

# Advancing geomechanics using DEM

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# Information

This is an edited pdf of the presentation I delivered at IS Cambridge  
(<http://is-cambridge.eng.cam.ac.uk/>) in Sept 2014

More detailed information is given in the keynote paper itself:

O'Sullivan, C. (2014) "Advancing Geomechanics using DEM"  
*Geomechanics from Micro to Macro Proceedings of IS-Cambridge, Vol. 1, 2014, Soga, K., Kumar, K., Biscontin, G., Kuo, M. (Eds.), CRC Press*

*Key references are given at the end of this pdf.*

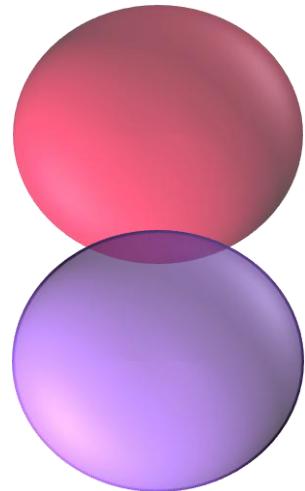
*For more information email me: [cath.osullivan@imperial.ac.uk](mailto:cath.osullivan@imperial.ac.uk)*

# Presentation Overview

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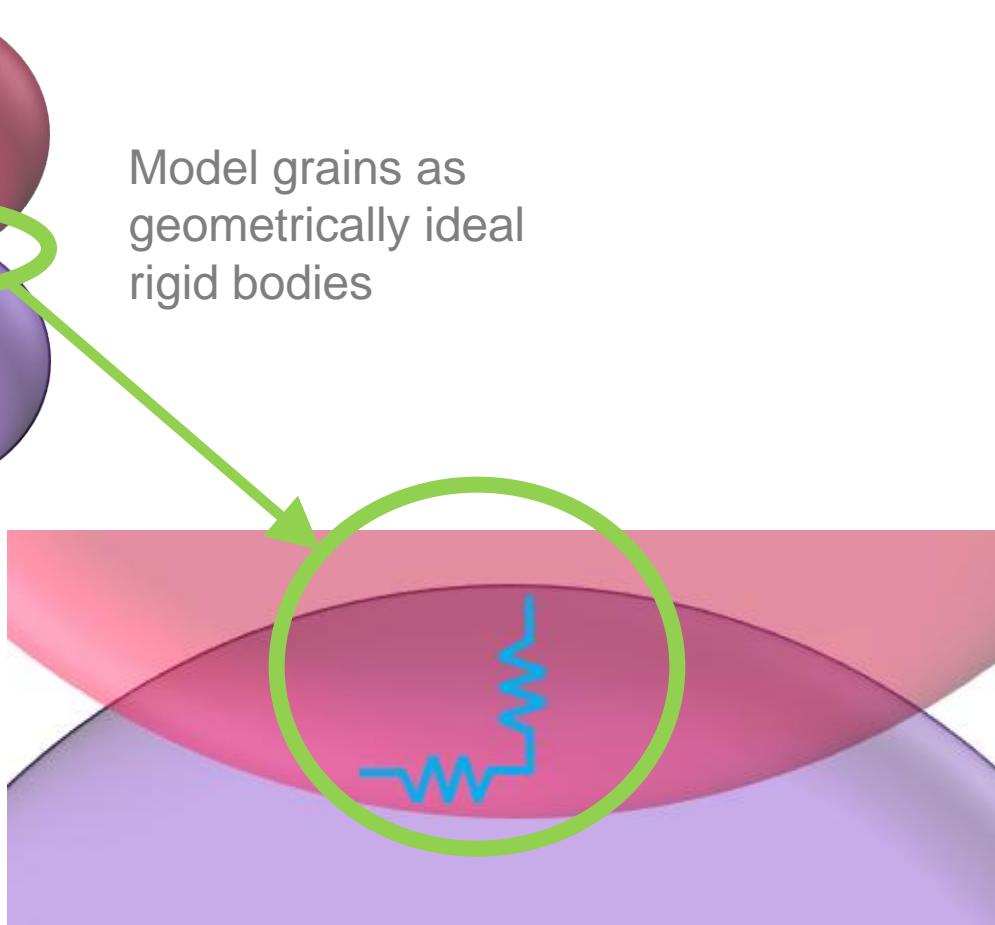
- Introduction to the Discrete Element Method (DEM)
- Use of DEM in Geomechanics
- Exploiting HPC
- Using the Critical State Line to assess quality of DEM simulation data
- Application: Studying soil response under a 3D stress state
- Application: Informing interpretation of laboratory test data
- Application: Internal erosion
- Application: Tunnelling-induced ground deformation

## Particulate DEM



Model grains as  
geometrically ideal  
rigid bodies

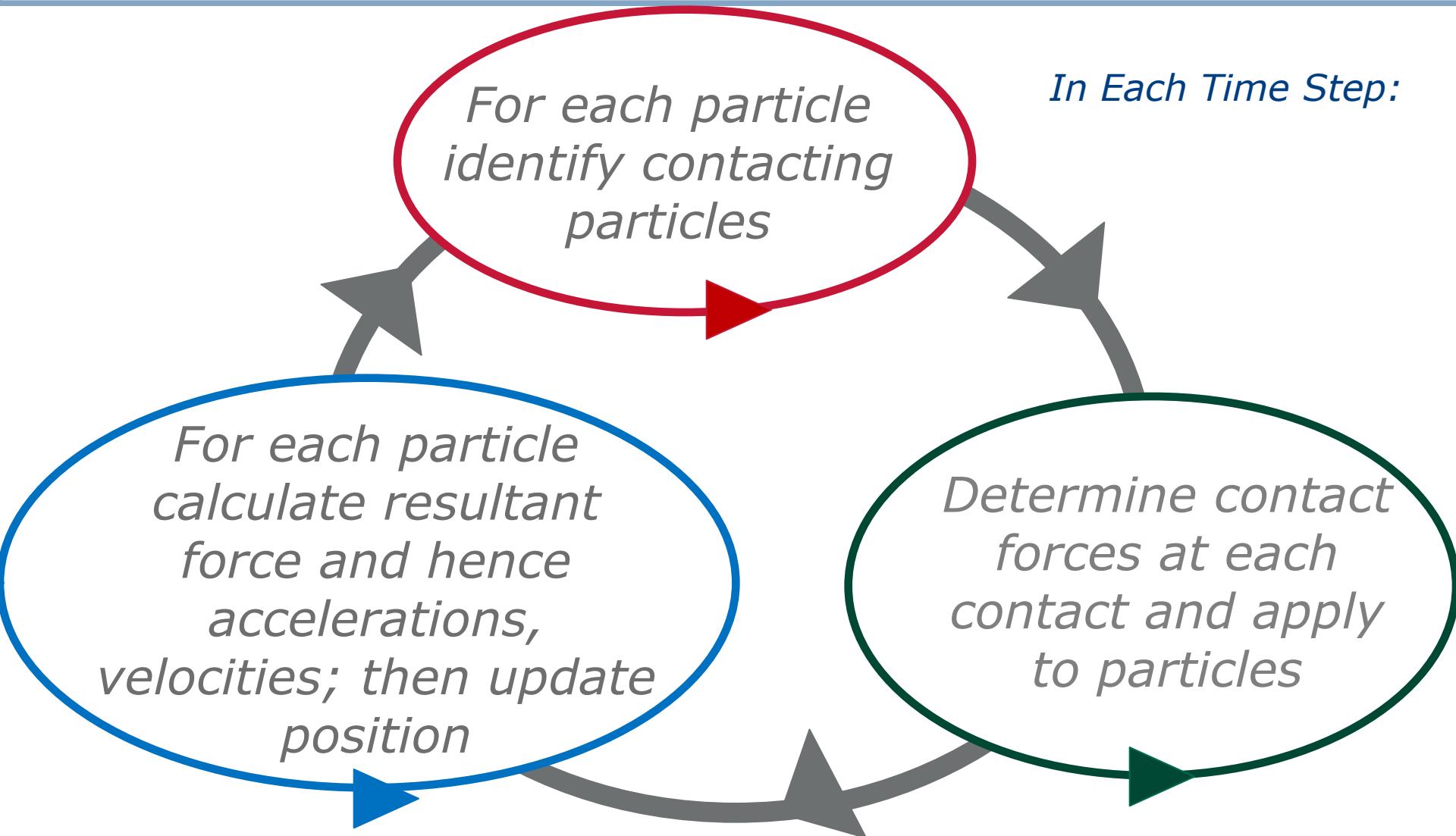
## Particulate DEM



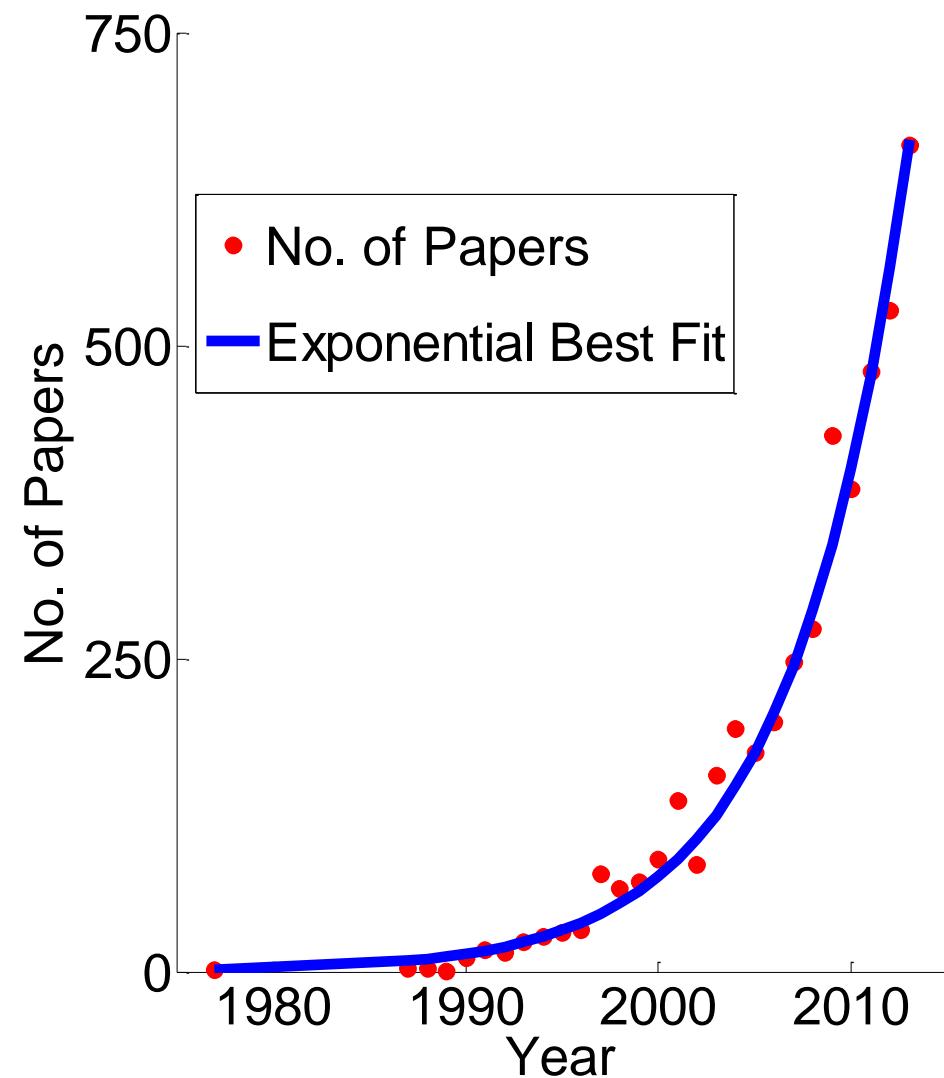
Model grains as  
geometrically ideal  
rigid bodies

Use orthogonal  
normal and  
tangential springs  
to determine  
contact forces

## Particulate DEM



## Use of DEM – All Scientific Disciplines



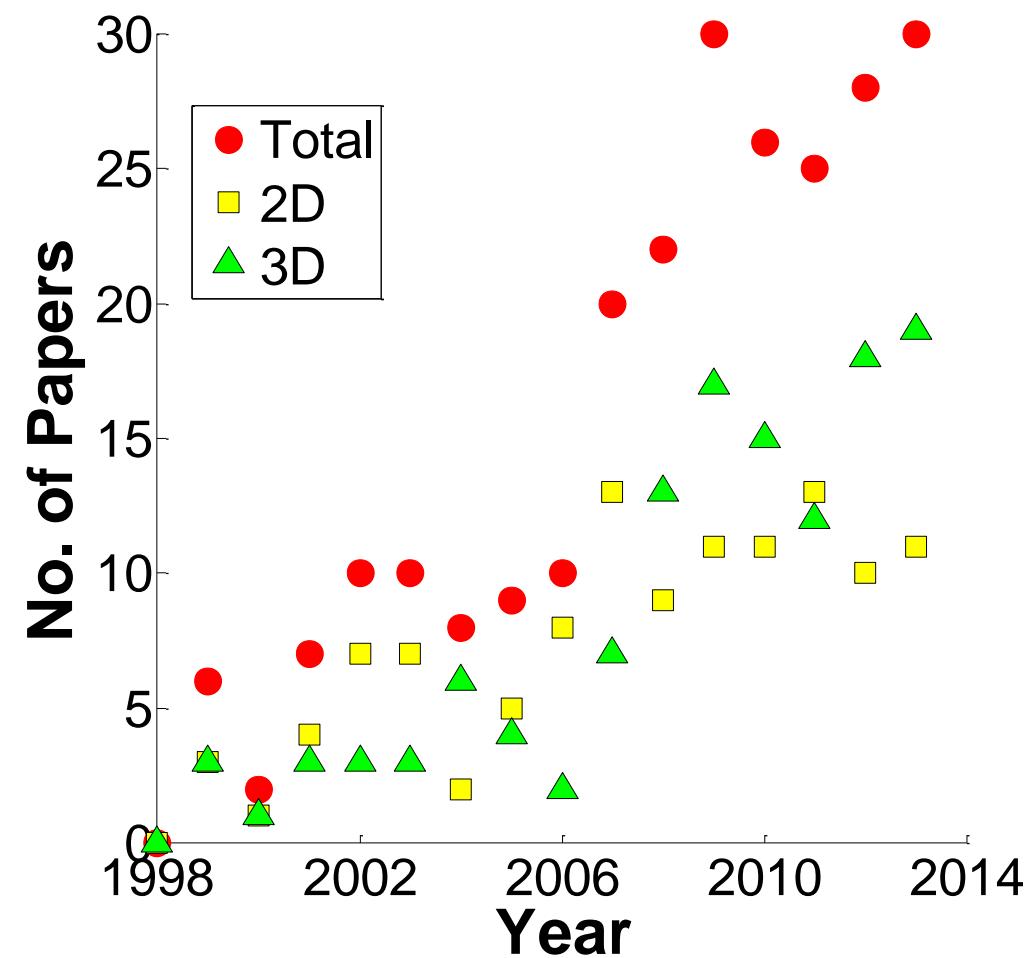
*Following approach of  
Zhu et al. (2007)*

*Web of Science (April 2014)*

*Keywords:*

- *Discrete element method/model*
- *Distinct element method/model*
- *Discrete particle simulation/method/model*
- *Granular dynamic simulation*

