from 1-phase tension. Dominant normal tensile forces on grain i are aligned in the direction of the applied tensile load. (b) Blue (gray) arrows correspond to forces acting on i from neighbor grains (forces from i acting on neighbor grains). (c) Depiction of the conservation rule: force flow out of node i = force flow into node i (for clarity, only the arcs transmitting the dominant forces are shown). (d) Conservation of tensile force flow evident in the symmetry of polar plots for normal tensile contact forces above and below the centroid of each grain (from stages 2 to 11 (47) for 1-phase tension (3-phase tension)).

4.1.3.1. Generic capacity function

The capacity function relevant to force transmission is the tensile bond strength given by Equation (3.1). For tensile force transmission, capacity rule is automatically satisfied by the bond breakage criterion in the DEM model which requires that the tensile force at any contact cannot exceed the bond strength F_{min}^n . From Equation (3.1), the contact capacity is thus given by

$$q_F(e) = F_{min}^n(e) = T_n(r_{min}(e))^2 = \frac{T_n(e)A_b(e)}{\pi}, \quad (4.1)$$

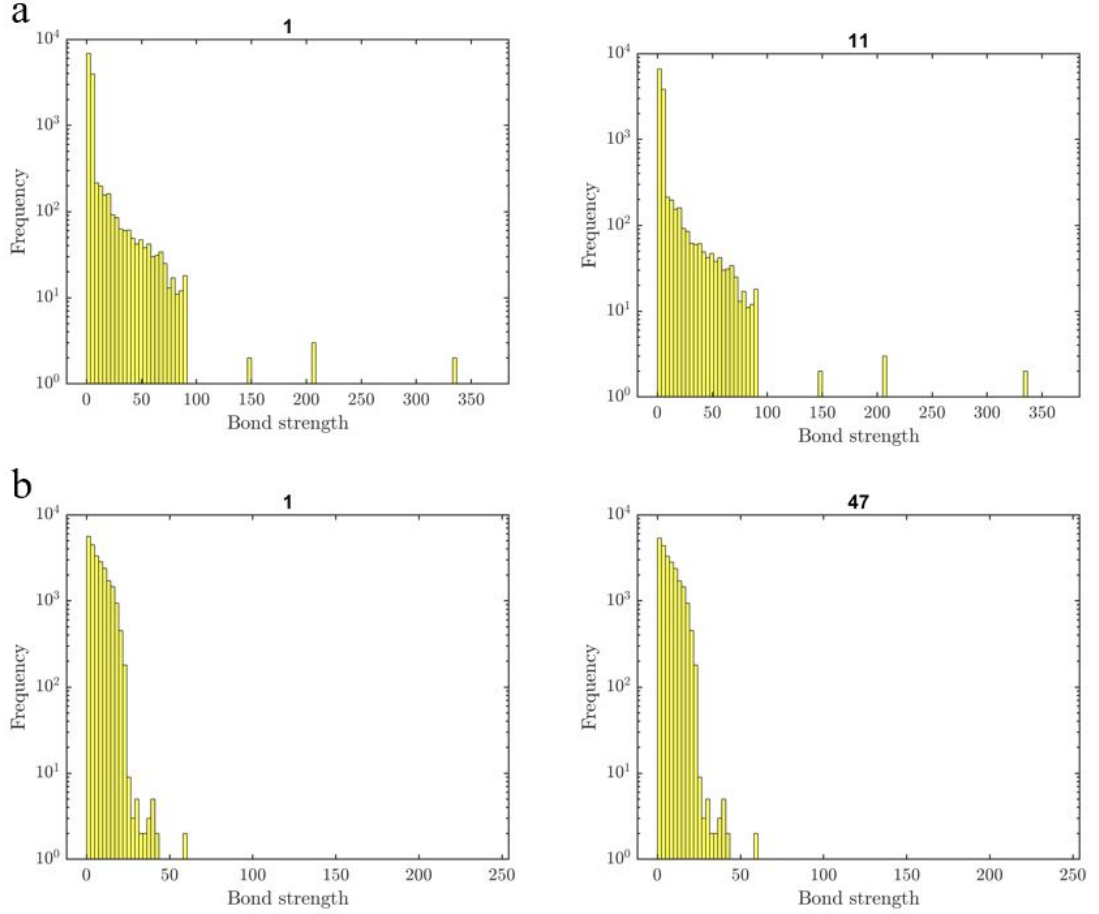


Figure 4.3.: Distribution of the contact capacity for force for (a) 1-phase tension and (b) 3-phase tension at the initial and final stage of the loading. Contact capacity for a bonded contact is constant throughout the loading. Distribution does not change much due to the limited bond breakages.

where A_b is the bond contact area $A_b = \pi r_{min}^2$. Flow network with this generic capacity function is referred to *force flow network* and denoted by $\mathcal{F}_F = (G, F_{min}^n, s, t)$.

Frequency distribution of the contact capacities given by Equation (4.1) is shown in Figure 4.3. Note that the contact capacity for a bonded contact is constant throughout the loading. Recall that these two tension samples do not contain many broken bonds. Therefore, distribution does not change much throughout the loading. Since many contracts have relatively high capacities, there is a possibility to change a cut with minimum capacity on it (sum of the capacities for the member contacts in the cut). This is due to the breakage of high capacity links in a cut that will result in a sudden decrease of the capacity and become the cut with minimum capacity. If this is the case, we should see this in the results from the minimum cut analysis.

4.1.3.2. Residual capacity function

We can extend the capacity function in Equation (4.1) to accommodate the loading state ϵ by using the current tensile contact forces. The contact capacity given by

$$\bar{q}_F(e) = F_{min}^n(e) - \|\vec{F}_n(e)\|, \quad (4.2)$$

where $\|\vec{F}_n\|$ is the magnitude of the normal tensile contact for the edge e . Flow network with this residual force capacity function is called a *residual force flow network* and denoted by $\bar{\mathcal{F}}_F = (G, F_{min}^n - \|\vec{F}_n\|, s, t)$.

4.1.3.3. Uniform capacity function

To demonstrate the effect on heterogeneity of capacity in network flow model, we use uniform contact capacity and given by

$$q(e) = C, \quad (4.3)$$

where C is a constant for every arc in $\mathcal{F}$. We use this as a reference flow network. Flow network with this uniform capacity function is called a *uniform capacity flow network* and denoted by $\mathcal{F}_C = (G, C, s, t)$.

4.1.3.4. Effect of a pre-factor in capacity function

Here we discuss the effect of pre-factor in capacity function, i.e., the effect of multiplying capacity by a constant for all the cases of capacity functions given above. This capacity function will not alter the distribution of contact capacities (shape of the distribution), i.e., this will preserve the relative values. Therefore, this will not affect the respective flow networks. Thus, results will not be changed with a pre-factor in capacity function.

4.1.4. Quantifying the global force transmission capacity

We propose a measure of global transmission capacity in the form of F^* , the maximum flow that the flow network $\mathcal{F}$ can sustain given its topology and link capacities. This involves solving an optimisation problem known as the *Maximum Flow Problem* (MFP). The MFP is equivalent to assigning force flows $x(e)$ to every arc e in $\mathcal{F}$, without violating the two constraints of conservation of flow and the capacity rule, such that the total amount of flow transmitted out of the source (or into the sink) in $\mathcal{F}$ is as high as possible.

Definition 1. Given a flow network $\mathcal{F} = (G, q, s, t)$, a flow x

$$x : A \rightarrow \mathbb{R}_+, e \mapsto x(e)$$

is called a *feasible (s, t) -flow*, if it satisfies:

(a) the conservation of flow

$$\sum_{e \in \delta^-(v)} x(e) = \sum_{e \in \delta^+(v)} x(e), \quad \forall v \in V - \{s, t\}, \quad (4.4)$$

where $e \in \delta^-(v)$ denotes arcs entering node v and $e \in \delta^+(v)$ denotes arcs leaving node v ; (b) the capacity rule

$$0 \leq x(e) \leq q(e), \quad \forall e \in A. \quad (4.5)$$

The *value of a flow* x , or net flow transmitted from the source s , is defined as

$$f(x) = \sum_{e \in \delta^+(s)} x(e) - \sum_{e \in \delta^-(s)} x(e). \quad (4.6)$$

We now have the following mathematical definition for our optimisation problem.

The Maximum Flow Problem (MFP): Given a flow network $\mathcal{F} = (G, q, s, t)$, find a feasible (s, t) -flow x such that $f(x)$ is maximum.

Since the applied tensile load is in the vertical direction, we select all nodes in contact with the top wall as sources, and all nodes in contact with the bottom wall as sinks. However, this results in a multiple source and sink flow problem, which our definition (above) does not incorporate. Fortunately, the multiple source and sink problem can be reduced to the classical maximum flow problem. We do this by selecting the top and bottom walls as two new nodes of G , i.e., the supersource and supersink, respectively; and then assigning infinite capacity to all contacts between walls and grains. In mathematical formalism we have the following:

Let $S \subset V$ and $T \subset V$ be disjoint sets of nodes of G . The quadruple (G, q, S, T) is called a *multiple-source, multiple-sink flow network*.

Definition 2. Given a multiple-source multiple-sink flow network (G, q, S, T) , a flow

$$x : A \rightarrow \mathbb{R}_+, \quad e \mapsto x(e)$$

is called a *feasible (S, T) -flow* if it satisfies:

$$\sum_{e \in \delta^-(v)} x(e) = \sum_{e \in \delta^+(v)} x(e), \quad \forall v \in V - (S \cup T); \quad (4.7)$$

$$0 \leq x(e) \leq q(e), \quad \forall e \in A. \quad (4.8)$$

The *value of a flow* x , or net flow transmitted from the supersource s , is defined as

$$f(x) = \sum_{e \in \delta^+(S)} x(e) - \sum_{e \in \delta^-(T)} x(e). \quad (4.9)$$

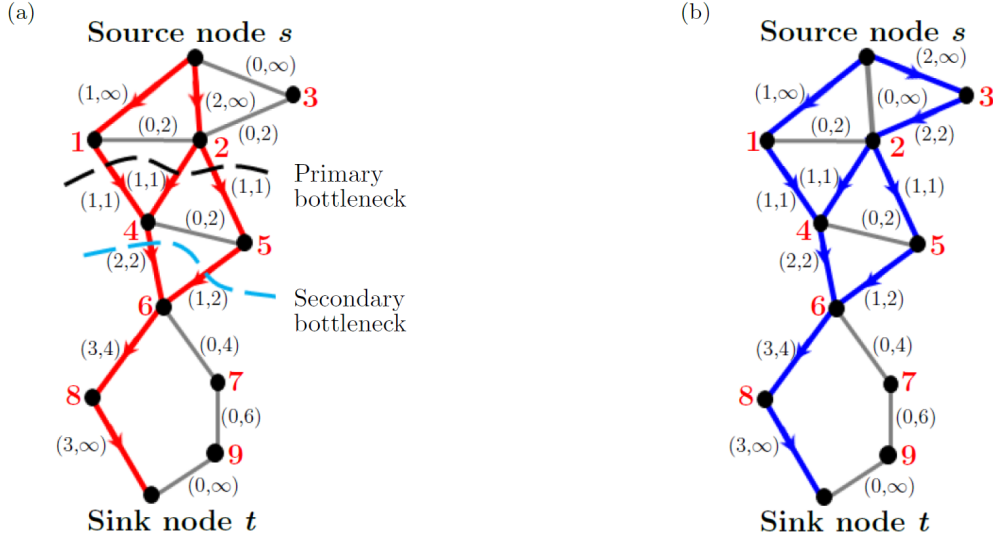


Figure 4.4.: A depiction of the multiple concepts discussed in sections 4.1.1-4.1.4. Two examples of a feasible (s, t) -flow with maximum flow $F^* = 3$. Link labels are of the form $(x(e), q(e))$. (a) Maximum flow pathways with unit cost $\mathcal{P}$ (red arcs), primary bottleneck or minimum cut (black dashed line), and secondary bottleneck (light blue dashed line). (b) Maximum flow pathways without cost (blue arcs). Gray arcs in (a) and (b) are not part of the maximum flow pathways: arcs with zero flow.

To solve the multiple-source multiple-sink maximum flow problem, we convert it to a (single source, single sink) Maximum Flow Problem as follows. Given (G, q, S, T) create a new node, the supersource s , and add an arc from s to every node in S . Similarly, create a new node, the supersink t , and add an arc from every node in T to t . Let the capacity of all new arcs be infinite. It can easily be shown that a maximum flow on the resulting flow network is a maximum flow on (G, q, S, T) when restricted to the arcs of G . Even for large networks, this problem can be solved efficiently by the use of existing algorithms (Ahuja *et al.* 1993).

Figure 4.4 is a toy example of a flow network showing two different flow assignments of equal value. Note that this figure serves to illustrate multiple aspects of the framework, both here and in future sections. Of relevance to the present discussion are the added arcs with infinite capacity from supersource s to nodes in S and from nodes in T to supersink t , where set S is $\{1, 2, 3\}$ and set T is $\{8, 9\}$. We use labels $(x(e), q(e))$ for each link e such that: $x(e)$ is the flow on e , $q(e)$ is the capacity of e , and each undirected link in the figure represents two arcs in opposite directions. The directed arcs which are not shown here correspond to zero flow. The maximum flow value F^* for this example is 3, as can be seen by summing the flows entering t or leaving s .

4.1.5. Predicting the preferential pathways for force transmission

As seen from Figure 4.4, solutions to the MFP are generally not unique. Depending on the algorithm used, different pathways may be used to transmit the flow through $\mathcal{N}$ from source to sink. In grain contact networks, there is a tendency for force chains to self-organise in quasilinear formation in alignment with the direction of the major principal stress axis (the vertical direction for the specimens studied here) (Nitka & Tejchman 2015). With respect to $\mathcal{N}$, such a pattern of self-organisation implies relatively short transmission paths. To capture this behaviour we extend our model to the *Minimum Cost Flow Problem* (MCFP). Solutions to this problem maximise total flow while also using paths that are as short as possible. We send the maximum flow F^* through the shortest possible paths to capture all the force chains (i.e., chains of high capacity links). If we push less than maximum flow F^* , we might not capture all the force chains. This is achieved by associating a unit cost with every arc in the network, and then solving the optimisation problem of finding a maximum flow through the network while also minimizing the total cost of all arcs used in the maximum flow. As with the MFP, there exist algorithms that can solve the MCFP for large networks (Ahuja *et al.* 1993).

In Figure 4.4, we depict two different maximum flow pathways: (a) maximum flow pathways with unit cost $\mathcal{P}$ (red arcs); (b) maximum flow pathways without cost (blue arcs). In Figure 4.4, grey arcs are not utilised in the flow pathways. As can be seen from Figure 4.4(a), the optimised routes $\mathcal{P}$ comprises the flow pathways $s - 1 - 4 - 6 - 8 - t$, $s - 2 - 4 - 6 - 8 - t$, and $s - 2 - 5 - 6 - 8 - t$. Each pathway has a length of 5 (5 arcs). The maximum flow value is 3 and the total cost (with the unit cost for each arc) is 15. In Figure 4.4(b) the flow pathways are $s - 1 - 4 - 6 - 8 - t$, $s - 3 - 2 - 4 - 6 - 8 - t$, and $s - 3 - 2 - 5 - 6 - 8 - t$. These paths have lengths 5, 6, and 6 and the maximum flow value is also 3. It is clear that $\mathcal{P}$ utilises shorter paths than the flow paths without cost. Note also that $\mathcal{P}$ is *not necessarily a subset* of the paths used in the MFP. From Figure 4.4(a), it is clear that link $(s, 2)$ is in $\mathcal{P}$, but not used in the flow of Figure 4.4(b). We now provide a formal definition of the MCFP.

The Minimum Cost Flow Problem (MCFP): The input of MCFP is a quadruple (G, q, b, c) , where $G = (V, A)$ is a directed graph,

$$q : A \rightarrow \mathbb{R}_+ \cup \{\infty\}$$

is a *capacity* function on arcs of G ,

$$b : V \rightarrow \mathbb{R}$$

is a *demand* function satisfying

$$\sum_{v \in V} b_v = 0,$$

and

$$c : A \rightarrow \mathbb{R}$$

is a *cost* function. We call b_v the *demand* (or *balance*) of v and $c(e)$ the *cost* of e . If $b_v \geq 0$ then v is a ‘demander’; if $b_v < 0$ then v is a ‘supplier’. Based on these, and the capacity $q(e)$ of arc e , the minimum cost flow problem is defined as follows.

We minimise the function

$$\sum_{e \in A} c(e)x(e),$$

subject to the net flow transmitted from any node v being given by

$$\sum_{e \in \delta^-(v)} x(e) - \sum_{e \in \delta^+(v)} x(e) = b_v, \quad \forall v \in V, \quad (4.10)$$

and

$$0 \leq x(e) \leq q(e), \quad \forall e \in A. \quad (4.11)$$

In our model, we let $c(e) = 1$ for all arcs e ; we let $b_v = 0$ for all $v \neq s$ and $v \neq t$; and we let $b_s = -F^*$ and $b_t = F^*$ where F^* is the maximum flow in G . Since the cost $c(e)$ of every arc is the same, solving the MCFP with these parameters creates an (s, t) -flow of value F^* while using flow paths that have as few arcs as possible.

4.1.6. Predicting the preferential pathways for damage propagation

Next, we look at the so-called ‘cuts’ of a network. A *cut* of a flow network is simply a partition of the nodes of the network so that the source is in one part of the partition and the sink in another. The capacity of a cut is the sum of the capacities of all arcs that leave the set of nodes containing the source and enter the set of nodes containing the sink. The cut with the minimum capacity is called the *minimum cut*. The minimum cut identifies the flow *bottleneck*. We find the preferential pathways for damage propagation from the flow bottlenecks, sites in the flow network that are highly prone to congestion. Pseudo-code for detecting flow bottleneck is given in Algorithm 1. The bottleneck is highly prone to congestion and is thus the most vulnerable part of a transmission network.

In a grain contact network, a cut can be visualised as a literal partition of the set of grains by means of a crack. In this sense, the capacity of the cut is the sum of the contact strengths (here bond strengths) between the grains separated in the crack. Therefore, the capacity of the cut is the fracture strength of the cut, i.e., the sum of the individual bond strengths required to break apart the bonds connecting the grains on either side of the cut. In Figure 4.4 (a) we depict two distinct cuts in a contact network using

dashed lines. The first cut is the minimum cut (the primary bottleneck), highlighted by the black dashed curve. It partitions the set of grains into two sets $\{1, 2, 3\}$ and $\{4, 5, 6, 7, 8, 9\}$. The links in this cut are $(1, 4)$, $(2, 4)$, and $(2, 5)$, each with a capacity of 1. The total capacity of this cut is, therefore, 3. The second cut, highlighted by the light blue dashed curve, partitions the network into $\{1, 2, 3, 4, 5\}$ and $\{6, 7, 8, 9\}$. The links in this cut are $(4, 6)$ and $(5, 6)$, each with the capacity of 2. The total capacity of this cut is, therefore, 4. We call this the secondary bottleneck since this cut has the second-lowest capacity: that cut with a capacity closest to the minimum cut capacity.

There is a useful relationship between the maximum flow F^* and the problem of finding the bottleneck. This arises from the famous Maximum-flow minimum-cut theorem in graph theory (Ahuja *et al.* 1993). The maximum flow and the minimum cut hold a dual relationship, namely, the maximum amount of flow that can be transmitted through a given flow network is equal to the capacity of the minimum cut. Now we define network cuts formally and give a mathematical description of the Maximum-flow minimum-cut theorem.

For $W \subset V$, denote $\overline{W} := V - W$. The sets W and $\overline{W}$ form a partition of V , and the set of arcs from W to $\overline{W}$, denoted by

$$\delta^+(W) = \{(v, w) \in A : v \in W, w \in \overline{W}\},$$

is called a *cut* of G induced by W . If the source $s \in W$, then $\delta^+(W)$ corresponds to the set of arcs leaving the set of nodes containing the source.

Definition 3. A cut $\delta^+(W)$ such that $s \in W$ and $t \in \overline{W}$ is called an (s, t) -cut of the flow network (G, q, s, t) . The *capacity* of such a cut is defined to be

$$q(\delta^+(W)) := \sum_{e \in \delta^+(W)} q(e).$$

The Minimum Cut Problem (MCP): Given a directed graph $G = (V, A)$ with two specific nodes, s (source) and t (sink), and a capacity $q(e) \geq 0$ on each arc $e \in A$, find an (s, t) -cut $\delta^+(W)$ with minimum capacity $q(\delta^+(W))$.

The Minimum Cut Problem is equivalent to the MFP by the following theorem.

Theorem 1. Maximum-flow minimum-cut theorem: In any network (G, q, s, t) , the maximum value of a feasible (s, t) -flow is equal to the minimum capacity of an (s, t) -cut. That is,

$$\max\{f(x) : x \text{ a feasible } (s, t)\text{-flow}\} = \min\{q(\delta^+(W)) : \delta^+(W) \text{ an } (s, t)\text{-cut}\}.$$

Algorithm 1 Detection of flow bottleneck

- 1: Consider the contact network $\mathcal{N}$ for a given stage of the loading.
 - 2: Construct a directed network G from $\mathcal{N}$.
 - 3: Determine the edge capacities and assign them to the corresponding links in G .
 - 4: Find grains attached to the top and bottom walls. Select two artificial nodes called super source s and super sink t . Connect s to grains attached to the top walls with infinite capacity. Connect grains attached to bottom walls to t with infinite capacity.
 - 5: Called the resultant network as the flow network $\mathcal{F}$.
 - 6: Run inbuilt maximum flow minimum cut algorithm in Python comes from networkX package, on $\mathcal{F}$.
 - 7: **return** Set of contacts which partition the system into two connected components such that s is one component and t is the other if removed. Called the flow bottleneck.
-

We can see that the minimum cut set B is a subset of $\mathcal{P}$. Forward arcs in the minimum cut must be saturated (each arc has flow value equal to its capacity). If any arc in the minimum cut is not saturated, then F^* is not the maximum flow as the flow can be further increased. As mentioned, all the above optimisation problems can be solved efficiently, and several polynomial-time algorithms for them have been discovered, as discussed in (Ahuja *et al.* 1993). For the MCFP, we used a version of the Ford-Fulkerson algorithm called the Edmonds-Karp Algorithm. The Ford-Fulkerson is relatively simple to describe. The algorithm keeps looking for a path from the source to the sink which has unused capacity on every link (such paths are called augmenting paths). It then increases the flow on this path and repeats this process until there are no more augmenting paths. The complexity of the Edmonds-Karp algorithm is $O(nm^2)$, where n is the number of nodes and m is the number of arcs. This is a polynomial complexity and is therefore considered efficient.

4.1.7. Minimum edge cut

This is a special case of the minimum cut problem discussed above. Here the idea is to find the cut with the least number of member contacts. The cut with the least number of bonds is called the minimum edge cut (Kirkpatrick 1984). To do that, we assign uniform capacity for every arc when creating the flow network as discussed in section 4.1.3.3. Then a bottleneck of this flow network is simply a cut-set with the minimum number of links. One might think the cut with a minimum number of member contacts should predict the location of the ultimate macrocrack. Here we use minimum edge cut to show that this is not the case for disordered and heterogeneous bonded granular materials. This also emphasises the effect of the heterogeneity of the contact capacity in predicting the final macrocrack location. Moreover, this gives us a maximum number of available transmission pathways from the source to the sink.

4.2. Methods for modelling energy propagation

Here we develop a framework for modelling the transmission of elastic energy in tension samples. Similar to force transmission, the key idea is to represent the transmission of elastic energy in the specimen as ‘flows’ through the contact network. This representation is valid and fit for purpose since the physical laws that govern the transmission of elastic energy in the specimen satisfy the constraints of the underlying optimisation problem for the scalar flows in the flow network. We solve a set of optimisation problems on this network at each time stage ϵ . For each time stage, the *input* comprises data on the contact bond strengths (fracture energy) and the contact network topology, and the *output* is the maximum flow and the preferential paths for energy and damage.

As we already covered most of the basic concepts in the previous section, we give more detail where the differences exist. The structure of this section is similar to the previous section.

4.2.1. Flow network and principal direction of flow

Construction of flow network is already discussed in section 4.1.1. However capacity function q will be different as we will discuss in section 4.2.3. The selection of the source and the sink node will be the same as force transmission.

The major force transmission pathways, i.e., tensile force chains are aligned with the applied tensile load (namely, vertical for the samples studied here). Intuitively, this implies that the paths which transmit elastic energy also align with the applied load. This is a direct result of the fact that elastic energy is calculated in terms of tensile normal contact force. Figure 4.5 confirms that elastic energy for approximately vertical contacts is dominant.

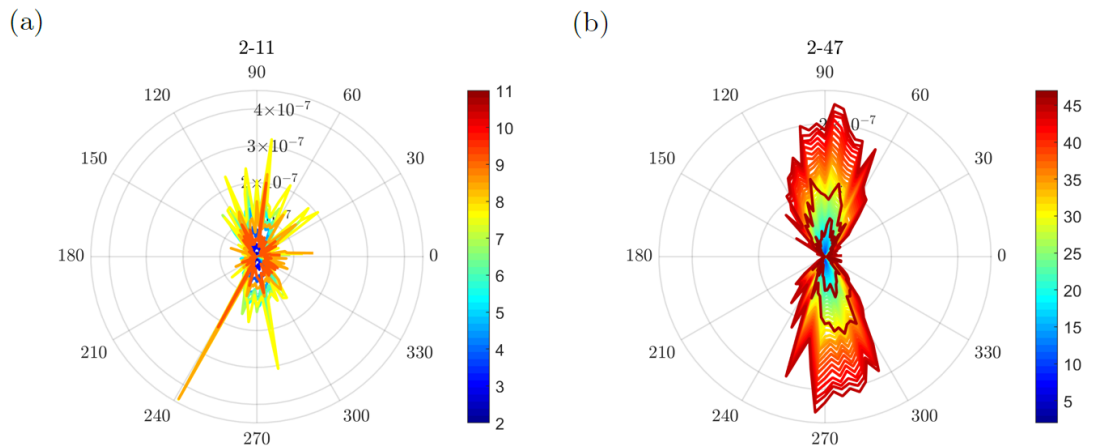


Figure 4.5.: Conservation of elastic energy flow evident in the symmetry of polar plots for elastic strain energies above and below the centroid of each grain (a) 1-phase tension and (b) 3-phase tension.

4.2.2. Conservation of flow

Recall that the conservation of flow requires that for any node in $\mathcal{F}$ except the source s and the sink t , the sum of the flows entering the node must equal the sum of the flows leaving the node. As can be seen from Figure 4.5, on average, flow conservation is satisfied at the grain level. This is mainly due to the fact that the energy of the contacts above any given node is approximately equal to the energy of the contacts below the node. We also calculated the percentage error of energy balance in the vertical direction for each grain and found out that the mean error is at most 25%.

4.2.3. Capacity rule

Recall that the capacity rule dictates that the amount of flow $x(e)$ transmitted through any arc e in $\mathcal{F}$ is limited by the corresponding link capacity $q(e)$, i.e., $x(e) \leq q(e)$. Next, we discuss the contact capacity function relevant to elastic energy transmission.

4.2.3.1. Generic capacity function

The capacity function relevant to elastic energy transmission is the maximum elastic energy given by Equation (3.1). In the DEM model when elastic energy reaches the maximum elastic energy (fracture energy, γ), bonds break. Therefore, data automatically obey the capacity rule. The contact capacity function which relevant to elastic energy transmission given by

$$q_E(e) = \gamma(e) = E_{max}(e) = 0.5(F_{min}^n(e))^2/K_n(e), \quad (4.12)$$

where F_{min}^n is given in Equation (3.1) and the normal contact stiffness k_n is given by

$$k_n = \frac{E(2r_A r_B)}{(r_A + r_B)},$$

where E is the Young's modulus and r_A, r_B are radii of two grains in contact. We denote the minimum of r_A and r_B by r in the future for convenience. The flow network with this energy capacity function is called a *energy flow network* and denoted by $\mathcal{F}_E = (G, \gamma, s, t)$.

Frequency distribution of the contact capacities given by Equation (4.12) is shown in Figure 4.6. Note that the contact capacity for a bonded contact is constant throughout the loading. Recall that these two tension samples do not contain many broken bonds. Therefore, distribution does not change much throughout the loading. Unlike the distribution of contact capacities for force (Figure 4.3), this has wide distribution with concentrated relatively low capacities. Note also there is a significant difference between the number of contacts with the lowest contact capacities and the second-lowest. Most of the capacities are in the lower end of the distribution and comparable, a possibility to change a cut with minimum capacity on it (sum of the capacities for the

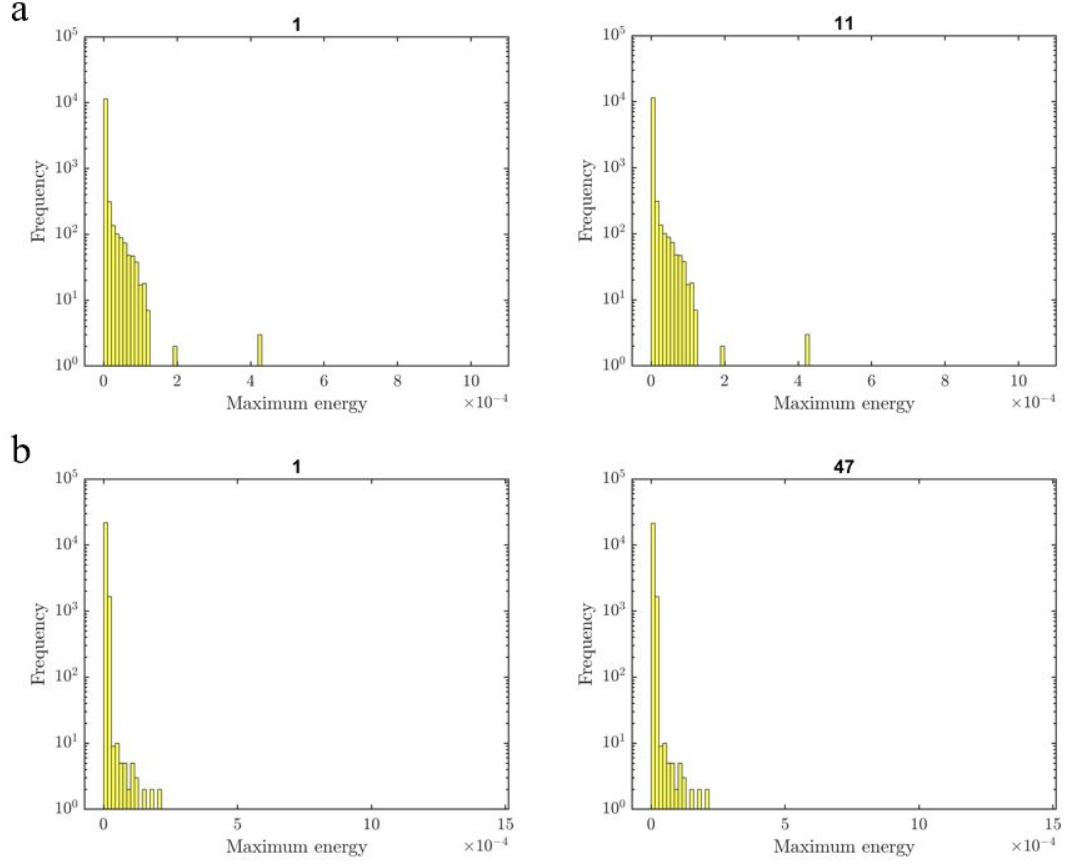


Figure 4.6.: Distribution of the contact capacity for energy for (a) 1-phase tension and (b) 3-phase tension at the initial and final stage of the loading. Contact capacity for a bonded contact is constant throughout the loading. Distribution does not change much due to the limited bond breakages.

member contacts in the cut) is minimum. If this is the case, we should see this in the results from the minimum cut analysis.

4.2.3.2. Residual capacity function

Similar to residual capacity for force as discussed above, we can incorporate the loading state to generic capacity function for energy transmission by using the realised (actual) energy E_r of the bonded contact. The contact capacity function is given by

$$\bar{q}_E(e) = E_{max}(e) - E_r(e). \quad (4.13)$$

The flow network with this residual energy capacity function is called a *residual energy flow network* and denoted by $\tilde{\mathcal{F}}_E = (G, E_{max}(e) - E_r(e), s, t)$.

4.2.4. Quantifying the global energy transmission capacity

Similar to force transmission, here we propose a measure of global transmission capacity in the form of maximum flow F_E^* for energy. Details are similar to that in section 4.1.4 except the contact capacity function.

4.2.5. Predicting the preferential pathways for energy transmission

Here idea is to find the shortest possible pathways that can transmit maximum flow for elastic energy with the minimum cost. The method is similar to that given in section 4.1.5 except the capacity function.

4.2.6. Predicting the preferential pathways for damage propagation

Here idea is to find the minimum cut of energy flow network $\mathcal{F}_E = (G, \gamma, s, t)$ which identifies the energy flow bottleneck. The method is similar to section 4.1.6 except the capacity function. As the contact capacity function is the fracture energy for contact (bond), the minimum cut (energy flow bottleneck) corresponds to the path with minimum fracture energy.

4.3. A source-sink independent maximum flow method for predicting crack/failure patterns in granular materials

We discussed a method to predict the location of the ultimate macrocrack as force bottlenecks and energy bottlenecks in the previous two sections for tension samples. A limitation of classical maximum flow minimum cut analysis in this context is the necessity of assigning a source and a sink, which requires an assumption to be made upfront on the direction of force/energy transmission. Crack patterns or failure zones that do not separate an assigned source and sink cannot be reliably predicted using classical maximum flow minimum cut analysis.

For the compression samples presented in Chapter 3, crack pattern passes through the top and bottom walls which we assigned as the source and the sink respectively. We assign the source and the sink according to the direction of the applied force as discussed above. If we use classical maximum flow minimum cut analysis, there is no way to predict the entire crack. This requires a new method. Here we proposed a method to do so. This method utilises Gomory-Hu trees. We discuss this method in detail next.

In the Gomory-Hu trees calculation, we find all possible source-sink pair minimum cuts. The minimum cut is already discussed in section 4.1.6. Therefore, we will only focus on Gomory-Hu trees. As we find all possible source-sink pair minimum cuts, capacity function plays a major role.

4.3.1. Gomory-Hu trees (GHT)

Consider the contact network $\mathcal{N}$ of the granular specimen where each grain is mapped to a node and each contact to a link. We denote the set of nodes of $\mathcal{N}$ by V , and the set of links at a given time step by A . We now associate every link e with a non-negative capacity $q(e)$ which corresponds to the bond strength. The capacity function for all of A is then written as

$$q : A \rightarrow \mathbb{R}_+.$$

From $\mathcal{N}$ we then derive the network $G := (V, A, q)$, which we call a *capacitated network*.

Let n be the number of nodes in G . The Gomory-Hu tree (GHT) is a structure which, for every pair of nodes u, v in G , stores the minimum cut of G that separates u and v . There are $O(n^2)$ pairs of nodes in G , however, the construction of the GHT shows that the minimum cuts for certain pairs of nodes coincide. In fact, the GHT contains exactly $n - 1$ distinct minimum cuts (Gomory & Hu 1961).

Now, we define above concepts more formally,

Let $G = (V, A, q)$ be a capacitated graph. For $S \subset V$, denote $\bar{S} := V - S$. The

sets S and $\bar{S}$ form a partition of V , and the set of edges from S to $\bar{S}$, denoted by

$$\delta(S) = \{(u, v) \in A : u \in S, v \in \bar{S}\},$$

where $\delta(S)$ denotes edges that have one endpoint in the set S and the other endpoint in the complement set $\bar{S}$ and is called a *cut-set* of G induced by S . The *capacity* of such a cut is defined to be

$$q(\delta(S)) := \sum_{e \in \delta(S)} q(e).$$

Definition 4. For a given capacitated network, $G = (V, A, q)$, a tree T_G is a Gomory-Hu tree (GHT) if the following holds:

1. The nodes of T_G coincide with the nodes of G ,
2. Each edge e in T_G has a non-negative weight $w(e)$,
3. For each pair of nodes u, v in T_G let e_{uv} be the edge of minimum weight on the path joining u and v in T_G . Then $w(e_{uv})$ is equal to the capacity of the minimum cut separating u and v in G .

The key property of the GHT that we need is the fact that a minimum capacity cut partitioning G can be found in linear time by simply finding the smallest capacity edge, say e , in T_G . The nodes in the two components of $T_G - e$ constitute the minimum cut of G . Similarly, using T_G one can calculate the k smallest capacity cuts in G for any k . Note that these cuts do not depend on an upfront selection of source and sink, and therefore an assumption about the direction of flow in the network is not needed.

In Figure 4.7, we show a toy contact network with $n = 9$ grains and corresponding GHT. As can be seen, there are 8 distinct minimum cuts. For an example, consider the minimum cut separating nodes $v = 2$ and $w = 5$. According to the Definition 4, the minimum cut separating them corresponds to the removal of edge $(2, 4)$ in the GHT as it gives the minimum capacity in the path from $v = 2$ to $w = 5$. The capacity of the minimum cut is 3 and corresponding two components upon the removal of edge $(2, 4)$ in the GHT are $\{1, 2, 3\}$ and $\{4, 5, 6, 7, 8, 9\}$. This partitions the GHT into two distinct components as well as the original network. Note also that, to obtain this partition, we need to remove links $(1, 4)$, $(2, 4)$, and $(2, 5)$ in the original network, which together has a capacity of 3. These three links together constitute the minimum cut-set separating nodes $v = 2$ and $w = 5$. The absolute (global) minimum cut of the original network (Figure 4.7 (a)) partitions the network into two distinct components such that one component contains only node 3 while the rest in the other component. The corresponding minimum cut-set contains only edge $(2, 3)$ which results in the cut

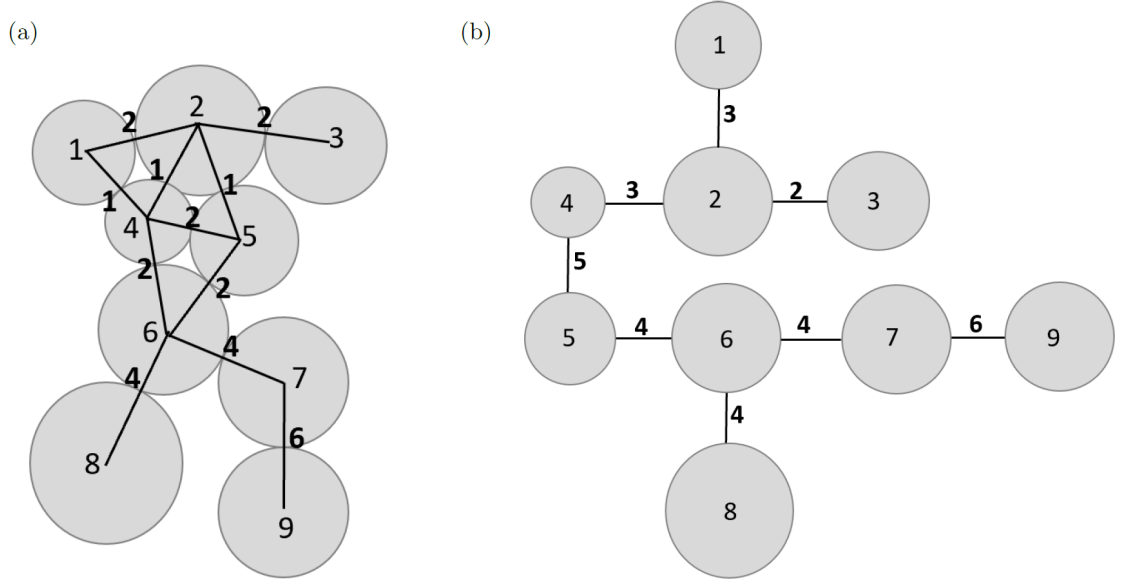


Figure 4.7.: (a) A toy contact network with $n = 9$ grains. Edge weights (capacities) are shown for the contacts are chosen arbitrary to illustrate the concepts. (b) Corresponding Gomory-Hu tree for the contact network in (a). The GHT contains 8 distinct minimum cuts, where the capacities of the minimum cuts label the edges.

capacity of 2. As can be seen from Figure 4.7 (a), the global minimum cut in the GHT sits on the edge (2,3). The removal of edge (2,3) in the GHT results in the global minimum cut in the original network. The global minimum cut in the network is included in the GHT together with other possible source-sink pairs minimum cut. Hence the user has the freedom to select a minimum cut according to their requirement.

