Modern Trends in Geomechanics IV **Assisi, May 2016**

DEM modelling of cohesive and cementitious materials

model conceptualisation, calibration & validation

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Granular Mechanics & Industrial Infrastructure Group

- Started in 1989 with initial focus on design of silos and bulk materials handling
- Greatly expanded into research and consultancy on multiphase particulate systems and industrial infrastructure
- Focus: developing scientific insights to underpin industrial innovation

Examples of impact on practice:

- EDEM (DEM Solutions Ltd)
- P4 (Particle Analytics Ltd)
- Uniaxial testers (ECT, EPT, Freeman UPT)
- Major contributions to Eurocodes

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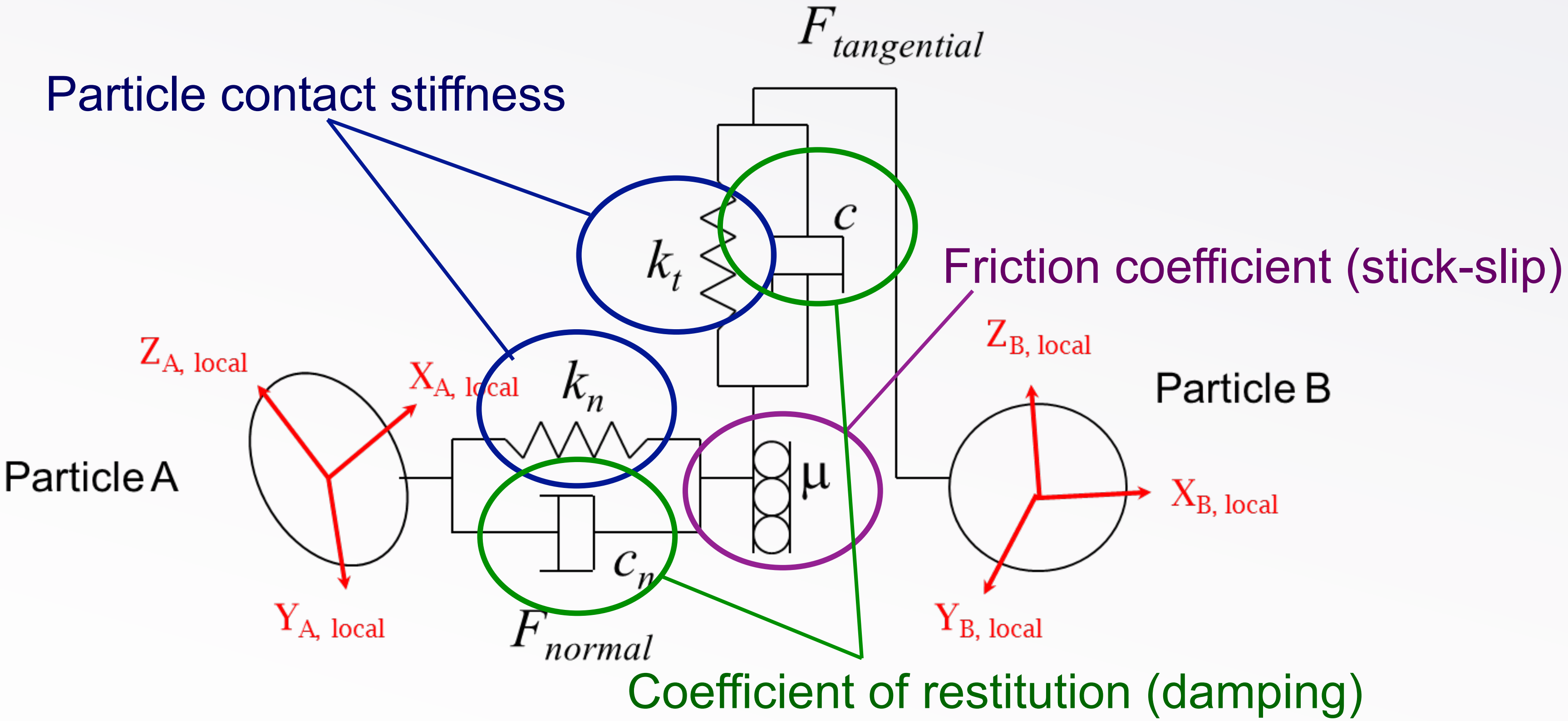
Introduction

- DEM modelling is increasingly popular for studying granular mechanics problems
- DEM modelling of cohesive and cementitious materials – faces significant challenges in producing realistic predictions
- What do we need to produce satisfactory predictions for bulk handling applications?
- Our focus: develop mesoscopic DEM with appropriate scaling laws to capture the bulk behaviour under different flow regimes

Particle contact force model: *cohesionless*



n = normal to the contact surface

t = tangential to the contact surface

DEM input parameters: *cohesionless*

Physical properties

- Mass, volume, shape, size distribution

Mechanical properties

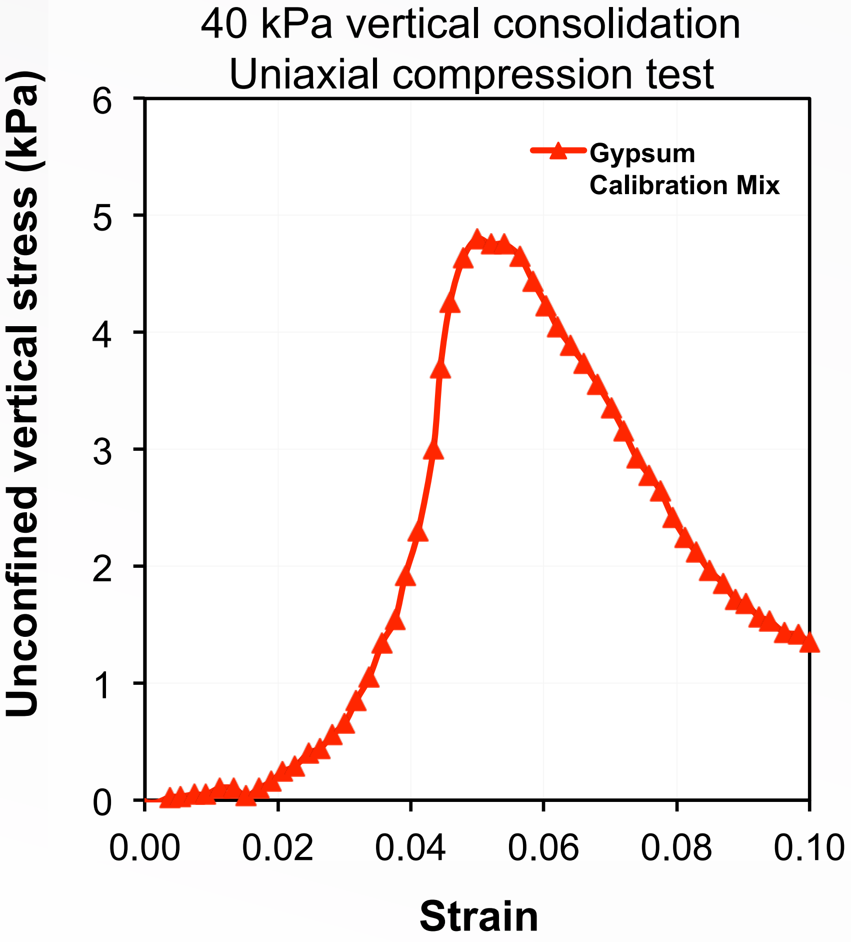
- Contact stiffness
- Contact friction (particle-particle, particle-wall)
- Coefficient of restitution (particle-particle, particle-wall)

Modelling bulk cohesion

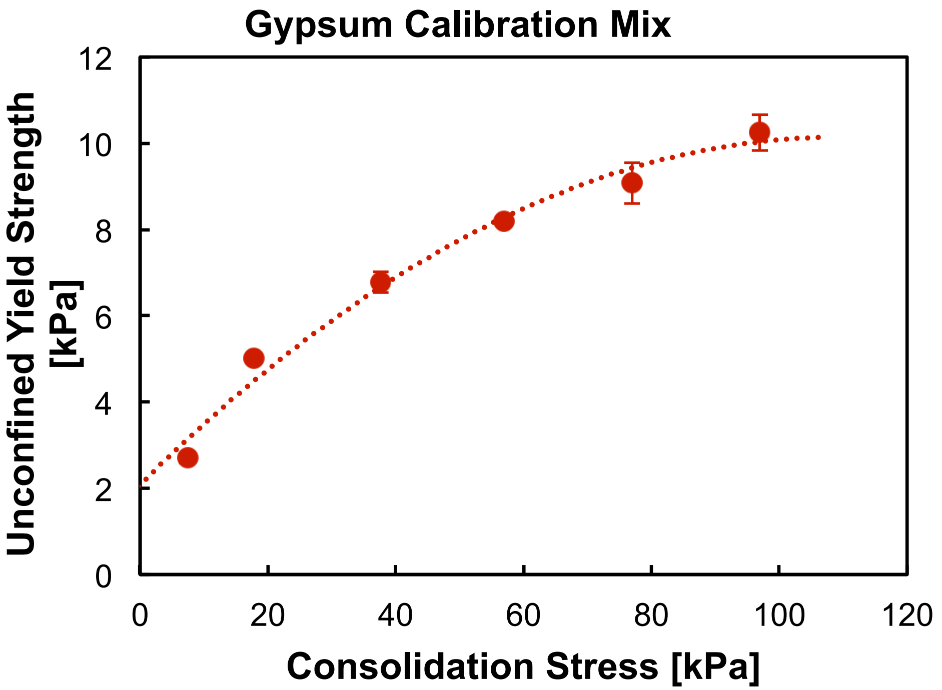
- Where does bulk cohesion arise from?
- Contact adhesion at particle level: surface and field related forces (e.g. van der Waals, electrostatic), solid and liquid bridge related forces (c.f. Tomas, 2006)
- Could also arise from changes in interstitial pressure
- Contact models such as JKR, DMT models have been used to model cohesive powders
- These models may have difficulty to capture **stress history dependence** and **over-consolidated** behaviour as seen in flow characterisation experiments

