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14. ABSTRACT We have recently established, in close collaboration with experimentalists (from geology, physics, geotechnical and agricultural engineering), a comprehensive first-of-a-kind knowledge base for state-of-the-art data, characterization and modelling of the behaviour of dense granular systems under quasi-static loading conditions. This behaviour is intrinsically multiscale and is arguably one of, if not, the most challenging to characterize and model of the gamut of granular behaviour encountered in practice. In particular, it exhibits self-organized pattern formation and					
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Report Title

Multiscale phenomena in the solid-liquid transition state of a granular material: Analysis and Modelling of Dense Granular Materials

ABSTRACT

We have recently established, in close collaboration with experimentalists (from geology, physics, geotechnical and agricultural engineering), a comprehensive first-of-a-kind knowledge base for state-of-the-art data, characterization and modelling of the behaviour of dense granular systems under quasi-static loading conditions. This behaviour is intrinsically multiscale and is arguably one of, if not, the most challenging to characterize and model of the gamut of granular behaviour encountered in practice. In particular, it exhibits self-organized pattern formation and co-evolution of emergent functional structures in the mesoscopic scale. Therefore, one of the great challenges in the field is to decipher a granular material's "inherent" structural design principles as it deforms in response to external loads. Herein we summarize key achievements from this research program, including those above and beyond what was originally proposed.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

<u>Received</u>	<u>Paper</u>
2011/08/30 0: 18	Sebastian Pucilowski, David M. Walker, Antoinette Tordesillas. A COMPLEX NETWORK ANALYSIS OF GRANULAR FABRIC EVOLUTION IN THREE-DIMENSIONS, Dynamics of Continuous Discrete and impulsive systems series, (09 2011): 0. doi:
2011/08/30 0: 9	David M. Walker, Antoinette Tordesillas, Itai Einav, Michael Small. Complex networks in confined comminution, Physical Review E, (08 2011): 0. doi: 10.1103/PhysRevE.84.021301
2011/08/30 0: 16	Antoinette Tordesillas, David M. Walker, Qun Lin. Force cycles and force chains, Physical Review E, (01 2010): 1. doi: 10.1103/PhysRevE.81.011302
2011/08/29 0: 15	G. W. Hunt, A. Tordesillas, S. C. Green, J. Shi. Force-chain buckling in granular media: a structural mechanics perspective, Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences, (01 2010): 249. doi: 10.1098/rsta.2009.0180
2011/08/29 0: 14	A. Tordesillas, S. D.C. Walsh, M. Muthuswamy. The Effect of Local Kinematics on the Local and Global Deformations of Granular Systems, Mathematics and Mechanics of Solids, (01 2010): 3. doi: 10.1177/1081286508089844
2011/08/29 0: 13	David M. Walker, Antoinette Tordesillas. Topological evolution in dense granular materials: A complex networks perspective, International Journal of Solids and Structures, (03 2010): 624. doi: 10.1016/j.ijsolstr.2009.10.025
2011/08/29 0: 12	J. Zhang, T. S. Majmudar, A. Tordesillas, R. P. Behringer. Statistical properties of a 2D granular material subjected to cyclic shear, Granular Matter, (03 2010): 159. doi: 10.1007/s10035-010-0170-2
2011/08/24 0: 10	Antoinette Tordesillas, Jingyu Shi, Timothy Tshai kiwsky. Stress-dilatancy and force chain evolution, International Journal for Numerical and Analytical Methods in Geomechanics, (02 2011): 264. doi: 10.1002/nag.910
2011/08/24 0: 8	David M. Walker, Antoinette Tordesillas, Colin Thornton, Robert P. Behringer, Jie Zhang, John F. Peters. Percolating contact subnetworks on the edge of isostaticity, Granular Matter, (02 2011): 233. doi: 10.1007/s10035-011-0250-y
2011/08/23 0: 7	Jingyu Shi, Giles Hunt, Antoinette Tordesillas. A characteristic length scale in confined elastic buckling of a force chain, Granular Matter, (02 2011): 0. doi: 10.1007/s10035-011-0252-9
2011/01/30 1: 6	Antoinette Tordesillas. Structural stability and jamming of self-organized cluster conformations in dense granular materials, Journal of the Mechanics and Physics of Solids, (02 2011): . doi:
2010/03/22 1: 2	O. Ben-Nun, I. Einav, A. Tordesillas. Force Attractor in Confined Comminution of Granular Materials, Physical Review Letters, (03 2010): . doi:

TOTAL: 12

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

<u>Received</u>	<u>Paper</u>
2011/09/04 1: 28	R. S. ANDERSSSEN, R. HARASZI, A. TORDESILLAS. A FORCE TRANSMISSION AND COMMUNITIONINTERPRETATIONOF THE RHEOLOGY OF GRAIN HARDNESS, Rheologica Acta, (10 2010): 0. doi:

TOTAL: 1

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

- 2011/08/30 0: 25 Fernando Alonso-Marroquin, Sergio-Andres Galindo-Torres, Antoinette Tordesillas, Yucang Wang. New perspectives for Discrete Element Modeling: Merging Computational Geometry and Molecular Dynamics, POWDERS AND GRAINS 2009: PROCEEDINGS OF THE 6TH INTERNATIONAL CONFERENCE ON MICROMECHANICS OF GRANULAR MEDIA. 2009/06/30 10:00:00, Golden (Colorado). : ,
- 2011/08/30 0: 24 J. Zhang, J. Ren, S. Farhadi, R. P. Behringer, T. S. Majmudar, A. Tordesillas. A Dense 2D Granular Material Subject to Cyclic Pure Shear, POWDERS AND GRAINS 2009: PROCEEDINGS OF THE 6TH INTERNATIONAL CONFERENCE ON MICROMECHANICS OF GRANULAR MEDIA. 2009/06/30 10:00:00, Golden (Colorado). : ,
- 2011/08/30 0: 17 Antoinette Tordesillas, Luc Sibille, Sebastian Pucilowski, Francois Nicot, Felix Darve. MICROSTRUCTURAL EVOLUTION IN DIFFUSE GRANULAR FAILURE: FORCE CHAINS AND CONTACT CYCLES, International Symposium on Computational Geomechanics. 2011/04/26 10:00:00, . : ,

TOTAL: 3

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received Paper

- 2011/08/30 0: 22 Antoinette Tordesillas, Giles Hunt , Jingyu Shi. A characteristic length scale in confined elastic buckling of a force chain, Granular Matter (08 2011)
- 2011/08/30 0: 21 David M. Walker, Antoinette Tordesillas, Sebastian Pucilowski, Qun Lin, Amy L. Rechenmacher, Sara Abedi. Analysis of grain-scale measurements of sand using kinematical complex networks, International Journal of Bifurcation and Chaos (08 2011)
- 2011/08/30 0: 20 Antoinette Tordesillas, Jingyu Shi, John F Peters. Isostaticity in Cosserat Continuum, Granular Matter (08 2011)
- 2011/08/30 0: 19 Tracy Rushmer, Antoinette Tordesillas, David M. Walker. Core Formation in Partially Molten Planetesimals: A Complex Network Analysis of Growth and Mixing Dynamics in Natural Metal-Silicate Systems, Physics of the earth and planetary interiors (08 2011)
- 2010/09/22 1: 4 . A Complex Network Analysis of Granular Fabric Evolution in Three-Dimensions , (09 2011)
- 2010/09/22 1: 3 David M. Walker · Antoinette Tordesillas · Colin Thornton, Robert P. Behringer · Jie Zhang · John F. Peters. Percolating contact subnetworks on the edge of isostaticity, (09 2010)
- 2008/09/17 0: 1 A. Tordesillas, M. Muthuswamy. A Thermomicromechanical Approach to Multiscale Continuum Modeling of Dense Granular Materials, (07 2008)

TOTAL: 7

Number of Manuscripts:

Books

Received

Paper

2011/09/04 11:26 Antoinette Tordesillas, David M. Walker, Amy Rechenmacher, Sara Abedi. Discovering community structures and dynamical networks from grain-scale kinematicsof shear bands in sand, Dordrecht: Springer, (07 2011)

TOTAL: 1

Patents Submitted

Patents Awarded

Awards

Graduate Students

<u>NAME</u>	<u>PERCENT_SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Names of Post Doctorates

<u>NAME</u>	<u>PERCENT_SUPPORTED</u>
David M Walker	0.50
Jingyu Shi	0.30
Qun Lin	0.20
FTE Equivalent:	1.00
Total Number:	3

Names of Faculty Supported

<u>NAME</u>	<u>PERCENT_SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Names of Under Graduate students supported

<u>NAME</u>	<u>PERCENT_SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields: 0.00

Names of Personnel receiving masters degrees

NAME

Total Number:

Names of personnel receiving PhDs

NAME

Total Number:

Names of other research staff

NAME

PERCENT SUPPORTED

FTE Equivalent:

Total Number:

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

We have opened up new areas of exploration in granular media science and have introduced new methods for analysis of experimental and simulation data – that go beyond the retrospective assessment of granular behaviour. Our publications in recent years have demonstrated the capabilities of these methods to deliver prospective information and knowledge on granular rheology at unprecedented levels of detail. Together with our experimental collaborators, we have been the first to:

- o Develop a unified approach for predictive continuum modelling of dense granular materials using a first-principles, physics-based approach within the framework of thermodynamics. This approach is unique in that it provides a formalism by which governing mechanisms on the mesoscopic scale, responsible for bulk deformation and failure of the material, can be explicitly accounted for via measurable quantities.
- o Map out the evolution of failure processes from the microscale to the macroscale based from the only available experimental data on interparticle contact forces in a deforming granular material
- o Map out conformational and conformational transition dynamics, and associated stability and energy landscapes, of emergent functional structures from their nucleation to collapse. This has revealed transition dynamics reminiscent of “magic numbers” seen in chemical and biological clusters.
- o Develop tools that characterize and model self-organization at an unprecedented level of detail, unveiling more intricate levels of co-evolution and cooperative behaviour among emergent functional structures at multiple length scales. The tools for material characterization have been shown to comprehensively mine information from experimental data and explicitly link observed behaviour and dynamics in the bulk to its respective origin at the finer (mesoscopic, microscopic) scales.
- o Develop tools that identify interconnections in topology, structural stability, dynamics and function from synergistic blends of techniques from various disciplines, i.e. Complex Networks, Structural Mechanics, Dynamical Systems, Optimization and Optimal Control, nearly all of which are seeing their first applications to granular mechanics and physics
- o Demonstrate potential applications to Sensor Networks and other areas of Complex Systems Science (eg communications, mining processes, seismology and epidemic spread).

Technology Transfer

US Army Research Office (ARO) grant

2007-2010

“Multiscale phenomena in the solid-liquid transition state of a granular material: Analysis, Modelling and Experimentation”

In this final report, I highlight some key achievements from this research program, beginning with an overview of research activities, including those above and beyond what was originally proposed. To support these, I have provided a brief discussion of some of the recent key papers from our group, describing how they have advanced knowledge in the broad science of granular materials. The past two years have been particularly fruitful and publications from this period are highlighted.

A. Statement of the problem studied from the ARO proposal

Understanding the nature of the upper soil surface – a form of granular material – is of paramount importance to the US Army. In this program, we are to integrate analytical, experimental and modeling techniques to characterise the solid-liquid transition regime in granular media. This regime is highly relevant to at least two key aspects of the Army's operations: off-road vehicle mobility and soil stability. Understanding soil stability and vehicle mobility is also crucial for a related strategic mission of the United States, namely the manned exploration of the Moon and Mars. With the Army's increasing reliance on modeling and simulation for decision-making, the next generation of constitutive models for granular materials must reliably predict dominant mechanisms at the relevant scales. The key to achieving this level of predictive capability is an in-depth knowledge of force transmission, energy dissipation and kinematics in granular assemblies across *multiple spatial and temporal scales*. Accordingly, the specific objectives of this program are twofold: (i) examine these three factors experimentally in conjunction with particle-based computer simulations (*i.e.* discrete element method or ‘DEM’) and, using knowledge from these, (ii) develop a new breed of micromechanical continuum models with predictive capabilities for multiscale phenomena in the solid-liquid transition regime. With current DEM simulations being limited to a few million particles (roughly the number of particles in a handful of sand), these continuum models fill an important niche in engineering practice, *viz.* large-scale applications such as soil–structure/machine interaction systems.

A quantitative understanding of granular behavior from the microscopic (particle) scale to the macroscopic engineering scale is an essential step toward delivering models whose predictive capabilities are of sufficient reliability for design, optimisation and control of granular material behaviour. Systems and processes involving granulates are complex, and due to inadequate understanding and modeling capabilities, rarely reach more than 60% of design performance. Given the prominence of these materials in a wide range of civilian and defense engineering operations, the potential of this proposed program to advance a myriad of “dual-use”

technologies (including the processing and handling of grains, aggregates and powders) is significant.



Figure 1. A summary of the key elements of the research program of A Tordesillas (University of Melbourne) in collaboration with RP Behringer (Duke University).

B. Achievements from the ARO program

Breaking new ground in Granular Matter

Despite their sheer prevalence in everyday life, the behaviour of granular material remains poorly understood – and, consequently, difficult to predict and control. Observed bulk mechanical behaviour of these materials – i.e. how they deform, how much load they can carry before failure – is a manifestation of processes that operate over a vast range of length and time scales. A complete understanding and thus prediction of this behaviour requires theoretical and computational tools that span: the microscopic (i.e. basic unit of two interacting grains in contact), the wide range of length scales encountered in the mesoscopic domain and, finally, the bulk or macroscopic scale. A further complication is that the mesoscopic and macroscopic domains vary considerably and depend on the system under consideration. For example, the current largest granular system for which properties down to the grain contacts have been

measured experimentally comprises around 1000 particles: here the mesoscopic is anywhere between the basic unit of two interacting grains and the bulk material. Compare this to a typical geological fault zone where the mesoscopic granular domain extends from hundreds to thousands of kilometres.