4.3.1.1. How to predict the major crack?

We first define so-called ‘connected cuts’ of a capacitated graph G . A *connected cut* of a graph is a partition of the nodes of the graph into two disjoint subsets such that each subset induces a connected component (a set of nodes in a graph such that there exists a path between every pair of nodes) of G .

In a grain contact network corresponding to a bonded granular sample (for example, concrete), a crack is equivalent to a connected cut in the sample. In bonded samples, there is a tendency for the major (dominant) crack to partition the sample into two connected components. Moreover, these two components are usually comparable in size (number of grains) i.e, the major crack usually breaks the sample into two large pieces. In general, concrete samples under compression produce a complicated crack pattern with some other minor cracks. But, in our analysis, we are interested in predicting the major crack (large pieces). Thus, we incorporate this fact into our analysis by imposing that the cut to be connected and two components are relatively large.

Let r_Γ be the ratio of the number of nodes in the smallest component to the largest component upon the removal of an edge e in the GHT. Now we pointed out some implications of r_Γ . If r_Γ is small (for an example, $r_\Gamma < 0.3$), we have small cuts i.e., one component contains few nodes while the rest of the nodes in the other. This translates to the minor cracks in the physical systems. If r_Γ is relatively large (for an example, $0.3 \leq r_\Gamma \leq 1.0$), we have relatively large cuts. This translates to the major cracks in the physical systems. A user has the freedom to select r_Γ according to their requirement i.e., whether they are interested to predict large cracks or small cracks. Since we are interested in predicting the major crack, in our analysis, we choose $0.3 \leq r_\Gamma \leq 1.0$ for more realistic predictions.

It was found in our classical maximum flow minimum cut analysis that cracks forms where force/energy congests i.e., the bottleneck in force/energy transmission. Therefore, we find the minimum cut within the proscribed ratio r_Γ as it gives a bottleneck. This is our prediction for the major crack. This procedure in detail is given in Algorithm 2.

Algorithm 2 The major crack prediction algorithm

- 1: Let T_G be a GHT constructed for a capacitated graph G with n nodes
 - 2: Set $[r \ w \ e]$ to an $(n - 1) \times 3$ null matrix (a matrix all of whose entries are zero)
 - 3: **for** $i := 1 : n - 1$ **do**
 - 4: Remove an edge e_i in T_G
 - 5: Compute the ratio $r(e_i)$ upon the removal of the edge e_i and set $[r \ w \ e][i] := [r(e_i) \ w(e_i) \ e_i]$ where $w(e_i)$ is the weight of the edge e_i in T_G
 - 6: **end for**
 - 7: **return** The minimum capacity edge e_i found in $0.3 \leq r \leq 1.0$. Remove e_i in T_G to get corresponding two partitions
-

Table 4.1 summarises the ratio r_Γ and the capacity of the cuts with the removal of edges in the GHT shown in Figure 4.7 (b). As can be seen from it, there are 3 minimum cuts within the ratio of $0.3 - 1.0$. These correspond to the removal of edges (2, 4), (4, 5), and (5, 6) in the GHT. Capacities are 3, 5, and 4 respectively. Thus, the removal of edge (2, 4) gives rise to the minimum cut within the prescribed ratio. Two partitions are $\{1, 2, 3\}$ and $\{4, 5, 6, 7, 8, 9\}$. This also corresponds to the global minimum cut of the network (Figure 4.4 (a), results from the classical multiple-source multiple-sink minimum cut analysis). But, this is not necessarily true for large networks (networks containing thousands of nodes).

4.4. Proposed fracture criterion and failure criterion

In this research, we proposed a fracture criterion to predict the location of the ultimate macrocrack/failure in disordered and heterogeneous bonded granular materials. Moreover, we also proposed a failure criterion to indicate the time of failure. Our proposed

Table 4.1.: Ratio r_Γ and capacity of the minimum cuts due to removal of edges in the GHT given in Figure 4.7 (b).

Edge removed	Ratio (r_Γ)	Capacity of the minimum cut
(1,2)	0.1250	3
(2,3)	0.1250	2
(2,4)	0.5000	3
(4,5)	0.8000	5
(5,6)	0.8000	4
(6,7)	0.2857	4
(6,8)	0.1250	4
(7,9)	0.1250	6

fracture criterion is *the minimum force and energy capacity criterion*. Here we claim that failure happens where force and energy congest (force and energy bottlenecks) in the system. We used the *maximum flow (global transmission capacity)* as an indicator of failure. We claim that when the actual flow (sum of the force/energy for the contacts in the bottleneck) reaches the maximum flow, materials fail. We will show that the efficacy of our proposed fracture criterion by using the laboratory scale data discussed in Chapter 3 and a data set from direct observation (field-scale data).

This simple question is surprisingly difficult to answer experimentally: measuring forces in three dimensions, between deeply buried grains, is challenging.

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5. Optimal routes for force transmission and their connection to force chains

As discussed in section 4.1.5 of Chapter 4, the solution to the MAXIMUM FLOW MINIMUM COST analysis is a set of percolating paths that represent the preferred pathways for force transmission. Our hypothesis is that most of the force chains form along these paths. If indeed this is the case, then: (a) our method can be used to identify where force chains form without needing information on contact forces, and (b) we will have uncovered the rule that potentially underlies force chain formation. Here we test this hypothesis for the data presented in Chapter 3. A summary is shown in Figure 5.1.

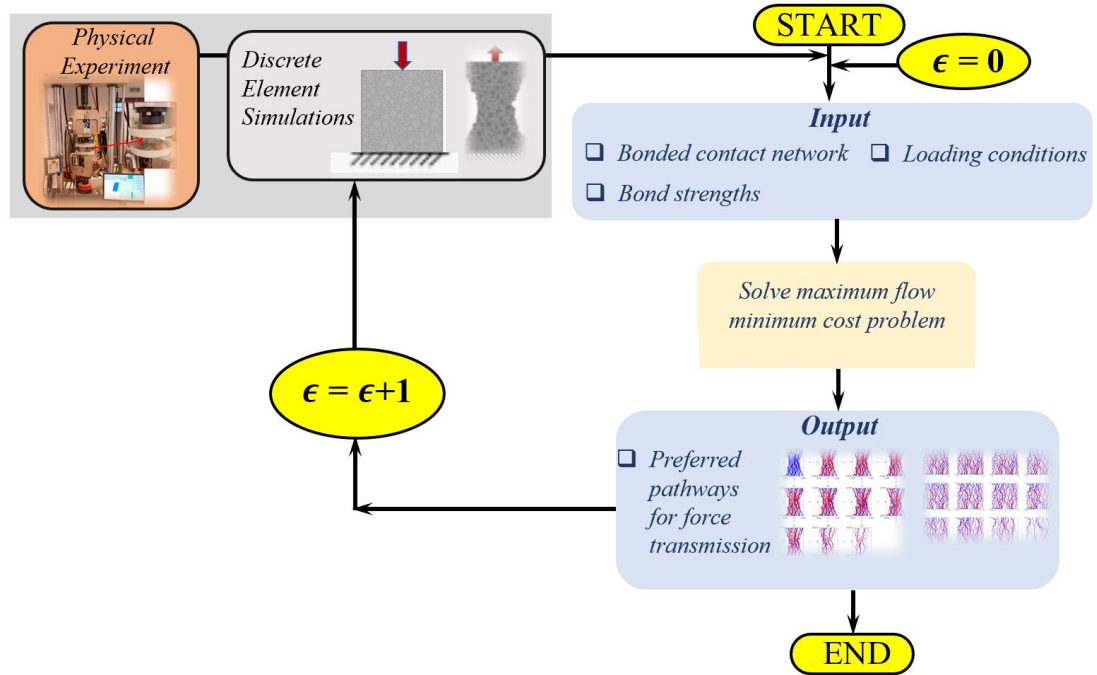


Figure 5.1.: A summary of the input data, methods used and the results.

This chapter is organised as follows. In section 5.1, we first identify all the tensile force chains as well as the compressive force chains in the uniaxial tension and compression tests, by modifying the force chain classification algorithm that was originally developed in Peters *et al.* 2005; Muthuswamy & Tordesillas 2006. We then use this force chain data to assess the extent to which the preferred paths for force from the network flow analysis in section 5.2 can predict the force chains. A brief conclusion is given in section 5.3.

5.1. Existence of force chains

For samples studied, we found the force chains and observed that the co-existence of tensile force chains as well as compressive force chains (see Appendix C for more details). Visuals of force chains revealed that tensile force chains (TFCs) in tension samples are dominant and are aligned with the direction of the applied tensile load. Similarly, compressive force chains are dominant in compression samples and are aligned with the direction of the applied compressive load. To detect force chains, we used the algorithm discussed in Appendix B. This utilises the information on contact forces. The experimental measurement of contact forces is still limited.

5.2. Predicting force chains from $\mathcal{P}$

Here, we discuss the results from preferential pathways for force transmission. Attention is paid to preferential pathways in tension samples. The spatio-temporal evolution of tensile force chains in $\mathcal{P}$ are shown in Figures 5.2 and 5.3. Note that $\mathcal{P}$ contains percolating paths from the top wall to bottom wall (blue links) while tensile force chains (red links) are not necessarily percolating from the top wall to bottom wall. Therefore, we can expect more links in $\mathcal{P}$ compared to tensile force chains. For 1T, on average, $\mathcal{P}$ comprises around 21% of $\mathcal{N}$ links before the peak and around 5% after peak load as shown in Figure 5.4. That for 3T is around 46% of $\mathcal{N}$ links before the peak and around 7% after peak load. A high percentage of $\mathcal{P}$ links for 3T in the prefailure is mainly due to the many more contacts between large coarse aggregate grains and small cement matrix grains (see Figure 1.2 for example). We observed three important trends common to 1T and 3T.

1. The majority of tensile force chain contacts are in $\mathcal{P}$ in the prefailure regime (Figure 5.5). For 1T, there are around 73% across stages 2 – 9. That for 3T is 91% across stages 1 – 45. A higher capture rate in 3T may be due to a high percentage of $\mathcal{P}$ links.
2. While scalar force flows cannot generally be used to predict the magnitudes of the vectorial contact forces, the direction of the normal tensile contact force anisotropy of grains in tensile force chains (vertical, as shown in Figure 4.2 (b)) is consistent with the *orientation* of the preferred flow path. In this study, we only use force flows to visualise flow pathways in Figures 5.2 and 5.3 where they serve solely to highlight the orientation of the preferential paths for force flow. Note that the thickest links (highest force flows) generally align with the vertical direction. This is expected as the Minimum Cost Flow Problem (MCFP) sends global force transmission capacity (maximum flow) through the most direct paths (i.e., paths

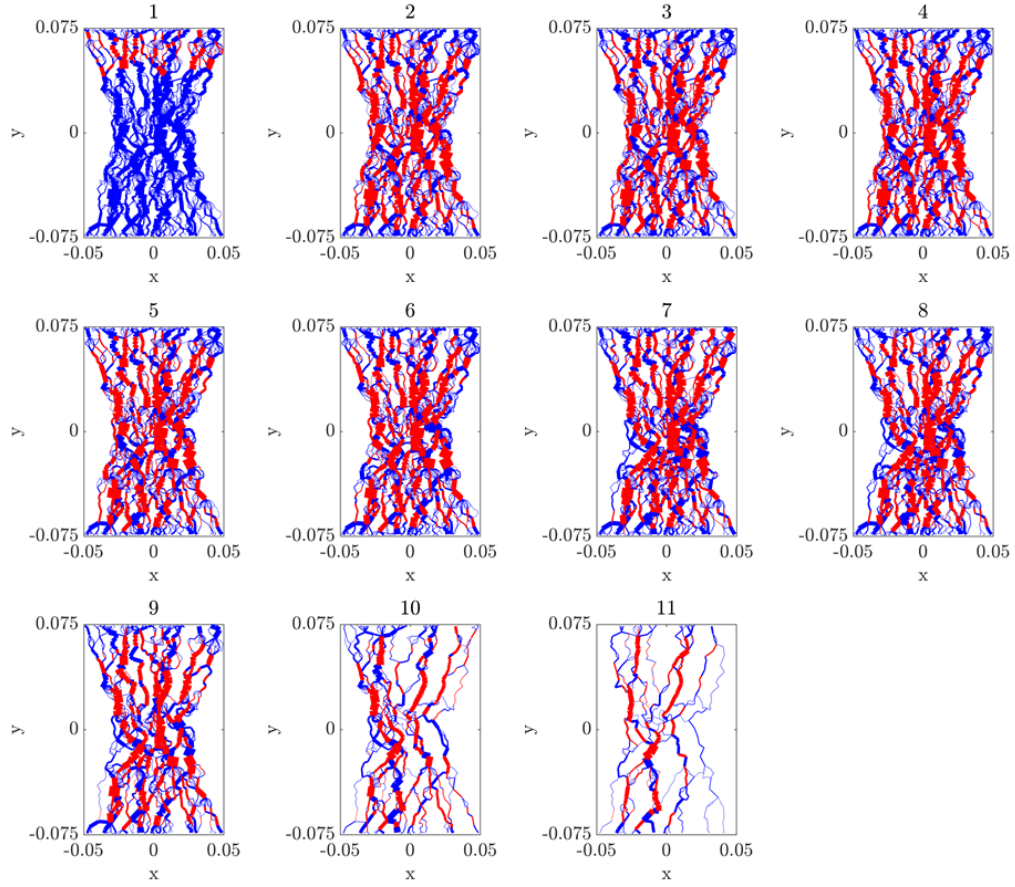


Figure 5.2.: *1T*: Most tensile force chains lie along the shortest possible routes that transmit the global capacity in the direction of the applied tensile load. Optimised routes $\mathcal{P} \in \mathcal{N}$ are the interconnected blue and red links that form percolating transmission pathways through $\mathcal{N}$. Link thickness is proportional to the force flow across each link. Links between grains in tensile force chains are coloured red; otherwise, the link is coloured blue. Residual strength due to $\mathcal{P}$ links along the left side of the specimen. Note system spanning tensile force chains are first established at stage 2 (Figure C.1).

with least cost or fewest member links) from the source to the sink. Thus, those contacts or links in alignment with the direction of flow (vertical for our samples) are preferred over those aligned in the transverse direction, which are either not used (links not in $\mathcal{P}$ with zero flow) or have smaller force flow values. Most links in $\mathcal{P}$ are strong contacts, i.e., transmit force above the global mean tensile force magnitude (Figure 5.6).

3. We see the degradation of pathways in $\mathcal{P}$ coincides in space and time with that for tensile force chains in the postpeak softening regime (stages 10 – 11 for 1T and 46 – 47 for 3T): observed that loss of $\mathcal{P}$ links along the right side of the specimen for 1T (left side of the specimen for 3T). Thus, the residual strength is mainly due to these remaining flow pathways in $\mathcal{P}$ along the left (right) side of the specimen

in 1T (3T).

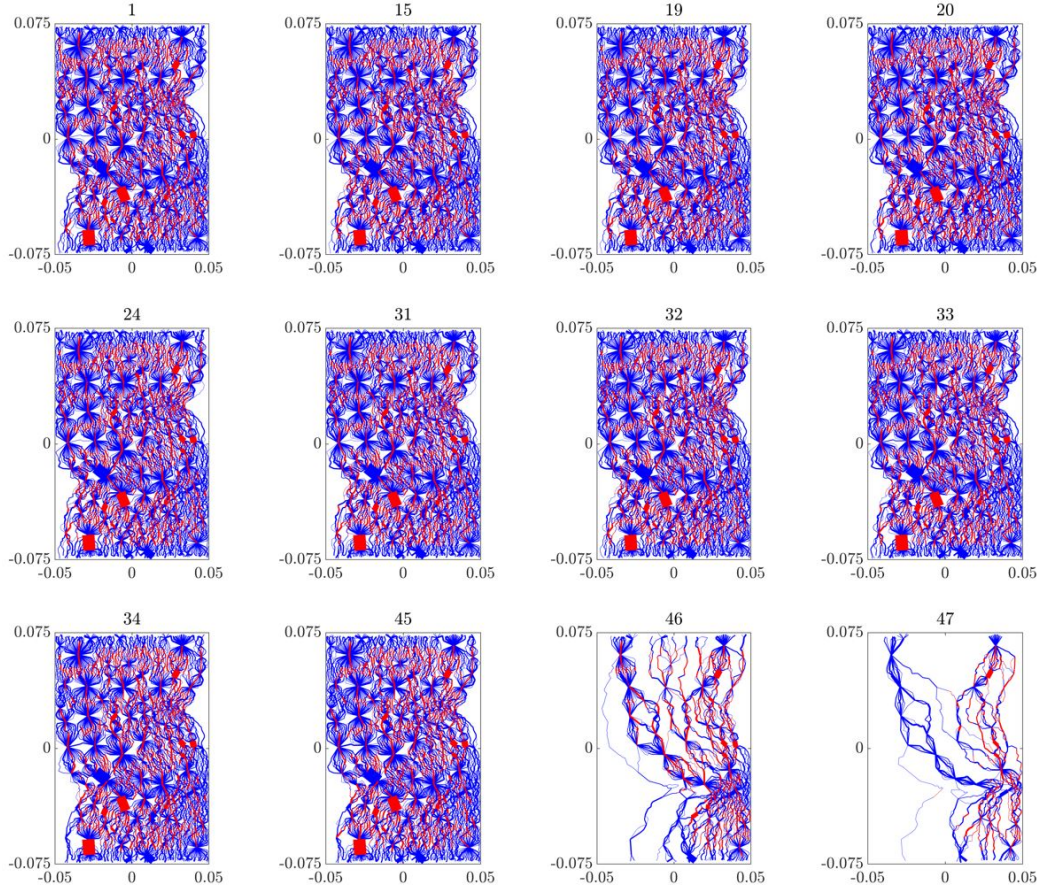


Figure 5.3.: 3T: Most tensile force chains: (i) lie along the shortest possible routes that transmit the global capacity in the direction of the applied tensile load, and (ii) are well-supported on either side by alternative channels for force transmission. This shows the optimal routes $\mathcal{P} \in \mathcal{N}$: interconnected blue and red links that form percolating transmission pathways through $\mathcal{N}$. Link thickness is proportional to the force flow across each link. Links between grains in tensile force chains are coloured red; otherwise, the link is coloured blue. Residual strength in postfailure regime is due to $\mathcal{P}$ links along the right side of the specimen.

Relative to 1T, 3T shows a much wider distribution of grains (the much higher ratio of fine cement matrix to coarse aggregate grains, with some aggregates being bigger and some cement grains being smaller). This leads to one important difference between the optimal routes $\mathcal{P}$ in the two specimens: a relative abundance of supporting contacts (blue) on either side of tensile force chain contacts (red) in the prefailure regime in 3T, as shown in Figure 5.3. That is, there are many more supporting contacts for tensile force chains that prevent the overloading of force chains contacts by distributing forces among them. Thus, this specimen is stronger in tension and more resistant to damage compared to the specimen in 1T.

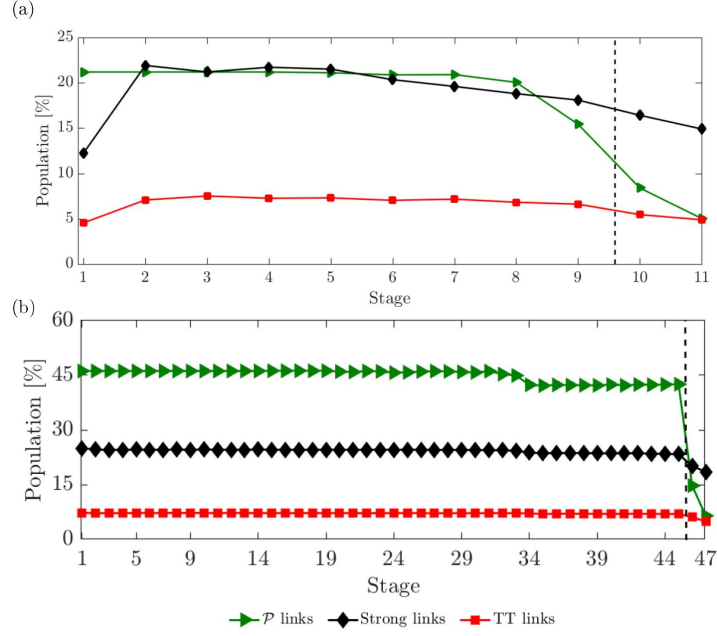


Figure 5.4.: Percentage population of tensile force chain contacts (TT links) in $\mathcal{N}$ remains essentially constant across stages (a) 2-9 for 1T and (b) 1-45 for 3T of the prefailure regime. This plot shows the evolution of the percentage population of links in various subsets of $\mathcal{N}$: $\mathcal{P}$ links, strong links, and TT links. Note that the system spanning force chain network is first established at stage 2 for 1T. Dashed vertical line marks the stage at peak load.

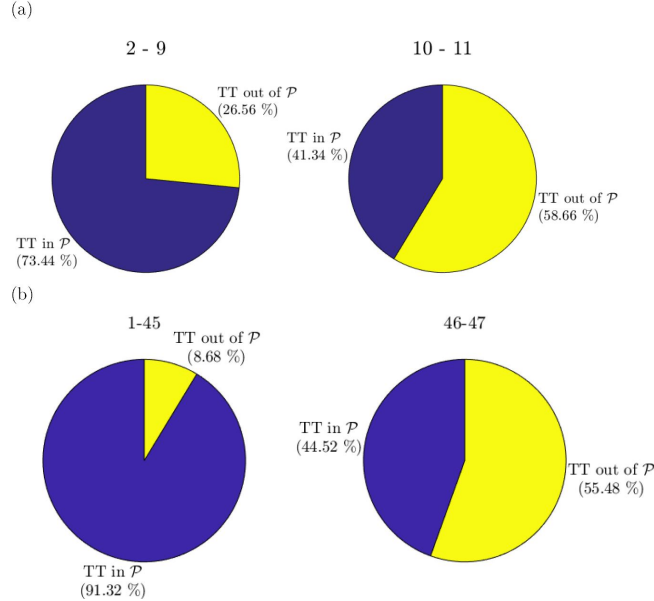


Figure 5.5.: Most TT links are in $\mathcal{P}$ in the prefailure regime. Percentage population of TT links in versus out of $\mathcal{P}$, averaged over the prepeak regime and postpeak softening regime for (a) 1T and (b) 3T. Note that the system spanning tensile force chain network first established at stage 2 for 1T (Figure C.1)

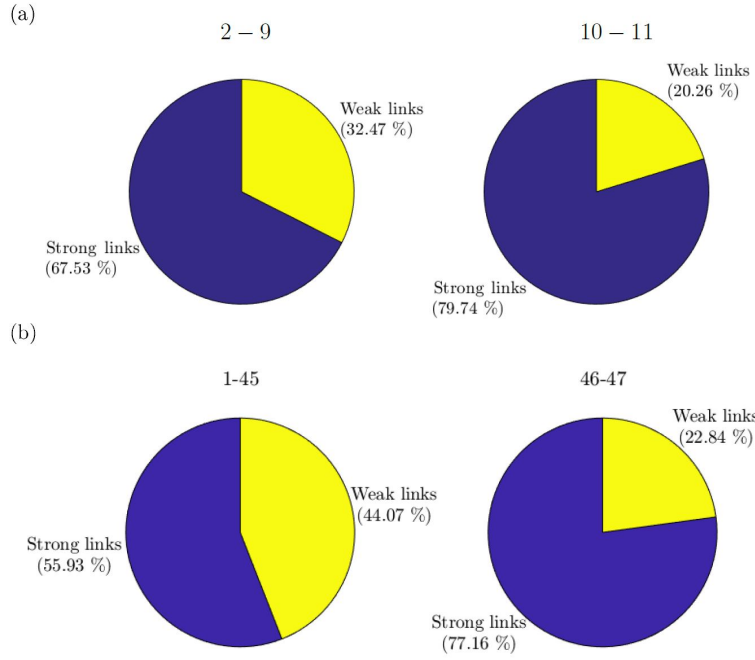


Figure 5.6.: *Most links in $\mathcal{P}$ are strong.* Composition of $\mathcal{P}$ classified according to strong and weak links, averaged over the prepeak regime and postpeak softening regime for (a) 1T and (b) 3T.

Similarly, we find that at least 70% of compressive force chains threat through optimal routes in 1C. The spatio-temporal evolution of compressive force chains in $\mathcal{P}$ is shown in Figures 5.8.

As mentioned before $\mathcal{P}$ contains percolating paths whereas the force chains network is not necessarily contains percolating paths. Note also that, to detect the force chains, we used the information on contact forces while $\mathcal{P}$ depends on the contact capacities. Moreover, $\mathcal{P}$ is aligned with the direction of applied loading (vertical) regardless of the time stage due to the nature of the optimisation problem that we solved. Therefore, not necessarily all the force chain contacts are in $\mathcal{P}$. In the failure regime, we can see some inclined force chains and this is consistent with the observation in [Jiang *et al.* 2011](#). Thus, in the failure regime, we can see a decrease in the force chain capture rate.

5.3. Conclusion

In conclusion, we have tested whether most of the force chains form along the preferred pathways for force transmission. Results revealed that, in the prefailure regime, force chains develop along the shortest possible paths through the sample, in alignment with the major principal stress axis. This gives insights into the self-organisation rules that underlie the formation of force chains. These results have laid a foundation to develop a reliable network flow model for force transmission to identify the location of the ultimate

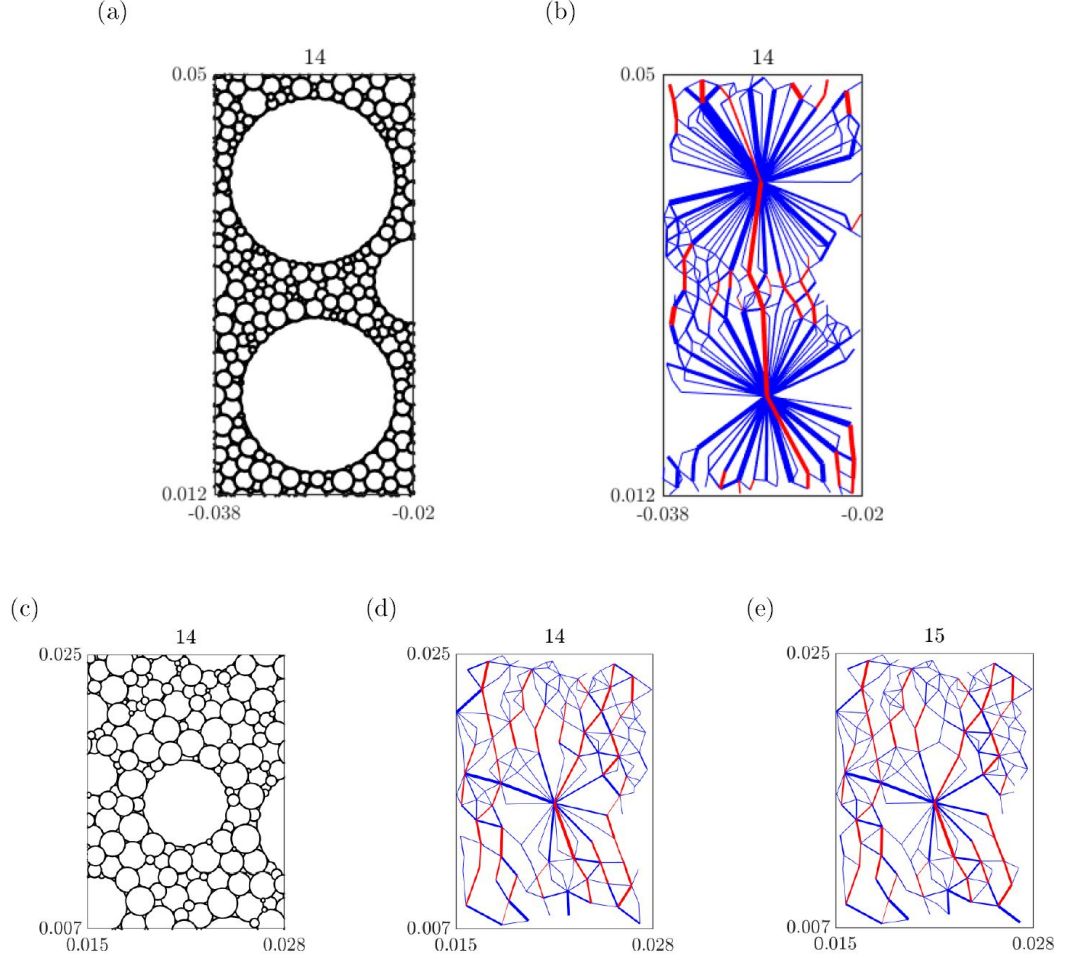


Figure 5.7.: *3T: The high fine to coarse grain ratio in the specimen results in a robust transmission system. The preferential force transmission pathways in $\mathcal{P}$ are surrounded by redundant alternative routes for backup transmission of force in the presence of damage.* (a) Representative zoomed-in view between aggregates (top left of specimen, stage 14) and (b) the corresponding pathways in optimal routes $\mathcal{P} \in \mathcal{N}$. (c) Representative zoomed-in view around an aggregate (middle right of the specimen, stage 14) and its corresponding pathways in optimal routes $\mathcal{P} \in \mathcal{N}$: (d) before damage at stage 14 and (e) after damage at stage 15. Links between grains in tensile force chains are coloured red; otherwise, the link is coloured blue.

macrocrack path similar to past studies of unbonded granular materials. This facilitates to characterise the coupled evolution of force and damage propagation. The results are discussed in the next chapter.

5.3. CONCLUSION

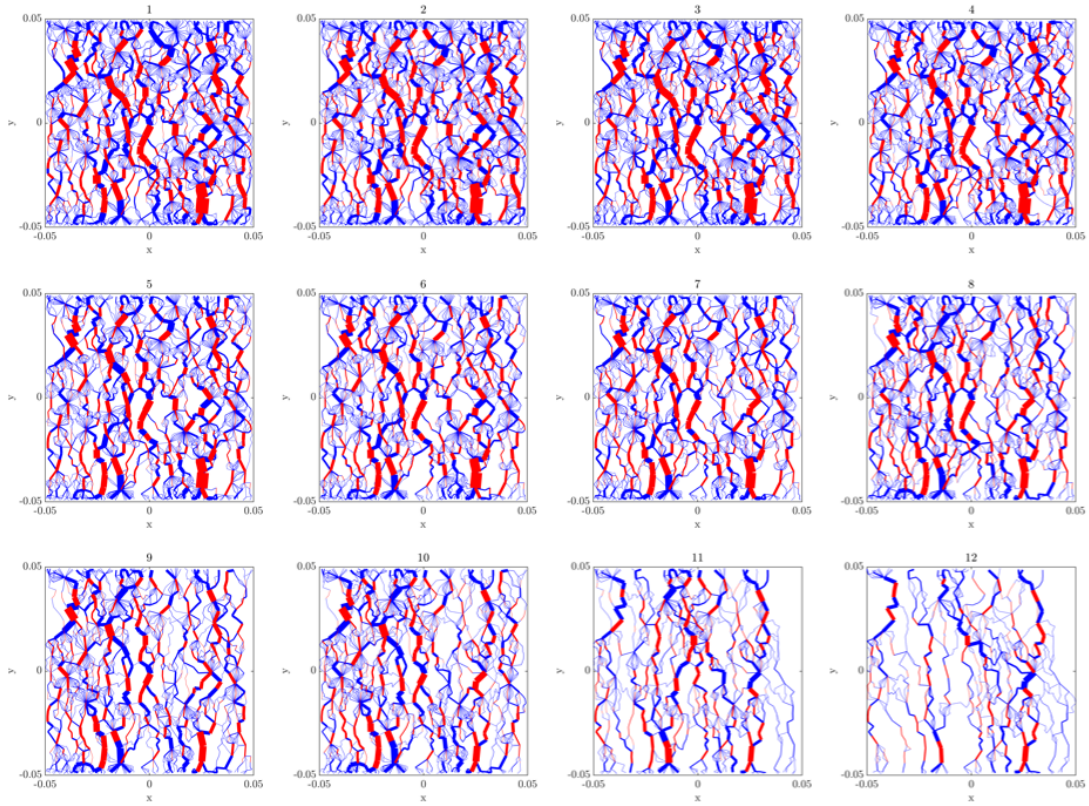


Figure 5.8.: *1C: Most compressive force chains lie along the shortest possible routes that transmit the global capacity in the direction of the applied tensile load.* Optimal routes $\mathcal{P} \in \mathcal{N}$ are the interconnected blue and red links that form percolating transmission pathways through $\mathcal{N}$. Link thickness is proportional to the force flow across each link. Links between grains in compressive force chains are coloured red; otherwise, the link is coloured blue.

6. Characterising and modelling the coevolution of damage and force transmission

Here we present the results for the preferred paths for damage, as determined using the *force bottleneck*. As discussed in Chapter 4, the fracture pattern can be predicted from the flow bottleneck, which forms the solution to the MAXIMUM FLOW MINIMUM CUT analysis. Results here focus on the uniaxial tension test data that was discussed in section 3.1 of Chapter 3. We choose these data because the failure pattern is simpler compared to the compression test. Here bonds fail mainly in tension and no new contacts form from grain rearrangements before failure. That is, each specimen responds to damage only by ‘rerouting’ forces to alternative pre-existing pathways. In our discussion, we pay attention to *redundancy*, i.e., the presence of multiple feasible paths for force transfer, and associated stress redistributions that result when these alternative paths are present. A summary is shown in Figure 6.1.

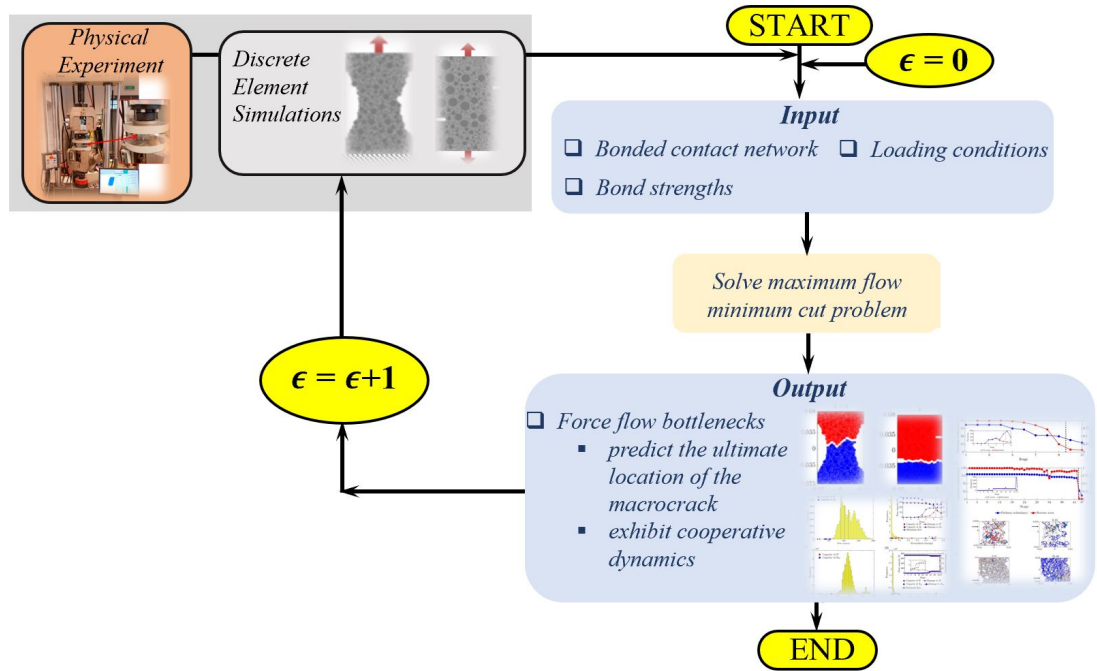


Figure 6.1.: A summary of the input data, methods used and the results.

This chapter is organised as follows. In section 6.1, we quantify the global force

transmission capacity by the maximum flow through the specimen. In section 6.2, we present the results on the force bottleneck which we use to predict the location of the ultimate macrocrack. We present two measures to quantify the robustness in section 6.3 and the cooperative interaction among the various sites of damage during the prefailure regime in section 6.4. Evidence for cascading failure is presented in section 6.5. Concluding remarks are given in section 6.6.

6.1. Quantifying transmission strength from F^*

In the bonded systems, bond breakage disrupts and decreases the feasible force transmission pathways (Figures 5.2, 5.3). As a result, the force transmission degrades. This is confirmed in Figure 6.2, where the maximum flow F^* , the highest normal tensile force flow that can be transmitted through the bonded contact network, varies inversely with the spread of damage. This trend highlights an underlying degradation in force transmission in $\mathcal{N}$ and of the robustness of $\mathcal{N}$, consistent with the progressive spread of damage. The highest drop in F^* accurately marks the transition from prefailure to failure regime: stages 9 – 10 for 1T and stages 45 – 46 for 3T, as seen in Figure 6.2 (see also the evolution of the macroscopic vertical tensile load in Figures 3.4, 3.5).

Note also that the relative tensile strengths of the specimens are well predicted by the *initial* maximum flow values: the ratio of peak tensile load for 1T to that of 3T is $130.3/233.5 = 0.56$, while the ratio of their *initial* maximum flow values is $418/733 = 0.57$.