Observed behaviour of cohesive solid : *stress history dependence*

Typical overconsolidated behaviour

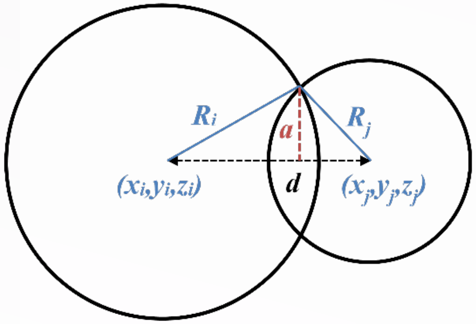


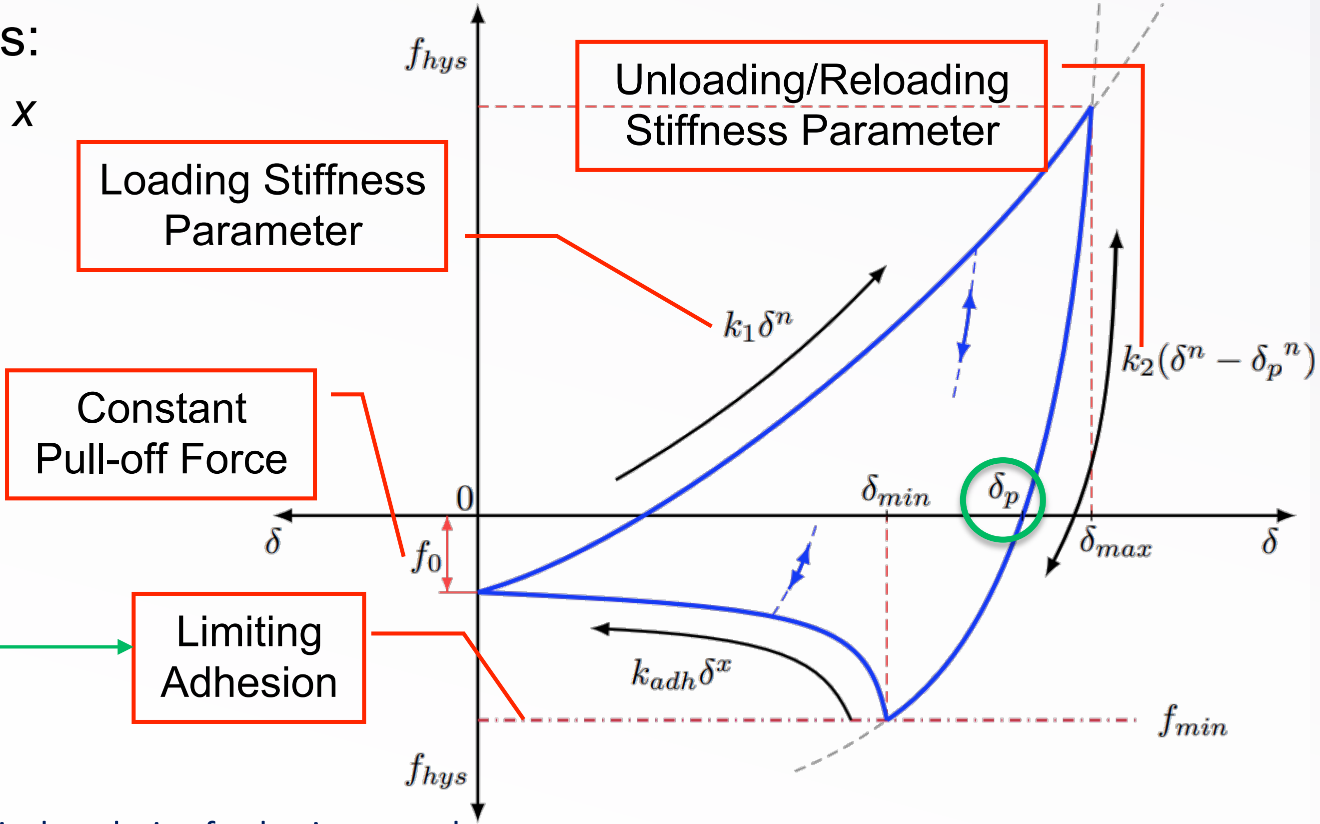
Increasing unconfined strength with consolidation stress - flow function



Proposed adhesive-frictional contact model – nonlinear

- Linear/Non-linear spring model for elastic-plastic deformation
- Model includes adhesion as a function of plastic deformation
- Model parameters:
  - f_0, k_1, k_2, $\Delta\gamma$, n, x





Unloading/Reloading Stiffness Parameter

Loading Stiffness Parameter

Constant Pull-off Force

Limiting Adhesion

Limiting adhesion is dependent on plastic deformation, δ_p

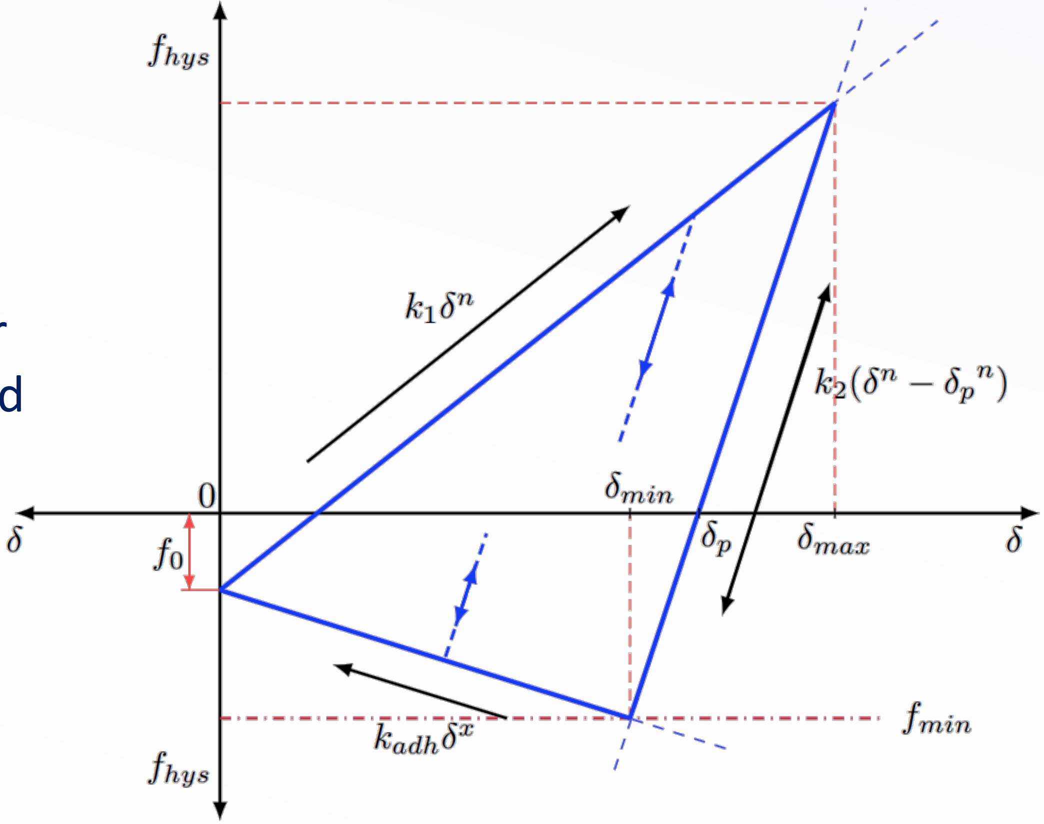
Thakur, et al. (2014) Micromechanical analysis of cohesive granular materials using the discrete element method with an adhesive elasto-plastic contact model. *Granular Matter*.

Proposed adhesive-frictional contact model – linear

- Linear/Non-linear spring model for elastic-plastic deformation
- Model includes adhesion as a function of plastic deformation
- Model parameters:
  - f_0, k_1, k_2, $\Delta\gamma$, n, x

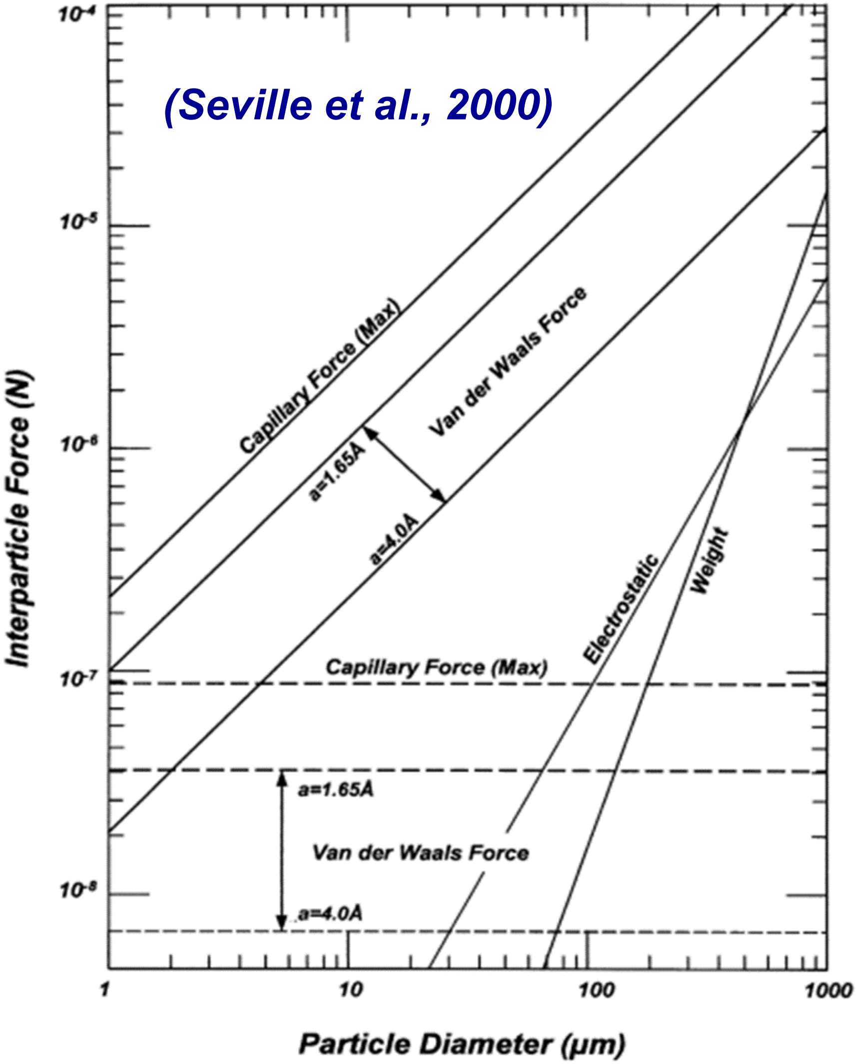
→n=1 (Thakur, et al., 2013), The model becomes linear and similar to Walton and Johnson (2009) and Luding's (2001): f_0,k_1,k_2,k_{adh}-four variable

Work on non-linear model published in Morrissey (2013)



Thakur, et al. (2014) Micromechanical analysis of cohesive granular materials using the discrete element method with an adhesive elasto-plastic contact model. *Granular Matter*.

