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DE CATALUNYA
BARCELONATECH

Microscopic calibration of rolling friction to mimic particle shape effects in DEM

Riccardo Rorato

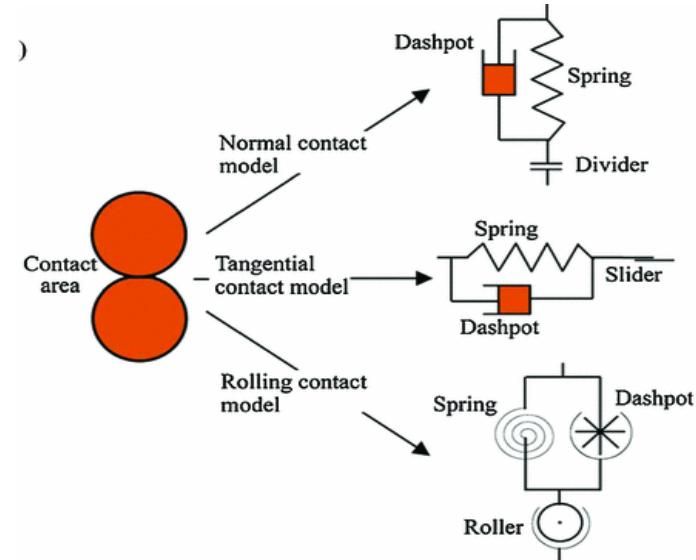
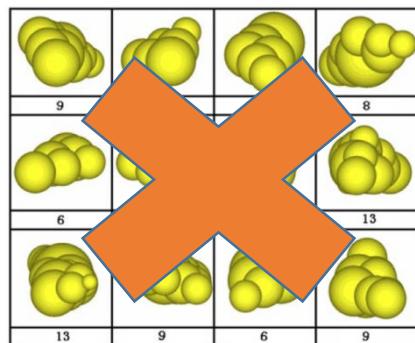
UPC: Marcos Arroyo, Antonio Gens

UGA: Edward Andò, Cino Viggiani

Itasca Symposium 2020
University of Vienna
19/02/2020

Objective:

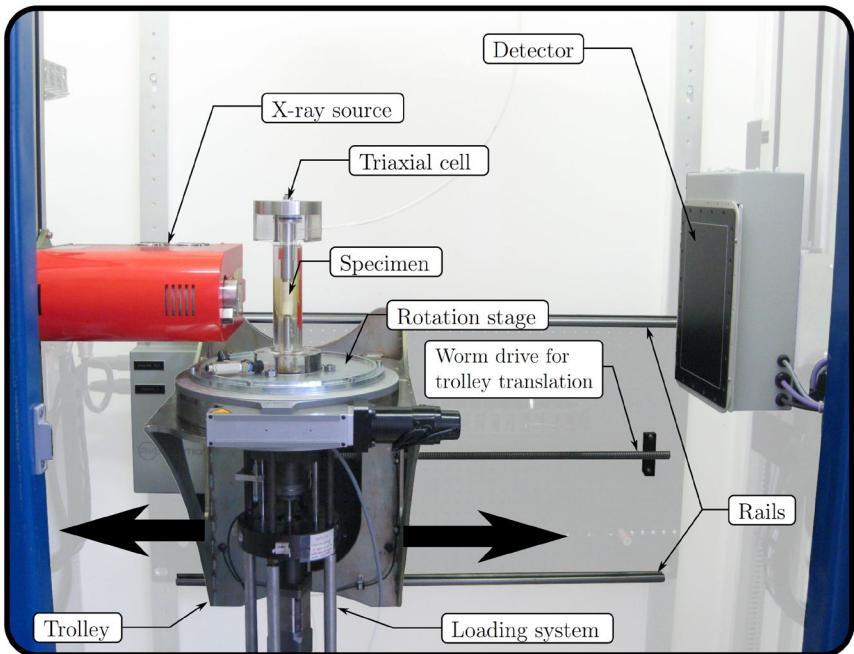
Enhance DEM simulations taking into account the shape of particles without dramatically increase the computational time



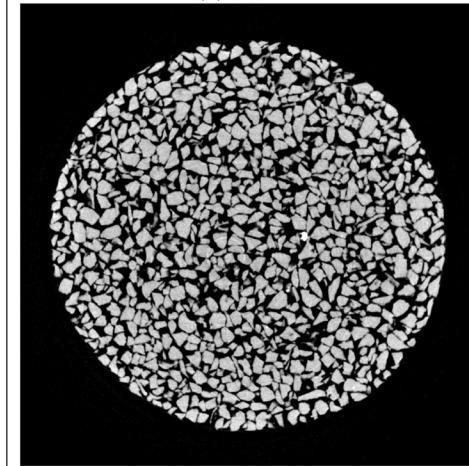
Tasks:

- Evaluate and quantify the 3-D shape of sand particles (x-rays μ -CT)
- Investigate the relationship between particle shape and kinematics
- Implement and calibrate a new constitutive model for DEM
(based on the rolling resistance concept)
- Test and exploit the constitutive model for larger DEM simulations
(e.g. CPT in the VCC)