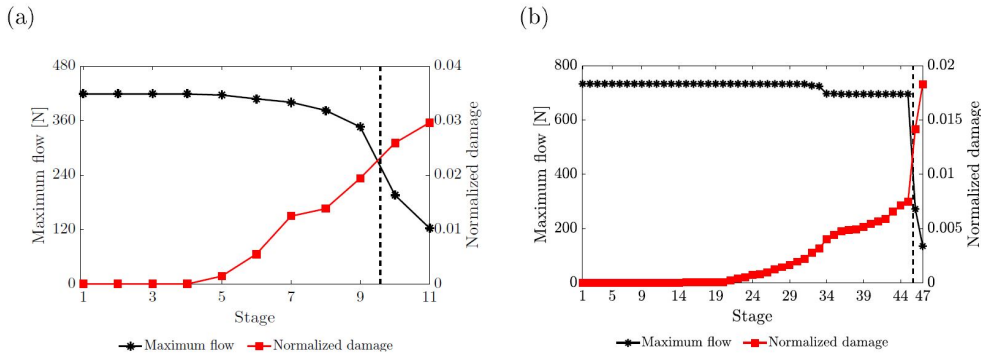


Figure 6.2.: 1T, 3T: Maximum flow quantifies the global transmission capacity of the bonded contact network. Evolution of the maximum flow F^* and the normalized damage (number of broken bonded contacts relative to the initial number of bonded contacts) in the bonded contact network $\mathcal{N}$ for: (a) 1T and (b) 3T. Dashed vertical line marks the stage at peak load.

6.2. Predicting the location of the ultimate macrocrack and crack interaction from force bottleneck $B(\mathcal{F}_F)$

By using the method described in section 4.1.6 of Chapter 4, we identify the force bottlenecks. The spatial-temporal distribution of force bottleneck is shown in Figure 6.3. It depicts that the force bottleneck (minimum cuts) accurately and reliably predict the location of the ultimate macrocrack. Two bottlenecks emerge throughout the loading history. For 1T, the first bottleneck (primary bottleneck B^*) emerges at stage 1 and persists in the middle of the gauge region and coincides with the location of the ultimate macrocrack. The second bottleneck (secondary bottleneck B_8) in the lower portion of the sample emerges in the stage 8. This coincides with the secondary crack which appears momentarily at stage 8. Note that this crack is then closed. Similar trends apply in 3T: the primary bottleneck B^* persists for stages 1 – 31 (lower section), while the secondary bottleneck B_{32} forms at stages 32 – 33 (upper section).

In a model to analyse fracture pattern in deforming rock using numerical simulation, which borrows dislocation theory, Ord & Hobbs 2010 used the concept of mobile versus immobile to describe the damage in their systems. According to their definition, the mobile defects are cracks forming at lower stress and immobile cracks are cracks forming at higher stress. Similarly, here we also consider two classes of broken bonds: *mobile links* versus *immobile links*, which correspond to the broken bonds that form relatively easily at low stress and high stress respectively. With this definition, the bonds that break in the primary bottleneck are immobile and bonds that break outside of the primary bottleneck are mobile. Consequently, we define immobile (mobile) links to be the set of all bonds that break in the primary bottleneck (outside the primary bottleneck) across all observed stages (1 – 11 for 1T, 1 – 47 for 3T). Note that not all bonds in the bottlenecks break. We observed that most of the prefailure damage is mobile, i.e., they lie outside the primary bottleneck B^* (Figure 6.4 (b,d)). Therefore, in the prefailure regime, sites of high concentrations of damage do not accurately indicate where the dominant macrocrack will likely form.

In what follows, we examine the properties of the minimum cut. To find what is special about the minimum cut, we have generated 10,000 random cuts in $\mathcal{N}$ that slice the sample from left to right. For 1T, capacities of these arbitrary cuts together with the capacities of primary bottleneck B^* and secondary bottleneck B_8 across all 11 stages are shown in Figure 6.5 (a). As can be seen from it, capacities of B^* and B_8 are low and lie outside of the distribution of capacities of random cuts. This explains why the bottlenecks are the critical location where force congests and why they exhibit a distinguished pattern of damage evolution relative to those of other feasible cuts (Figure 6.5 (b)). Similar trends have been observed for 3T (see Figure 6.5 (c, d)).

Damage to primary bottleneck B^* , secondary bottleneck $B_8(B_{32})$ and random cuts

6.2. PREDICTING THE LOCATION OF THE ULTIMATE MACROCRACK AND CRACK INTERACTION FROM FORCE BOTTLENECK $B(\mathcal{F}_F)$

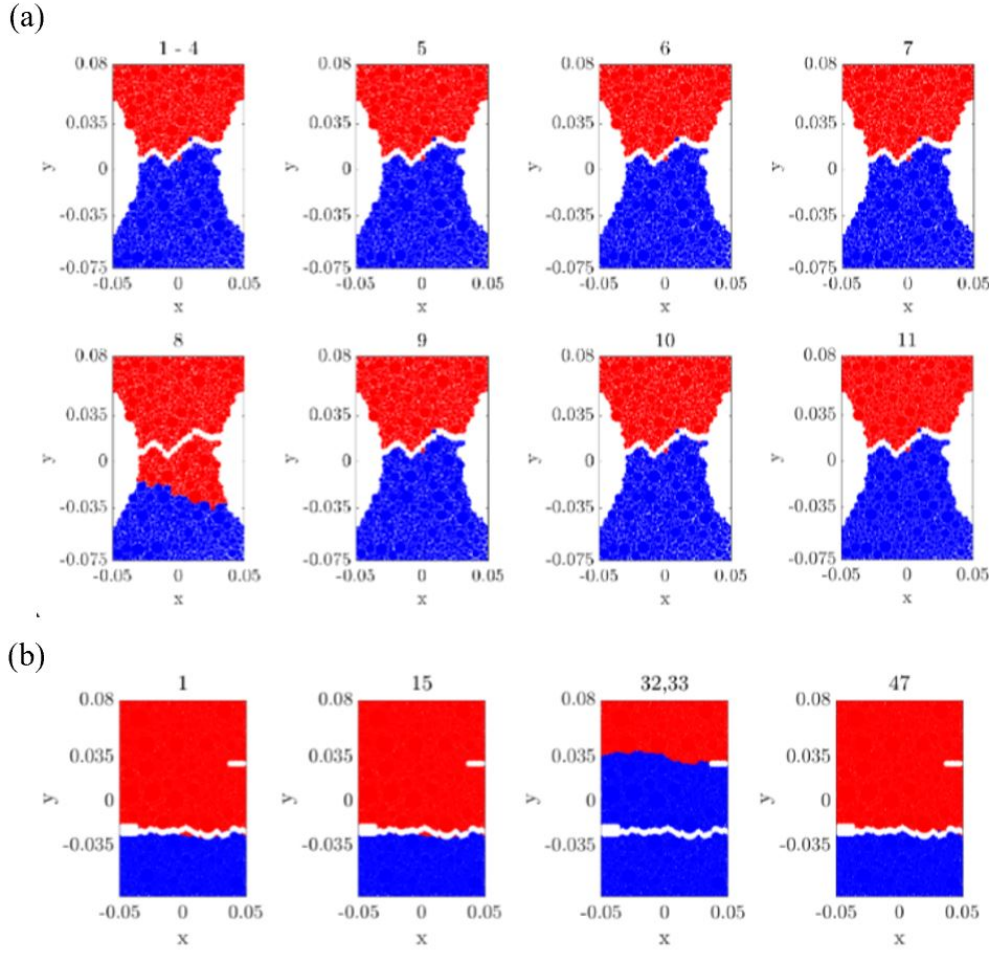


Figure 6.3.: *1T, 3T: Force bottlenecks $B(\mathcal{F}_F)$ provide an early prediction of the location of the ultimate macrocrack.* Spatial distribution of the bottlenecks $B(\mathcal{F}_F)$ with contact capacity function given by Equation (4.1) for (a) 1T and (b) 3T. Grains on either side of the ultimate macrocrack are artificially separated to aid visual comparison of the bottleneck versus the actual macrocrack location. Prediction persists for all stages except stage 8 (stages 32, 33) for 1T (3T), where it predicts the secondary or competing bottleneck. Stage corresponds to the peak force in between stages 9 and 10 (45 and 46) for 1T (3T). Note also that for 3T, we have only included a prediction for selected stages. Other stages have a similar prediction.

across all 11(47) stages are shown in Figure 6.5 (b (d)) for 1T (3T). In 1T, in the prefailure regime (up until stage 9), the greatest damage occurs initially in the secondary bottleneck B_8 . In contrast, in the postpeak softening regime, damage concentrates in the primary bottleneck B^* (Figure 6.5 (b) inset) where the macrocrack ultimately forms (recall Figure 6.3 (a)). In 3T, more damage concentrates in the secondary bottleneck B_{32} across stages 30-34 (note only 1 bond breaks in B^* and in B_{32} prior to stage 30). But, as the applied tensile force increases, damage in B^* also rises. This eventually matches that of B_{32} across stages 35 – 36, before the catastrophic of bond failures

6.2. PREDICTING THE LOCATION OF THE ULTIMATE MACROCRACK AND CRACK INTERACTION FROM FORCE BOTTLENECK $B(\mathcal{F}_F)$

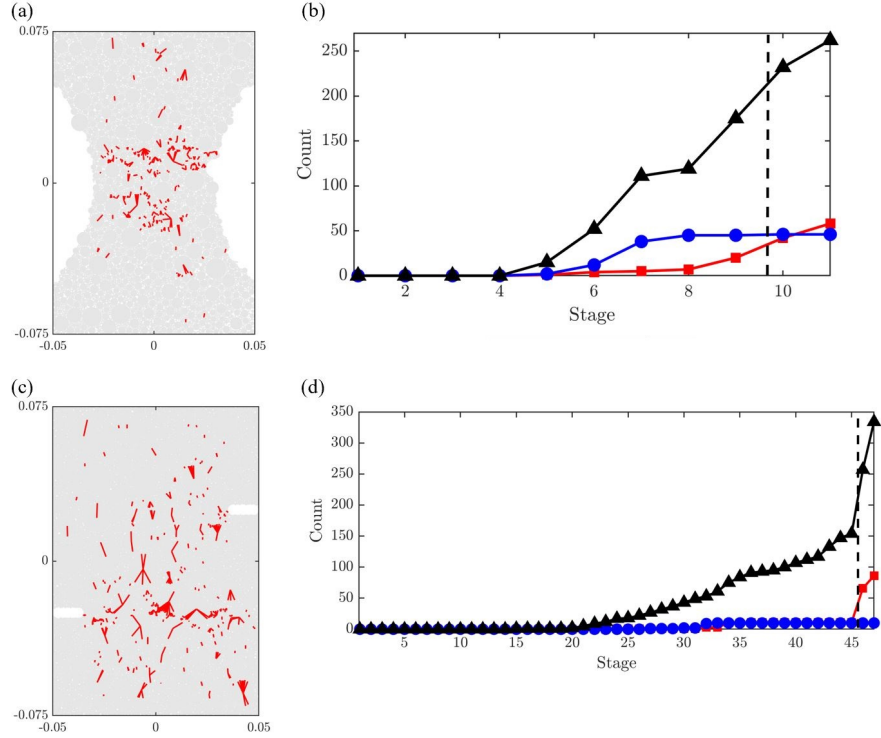


Figure 6.4.: *1T, 3T: Primary bottleneck is protected in the prefailure regime.* (a,b) 1T and (c,d) 3T. (a,c) Spatial distribution of mobile links that are not in the secondary bottleneck. (b,d) Evolution of the number of broken bonds in B^* (red), the secondary bottleneck (blue) and elsewhere (black). Dashed vertical line marks the stage at peak load.

across stages 45 – 47.

The flow capacity and damage is shown in inset of Figures 6.5 (b) and (d) for 1T and 3T respectively. Recall from Maximum-flow minimum-cut theorem (Theorem 1) that the flow capacity of the minimum cut (bottleneck) equals to the maximum flow. This sets the upper bound on the force flow that can be transmitted through the contact network $\mathcal{N}$. Therefore, damage to the contact in the bottleneck leads to the greatest reduction in global transmission capacity. Hence, the bottleneck is the most vulnerable as well as the most critical part of the sample. Corresponding values for the secondary bottleneck in stages 1 – 11 are also shown for comparison. Note that the bottleneck corresponds to the minimum cut. This cut is a subset of contacts, which partition the flow network into two if removed, such that the sum of its member capacities is a minimum. This, along with the rapid spread of damage in the lower portion of the sample in the preceding stage 7 (recall Figure 3.7), explains why the secondary bottleneck in the lower portion of the sample becomes the true bottleneck in stage 8 for 1T. A similar trend applies to 3T.

The evolution of the distributions in cut capacities and attendant damage in Figure 6.5 also provides new insight into crack interaction in the presence of damage. Recall that

6.2. PREDICTING THE LOCATION OF THE ULTIMATE MACROCRACK AND CRACK INTERACTION FROM FORCE BOTTLENECK $B(\mathcal{F}_F)$

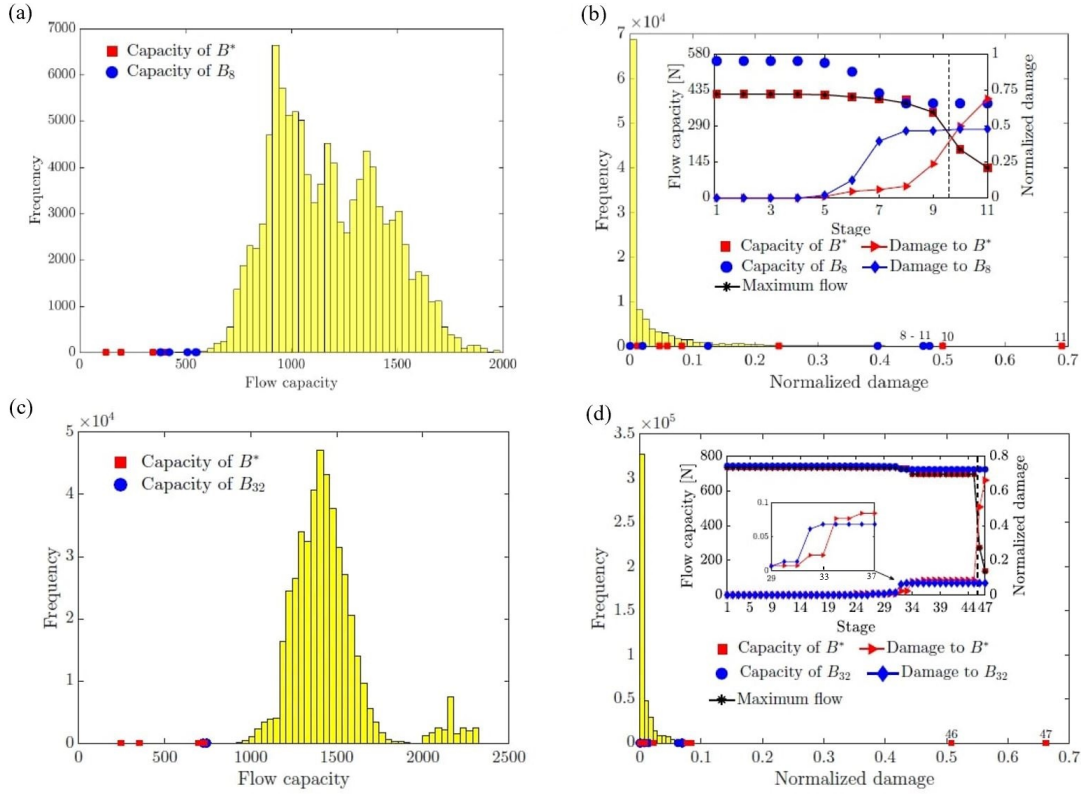


Figure 6.5.: *1T, 3T: Cut capacity distinguishes the bottlenecks and their damage evolution.* (a,b) 1T and (c,d) 3T. Frequency distribution for (a,c) the capacities of 10,000 random cuts of $\mathcal{N}$, and (b,d) their normalized damage across *all* observed stages of loading. The capacities of the primary bottleneck B^* (secondary bottleneck B_8 for 1T or B_{32} for 3T) are marked by the red squares (blue circles). Normalized damage in a given bottleneck is the number of broken bonded contacts relative to the number of bonded contacts in the initial stage 1. Damage in bottlenecks prior to stage 30 is confined to one broken bond at: stage 24 in B^* and stage 27 in B_{32} . Inset shows crack interaction from the perspective of the coevolution of the capacities and damage in the bottlenecks: dashed vertical line marks the stage at peak load.

the fact that the global transmission capacity F^* is equal to the minimum cut capacity. Together this and distributions of cut capacity and damage shown in Figure 6.5, we can consider the following two possible cases in the prefailure regime for 1T.

1. The capacity of the minimum cut is much smaller than any other cut (e.g., B^* in stages 1-6, Figure 6.5 (a)). In this case, a single recurring force bottleneck is likely to develop (see stages 1 – 6, Figure 6.3 (a)). This is possible as a few links can be lost to other cuts without change to minimum cut (see stages 5 – 7, Figure 6.5 (b)).
2. The capacities of few cuts are close to the minimum value meaning to say multiple potential force bottlenecks exist (e.g., B_8 in stages 7 – 9, Figure 6.5 (b) inset). In this case, we can expect changes to the bottlenecks (stages 7 – 9, Figures 6.3 (a),

6.5 (a,b)). This is possible as breakages of few links in another cut with only a slightly higher-capacity may suffice to reduce its cut capacity to the global minimum. As a result, this cut may become the new minimum cut (bottleneck). This can be seen in the switches in bottlenecks: from B^* to B_8 across stages 7 – 8, and vice versa across stages 8 – 9. Here the primary bottleneck is protected by a secondary bottleneck by sacrificing its links. This prevents a reduction in maximum flow (damage to links in previous minimum cut guarantees a reduction in global transmission capacity F^*). This process ensures that the inevitable reduction in global transmission capacity F^* is either delayed or at least minimised, as damage spreads.

Qualitatively similar trends have been observed between B^* and B_{32} in 3T. In summary, results here suggest that *multiple crack interaction in the prefailure regime can be viewed as a cooperative process among force bottlenecks to minimise the inevitable reduction in global force transmission capacity due to damage.*

The cooperative interaction between two force bottlenecks contributes to maximise force transmission while keeping damage in the force bottlenecks to a minimum. This is especially evident in the primary bottleneck B^* , where the majority of force transfer across B^* prior to peak-load is routed through its high capacity links. Consequently, low capacity links break in the prefailure regime. Since the maximum flow F^* is the sum of the link capacities in the bottleneck, this has the effect of minimising the reduction in the maximum flow due to the damage (Figure 6.6).

6.3. Quantifying robustness from $\mathcal{P}$, B and B_{min}

A system's robustness to damage depends crucially on redundancy in force transmission pathways. Here we propose two measures to quantify system robustness. The first measure purely depends on topological connectivity (available number of transmission paths). The second measure is based on how redundancy facilitates to redistribute forces when bonds break.

6.3.1. Pathway redundancy p_{min}

A measure of robustness must necessarily consider the pathway redundancy in $\mathcal{N}$. Pathway redundancy focuses on the multiplicity of paths from source to sink in G with respect to the topology of the uncapacitated directed links of $\mathcal{N}$. Transmission robustness, in analogy to maximum flow, has a useful duality property: (1) the maximum number of percolating link-disjoint paths (paths that do not overlap or share links) through $\mathcal{N}$ between the source and the sink is equal to (2) the minimum number of links whose removal would disconnect the source and the sink from each other. We refer to (1) as

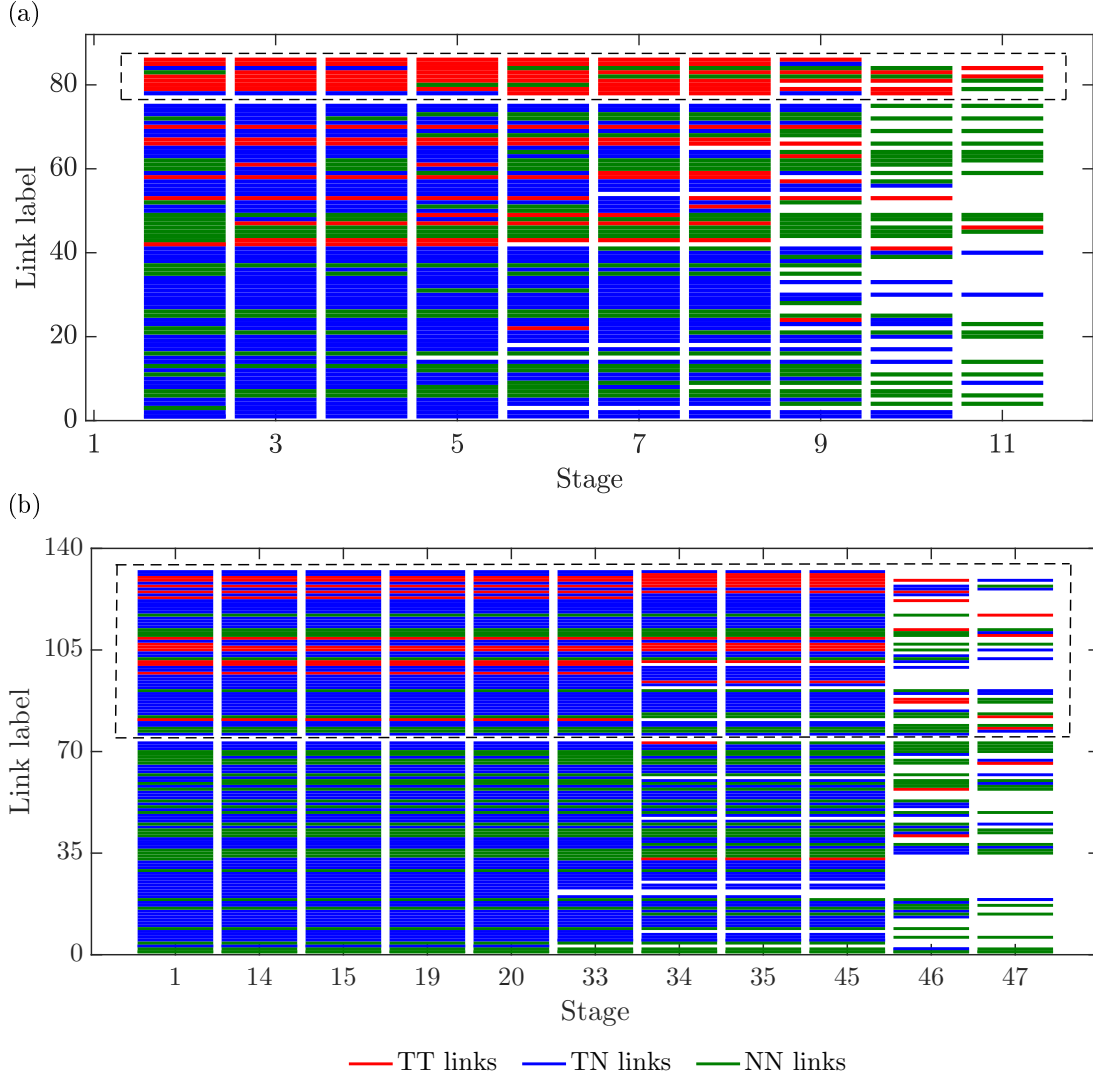


Figure 6.6.: *1T, 3T: Despite being prone to congestion, tensile force chains endure in the bottleneck due to damage being confined to low capacity links in the prefailure regime.* The evolution of link type for each of the k member links of B^* is shown for (a) 1T where $k = 84$, and (b) 3T where $k = 130$. Links in B^* are ranked from lowest (1) to highest tensile bond capacity (k) at that stage when the tensile force chain network is first established (stage 2 for 1T and stage 1 for 3T). Link type is represented by a horizontal bar coloured according to the type of grains in contact: red (TT- tensile force chain grains), green (NN- neither is a tensile force chain grain), blue (TN- one is a tensile force chain grain, the other is not). Dashed rectangle highlights links with above the global mean capacity. A transition to a different link type manifests as a change in the colour of the bar. No bar is shown for a link that breaks. See Appendix A for classification of contacts.

the *pathway redundancy* p_{min} of G . The dual quantity (2) is referred to as the *link-connectivity* of G , and is equal to the minimum number of links in any cut separating the source and the sink. The pathway redundancy p_{min} is given by the bottleneck of

the uniform capacity flow network $\mathcal{F}_C = (G, C, s, t)$, $\mathcal{B}(\mathcal{F}_C)$.

In the tension samples, multiple link-disjoint pathways are available to transmit the applied tensile load in the vertical direction. The number of such pathways is shown in Figure 6.7 (a,b). As damage progress in $\mathcal{N}$, the number of available transmission pathways decreases. This is evident in monotonic decrease in p_{min} .

6.3.2. Reroute score R_{re}

When a bonded contact breaks, certain paths will be ceased and no longer be available for force transmission. However, if there are many more pathways for force transfer in the network, then flow can be diverted to other available pathways without significantly affecting the maximum flow F^* . That is, redundancy facilitates to prevent overloading of the contacts in the bottleneck by diverting flow elsewhere. We quantify the capability to reroute flow through a *reroute score*, denoted by R_{re} , given by

$$R_{re} = \rho \left(1 - \frac{|\alpha - \beta|}{(\alpha + \beta + 1)} \right), \quad (6.1)$$

where ρ ($0 \leq \rho \leq 1$) is the ratio of the number of links in $\mathcal{P}$ relative to its initial value, $\alpha \geq 0$ is the number of replacement links to which flow is diverted, and $\beta \geq 0$ is the number of links that cease to be part of $\mathcal{P}$ (links that leave $\mathcal{P}$ either to join the complementary set $\bar{\mathcal{P}}$ in $\mathcal{N}$ or are damaged). The reroute score is maximum when a replacement contact from $\mathcal{N}$ is found for every contact lost to $\mathcal{P}$: $R_{re} = \rho$ if $\alpha = \beta$, where $\rho = 1$ when there is no damage to $\mathcal{N}$.

When bonded contact break, some of the previously used links leave and new links enter $\mathcal{P}$ from $\mathcal{N}$ as shown in Figure 6.7. An old link leaves $\mathcal{P}$ can be either damaged (link at stage t-1 but does not exist in $\mathcal{N}$ at stage t) or is in the complement set of $\mathcal{P}$ (exists in $\mathcal{N}$). Reroute score R_{re} accurately capture the transition from prefailure to failure as can be seen from Figure 6.7 (a,b).

For 1T, when pathway redundancy is high, across stages 1–8, the system compensates for the disruptions to transmission by finding replacement contacts in $\mathcal{N}$ for almost every contact that leaves $\mathcal{P}$. By contrast, when pathway redundancy is low, across stages 9–11, we observe a sudden degradation in $\mathcal{P}$ without a matching recovery. This can be seen from the increasing number of contacts that leave $\mathcal{P}$ at the same time decreasing the number of contacts that enter $\mathcal{P}$ from $\mathcal{N}$, as shown in Figures 6.7 (a,c), 6.8. Force rerouting patterns exhibit the cooperative behaviour in the bottlenecks in the early stages of the prefailure regime, as discussed previously. B_8 sustains most of the damage and, consequently, force reroutes up until stage 8 (Figure 6.9 (a)). This leaves B^* essentially intact with minimal damage and change to its tensile force chain membership across stages 1–8 (Figure 6.6 (a)). Moreover, the contacts with the above mean capacity (strong links) are preserved. Therefore, these preserved high capacity

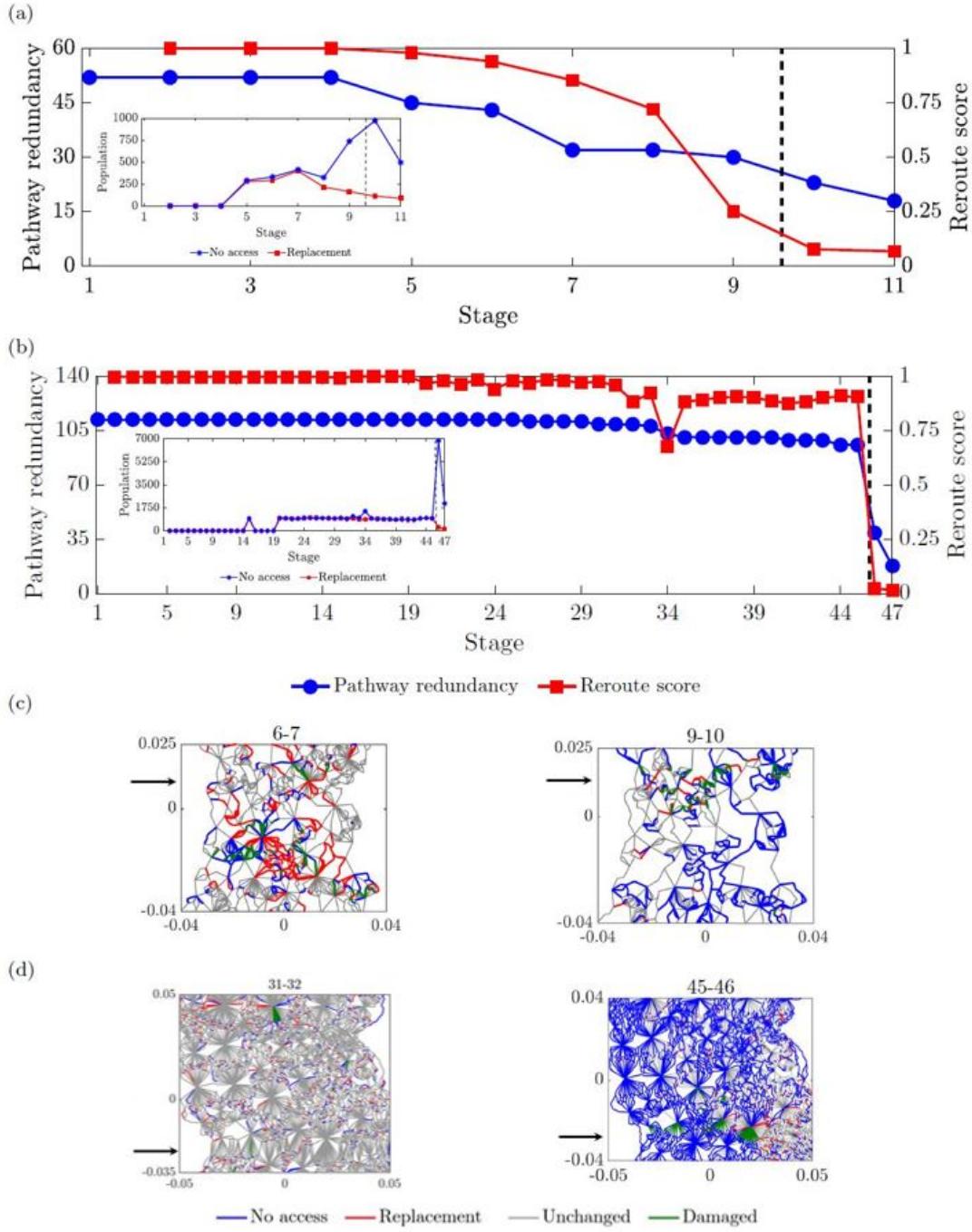


Figure 6.7.: 1T, 3T: Pathway redundancy, which allows rerouting of forces to alternative paths, underpins robustness of $\mathcal{N}$. (a,c) 1T and (b,d) 3T. (a,b) Evolution of the pathway redundancy p_{min} and the reroute score R_{re} ($R_{re} = 1$ is maximum when a new replacement link from $\mathcal{N}$ is found for every old link that is no longer accessed in $\mathcal{P}$) for 1T. Inset shows the evolution of the number of links that leave $\mathcal{P}$ but remain in $\mathcal{N}$ (no access) and enter $\mathcal{P}$ (replacement) due to rerouting. Dashed vertical line marks the stage at peak load. (c,d) Spatial distribution of rerouted and damaged links in $\mathcal{P}$. Black arrow marks the general location of the macrocrack.

contacts and tensile force chain contacts will release a large amount of energy when they break. 3T manifests similar trend except, in the entire prefailure regime (stages 1 – 45), it finds replacement contacts in $\mathcal{N}$ for almost every contact that is no longer accessed in $\mathcal{P}$ whereby maintaining high reroute score. This is possible due to a high level of redundancy.

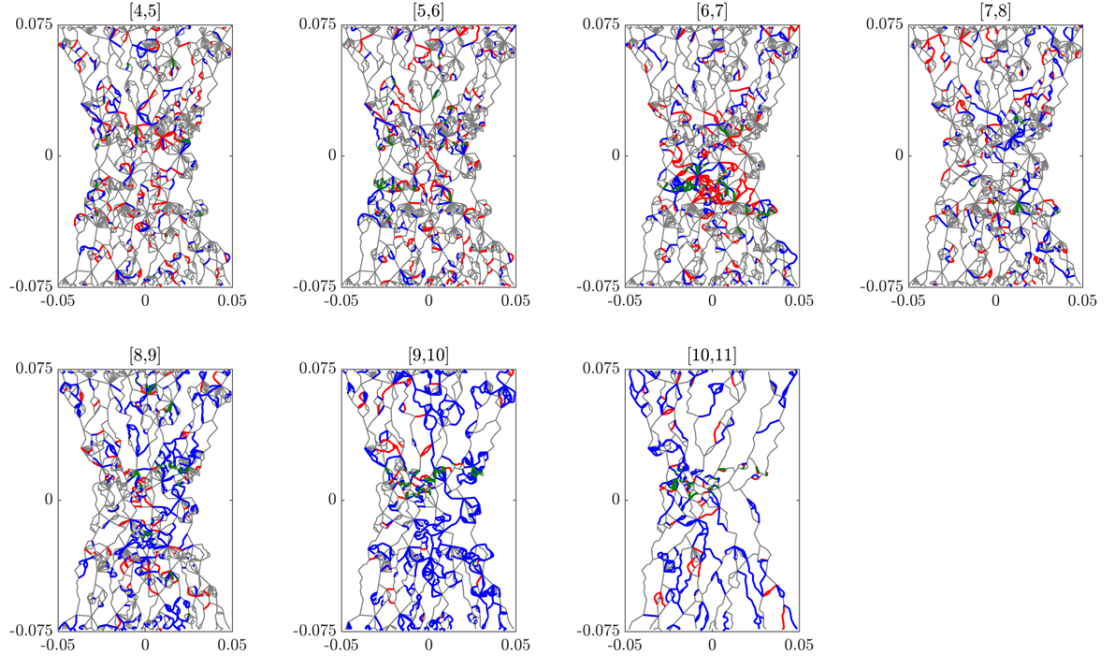


Figure 6.8.: *1T: Disruptions to force transmission, due to damage, lead to continual reconfigurations in force pathways.* Spatial distribution of rerouted and damaged links in $\mathcal{P}$ across the preceding time step at key stages $[t-1, t]$: blue links leave $\mathcal{P}$ but remain in $\mathcal{N}$, red links enter $\mathcal{P}$ to replace the blue links, gray links undergo no change, and green links are the contacts that break. Damage and rerouting initiate across stages 4-5.

For 3T, across stages, 1 – 45, the high level of redundancy in $\mathcal{N}$ enables significant force redistributions (i.e., changes in the force magnitudes) across the different contacts in $\mathcal{P}$ with minimal bond breakage (Figure 6.10). This and the significant number of alternative pathways surrounding tensile force chains in $\mathcal{P}$, as shown in Figure 5.3 result in minimal damage to the bottlenecks as the damage occurs elsewhere in the sample as can be seen from Figure 6.4 (d) (only one damaged link in each until stage 30), and a weaker interaction among the bottlenecks. Across stages 30 – 34, B_{32} sustains greater damage and number of undamaged links that are lost to $\mathcal{P}$ (no access links, Figure 6.9 (b)). This leaves B^* essentially intact with minimal damage and change to its tensile force chain membership across stages 1 – 35 (Figure 6.6 (b)). Across stages 36 – 45, the damage is diverted away from both bottlenecks due to the high level of redundancy, before a cascade of bond breakages occur in B^* across stages 45 – 47.

6.4. COOPERATIVE INTERACTION BETWEEN MOBILE AND IMMOBILE CONTACTS

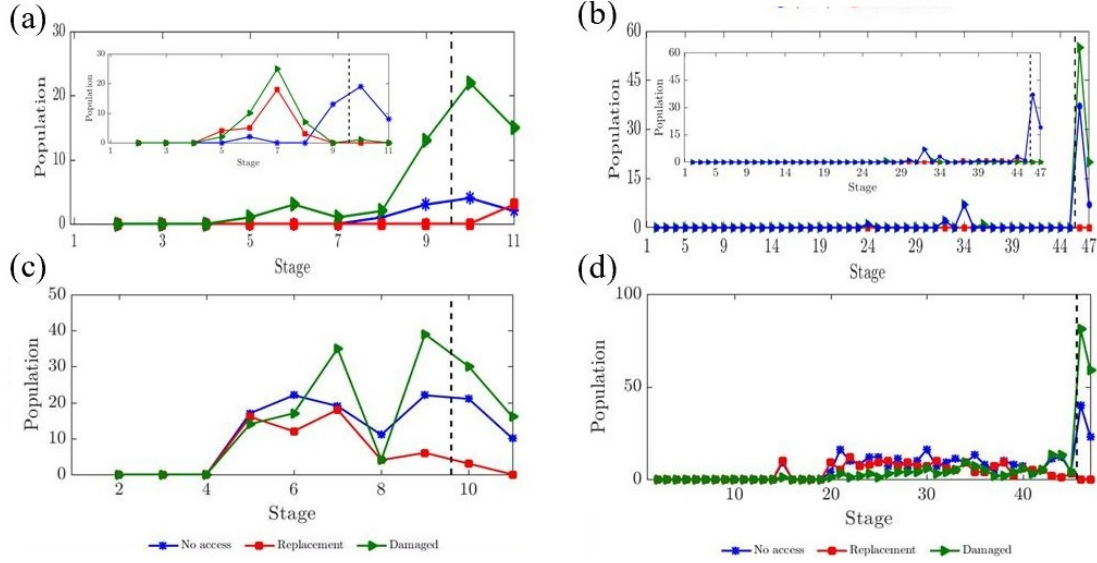


Figure 6.9.: $1T$, $3T$: Force reroutes in the bottlenecks relative to $\mathcal{P}$. (a,c) $1T$ and (b,d) $3T$. Population of no access, replacement, and damaged links across the preceding time step $[t-1, t]$: (a,b) in B^* and the secondary bottleneck (inset); and (c,d) in the mobile links outside of bottleneck. Dashed vertical line marks the stage at peak load.

6.4. Cooperative interaction between mobile and immobile contacts

To get a better understanding of the cooperative dynamics between the sites of damage, and their coevolution with the preferential force pathways $\mathcal{P}$, we extended our study to all the sites of damage. For $1T$, we find the mobile links sustain most of the force reroutes up until stage 8 (Figures 6.9 (a) inset, 6.9 (c) and 6.11). This is consistent with the earlier finding that prefailure damage mainly happens outside B^* , which are the mobile links. Consequently, this protects B^* . Note also that all of its contacts used entirely in the preferred force pathways $\mathcal{P}$ until stage 8 (Figure 6.9 (a)). However, the damage that occurs across stages 8–9 in B^* significantly reduces the available pathways for force reroutes. This is evident in the marked reduction in the reroute score. This also reduces the global force transmission capacity, but we see the highest drop across stages 9–10. This is consistent with the greatest damage to B^* in this time interval (Figure 6.2 (b)).