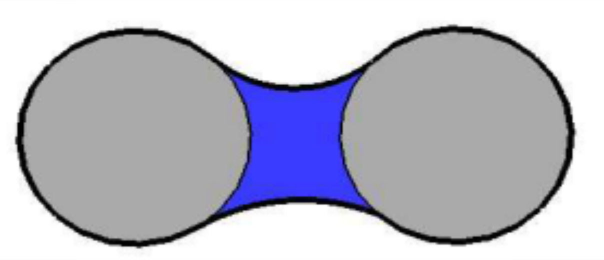
Challenges of modelling at particle scale



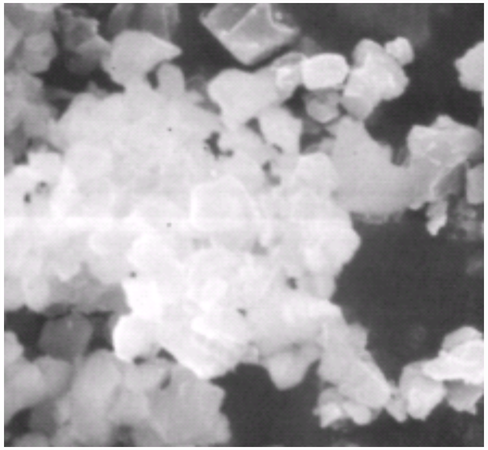
- Magnitude of adhesion can be large but effective range is extremely small (~nm)
- Dotted line shows contact radius based on surface asperity
- Modelling particle contact adhesion based on particle radius (smooth sphere) can be erroneous for real solids with surface roughness

Modelling strategy

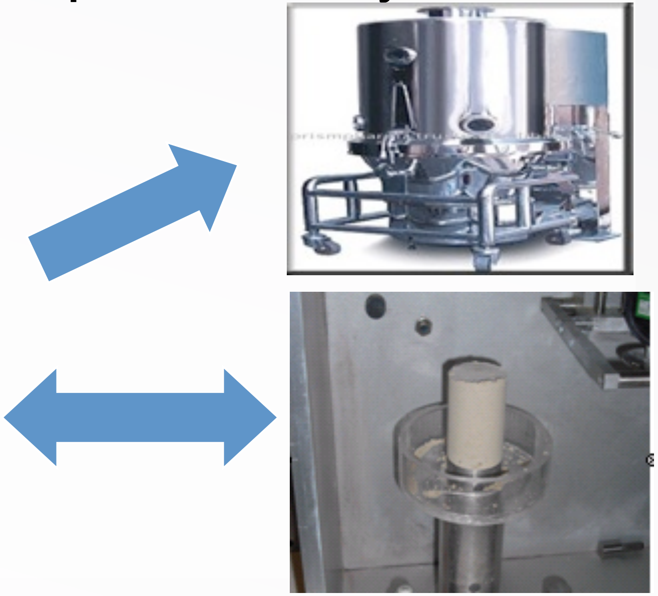
- Not attempting to model at individual particle scale
- Strategy is to model at an intermediate length scale that can reproduce bulk characteristics including stress history dependent cohesion
- Capture key observed phenomena important for your problems



Micro (Particle scale)



Meso (Intermediate scale)



Macro (Bulk Scale)

Capturing material compressibility, shear and cohesive response

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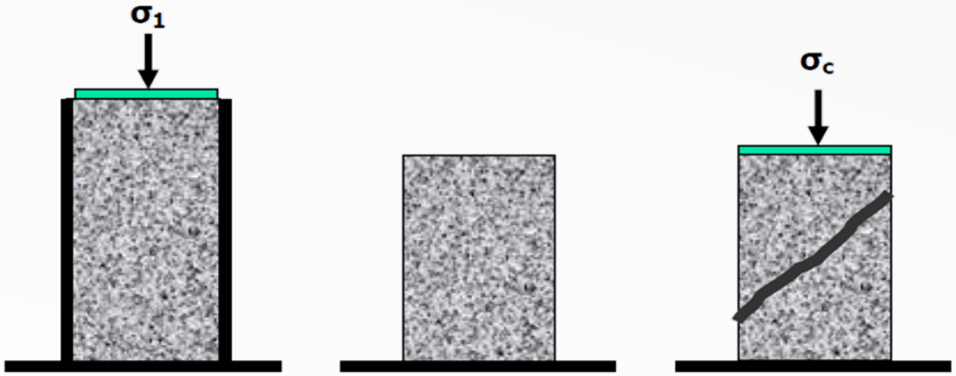
Edinburgh Powder Tester (EPT)

- First developed jointly with DuPont: Bell et al (2007) “Evaluation of the Edinburgh Powder Tester” Proc, PARTEC 2007, Nuremberg.

Edinburgh Powder Tester



a) Confined consolidation **b) unconfined state** **c) unconfined failure**

EPT functionalities

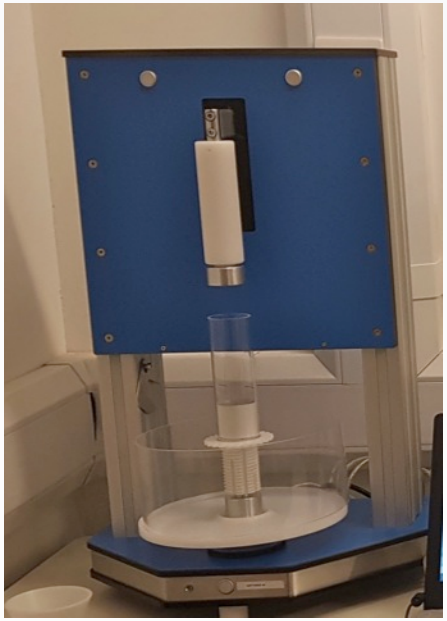
- EPT provides rapid and reproducible measurements of :
  - Filled porosity / packing density
  - Compressibility under confined compression
  - Unconfined yield strength as a function of prior consolidation stress
  - Stress-strain response to failure under uniaxial loading
- Measures "flow function"/caking strength, and stress-strain response, with time consolidation

J. Morrissey, J. Sun, J.F. Chen, J.Y. Ooi, K. Tano, G. Horrigmoe (2012) "An experimental and DEM study of the behavior of iron ore fines" 7th Int. Conf. Conveying and Handling of Particulate Solids, Friedrichshafen, Germany, September 2012, 9pp.

S. C. Thakur, H. Ahmadian, J. Sun and J. Y. Ooi "An experimental and numerical study of packing, compression, and caking behaviour of detergent powders" Particuology 2013.

Freeman UPT Tester

- A version of the Edinburgh Powder Tester has been licensed to Freeman Technology
- Launched this year as the Freeman UPT Tester – available worldwide

