Particle scale insights into the load:deformation behaviour of sand

Catherine O’Sullivan

Kevin Hanley, Xin Huang, Masahide Otsubo
Discrete Element Method
Idealizes particle shape and contact behaviour

Conceptually simple algorithm – transient analysis – step forward in time

Identify contacting particles
Determine contact forces
Update positions
Forces on particles → accelerations + velocities

High performance computers enable larger samples to be simulated
Direct Shear Test – illustration of benefits of DEM

Grade 25 steel precision balls
Diameter 0.992 mm

Cui and O’Sullivan (2006)
Géotechnique

DEM model: 11700 Spheres

Mean $\mu_{\text{surface}}$ 5.5°
Mean $\mu_{\text{surface}}$ 5.7°
Direct Shear Test

Lab

DEM

Stress ratio, $\tau / \sigma_n$

Global shear strain: %

Stress ratio, $\tau / \sigma_n$

Global shear strain: %

Vertical strain: %

Vertical strain: %

Direct Shear Test
Direct Shear Test

\[ \phi'_p = \text{peak angle of shearing resistance} = \text{peak “friction” angle} \]

\[ e_0 = \text{initial void ratio} \]
Stress ratio $\tau / \sigma_n$

Global shear strain: %

Vertical strain: %

Contact Normal Forces (Normalized)
Global shear strain: %

Stress ratio $\tau/\sigma_n$

Contact Normal Forces (Normalized)

Vertical strain: %
DEM and sand behaviour

- Even using spherical particles and simple contact models, DEM simulations can capture many of the complex mechanical response characteristics of sand.

- The demonstrated ability to capture this behavior means that DEM can be used:
  - To advance understanding of the fundamental mechanisms that underlie the observed response in laboratory element tests.
  - In parametric studies to better understand how various particle-scale parameters influence the overall load:deformation response.
  - To complement experimental studies e.g. by considering stress and strain states that cannot be attained in experiments.
DEM can capture stress-dependant/frictional strength

Direct shear test simulations
Modified version of Trubal
Dr. L. Cui
DEM can capture the existence of a critical state

\[ \psi_0 = \begin{cases} 
0.0412 & \text{loose (wet)} \\
0.0245 & \\
0.0171 & \\
\end{cases} \]

\[ \psi > 0 \quad \text{loose (wet)} \]
\[ \psi = 0 \quad \text{critical state} \]
\[ \psi < 0 \quad \text{dense (dry)} \]

Triaxial test simulations
Granular LAMMPS
Mr. X. Huang
DEM can capture sensitivity of $\Phi_p$ to void ratio (state)

Triaxial test simulations
Granular LAMMPS
Mr. X. Huang
Dr. K. Hanley

Toyoura Grading
Dunkirk Grading

Peak angle of shearing resistance, $\phi_p$

Initial state parameter, $\psi_0$
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

- Triaxial test simulation
  - Parallel Bond Contact Model
  - PFC 3D spheres
  - Dr. G. Cheung
DEM can capture the stress-dependency of soil stiffness

\[ G_{xy} \propto \sigma_0^{0.39} \]
\[ G_{yz} \propto \sigma_0^{0.4} \]
\[ G_{zx} \propto \sigma_0^{0.38} \]

Bender element test simulation, cubical cell
FCC packing
Simplified Hertz-Mindlin Contact Model
PFC 3D spheres
Dr. J. O’Donovan
DEM can capture hysteresis in cyclic loading

Strain controlled triaxial tests
Simplified Hertz-Mindlin Contact Model
Modified Trubal, spheres
Dr. L. Cui
DEM can capture strain softening and localization

Biaxial compression - 12,512 disks
PFC 2D: Flexible membrane boundary

Disk rotation (rad)
Axial strain=3.7%
DEM can capture 3D stress-space failure criterion

Intermediate principal stress ratio

\[ b = \frac{\sigma_2 - \sigma_3}{\sigma_1 - \sigma_3} \]