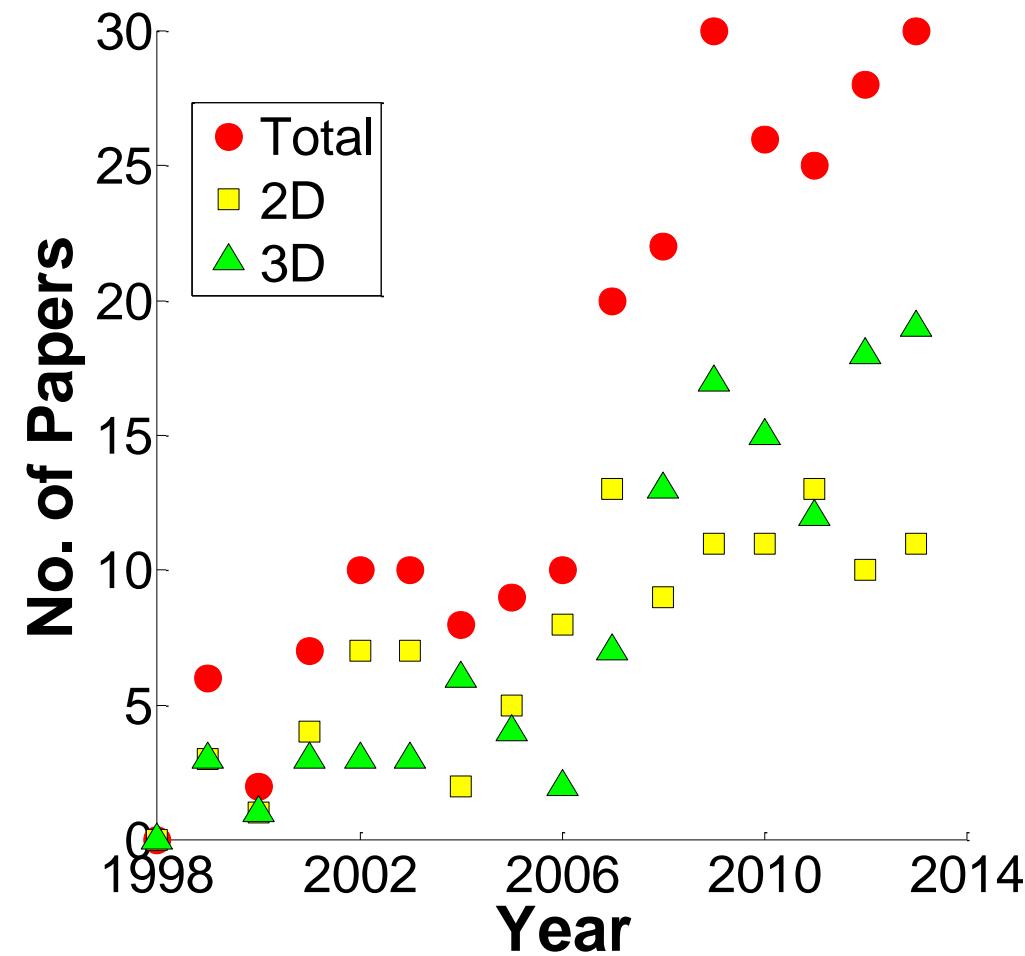
## Use of DEM – Geomechanics



### *Journals Considered:*

- Canadian Geotechnical Journal
- Computers and Geotechnics
- Geomechanics and Geoengineering
- Géotechnique
- Int. J. Num. and Analt. Methods in Geomechanics
- Int. J. of Geomechanics (ASCE)
- Int. J. of Rock Mechanics and Mining Sciences
- J. Geotech and Geoenvrn Engineering(ASCE)
- Soils and Foundations

## Use of DEM – Geomechanics



*Approx. 60% element test simulations*

*Approx. 20% code/algorithm development*

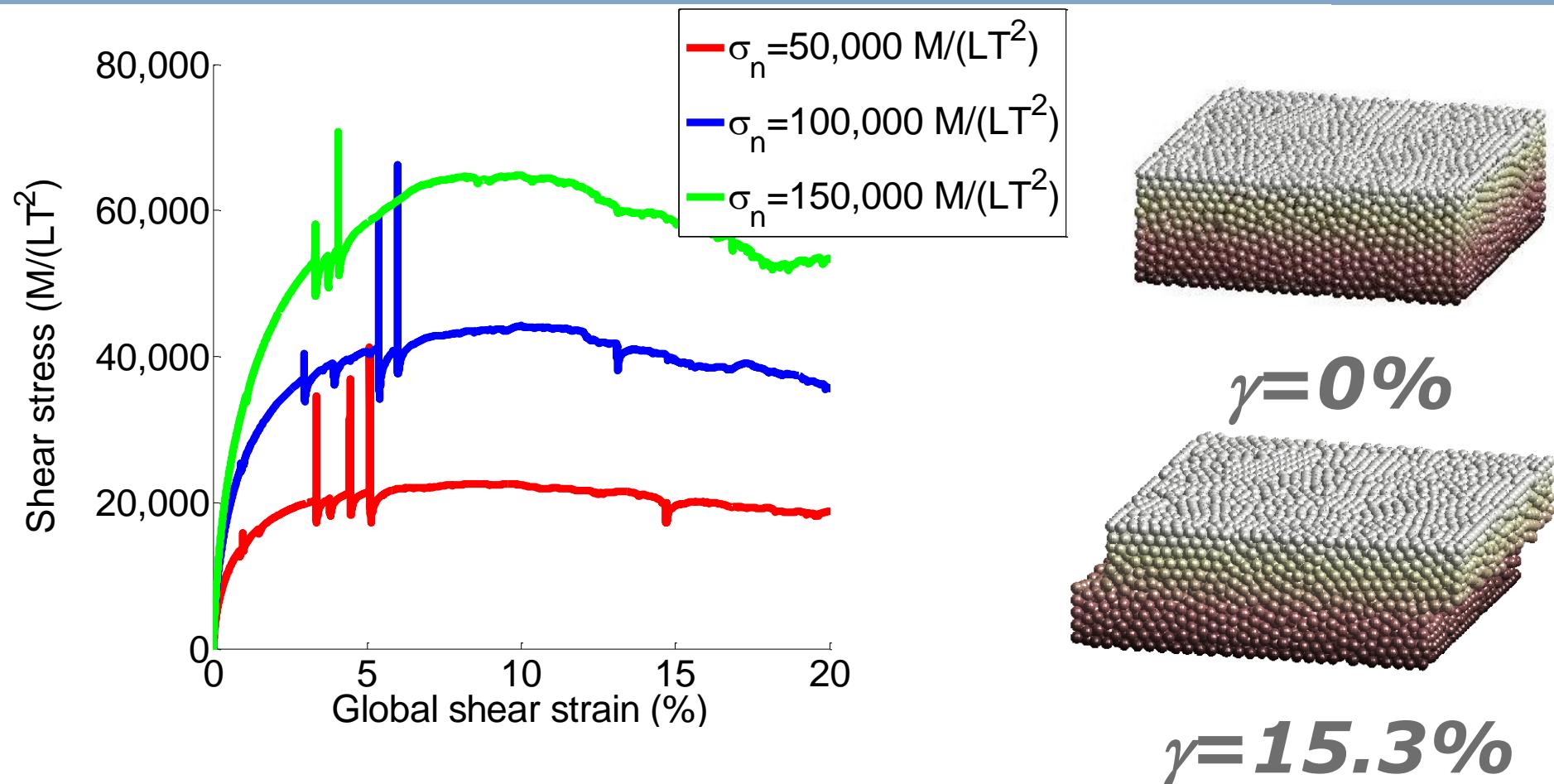
*Approx. 20% field scale / boundary value problems*

## Use of DEM – Geomechanics

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DEM can capture many mechanical response characteristics that are unique to granular materials

## DEM can capture stress-dependant/frictional strength

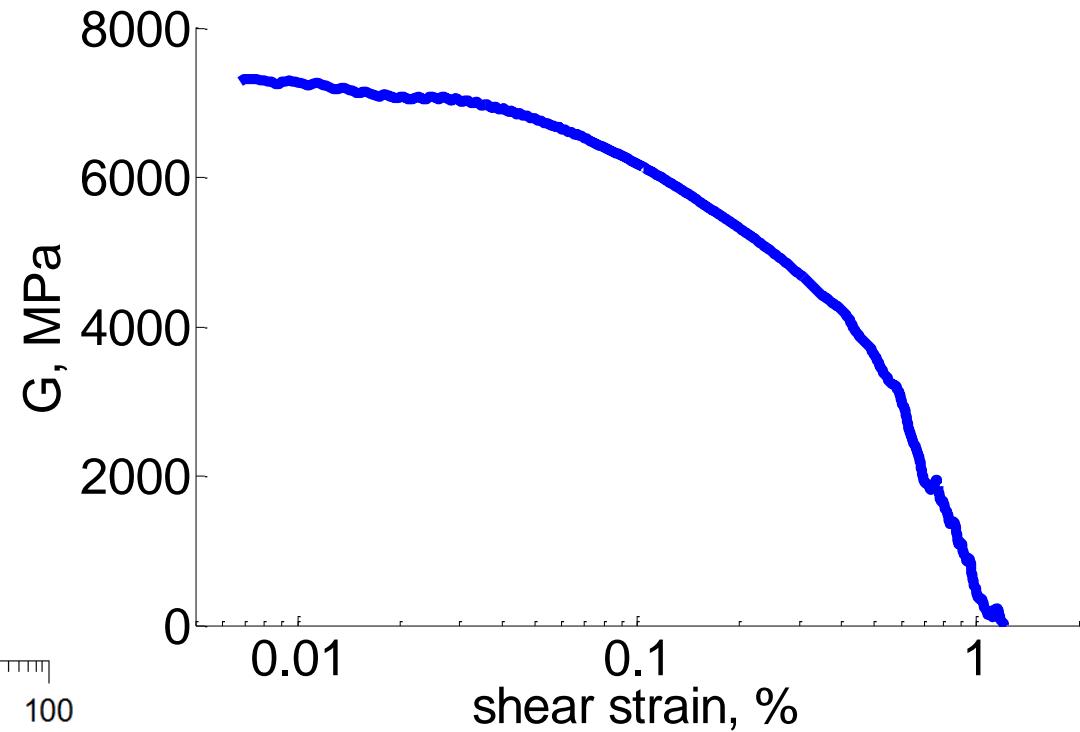
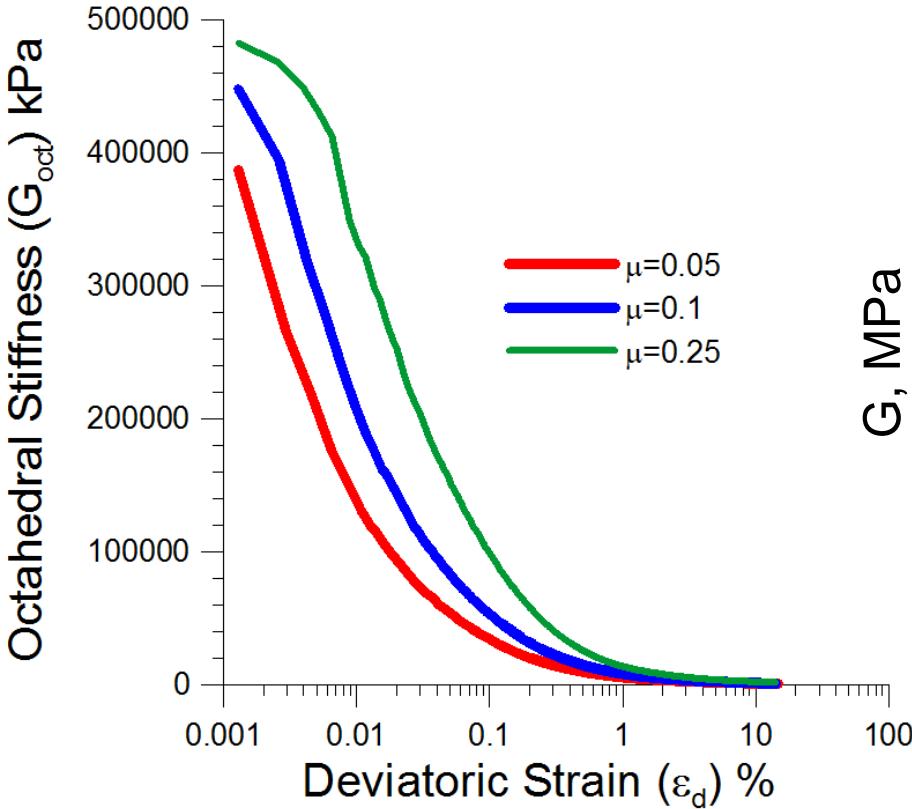


*Direct shear test simulations*

*Modified version of Trubal*

*Dr. L. Cui (Cui and O'Sullivan, 2006)*

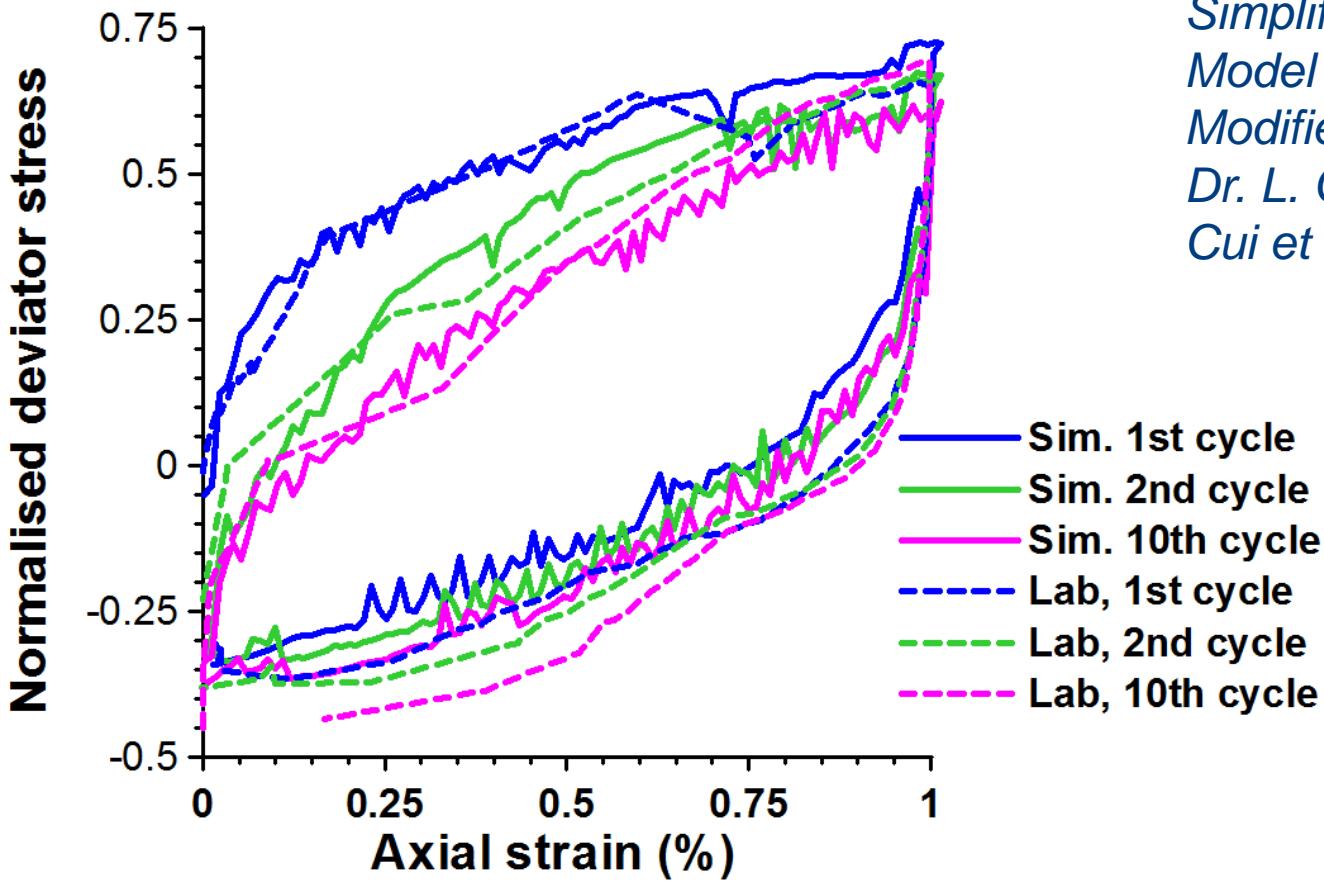
## DEM can capture the non-linear nature of soil stiffness



*Triaxial test simulations*  
*Simplified Hertz-Mindlin Contact Model*  
*Modified Trubal, periodic cell, spheres*  
*Dr. D. Barreto (Barreto and O'Sullivan, 2012)*

*Triaxial test simulation*  
*Parallel Bond Contact Model*  
*PFC 3D spheres*  
*Dr. G. Cheung (Cheung et al., 2013)*

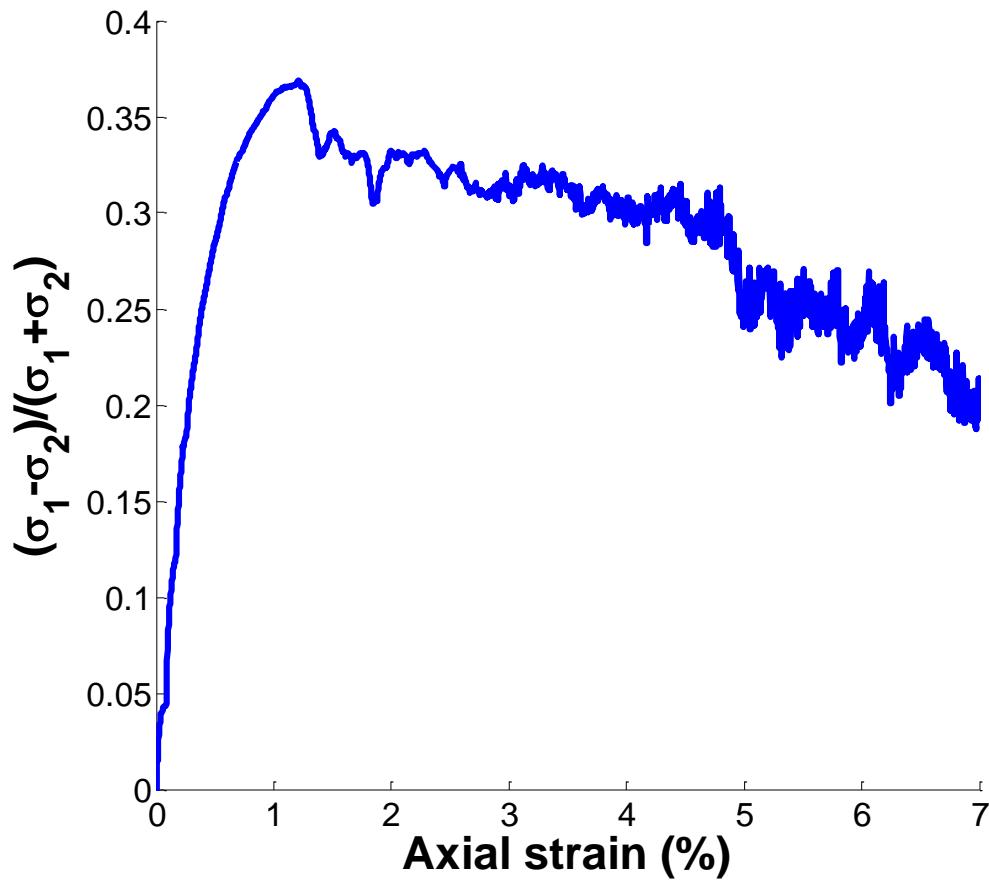
## DEM can capture hysteresis in cyclic loading