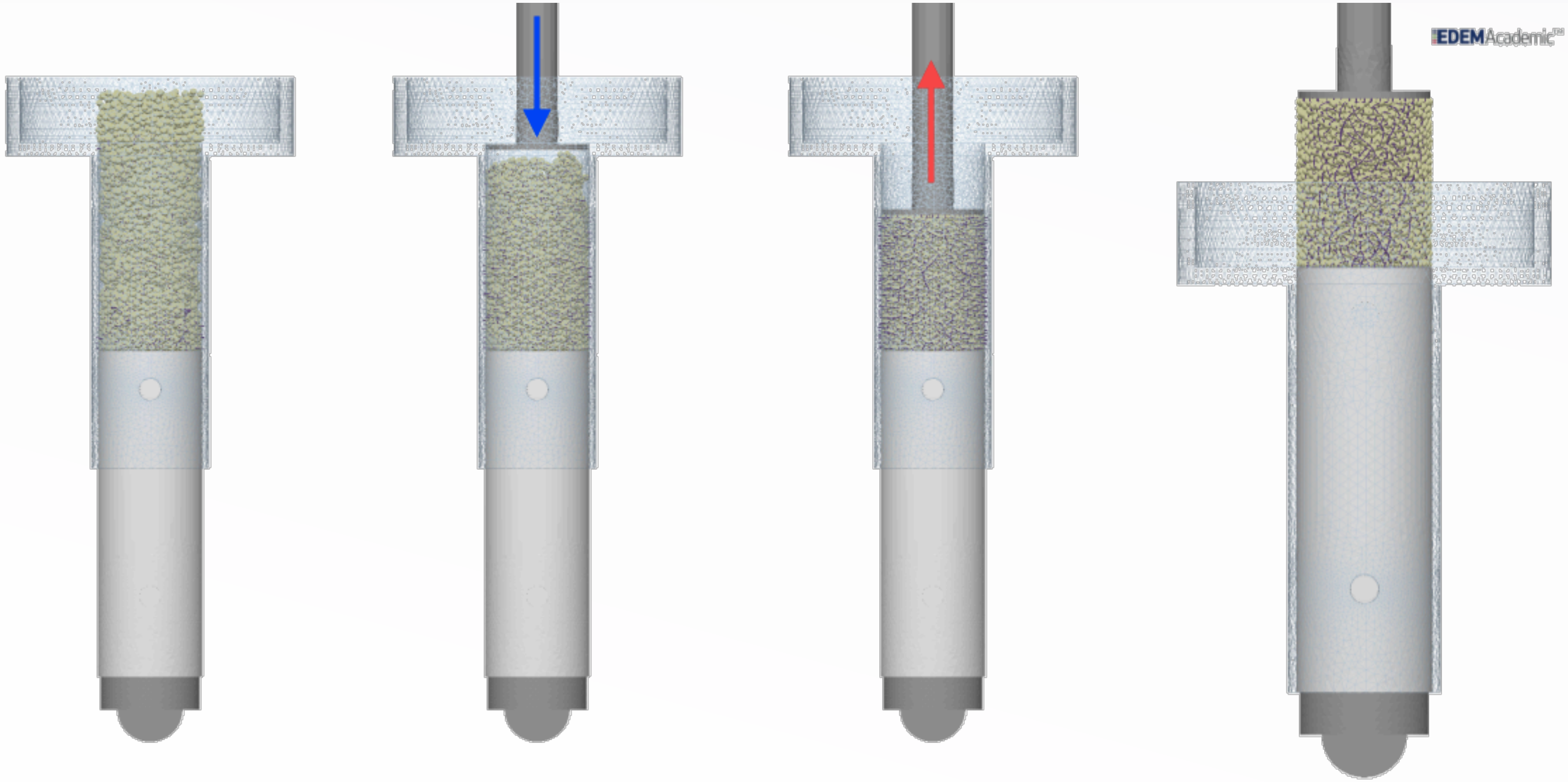


Modelling EPT uniaxial test

- Target is for the model to produce the key observed phenomena (problem dependent):
- Filled porosity/packing density
- Compressibility under confined compression
- Stress-strain response to failure under uniaxial loading
- Unconfined yield strength as a function of prior consolidation stress

Modelling EPT uniaxial test

- DEM Simulation Sequence:



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Sample failure mode

Model is capturing the development of conjugate shear bands (planar model comparison)

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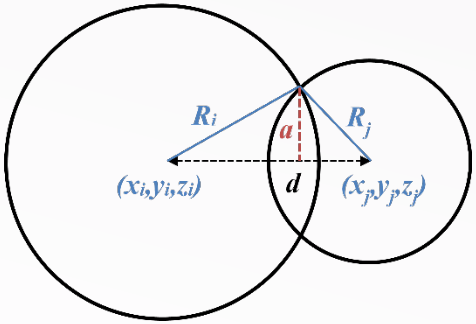
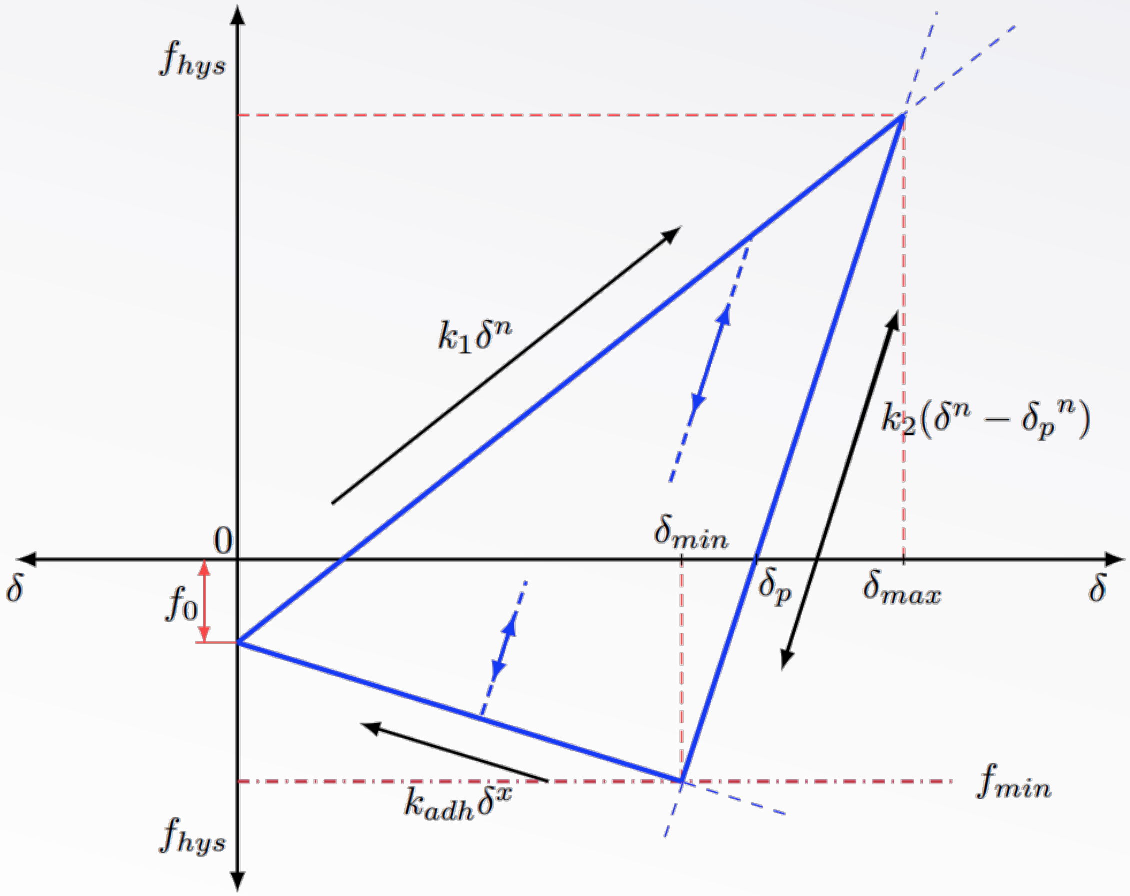
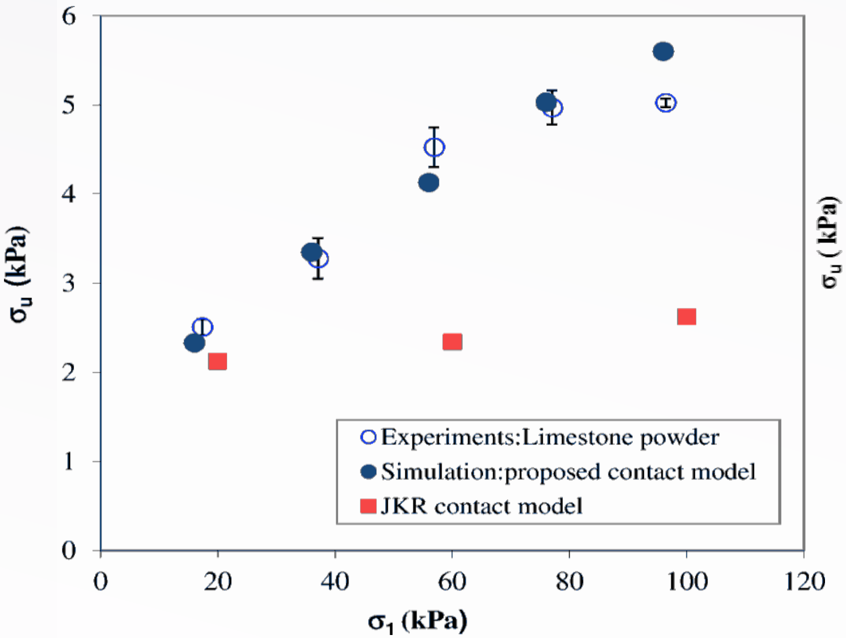
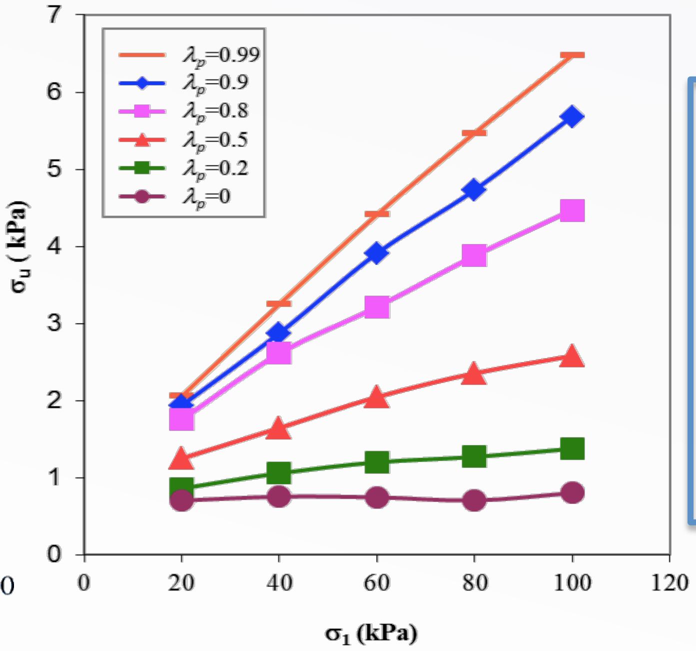
Adhesive-frictional contact model