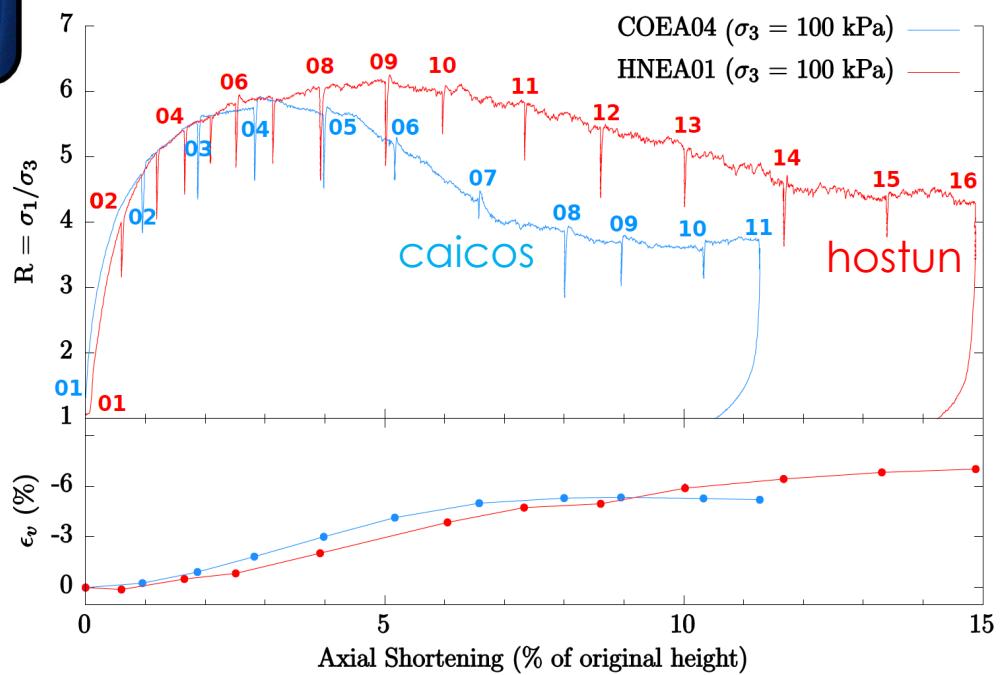
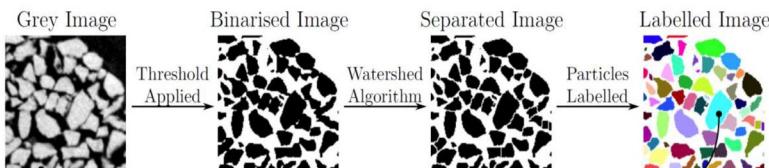
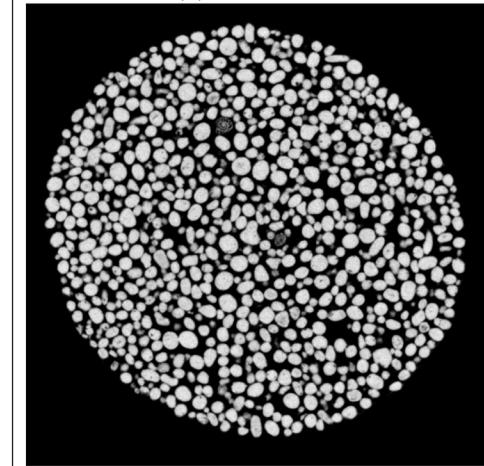
X-rays micro-tomography for geomaterials



HOSTUN sand

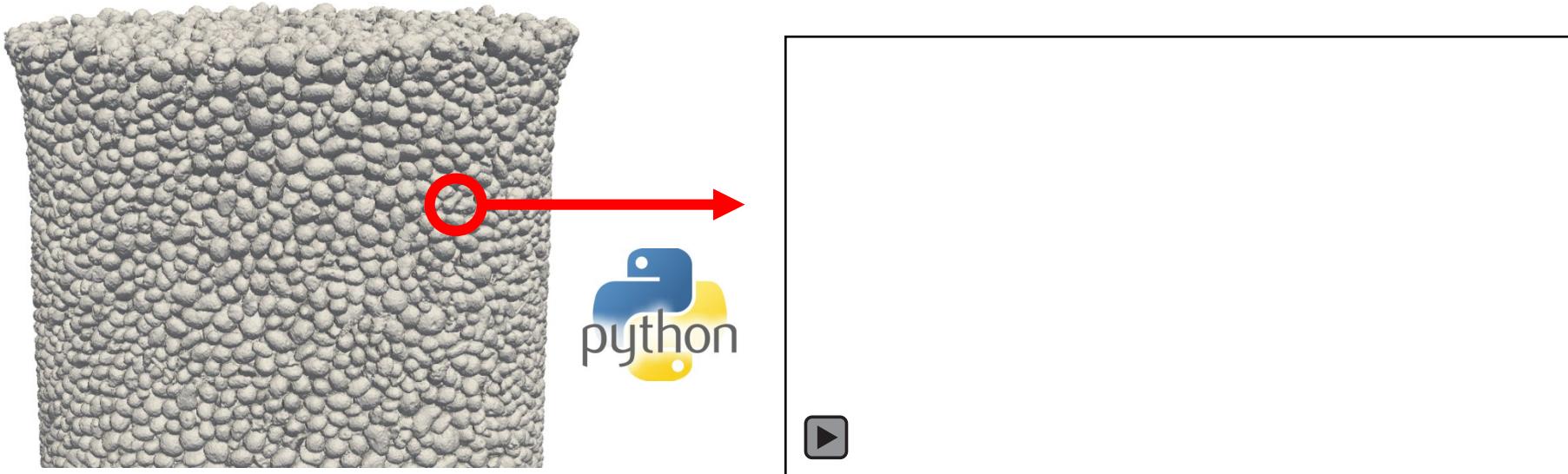


CAICOS ooids



(Edward Andò, 2013)

Numerical quantification of particle geometry



Geometrical properties numerically measured:

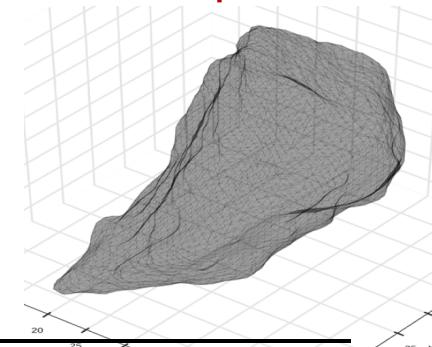
- Volume (summing up all the voxels)
- Surface area (Marching Cubes algorithm, after Gaussian filter)
- Equivalent sphere properties (i.e. equivalent grain diameter, surface area of the equivalent sphere, etc.)
- Short, intermediate, longest axis
- Convex hull
- Maximum (and Minimum) inscribed (circumscribed) sphere
- Eigenvalues / Eigenvector of inertia tensor

NB: All the algorithms have been validated against ideal cases (i.e. spheres, spheroids, ellipsoids)

Numerical quantification of particle shape descriptors

The previous properties can be combined together in order to create some shape descriptors

Grain
46972 of
specimen
HNEA01

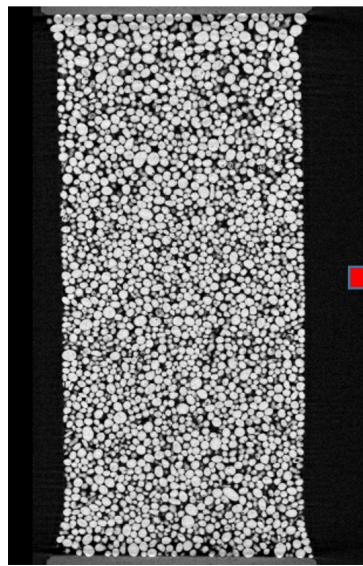


Shape descriptor	Equation	
Degree of true sphericity, Ψ	$\frac{S_n}{S}$	0.7427
Flatness index, FI	c/b	0.4982
Elongation index, EI	b/a	0.7496
Intercept sphericity, Ψ_{int}	$\sqrt[3]{\frac{bc}{a^2}} = \sqrt[3]{FI(EI)^2}$	0.6542
Operational sphericity, Ψ_{op}	$\sqrt[3]{\frac{V}{V_{CS}}}$	0.5661
Convexity, Co	V/V_{CH}	0.8274
Alshibli Sphericity, Ψ_{al}	$\frac{V}{V_{d=c}}$	3.8868

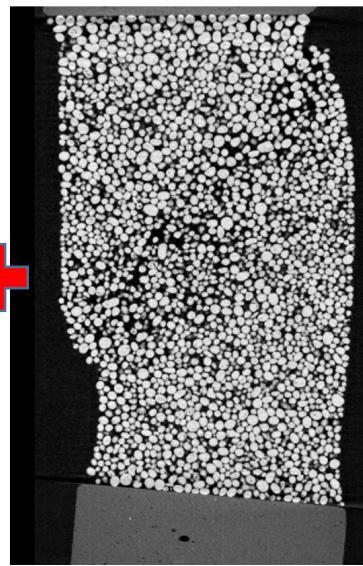
→ Statistical distribution of shape parameters

3D Digital Image Correlation: TomoWarp2 (Discrete)

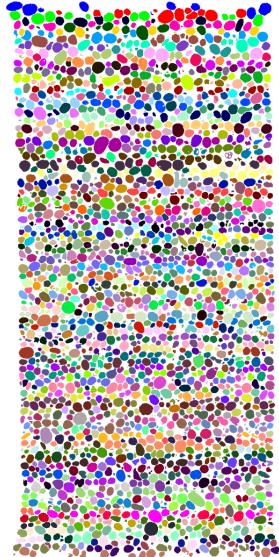
4
I
N
P
U
T
S



Step "01"

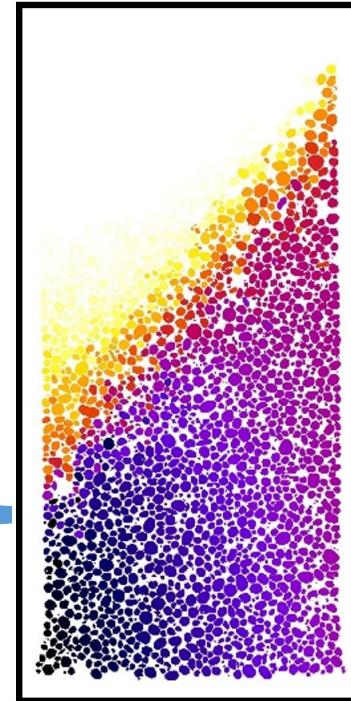


Step "12"
(can be any)