My research activities in recent years have fused state-of-the-art developments in areas of pure and applied mathematics and statistics with cutting-edge experimental developments in physics, geology and engineering – to understand and predict the multiscale behaviour of granular materials. Several pioneering achievements have led to breakthroughs related to the fundamental and interconnected issues of stability, failure and energy dissipation, either in the presence or absence of particle breakage.

Purpose of the Research

We have recently established, in close collaboration with experimentalists (from geology, physics, geotechnical and agricultural engineering), a comprehensive first-of-a-kind knowledge base for state-of-the-art data, characterization and modelling of the *behaviour of dense granular systems under quasi-static loading conditions*. This behaviour is intrinsically *multiscale* and is arguably one of, if not, the most challenging to characterize and model of the gamut of granular behaviour encountered in practice. In particular, it exhibits self-organized pattern formation and co-evolution of emergent functional structures in the mesoscopic scale. Therefore, one of the great challenges in the field is to decipher a granular material's “inherent” structural design principles as it deforms in response to external loads.

Research Trends: Cycling between lab bench - modelling - and simulation

My group has pioneered the development of:

- A focussed and highly integrated experimental, simulation and theoretical program of research for a wide range of *real* granular materials – both natural (e.g. soil, rocks, grains) and synthetic (e.g. glass beads, photoelastic particles).
- A program that brings to bear recent developments from the mathematics and statistics of complex systems on fundamental and applied problems relating to granular rheology.
- A unified thermodynamically consistent approach for predictive continuum modelling of dense granular materials, that has demonstrated predictive capability for observed behaviour down to the fine scale of a few grains.
- Theoretical tools that can mine information from experimental data – as they are generated. This requires close coherent effort that intertwines state-of-the-art theory and experiment.
- Theoretical tools for data analysis with *predictive* capability to answer "How is a given granular material *most likely* to respond to a given load – and why?" as well as enable new rheological questions to be answered accurately and at unprecedented levels of detail.

Specific outcomes from research work

We have opened up new areas of exploration in granular media science and have introduced new

methods for analysis of experimental and simulation data – that go beyond the retrospective assessment of granular behaviour. Our publications in recent years have demonstrated the capabilities of these methods to deliver *prospective* information and knowledge on granular rheology at unprecedented levels of detail. Together with our experimental collaborators, we have been the first to:

- Develop a unified approach for predictive continuum modelling of dense granular materials using a first-principles, physics-based approach within the framework of thermodynamics. This approach is unique in that it provides a formalism by which governing mechanisms on the mesoscopic scale, responsible for bulk deformation and failure of the material, can be explicitly accounted for via measurable quantities.
- Map out the evolution of failure processes from the microscale to the macroscale based from the only available experimental data on interparticle contact forces in a deforming granular material
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- Develop tools that characterize and model self-organization at an unprecedented level of detail, unveiling more intricate levels of co-evolution and cooperative behaviour among emergent functional structures at multiple length scales. The tools for material characterization have been shown to comprehensively mine information from experimental data and explicitly link observed behaviour and dynamics in the bulk to its respective origin at the finer (mesoscopic, microscopic) scales.
- Develop tools that identify interconnections in topology, structural stability, dynamics and function from synergistic blends of techniques from various disciplines, i.e. Complex Networks, Structural Mechanics, Dynamical Systems, Optimization and Optimal Control, nearly all of which are seeing their first applications to granular mechanics and physics
- Demonstrate potential applications to Sensor Networks and other areas of Complex Systems Science (eg communications, mining processes, seismology and epidemic spread).

The combination of emerging techniques from mathematics (complex networks, nonlinear dynamics and systems theory and optimization), together with structural mechanics and constitutive theory – forms the beginnings of a new direction and focus in micromechanics of granular media. To the best of our knowledge, this is the first attempt to integrate these techniques into one coherent nexus that allows information from material characterization to be synchronized with and directly brought to bear and tested on models and simulations of phenomena – across multiple length scales – and in 2D as well 3D systems. This unique collection of techniques has revolutionized the field since we can now probe the inner workings of granular systems at the highest level of resolution to gain insights into the fundamental origins of stability, pattern formation and failure of granular materials. The research program thus paves the way for breakthrough applications in the characterization of material behavior at multiple length scales, and to the reliable prediction of the mechanical response of granular materials in a wide range of loading conditions.