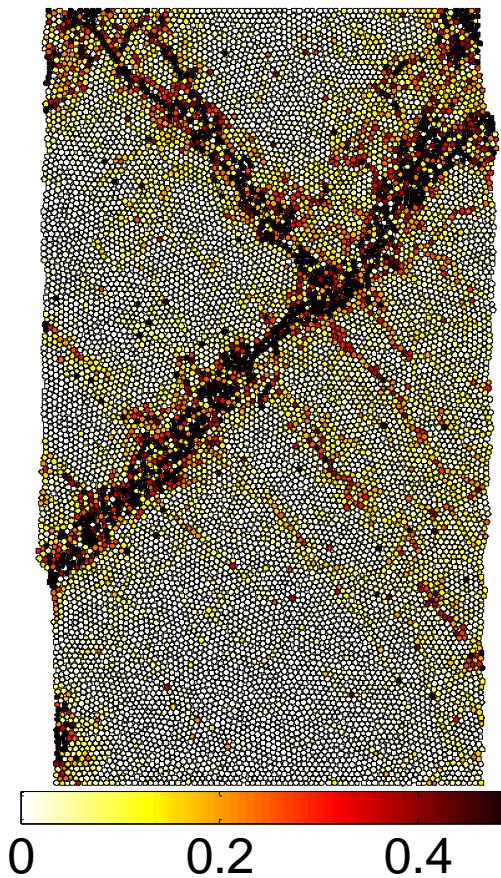
*Strain controlled triaxial tests  
Simplified Hertz-Mindlin Contact  
Model  
Modified Trubal, spheres  
Dr. L. Cui  
Cui et al. (2007)*

## DEM can capture strain softening and localization

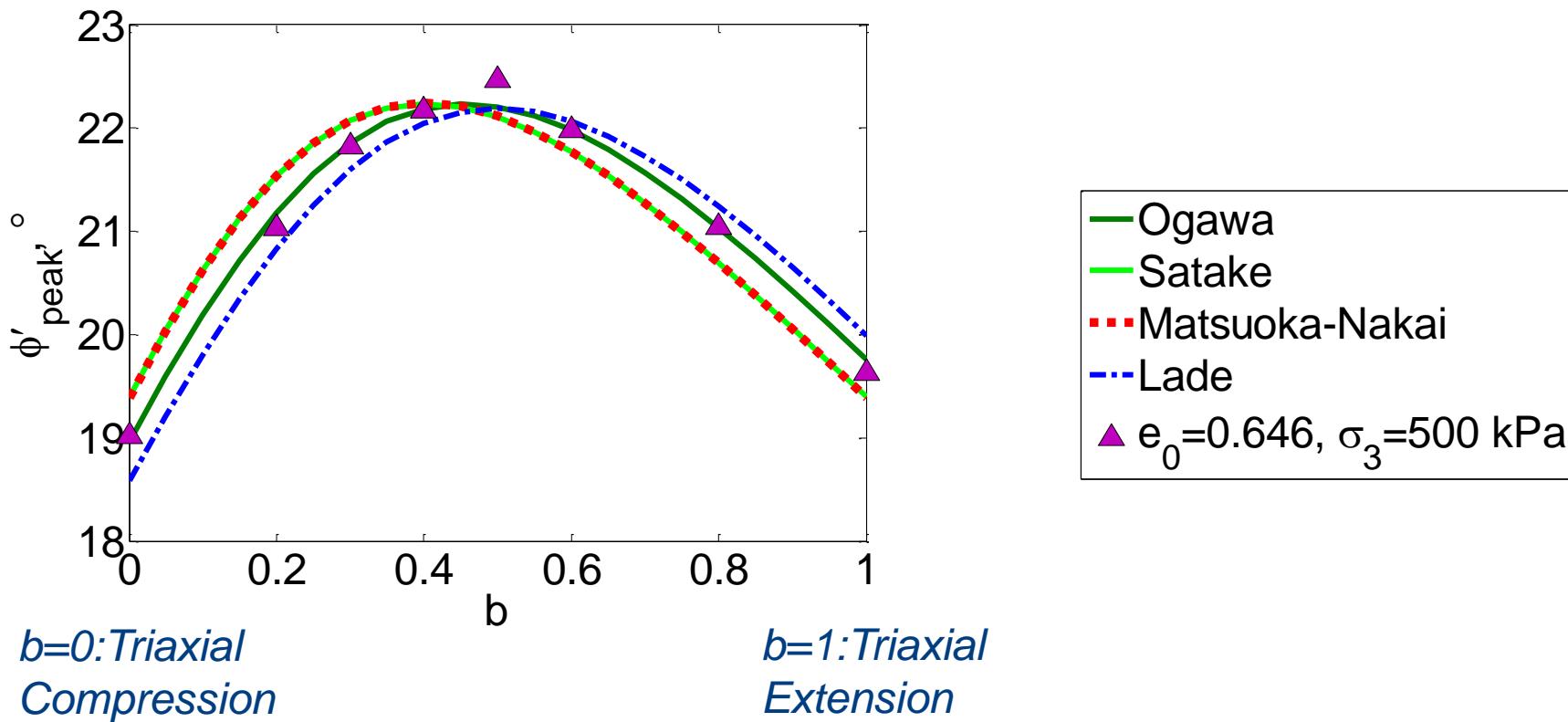
Biaxial compression - 12,512 disks  
PFC 2D: Flexible membrane boundary  
O'Sullivan et al. (2003)



Disk rotation (rad)  
Axial strain=3.7%



## DEM can capture 3D stress-space failure criterion



$$b = \frac{\sigma_2 - \sigma_3}{\sigma_1 - \sigma_3}$$

Intermediate  
principal stress  
ratio

Granular LAMMPS  
Mr. X. Huang  
Huang et al. (2014a)

## Use of DEM – Geomechanics

*DEM can capture many mechanical response characteristics that are unique to granular materials. DEM enables creation of useful abstractions of real soil.*

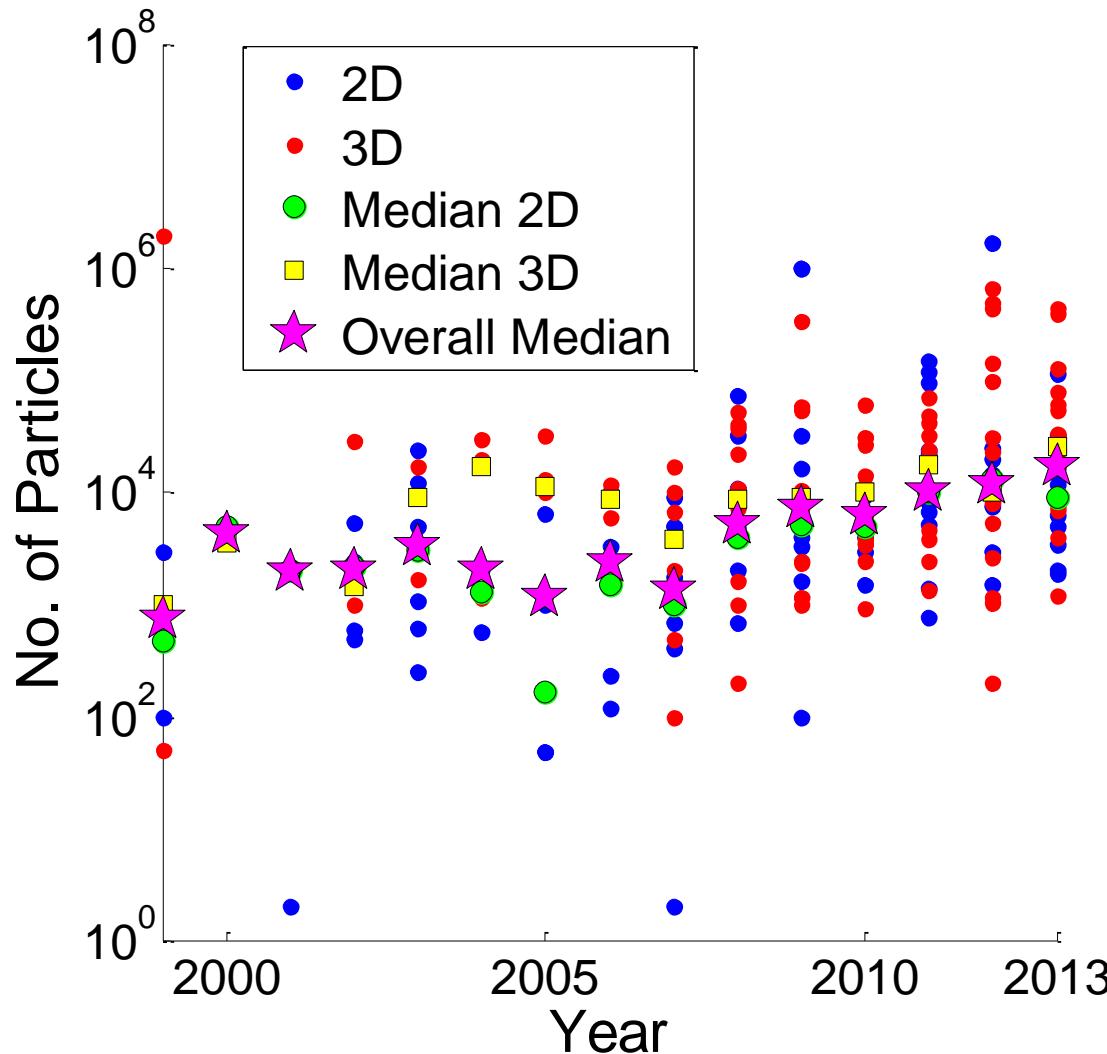
Ideal tool for:

- Extending existing constitutive models (fill gaps in testing),
- Fundamental micro-macro studies
- Parametric studies
- Examining particle-level phenomena (e.g. crushing)

But:

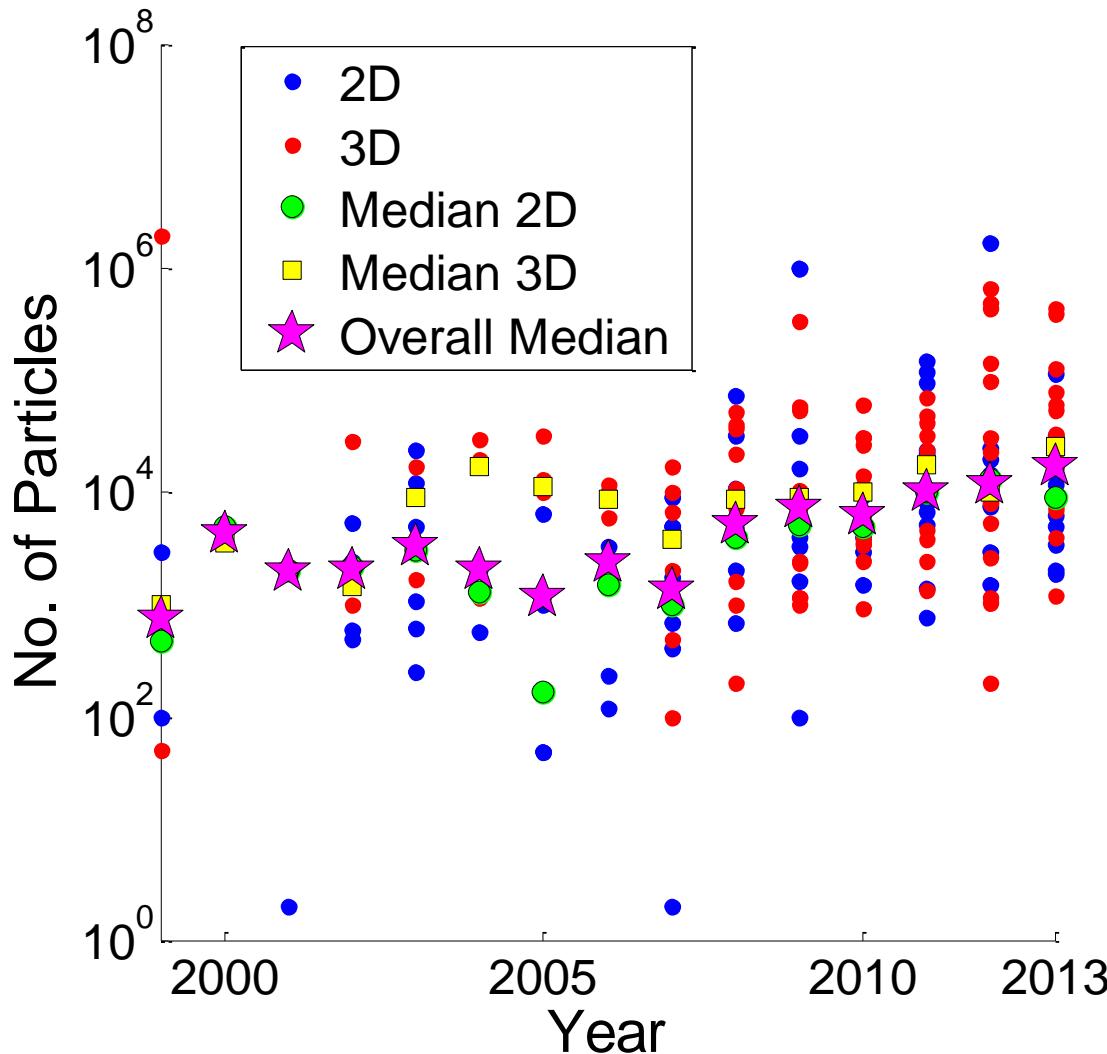
Computational cost limits to small numbers of particles, ideal geometries, relatively simple contact models.