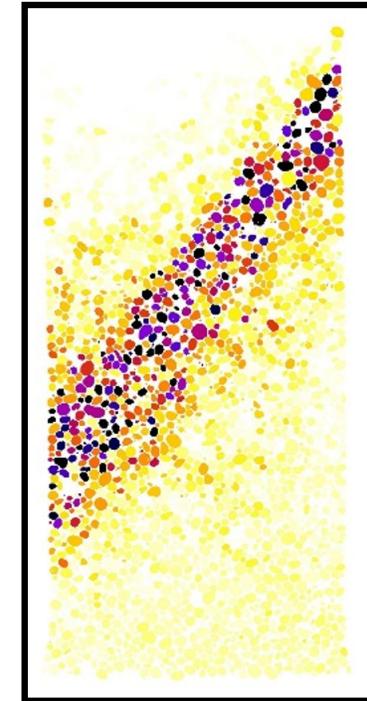


+
File containing
the
displacements of
the previous
correlation

Accumulated
Z-displacement



Accumulated
Total rotation

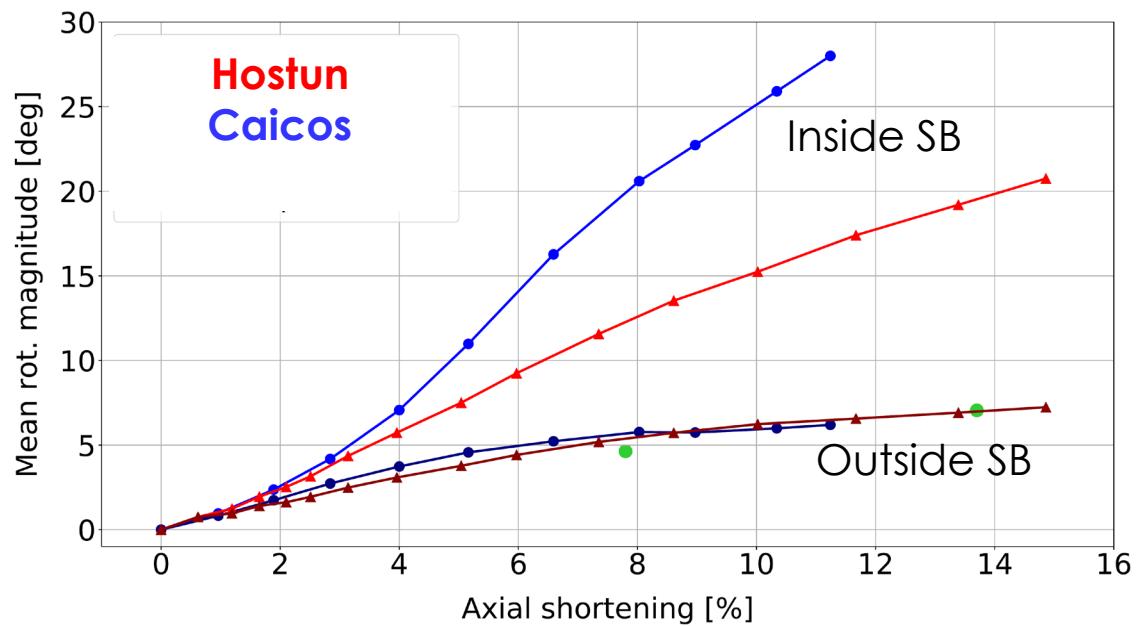


2
O
U
T
P
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T
S

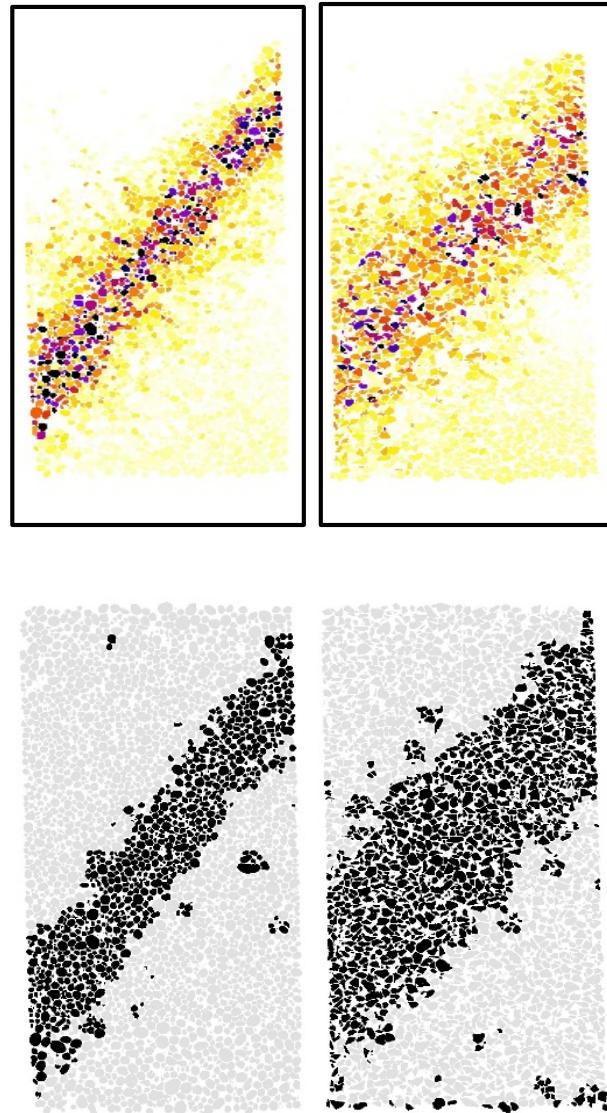
0 pixels (vertical displacement)
0° (rotation)

-200 pixels (vertical displacement)
60° (rotation)