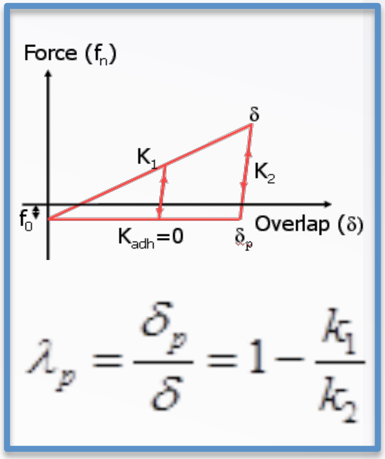




Stress history dependency: comparison with experiments



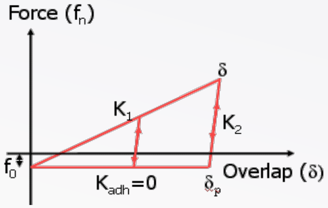




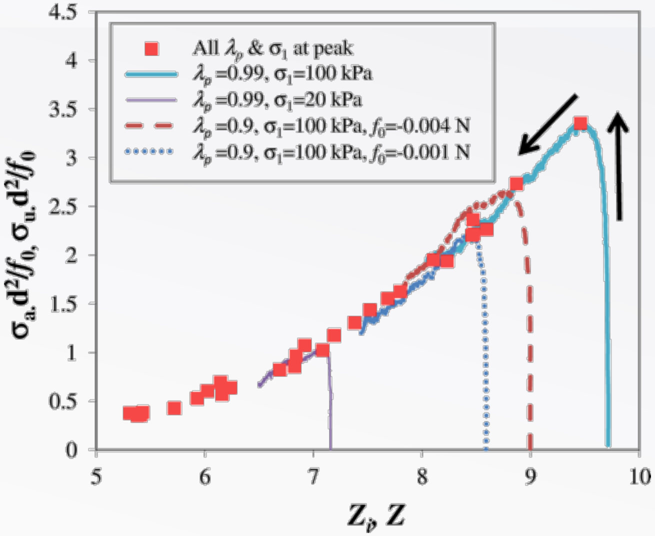
$$\lambda_p = \frac{\delta_p}{\delta} = 1 - \frac{k_1}{k_2}$$

- The model is capable of reproducing experimental flow function
- Cohesion arises from contact plasticity. For elastic contact, history dependence largely disappears
- What is the micromechanics behind bulk cohesive strength?

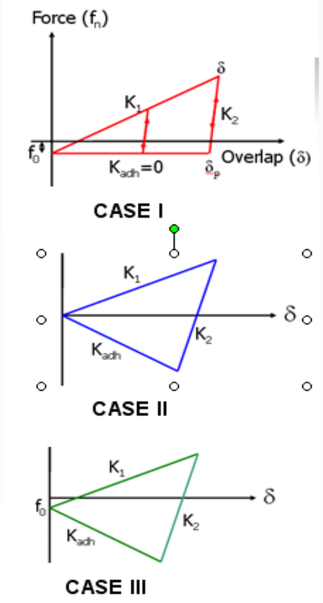
Microstructural investigation

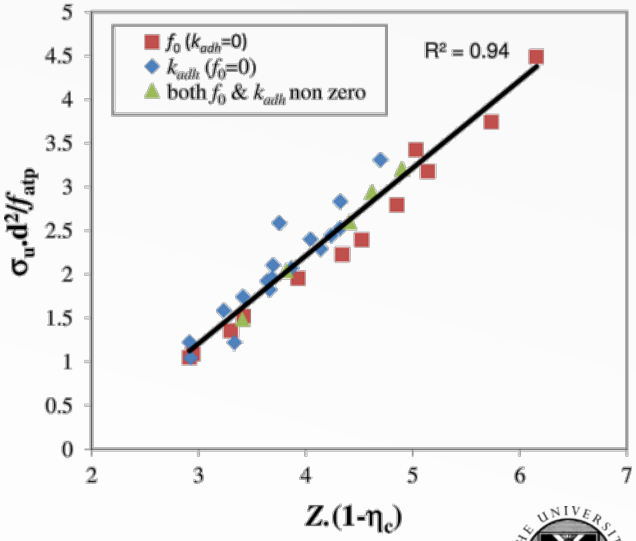


$\sigma_{u=}$ Unconfined strength
d=Particle diameter
f_0= Initial adhesive strength
Z=Co-ordination number
η_c=Consolidated porosity
$f_{atp=}$= average tensile strength at peak



- Plasticity leading to microstructural evolution of CN is the reason for stress history dependence





- Unconfined strength is a function of CN, porosity, particle size, and adhesive force.

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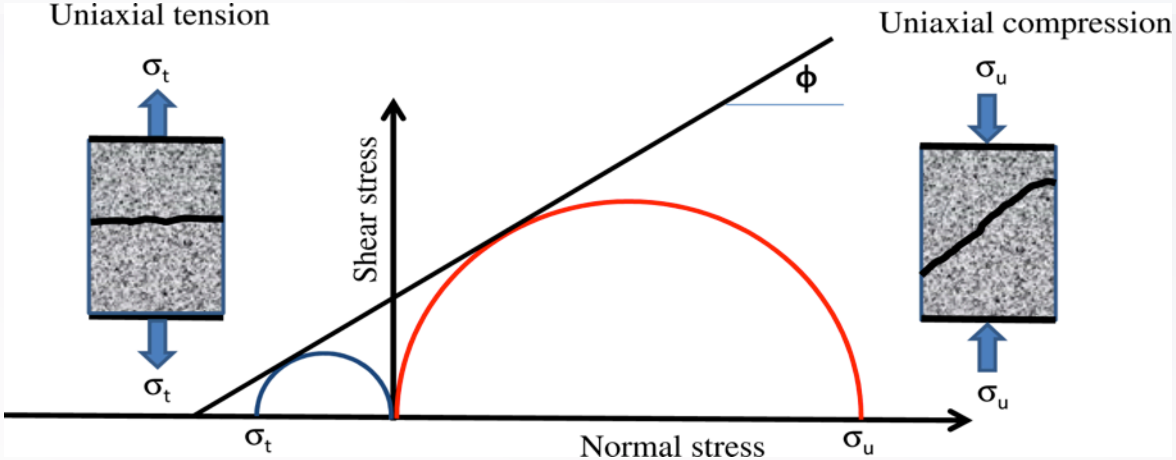
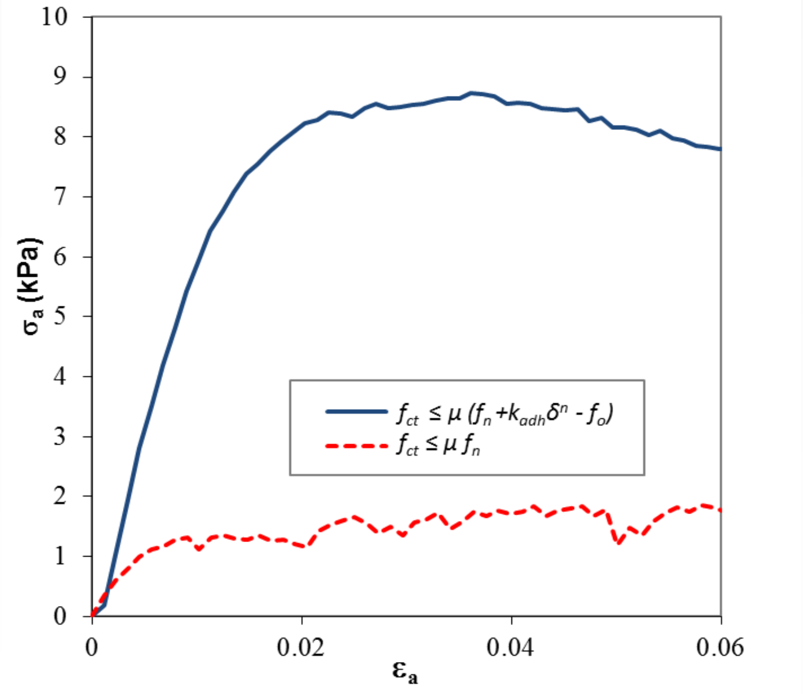
Physical interpretation



$$\sigma_u = \frac{1+\sin\phi}{1-\sin\phi}\sigma_t$$

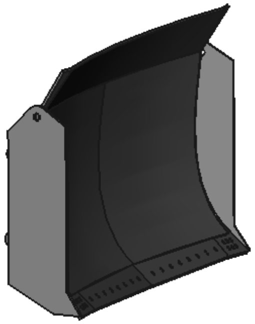
$$\frac{\sigma_u}{(f_{atp}/d^2)} \propto (1-\eta_c)z$$

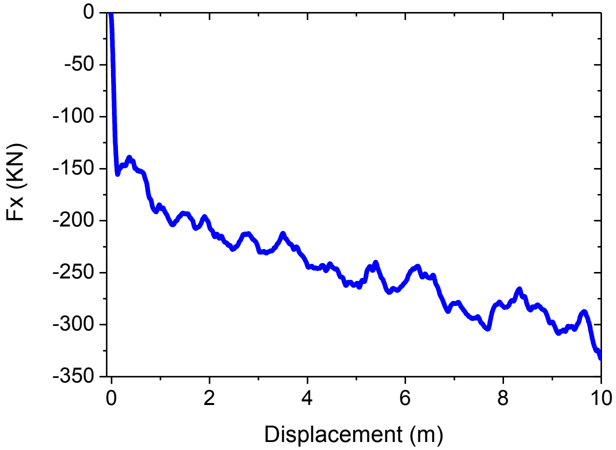


The contribution of adhesive force to limiting frictional resistance at the contacts is the major source of unconfined strength but not the adhesive (tensile) force itself

Analysis of large scale simulations

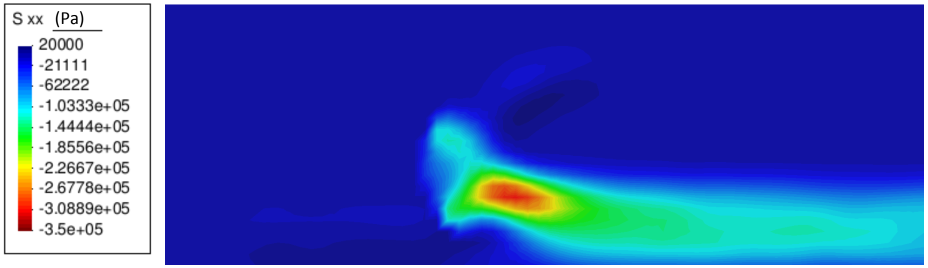
- **Reaction forces on the blade** are analysed during the process :
  - Related to **energy consumption**.