## No. of particles in geomechanics DEM simulations



- If  $e=0.563$ , there are over 150,000 no. 200  $\mu\text{m}$  spheres in a  $10\text{mm} \times 10\text{mm} \times 10\text{mm}$  cube

## No. of particles in geomechanics DEM simulations

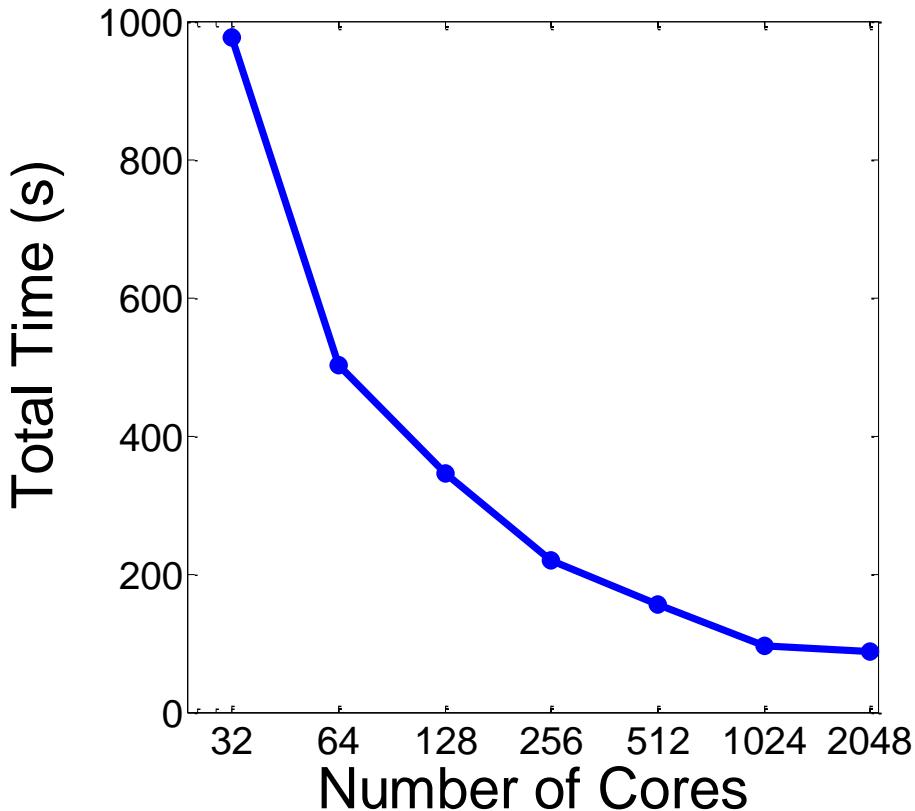


- *Serial codes dominate: 67% of publications in 2010-2013 used PFC2D/3D, a number of groups are using derivatives of Trubal*
- *Processor speeds no longer double every two years*
- *Multicore computers now widely available*
- *University clusters*
- *Shared use facilities exist and are expanding, e.g. UK £43 million investment into ARCHER in 2011*

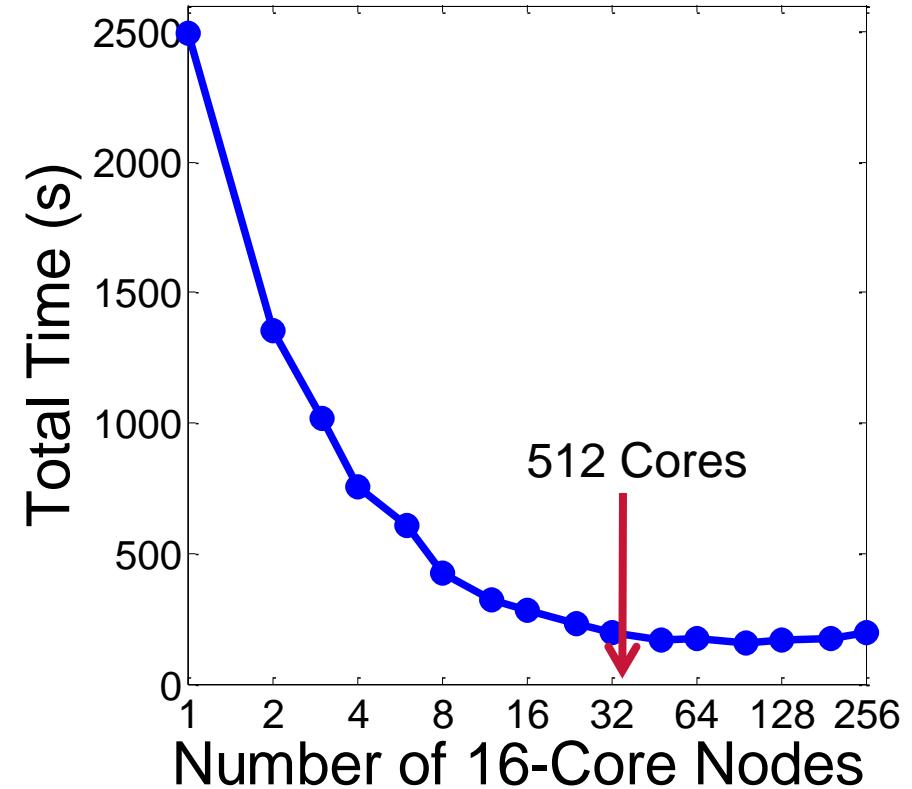
## Use of multiple processors in DEM simulations

- YADE (2008) – based on OpenMP – shared memory systems
- PFC version 5 – multi core
- For larger shared, use High Performance Computing (hpc) systems – need a code that works with distributed memory / MPI
- MPI Codes: LAMMPS, LIGGGHTS, EYS
- LAMMPS (<http://lammps.sandia.gov/>)
  - Uses spatial decomposition
  - Classical molecular dynamics code that can be used for DEM
  - Researchers at IC (Marketos, Hanley) have been working to modify the granular LAMMPS package
  - Modified contact models
  - Implemented stress-controlled periodic boundaries (as in Trubal)

## Scaling of granular LAMMPS

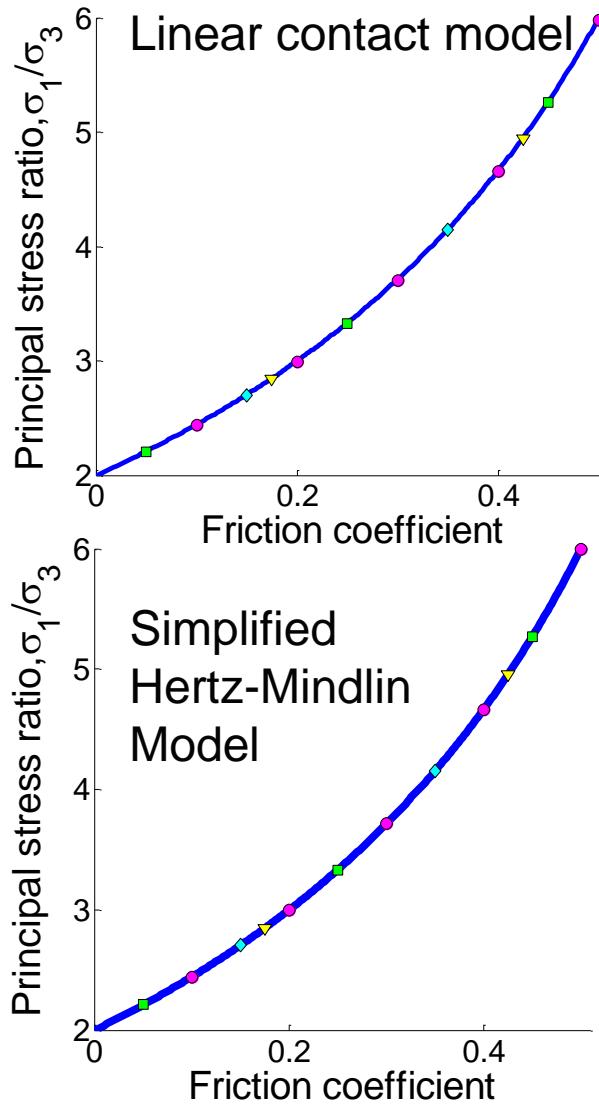


*FCC simulation, 125,000 uniform spheres, 100,000 time steps, HECToR Phase 3*

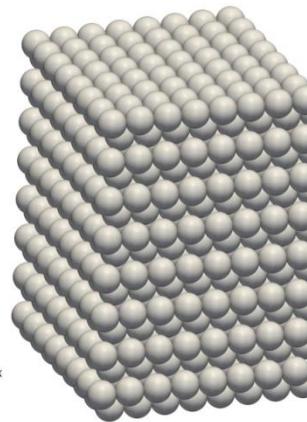
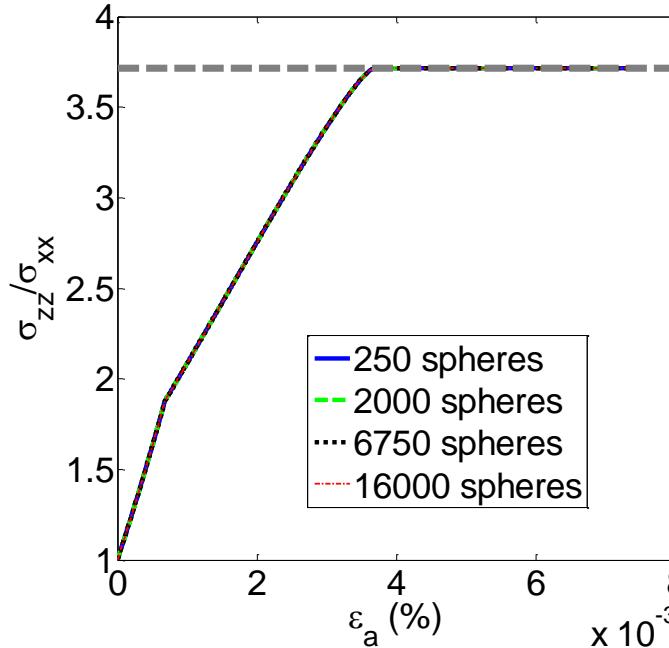


*Polydisperse sample, 351,248 spheres, 100,000 time steps, Hartree Blue Joule*

# Use of Analytical Solution to Validate DEM code LAMMPS



- Analytical Solution
- Serial (No Damping)
- ◆ Serial (Local Damping)
- Serial (Viscous Damping)
- ▽ HECToR



Solution documented in Thornton (1979)

K. Hanley and X. Huang

## Current and future DEM use

The ability of DEM to capture complex soil behaviour is well established

There is a growth in DEM use in geomechanics, however models remain relatively simple/small

There is a clear transition to multi-core capable DEM codes.

Validation of such codes is important

## Assessing DEM simulation quality: Sample size and CSL

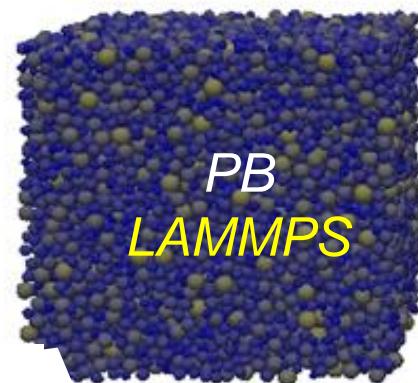
Grading - similar to Toyoura Sand

Simplified Hertz Mindlin Contact Model

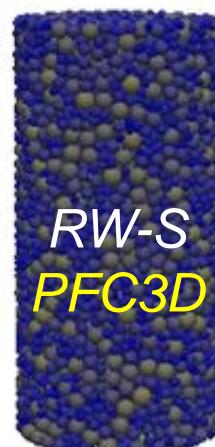
Drained triaxial compression tests

$\mu$  (friction coeff) 0.25

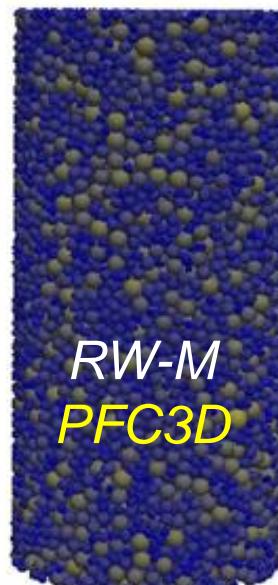
5.25mm cube



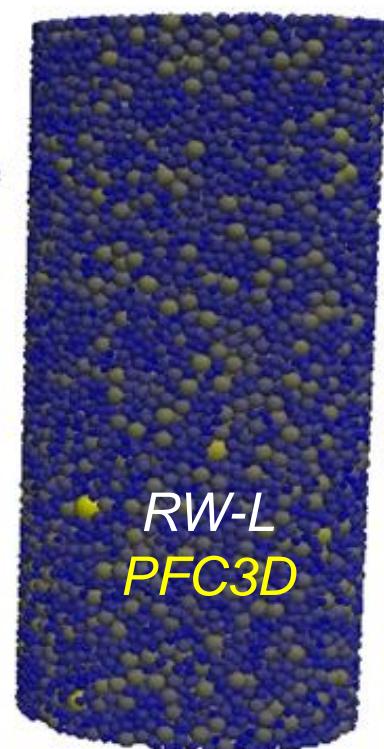
3x6.8 mm



4x8.8 mm



5x11.0 mm



Mr. X. Huang

Huang et al. (2013)

$(\text{Dimension})_{min}/D_{50} =$

25

14

19

24

No. Particles =

20,164

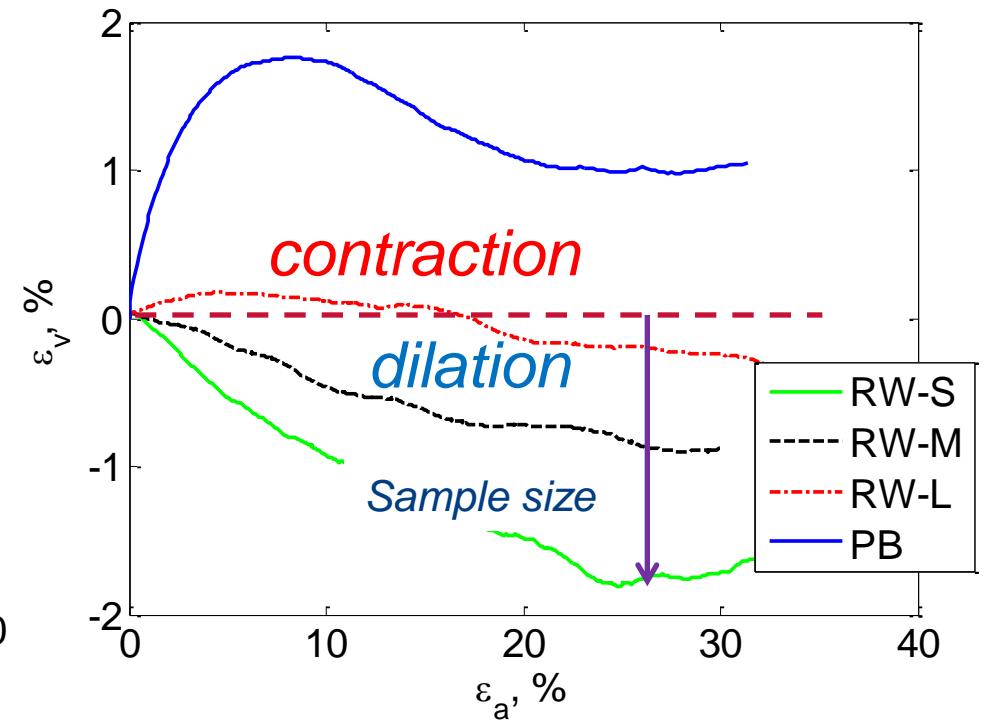
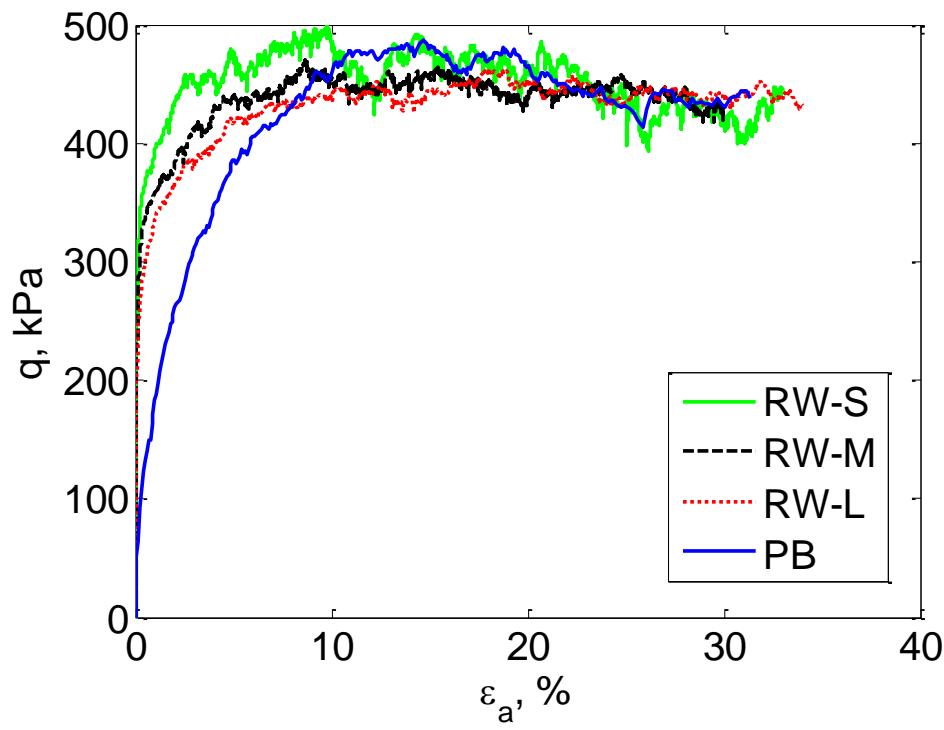
6,783