- \( b = 0 \): Triaxial Compression
- \( b = 1 \): Triaxial Extension

Granular LAMMPS
Mr. X. Huang

\[ e_0 = 0.646, \sigma_3 = 500 \text{ kPa} \]
DEM can capture anisotropy of strength

![Graph showing the angle of shearing resistance vs principal stress orientation.](image)

- K<sub>0</sub> compressed samples
- Modified Trubal
- Dr. D. Barreto
DEM can capture the non-coaxiality of stress and strain increments

\[ \Delta \alpha = \text{angle between principal stress direction and principal strain increment direction} \]

Simple shear test simulations
PFC 2D
Dr. C. K. Shen
DEM can be calibrated to model sandstone

70 MPa Triaxial

Contact bond at ball-ball contact
DEM can be calibrated to model sandstone
DEM can be used to simulate interbedded rock layers.
DEM can be used to simulate interbedded rock layers

Contact bond at ball-ball contact

Parallel bond

$\alpha_{\text{bond}}^2 R_{\text{min}}$

Sandstone

Siltstone

Contact bond at ball-ball contact

Parallel -bond

$R_{\text{min}}$

$\alpha_{\text{bond}}^2 R_{\text{min}}$

$q_{\text{max}}^{\text{strong}} / q_{\text{max}}^{\text{weak}} = 1.75$

$q_{\text{max}}^{\text{strong}} / q_{\text{max}}^{\text{weak}} = 3.47$

$q_{\text{max}}^{\text{strong}} / q_{\text{max}}^{\text{weak}} = 5.00$

Tzillas et al (2013)

Zainab et al (2007)
DEM and sand behaviour

- Even using spherical particles and simple contact models, DEM simulations can capture many of the complex mechanical response characteristics of sand.

- The demonstrated ability to capture this behavior means that DEM can be used:
  - To advance understanding of the fundamental mechanisms that underlie the observed response in laboratory element tests.
  - In parametric studies to better understand how various particle-scale parameters influence the overall load:deformation response.
  - To complement experimental studies e.g. by considering stress and strain states that cannot be attained in experiments.
Advancing understanding of load:deformation behaviour.

Three fundamental questions

1. What determines the nature of the stress:stiffness relationship?

2. Does the state parameter concept hold under a general stress state?

3. At a given stress level why do we see more crushing in shearing than in compression?
Pressure-Stiffness Relationship

- Elastic theory explains pressure dependency: contact area increases as pressure increases – larger area gives a larger stiffness

- Elastic theory predicts that $G_0 \propto (p')^{1/3}$

- Experimental data for sand gives $G_0 \propto (p')^{1/2}$

Otsubo and O’Sullivan S+F (2018)
Roughness-dependant contact behaviour

Contact between smooth elastic spheres: Hertzian behaviour

$N \propto \delta^{3/2}$

Contact between rough spheres:

- Asperity dominated
  - $\delta_1 = 0.82 S_q^*$
  - $\delta_2 = 1.24 S_q^*$
  - $\delta_{T1} = 2.11 S_q^*$
  - $\delta_{T2} = 24.47 S_q^*$

Transitional

Hertzian
Controlling and Surface Roughness

Ballotini + Toyoura Sand

Used spherical glass beads to isolate roughness from shape (form) effects

Measured roughness using interferometry
Roughened Ballotini

$S_q = 58$ nm

$S_q = 127$ nm

$S_q = 267$ nm

$S_q = 612$ nm

(Otsubo, 2017)
Quantifying Stiffness in Laboratory

Shear plates (Transmitter) → Specimen $\phi = 50$ mm → Shear plates (Receiver)

Function generator → Oscilloscope → Amplifier → Output

(Otsubo, 2017)
Simulating Tests using DEM

- DEM code: LAMMPS
- 155,165 particles
- Diameter: $D = 2.54$ mm (mono-size)
- Particle shear modulus: $G_p = 25$ GPa
- Particle Poisson’s ratio: $\nu_p = 0.2$
- Inter-particle friction:
  - $\mu = 0.0$ (dense) 0.15 (loose)
- $p' = 100$ kPa to 10 MPa
- Planar shear waves