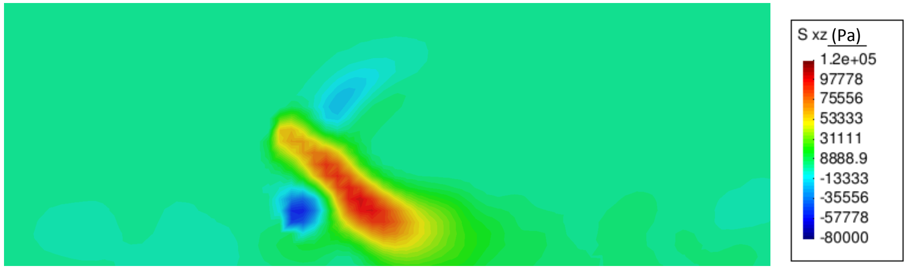


- **Coarse-graining** of DEM results using P4 is used to analyse **bulk properties:**

<u>Horizontal normal stress</u>



<u>Shear stress</u>

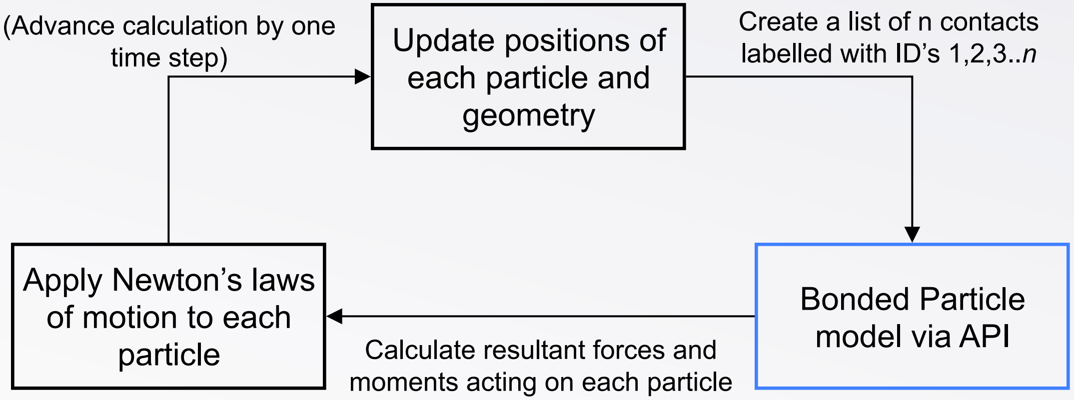


Modelling cementitious materials

Development of a new bonded particle model

Modelling cementitious materials such as rock or concrete

Materials idealised as a dense assembly of bonded discrete particles



Update positions of each particle and geometry

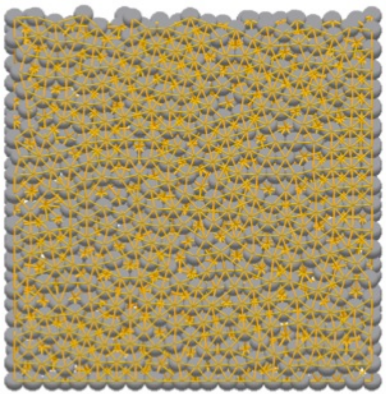
Create a list of n contacts labelled with ID's 1,2,3..*n*

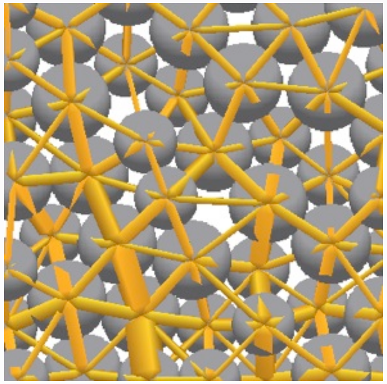
Bonded Particle model via API

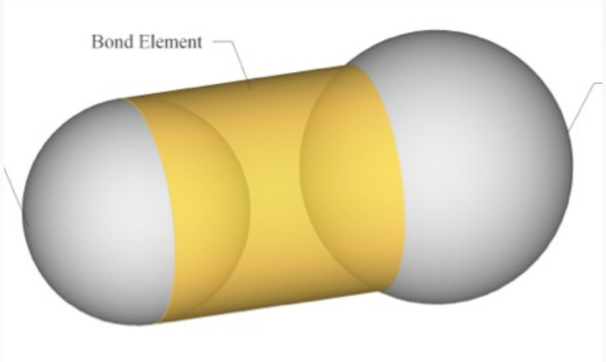
Calculate resultant forces and moments acting on each particle

Apply Newton's laws of motion to each particle

(Advance calculation by one time step)

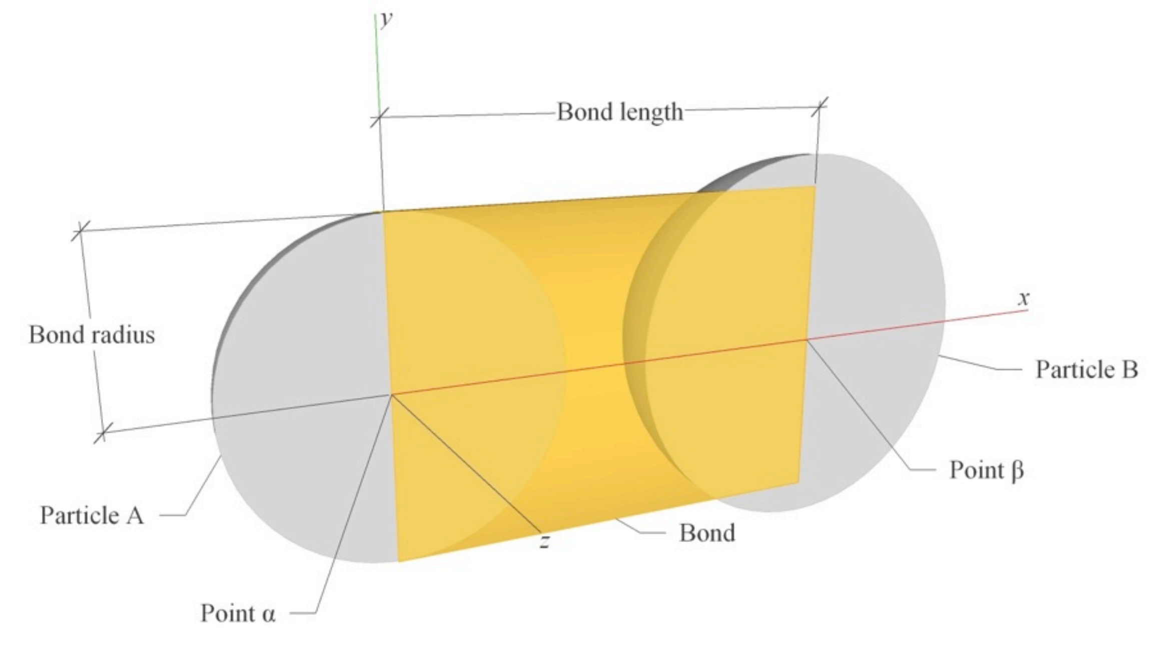






Formulation of bonded-contact model

- Based on the Timoshenko beam theory (suitable for short members)
- Each bond transmits forces and moments across itself
- Each bond behaves in a linear elastic manner
- When failure criteria are met the bond breaks and cannot be reintroduced
- Beams experience displacement loading from the particles they connect

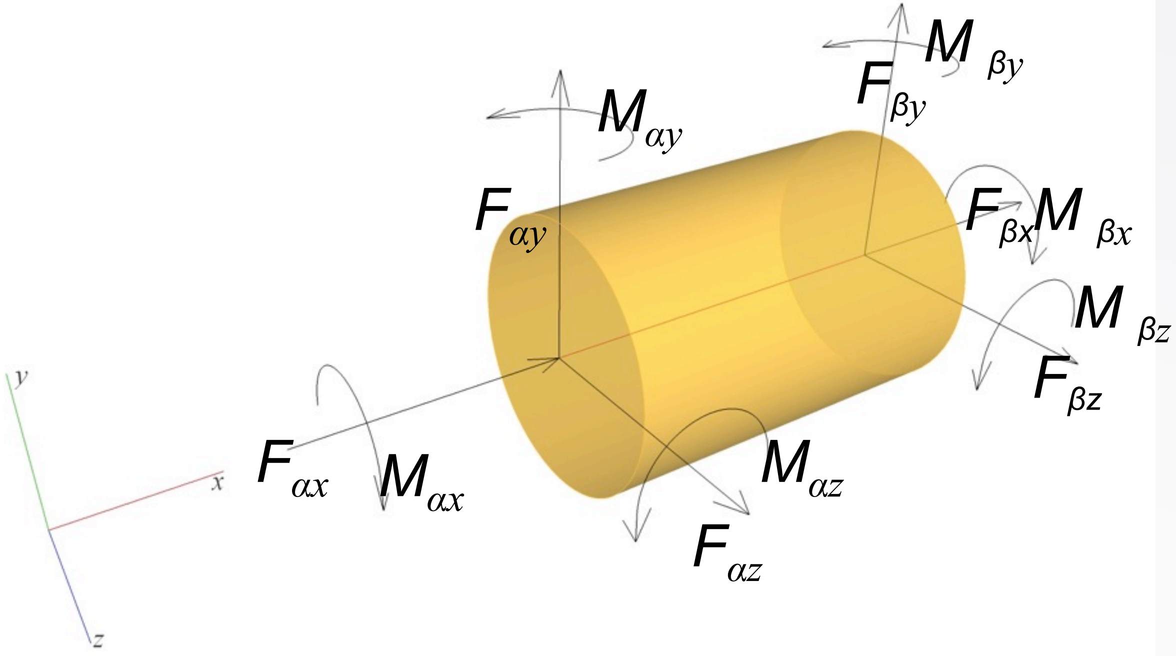


Brown et [illegible] erials and deformable structures" under review in Granular Matter

Bond forces and moments: Timoshenko Beam

The 6 forces and 6 moments acting on the bond $\{F_i\}$ are calculated from the local displacement of the ends using a stiffness matrix $[K]$.