B. Research publications and highlights

In the past two decades, mathematicians together with physicists, chemists and biologists have made considerable strides in understanding self-organized pattern formation in many forms of complex systems. Over this period, we have also come to realize how richly nuanced this subject can be and how significant are the challenges that remain. However, there is tremendous potential and opportunity for some of the mathematical advances to enrich our understanding of an even wider range of phenomena. The return on such an investment for many sectors of science and industry cannot be understated, and there is perhaps no better example than in the characterisation and modelling of granular processes.



Figure 2. A key focus of our program is on self-organization in granular matter with respect to topology, stability, dynamics and function.

In the past two years, we have shown that the fusion of state-of-the-art advances in non-invasive laboratory tests at increasing levels of resolution, when combined with a judicious and systematic application of complex systems methods, from network analysis to data mining and modelling paradigms – can deliver deep and potent insights into granular material behaviour. Our strategy is to consider the granular body as a complex dynamical structure that continually adapts to the forces imposed on it. We employ a multidisciplinary approach to the characterization and modelling of its response to forces. This embodies synergistic blends of principles and techniques from nascent as well as classical subdisciplines within mathematics, physics and mechanics including: Complex Networks, Nonlinear Dynamical Systems, Statistical Physics and Stochastic Processes, Sensor Networks, Structural Mechanics, Data Mining, Information Theory, Optimization and Optimal Control. Many of the techniques we are employing are seeing their first application to granular systems. Moreover, these techniques have in the past existed as separate entities, but for the first time our group has successfully fused some of these together to form one coherent theoretical platform with novel and unmatched predictive capabilities.

(4A) Published Work Completed in 2009-2010

Each has a brief summary (and where available, 2009 impact factor and citations as of November 30, 2010 from Thomson's ISI). Papers with a * are given in section 5.

Topology, Dynamics and Function

- [1] Walker, DM, Tordesillas, A (2010) "Topological evolution in dense granular materials: A complex networks perspective" *International Journal of Solids and Structures* **47** pp 624-639.

Inspired by developments in biological networks, this is the first study to use Complex Networks to fully characterize topological evolution of contact and contact forces in a deforming assembly in the stages leading up to and during failure. (*Impact factor 1.809, 1 citation*)

- [2] * Tordesillas, A, O'Sullivan P, Walker DM, Paramitha (2010) "Evolution of functional connectivity in contact and force chain networks: feature vectors, k-cores and minimal cycles," *Comptes-Rendus Mecanique. Comptes Rendus de l'Academie des Sciences, Proceedings of the French Academy of Sciences* **338** pp 556-569.

This is the first incisive study into granular rheology under shear, i.e. 'granular friction', and quantifies the ability of a material to resist forces that splits the bulk material into sub-domains which can then slide against each other. Together with two third year students (O'Sullivan & Paramitha), we followed the footsteps of Charles Augustin Coulomb who published in the same journal his now famous 'Coulomb's law of friction' in "*Essai sur la theorie du frottement*" for solid bodies. Armed with the modern tools of Complex Networks, we uncovered mechanisms underpinning 'granular friction' from the standpoint of topology, structure and function. (*Impact factor 0.667; 7 citations*)

- [3] Tordesillas, A, Pucilowski, S, Walker, DM, Peters, J, Hopkins, M (2010) "A complex network analysis of granular fabric evolution in three-dimensions" *Dynamics of Continuous, Discrete and Impulsive Systems-B*. (In press)

The techniques in [1]-[2] are extended to three-dimensional systems where patterns of failure are significantly more complex and intricate. (*Impact factor 0.972*)

- [4] Tordesillas A, Walker, DM (2011) "Deciphering D'Alembert's dream: new tools for uncovering rules for self-organized pattern formation in geomaterials" *Proceedings, 2011 International Workshop on Bifurcations and Degradations in Geomechanics*. (In press)

The techniques in [1]-[2] are extended to a broader range of experimental and simulation data sets to demonstrate that the techniques and findings are robust.

Experiments to test and guide theoretical development

- [5] Tordesillas, A, Zhang, J and Behringer, RP (2009) “Buckling force chains in dense granular assemblies: physical and numerical experiments” *Geomechanics and Geoengineering* **4**(1) pp 3-16.

The first quantitative characterization of force chain evolution and failure by buckling in a monotonic biaxial compression test.

- [6] Zhang, J, Ren, J, Farhadi, S, Behringer, RP, Majmudar, TS, Tordesillas, A (2009) “A dense 2D granular material subject to cyclic pure shear” *Powders & Grains AIP Conference Proceedings* **1145**, pp 553-556.
- [7] Zhang, J, Majmudar, T, Tordesillas, A, Behringer, RP (2010) “Statistical properties of a 2D granular material subjected to cyclic shear” *Granular Matter* **12** pp 159-172.