(Otsubo, 2017)
Roughness-dependant contact behaviour

DEM Contact Model

Contact between roughened spheres

\[ \delta_1 = 0.82 S_q^* \]
\[ \delta_2 = 1.24 S_q^* \]
\[ \delta_{T1} = 2.11 S_q^* \]
\[ \delta_{T2} = 24.47 S_q^* \]
Surface Roughness and Stiffness

Experiments

- $p' = 50$ kPa
  - $e = 0.605, 0.599, 0.597, 0.594$

- $p' = 200$ kPa
  - $e = 0.602, 0.597, 0.594, 0.591$

- $p' = 750$ kPa
  - $e = 0.598, 0.594, 0.589, 0.586$

DEM simulations

- $p' = 50$ kPa
  - $e = 0.636, 0.635, 0.634, 0.633$

- $p' = 200$ kPa
  - $e = 0.634, 0.633, 0.633, 0.632, 0.630$

- $p' = 800$ kPa
  - $e = 0.630, 0.629, 0.629, 0.628, 0.626$

(Otsubo, 2017)
Surface Roughness and Stiffness

\[ F(e) = \frac{(1.28-e)^2}{1+e} \]

![Graph showing relationship between surface roughness and stiffness](image)

**Lab**

- \( n = \frac{1}{3} \)
- \( n = \frac{1}{2} \)

**Materials**

- \( S_q = 58 \) nm \( (n = 0.385) \)
- \( S_q = 127 \) nm \( (n = 0.439) \)
- \( S_q = 267 \) nm \( (n = 0.499) \)
- \( S_q = 586 \) nm \( (n = 0.534) \)

**DEM**

- \( S_q = 0 \) nm \( (n = 0.368) \)
- \( S_q = 70 \) nm \( (n = 0.404) \)
- \( S_q = 140 \) nm \( (n = 0.427) \)
- \( S_q = 280 \) nm \( (n = 0.484) \)
- \( S_q = 600 \) nm \( (n = 0.566) \)
DEM data on Contact Evolution

- **Asperity**
- **Transitional**
- **Hertzian**

\[ S_q = 70 \text{ nm} \]

\[ S_q = 280 \text{ nm} \]
What determines the nature of the stress:stiffness relationship?

- Complementary DEM + experimental research study showed that the exponent in the stress:stiffness relationship is influenced by surface roughness.

- Conclusions are robust as they are confirmed in lab and with simulations.

- DEM provided insight beyond that attainable in the laboratory by enabling classification of the contacts in each virtual sample.
Does the state parameter concept hold under a general stress state?

- Been and Jefferies state parameter concept is integrated in many constitutive models for sand behaviour.

- It is not easy to experimentally explore whether the quantitative relationships proposed by Been and Jefferies hold in a general stress state.

- This lack of understanding compromises our ability to use the developed constitutive models outside of axi-symmetric (triaxial) stress states.
Critical state is a state where the soil deforms at constant stress and constant void ratio.

Been and Jefferies (1985) Géotechnique

Critical state locus (CSL) for Toyoura sand Verdugo (1992) Géotechnique

Observations from direct shear tests:
• Peak friction angle ($\phi'$) depends on $e$
• Dilatancy depends on stress level
State Parameter for Sand: $\Psi$

Void ratio $e$

Deviatoric stress $q$

Mean effective stress $p'$

$q = \sigma'_1 - \sigma'_3$

$p' = \frac{1}{3}(\sigma'_1 + 2\sigma'_3)$ (triaxial case)

Been and Jefferies (1985)

Géotechnique
Variation in $\Phi'_p$ with $\Psi_0$

Experimental data from Jefferies and Been (2006)

$\Phi'_p$ = peak angle of shearing resistance
$\Psi_0$ = peak “friction” angle
$\Phi'_p$ = peak angle of shearing resistance
$\Psi_0$ = initial state parameter
Variation in $\Phi'_p$ with $\Psi_0$
In Situ Stresses