$$\{F_i\} = \left\{ \begin{matrix} F_{\alpha xi} \\ F_{\alpha yi} \\ F_{\alpha zi} \\ M_{\alpha xi} \\ M_{\alpha yi} \\ M_{\alpha zi} \\ F_{\beta xi} \\ F_{\beta yi} \\ F_{\beta zi} \\ M_{\beta xi} \\ M_{\beta yi} \\ M_{\beta zi} \end{matrix} \right\} = [K] \cdot \left\{ \begin{matrix} d_{\alpha x} \\ d_{\alpha y} \\ d_{\alpha z} \\ \theta_{\alpha x} \\ \theta_{\alpha y} \\ \theta_{\alpha z} \\ d_{\beta x} \\ d_{\beta y} \\ d_{\beta z} \\ \theta_{\beta x} \\ \theta_{\beta y} \\ \theta_{\beta z} \end{matrix} \right\}$$



Bond failure criteria

The bond fails (and is removed from the simulation) if one of the three failure criteria are met. Spring contact takes over (e.g. Hertz-Mindlin model)

The compressive stress exceeds the compressive strength

$$\sigma c_{i\max} = \frac{F_{ix}}{A} - \frac{M_i r}{I}$$

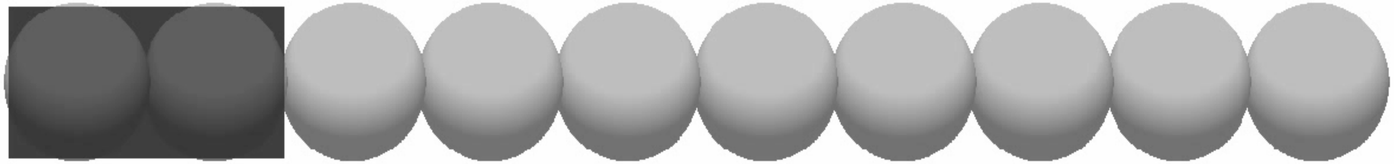
The tensile stress exceeds the tensile strength

$$\sigma t_{i\max} = \frac{F_{ix}}{A} + \frac{M_i r}{I} \qquad i = \alpha, \beta$$

The shear stress exceeds the shear strength

$$\tau_{i\max} = \frac{4S_i}{3A} + \frac{M_{ix} r}{2I}$$

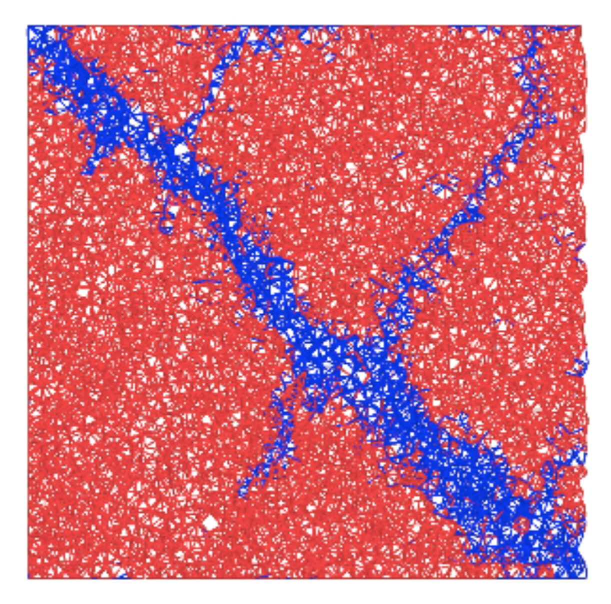
Verification – Cantilever beam

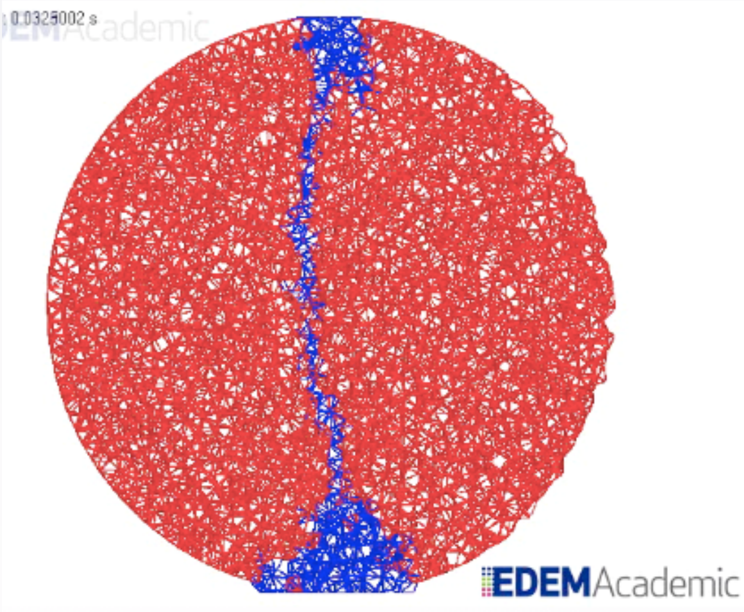


Verified against theoretical solutions for both static loading and dynamic loading

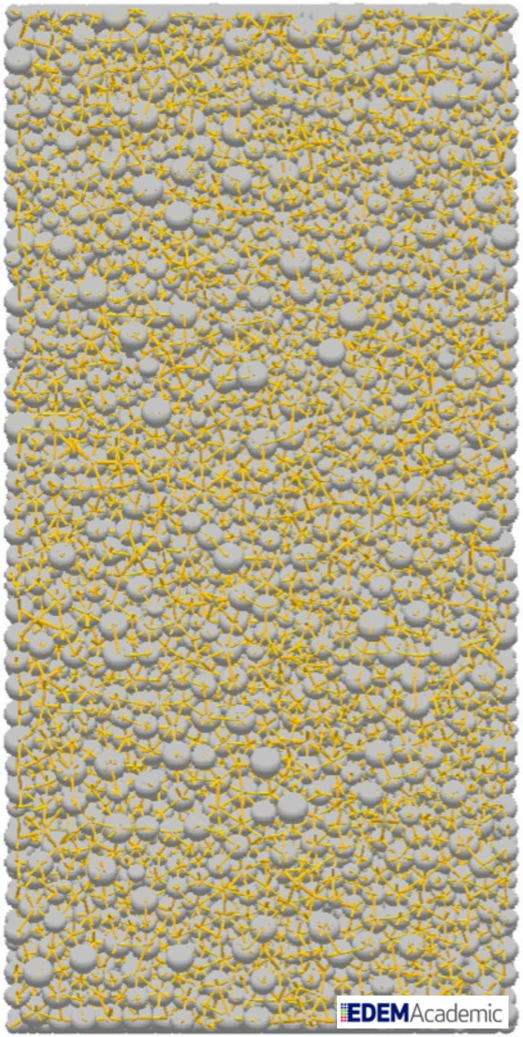
- Brown et al “A bond model for DEM simulation of cementitious materials and deformable structures” under review in Granular Matter
- N. Brown, PhD Thesis (2013)

Modelling cementitious material





Modelling concrete

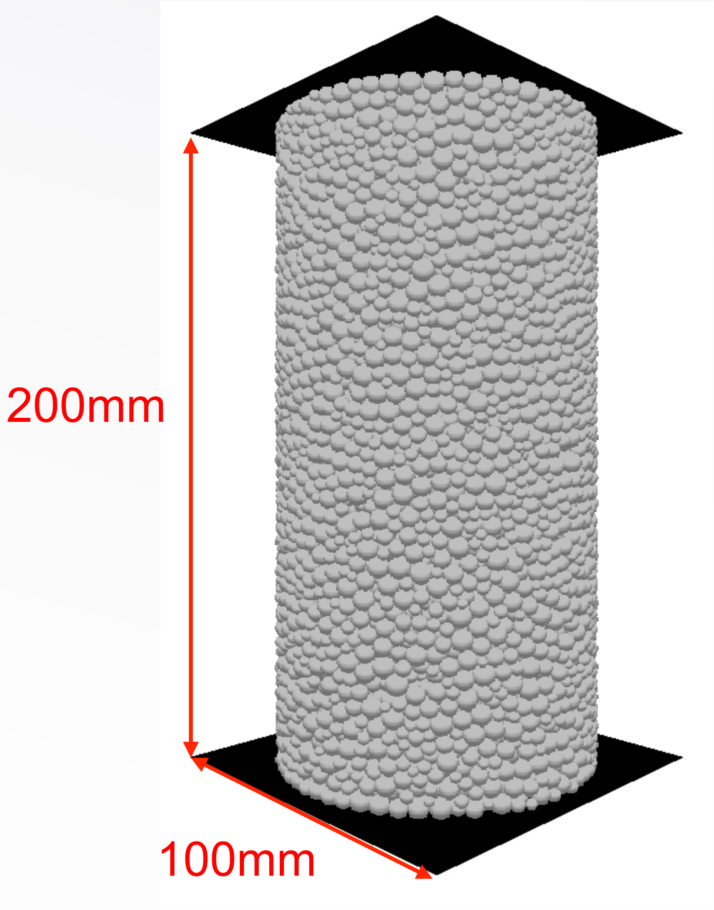


(Orthographic slice through the centre of a cylinder)

- Create a dense assembly of particles (grey)
- Form bonds (yellow) between eligible particles capable of resisting compression, shear, tension and bending forces, dealt with using a bonded-contact model
- Apply a load via displacement of boundaries

Uni-axial compression of concrete

DEM Set-up



Specimen characteristics	
Total number of particles	20,561
Average particle radius (mm)	2.14
Minimum particle radius (mm)	1.28
Maximum particle radius (mm)	3.02
Porosity	0.37
Average number of bonds per particle	9.58
Bonded contact parameters	
Bond Young's modulus (GPa)	35
Bonds Poisson's ratio	0.2
Bonds tensile strength (MPa)	50
Bonds shear strength (MPa)	100
Strength coefficient of variation	0.9
Non-bonded contact parameters	
Particle shear modulus (GPa)	16
Particle Poisson's ratio	0.25
Coefficient of restitution	0.5
Coefficient of static friction	1