16,073

31,392

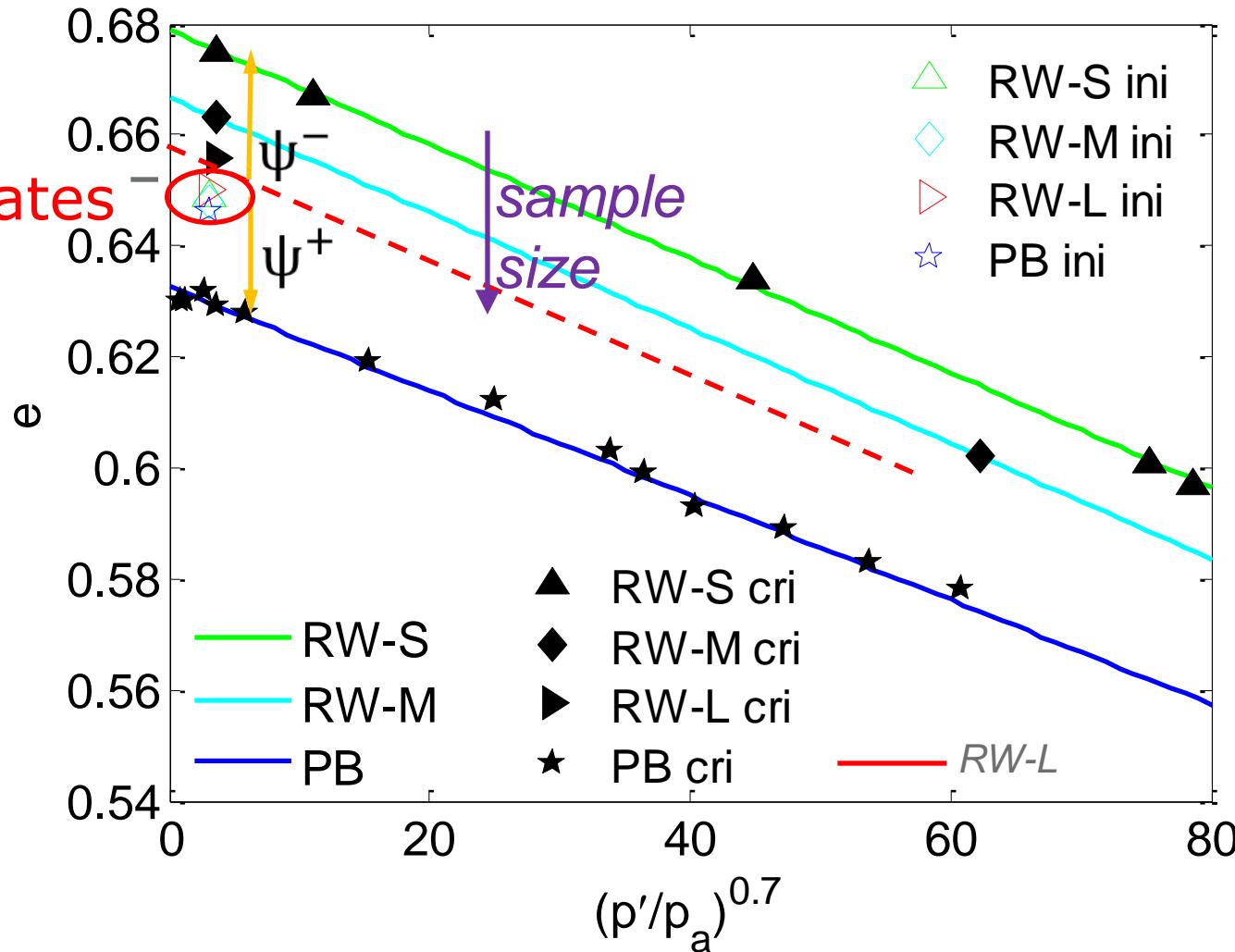
# Assessing DEM simulation quality: Sample size and CSL

$$e_0 = 0.646, \sigma'_{3,0} = 500 \text{ kPa}$$

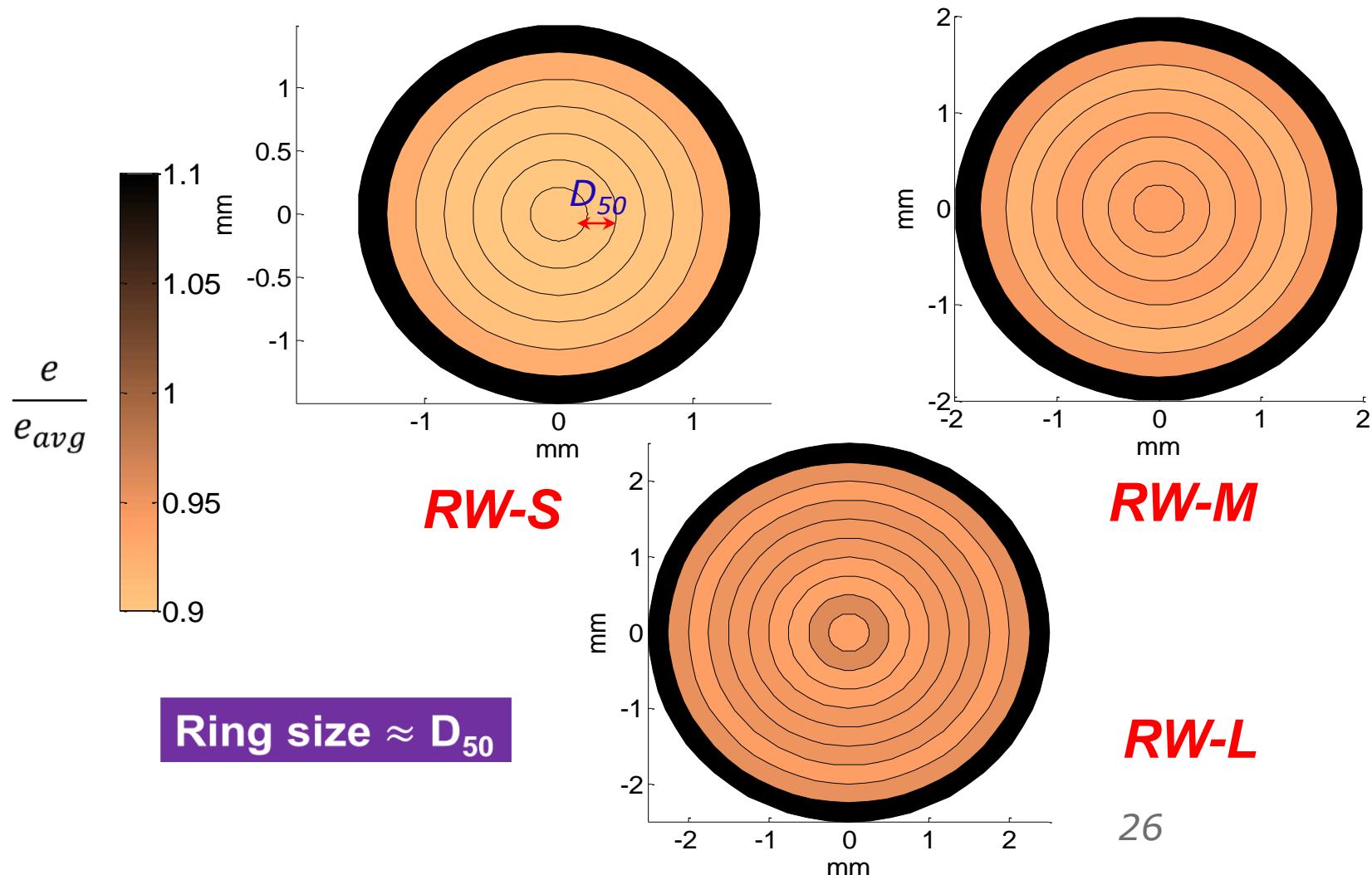


## Assessing DEM simulation quality: Sample size and CSL

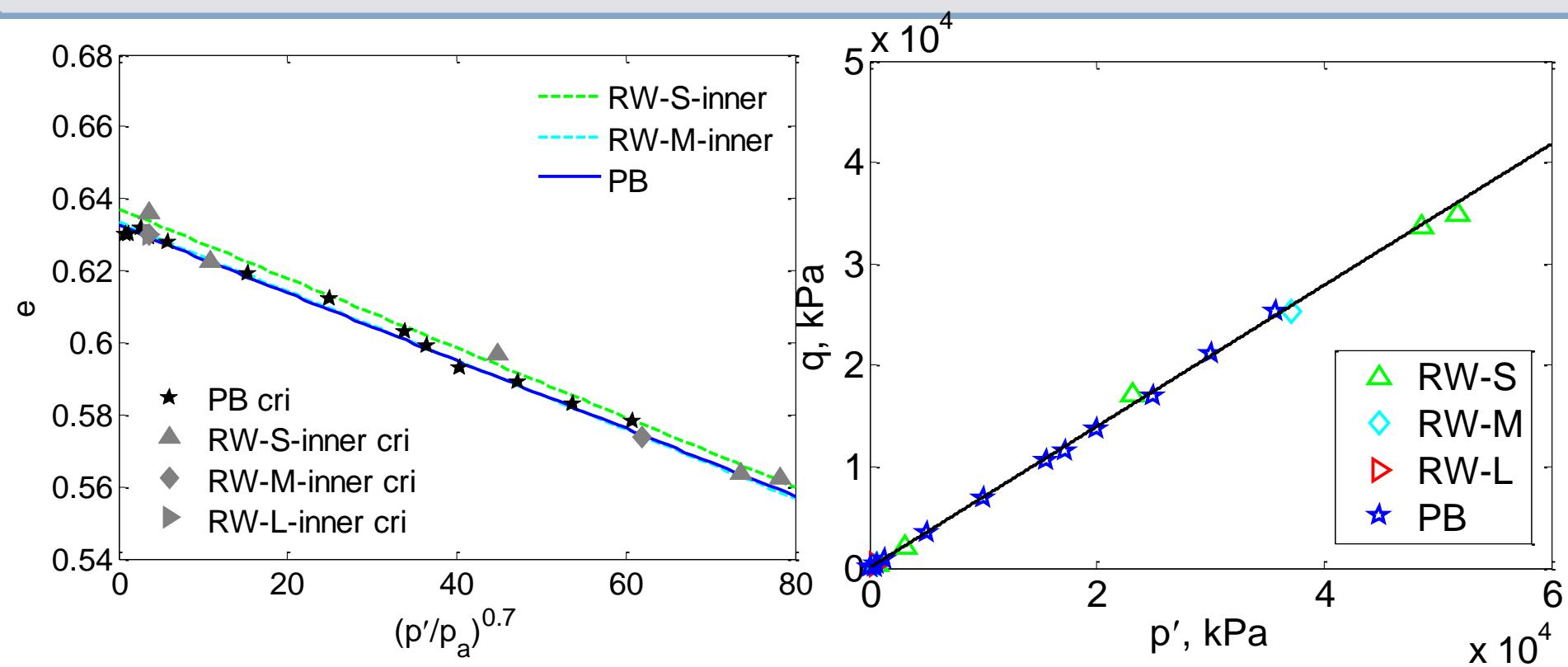
Initial States



## Assessing DEM simulation quality: Sample size and CSL

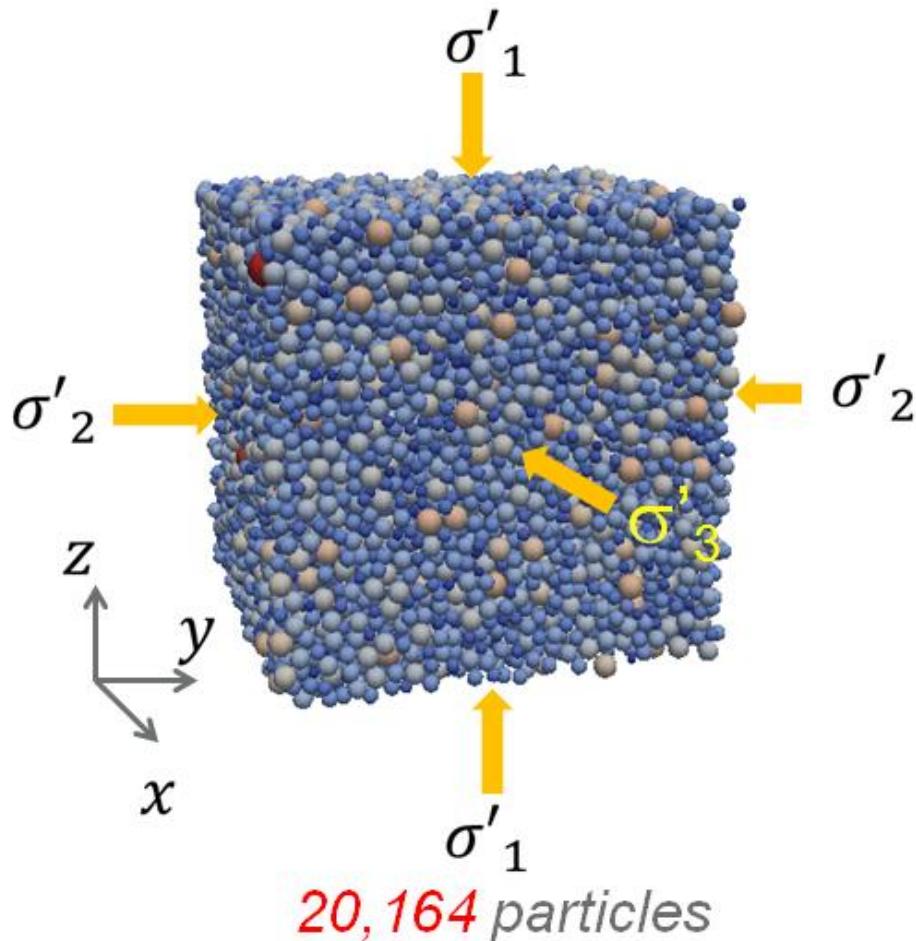


## Assessing DEM simulation quality: Sample size and CSL



CSL for homogeneous inner regions

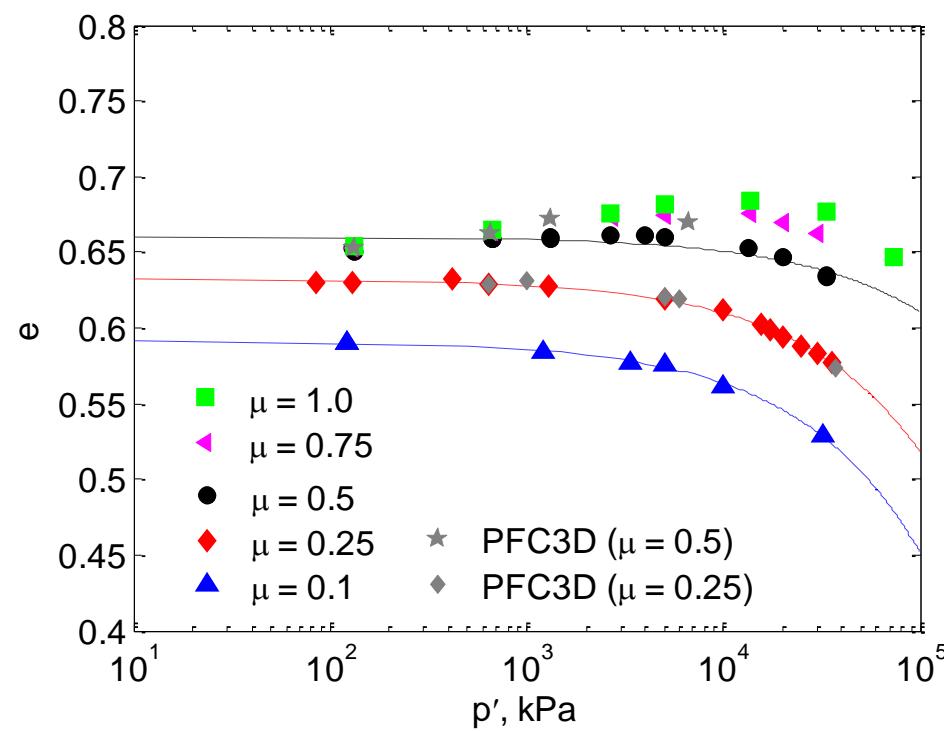
## Assessing DEM simulation quality: Choice of $\mu$ and CSL



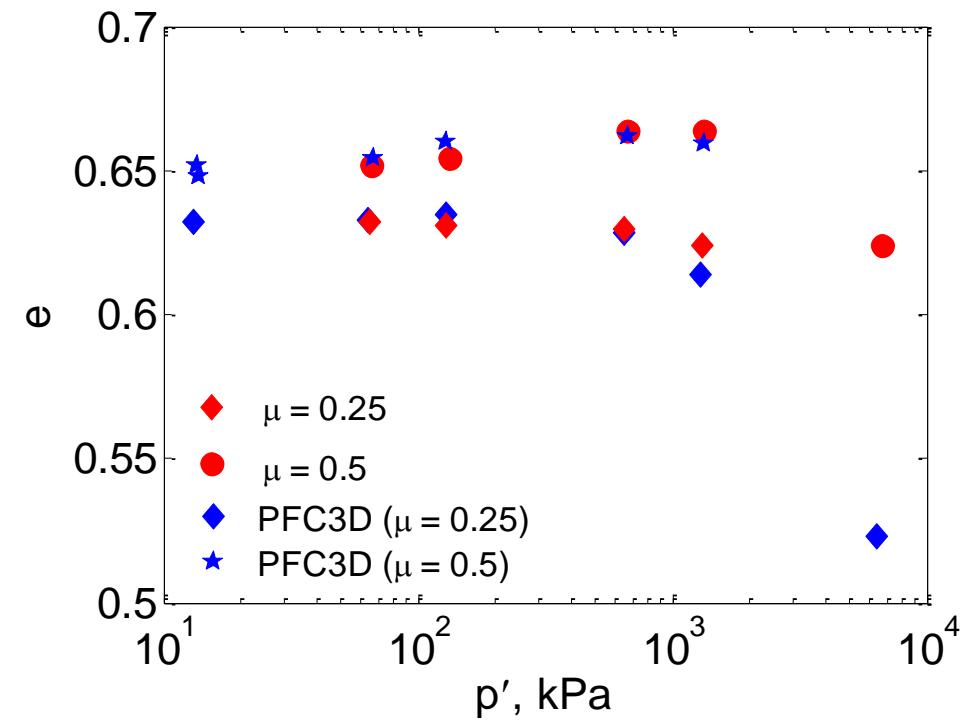
- *Periodic boundaries*
- *Grading similar to Toyoura sand*
- *Varied inter-particle friction value,  $\mu$*
- *Most of simulations used LAMMPS*
- *Mr. X. Huang*
- *Huang et al. (2014b)*