History of mean grain rotations



CAICOS HOSTUN

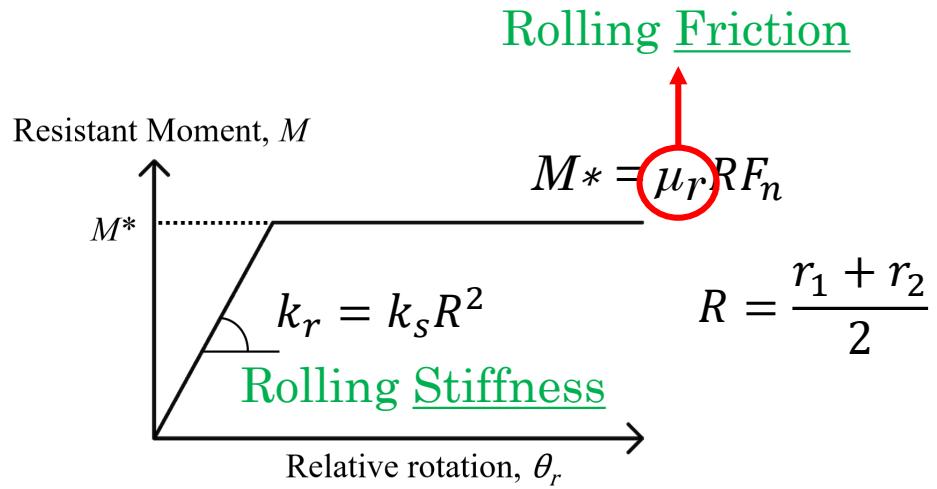
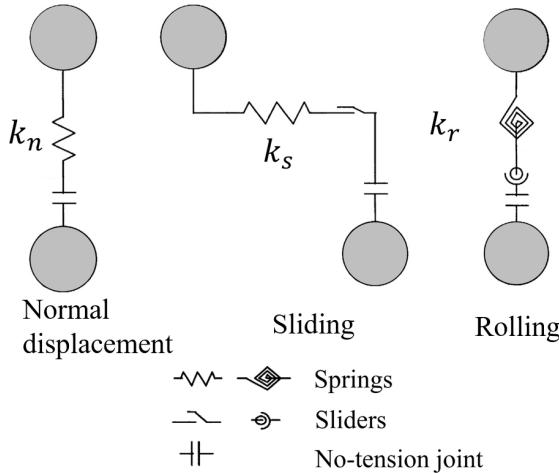


Relating rolling resistance and particle shape

Goal: Relate Particle Shape (?) → Rolling Resistance (?)

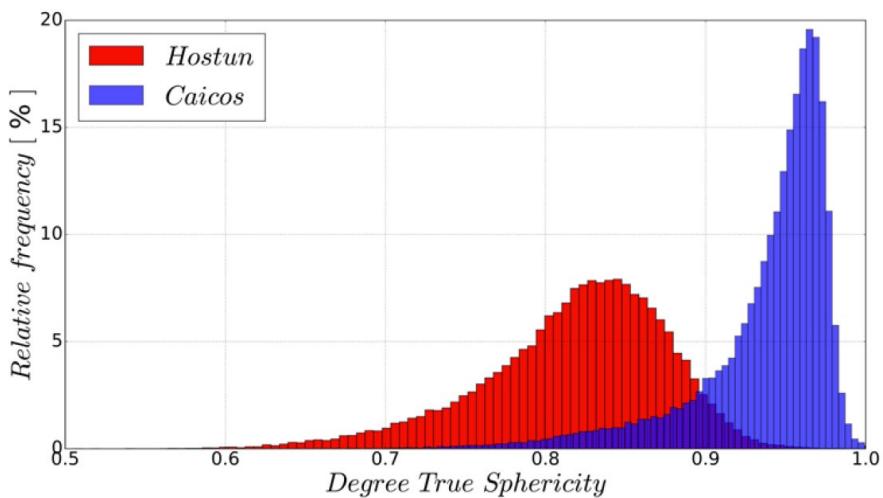
Assumptions:

- Linear contact model in the normal/shear direction
- Simplified Iwashita & Oda CM (no additional viscous dissipations) in the rolling direction (implemented in PFC5)



Particle Shape

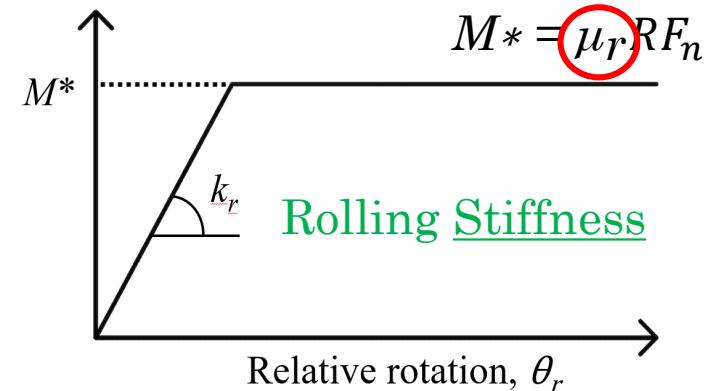
From the experiments, we know the “*degree of true sphericity (Ψ)*” is the shape parameter that most affects particles rotations



Rolling Resistance

Resistant Moment, M

Rolling Friction



Rolling Stiffness

A blue curved arrow points from the bottom left towards a central box. Inside the box is the equation $\mu_r = a \psi^b$, where a and b are red variables.