Stress increments beneath a circular footing on isotropic, linear elastic foundation

Contours of
\[
\frac{\Delta \sigma'_2 - \Delta \sigma'_3}{\Delta \sigma'_1 - \Delta \sigma'_3}
\]

\(\sigma'_1\) = major principal stress
\(\sigma'_2\) = intermediate principal stress
\(\sigma'_3\) = minor principal stress
\(\sigma'_1 > \sigma'_2 > \sigma'_3\)

Along CL:
- \(\Delta \sigma'_2 = \Delta \sigma'_3\)
- Triaxial conditions

Hight (1983)
Variation in Soil Strength with $b$

- **University of Bristol Cubical Cell**
- **Can control $b$**
  - $b=1$: Triaxial extension
  - $b=0$: Triaxial compression
  - $b\approx0.5$: Plane strain

$$b = \frac{\sigma'_{2}-\sigma'_{3}}{\sigma'_{1}-\sigma'_{3}}$$

- $\phi'_p$: peak angle of shearing resistance
- $\phi'_p = \text{peak "friction" angle}$

O’Sullivan et al. (2015); Géotechnique
DEM Analysis of $\psi$ for a 3D Stress State

- 20,164 spherical particles
- Periodic boundaries
- Grading similar to Toyoura sand
- Friction coefficient $\mu=0.25$
- Controlled $b$
- Deformed to large strain
- Varied initial state parameter ($\psi_0$)
- Most of simulations used LAMMPS

Huang et al. (2014)
Géotechnique
Variation in $\Phi'_p$ and $\Phi'_cs$ with $b$

$b=0$: Triaxial Compression  
$b=1$: Triaxial Extension

Huang et al. (2014)  
Granular Matter

$\Phi'_p$, $\Phi'_cs$ with $b$

$\Phi'_p = \frac{\sigma'_2 - \sigma'_3}{\sigma'_1 - \sigma'_3}$

Legend:
- Ogawa
- Satake
- Matsuoka-Nakai
- Lade
- $e_0 = 0.646, \sigma'_3 = 500$ kPa
- $e_0 = 0.533, \sigma'_3 = 100$ kPa
- $e_0 = 0.612, \sigma'_3 = 5000$ kPa
- $e_0 = 0.625, \sigma'_3 = 2000$ kPa
- $e_0 = 0.625, \sigma'_3 = 1000$ kPa
- $e_0 = 0.646, \sigma'_3 = 500$ kPa
Sensitivity of CSL locus to $b$
State-Dependent Response

Ψ > 0  loose  \( q = \sigma_1' - \sigma_3' \)
Ψ < 0  dense  \( p' = \frac{1}{3}(\sigma_1' + 2\sigma_3') \)
(triaxial)

Huang et al. (2014)
Géotechnique
Variation in $\Phi'_p$ with $\psi_0$

Experimental data from Jefferies and Been (2006)
Variation in $\Phi'_p$ with $\psi_0$

Huang et al. (2014)
Géotechnique
Variation in $\Phi'_p - \Phi'_{cs}$ with $\Psi_0$

Experimental data from Jefferies and Been (2006)
Variation in $\Phi'_p - \Phi'_{cs}$ with $\Psi_0$

Huang et al. (2014)
Géotechnique
Variation in $D_p$ with $\psi_0$

Dilatancy at Peak, $D_p$

Experimental data from Jefferies and Been (2006)
Variation in $D_p$ with $\psi_0$

- Jefferies and Been
- DEM $b=0$
- DEM $b=0.2$
- DEM $b=0.3$
- DEM $b=0.4$
- DEM $b=0.5$
- DEM $b=0.6$
- DEM $b=0.8$
- DEM $b=1.0$
- DEM Plane Strain

Huang et al. (2014) Géotechnique
Consideration of NORSAND model

Dense Sample:
\[ \sigma_3' = 300 \text{ kPa}, \psi_0 = -0.0823 \]

Loose Sample:
\[ \sigma_3' = 500 \text{ kPa}, \psi_0 = 0.0171 \]

Huang et al. (2014)
Geotechnique
Does the state parameter concept hold under a general stress state?