Papers in [6]-[7] present the first quantitative characterization of force chain evolution and failure by buckling in a cyclic shear test. (*Impact factor of [7] 1.330, 1 citation*)

Theory providing feedback to particle-based simulations

- [8] Alonso-Marroquín, F, Galindo-Torres, S-A, Tordesillas, A, Wang, Y (2009) “New perspectives for discrete element modelling: Merging computational geometry and molecular dynamics.” *Powders & Grains AIP Conference Proceedings* **1145**, pp 825-828.

This paper presents novel method for accounting for complex particle shapes in discrete element simulation.

Topology, Structural Stability, Dynamics

- [9] * Tordesillas, A, Muthuswamy, M (2009) “On the modelling of confined buckling of force chains” *Journal of Mechanics and Physics of Solids* **57** pp 706-727.

The first rigorous mathematical analysis of the fundamental mechanism of failure for dense materials, confined buckling of force chains, and its connection to the defining behaviour of dense systems at the macroscopic scale – i.e. loss of load-carrying capacity of the material as it expands in bulk volume. This study tracks the evolution of a force chain ‘from birth to death’ (*Impact factor 3.317; 13 citations*)

- [10] Tordesillas, A, Lam, E, Metzger, P (2009) “Hyperstaticity and loops in frictional granular packings” *Powders & Grains AIP Conference Proceedings* **1145**, pp 325-328.

Densely packed frictional granular materials are hyperstatic (i.e. redundantly constrained). This is the first paper to report on the origins of hyperstaticity.

- [11] Hunt, G, Tordesillas, A, Green, S, Shi, J (2010) “Force chain buckling in granular media: A structural mechanics perspective” *Philosophical Transactions of the Royal Society A* **368** pp 249-262.

In this paper, we demonstrate commonalities in the design principles employed by the material and those seen in man-made structures. Parallels are drawn between the response of a discrete strut on a linear elastic foundation and force-chain buckling in a constrained granular medium. (*Impact factor 2.295, 3 citations*)

- [12] Tordesillas, A, Hunt, G, Shi, J (2010) “A characteristic length scale for confined elastic buckling of force chains” *Granular Matter*. (In press)

From anonymous reviewers:

“This paper presents a brilliant idea for the explanation of the well-known experimental observation that the shear band thickness is roughly around 5-10 average particle diameters.”

“The manuscript is an outstanding contribution to the description of shear band formation, instabilities of granular materials and it is an important advance to the development of micropolar continua.”

(*Impact factor 1.330*)

- [13] * Tordesillas, A, Walker DM, Lin Q (2010) "Force cycles and force chains" *Physical Review E* **81**, 011302.

This presents the discovery and first quantitative characterization of *cyclic building blocks* for self-organization of granular materials and their synergetic co-evolution with the *linear building blocks*, the primary load-bearing force chains. Stabilizing agents in the form of truss-like 3-cycles provide the column-like load-bearing force chains dual resistance against buckling: 3-cycles: i) prop-up force chains, and ii) frustrate particle rotation. (*Impact factor 2.400, 1 citation*)

- [14] Tordesillas A, Lin Q, Zhang J, Behringer, RP, Shi, J (2010) “Structural stability and jamming of self-organized cluster conformations in dense granular materials” *Journal of the Mechanics and Physics of Solids*. (In press DOI:10.1016/j.jmps.2010.10.007)

This paper presents the first quantitative criterion for a self-organized granular cluster conformation to be “structurally stable” and the first characterization of the stability of linear and cyclic building blocks, first reported in [13], for dense granular media.

From anonymous reviewers:

“The paper contains many original and significant derivations and results. It is exceedingly well written and was a pleasure to review. The authors present the following important developments: a clear definition of the internal structural stability of granular media, both local and global; a clear criterion for determining stability and a proof that it satisfies the definition; a clear presentation of the stiffness matrix for a 2D cluster, based upon the work of

Bagi; a proposed set of upper and lower bounds for the stability of a non-conservative system; and a fascinating set of DEM simulations and photoelastic experiments. The experiments yield a number of important results: a correlation between the Krut-Rothenburg and Thornton-Antony measures of determinacy; a finding that internal instability can be adequately captured at lengths scales less than seven particle diameters, obviating the need for a more computationally intensive search; an experimentally-based description of the role of 3-cycles in promoting force chains; and a conclusive finding that shear bands are associated with internal structural instability.”