Applied to all particles involved in the simulations

Ψ is a particle property

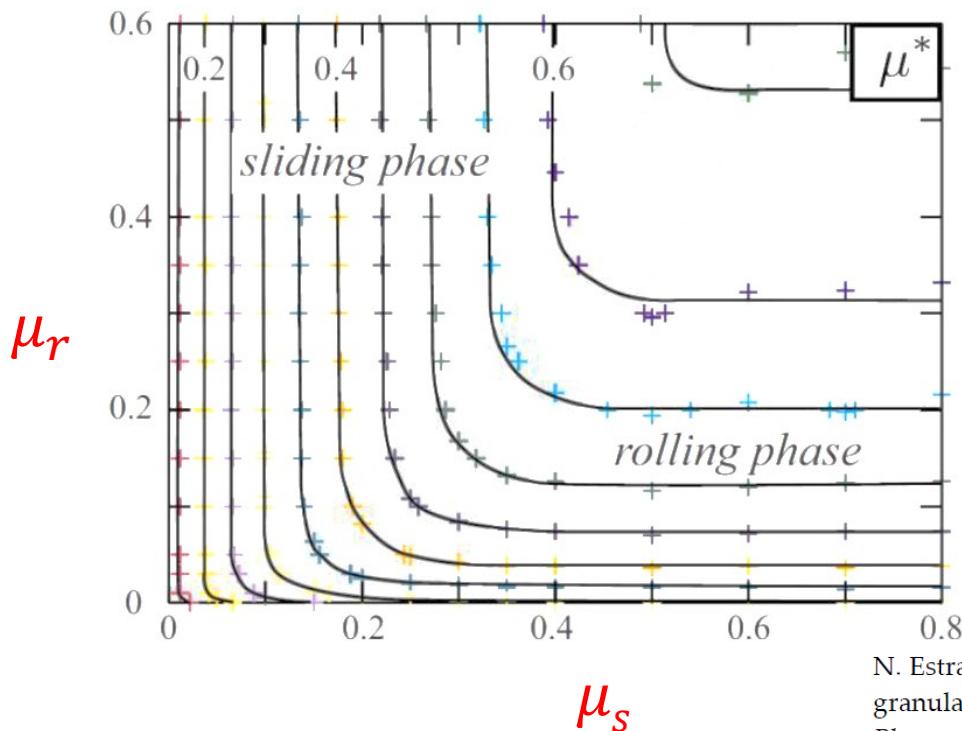
$$\mu_r = \min(\mu_{r,1}, \mu_{r,2})$$

μ_r is a contact property

→ Try to find the set of parameters (a , b and μ_s , by trial & error) that best match the triaxial responses of HNEA01/COEA04 in terms of:

- 1) Stress-strain response
- 2) Volumetric response
- 3) **Rotations inside shear band**

$$\left. \begin{array}{l} \mu_r = a \psi^b \\ \mu_s \end{array} \right\}$$



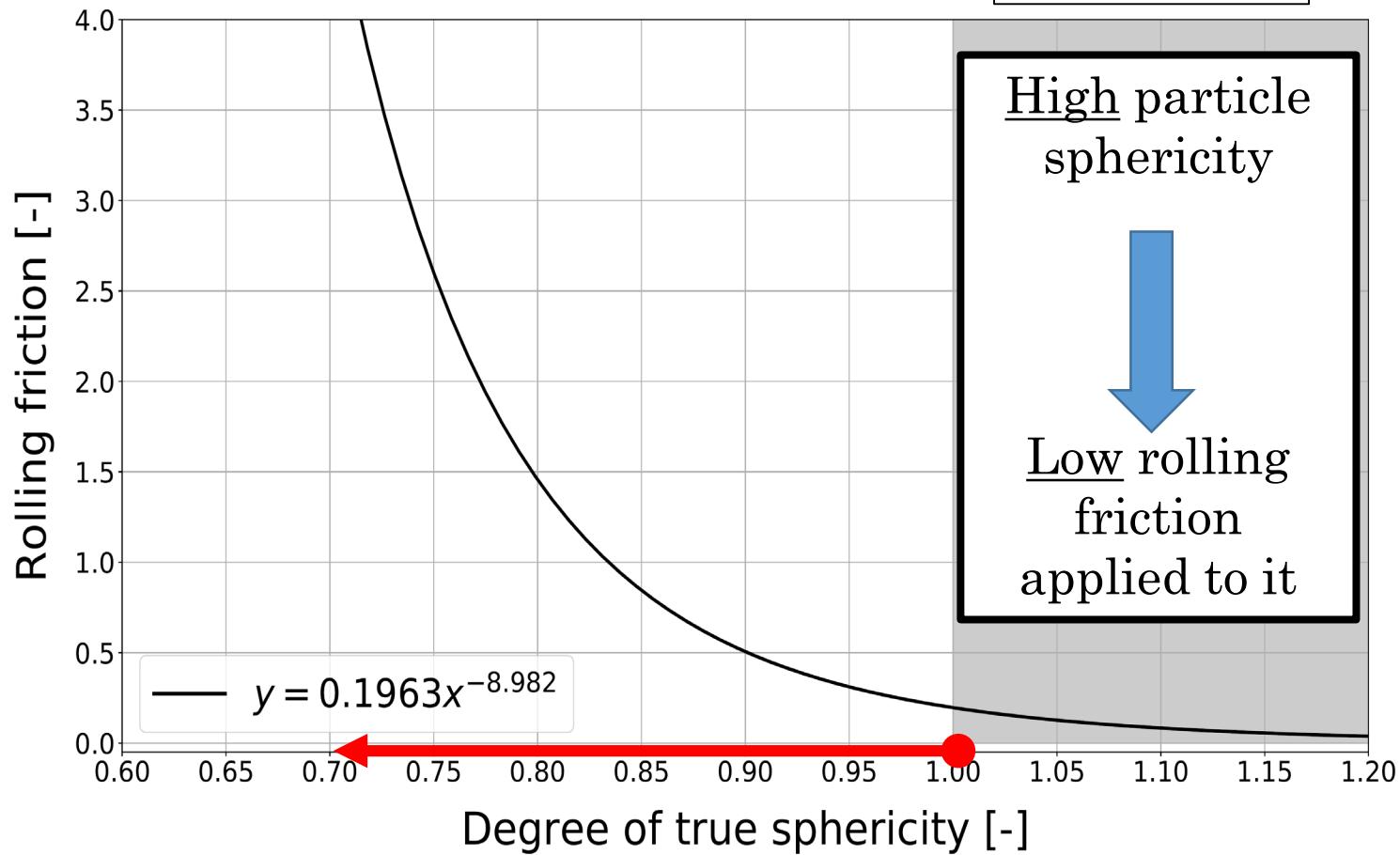
The same macro-mechanical response can be obtained by using several sets of parameters, but the rotation information (from DVC) provides a UNIQUE solution

Calibration procedure

Macro-mechanical responses
(TX tests Hostun/Caicos at 100kPa)

- Match **Granulometry** and **porosity** → Scale 1:1
- **Compress isotropically** at 100kPa confining pressure
 - (with rigid-walls and servo-controlled mechanism)
- Shear the sample at low rate (small “*Inertial number*”)