By contrast, $3T$ maintains a high reroute score for all of the prefailure regime due to the high level of redundancy in $\mathcal{N}$ and only drops at the same time (between stages 45–56) as the global transmission capacity drops (Figures 6.7 (b), 6.9 (b,d)). Before this, there was limited bond breakage in B^* and therefore, the maximum flow remained constant (Figures 6.4 (d), 6.5 (d) inset). In the entire prefailure regime, damage occurred mainly outside of B^* (i.e., mobile links). This is due to the high level of redundancy. There are many available redundant pathways to replace the broken bonds whilst main-

6.5. BRITTLE FAILURE: SUPPRESSED FOLLOWED BY CASCADING FAILURE IN THE FORCE BOTTLENECK

taining maximum flow. However, breakage of the edges in the bottleneck, which are at or close to full capacity in this peak stress regime, results in a greater reduction in maximum flow and reroute capability.

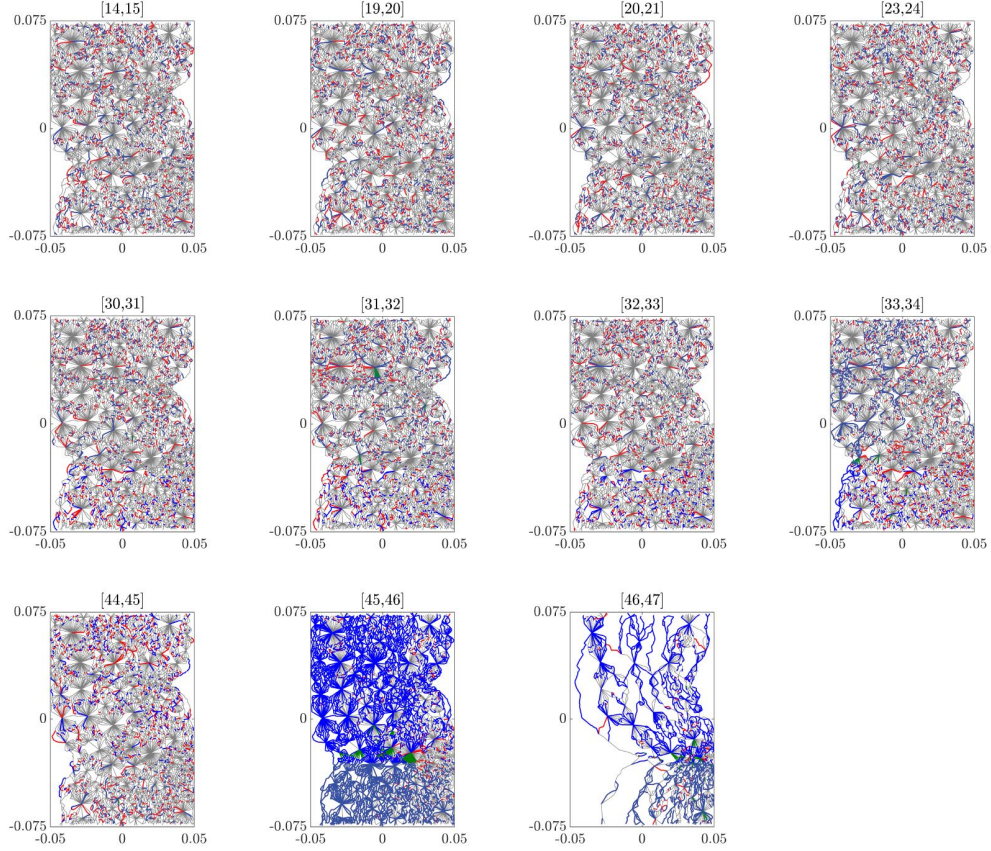


Figure 6.10.: *3T*: Disruptions to force transmission, due to damage, lead to continual reconfigurations in force pathways. Spatial distribution of rerouted and damaged links in $\mathcal{P}$ across the preceding time step at key stages $[t-1, t]$: blue links leave $\mathcal{P}$ but remain in $\mathcal{N}$, red links enter $\mathcal{P}$ to replace the blue links, grey links undergo no change, and green links are the contacts that break. Damage and rerouting initiate across stages 14-15.

6.5. Brittle failure: suppressed followed by cascading failure in the force bottleneck

The evolution of link type in B^* is shown in Figure 6.6. In both specimens, apart from a few exceptions, the tensile force chain contacts (TT) are mostly preserved in the prefailure regime, i.e., TT contacts (red) maintain their type. Further supporting evidence can be found in the evolution of damaged versus undamaged contacts in B^* (Figures 6.12, 6.13 (c,d)).

We see evidence of an optimal force transmission relative to the contact (bond) capacities. As the applied load is increased in the prefailure regime, a regulated increase

6.5. BRITTLE FAILURE: SUPPRESSED FOLLOWED BY CASCADING FAILURE IN THE FORCE BOTTLENECK

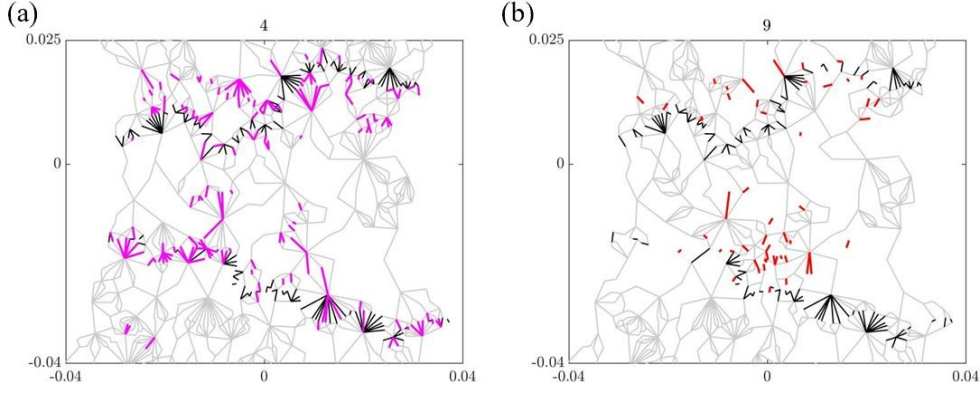


Figure 6.11.: *1T*: Force reroutes in $\mathcal{P}$. (a) Spatial distribution of $\mathcal{P}$ in the region of the bottlenecks at stage 4: mobile links (magenta), other bottleneck contacts (black). (b) Spatial distribution of mobile links used to replace links lost to $\mathcal{P}$ across stages 4-9 (red) shown with other bottleneck contacts (black). All other links of $\mathcal{P}$ are shown in grey.

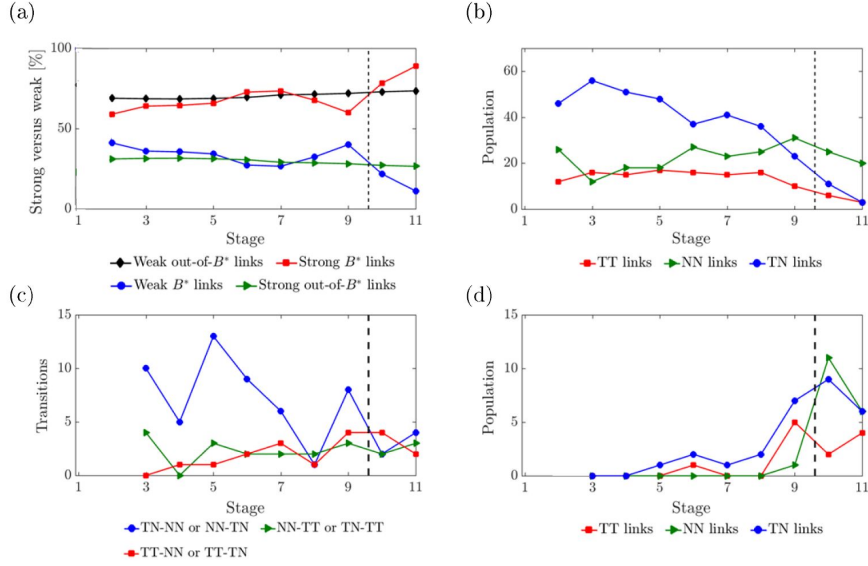


Figure 6.12.: *1T*: In B^* , most contacts are strong and support a tensile force chain grain (TN links) with damage mainly confined to these contacts. This leaves tensile force chain contacts largely intact (TT links) in the prefailure regime. These plots show the evolution of links in B^* (initial population is 84). (a) Percentage population of B^* links classified as strong versus weak; corresponding values for links outside of B^* are shown for comparison. (b) Number of links according to type: on average, around 58% of TN and NN links are strong contacts. (c) Evolution of transitions in link types: e.g., TN-NN at stage t means the number of link transitions from TN to NN during the preceding interval $[t-1, t]$. (d) Number of links of a given type that break during the preceding interval $[t-1, t]$. Note that (c) and (d) start at stage 3 since the percolating tensile force chain network is first established at stage 2. Dashed vertical line marks the stage at peak load. The method used to classify the different types of links or contacts relative to tensile force chains is described in Appendix A.

6.5. BRITTLE FAILURE: SUPPRESSED FOLLOWED BY CASCADING FAILURE IN THE FORCE BOTTLENECK

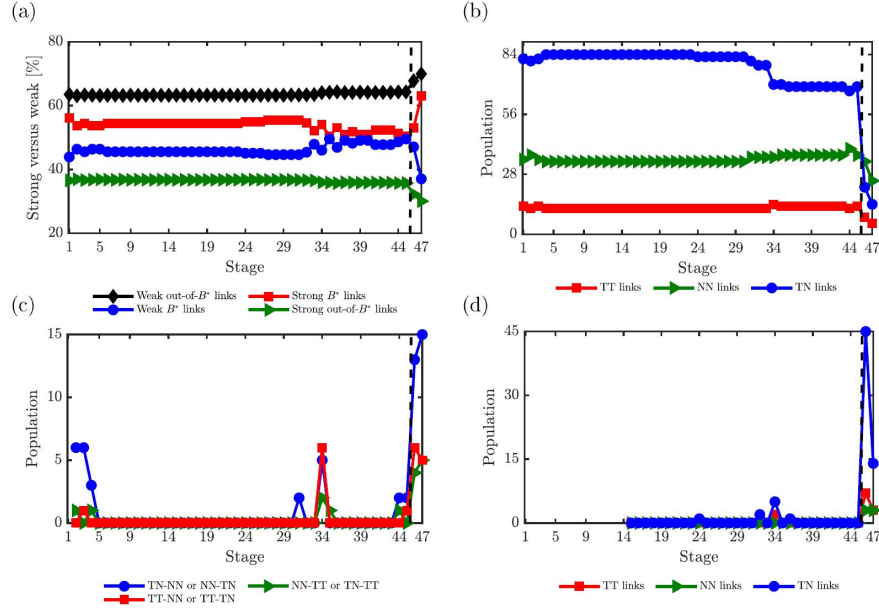


Figure 6.13.: *3T*: In B^* , most contacts are strong and support a tensile force chain grain (TN links) with damage mainly confined to these contacts. This leaves tensile force chain contacts largely intact (TT links) in the prefailure regime. These plots show the evolution of links in B^* (initial population is 130). (a) Percentage population of B^* links classified as strong versus weak; corresponding values for links outside of B^* are shown for comparison. (b) Number of links according to type: on average, around 52% of TN and NN links are strong contacts. (c) Evolution of transitions in link types: e.g., TN-NN at stage t means the number of link transitions from TN to NN during the preceding interval $[t-1, t]$. (d) Number of links of a given type that break during the preceding interval $[t-1, t]$. Dashed vertical line marks the stage at peak load. The method used to classify the different types of links or contacts relative to tensile force chains is described in Appendix A.

in the contact forces in the system can be observed to prevent damage in the bottleneck. Recall that damage in the bottleneck results in the greatest reduction in the maximum flow F^* . Note also that all bottleneck contacts belong to the optimised flow routes $\mathcal{P}$. Thus, bottleneck contacts play a major role in force transmission. The most critical parts of the sample are those contacts in tensile force chains (type TT) that lie in the bottleneck region. These contacts carry the majority of applied load, they are especially prone to becoming congested. For 1T, this can be seen from the accumulated load in the TT contacts relative to the supporting contacts TN and NN in Figure 6.14. Remarkably, in the prefailure regime, except the final stage, tensile force chain contacts in the bottleneck are protected. This is archived through a mechanism that spreads out the force across a web of predominantly strong contacts supporting the tensile force chains in the primary bottleneck B^* . We observed a similar trend for 3T with some exceptions enables through the high level of redundancy. Tensile force chain contacts are protected in the entire prefailure regime (Figures 6.6 (b), 6.13 (b,d)). For both samples,

6.5. BRITTLE FAILURE: SUPPRESSED FOLLOWED BY CASCADING FAILURE IN THE FORCE BOTTLENECK

we observed a disproportionately large number of member contacts in B^* transmitting at least the average tensile force as opposed to the complementary set of contacts that lie outside B^* (Figures 6.12 (a), 6.13 (a)).

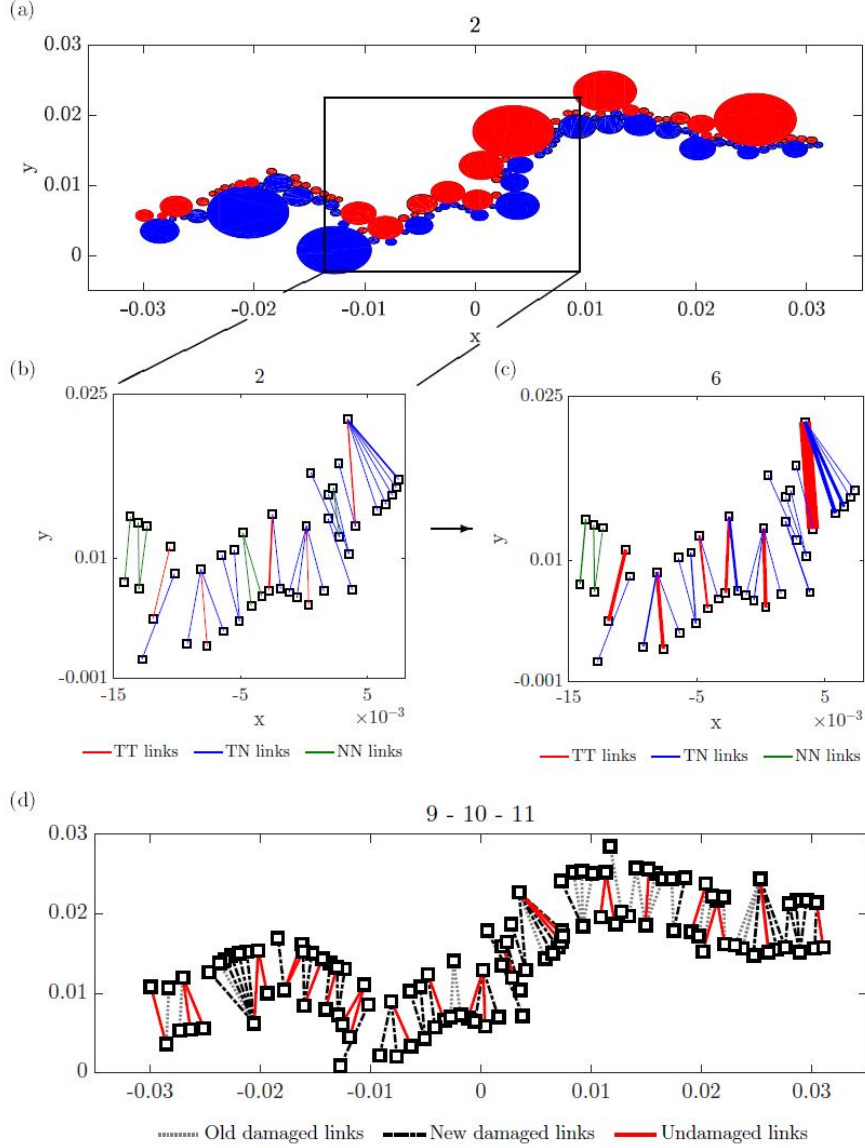


Figure 6.14.: *1T: Heightened interdependency among contacts in B^* predispose them to cascading failure.* (a) Grains coloured red (blue) belong to the upper (lower) portion of the specimen in 1T. Contact types for the highlighted region in (a) at: (b) stage 2 and (c) stage 6. Recall that Stage 2 is when the tensile force chain network is first established and stages 2 – 6 see a steady increase in the applied tensile load. Line thickness is proportional to the magnitude of the contact force. (d) Evolution of bonds as failure cascades in B^* across stages 9 – 11 in 1T. Similar trends apply to 3T (not shown).

In 1T, as can be seen from Figure 6.12 (d), the damage in B^* is mainly sustained by those contacts directly supporting force chains (TN). With respect to undamaged

6.5. BRITTLE FAILURE: SUPPRESSED FOLLOWED BY CASCADING FAILURE IN THE FORCE BOTTLENECK

contacts, we observed significant non-identity reconfigurations among the supporting contacts, i.e., TN-NN and NN-TN, followed by supporting contacts becoming force chains, NN-TT and TN-TT (Figure 6.12 (c)). These transitions occur even before the initiation of damage at stage 5. Demotion of TT contacts to TN or NN are rare (confined to 1 or 2 contacts) until stage 9 when a cascade of bond failures occur across stages 9 – 19 (Figure 6.15 (a)). In 3T, the high level of redundancy in $\mathcal{N}$ leads to a more robust specimen. Prefailure transitions in B^* are rare and occur only when bonds at TN contacts that support tensile force chains break ((Figure 6.13 (c,d))).

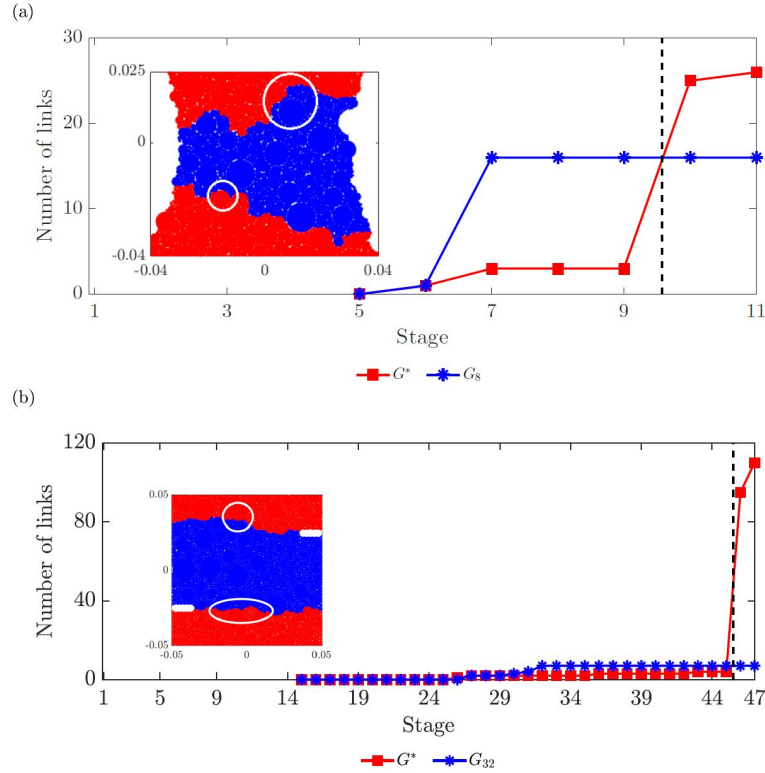


Figure 6.15.: *1T, 3T: Suppressed failure followed by cascading failure in the primary force bottleneck.* Crack interaction as described by the evolution of the size (number of links) of the two largest components of the damage network D_N for (a) 1T and (b) 3T. Dashed vertical line marks stage at peak load. Inset (a): general location at stage 11 of G_8 (lower circle) and G^* (upper circle) shown with the primary and secondary bottlenecks (red-blue interfaces). Inset (b): general location at stage 47 of G_{32} (upper circle) and G^* (lower circle) shown with the primary and secondary bottlenecks (red-blue interfaces).

Further evidence of minimal damage to the primary bottleneck B^* in the prefailure regime can be found in the evolution of the damaged network D_N for both specimens (Figure 6.15). In D_N , the links represent the broken bonds and the nodes are the damaged grains, i.e., those with at least one broken bond (see Appendix A for more detail). Prior to the peak load, the largest and second-largest connected components of

D_N , G_8 (or G_{32}) and G^* , respectively lie in the region of the bottlenecks B_8 (or B_{32}) and B^* . This is consistent with the damage maps in Figures 3.7, 3.8.

In particular, in 1T, G_8 is larger than G^* across stages 5 – 9 as can be seen from Figure 6.5 (b). This further consolidates that B_8 initially sustains most of the damage. However, as tensile forces increase towards the bond capacities, a critical point is reached when even a small increase in force triggers a cascade of bond failures across multiple interconnected contacts in B^* (inset Figure 6.15). Consequently, G^* outgrows G_8 and becomes the giant component in the postpeak softening regime. Recall from Figure 5.2 that the relatively sparse $\mathcal{P}$ links on the right side of the specimen for stages 10–11. This coincides with G^* being on the right side of B^* and explains why the residual strength of this specimen is mainly due to the $\mathcal{P}$ links on the left side of the specimen. All of these trends similarly hold for 3T, except that G^* is on the left side of B^* , consistent with the highly degraded and sparse $\mathcal{P}$ pathways on the left side of the specimen during failure (stages 46 – 47, Figure 5.3).

6.6. Conclusion

In conclusion, the force bottlenecks (minimum cuts) accurately and reliably predict the location of the ultimate macrocrack, except where it predicts the secondary crack, for the tension samples. We also observed a cooperative behaviour between force bottlenecks, which enables by redundancy, to minimise the inevitable reduction in global force transmission capacity due to damage. Results showed that sites, where damage and high stresses concentrate in the prefailure regime are not reliable indicators of where the dominant macrocrack will likely form. Moreover, the system is robust to damage up to a point due to many available paths (redundancy) for force transmission. After redundancy is depleted, a small change in the network triggers cascading failure along the primary bottleneck.

both of the Rankine and the Tresca criteria predict the failure that corresponds to the elasticity breakdown occurring at some critical states.

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7. Energy transmission and comparison of our fracture criteria with some classical fracture mechanics criteria

Here we present the results for the preferred paths for damage, as determined using the *energy bottleneck*. The methods behind these results were presented in section 4.2 of Chapter 4. We wish to compare our model's predictive capacity with four commonly used fracture mechanics criteria: (a) the minimum total energy functional (Francfort & Marigo 1998), (b) the critical minimum strain energy density (Sih 1973), (c) the maximum energy release rate (Palaniswamy & Knauss 1972) and (d) the maximum normal stress (Rankine stress) (Rankine 1857). A summary is shown in Figure 7.1.

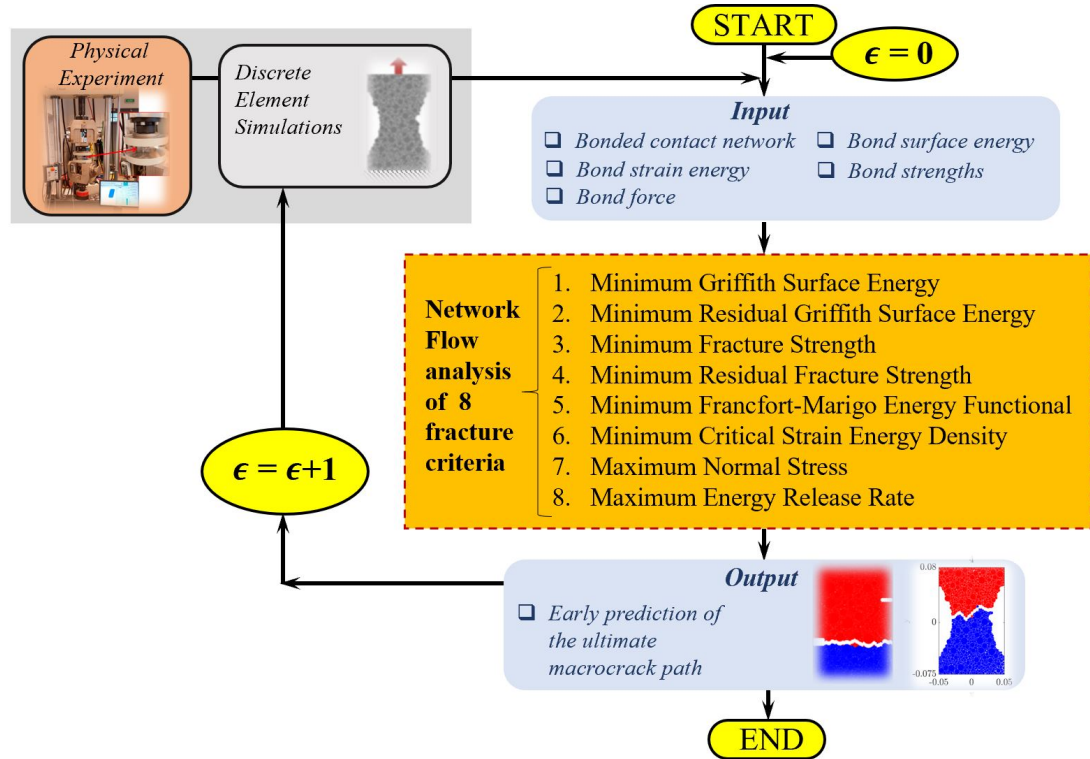


Figure 7.1.: A summary of the input data, methods used and the results.

This chapter is organised as follows. In section 7.1, we discuss the fracture criteria tested. In section 7.2, we establish a closed-form relationship between these fracture criteria. Finally, we present the results in section 7.3 before concluding in section 7.4.

7.1. Fracture criteria tested

Criterion 1: The energy flow bottleneck as the path of minimum Griffith's fracture surface energy

According to Griffith theory, a crack will propagate when there is sufficient stored potential energy to overcome the fracture surface energy of the material. The outstanding question is: *Once this condition is met, along which path $\mathcal{C}$ will the ultimate macrocrack propagate?* Here we propose that this path is given by $B(\mathcal{F}_E)$, the bottleneck of the flow network $\mathcal{F}_E = (G, s, t, \gamma)$: the cut where Griffith's fracture surface energy $\gamma(\Gamma)$ is minimum over all feasible cuts Γ of $\mathcal{F}_E$. This is also to test our model's fracture criterion, i.e., the minimum energy capacity criterion.

Criterion 2: The residual energy flow bottleneck

Criterion 1 can be extended to account for the loading stage ϵ , by incorporating the realised (actual) strain energy for the bond E_r in the capacity function: $\bar{q}_E(\epsilon) = \gamma - E_r$. Thus, an alternative criterion for the crack path is the path which is closest to breaking point relative to the fracture surface energy of the system: the bottleneck $B(\bar{\mathcal{F}}_E)$ of the flow network $\bar{\mathcal{F}}_E = (G, s, t, \gamma - E_r)$. As we discussed in Chapter 4, the energy flow is only approximately conserved in $\mathcal{N}$. Therefore, $B(\mathcal{F}_E) \approx B(\bar{\mathcal{F}}_E)$.

Criterion 3: The force flow bottleneck as the path of least resistance to fracture

The path of least resistance to fracture is given by the force bottleneck $B(\mathcal{F}_F)$. We reported on this in the previous chapter.

Criterion 4: The residual force flow bottleneck

The path that is closest to breaking point relative to the fracture strength of the system can be established from the bottleneck $B(\bar{\mathcal{F}}_F)$. The same argument from Criterion 2 applies. As we discussed in Chapter 4, the force flow is only approximately conserved in $\mathcal{N}$. Thus, $B(\mathcal{F}_F) \approx B(\bar{\mathcal{F}}_F)$.

Criterion 5: The path of minimum Francfort-Marigo energy functional (Francfort & Marigo 1998)

Francfort and Marigo [Francfort & Marigo \(1998\)](#) proposed that the macrocrack develops along the path where the total energy functional E_{tot} is minimum. Recall from section 2.2.1.2 of Chapter 2

$$E_{tot}(\Gamma, \epsilon) = E_d(\Gamma \setminus \mathcal{N}, \epsilon) + E_s(\Gamma). \quad (7.1)$$

Equation (7.1) can be expressed as

$$E_{tot}(\Gamma) = \sum_{e \in A \setminus \Gamma} E_r(e) + \sum_{e \in \Gamma} \gamma(e) = \sum_{e \in A} E_r(e) + \sum_{e \in \Gamma} (\gamma(e) - E_r(e)). \quad (7.2)$$

Since $\sum_{e \in A} E_r(e)$ does not depend on Γ , E_{tot} is minimized when $\sum_{e \in \Gamma} (\gamma(e) - E_r(e))$ is minimized. This path is given by the bottleneck $B(\bar{\mathcal{F}}_E)$ of the flow network $\bar{\mathcal{F}}_E = (G, s, t, \gamma - E_r)$ from Criterion 2.

Criterion 6: The path of minimum critical strain energy density

Building on Criterion 1, the capacity function given in Equation (4.12) can instead be expressed in terms of the critical strain energy density in the spirit of Sih (Sih 1973): $q(e) = \hat{\gamma} = \frac{\gamma(e)}{\pi(r(e))^2}$. This yields a new potential crack path which is given by the minimum cut of the flow network $\mathcal{F} = (G, s, t, \hat{\gamma})$. Thus, the path where the Griffith's fracture surface energy density $\hat{\gamma}(\Gamma)$ is minimum is given by the minimum cut of $\mathcal{F} = (G, s, t, \frac{\gamma}{\pi r^2})$, $B(\mathcal{F})$.

Criterion 7: The path of maximum energy release rate (Palaniswamy & Knauss 1972)

To find the path along which the maximum potential energy is released in $\mathcal{N}$, we solve for the maximum cut (see Appendix D for maximum cut algorithm) Γ_{max} of $\mathcal{F}_E$ such that

$$q(\Gamma_{max}) = \text{Maximize} \left\{ \sum_{e \in S(\Gamma)} \gamma(e) \right\},$$

where $S(\Gamma(\epsilon))$ is the set of saturated edges of $\Gamma(\epsilon)$. That is, $S(\Gamma(\epsilon))$ comprises those broken bonds in $\Gamma(\epsilon)$ as a result of the actual energy at $\epsilon - 1$ reaching its respective Griffith's fracture surface energy, $E_r(\epsilon - 1) = \gamma(\epsilon - 1)$.

Criterion 8: The path maximum normal stress (Rankine stress criterion (Rankine 1857))

To find the path that satisfies the Rankine stress criterion in $\mathcal{N}$, we solve for the maximum cut (see Appendix D for maximum cut algorithm) Γ_{max} of $\mathcal{F}_F$ such that

$$q(\Gamma_{max}) = \text{Maximize} \left\{ \sum_{e \in \Gamma} \frac{\|\vec{F}_n(e)\|}{\pi(r(e))^2} \right\}.$$

7.2. Closed-form relationships between criteria

Recall from Chapter 4 that the actual strain energies and tensile force magnitudes realised in the DEM simulations are only approximately conserved in $\mathcal{N}$. Here we

assume that conservation of flow is exactly satisfied. Therefore, the total flow across any two feasible cuts of a flow network is the same and the bottleneck of any two flow networks with capacities that differ only by a multiplicative constant is the same as discussed in Chapter 4. Below, subject to these two conditions, we establish closed-form relationships between the energy flow bottleneck $B(\mathcal{F}_E)$ from Criterion 1, the force flow bottleneck $B(\mathcal{F}_F)$ from Criterion 3, and the paths corresponding to all the other fracture criteria. Note that corollaries 1 – 5 apply to all stages of loading history, whereas corollary 6 is confined to the postpeak softening regime.

Corollary 1: The path of least resistance to fracture is the path closest to fracture, with respect to either the fracture strength or the fracture surface energy of the system: $B(\bar{\mathcal{F}}_E) = B(\mathcal{F}_E)$ and $B(\bar{\mathcal{F}}_F) = B(\mathcal{F}_F)$.

To prove this, we use the definition of the minimum cut (section 4.1.6 of Chapter 4). By definition we have

$$q(B(\bar{\mathcal{F}}_E)) = \text{Minimize} \left(\sum_{e \in \Gamma} (\gamma(e) - E_r(e)) \right) = \text{Minimize} \left(\sum_{e \in \Gamma} \gamma(e) - \sum_{e \in \Gamma} E_r(e) \right).$$

Due to the exact conservation of flow, the energy flow for any feasible path Γ in $\mathcal{F}_E$ is the same: $\sum_{e \in \Gamma} E_r(e)$ is the same for any Γ . Therefore, $\sum_{e \in \Gamma} \gamma(e) - \sum_{e \in \Gamma} E_r(e)$ is minimised when $\sum_{e \in \Gamma} \gamma(e)$ is minimised. But $\sum_{e \in \Gamma} \gamma(e)$ is minimised at $B(\mathcal{F}_E)$. Thus, $B(\bar{\mathcal{F}}_E) = B(\mathcal{F}_E)$. By the same argument, $B(\bar{\mathcal{F}}_F) = B(\mathcal{F}_F)$.

Corollary 2: The path with the minimum total energy as defined by Francfort and Marigo is the path with the minimum fracture surface energy.

As we have shown in Criterion 2, the path which minimises E_{tot} is the bottleneck of the residual energy flow network. As shown in Corollary 1, it is given by $B(\mathcal{F}_E)$ from Criterion 1.

Corollary 3: If the bonds are uniformly sized, then the path with the minimum critical strain energy density is the path with the minimum fracture surface energy.

When the bonds are uniformly sized, the capacity function of two flow networks $\mathcal{F} = (G, s, t, \frac{\gamma}{\pi r^2})$ and $\mathcal{F} = (G, s, t, \gamma)$ differs only by a constant multiple. Therefore, they have the same bottleneck. That is, the critical strain energy density is minimised along $B(\mathcal{F}_E)$ from Criterion 1.

Corollary 4: When the bonds have the same critical tensile bond stress, then the path that satisfies the Rankine stress criterion is the path with the minimum fracture strength.

As flow is conserved, the tensile normal force flow across any feasible cut of $\mathcal{F}_F = (G, s, t, F_{min}^n)$ is the same. Therefore, the path which maximises the tensile normal stress is the path with the least total bond area. This path is given by $B(\mathcal{F})$, the minimum cut of the flow network $\mathcal{F} = (G, s, t, A_b)$ with edge capacity equal to the area of the corresponding bond A_b . Recall $F_{min}^n(e) = \frac{T_n(e)}{\pi} A_b(e)$. If the critical tensile stress T_n is uniform, then the capacity function of two flow networks $\mathcal{F}_F = (G, s, t, F_{min}^n)$ and $B(\mathcal{F} = (G, s, t, A_b))$ differs only by a constant multiple. Therefore, they have the same bottleneck. That is, when the critical tensile stress T_n is uniform in $\mathcal{N}$, the path that satisfies the Rankine stress criterion is the force bottleneck $B(\mathcal{F}_F)$ from Criterion 3.

Corollary 5: When bond properties are uniform, and the only source of heterogeneity is the bond connectivity, i.e., disordered but otherwise homogeneous network, then all the fracture criteria except for the maximum energy release rate (criterion 7) are satisfied along the path with the least number of bonds.

In the special case when bond properties are uniform in $\mathcal{N}$, the capacity functions q_E and q_F are both constants. As we discussed in section 4.1.7 of Chapter 4, $B(\mathcal{F}_E) = B(\mathcal{F}_F)$ and is a minimum edge cut. Moreover, the paths from Criteria 1-6 and 8 converge to one path, which is the minimum edge cut. The number of bonds in this cut, p_{min} , gives a measure of path redundancy in $\mathcal{N}$ as discussed in the previous chapter.

Corollary 6: In the postpeak softening regime, when the maximum flow is reached, then the path of maximum energy release rate is the same as the path with the minimum fracture surface energy.

As can be seen from Figure 7.2, the realised flow is close to the maximum flow in $\mathcal{F}_E$ in the postpeak softening regime. Let $\Theta(\Gamma(\epsilon))$ be defined as the total flow from the saturated edges in Γ : $\Theta(\Gamma) = \sum_{e \in S(\Gamma)} x(e) = \sum_{e \in S(\Gamma)} \gamma(e)$. Since $x(\Gamma)$ is the total flow across Γ , $\Theta(\Gamma) \leq x(\Gamma)$. By flow conservation, the total flow through any feasible cut is the same, $x(\Gamma) = x(\Gamma_{min})$. Since Γ_{min} is a minimum cut, every edge of Γ_{min} is saturated when the maximum flow is reached in $\mathcal{N}$. That is, $S(\Gamma_{min}) = \Gamma_{min}$ and $\Theta(\Gamma_{min}) = \sum_{e \in \Gamma_{min}} x(e) = \sum_{e \in \Gamma_{min}} \gamma(e) = x(\Gamma_{min})$. Thus $\Theta(\Gamma) \leq \Theta(\Gamma_{min})$. Given Γ is arbitrary, this implies that at those stages where the realized flow in $\mathcal{N}$ reaches the maximum flow F_E^* , the energy release is maximized along $B(\mathcal{F}_E)$ from Criterion 1.

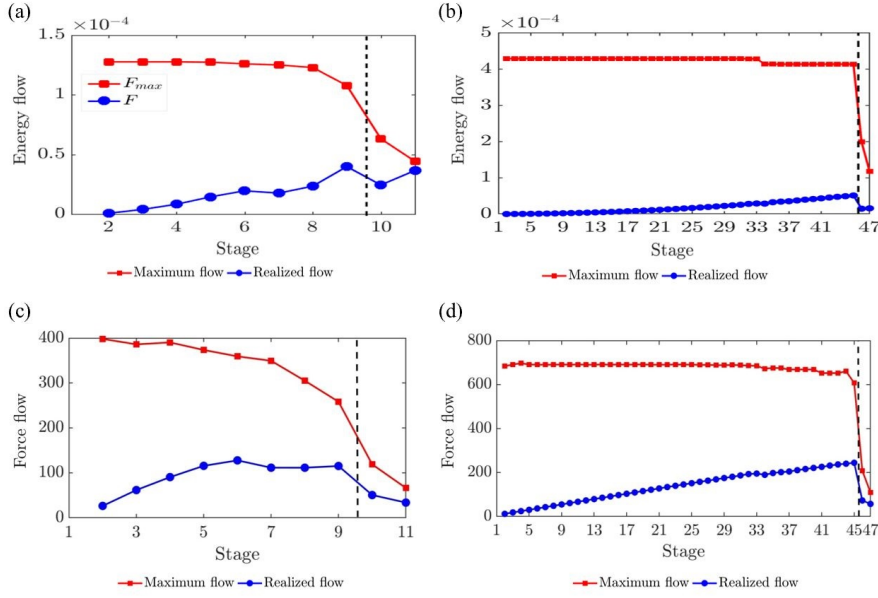


Figure 7.2.: 1T, 3T: *Failure is characterized by the transmission of energy and force near the global flow capacity of the bond network.* (a, c) 1T. (b, d) 3T. Evolution of the realized flow and the maximum flow in $\mathcal{N}$: energy flow (a, b), force flow (c, d). Dashed vertical line marks the stage at peak load. Note that the sample is only partially split and some bonds remain in the macrocrack path at the final stage m .