# Assessing DEM simulation quality: Choice of $\mu$ and CSL

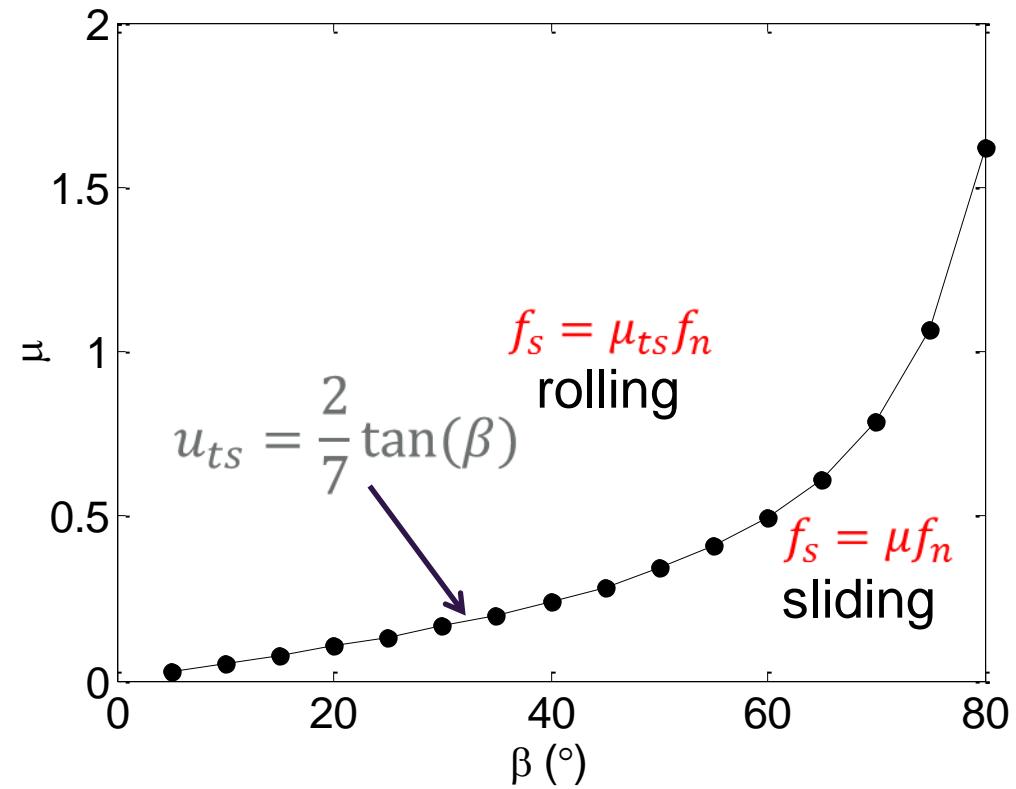
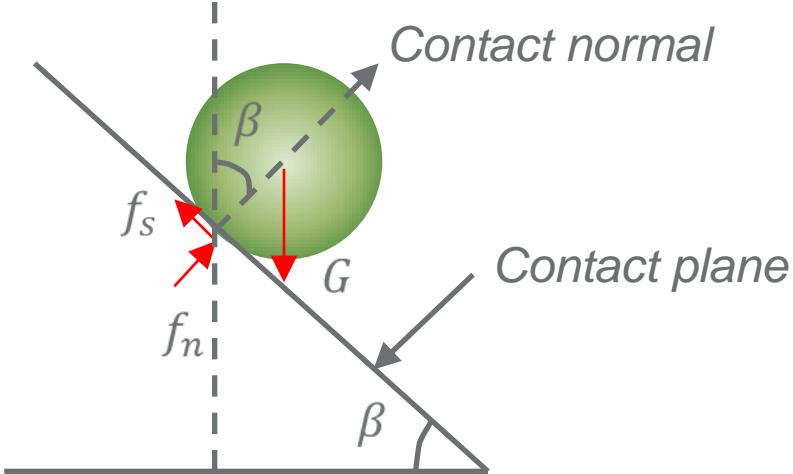
*Simplified Hertz-Mindlin contact model*



*Linear elastic contact model*



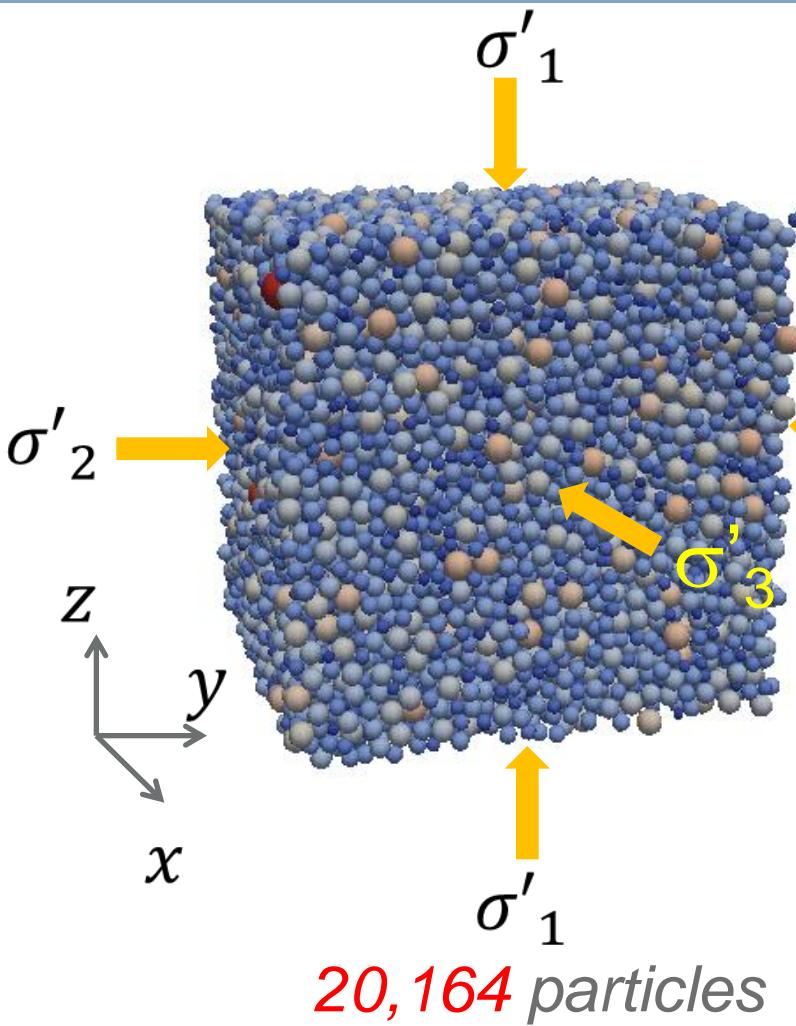
## Assessing DEM simulation quality: Choice of $\mu$ and CSL



## Assessing DEM simulation quality: CSL

Plotting the critical state line and understanding the sensitivity of the critical state line to DEM model parameters is a useful quality check on a DEM model

## Application: Studying soil response under a 3D stress state

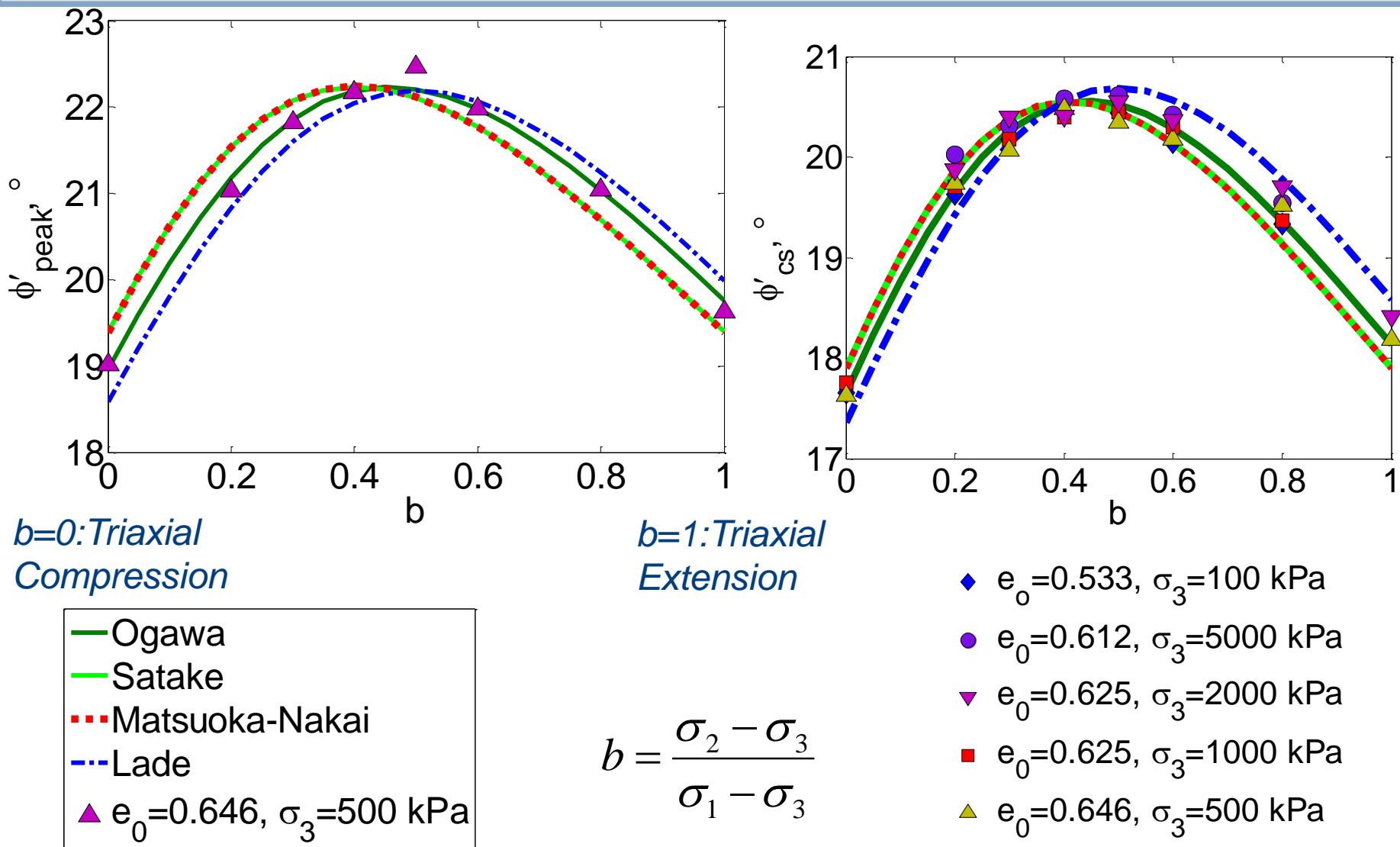


- Periodic boundaries
- Grading similar to Toyoura sand
- Most of simulations used LAMMPS
- Friction coefficient  $\mu=0.25$
- Controlled  $b$
- Deformed to large strain

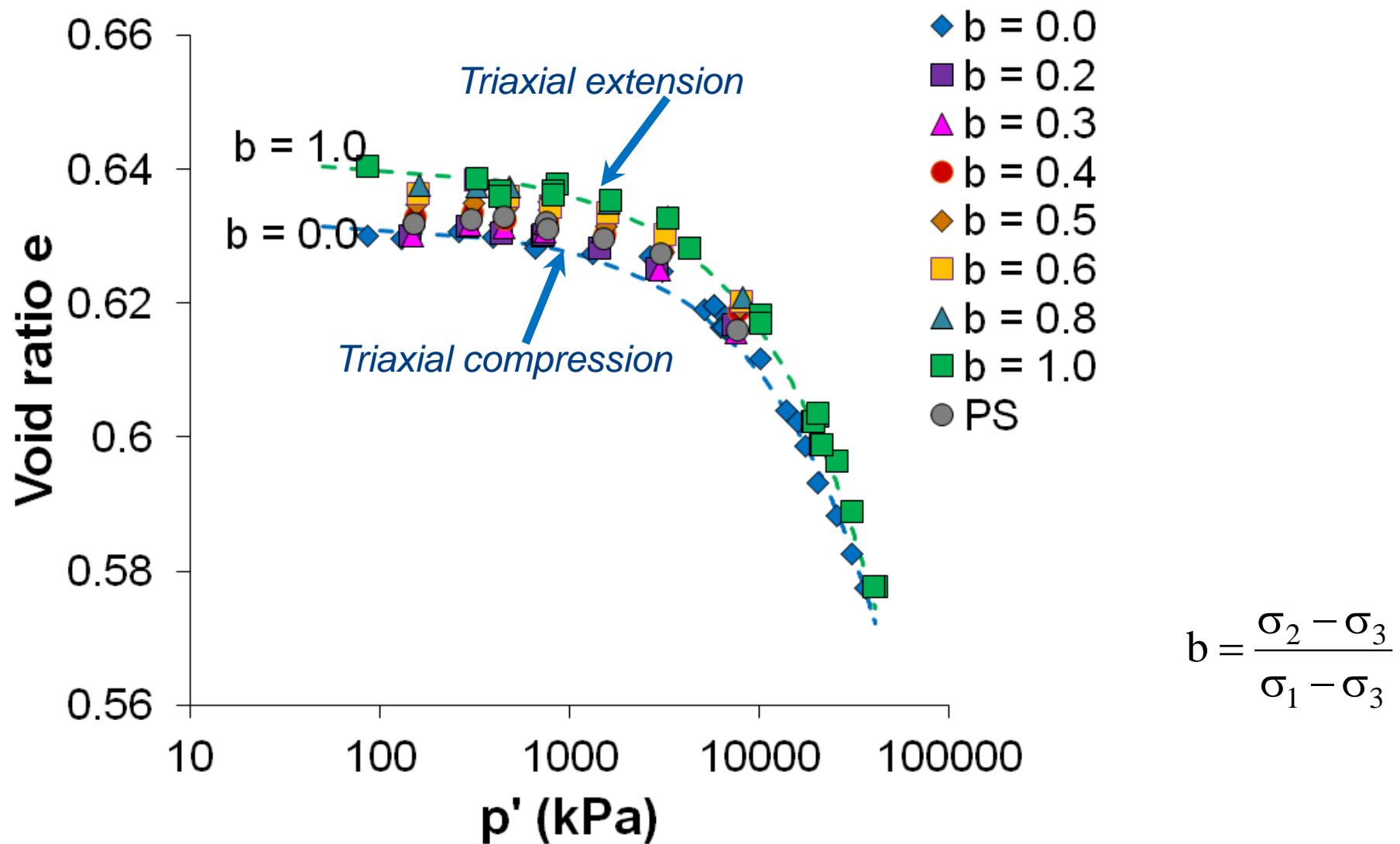
Mr. X. Huang

Huang et al. (2014a)

## Application: Studying soil response under a 3D stress state



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## Application: Studying soil response under a 3D stress state

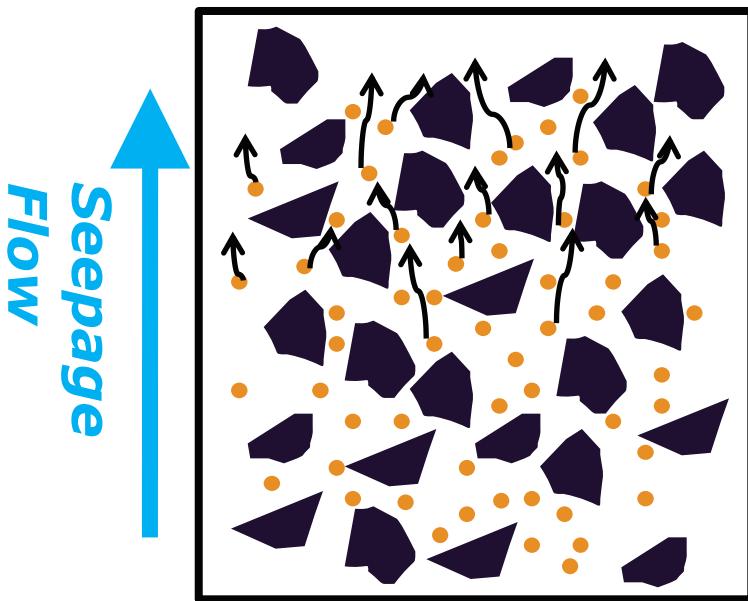
DEM can capture the dependence of  $\phi'$  on  $b$

DEM can capture the dependence of the material response on  $\psi$

DEM can be used to extend and develop constitutive models within the critical state soil mechanics framework