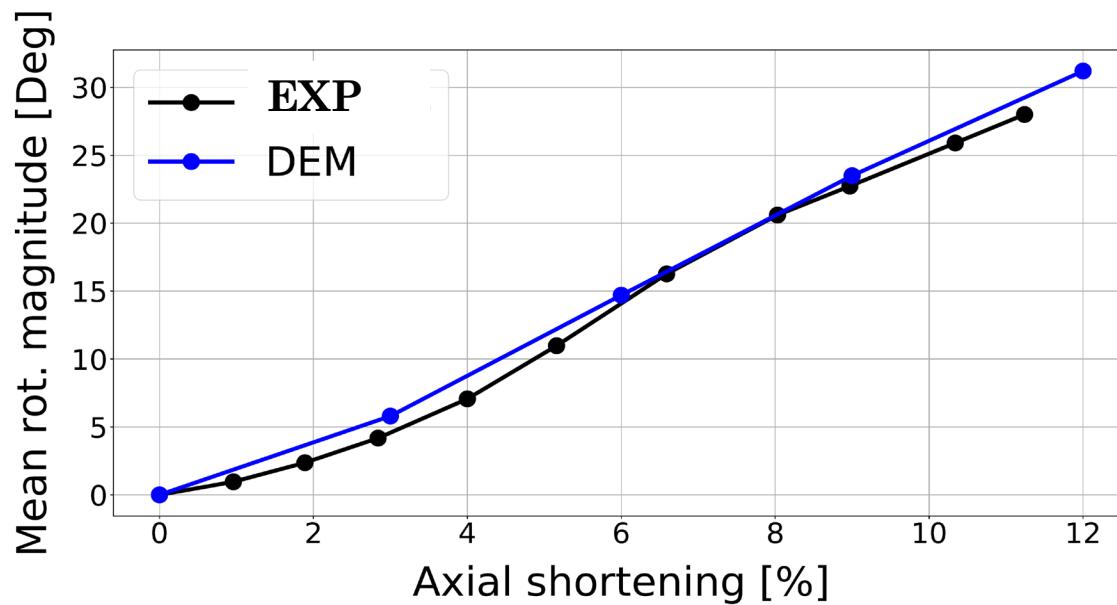
$$\mu_r = \alpha \psi^b$$



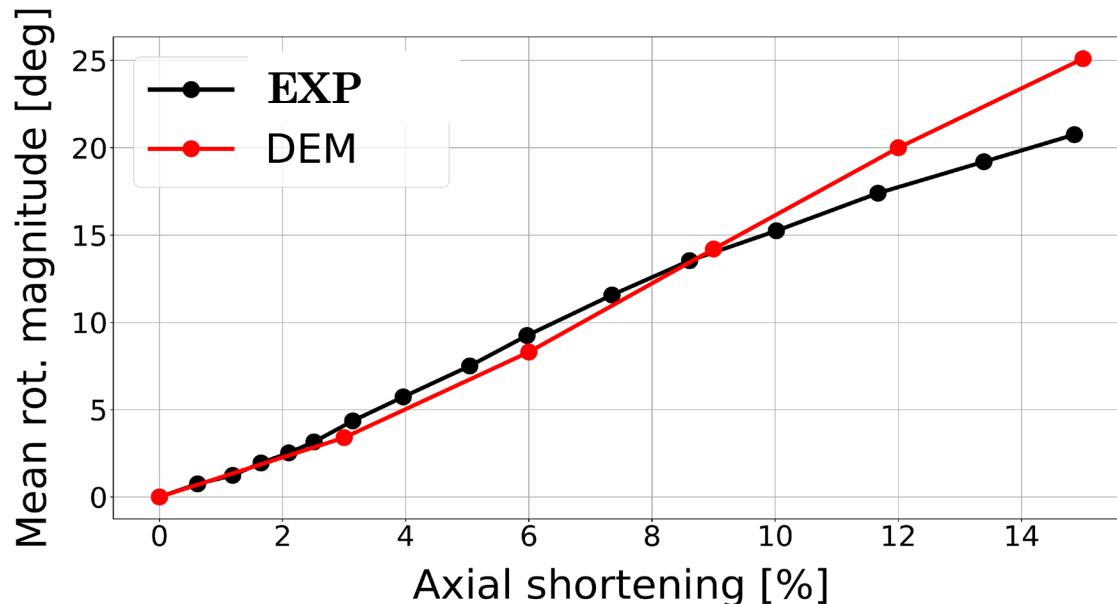
Calibrated for two sands but meant to be “universal”!