7.3. Results

Here, we seek to address an open question: Can the path of the crack that leads to failure be predicted from known microstructural properties and, if so, how far in advance of peak strength? In particular, we want to check whether our model's fracture criterion (minimum energy capacity) can predict the location of the ultimate macrocrack path. This path corresponds to the bottleneck from Criterion 1. This path is shown in Figure 7.3. As can be seen, minimum capacity cut, reliably predict the location of the ultimate macrocrack from the beginning of the loading history for both 1T and 3T. Furthermore, the prediction persists and is robust. This model did not predict the competing (secondary) cracks as in the case of force bottlenecks.

It is essential to check the evolution of the bottleneck (minimum cut) capacity relative to arbitrary cuts to answer why this model did not predict the secondary crack. As can be seen from Figure 7.4, capacity for the bottleneck is much smaller than other cuts. In this case, a single recurring energy flow bottleneck is likely to emerge. This is possible as breakage of few links in other cuts will not sufficient to become new minimum cut. To get further insight, we compute the cut capacity for recurring energy flow bottleneck $\mathcal{B}_E$ and the competing force bottleneck B_8 (B_{32}) (this is the secondary bottleneck reported in the previous chapter in 1T (3T)). As can be seen from Figure 7.5, the cut capacity

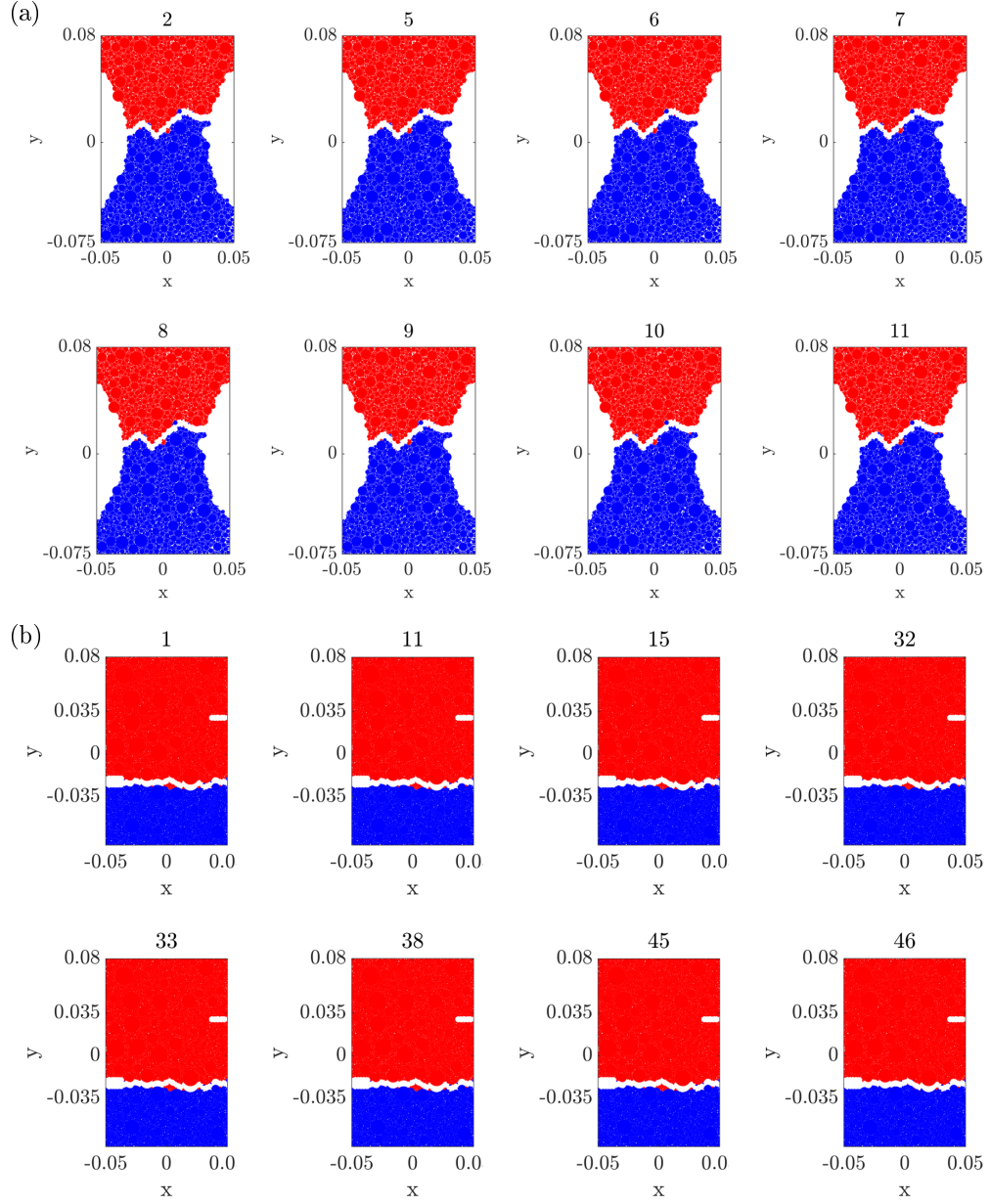


Figure 7.3.: $1T$, $3T$: Energy flow bottlenecks $\mathcal{B}_E$, like the force flow bottlenecks $\mathcal{B}_F$, provide an early prediction of the ultimate crack pattern. Spatial distribution of the bottlenecks with edge capacity function given by Equation (4.12) (red-blue interface). Grains on either side of the ultimate macrocrack are artificially separated to aid visual comparison of the bottleneck versus the actual macrocrack location. Note prediction persists for all stages. Note also that we have only included the prediction for selected stages. Other stages have a similar prediction.

clearly distinguishes these two. We see that clear difference in the cut capacities and that for B_8 is higher. This is consistent with the discussion in section 4.2.3.1 of Chapter 4. This explains why the energy bottleneck only predicts the ultimate macrocrack. It also shows that the maximum flow (red line) accurately marks the transition from prefailure

7.3. RESULTS

to failure as in the case with force bottlenecks. This highlights the accuracy of our failure criterion.

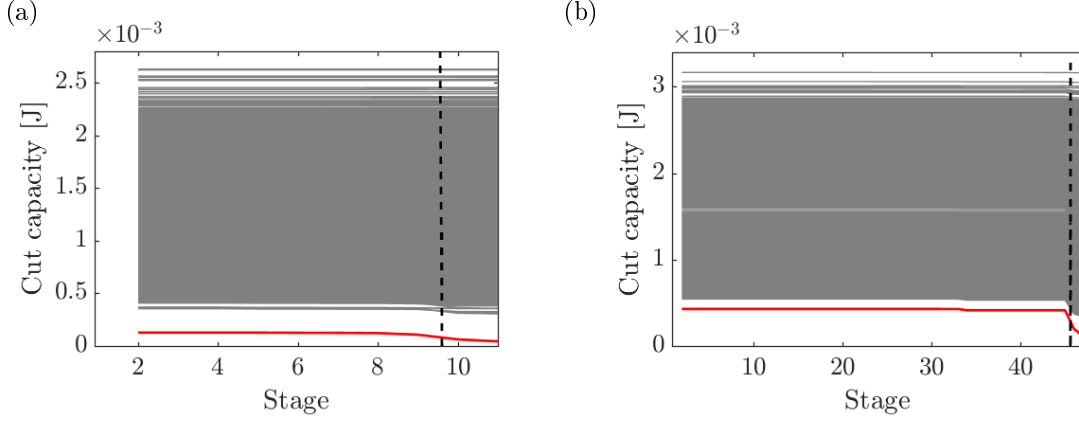


Figure 7.4.: *1T, 3T: Cut capacity distinguishes the bottleneck from other arbitrary cuts.* Evolution with the stage of cut capacity computed for 10,000 arbitrary cuts (grey) and the bottleneck (red) for (a) 1T and (b) 3T. Dashed vertical line marks strain at peak load.

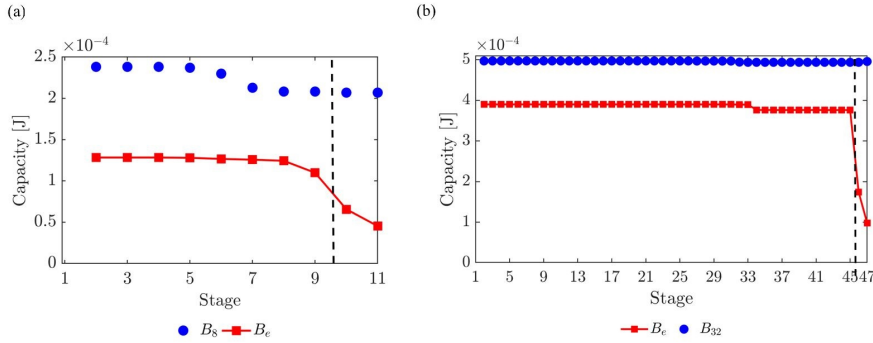


Figure 7.5.: *1T, 3T: Energy bottlenecks do not predict the competing crack.* The evolution of the capacities of the energy flow bottleneck $\mathcal{B}_E$ (red) with secondary force bottleneck $B_8(B_{32})$ (blue circle) for (a) 1T and (b) 3T. Dashed vertical line marks the stage at peak load.

Next, we investigate the performance of each criterion. For each criterion, we quantified the error between the predicted location and the actual location of the macrocrack as follows:

$$P = \frac{|(V_{B_u} \setminus V_{\mathcal{C}_u}) \cup (V_{\mathcal{C}_u} \setminus V_{B_u})|}{|V_T|} \times 100\%, \quad (7.3)$$

where V_{B_u} , $V_{\mathcal{C}_u}$ are the set of grains in the upper part of the bottleneck and the macrocrack respectively, V_T is the set of all the grains in the sample, and $|\cdot|$ denotes the cardinality (number of grains). Hence P_e quantifies the number of offset grains in the prediction relative to the macrocrack, normalized by the total number of grains.

1. As can be seen from Figures 7.6 and 7.7, the bottlenecks of the energy/force flow networks and residual energy/residual force flow network are essentially the same. As shown above, this implies that at any given stage of loading, the bottlenecks distinguish themselves from all other feasible crack paths in two respects: by having the least total capacity and by being closest to fracture, with respect to fracture strength or fracture surface energy. That is, the fracture criterion that delivers an early prediction for the location of the ultimate macrocrack path must be related to the flow bottleneck. On the other hand, the realised (actual) flows are an outcome of an optimised transmission process that maximises the global throughput subject to the redundancies of, and the capacities of member segments or bonds along, the percolating paths through the specimen. Results here are consistent with recent experiments on ceramics (Kondo *et al.* 2019; Daniel *et al.* 2019), metallic glasses (Qu *et al.* 2016) and graphite Hug *et al.* (2020).
2. As judged from the prediction error, the best of the eight fracture criteria is the force residual bottleneck (Criterion 4). This makes sense because: (i) it uses the actual bond capacities from the DEM model; and (ii) it accounts for the loading stage of the material through the actual bond force realized. Note that since the bottleneck for Criterion 5 is found by solving the same minimum cut in Criterion 2, their errors are the same.

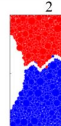
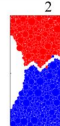
Criterion Regime	1	2	3	4	5	6	7	8
Pre-peak								
Pre-peak error (%)	1.051	0.526	1.032	0.425	0.526	9.409	26.986	12.586
Post-peak (softening)								
Post-peak error (%)	0.465	0.627	0.424	0.344	0.627	0.465	2.645	2.986

Figure 7.6.: 1T: *Early prediction of the location of the ultimate macrocrack path $\mathcal{C}$ by the energy, force and residual bottlenecks.* Summary of crack path predictions (red-blue interface) for the eight fracture criteria and their maximum error in the prepeak and postpeak softening regimes (to aid visual, an artificial separation shows $\mathcal{C}$). Representative stages shown are stage 2 when the system spanning force chain network is first established and the final stage of loading. Criterion 8 starts at stage 5 as there are no broken bonds until then.

3. Our results revealed that minimum critical strain energy density, maximum energy

7.3. RESULTS

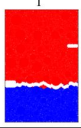
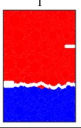
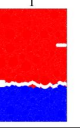
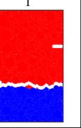
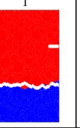
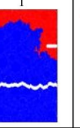
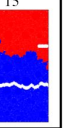
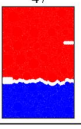
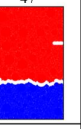
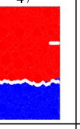
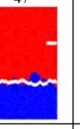
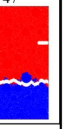
Criterion \ Regime	1	2	3	4	5	6	7	8
Pre-peak								
Pre-peak error (%)	0.719	0.708	0.696	0.672	0.708	0.732	55.045	24.854
Post-peak (softening)								
Post-peak error (%)	0.240	0.216	0.191	0.192	0.216	0.360	3.765	3.856

Figure 7.7.: 3T: *Early prediction of the location of the ultimate macrocrack $\mathcal{C}$ by the energy, force and residual bottlenecks.* Summary of crack path predictions (red-blue interface) for the eight fracture criteria and their maximum error in the prepeak and postpeak softening regimes (to aid visual, an artificial separation shows $\mathcal{C}$). Representative stages shown are stage 1 when the system spanning force chain network is first established and the final stage of loading. Criterion 8 starts at stage 15 as there are no broken bonds until then.

release rate and maximum normal stress (Criteria 6-8) do not provide a reliable early prediction for the location of the ultimate macrocrack. This is due to these criteria do not capture the path redundancy in $\mathcal{N}$ in the prefailure regime. Redundancies in transmission paths facilitate to reroute energy and force to higher capacity bonds to prevent bond breakage. As shown in the previous chapter, damage in the early stages of the prefailure regime mainly occurs away from the macrocrack path $\mathcal{C}$. Similar stress redistributions around strain concentration sites have been observed to divert damage away from the crack path into the bulk of the sample (Peng *et al.* 2020; Papanikolaou *et al.* 2019). Given the macrocrack path $\mathcal{C}$ essentially coincides with the energy bottleneck $B(\mathcal{F}_E)$, this may initially seem counterintuitive given the close proximity to fracture of the bonds in $B(\mathcal{F}_E)$. It turns out there is an interplay between force chain stability in the energy bottleneck and path redundancy, as we now demonstrate.

- We reported the interplay between force chain stability in the force bottleneck and path redundancy in the previous chapter. Same holds for the energy bottleneck as they are essentially the same.
- The bottleneck force chains are the most obvious suspect location for failure. However, we find these preserved in the prefailure regime. Moreover, the damage is confined to the low capacity link leaving high capacity links in the bottleneck intact (Figure 7.8-inset). This suggests that forces are spread out

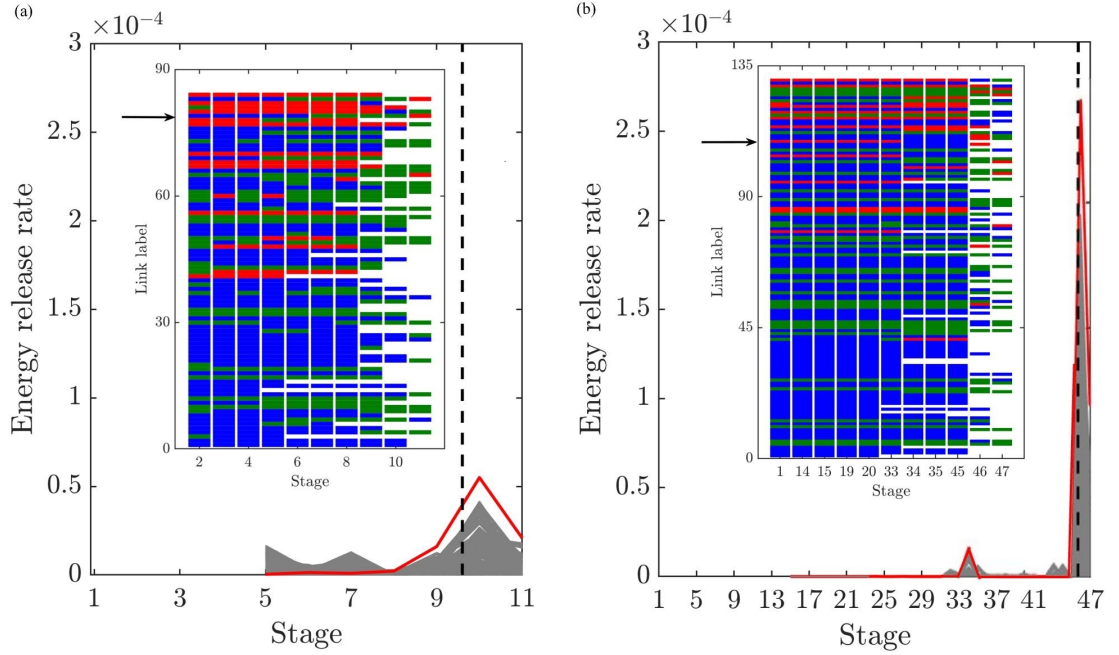


Figure 7.8.: Evolution of energy release rate for all 10,000 random cuts (grey) and bottlenecks (red) for (a) 1T and (b) 3T. No broken bonds until stage 5 for 1T and stage 15 for 3T. Insets show the evolution of link type for each of the k member links of the energy bottleneck $B(\mathcal{F}_E)$. For 1T, $k = 84$; for 3T, $k = 130$. Links in B are ranked from lowest to highest fracture surface energy (labelled 1 to k) at that stage when the tensile force chain network is first established (stage 2 for 1T and stage 1 for 3T). Link type is represented by a horizontal bar coloured according to the type of grains in contact: red (TT- tensile force chain grains), green (NN- neither is a tensile force chain grain), blue (TN- one is a tensile force chain grain, the other is not). See Appendix A for the classification of link type. Bonds having above the global mean fracture surface energy lie above the black arrow. A transition to a different link type manifests as a change in the colour of the bar. No bar is shown for a link that breaks.

across member contacts (Figure 6.14 (a-c)). Therefore, when these contacts break, the sample releases the greatest amount of energy (Figure 7.8). We believe this process may prove to be a contributing factor to the so-called ‘crack shielding’ or crack toughening that has been reported in the literature on granular composites [Tang *et al.* \(2020\)](#); [Peng *et al.* \(2020\)](#); [Papanikolaou *et al.* \(2019\)](#).

4. The process described above and the previous chapter protect the bottleneck from damage in the prefailure regime. However, it has the opposite effect in the softening regime by predisposing the bottleneck to rapid fracture. As path redundancy is depleted with the spread of damage, the remaining bottleneck bonds are collectively brought closer and closer to their respective breaking points. This results in a cascading of bond failure along the bottleneck in the transition to postpeak

softening regime, with two attendant mechanisms *in the bottleneck* $B(\mathcal{F}_E)$:

- energy release rate becomes maximum (Figure 7.8). This shows a peak in the energy released in the transition to prefailure to failure and also a higher energy release rate during postpeak softening regime. This can be explained by the remaining high capacity bonds of tensile force chains and their lateral supports, since these stores the highest levels of potential strain energy while being closest to fracture (Figure 6.14). In contrast, concurrent energy release rates in all other feasible crack paths are much less, due to member bonds being further away from their respective fracture surface energies and hence can support an increase in strain energy without breaking. The higher pathway redundancy for 3T supports the earlier finding that tensile force chain contacts in $\mathcal{P}$ are significantly more supported than those in 1T (recall from Chapter 5). This enables the bottleneck in 3T to support and store much higher energies than 1T before the onset of cascading failure. This is consistent with the observed results (Figure 7.8). This influence of connectivity on the stability of force chains was recently observed by Tang *et al.* 2020 in their study of packing and grain size distribution for optimal performance of reactive materials like aluminumpolytetrafluoroethylene (Al-PTFE) granular composites.
- normal stress becomes maximum as the tensile force flow through the bottleneck becomes close to the maximum force flow while the total bond area becomes minimum.

5. In the previous section, we derived closed-form relationships based on the result that force and energy bottlenecks provide an early and accurate prediction of the ultimate crack path $\mathcal{C}$. These relationships naturally shed light on the specific influences of heterogeneities in bond geometry, strength and surface energy, a topological disorder in the bond network, as well as the stage of loading on the ultimate crack path, as outlined in the previous section. Additionally, it can help explain why all eight fracture criteria approximately agree in their prediction of $\mathcal{C}$ in the postpeak softening regime. This is mainly due to the collective breakage of bonds along $\mathcal{C}$ in this regime. Criterion 7 identifies $\mathcal{C}$ due to corollary 6. Criterion 8 identifies $\mathcal{C}$ due to corollary 4 as $\mathcal{C}$ becoming the path with the least total bond area. Criterion 6 identifies $\mathcal{C}$ as $\mathcal{C}$ becoming the path with the least number of bonds.

7.4. Conclusion

In conclusion, we have shown that our model's fracture criterion, i.e., minimum energy capacity, provides an early prediction of the path of the mode I crack that leads to failure. We have shown that the effect of disorder in the bonded contact network, heterogeneities in bond properties and state of loading on the macrocrack path. These flow bottlenecks were also related to widely used fracture criteria into a unified framework of network flow. This data-driven study now paves the way for examination of more complex loading conditions, which we address in the next chapters.

The crack in tension appears abruptly at the stress peak and involves almost no secondary cracks along its path. In contrast, the main cracks in compression are thicker and involve numerous secondary cracks produced during crack growth.

Topin *et al.* 2007

8. Preliminary results on the prediction of crack patterns in compression samples

In the previous two chapters, we presented the results for the uniaxial tension tests where the cracks do not pass through the source and sink of the flow network, namely, the top and bottom walls of the sample. Here we focus on the compression samples, discussed in section 3.2 of Chapter 3, where not only is the crack pattern more complex but also the cracks intersect the source and sink of the flow network. This is a problem since in a classical network flow analysis, the bottleneck cannot pass through these nodes. Consequently, we use the method proposed in section 4.3 of Chapter 4 to predict the crack pattern. In assessing the performance of this new method, we compare our results with four commonly used fracture criteria, to complement the discussion in Chapter 7. A summary is shown in Figure 8.1.

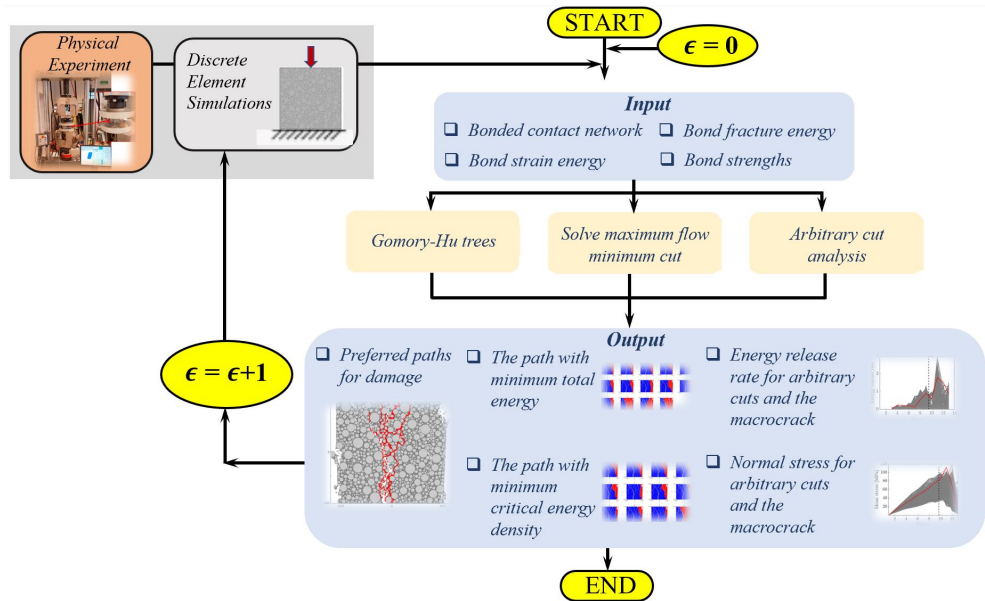


Figure 8.1.: A summary of the input data, methods used in this chapter and the results.

This chapter is organised as follows. In section 8.1, we present the predicted crack locations. In section 8.2, we compare our results with four commonly used classical fracture mechanics criteria. A brief conclusion is given in section 8.3.

8.1. Force and energy bottlenecks

Here we test the performance of our proposed method in predicting complicated and vertical crack patterns (align with applied load and hence passes through the source and the sink assignment in the classical maximum flow minimum cut analysis) in compression samples. Here we use the method discussed in section 4.3 of Chapter 4. Firstly, we present the results from force bottlenecks. Secondly, we present the results from energy bottlenecks. Next, we will discuss the results for compression samples. The attention is paid to 1C.

8.1.1. Bottleneck derived from tensile bond strength

As discussed in Chapter 2, the main bond failure mode is tension even in a system subjected to compression. Moreover, for data we studied, The essential microscale mechanism for damage in the prefailure regime is bond breakage in tension Nitka & Tejchman (2015). Therefore, it is intuitive to use tensile bond strength as the contact capacity function. The contact capacity function is given by

$$q = F_{min}^n = T_n r^2, \quad (8.1)$$

where T_n is the critical tensile normal stress and r is the radii of the smaller of the two spherical grains in bonded contact. Here we seek to answer the question *can the crack pattern be predicted using known tensile bond strength? If so how early in the loading history?*

The spatial distribution of the accumulated predicted location for the final crack with the contact capacity given by Equation (8.1) is shown in Figures 8.2 and 8.3 for 1C and 3C respectively. Note that this capacity function did not give any prediction until stages 8 (15) for 1C (3C). It predicts the partial boundaries of the major crack and other minor cracks for most of the loading history.

8.1. FORCE AND ENERGY BOTTLENECKS

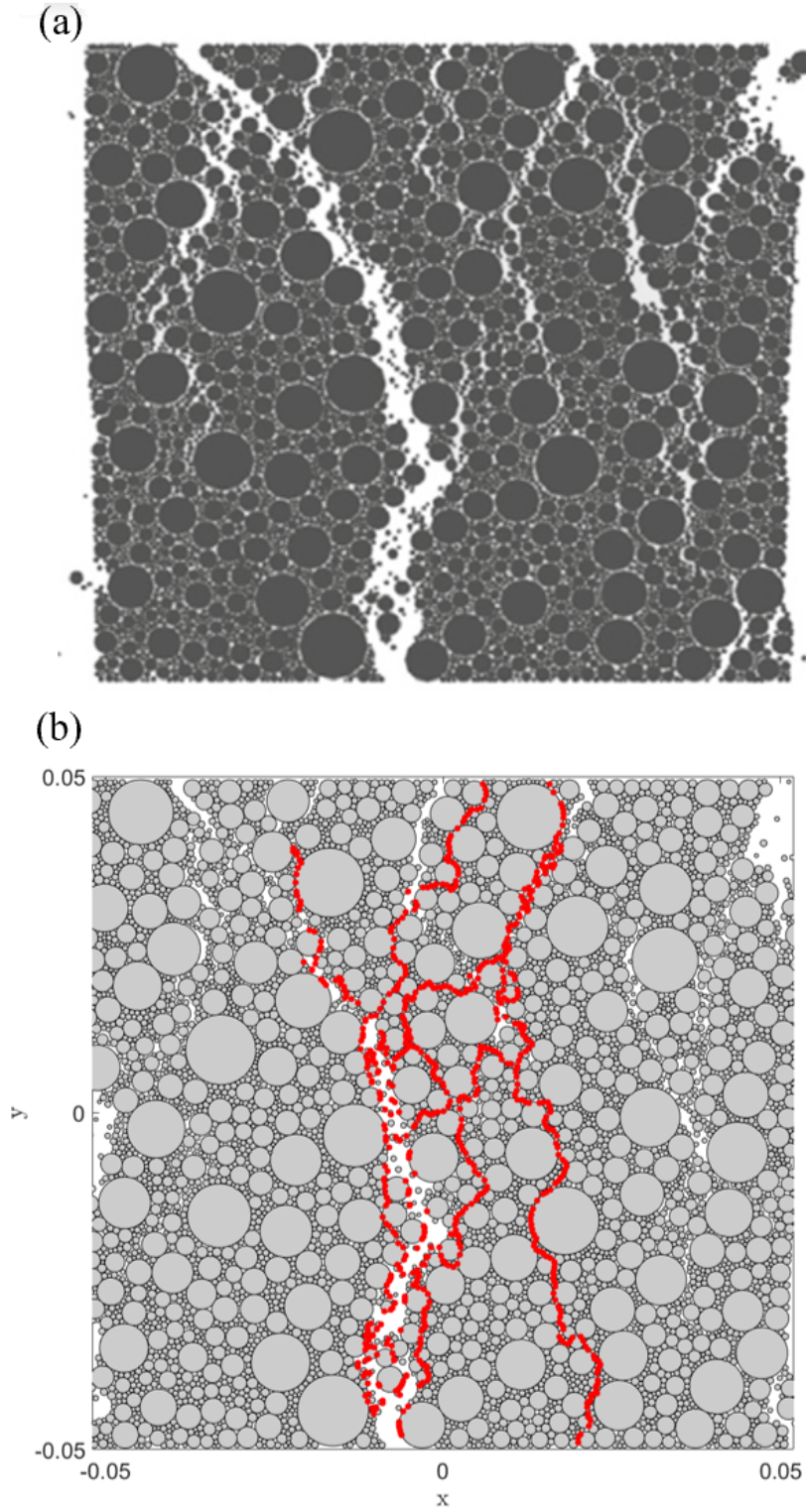


Figure 8.2.: 1C: Spatial distribution of prediction form GHT with contact capacity function given by Equation (8.1). (a) The final crack pattern from the DEM data. (b) Accumulated distribution of predicted location is plotted as the contact point of the edges in the cut (red). Use the grain positions information at the final stage of loading. No prediction until stage 8. The strain stage correspond to peak force is between states 9 and 10.

8.1. FORCE AND ENERGY BOTTLENECKS

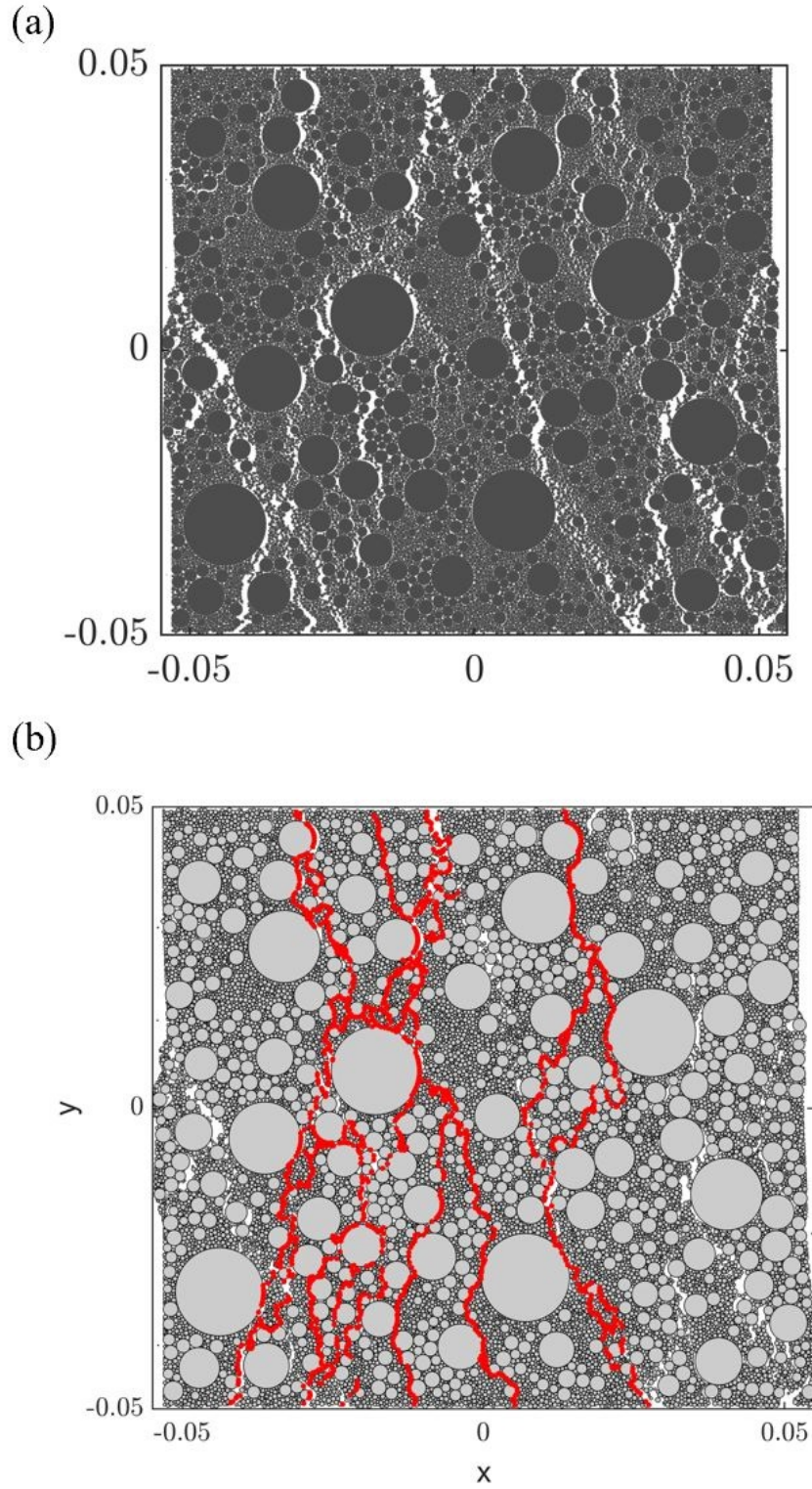


Figure 8.3.: 3C: Spatial distribution of prediction form GHT with contact capacity function given by Equation (8.1). (a) The final crack pattern from the DEM data. (b) Accumulated distribution of predicted location is plotted as the contact point of the edges in the cut (red). Use the grain positions information at the final stage of loading. No prediction until stage 15. The strain stage correspond to peak force is between states 15 and 16.

8.1.2. Bottleneck derived from maximum energy

The majority of classical fracture mechanics criteria are based on energy, as discussed in Chapter 2. Results from the previous chapter confirmed that energy-based contact capacity functions reliably and robustly predicted the location of the ultimate macrocrack path in tension samples. Similarly, here we test the prediction from energy capacity function which only consider the tensile bond failure mode. This contact capacity function is given by

$$q = \frac{0.5(F_{min}^n)^2}{K_n}, \quad (8.2)$$

where $K_n = E \frac{2r_A r_B}{r_A + r_B}$ is the normal contact stiffness. E is the Young's elastic modulus of the contact, r_A and r_B are the radii of the grains sharing the bond such that $r = \min(r_A, r_B)$. These are known material parameters for each contact. Here we seek to find an answer for the question *can the crack pattern be predicted by using only the tensile failure mode? If so how early in the loading history?*

For 1C, the spatial distribution of accumulated predicted location for the final crack pattern with this capacity function is shown in Figure 8.4. Similar to previous capacity function tested, this did not give any prediction until stage 8. As this capacity function fails to give a reasonable prediction for 1C, we did not test this capacity function for 3C. From the above results, we can see that the prediction is not reasonably good if we consider only tensile bond failure mode.

Even though the essential microscale mechanism for damage in the prefailure regime is bond breakage in tension Nitka & Tejchman (2015), the majority of contacts are in compression. Furthermore, bonds can fail by shear. Therefore, it is not immediately clear the effect of assigning tensile bond strength for those contacts under compression. Since force is a vector quantity, we cannot combine two types of forces in our analysis. To avoid this, we turn into a capacity function that is based on energy as discuss next.

Regardless of the main bond failure mode being tension, the majority of contacts are in compression. Thus, we used a combination of contact capacity function: maximum shear energy for compressive contacts and maximum elastic energy for tensile contacts. This contact capacity function is given by

$$q = \begin{cases} \frac{0.5(F_{min}^n)^2}{K_n}, & \text{for tensile contacts,} \\ \frac{0.5(F_{max}^s)^2}{K_s}, & \text{for compressive contacts,} \end{cases} \quad (8.3)$$

where $K_s = \nu E \frac{2r_A r_B}{r_A + r_B}$ is the tangential contact stiffness and $F_{max}^s = Cr^2$ is the maximum shear force (strength at bond fail by shear). C is the maximum shear stress and ν is the Poisson's ratio. These are known material parameters for each contact.

The spatial distribution of accumulated energy bottlenecks derived from the Equation (8.3) is shown in Figures 8.5 and 8.6 for 1C and 3C respectively. It shows that

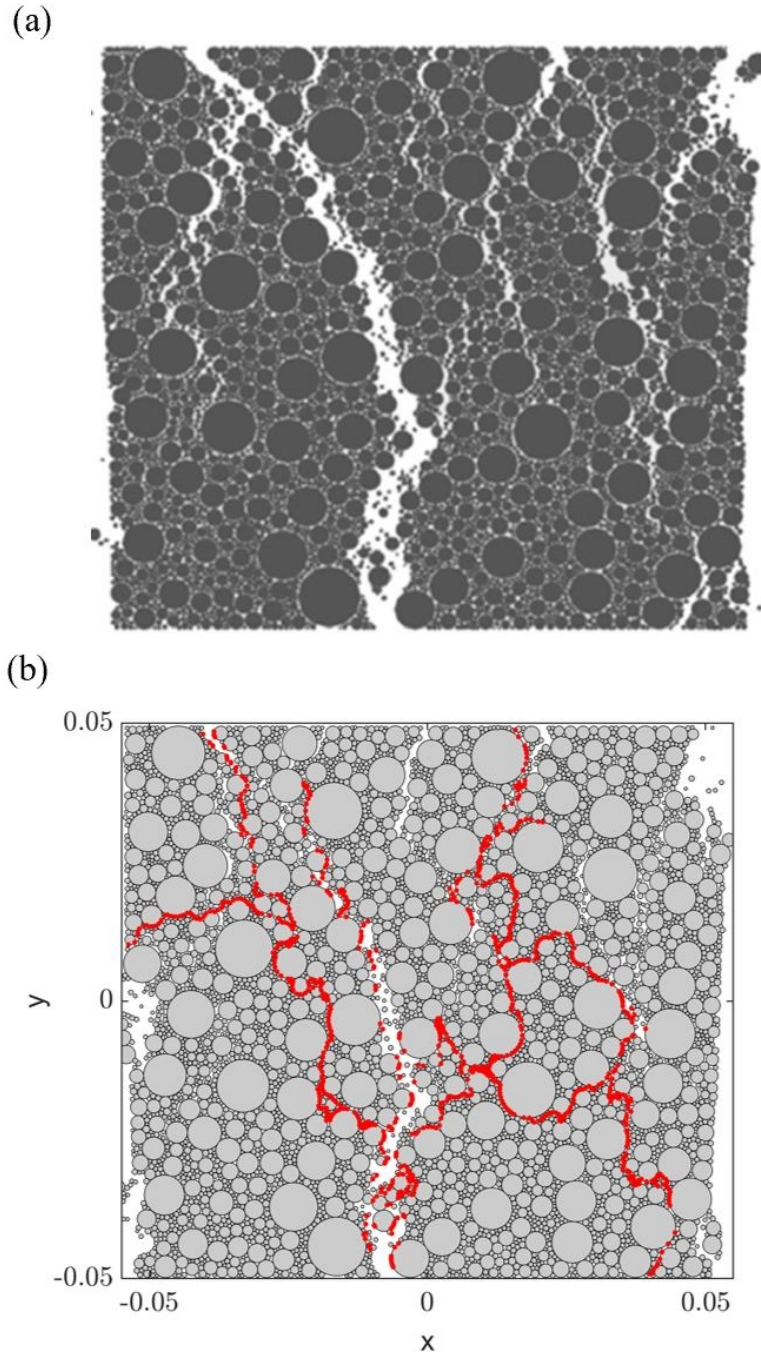


Figure 8.4.: 1C: Spatial distribution of prediction from GHT with contact capacity function given by Equation (8.2). (a) The final crack pattern from the DEM data. (b) Accumulated distribution of predicted location is plotted as the contact point of the edges in the cut (red). Use the grain positions information at the final stage of loading. No prediction until stage 8. The strain stage correspond to peak force is between states 9 and 10.

energy bottlenecks predict the complicated crack pattern quite well from the beginning of the loading history.