## Application: Internal Erosion

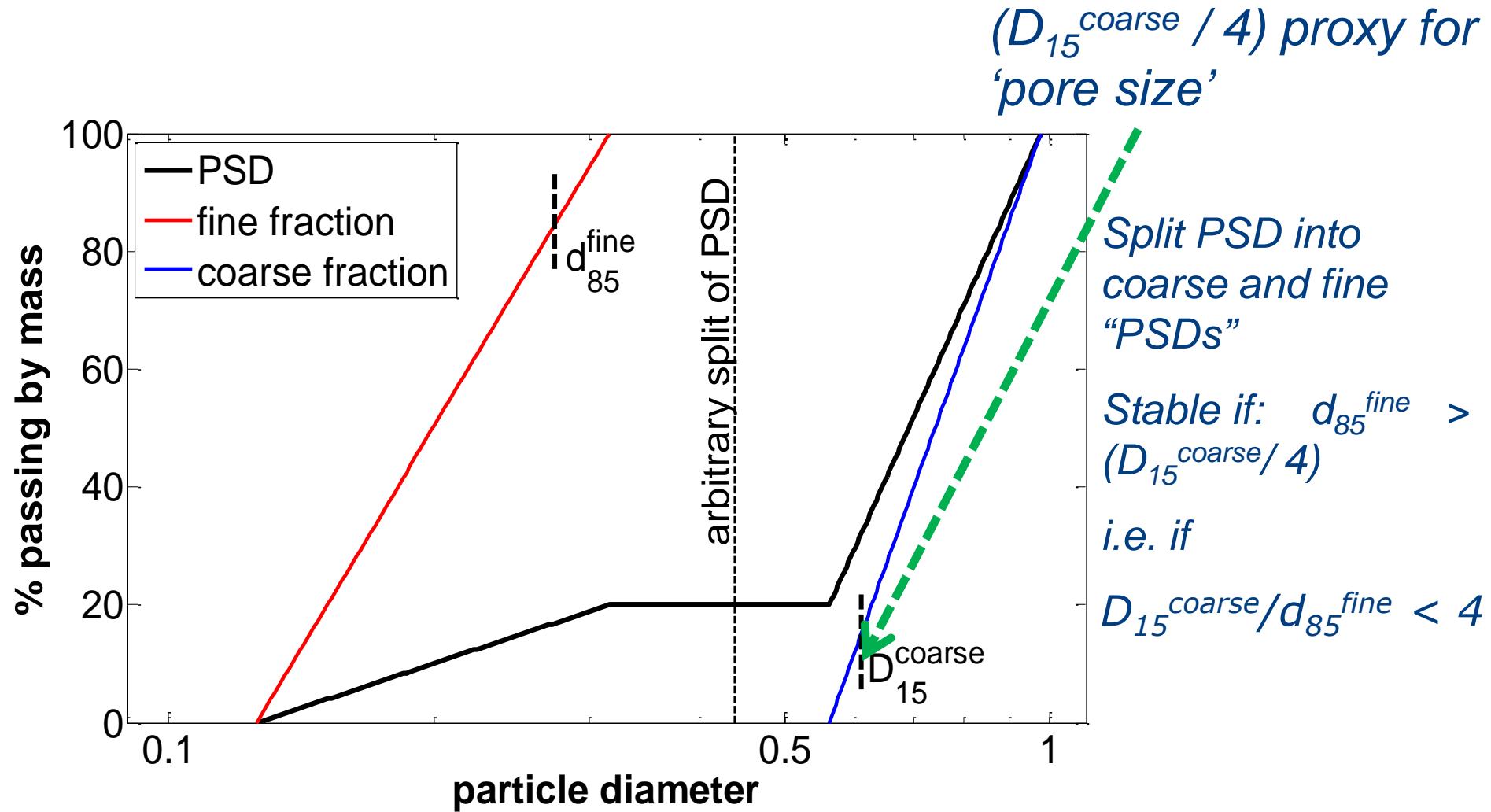
- Cohesionless fines in gap graded materials are known to influence internal stability
- Internal stability = ability of coarse fraction to prevent erosion of finer fraction under seepage



(from Muir Wood, 2007)

PhD student Dr. Tom Shire  
Shire et al. (2014)

# Filter Criteria: Kézdi (1979)



## Stress partition - $\alpha$

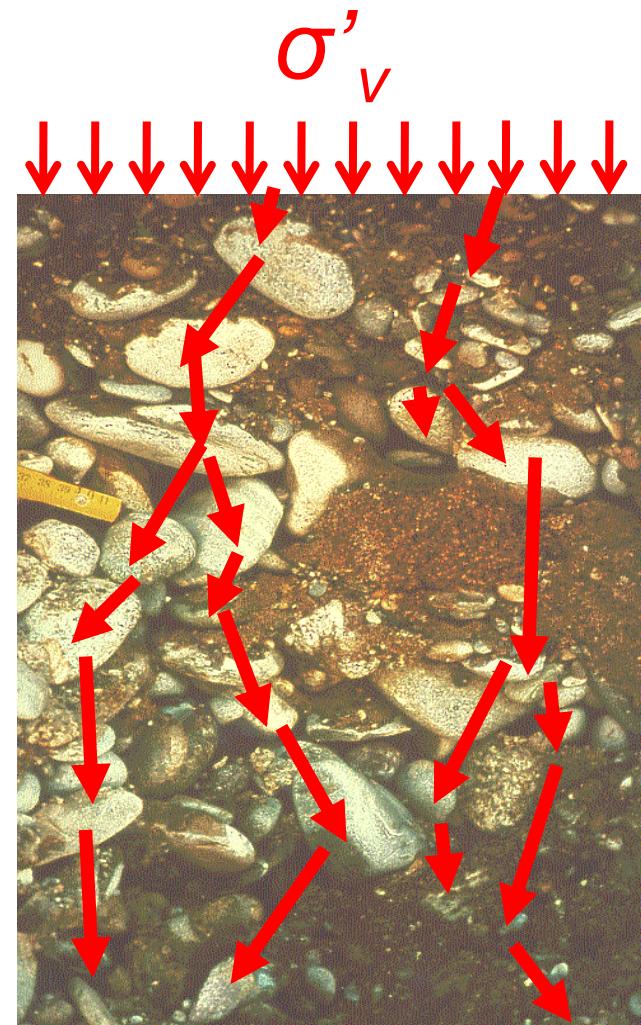
Skempton and Brogan (1994):  
Micromechanical hypothesis to explain  
why  $i_{crit} < -1$ :

Coarse matrix transfers overburden

Fines carry reduced effective stress:

$$\sigma'_{fines} = \alpha \times \sigma'$$

$$i_{crit} = \alpha \times i_{crit(\text{heave})}$$



## Stress partition – $\alpha$ – DEM calculations

$$\alpha = \frac{p'_{fine}}{p'}$$

$$p' = \frac{1}{V} \sum_{p=1}^{N_p} (p^p V^p)$$

$$p'_{fine} = \frac{(1-n)}{\sum N_{p,fine} V^p} \sum_{p=1}^{N_{p,fine}} (p^p V^p)$$

- $p^p$ =average particle stress
- $V^p$ = particle volume
- $V$ =total volume
- $n$ =porosity
- $N_p$ =No. of particles
- $N_{p,fine}$ =No. of fine particles

$p^p$  calculated from summation of products of contact vectors and contact forces – (Potyondy and Cundall, 2004)

## Application: Internal Erosion

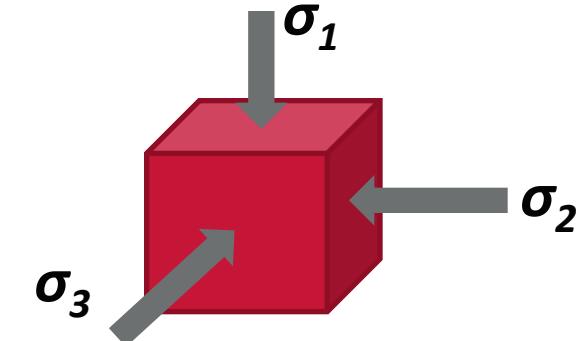
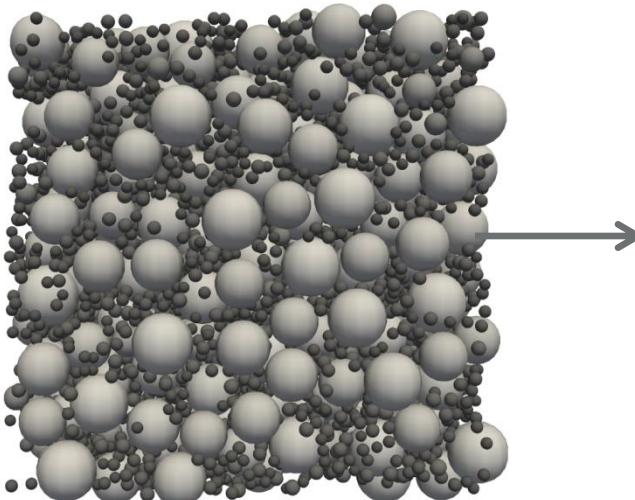
Isotropic compression at to  $p' = 50\text{kPa}$

Sample density controlled using  
interparticle friction:

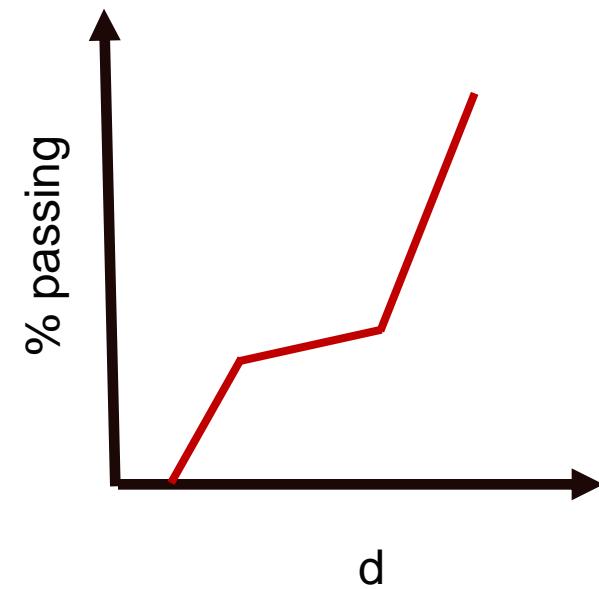
$\mu = 0.0$  (Dense),  $\mu = 0.1$  (Medium dense),  
 $\mu = 0.3$  (Loose)

DEM code granular LAMMPS up to 304,205  
particles

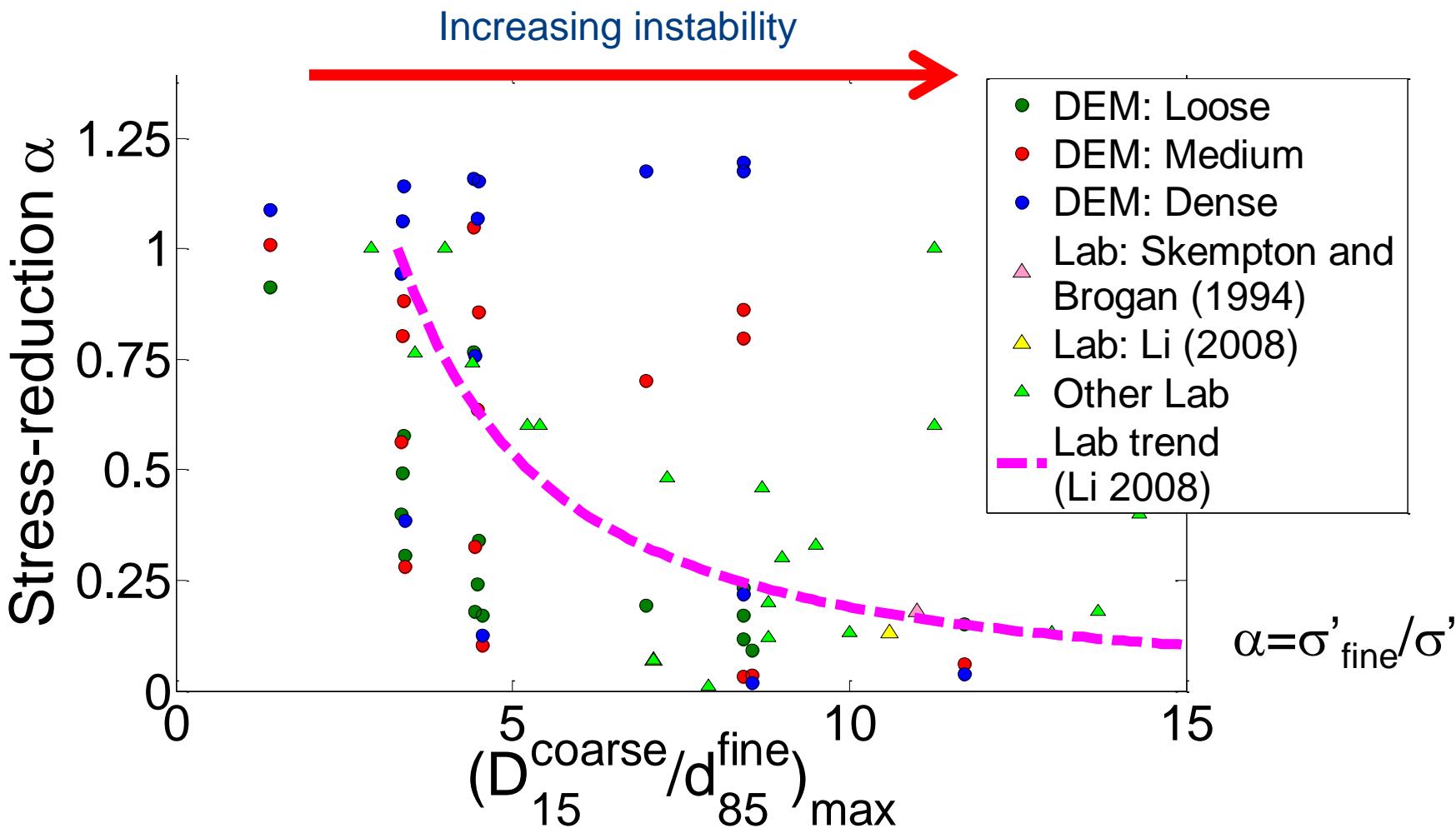
Periodic boundaries



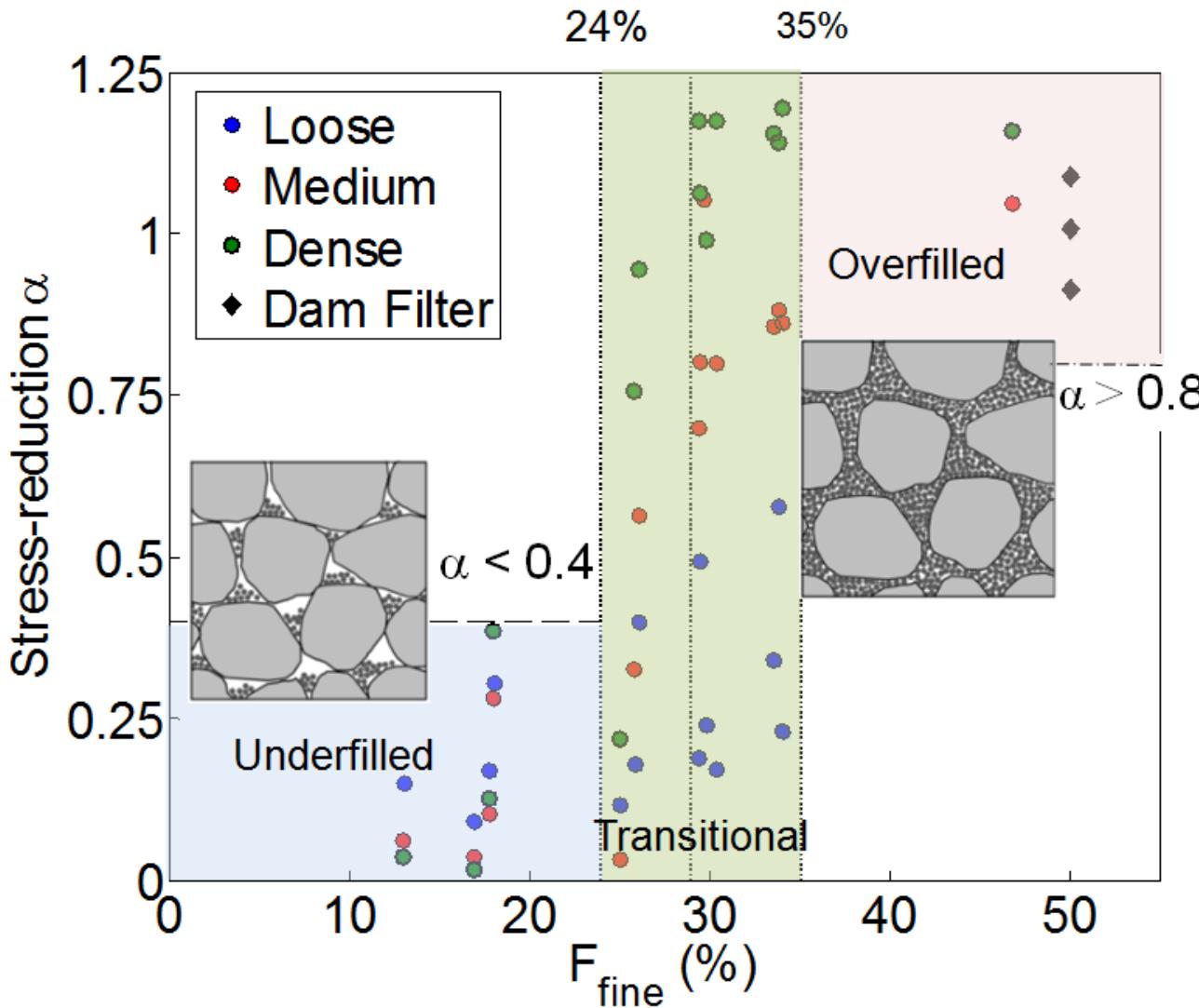
Range of gap graded  
materials considered