“Within the field of granular mechanics, the manuscript is among the best that the Reviewer has encountered in the past several years. The paper is of eminent interest to the journal's readers.” (*Impact factor 3.317*)

[15] Walker, DM, Tordesillas A, Thornton, C, Behringer, RP, Zhang J, Peters JF “Percolating contact subnetworks on the edge of isostaticity” *Granular Matter*. (In press)

Experimental observations have long suggested that the strong particle network comprising the load-bearing force chains, may be an isostatic backbone embedded within the hyperstatic particle system. We show this is highly plausible by finding the minimal spanning trees of a graph -- optimized to bear properties exhibited by force chains, delivers such a network. We find that the strong truss-like 3-force-cycles discovered in [13], when added to the spanning trees, introduces a level of redundancy required to achieve a network that is almost if not isostatic. (*Impact factor 1.330*)

Past, present and future: Overview of theory and experiment

[16] Tordesillas, A, Behringer, RP (2009) “Are we there yet? Following the energy trail in cohesionless granular solids” pp 47-84. Proceedings of the *Mechanics of Natural Solids*. Eds. Kolymbas D. and Viggiani G. Springer-Verlag, Berlin ISBN 978-3-643-03577-7.

There is no other topic in the broad science of granular media that draws together the two disciplines of physics and mechanics more than that of force transmission. Behringer’s group remains the first and only group in the world today that can deliver complete information in a deforming granular material including contact forces between grains: this remarkable achievement is published in *Nature* (2005). Here we review recent developments from our combined studies on force chain evolution, covering the three fronts of experiment, modelling and simulation.

Spreading the news and excitement of research on granular materials

[17] *Tordesillas, A, Kirszenblat, D, Mangelsdorf, C (2009) “Taming the complexity of granular materials with Vector Calculus” *Australasian Journal of Engineering Education* **15** (2) pp 85-94. ISSN 1324-5821.

I take a colleague and a second year mathematics student on a small exploratory program that brings to life the topic of Vector Calculus in the classroom in the context of granular materials. (Vector Calculus is a second year subject both in the heritage degree and Melbourne model

program).

Analysis of kinematics: Transitioning to predictive continuum modelling

- [18] Tordesillas, A, Walsh, SDC, Muthuswamy, M (2009) "The effect of local kinematics on the local and global deformations of granular systems" *Mathematics and Mechanics of Solids* **15** pp 3-41.

Presents a novel measure of local deformation that accounts for particle rotations, and uncovered new insights into the influences of distinct contact modes on local and global kinematics. This is the first step that would enable us to inject the relevant lessons learned on material characterization, i.e. from the standpoints of topology, structure, dynamics and function, into predictive continuum modelling for large-scale systems. (*Impact factor 1.065, 1 citation*)

Predictive continuum model: development and tests of its veracity

- [19] Tordesillas, A, (2009) "Thermomicromechanics of dense granular materials" *Powders & Grains* AIP Conference Proceedings **1145**, pp 51-55.

In this *keynote* paper for the premier conference in the field Powders and Grains, I report on the first high-resolution thermomicromechanical continuum model for granular media. The most advanced model of its kind can capture phenomena down to the scale of only a few particles.

- [20] Tordesillas, A, Shi, J (2009) "Micromechanical analysis of failure propagation in frictional granular materials" *International Journal of Numerical and Analytical Methods in Geomechanics* **33** pp 1737-1768.

Demonstrates the veracity of the first of its kind high-resolution predictive continuum model for dense granular materials in [19]. This study shows the model can capture the spatio-temporal propagation of failure at an unprecedented level of detail, across spatial resolutions from only a few grains to the bulk. (*Impact factor 1.301; 3 citations*)

- [21] Tordesillas, A, Shi, J, Muhlhaus, HB (2009) "Non-coaxiality and force chain evolution" *International Journal of Engineering Science* **47** (2009) pp 1386–1404.

Noncoaxiality is a defining behavior of dense granular systems on the macroscopic scale. We show for the first time that the underpinning mechanism for this trend is force chain evolution and that the model in [19] can successfully reproduce this trend. (*Impact factor 1.360; 4 citations*)

- [22] * Tordesillas, A, Shi, J, Tshaikiwsky, T (2010) "Stress-dilatancy and force chain evolution", *International Journal of Numerical and Analytical Methods in Geomechanics* (In press: DOI: 10.1002/nag.910)

‘Reynolds dilatancy’, a cornerstone of Soil Mechanics, is another defining behavior of dense granular systems on the macroscopic scale. This phenomenon was named after Osborne Reynolds who observed it while walking along the beach and reported it in *Philosophical Magazine* in 1885. We show for the first time that the underpinning mechanism for dilatancy is force chain evolution and that the model in [19] can successfully reproduce this trend. (*Impact factor 1.301*)

Predictive modelling: Discrete, cellular automata with applications to seismology

- [23] Tordesillas, A, Muthuswamy, M (2009) “Stick-slip and force chain buckling” *Powders & Grains* AIP Conference Proceedings **1145**, pp 313-316.