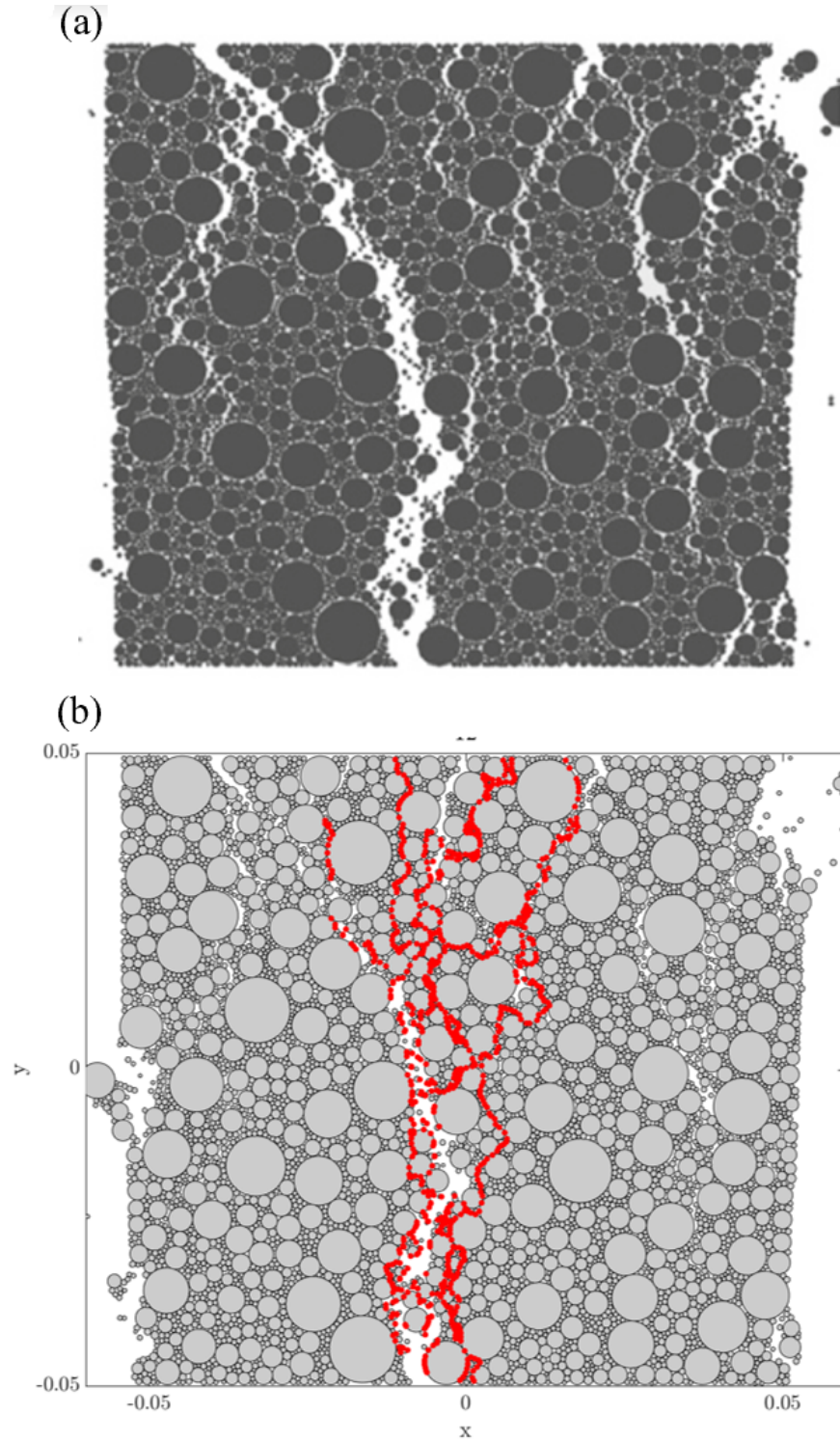


Figure 8.5.: 1C: Spatial distribution of prediction from GHT with the edge capacity model given by Equation (8.3). (a) The final crack pattern from the DEM data. (b) Accumulated distribution of predicted location is plotted as the contact point of the edges in the cut (red). Use the grain positions information at the final stage of loading.

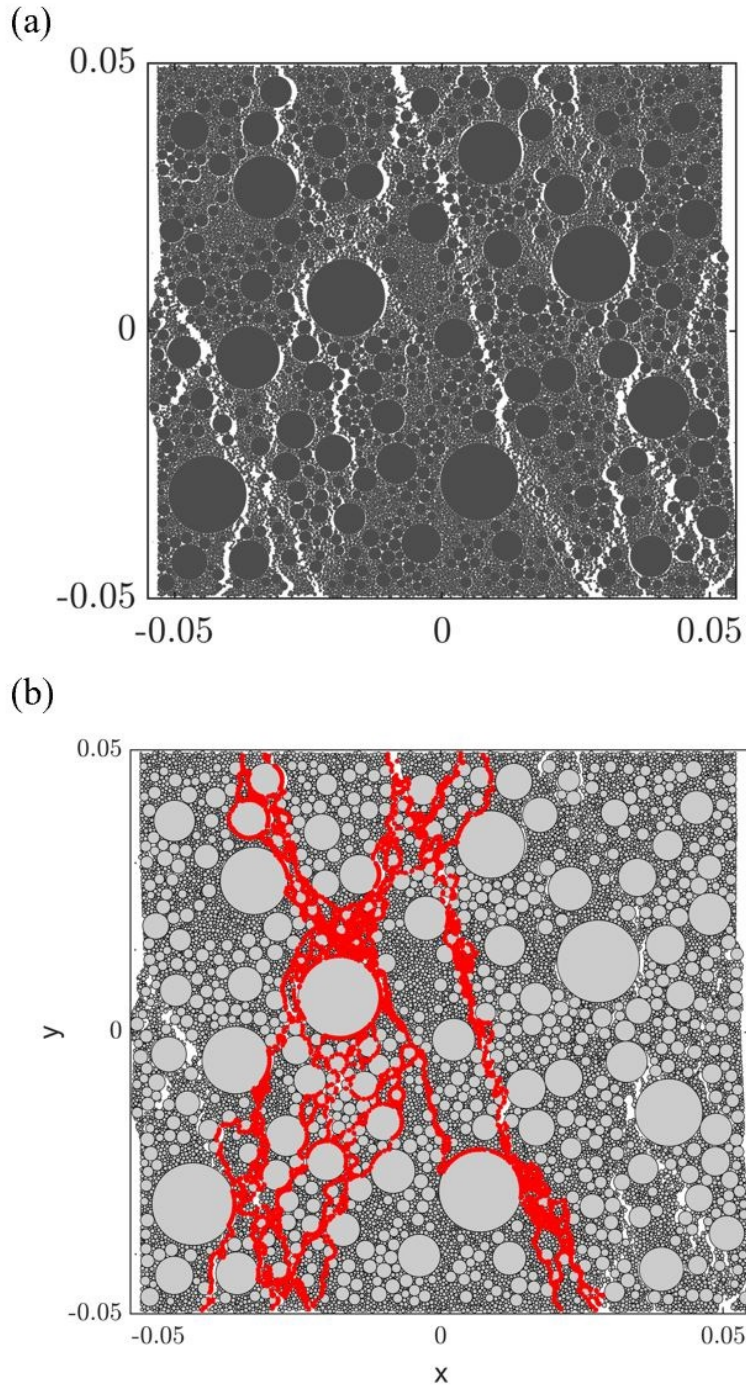


Figure 8.6.: 1C: Spatial distribution of prediction from GHT with the edge capacity model given by Equation (8.3). (a) The final crack pattern from the DEM data. (b) Accumulated distribution of predicted location is plotted as the contact point of the edges in the cut (red). Use the grain positions information at the final stage of loading.

When we compare prediction from tested contact capacity function, a combination of energy contact capacity function performs well. But, still, there exist many cuts with close-cut capacity (competing cuts) and hence GHT fails to give a persistent prediction.

8.2. COMPARISON WITH THE CLASSICAL FRACTURE MECHANICS CRITERIA

Therefore, the breakage of a few links in another cut results in a minimum capacity cut and becomes the new minimum cut. That is why the predicted location keeps changing. The results also revealed that shear failure and compressive contacts have a major influence in predicting the crack pattern.

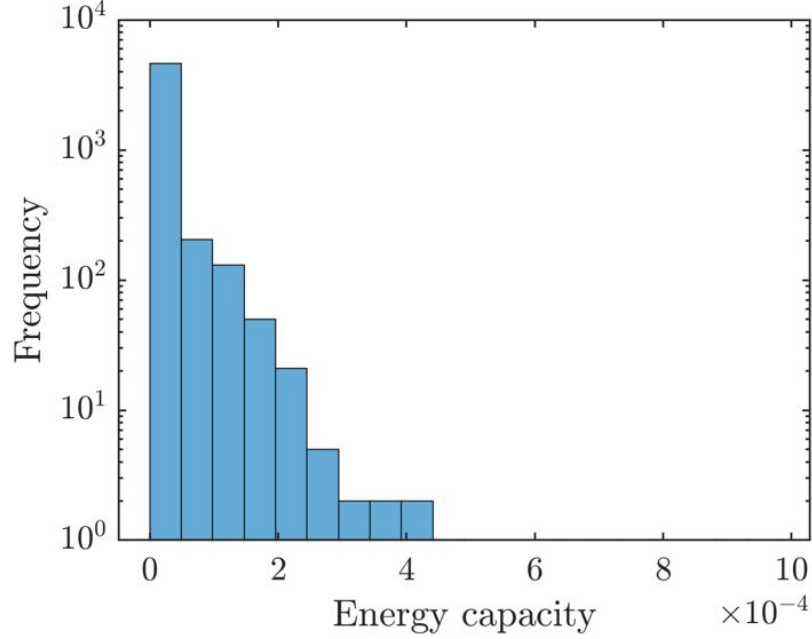


Figure 8.7.: 1C: Frequency distribution of minimum cut capacity at stage 11 with edge capacity model given by Equation (8.3). There are 5,015 minimum cuts in the GHT. Other stages show similar results. This shows that there are many cuts with close cut capacity in this sample.

To assess the predictive capability of our proposed method, it is important to check the performance of existing classical fracture mechanics criteria for these compression samples. Therefore, we will test the performance of four commonly used classical fracture mechanics criteria next.

8.2. Comparison with the classical fracture mechanics criteria

Similar to the previous chapter, here we test four classical fracture mechanics criteria for 1C. Note that we did not use the GHT method with these criteria. The location of the final crack is available as a part of the data. We do not input the final crack in the proposed method and only used to compare the results. It is easy to test the predictive capability of classical fracture mechanics criteria, as the orientation of the final crack pattern is known as will discuss next.

8.2.1. prediction from Francfort-Marigo energy functional

As discussed in the previous chapter, we can use the maximum flow minimum cut theorem to find the path Γ , which minimises the total energy E_{tot} of the system. To do that, we set the contact capacity function $q = E_{max} - E_r$, as discussed in section 2.2.1.2 of Chapter 2. Since the actual crack path for 1C is vertical, we assign the grains attached to the left and right walls as the source and the sink respectively. Note here that we use maximum flow minimum cut theorem purely to find the vertical cut with the minimum residual capacity. We *do not* pose the question as modelling force transmission. Therefore, the physical meaning is not important here. However, maximum flow minimum cut analysis implicitly assumes the conservation of flow and outputs the cut with minimum capacity. Thus, the bottleneck of $\tilde{\mathcal{F}}_E = (G, E_{max} - E_r, s, t)$ should be the vertical path which minimises the total energy E_{tot} in Equation (7.1) as discussed in the previous chapter.

The vertical cut which minimises the total energy is shown in Figure 8.8, as a red-blue interface. As can be seen, the predicted path does not coincide with the major crack until stage 12. The results after stage 14 are similar to that for stage 14. Next, we will test the performance of the minimum critical energy density criterion.

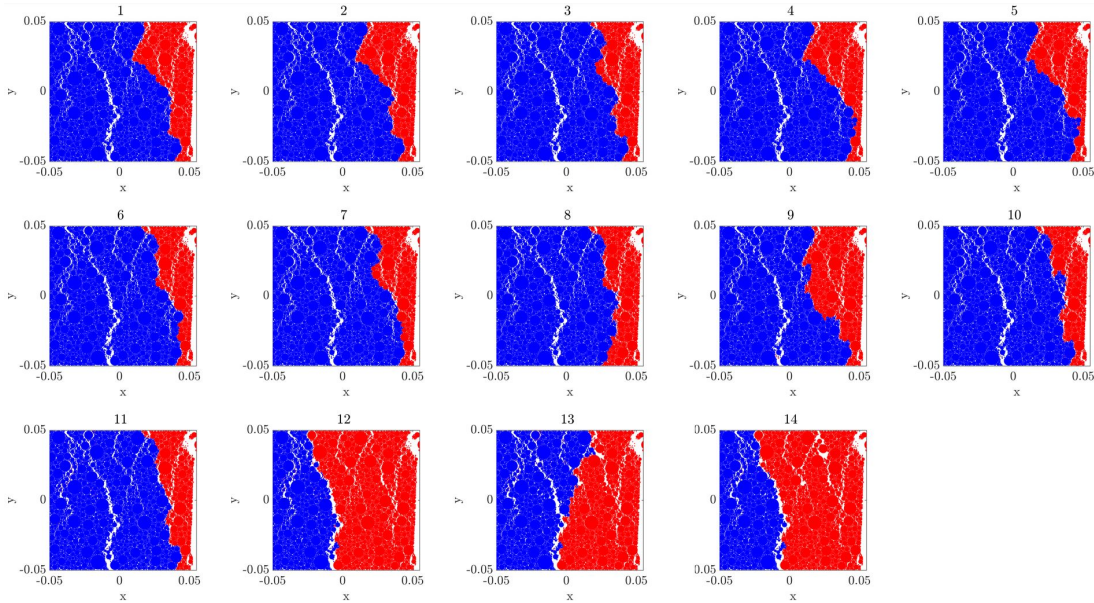


Figure 8.8.: 1C: Spatial distribution of vertical path (red-blue interface) which minimises the total energy given by Equation (7.1). Used grain position information at the final stage (21) to aid visual comparison with predicted location with the actual crack pattern.

8.2.2. prediction from critical minimum energy density criterion

Our aim here is to see whether this criterion predicts the major crack path or not. Therefore, to find the vertical path with minimum critical energy density given in

8.2. COMPARISON WITH THE CLASSICAL FRACTURE MECHANICS CRITERIA

Equation (2.15), we carried out maximum flow minimum cut analysis with the contact capacity function $q = \frac{E_{max}}{\pi r^2}$ and the left and right walls as the source and sink respectively as the same reasoning given above. This means the bottleneck of the flow network $\mathcal{F} = (G, \frac{E_{max}}{\pi r^2}, s, t)$ should be the vertical path which minimises the critical energy density.

The predicted path is shown in Figure 8.9, as a red-blue interface. It depicts that this path does not coincide with the major crack until stage 12, as in the case of total energy. The results after stage 12 are similar to that for stage 12. We investigate the predictive capacity of the maximum energy release rate criterion next.

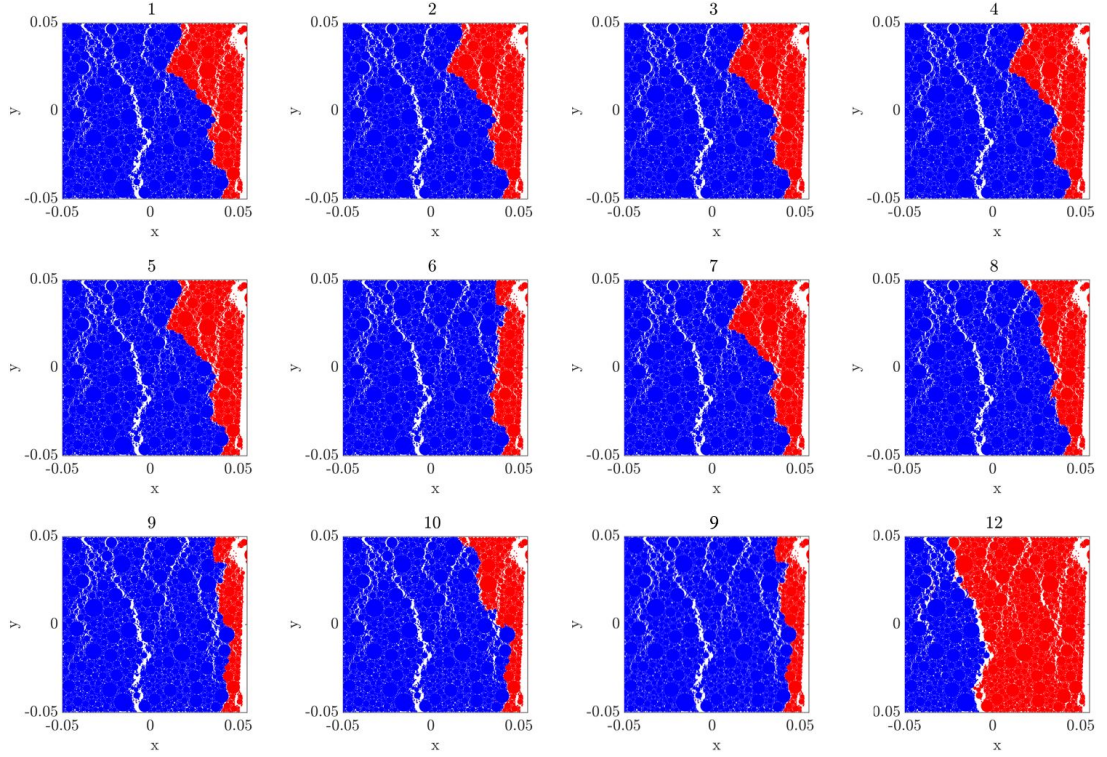


Figure 8.9.: 1C: Spatial distribution of vertical path (red-blue interface) which minimises the strain energy density. Used grain position information at the final stage (21) to aid visual comparison with predicted location with the actual crack pattern.

8.2.3. Prediction form maximum energy release rate criterion

As the maximum cut problem is NP-hard as mentioned in the previous chapter and approximation algorithm also computationally expensive, first, we calculated the energy release rate given in Equation (2.13) for 10,000 arbitrary cuts and the final crack. The result is shown in Figure 8.10. It shows that the energy release rate is not higher for the crack. Therefore, we did not employ the maximum cut algorithm to find the path which maximises the energy release rate. Similarly, we use arbitrary cut analysis to

check whether the final crack path has higher stress. The results are discussed next.

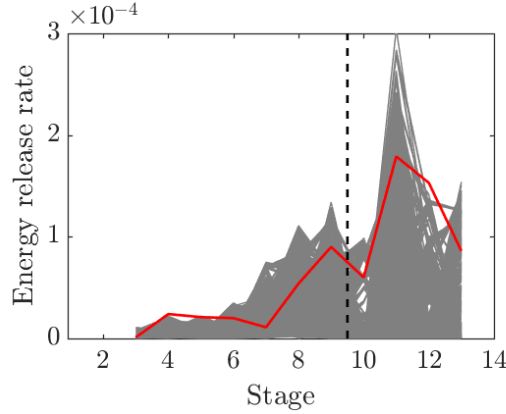


Figure 8.10.: 1C: Evolution with stage of energy release rate computed for 10,000 arbitrary cuts (grey) and the final crack. Dashed vertical line marks strain at peak load.

8.2.4. Prediction form Rankine stress criterion

To see whether the crack path has higher stress, we computed the mean stress for 10,000 arbitrary cuts and the final crack. The result is shown in Figure 8.11. We took the mean to avoid bias towards the cut with many member contacts. It depicts that the mean stress for the final crack lies in the distribution of arbitrary cuts. Hence, we can see that the final crack path does not have the maximum stress. Therefore, we did not employ the developed approximation algorithm to find the maximum cut.

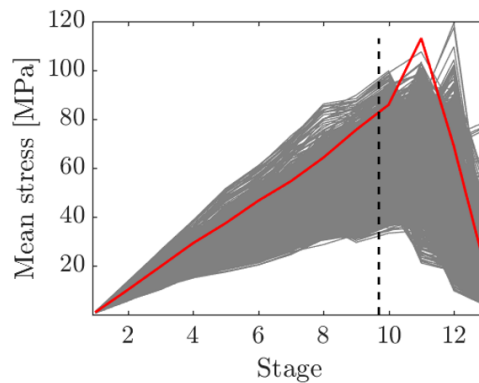


Figure 8.11.: 1C: Evolution with stage of the mean stress computed for 10,000 arbitrary cuts (grey) and the final crack. Dashed vertical line marks strain at peak load.

8.3. Conclusion

The preliminary results were presented to check the performance of the proposed method to find a crack that goes through the so-called source and the sink. The main advan-

tag of the proposed network flow model which uses Gomory-Hu tree over the classical minimum cut analysis is that an upfront selection of the source and sink is not needed. Hence, prior knowledge of the orientation of the crack and direction of flow is not required. Results revealed that this method performed quite well over the classical fracture mechanics criteria tested here. This may be due to the classical fracture mechanics criteria did not capture the disorder and heterogeneity as shown in the previous chapter. This warrants future study. This also paves a way to predict the failure location for real-world data where the orientation/location of the failure is not necessarily known before the actual failure. We will address such a case in the next chapter.

These statistics highlight the potentially devastating consequences of catastrophic rock avalanches and emphasize the importance of early-warning monitoring systems, such as those used at the Bingham Canyon mine.

Pankow *et al.* 2014

9. Preliminary results for field-scale predictions of a rockslide from radar data

So far, we have tested the performance of the network flow model to predict the location of the ultimate macrocrack in laboratory-scale numerical data presented in Chapter 3. Here we are seeking to answer: *can network flow method similarly predict the location of the failure zone for a real-world field scale data, from monitoring of a developing rock slide in an open pit mine? If so how far in advance?*

For the DEM data sets, the contact network as well as the bond strength needed to construct the flow network are directly available. But, for the radar data, the observation points are the cells or pixels of a regular fixed grid. Consequently, we create a flow network where the nodes are the pixels and adjacent pixels in the grid are linked. A capacity function is then formulated based on the ground motion data recorded at the corresponding pixels.

This chapter is organised as follows. In section 9.1, we present data studied. In section 9.2, we summarise our network flow method. We present results in section 9.3 before conclusion is given in section 9.4.

9.1. Data

Here we discuss the large field-scale data set from a rock wall in an open-pit mine (Figure 9.3) (Tordesillas *et al.* 2018). The mine operation, location and year of the rockslide are confidential. The rock slope expands around 200 m in length and 40 m in height. The cumulative displacement of 1803 pixel locations, which cover the rock face, was measured by using slope stability radar (SSR) technology (Dick *et al.* 2014). The movement of these locations was monitored over a period of three weeks: 10:07 May 31 to 23:55 June 21. The cumulative displacement of each monitored location was recorded at every six minutes, with high accuracy, relative to the stationary ground-based monitoring station. Therefore, we have time-series data from 1803 pixel locations at high spatial and temporal resolutions for the entire slope. A rockslide occurred on the western side of the slope on June 15, with a strike length of around 120 m. A global average peak velocity of 0.56 mm/min (33.61 mm/hr) was recorded at 13:10 June 15 which corresponds to time stage $\epsilon = 3,568$. The input data to our analysis consist of

the following system properties at each time state $\epsilon = 1, 2, \dots, m$:

- coordinates of observed locations $\ell = 1, 2, \dots, 1803$,
- displacement recorded at each location $d_\ell = d_1, d_2, \dots, d_{1803}$.

Here we analysis data until time stage $\epsilon = 3,600$.

9.1.1. Contact network

At each time stage, the cumulative displacement of 1,803 locations was measured. However, these observed points are not uniformly distributed in the physical domain (see Figure 9.1 (a)). Following Tordesillas *et al.* 2018 we discretised the physical domain into a regular grid as follows. Here we consider $5 \text{ m} \times 2 \text{ m}$ grid cells. We observed that some cells contain up to 15 pixels points and each cell contains three pixel points on average. Here we took the mean of the cumulative displacement of the pixel points in each cell and assign this value to newly created cells (coordinate at centre of the new cell). Now we have 611 points in a regular grid (see Figure 9.1 (b)). Thus, an intuitive way to create a contact network for this data is to connect the adjacent pixels which share a common boundary as shown in Figure 9.2. We create a contact network for each time stage. Note here that the contact network will be the same for each time stage. However, as we will discuss next, the contact capacity varies from time stage to stage.

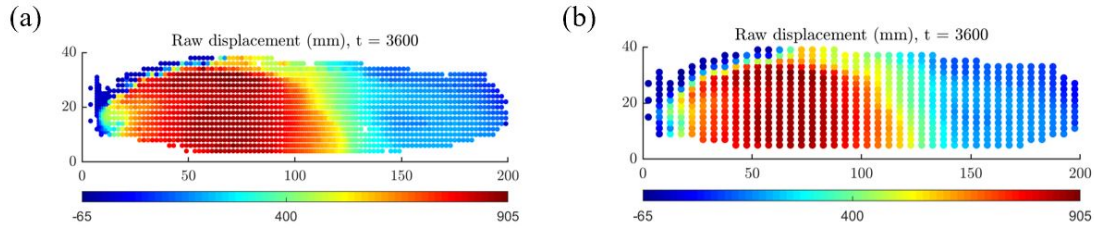


Figure 9.1.: Mine: This shows the cumulative displacement data at the final stage of loading for (a) observed 1,803 pixel points and (b) discretise domain of 611 grid points. Note that the failure boundary is the same.

9.1.2. Bond strength

For the DEM data, the information on bond strengths is available to us as part of the data. But, for this sample, as it comes from the actual measurement of displacement of the slope at various locations, we do not have the information on bond strength. That means, we have to model the contact strength. Here the idea is to use the relative displacement of two pixels in contact. If the relative displacement between two pixels in contact is greater, these two pixels either move in a different direction or move in the same direction with creating tension. This means that contact is about to break.

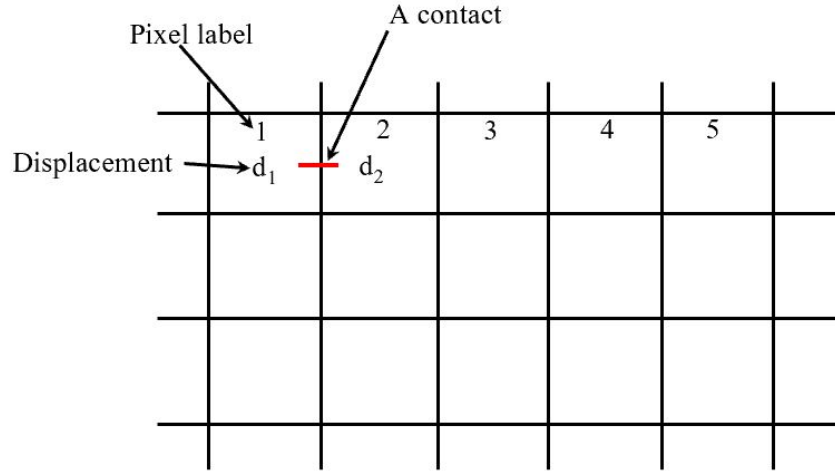


Figure 9.2.: Mine: An illustration of locations of discretised grid points and the proposed method to construct the contact network. There are 611 grid points. We connect two grid points (cells) if they share a common boundary (red link).

On the other hand, if the relative displacement is small, they are moving together and will not pull apart. Therefore, we propose a following contact capacity function which is purely based on the kinematics data and is given by:

$$q = \frac{1}{|\Delta u|^2}, \quad (9.1)$$

where $|\Delta u|$ is the magnitude of relative displacement for two pixels in contact (for example $|\Delta u| = |d_1 - d_2|$ for the contact between pixels 1 and 2 in Figure 9.2).

9.1.3. Failure zone

The final failure zone is shown in Figure 9.3 (b). Here we visualise raw displacement for an individual pixel at the final time stage. The failure zone takes a parabolic shape. Note that if we use raw displacement data, this failure pattern does not visible until the actual failure.

9.2. Method

As in the case of previous chapters, here we use a network flow analysis to predict the location of the failure. A rockslide happens due to the gravitational effect. Therefore, it is intuitive to use the top and bottom boundaries of the rock wall as the source and sink respectively in the maximum flow minimum cut analysis. But, the problem is, in reality, we do not know the exact failure pattern. Thus, we employ the Gomory-Hu trees to find the location of the source and the sink. Here the idea is similar to the previous chapter. First, we find the minimum capacity cut within the ratio of 0.3 – 1. Recall that GHT contains only $n - 1$ minimum cuts explicitly for a graph with n vertices.

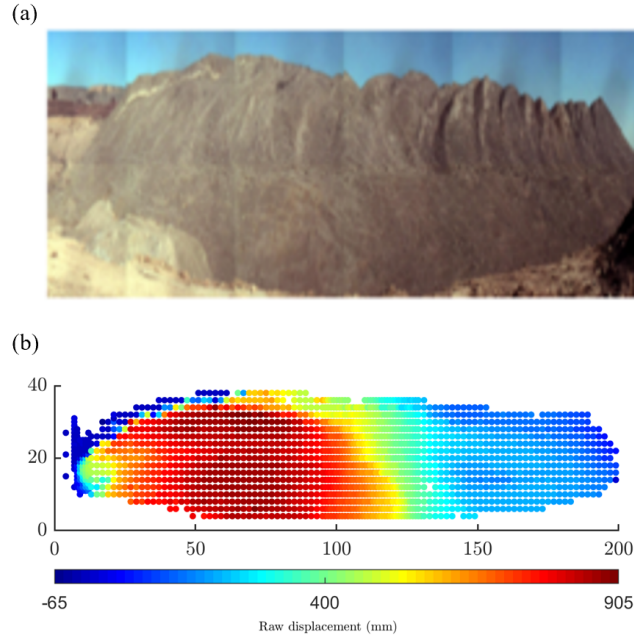


Figure 9.3.: Mine: (a) Monitored slope ([Tordesillas *et al.* 2018](#)). (b) Spatial distribution of displacement at $\epsilon = 3600$.

However, there are $n(n-1)/2$ minimum cuts in reality. The others can be inferred from the GHT. We find all possible combination of nodes which corresponds to the minimum capacity cut for each stage of loading. For each stage, we have at least one pair of nodes. All the nodes found from are then visualised. We see the clustering of nodes in the top and bottom boundaries as shown in Figure 9.4. Next, we carry out the classical maximum flow minimum cut analysis which identifies the force bottleneck and minimum cost flow problem which identifies the preferential paths for force transmission. These two methods are already discussed in Chapter 4.

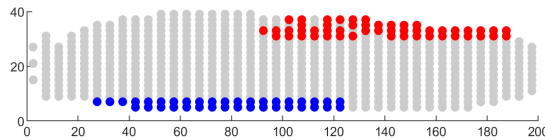


Figure 9.4.: Mine: Spatial distribution of nodes corresponds to the minimum capacity cut from GHT for all stages of loading. Note that clustering of nodes near top and bottom boundaries.

9.3. Results

Figure 9.5 shows that the minimum cut (bottleneck) derived from the kinematic data predicts the location of the failure for this field-scale data. Predicted location here is shown as the red-blue interface. This method indicates the failure location at least 13

9.4. CONCLUSION

days prior and it gives persistent prediction at least four days before the actual failure.

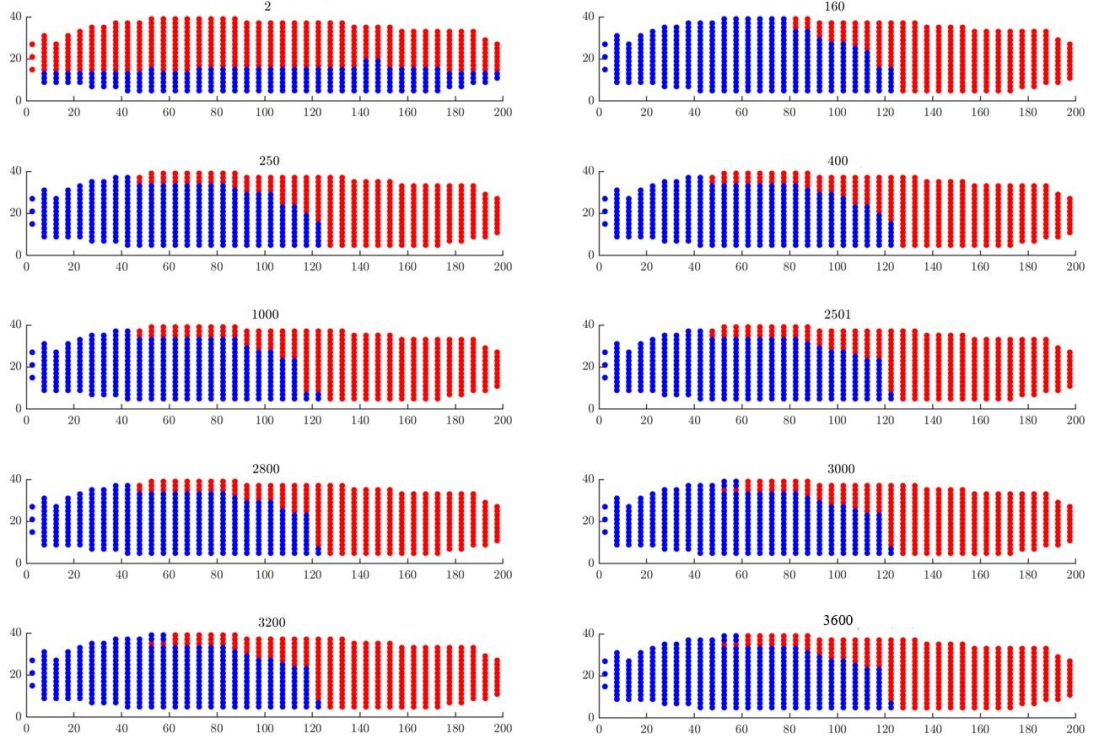


Figure 9.5.: Mine: Early prediction of the ultimate location of failure. Predicted landslide boundary is shown as red-blue interface. Note that consecutive time states are 6 minutes apart and the failure time is $\epsilon = 3568$. Note also that we have only shown the predicted location for selected time stages. There is no prediction until time stage $\epsilon = 250$. After that it indicates the general location of failure and predicted location persists after time stage $\epsilon = 2500$

Figure 9.6 shows the optimised routes for force transmission for selected time stages. These are the preferred paths for stress transfer in the system. Initially, the sites of high-stress concentration are not the region where ultimate failure will likely form as discussed in Chapter 6. Therefore, consistent with this, here we see a dense network of pathways for preferred paths initially. However, as time stages approach failure, these paths are beginning to concentrate around the failure zone, and we see a sparse network. In the failure regime, this network is even sparse and concentrated along the failure boundary, as the failure regime experience high stresses.

9.4. Conclusion

In conclusion, we have answered the question: Can the network flow method similarly predict the location of the failure zone for real-world data by using kinematics data? Results revealed that our network flow approach translates well into the field-scale, delivering an early prediction of the location of catastrophic failure well in advance of

9.4. CONCLUSION

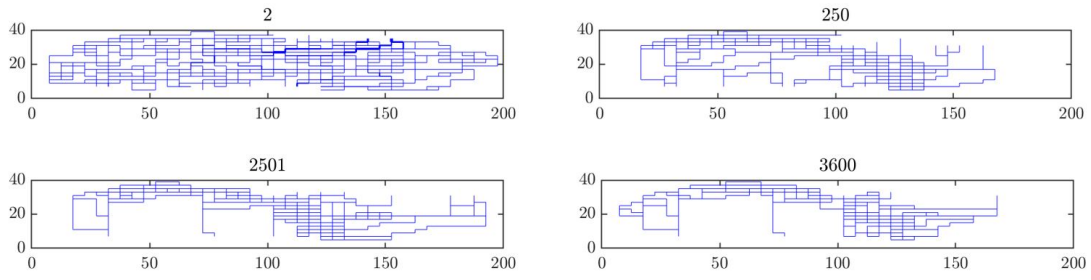


Figure 9.6.: Mine: Predicted preferential paths for force propagation (interconnected blue lines) for selected time stages. Line thickness is proportional to the magnitude of flow through that contact. Note that the failure time is $\epsilon = 3568$.

the event of two weeks prior to collapse for Mine. This warrants future study.

10. Conclusions and future research

In this thesis, we examined using Network Flow theory the transmission of force and energy and their coupled evolution with damage in disordered and heterogeneous bonded granular materials like concrete. We developed a data-driven framework for predicting the preferential paths for force and showed that force chains mostly form along these paths. We also showed that the preferred paths for damage can reliably predict the ultimate macrocrack path. The main findings of the thesis are summarised below.

1. That our models can provide a reliable prediction of force chains and crack paths suggests that force transmission processes in the class of materials studied here are optimised.
2. Persistent flow bottlenecks robustly predict the location of the ultimate macrocrack.
3. When redundant paths exist, the sites of damage and high-stress concentrations early in the prefailure regime are not reliable indicators of where the ultimate macrocrack will likely form. Forces and damage are redirected to alternative paths away from the flow bottleneck.
4. Recurring bottlenecks are precursors for cascading failure. This finding may prove beneficial in studies of other complex transmission systems, such as power grids, telecommunication and road networks.

Like with any model, there are limitations to the work presented here. In particular, a key assumption made was that no new contacts formed before the peak load. Therefore, the prefailure response to damage is mainly due to redistributions of the force in a network that is progressively losing contacts, since no new contacts can form from contact rearrangements. Thus, results reported here may not apply when grain rearrangements become important in the prefailure regime. Also we focussed only on the transmission of tensile forces. Future work aiming to model the transmission of both compressive and tensile forces would ultimately lead to a multi-commodity flow problem. This might improve the prediction for more complex tests like the 3-point and 4-point bending tests. On the other hand, there is a possibility to explore a probabilistic contact capacity function. It is also possible to use the MAXIMUM CUT PROBLEM as an alternative to the MINIMUM CUT PROBLEM provided an appropriate maximisation

problem for the fracture path can be identified. This alleviates the necessity of identifying the flow direction through the source-sink assignment and other constraints in the network flow minimum cut analysis.