## Application: Internal Erosion



## Application: Internal Erosion



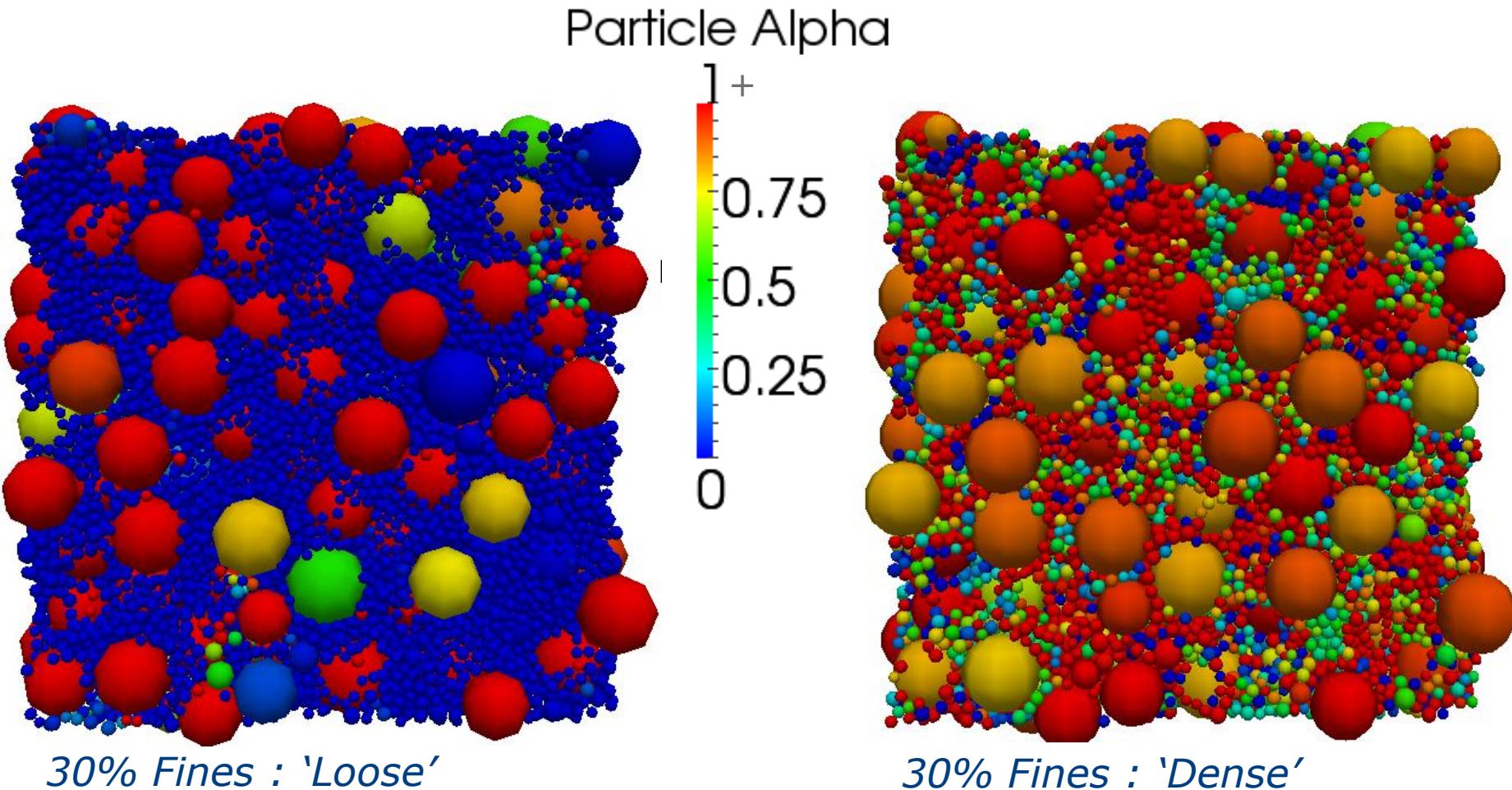
**Skempton and Brogan(1994):**

Critical fines content where fines just fill voids:  $F_{\text{fine}} = 24\text{-}29\%$

Finer fraction separates coarse fraction particles:  
 $F_{\text{fine}} = 35\%$

# Application: Internal Erosion

*Images of transition zone*



# Application: Internal Erosion

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Internal erosion is a particle scale problem that is well suited to DEM analysis

DEM can examine the hypotheses on which internal erosion guidelines are based

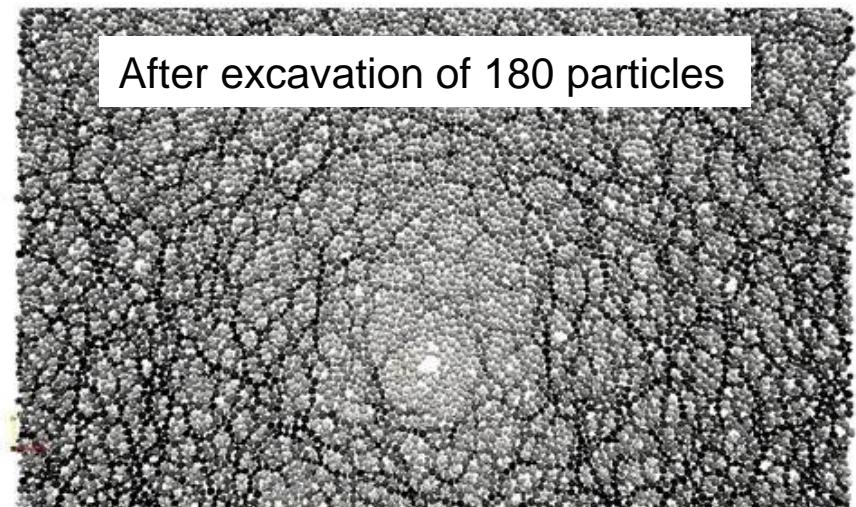
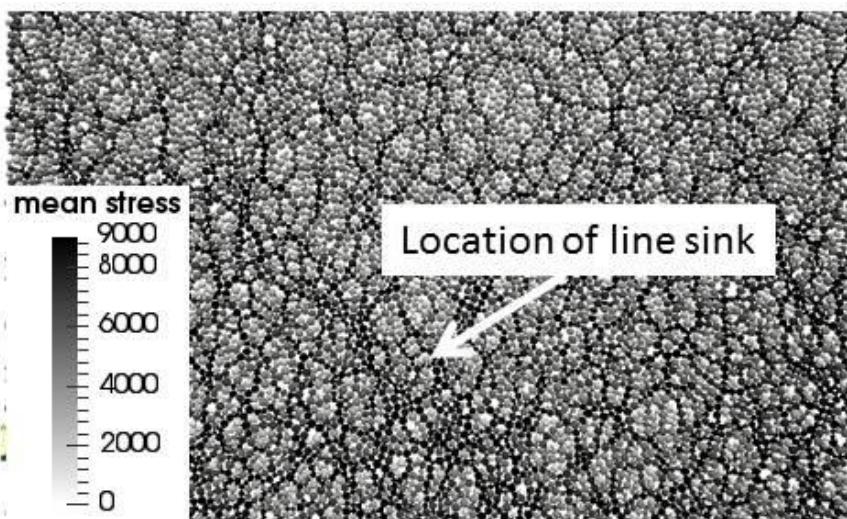
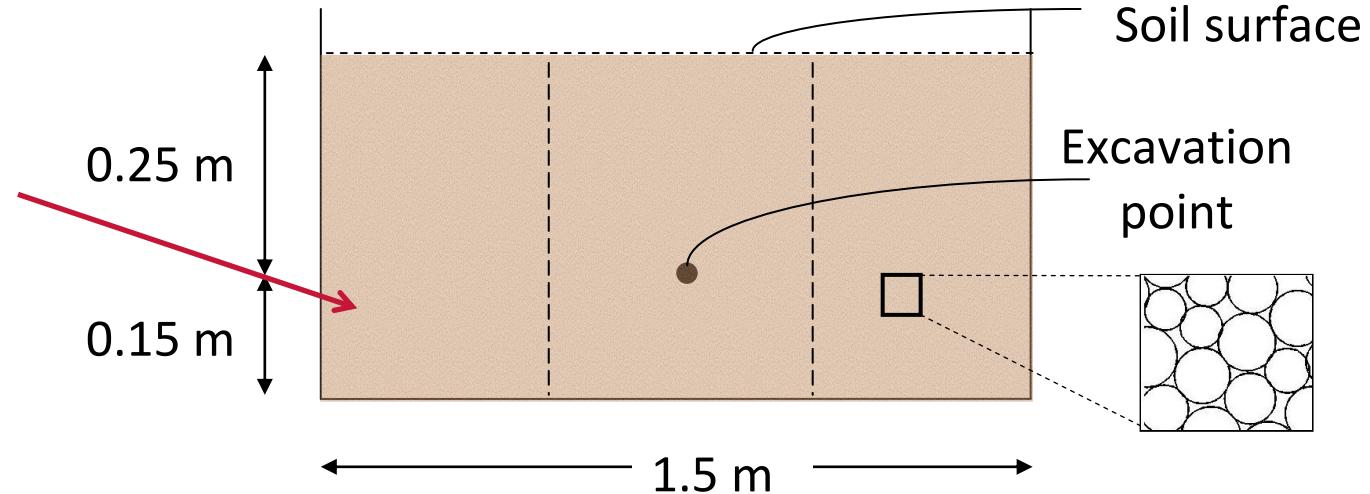
## Application: Tunnelling induced ground deformations

- Tunnelling paradox: surface settlement curve predicted in numerical models is highly sensitive to model parameters but field observations give remarkably consistent topologies.
- Model created using line-sink approach adopted in continuum analysis by Verruijt and Booker (1996)

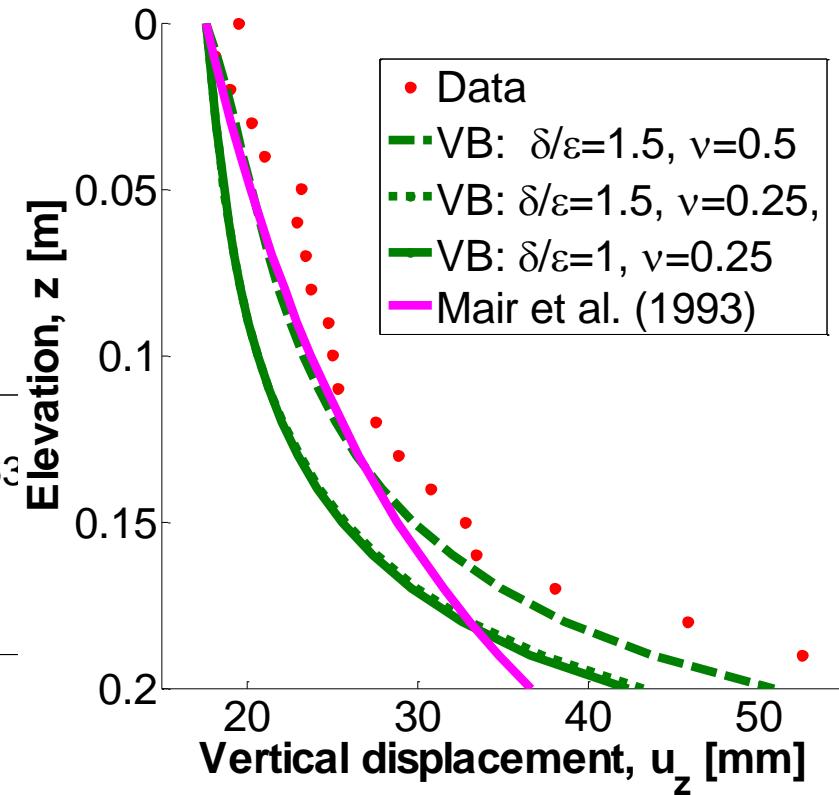
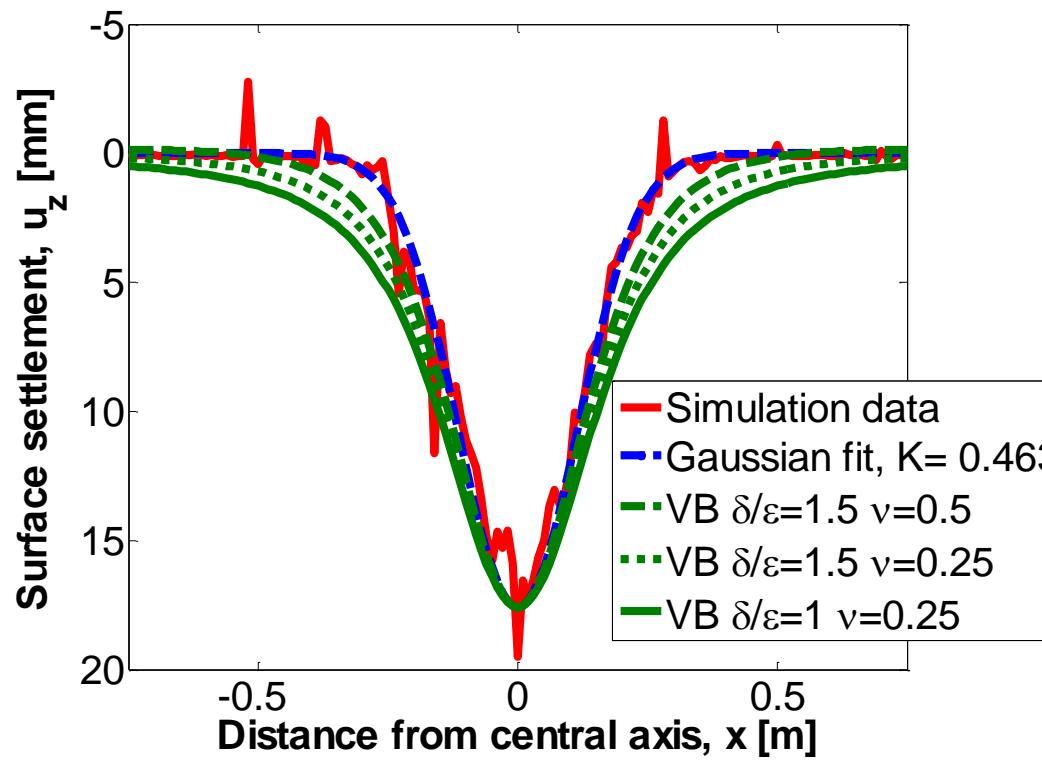
*Dr. George Marketos, Prof. J. Burland,  
Mr. T. Bym*

## Application: Tunnelling induced ground deformations

117,153 disks  
Granular LAMMPS  
Mr. T. Bym  
Dr. G. Marketos



## Application: Tunnelling induced ground deformations



VB=Verruijt and Booker Soln.

## Application: Tunnelling induced ground deformations

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Provided we can develop appropriate boundary conditions, even 2D DEM can provide insight into field-scale deformation mechanisms

## Conclusions

- DEM use in geomechanics continues to grow, though perhaps not as rapidly as in other disciplines
- Now proven as a tool that can reproduce characteristic mechanical behaviour of sand
- There is currently a transition towards the use of high performance computing to run DEM simulations in geomechanics
- Validation is important, plotting the critical state line can be useful to assess whether a model is reasonable
- DEM can allow us to explore stress states that are not easily attainable in the lab
- DEM can complement laboratory testing where interpretation is complex
- DEM can inform design guidelines for problems that are driven by particle-scale interaction
- When appropriate boundary conditions can be applied, DEM can inform field-scale soil deformation analysis

# Acknowledgements

## Collaborators:

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Prof. J. Burland, Imperial  
Dr. E. Ibraim, Bristol  
Prof. D. Muir Wood, Dundee  
Prof. J. Fannin, UBC

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1851

## Post-doctoral researchers:

Dr. K. Hanley (now in Edinburgh)  
Dr. G. Marketos (now in Utrecht)

## PhD students:

Dr. Liang Cui (now in Surrey)  
Dr. D. Barreto (now in Edinburgh Napier)  
Dr. J. O'Donovan (now in Buro Happold)  
Dr. T. Shire (now in Atkins)  
Dr. G. Cheung (now in ARUP)  
Dr. C. K. Shen (now in MottMcDonald)  
Mr. X. Huang (HKU / Imperial)

## Key references (in order of citation in presentation)

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