Seismic faults undergo “stick-slip” motion which is believed to be a key mechanism for earthquakes. Stick-slip involves sliding motion between two faults. Inspired by laboratory work from seismology on assemblies of glass beads, showing that the birth and death of force chains lead to stick-slip, we present here the first cellular automata of stick-slip motion based on force chain evolution developed in [9].

Broadening applications of theoretical tools: systems with particle breakage with potential applications to seismology, mineral extraction, and chemical processes.

- [24] * Ben-Nun, O, Einav, I, Tordesillas, A (2010) “Force attractor in confined comminution of granular materials” *Physical Review Letters* **104** 108001.

This reports on the discovery that the dynamics of contact forces in the process of comminution (i.e. particle breakage) is governed by a multiple-point attractor. The ultimate or long-term distribution of the contact forces follows a clear and unique log-normal distribution, distinctively different from previous observations in systems in the absence of particle breakage. (*Impact factor 7.328*)

Broadening applications of theoretical tools to naturally occurring granular materials: sand

- [25] * Tordesillas A, Walker, DM, Rechenmacher, A, Abedi, S (2011) “Discovering community structures and dynamical networks from grain-scale kinematics of shear bands in sand” *Proceedings, 2011 International Workshop on Bifurcations and Degradations in Geomechanics*. (In press)

This is the first application of Complex Networks and Dynamical Systems to high-resolution experimental measurements of grain scale displacement fields in sand. We discover a remarkable property of sand: the shear band (an emergent pattern that is regarded as the signature failure microstructure for dense sand) is a zone in which the spread of information to all other parts of the specimen is at its most efficient – i.e. follows routes of shortest paths. This discovery may ultimately lead to an improved understanding of self-organization, specifically the nature of

energy flow in what is known in Soil Mechanics as the “critical state regime” which occurs in the presence of persistent shear bands.

(4B) Research Manuscripts In Review Suitable for Publication

Broadening applications of tools to studies of wheat grain crushing

- [26] Anderssen, RS, Haraszi, R, Tordesillas, A “A force chain and comminution interpretation of the rheology of grain hardness” *Rheologica Acta*. (In review)

The work here presents the necessary first step in the development of the first rigorous definition and an associated rapid test for grain hardness that is tied to the rheological properties of wheat during crushing.

Broadening applications of tools to comminution with links to sensor networks and seismology

- [27] * Walker, DM, Tordesillas A, Einav, I, Small, M “Minimal cycle energy and robustness to attack in confined comminution contact networks” *Physical Review Letters*. (In review)

This is the first application of methods conceived from a fusion of Complex Networks and Dynamical Systems to a confined comminution system. We discover that the contact network at *the ultimate state* exhibits a scale-free degree distribution and small-world properties – implying that the majority of the nodes in the contact network have a very low number of connections while a small percentage of nodes has a very large number of connections (i.e. hubs). This means that the network is robust to random attacks but is vulnerable to systematic attacks.

New frontiers: Refining knowledge of rules for self-organization

- [28] * Tordesillas, A, Walker, DM, Froyland, G, Zhang, J, Behringer, RP “Transition dynamics in granular clusters” *Letters to Nature*. (In review)

Here we discover a remarkable property of dense granular systems – reminiscent of “magic number behaviour” exhibited by chemical as well as biological clusters. Here we uncover preliminary evidence that show the material under load is attempting to rearrange its constituent particles – so as to optimize the stability of the load-bearing force chains. This opens up an entirely new area for exploration in the science of granular matter that holds significant promise in our future ability to predict and thus ultimately control granular behaviour.

(4C) Research Manuscripts Suitable for Publication

Research manuscripts suitable for publication but which have not yet been submitted for review (currently being formatted to meet Journal specifications)

Broadening applications of tools to studies of mixing dynamics natural metal-silicate systems

- [29] Rushmer, T, Tordesillas A, Walker, DM, “A complex network analysis of growth and mixing dynamics in natural metal-silicate systems” *Geophysical Research Letters*.

The segregation of metallic cores from silicate mantles is one of the earliest, and most important, differentiation process involved in the evolution of terrestrial planetary bodies. Here, we have developed an innovative approach that combines experimental partial melting experiments on natural material with complex network analyses to elucidate and quantify the growth of metallic melt regions in a H6 chondrite (Kernouve).

Broadening applications of tools to studies of seismology

- [30] Tordesillas, A, Muthuswamy, M “Cellular automaton of stick-slip: model construction from micromechanics of force chain buckling. *Journal of Geophysical Research*
- [31] Tordesillas, A, Muthuswamy, M “Cellular automaton of stick-slip: validation against statistics of natural earthquakes” *Journal of Geophysical Research*