Modelling concrete

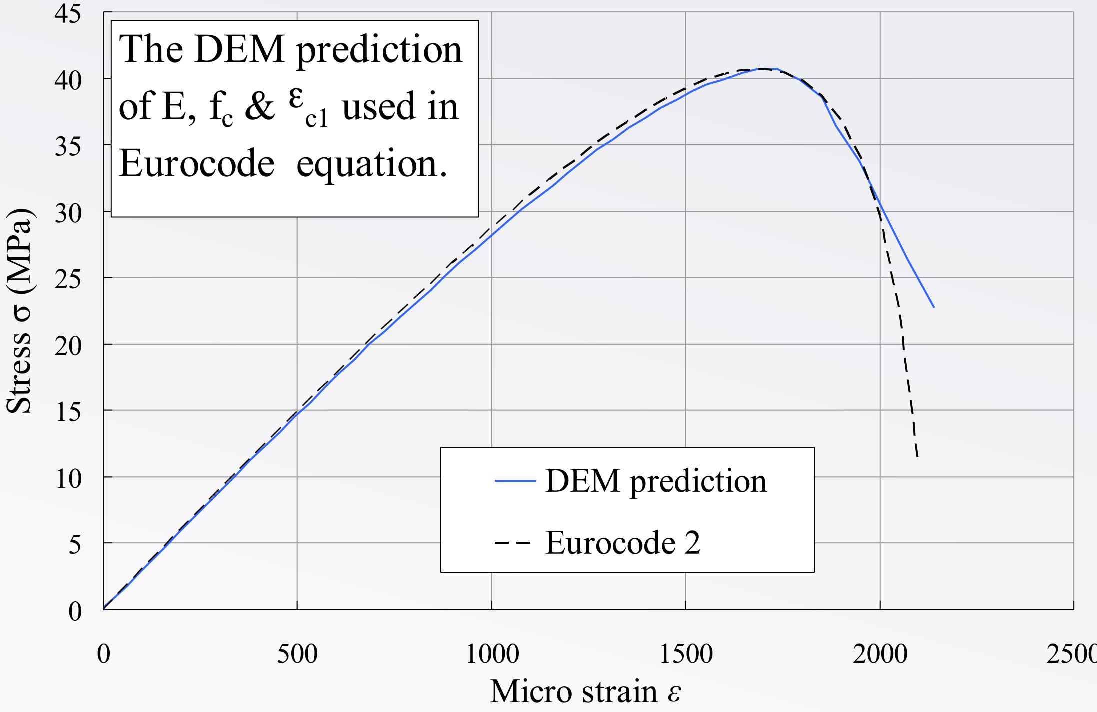
The bond parameters for a uniaxial compression test

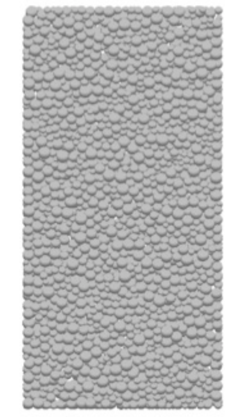
E_b = 35GPa

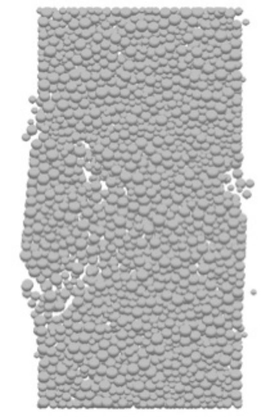
V_b = 0.2

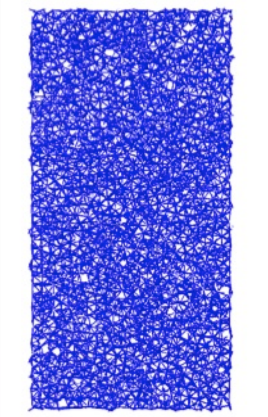
F_t = 50MPa

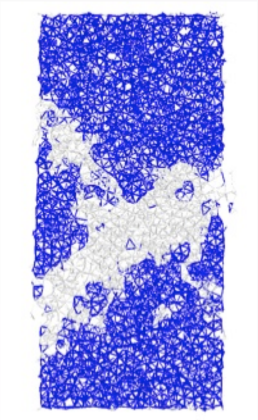
F_s =100MPa


The DEM prediction of E, f_c & ε_{c1} used in Eurocode equation.

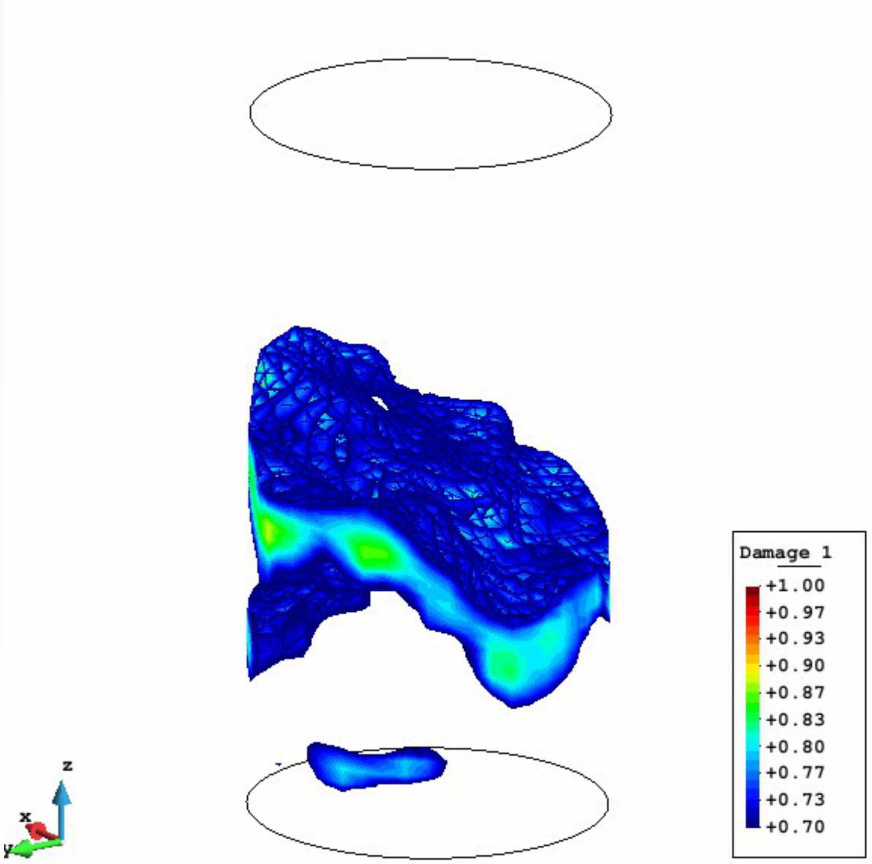

(a) Initial particle positions


(b) Post peak particle positions

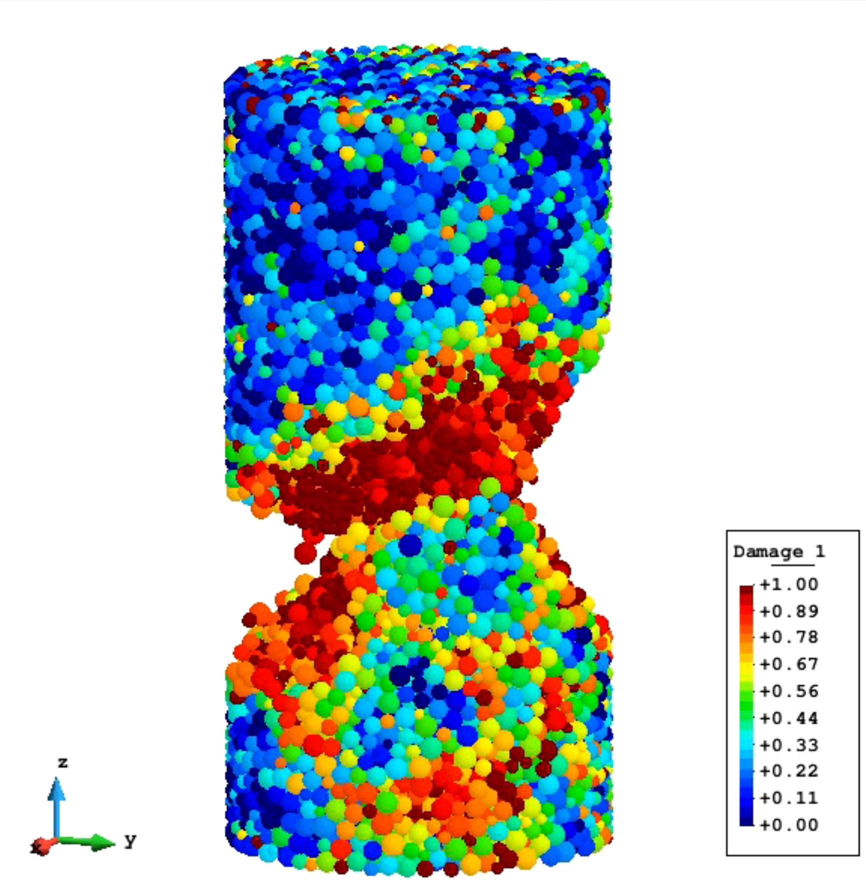

(c) Initial bond network


(d) *Post-peak bond network (blue=intact, grey=broken)*

Modelling concrete – Uniaxial Compression



Primary crack after peak load



Eventual particle arrangement

Acknowledgements

- Co-workers: J.P. Morrissey, S.C. Thakur, N. Brown, A. Janda, J.-F. Chen, Carlos Labra
- Funding and collaboration:
  - EC FP7 Marie Curie ITN (PARDEM, T-MAPPP), EPSRC, Univ. Edinburgh
  - P&G, LKAB, DEM Solutions, John Deere