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A. Classifications of nodes/links in the flow network and damaged network & its components

A.1. Classifications of nodes/links in the flow network

This contain how to classify nodes and links in the flow network $\mathcal{F} = (G, q, s, t)$. The source s and the sink t nodes are the top and bottom walls respectively. This assignment can be reversed without change to the results as flow is symmetric. Detailed description of classification of nodes/links can be found in the following sections.

A.1.1. Classifications of nodes

We classify nodes in the flow network into two groups: those belonging to tensile force chains (T) versus those that support the tensile force chains (N). Black and gray grains in Figure A.1 are T and N grains respectively and it is an example illustration.

A.1.2. Classifications of links as type TT, TN, and NN

We can also classify the contacts relative to tensile force chains, labelled as TT, TN, NN (see Figure A.1). TT contacts are those between two grains in tensile force chains; TN contacts are those between a grain in a tensile force chain and another grain that does not belong to a tensile force chain; NN contacts are those between two grains that are not in tensile force chains.

A.1.3. Classifications of links as strong versus weak

Force transmission in granular materials transmit force through a dual network of strong versus weak contacts [Radjai *et al.* \(1996\)](#). We can classify tensile contacts into strong versus weak contacts. The strong contacts comprise those transmitting at least the global average tensile force. Weak contacts transmit below the global average tensile force.

A.2. Damaged network and its components

Damaged network is a network where the links represent the broken bonds and the nodes are the damaged grains (i.e., those with at least one broken bond). This network

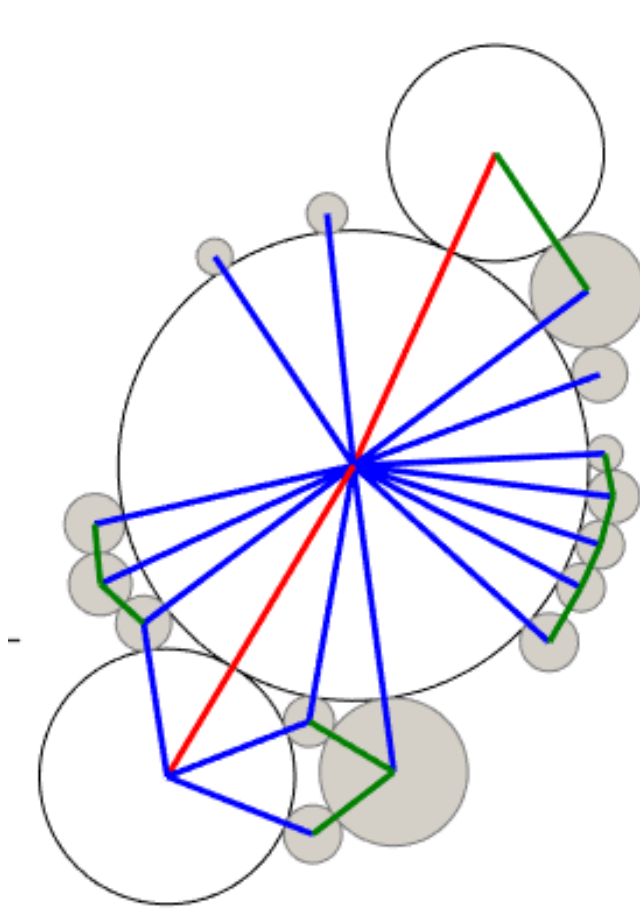


Figure A.1.: Illustration of classification of links/nodes. T grains (black outline) are the grains those belonging to tensile force chains and N grains (light gray) are the grains those do not belong to tensile force chains. TT (red links), TN (blue links), and NN (green links) are the contacts between two grains in tensile force chains (T grains), a grain in a tensile force chain (T grain) and another grain that does not belong to a tensile force chain (N grain), and two grains that are not in tensile force chains (N grains) respectively.

is not necessarily a single connected graph i.e., a graph such that nodes are connected to each other by paths. There might be multiple connected components. We refer to the largest connected component as giant component.

Blue links in Figure A.2 (a) and (b) show remaining bonded contacts for a selected region of the sample (with same grain ids) for stages 9 and 10 respectively. Red links in Figure A.2 (c) show the damaged network. Links in the damaged network are the broken bonds from stage 9 to 10. As can be seen from it, there are two connected components with the size (measured in terms of the number of links) of 20 (left) and 14 (right). Therefore giant component is the component with 20 links (left).

A.2. DAMAGED NETWORK AND ITS COMPONENTS

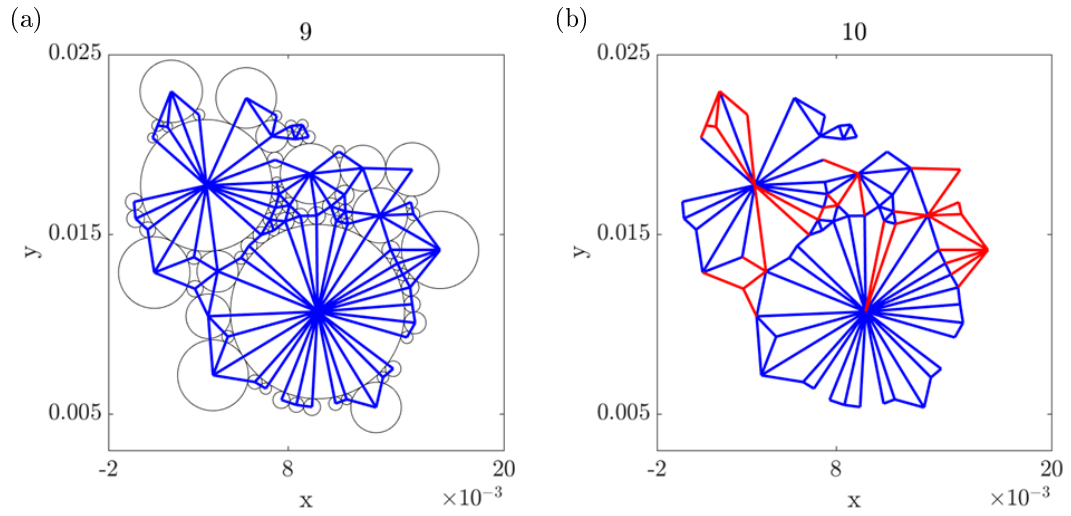


Figure A.2.: Illustration of damaged network. (a) Part of the 1-phase tension sample at stage 9 with remaining bonded contacts (blue). (b) Same part of the sample with remaining bonded contacts (blue) at stage 10 and broken bonds (red) from stage 9 to stage 10.

B. Method for detection of force chains in bonded granular media

The major difference between unbonded and bonded granular material is that bonded contact can accommodate both compressive and tensile forces whereas unbonded contact can only support compressive forces. Therefore we can expect the formation of compressive force chains (FCs) and tensile force chains (TFCs). Compressive (tensile) Force chains are quasi-linear chains of at least 3 grains, each carrying above-average compressive (tensile) particle load vector magnitude: these columnar chains are under axial compression (tension). [Muthuswamy & Tordesillas 2006](#) introduced a quantitative way to determine the FCs in unbonded granular materials. Here we extend this algorithm to find both FCs and TFCs in bonded granular materials.

Detection of force chains in bonded granular materials is two-fold. First, identify the grains experiencing tensile forces and compressive forces (Subsection [B.1](#)). Second, apply force chain detection algorithm (Subsection [B.2](#)). A detailed description of identifying grains and tensile force chain detection algorithm given below.

B.1. Classification of grains as T_e versus C_o

We classify each grain in the specimen according to its *particle load vector*, $\mathbf{P}$. This vector is derived from the local force moment tensor associated with each particle, defined as [Muthuswamy & Tordesillas 2006](#):

$$\hat{\sigma}_{ij} = \sum_{c=1}^N f_i^c r_j^c, \quad (\text{B.1})$$

where N is the number of contacting neighbours of the particle, f_i^c denotes the components of the contact force, and r_j^c denotes the components of the unit normal vector from the centre of the particle to the point of contact.

If all the contact forces acting on a particle are compressive (tensile), then all the eigenvalues of $\hat{\sigma}_{ij}$ are negative (positive). In general, there will be a mix of compressive and tensile forces acting on each grain and hence there may be a mix of positive and/or negative eigenvalues of $\hat{\sigma}_{ij}$. In this case, if compressive forces are dominant, the sign of the largest eigenvalue magnitude is negative and if the tensile forces are dominant, the sign of the largest eigenvalue magnitude is positive. Thus we use the sign of the largest

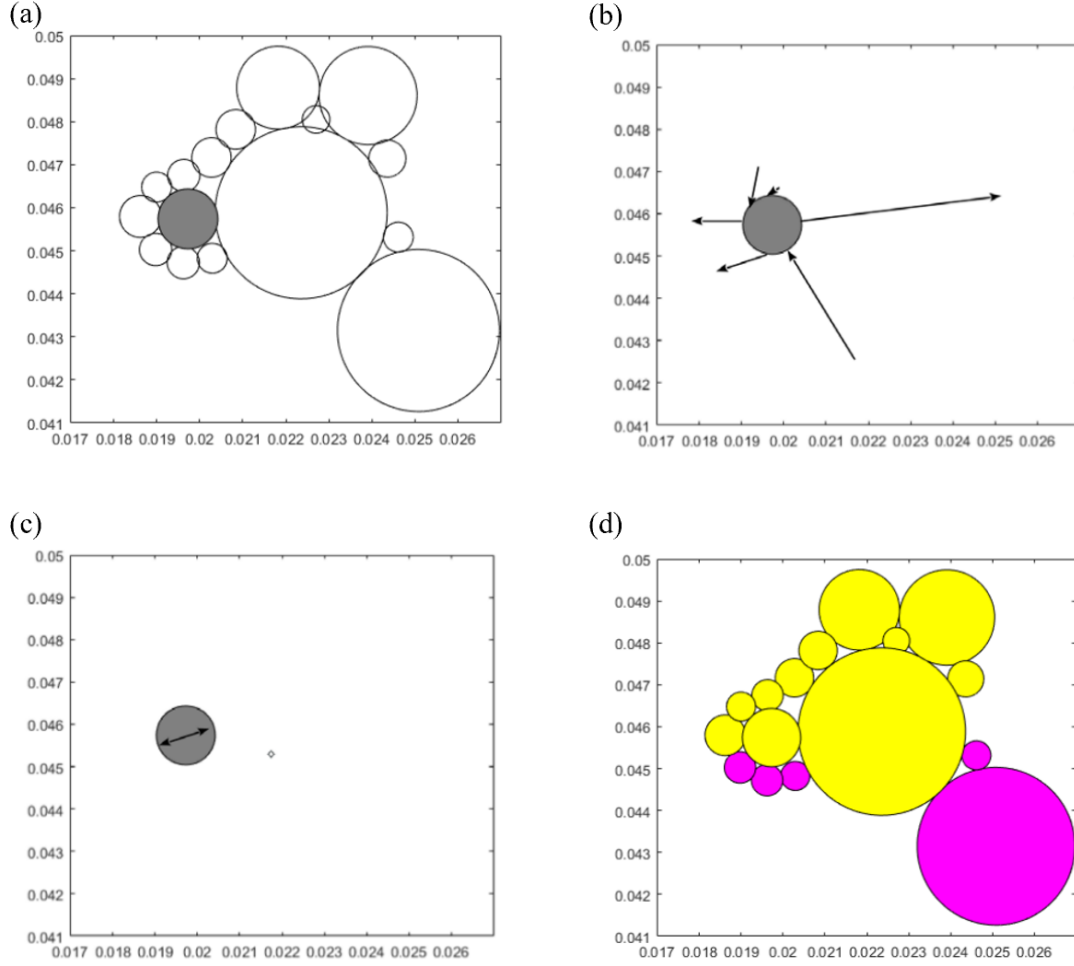


Figure B.1.: An algorithm for classifying grains as T_e versus C_o grains. (a) Selected grains at strain of 0.18% of 1-phase compression test with selected grain 808. (b) Forces acting on grain, 808. (c) Visual of particle load vector of grain, 808. (d) Classification of grains as T_e (yellow) versus C_o (magenta).

eigenvalue magnitude to classify the grains as tensile (T_e) grains versus compressive (C_o) grains. Once a grain is classified into a T_e versus a C_o grain, the magnitude and direction of the grain's *particle load vector*, $\mathbf{P}$ is defined by the largest eigenvalue magnitude of $\hat{\sigma}_{ij}$ and its corresponding eigenvector, respectively. A summary of the algorithm for classification of grains is given in Algorithm 3.

Let's calculate $\mathbf{P}$ for the grain 808 using the information in Tables B.1 and B.2 noticing that recorded forces in columns 3 – 6 in Table B.1 are acting on grains listed in column 1.

$$\hat{\sigma}_{ij} = \sum_{c=1}^6 f_i^c r_j^c$$

$$\hat{\sigma}_{ij} = \begin{bmatrix} 8.414012511516594 & 3.992532183494790 \\ 4.043466503626107 & -3.991042627856697 \end{bmatrix}$$

B.2. IDENTIFYING TENSILE FORCE CHAINS

Table B.1.: Contact data for the selected grain, 808 at strain of 0.18% of 1-phase compression test.

ID1	ID2	F_{n_x}	F_{n_y}	F_{t_x}	F_{t_y}
976	808	2.07767138	-0.10669269	-0.00630008	-0.12268414
4429	808	-0.49923467	0.50792185	0.79174205	0.77820058
808	3324	-0.10134039	-0.96052519	-1.99165690	0.21013013
808	4732	0.022774145	-0.237475589	-0.336560818	-0.032276518
808	82	7.35136023	0.40013275	-0.029160790	0.535750887
808	1645	-2.59257309	4.19252386	0.0821346241	0.0507904125

Table B.2.: Particle data for grains (ID1 and ID2) in Table B.1.

ID	X	Y	Radius
82	0.0223569452097	0.045882448582	0.00199848
808	0.0197278683225	0.045739348582	0.000695068
976	0.0186237253507	0.045796048582	0.000486
1645	0.0202928207579	0.044825748582	0.00034725
3324	0.0196206006776	0.044722648582	0.000375
4429	0.0190011142033	0.046478748582	0.00034725
4732	0.0196312108103	0.046747248582	0.000375

Eigenvalues of $\hat{\sigma}_{ij}$ are 9.601682395303929 & -5.178712511644032 and corresponding eigenvectors are $(0.958490384192462 \ 0.285124855827383)^T$ and $(-0.281820154612072 \ 0.959467248244789)^T$ respectively. Since sign of the largest eigenvalue magnitude is positive, grain 808 is a T_e grain (see Figure B.1).

B.2. Identifying tensile force chains

Note that the distribution of radii of the grains studied here is relatively wide. For the 1-phase tension sample, minimum radius of the grain is 2.7895×10^{-4} while the maximum radius of the grain is 5.3064×10^{-3} m. The definition of tensile force chains, ‘quasilinear particle assemblies carrying the majority of the tensile load’, is used to quantitatively identify force chains in accordance with the method proposed in [Muthuswamy & Tordesillas 2006](#). In the method proposed in [Peters *et al.* 2005](#), the particle stress tensor was used to calculate an estimate of the load carried by a particle. However, since the particle stress tensor is normalized by particle volume, this produced biased statistics (small particles were preferred). A summary of the algorithm for identifying tensile force chains is given in Algorithm 4. This algorithm, detailed below, is applied

Algorithm 3 Classification of grains as T_e versus C_o

- 1: Take all grains in the system.
 - 2: Calculate local force moment tensor associated with each grain, $\hat{\sigma}_{ij}$.
 - 3: Calculate eigenvalues of $\hat{\sigma}_{ij}$.
 - 4: Find sign of the largest eigenvalue magnitude.
 - 5: If sign is positive classify grain as T_e .
 - 6: If sign is negative classify grain as C_o .
 - 7: **return** Collection of T_e grains (T_e -class) and C_o grains (C_o -class) for the system at some state.
-

to the set of all T_e grains in the specimen (i.e., the T_e -class). In a nutshell, each grain must pass two consecutive criteria to be part of a tensile force chain.

Criteria 1: The mean $|\mathbf{P}|$ is calculated for T_e -class. T_e -grains whose particle load vector magnitude is less than or equal to this mean value are removed, Figure B.2 (b).

Criteria 2: The particle with the largest particle load vector magnitude is selected from the grains those pass the Criteria 1 as the start of a tensile force chain, Figure B.2 (c). Neighbouring candidate particles are considered in the direction of $\mathbf{P}$ within a prescribed tolerance angle, θ , Figure B.2 (d) (we selected θ to be 45°). The imposed *quasi-linearity* condition is:

$$\cos \theta < \frac{\mathbf{P} \cdot \mathbf{l}_c}{|\mathbf{P}| |\mathbf{l}_c|} \leq 1, \quad (\text{B.2})$$

where, $\mathbf{l}_c$ is the branch vector from the center of the particle to the neighbouring candidate. Any neighbouring candidate particle must lie within a θ° sector centered at the particle center (Figure B.2 (d)). A situation may occur where, although a candidate particle lies within the allowed region, the reverse may not be true. To avoid this, a *back check* is performed (Figure B.2 (e)). Once a match is selected, it is added to the tensile force chain and the process is repeated until the chain cannot grow further (Figure B.2 (f)). The algorithm then returns to the initial tensile force chain grain, and searches *backwards* in a similar fashion (Figure B.2 (g) & (h)). Grains found from the above iterations are removed from future tensile force chain candidacy. If three or more grains including the initial particle were found, the collection of grains is called a *tensile force chain* (Figure B.2 (i)). The algorithm repeats until no more candidate particles exist. Similarly by applying Algorithm 4 to C_o -class gives force chains.

B.3. Discussion

Force transmission in bonded granular media is governed by force chains (Potyondy & Cundall 2004; Qin & Zhang 2011). Here we presented a method to detect both compressive and tensile force chains in bonded granular materials. This is a prerequisite knowledge for delivering a reliable network flow model for force transmission. This will

Algorithm 4 Tensile Force chain detection algorithm

- 1: Set $\mathcal{T} :=$ to all T_e grains (i.e. the T_e -class) within the system at some strain state.
 - 2: Remove all T_e grains from $\mathcal{P}$ whose $|\mathbf{P}|$ is less than or equal to the mean $|\mathbf{P}|$ of T_e -class.
 - 3: Let all remaining particles in $\mathcal{P}$ be candidate particles $\mathcal{C}$.
 - 4: **while** $\mathcal{C}$ is not empty **do**
 - 5: Set $P :=$ particle with largest $|\mathbf{P}|$ in $\mathcal{C}$.
 - 6: Start a new tensile force chain with this particle $\mathcal{TFC} = P$.
 - 7: **repeat**
 - 8: Let $\mathcal{NE} :=$ neighbours of P which are quasi-linear.
 - 9: Remove from $\mathcal{NE}$ particles which fail back check to P .
 - 10: Select next particle P' from $\mathcal{NE}$.
 - 11: Add this particle to the tensile force chain $\mathcal{TFC} := \mathcal{TFC} + P'$
 - 12: Remove particle P from $\mathcal{C}$.
 - 13: Set $P := P'$.
 - 14: **until** $\mathcal{NE}$ is empty (no neighbour choices exist)
 - 15: Do the above loop again, growing the chain backwards from initial particle.
 - 16: Particles in $\mathcal{TFC}$ form tensile force chain, added to collection.
 - 17: **end while**
 - 18: **return** Collection of all tensile force chains for the system at some state.
-

help: (1) relate force chains to preferential force transmission paths in the system as uncovered from the maximum flow-minimum cost flow problem (we expect these two patterns to be spatially correlated), (2) explore coupled evolution of force transmission & crack propagation and (3) improve our understanding of why force chains form where they form.

B.3. DISCUSSION

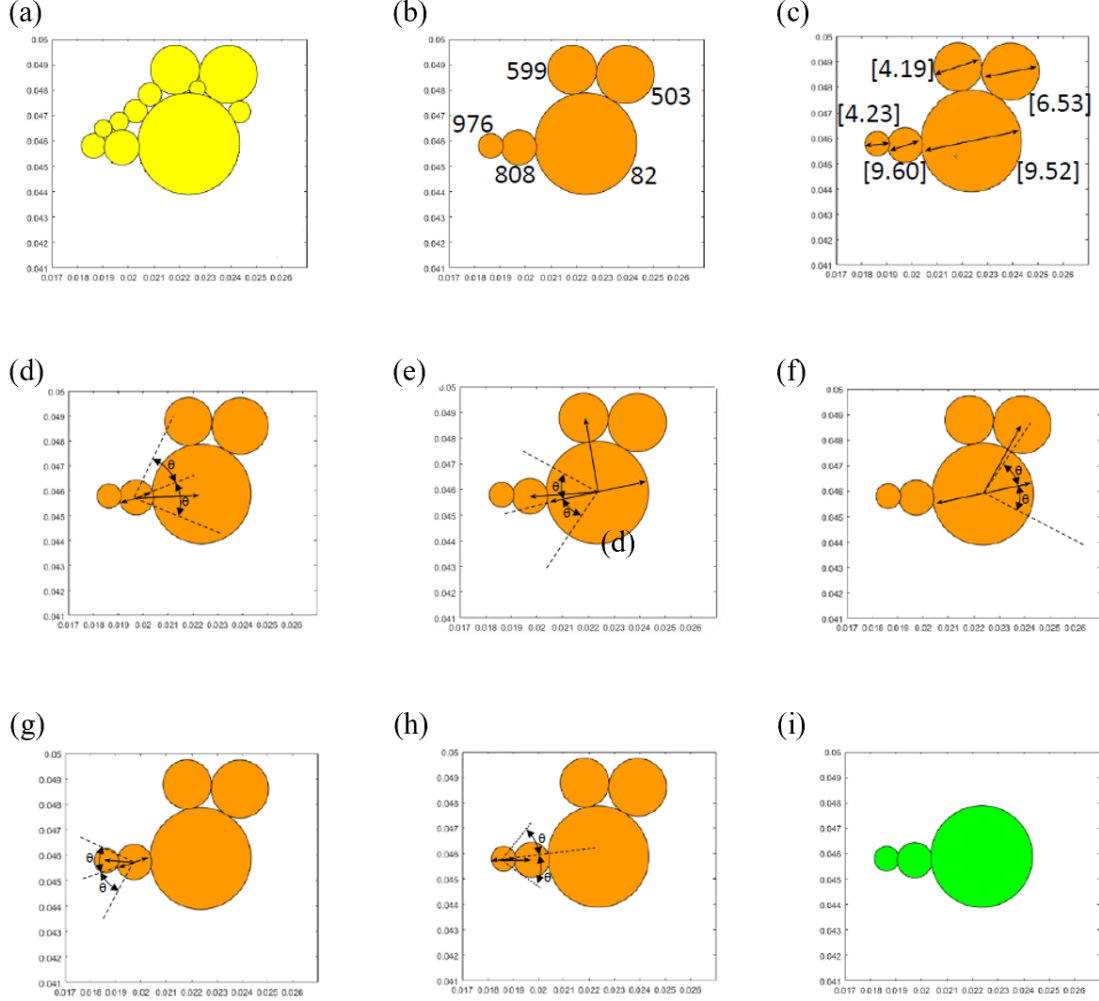


Figure B.2.: An algorithm for identifying tensile force chains. Double sided arrows through grains centers indicate the particle load vector, $\mathbf{P}$. Single-sided arrows joining grain enters denote branch vectors. (a) T_e -class is selected (selected grains are from T_e -class shown here). (b) Remove all T_e grains whose $|\mathbf{P}|$ fall below the mean $|\mathbf{P}|$ of T_e -class. (c) Grain with highest $|\mathbf{P}|$ is selected, 808. $|\mathbf{P}|$ is given inside the square bracket for each grain. (d) Look forward in the direction of $\mathbf{P}$ for contacting grains with a prescribed tolerance angle, 82. (e) Select 82. Back check pass as 808 lies within the tolerance angle, 82 forms the next particle in tensile force chain. (f) Look forward in the direction of $\mathbf{P}$ for contacting grains with a prescribed tolerance angle. None of contacting grains are not within the tolerance angle. (g) Initial grain, 808 is selected to grow tensile force chain backwards. Look backward in the direction of $\mathbf{P}$ for contacting grains with a prescribed tolerance angle, 976. (h) Select 976. Back check pass as 808 lies within the tolerance angle. (i) 976 – 808 – 82 forms a tensile force chain.

C. Results: Characterisation of force chains

Here we present results from force chain analysis for DEM data discussed in Chapter 3 in more detail. The attention is paid to 1-phase tension (1T) and 1-phase compression (1C). To detect force chains, we used the method discussed in Appendix B.

C.1. Force chains

By using newly developed force chain detection algorithm discussed in Appendix B, we identify the tensile force chains (TFCs) and compressive force chains (CFCs) for the bonded samples presented in Chapter 3. In these samples, as can be seen from Figures C.1 – C.8, we observed that the co-existence of CFCs and TFCs as reported in the literature (Buttlar & You 2001; Diederichs 2003; Potyondy & Cundall 2004; Khanal *et al.* 2005; Liu *et al.* 2017; Sinaie *et al.* 2018). TFCs are dominant in the samples subject to uniaxial tension (Figures C.1 and C.3). Moreover, TFCs are aligned with the direction of the applied load. CFCs mainly form in the failure regime and are normal to the applied load. On the other hand, CFCs are dominant in the samples subject to uniaxial compression and are aligned with the direction of the applied load (Figures C.5 and C.7). TFCs mainly form towards the failure and normal to the applied load. CFCs in compressive samples exhibit a similar trend those observed for the unbonded granular materials.

In the prefailure regime, distribution of force chains (TFCs in tension samples and CFCs in compressive samples) are uniform as observed in the literature (Su *et al.* 2017). This is mainly due to a built-in redundancy in the contact network representing the data. Despite the continuous damage to the bonds in the prefailure regime, forces are being rerouted to the other available pathways to protect the force chains. But, there is a threshold for this. When damage progresses towards failure, redundancy of the contact network get depleted and no longer possible to reroute the forces. Hence force chains break and degrade towards the failure. This is consistent with the visual of force chains. This explains why force chains degrade toward failure.

Now we analyse force chains in more detail attention paid to 1T and 1C. Note that 3T and 3C exhibit similar trends.

In 1-phase tension (1T): relative to the global sample, TFCs are in the minority and

C.1. FORCE CHAINS

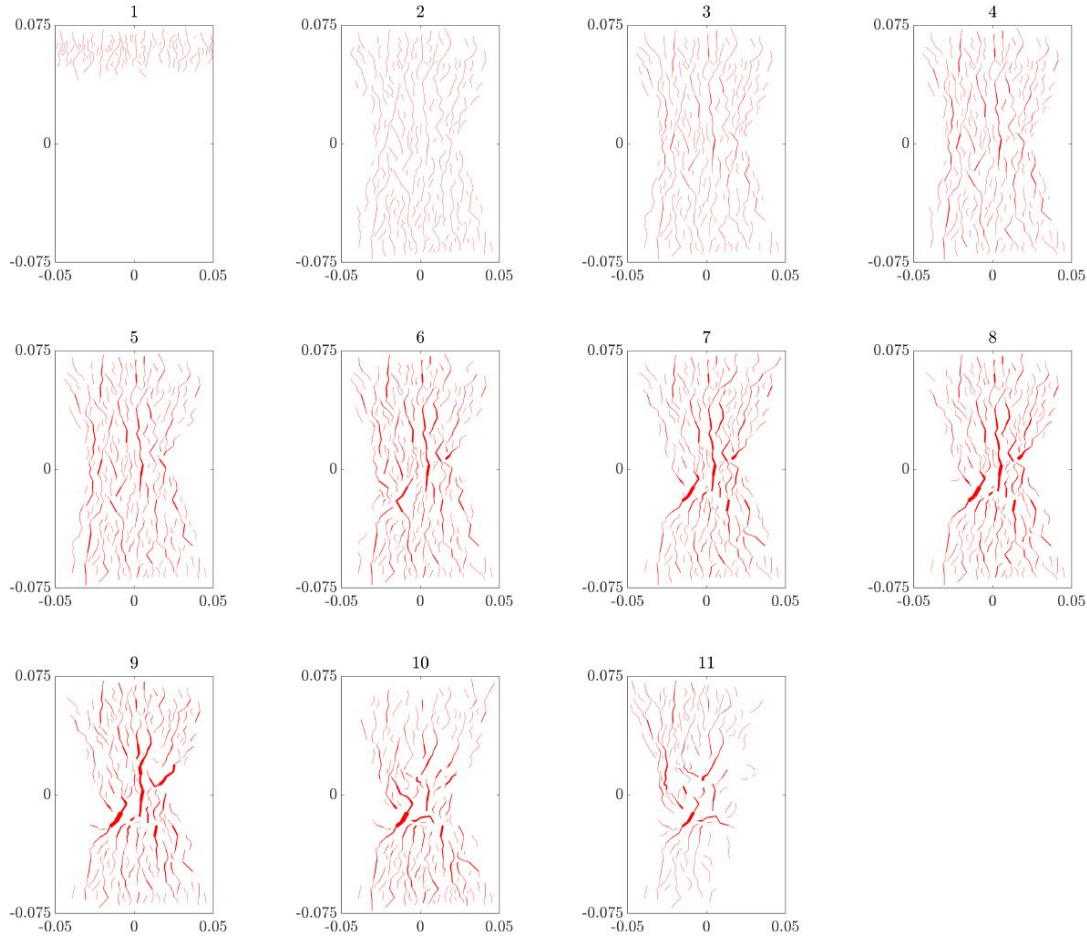


Figure C.1.: *1T*: Force transmission is governed by tensile force chains. The spatial distribution of tensile force chains at key stages is visualised here by the contact links (lines connecting the centroids of grains in the chain): link thickness is proportional to the magnitude of the tensile force transmitted at the contact. A percolating tensile force chain network is first established at stage 2.

CFCs are even less (Figure C.9 (a)). There is a small percentage of CFCs (maximum of 5%) that emerge after peak-force. The percentage of TFCs decreases with loading (peak value of 14% and the minimum value of 7%). While tensile force chains support the majority of the applied tension pre-peak, both tensile force chains and compressive force chains share comparable loads (albeit force chains carry slightly fewer loads) in the failure regime (Figure C.9 (b)). Moreover, despite the disproportionately low numbers of TFCs, they support the majority of the applied tensile load throughout loading history. This is evident in the average particle load vector (PLV) magnitude of TFCs which captures all the key features of the force-strain response (compare Figure C.9 (b) with Figure 3.4).

Next, we answer to a question *why compressive force chains form in tension tests?* Here we observed at least two mechanisms that will explain the emergence of CFCs in

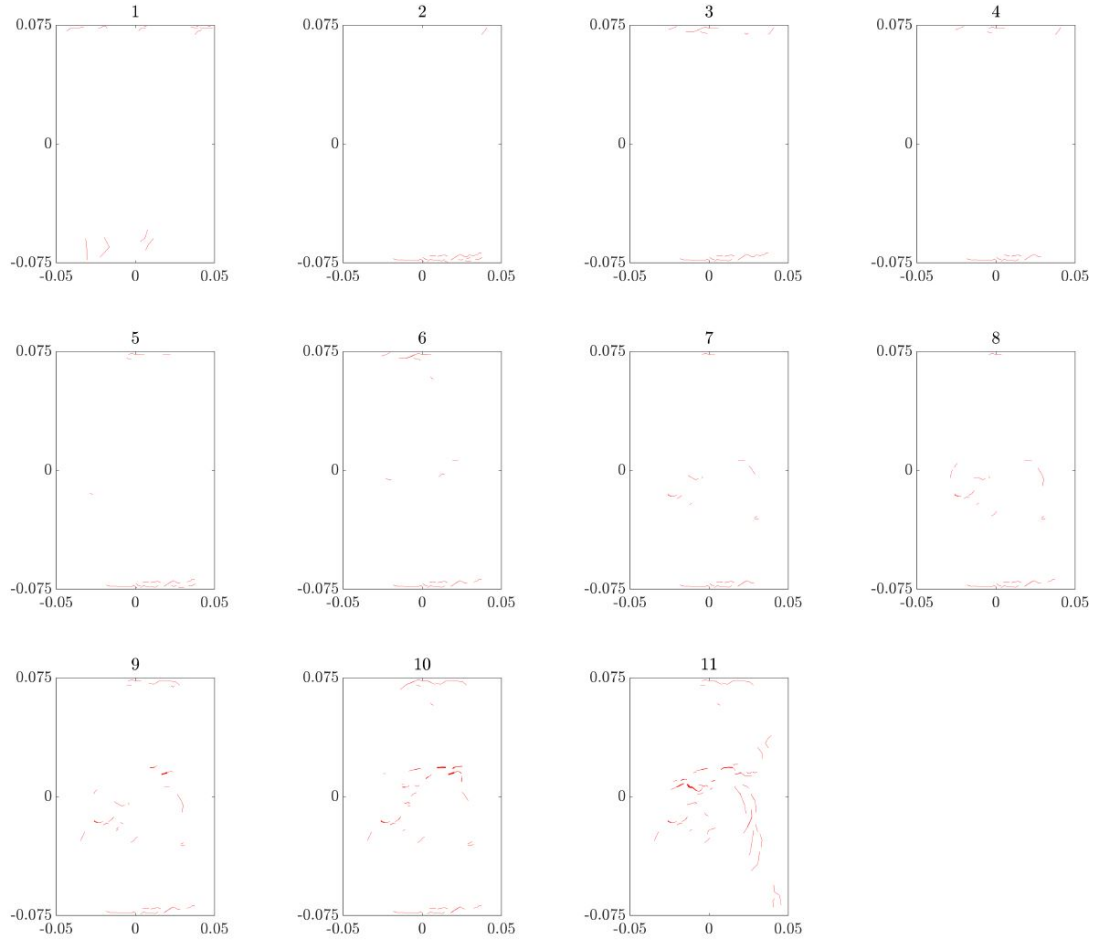


Figure C.2.: *1T*: A negligible number of compressive force chains form in the prefailure regime. The spatial distribution of compressive force chains at key stages is visualised here by the contact links (lines connecting the centroids of grains in the chain): link thickness is proportional to the magnitude of the compressive force transmitted at the contact using the same scale as that used to visualise the tensile force chains in Figure C.1 to allow direct comparison.

a tension test.

1. One mechanism is tied to *load eccentricity*. Appreciable load eccentricity develops due to the evolution of fracture in the stages leading up to peak-force: the upper region of the sample is pulled up and to the right, while the lower region is pulled to the left, causing the middle portion of gauge section of the dog-bone specimen to rotate in the clockwise direction. Consequently, there is a build-up of compressive stresses next to the lower right boundary, leading to the formation of force chains in this region (Figure C.10).
2. A second mechanism arises from *the applied load*. In the direction of applied load (vertical), chains of grains are axially stretched while in the perpendicular direc-

C.1. FORCE CHAINS

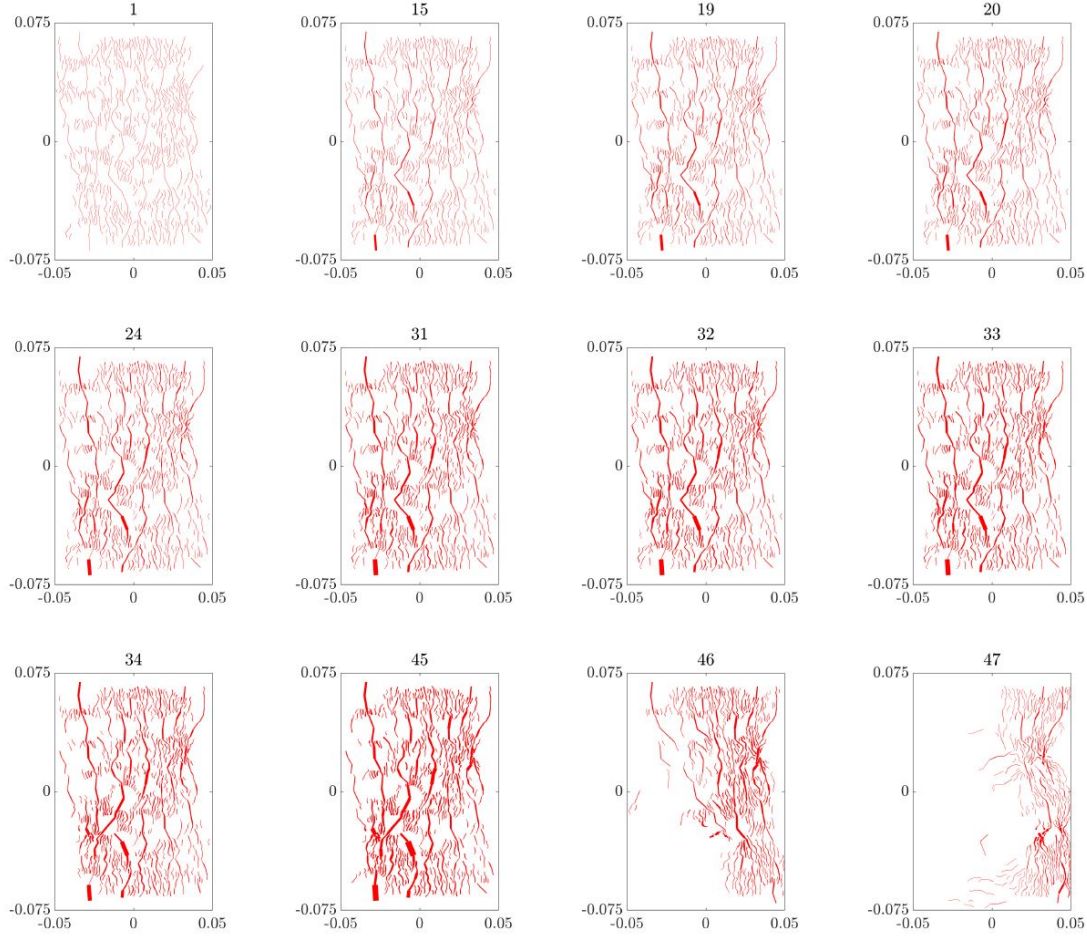


Figure C.3.: *3T*: Force transmission is governed by tensile force chains. The spatial distribution of tensile force chains at key stages is visualised here by the contact links (lines connecting the centroids of grains in the chain): link thickness is proportional to the magnitude of the tensile force transmitted at the contact. A percolating tensile force chain network is first established at stage 1.

tion, chains of grains are pushed toward and are thus subject to axial compression whereby forming CFCs.