• Been and Jefferies state parameter concept is integrated in many constitutive models for sand behaviour.

• DEM simulations show that the quantitative relationships proposed by Been and Jefferies hold in a true-triaxial stress state.

• Constitutive models can be calibrated to capture the DEM data and give confidence in their predictive capacity outside of axi-symmetric (triaxial) stress states.
At a given stress level why do we see more crushing in shearing than in compression?

- Can DEM capture the trends reported from experimental studies?

- Can the particle-scale data available in the DEM simulations explain the experimental observations?
Influence of crushing on load:deformation behaviour

Use of Hardin’s relative breakage to quantify crushing

\[ B_r = \frac{A_1}{A_1 + A_2} \]

Hanley et al S+F (2015)
Influence of crushing on load-deformation behaviour

\[ B_r = \frac{A_1}{A_1 + A_2} \]

Coop and Lee (1993)
Influence of crushing on load-deformation behaviour

Coop and Lee (1993)

1. Can a DEM simulation capture difference in extent of crushing on CSL when compared with NCL at the same stress level?

2. Can DEM simulation data explain the difference in extent of crushing?
Influence of crushing on load: deformation behaviour

- DEM simulations used particle size distribution similar to Dunkirk sand
- Isotropic compression in a periodic cell
- Strain controlled triaxial compression with a constant $\sigma'_3$
Influence of crushing on load:deformation behaviour

- Maximum force crushing criterion
- Particle shrunk to lose all contacts if criterion reached
Influence of crushing on load-deformation behaviour

Evolution of PSD with compression
Influence of crushing on load-deformation behaviour

- Maximum force crushing criterion
- Particle shrunk to loose all contacts if criterion reached
Influence of crushing on load deformation behaviour

Simulations without crushing

Simulations modelling crushing
Influence of crushing on load:deformation behaviour

Simulations without crushing

Simulations modelling crushing
Influence of crushing on load-deformation behaviour

Simulations without crushing

Simulations modelling crushing
Influence of crushing on load-deformation behaviour

\[ B_r = \frac{A_1}{A_1 + A_2} \]

---

Graph showing the percentage passing (by volume) against particle diameter (mm) for different pressure levels. The graph compares the PSD (Particle Size Distribution) before and after crushing.
Muir Wood and Maeda proposed that CSL moves downwards as crushing progresses.
Influence of crushing on load-deformation behaviour

Coop and Lee (1993)
Influence of crushing on load:deformation behaviour
Influence of crushing on load:deformation behaviour

Comparison of isotropic compression 8 MPa to 16 MPa and triaxial shearing at $\sigma_3=8$ MPa

Contact number ratio

\[ CNR = \frac{C_d}{C_0} \]

$C_d=$ total number of distinct contacts
$C_0=$ No. of contacts at start of simulation

Mean effective stress, $p'$ (kPa)
At a given stress level why do we see more crushing in shearing than in compression?

• DEM can capture the trends reported from experimental studies.

• The particle-scale data available in the DEM simulations show that there is significantly more variation in the forces experienced at contacts during shearing than during compression.

• The particle-scale data also show that contact evolution (formation of new contacts) is greater in shearing than in compression.
Conclusions

• DEM can capture many of the complex response phenomena associated with sand behavior.

• DEM can generate the particle scale data to explain the overall mechanical response observed in laboratory element tests.

• DEM can be used to complement experimental research by considering frameworks and constitutive models under stress states that cannot be attained experimentally.
Acknowledgements

• My former PhD students and Post-Docs
• Technicians at in Imperial College Soil Mechanics Laboratory
• Engineering and Physical Sciences Research Council
• Institution of Civil Engineers Research & Development Fund
• JASSO
• Dixon Scholarship Imperial College
• Royal Commission for Exhibition of 1851