In 1-phase compression (1C): Figure C.11 (a) shows that CFCs and TFCs comprise a small fraction of grains (less than 20%) at all stages. The percentage of CFCs rises from 12% to a peak value of 16%, then rapidly drops to around 6% during failure. TFCs emerge essentially only after peak-force and never exceeds 4%. Despite the disproportionately low numbers of CFCs, it is clear they support the majority of the applied compressive load throughout loading history. This is evident in the average particle load vector (PLV) magnitude of CFCs which captures all the key features of the force-strain response (compare Figure C.11 (b) with Figure 3.9). *This result together with those observed for 1T show that force chains are the most important pathways for*

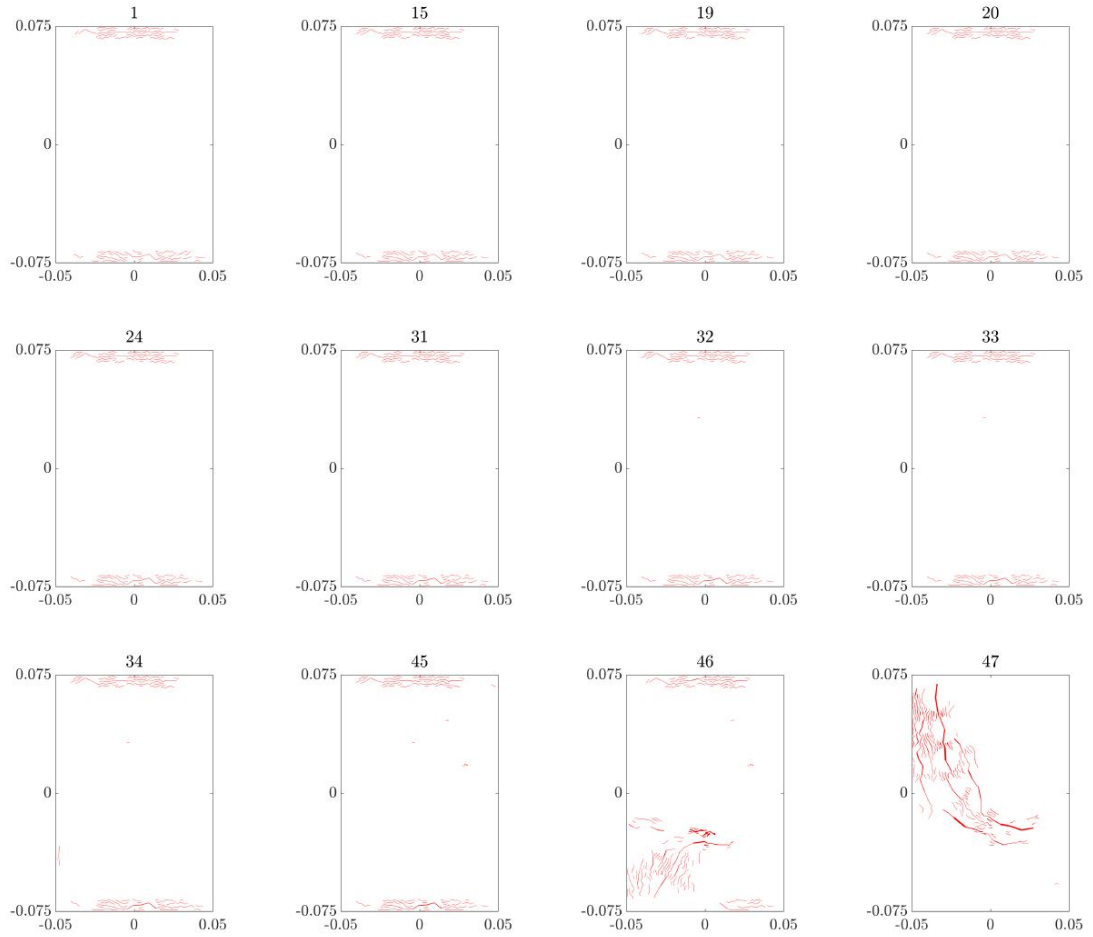


Figure C.4.: $3T$: A negligible number of compressive force chains form in the prefailure regime. The spatial distribution of compressive force chains at key stages is visualised here by the contact links (lines connecting the centroids of grains in the chain): link thickness is proportional to the magnitude of the compressive force transmitted at the contact using the same scale as that used to visualise the tensile force chains in Figure C.3 to allow direct comparison.

force transmission in bonded granular materials.

Now we turn into investigate *why tensile force chains form in compression tests?* Here we observed at least two mechanisms that will explain the emergence of TFCs in a compression test.

1. One mechanism is tied to the boundary conditions that develop around fragments, which maintain some bonded and frictional connections with other fragments: recall Figure C.12. These remaining connections mean that *significant interactions (i.e., stress transfer) occur between fragments. This results in them being subject to flexural and axial loads that are a combination of tensile, compression and shear loads.* Consequently, tensile as well as compressive force chains form inside

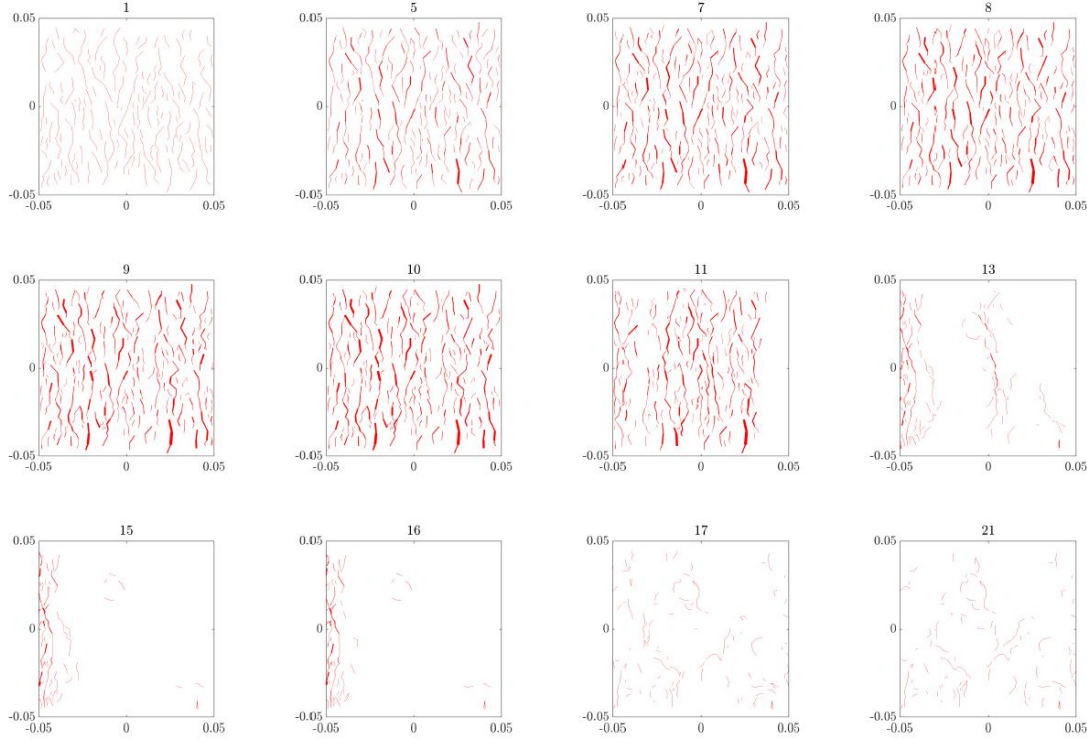


Figure C.5.: *1C: Force transmission is governed by compressive force chains.* The spatial distribution of compressive force chains at key stages is visualised here by the contact links (lines connecting the centroids of grains in the chain): link thickness is proportional to the magnitude of the compressive force transmitted at the contact. A percolating compressive force chain network is first established at stage 1.

these fragments. This explains why TFCs developed inside the fragments, and fragments experience a combination of compressive, tension and shear load as observed by [Potyondy & Cundall 2004](#); [Khanal *et al.* 2005](#).

2. A second mechanism arises along *shear crack zones*: *in one direction, chains of grains are axially compressed; in the perpendicular direction, chains of grains are pulled apart and are thus subject to axial tension.* We observed an evolution in which a chain of grains, under axial compression, initially forms a force chain in the direction of compression along a crack; this force chain then buckles as shear progresses, and then later member grains become subject to axial tension and form part of a tensile force chain (Figure [C.13](#)).

C.2. Buckling force chains and vortices

Force chain buckling is an event that relevant to a time interval. We say that a force chains at time stage $t - 1$ is buckled at time stage t if one or more contact in force chains

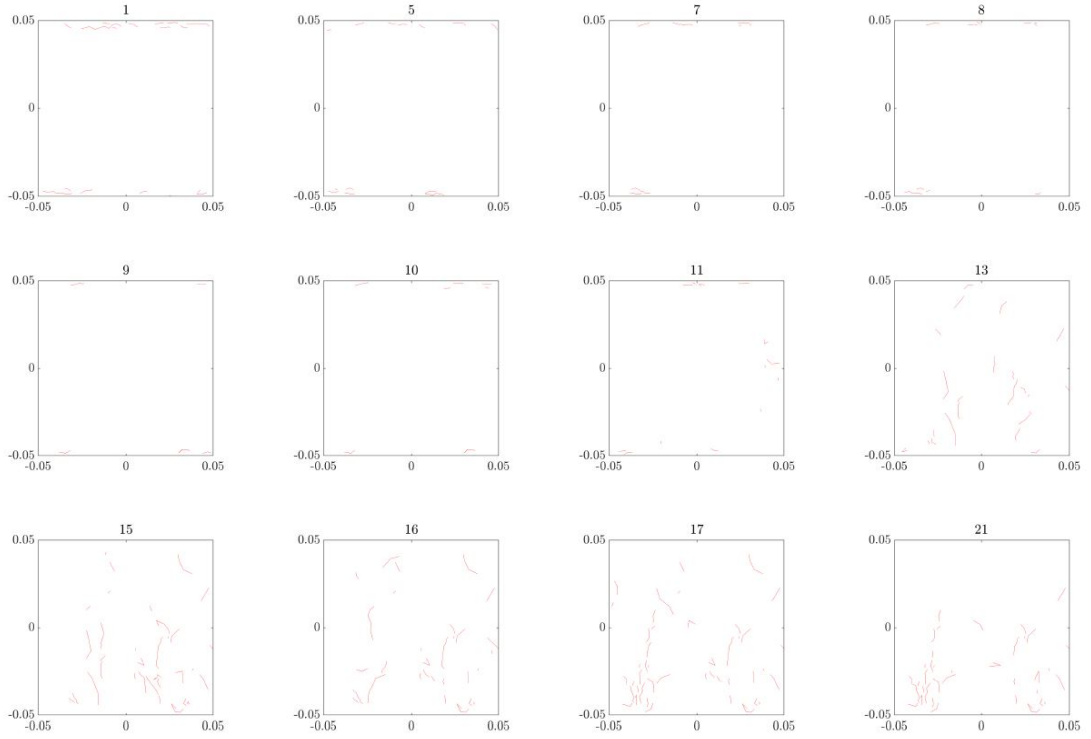


Figure C.6.: *1C*: A negligible number of tensile force chains form in the prefailure regime. The spatial distribution of tensile force chains at key stages is visualised here by the contact links (lines connecting the centroids of grains in the chain): link thickness is proportional to the magnitude of the tensile force transmitted at the contact using the same scale as that used to visualise the tensile force chains in Figure C.5 to allow direct comparison.

exceed the prescribed threshold value for buckling and experience reduction of contact forces (Tordesillas & Muthuswamy 2009). This threshold quantifies how straight force chain should be to avoid force chain buckling. In our buckling force chains analysis, the set threshold is 1° .

We also track buckling of compressive force chains (CFCs), Buckling is *not* relevant to TFCs. In general, we expect CFCs to fail by buckling and bond breakage, while TFCs fail by bond breakage only. Therefore buckling force chains analysis only applicable for compression samples. Failure analysis of CFCs in unbonded granular materials show that buckling is associated with vortical motion (Tordesillas *et al.* 2014, 2008; Tordesillas 2007). We explore this observation hold for the bonded granular materials.

First, to get an insight into the failure of TFCs, we investigate the connection between vortices and TFCs in compression samples. Vortices are identified by using the method developed by Tordesillas *et al.* 2016. This method identifies the centre (vortex core), radii and particles (grains) inside the vortex. An example of vortices is given in Figure C.14 for 1C at stage 9. Visual in Figure C.15 shows that TFCs are mainly

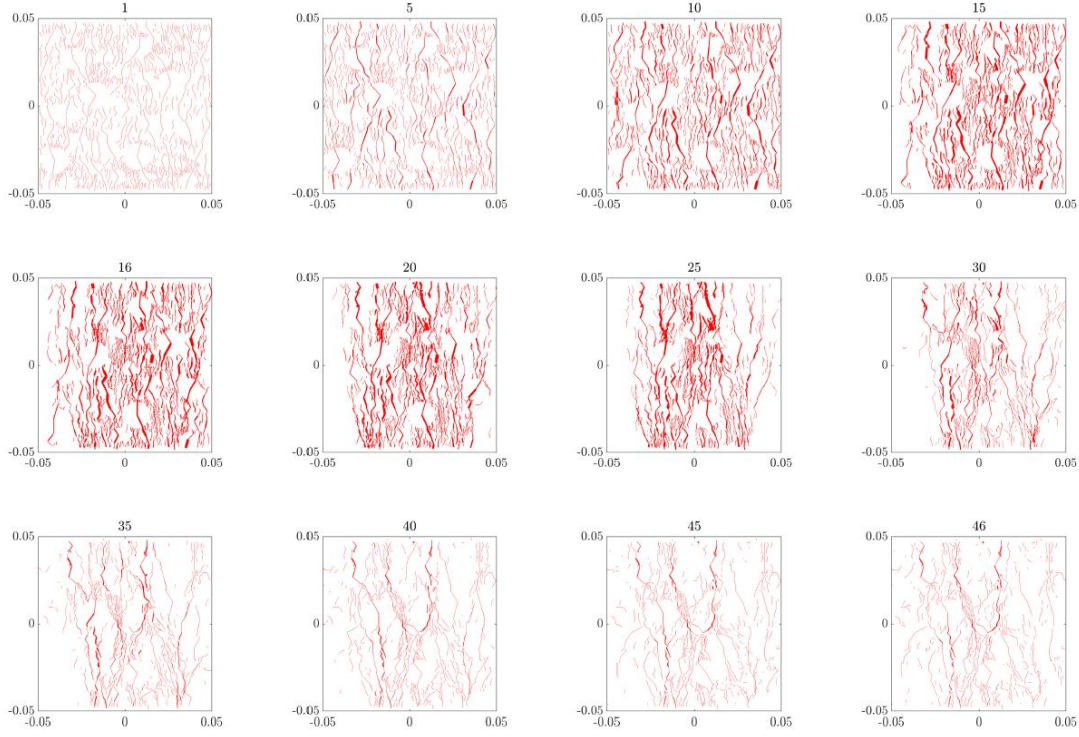


Figure C.7.: *3C: Force transmission is governed by compressive force chains.* The spatial distribution of compressive force chains at key stages is visualised here by the contact links (lines connecting the centroids of grains in the chain): link thickness is proportional to the magnitude of the compressive force transmitted at the contact. A percolating compressive force chain network is first established at stage 1.

outside vortices. We say that a TFC is in vortices if at least one of the grains in TFC is inside vortices. We observed that around 87% of TFCs are outside vortices for both 1C and 3C. Therefore we can conclude that TFCs do not fail by buckling. Furthermore, we did not observe any buckling force chains in tension samples. This further clarifies our claim that TFCs fail by bond breakage only. Moreover, TFCs form inside the fragments (Figure C.17 (b)).

Second, we investigate the relationship between BFCs and vortices. As mentioned earlier, vortical movements are responsible for CFCs fail by buckling. If this is true, then the majority of BFCs should be inside vortices. Accumulated BFC-segments together with accumulated vortices are shown in Figure C.16 for 1C and 3C. As can be seen from it, BFCs are mainly inside the vortices. To get a quantitative measure, we compute the percentage of accumulated BFCs that are in accumulated vortices at the final stage of loading. We say that a BFC is in a vortex if at least one grain of BFC is inside vortex. We found out that more than 65% of BFCs are in vortices for both 1C and 3C. Moreover, BFC-segments form next to fragment boundaries or along the fracture zones between fragments (Figure C.17 (a)). *Hence, BFCs delineate somewhat the macrocrack.*

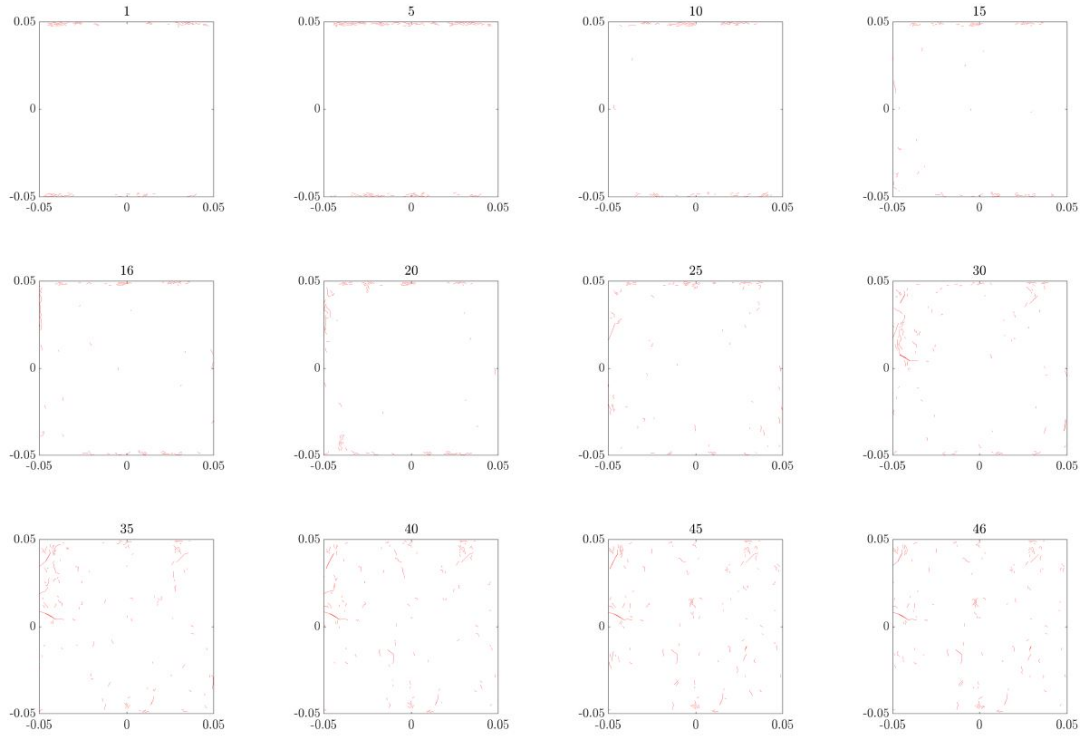


Figure C.8.: *3C*: A negligible number of tensile force chains form in the prefailure regime. The spatial distribution of tensile force chains at key stages is visualised here by the contact links (lines connecting the centroids of grains in the chain): link thickness is proportional to the magnitude of the tensile force transmitted at the contact using the same scale as that used to visualise the tensile force chains in Figure C.7 to allow direct comparison.

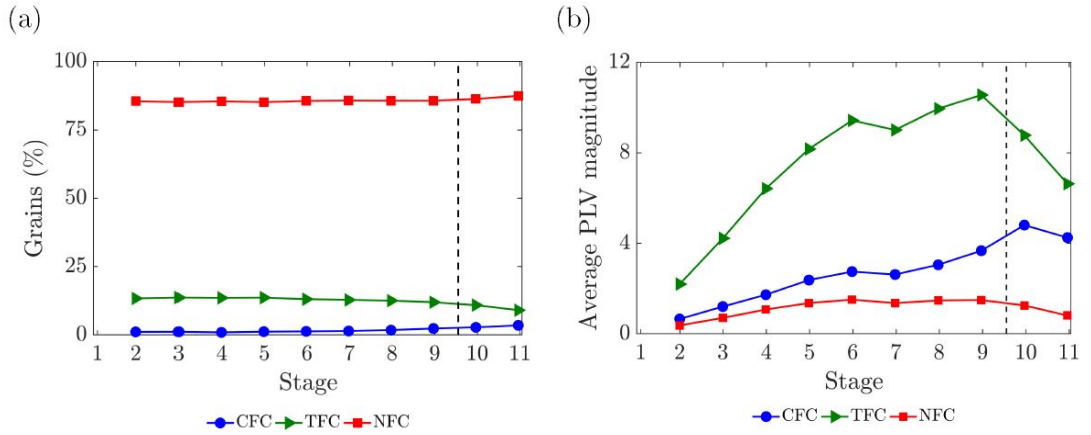


Figure C.9.: *1T*: (a) Evolution of percentage of CFC, TFC, and NFC grains (grains are not part of either compressive or tensile force chains. See Appendix A for more details about classification of nodes). (b) Evolution of average PLV magnitude of CFC, TFC, and NFC grains. Vertical dashed line indicates the strain state of the peak vertical force.

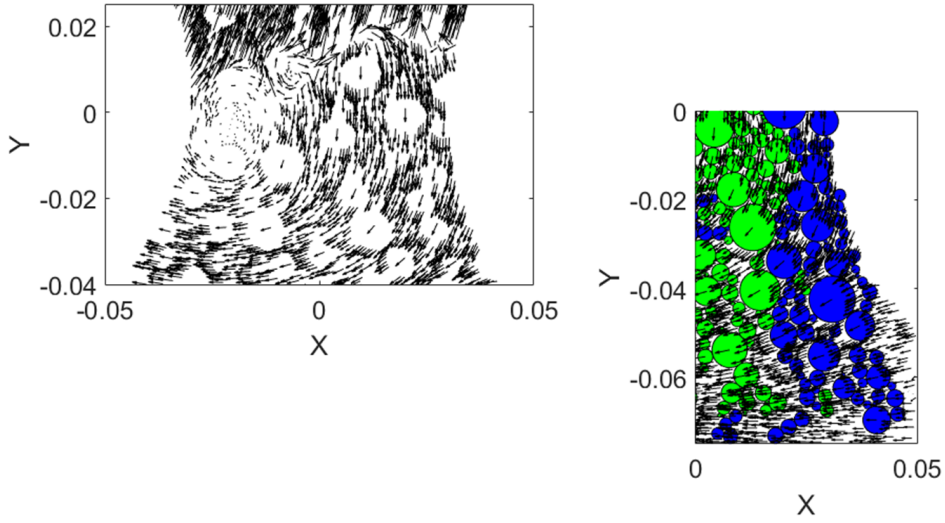


Figure C.10.: *1T*: Grain displacements in the fracture region in the gauge section just after the drop in peak force (left); a concentration of compressive force chains next to the right boundary of the specimen (blue grains) with tensile force chains (green grains) behind (or to the left of) the force chains.

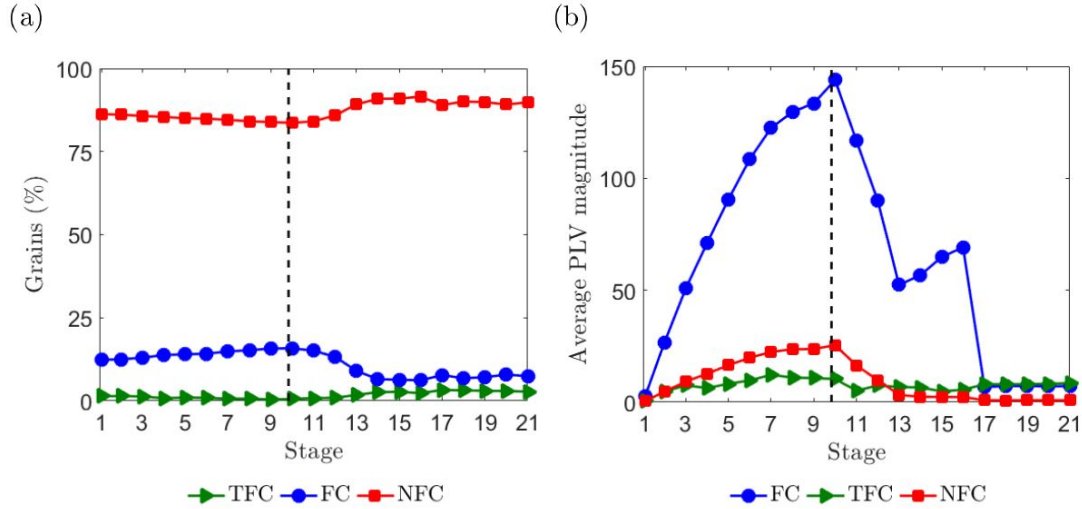


Figure C.11.: *1C*: Compressive force chains capture all the key features of the force-strain response. (a) Evolution of percentage of CFCs (grains in compressive force chains), TFCs (grains in tensile force chains), and NFCs grains. (b) Evolution of average PLV magnitude of FCs, TFCs, and NFCs grains (relative to their respective population). Vertical dashed line indicates the strain state of the peak vertical force.

Thus, compressive force chains disappear in the crack locations. This explains why force chains disappeared in the crack location as observed by [Su et al. 2017](#).

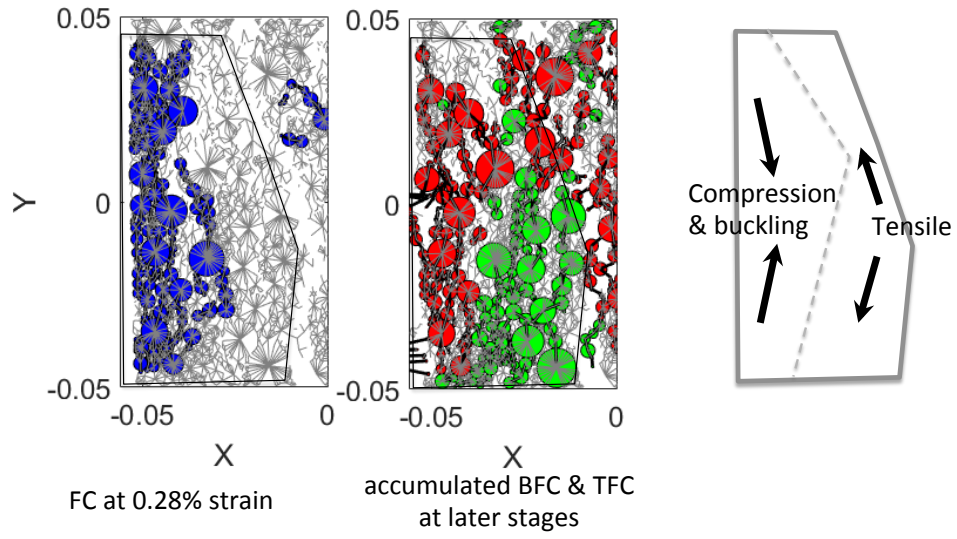


Figure C.12.: 1C: Flexural loads develop on lower left fragment in the post-peak force regime resulting in the formation of CFCs concentrating next to the left boundary of the sample (blue grains in left). Under the applied axial compression, these force chains subsequently buckle (red grains in middle), in turn, leading to the formation of TFCs behind (or to the right of) the BFCs (green grains in middle). Illustration of stress distribution on lower left fragment (right).

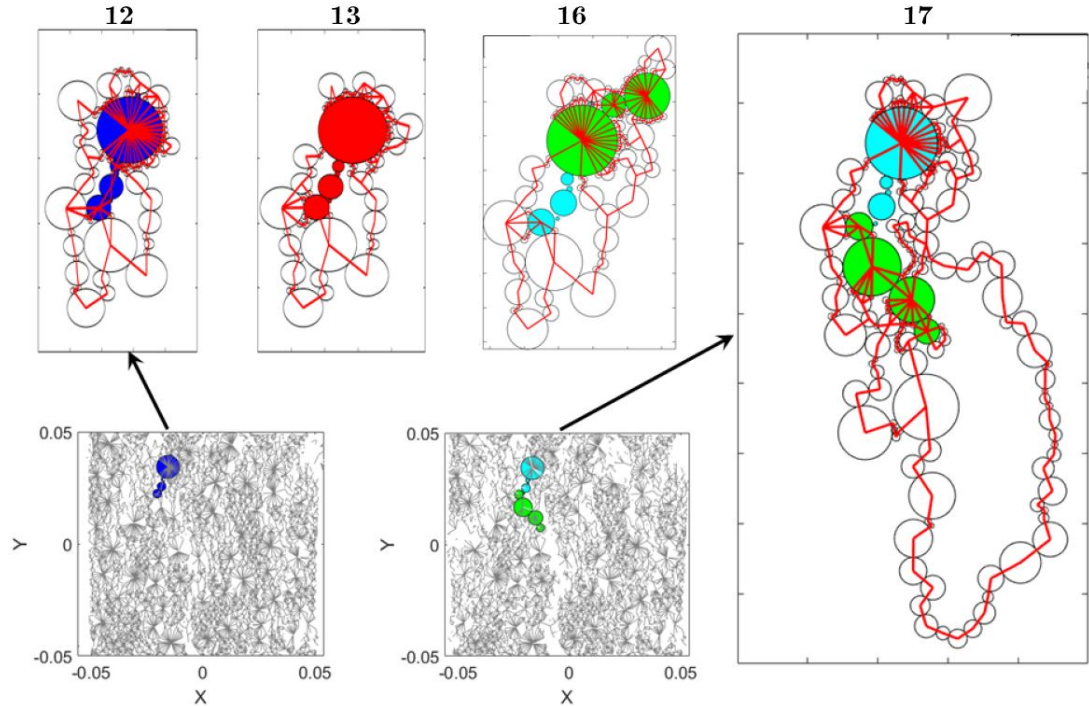


Figure C.13.: 1C: Evolution of a CFC (blue grains) to a BFC (red grains) to a TFC (green grains) with increasing strain along a shear crack in the top left corner of the sample, in between the lower left fragment and the middle top fragment in Figure 3.12. Cyan grains are the grains that are not part of force chains.

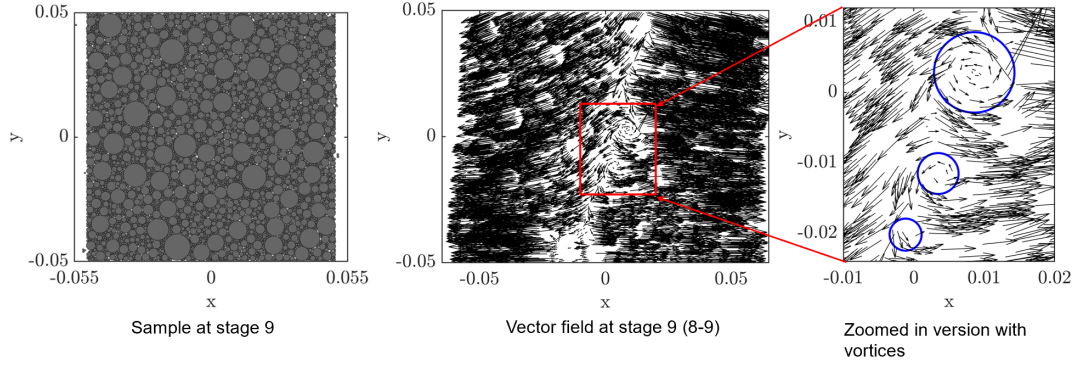


Figure C.14.: 1C: Visual of grains at stage 9 plotted according to grain size and grain position (left). Corresponding displacement field in the interval $[8, 9]$ (middle). Displacement is visualised as a vector plotted at the center of grain. Length of the vector is proportional to the magnitude. Zoomed in image of the location of sample highlighted with vortices (right).

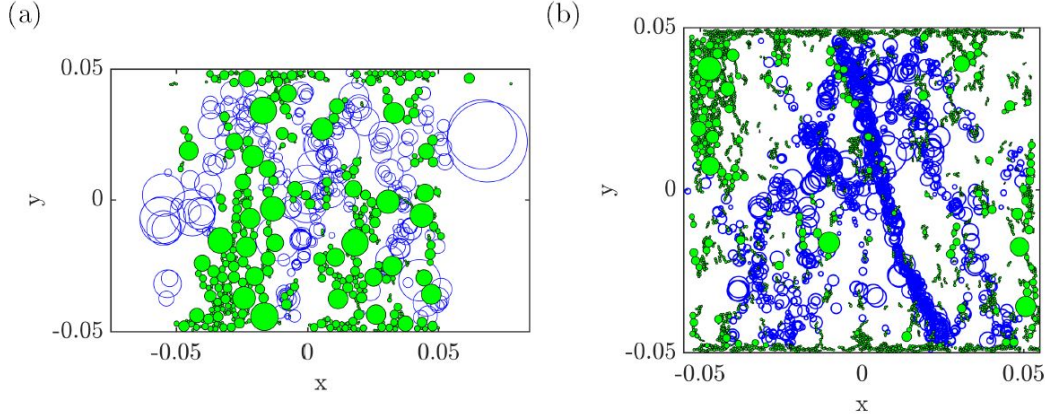


Figure C.15.: 1C, 3C: Tensile force chains are mainly lie outside the vortices. Spatial distribution of accumulated TFCs (green) and vortices (blue outlined circle) plotted with particle data at the final stage of loading for (a) 1C and (b) 3C. Vortices are visulaised with vortex core and radii.

C.3. Conclusion

We observed that TFCs (CFCs) are dominant in the tension (compression) samples and aligned in the direction of the applied tensile (compressive) load. Compressive force chains show similar trends those observed for the unbonded systems.

Buckling force chains analysis of CFCs of compression samples show that BFCs are along the fracture zone between fragments. Hence, BFCs somewhat delineate the macro-cracks. As BFCs form towards the failure, CFCs degrades in these regions. Results show that vortical movements are the mechanism which is responsible for force chains fails by buckling. This is consistent with the findings from the unbonded granular systems. Moreover, tensile force chains do not fail by buckling.

C.3. CONCLUSION

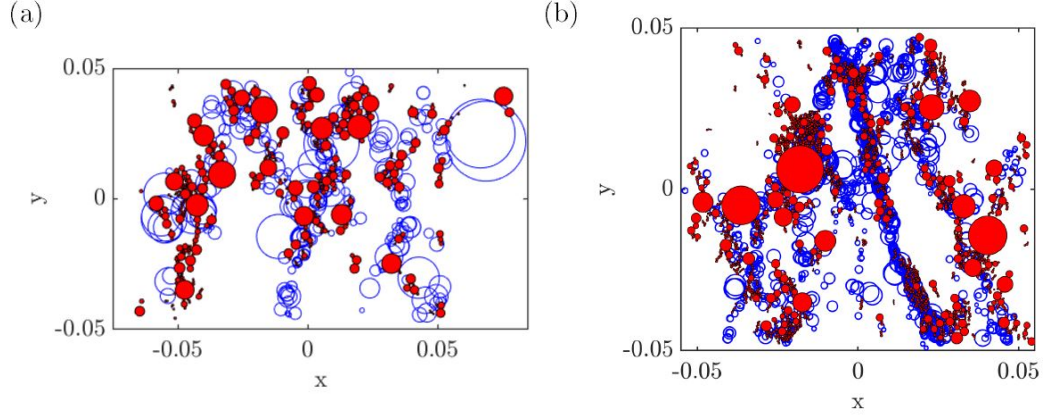


Figure C.16.: *1C, 3C: BFC grains mainly lie inside the vortices. Spatial distribution of accumulated BFC-segments (red) and vortices (blue outlined circle) plotted with particle data at the final stage of loading for (a) 1C and (b) 3C. Vortices are visualised with vortex core and radii.*

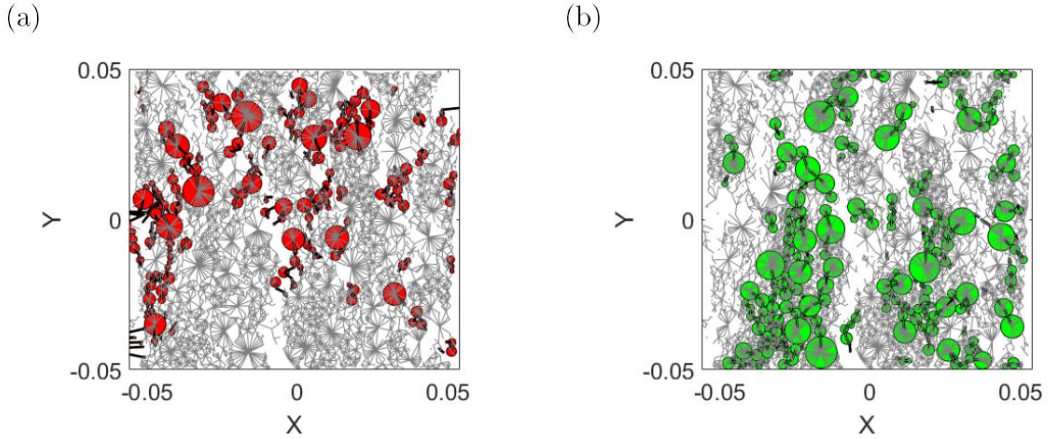


Figure C.17.: *1C: Buckling force chain delineate somewhat macrocrack and tensile force chains form inside the fragments. (a) Accumulated BFCs segments and (b) accumulated TFCs with the remaining bonds at the final stage of loading. Gray lines are the remaining bonds and red (green) grains are the grains in BFC segments (TFCs) shown for grain positions at the final stage of loading.*

D. Method to find maximum cut in a graph

As opposed to finding minimum cuts in a graph, finding maximum cuts is NP-complete (Khot *et al.* 2007). So we must use a heuristic method to find an approximate solution, i.e., not necessarily the global maximum. Here we use a probabilistic technique called “simulated annealing (SA)” for approximating the global maximum. This algorithm is known to converge to the global extrema if the cooling schedule is slow enough and the initial temperature is relatively high (Hromkovič 2013). Annealing technique is inspired by metallurgy which heat (metal or glass) and allow it to cool slowly, to remove internal stresses and toughen it. Simulated annealing is one of the best-known algorithms to find a global maximum or minimum (Khan *et al.* 1997). Initially, it searches through the entire solution space and accepts the worst solutions with some probability. But it keeps the best solution. In the next step, it starts with the current best solution and searches for a better solution. As temperature decreases the probability of accepting the worst solution decreases. At the end of the minimisation ($Temp = 0$), it compares all the best solution found in each step and outputs the best solution among them. Pseudo-code is given in Algorithm 5.

In the context of the maximum cut problem, the idea is to start with a random cut Γ and randomly move a node across the cut. The current cost is then compared with the previous cost and if the current cost is better than the previous cost, the new partition is accepted. Otherwise, this partition is accepted conditionally with some probability. Initially, this process starts at a higher temperature. This enables the algorithm to search through the entire domain. Then the temperature is gradually decreased. When we decrease the temperature, the probability of accepting the worst solution is low. Thus, this process converges to a better solution (Rutenbar 1989; Abramson 1991). During this process, the choice of initial temperature, cooling rate and the number of iterations play a major role.

Algorithm 5 Simulated annealing algorithm to find the maximum cut ([Hromkovič 2013](#))

- 1: Input: the contact network $\mathcal{N}$ for a given time stage ϵ of the loading
 - 2: Assign the edge weight (for instance energy release rate or the principal stress to all edges of $\mathcal{N}$)
 - 3: Randomly generate a cut (Γ)
 Select an initial temperature $Temp$
 Select a temperature reduction function f
 $Itter := 0$
while $Temp > 0$
 Begin randomly move a node across the cut
 Compute the new cut and the cost. Define $dE = \text{new cost} - \text{previous cost}$
 if $dE > 0$
 Accept new solution
 else
 Begin generate a random number $r \in (0, 1)$ uniformly
 if $r < e^{dE/Temp}$
 Move to the new solution with this probability
 end
 $Itter := Itter + 1$;
 $Temp := f(Temp, Itter)$
 end
 4: **return** Outputs the maximum cut.
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