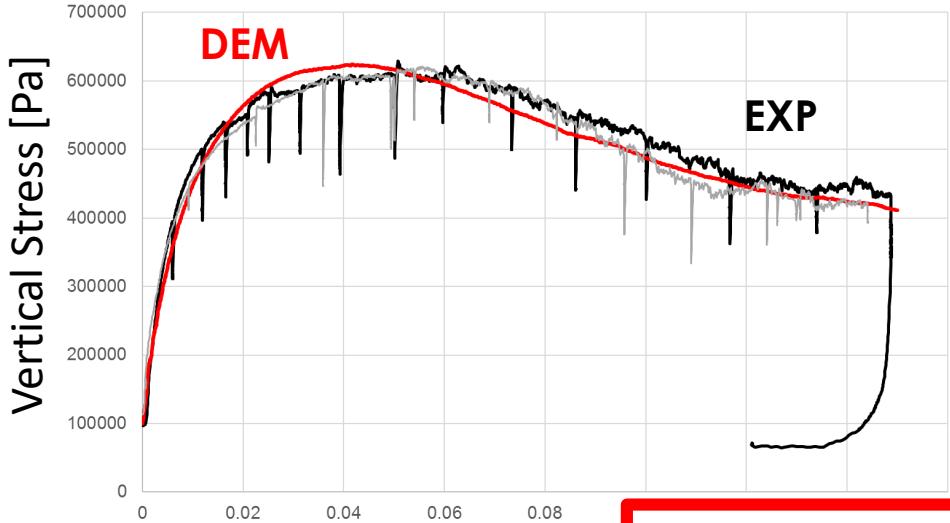
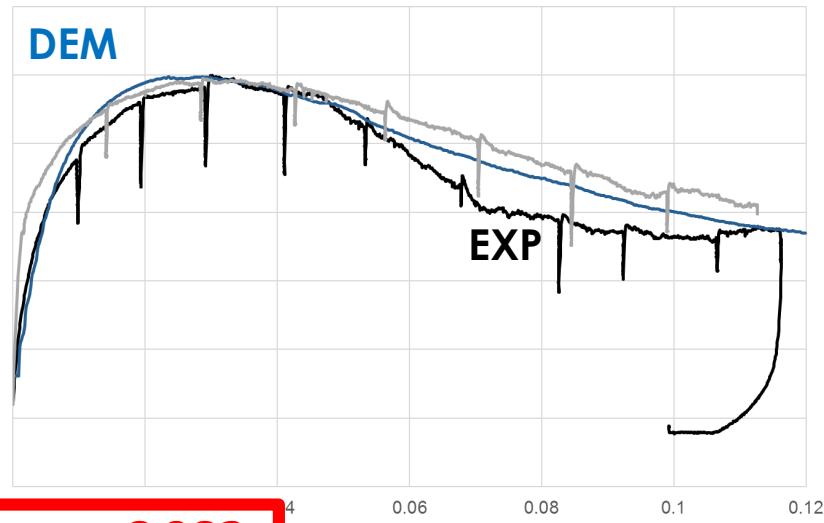
Histories of Mean Rotations (EXP vs DEM) inside the shear band

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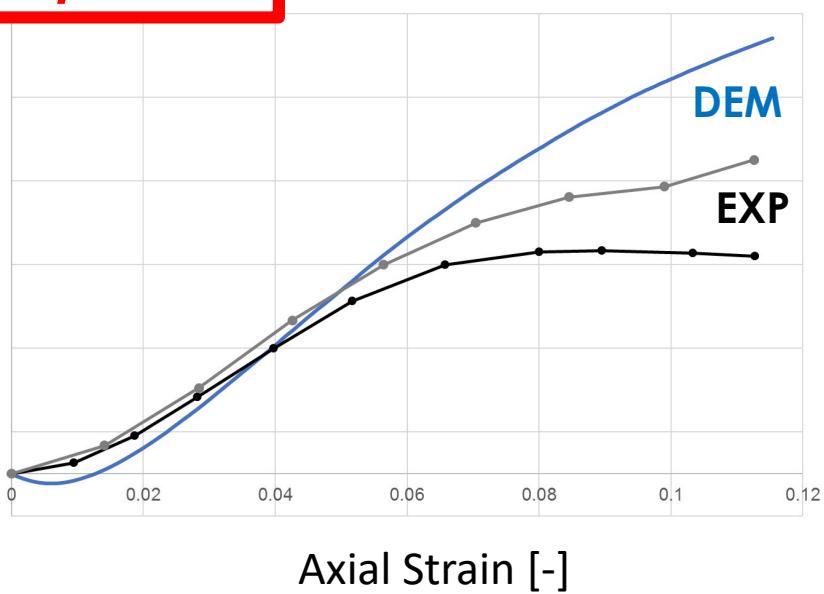
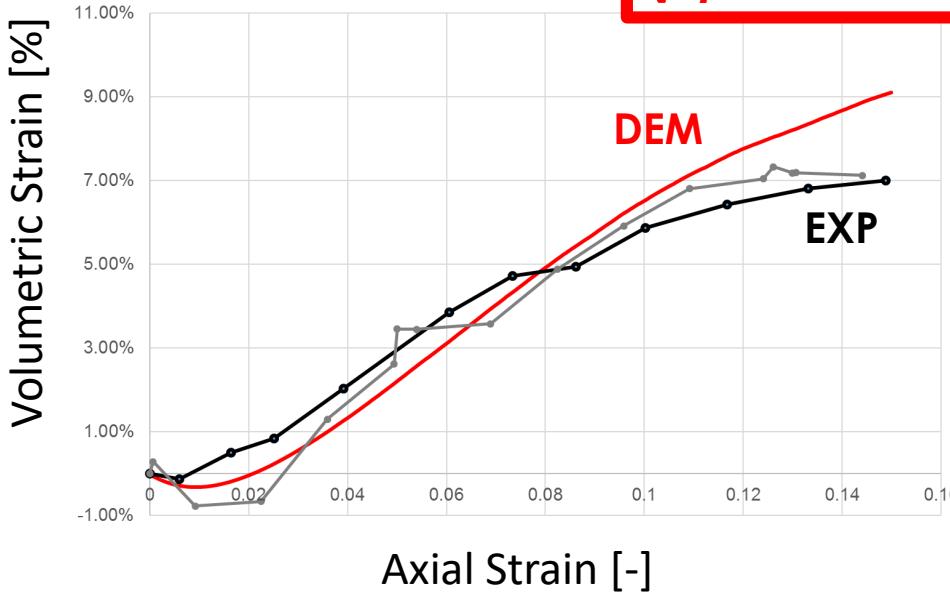


HOSTUN sand



HOSTUN sand $\mu = 0.55$ **CAICOS ooids** $\mu = 0.60$ 

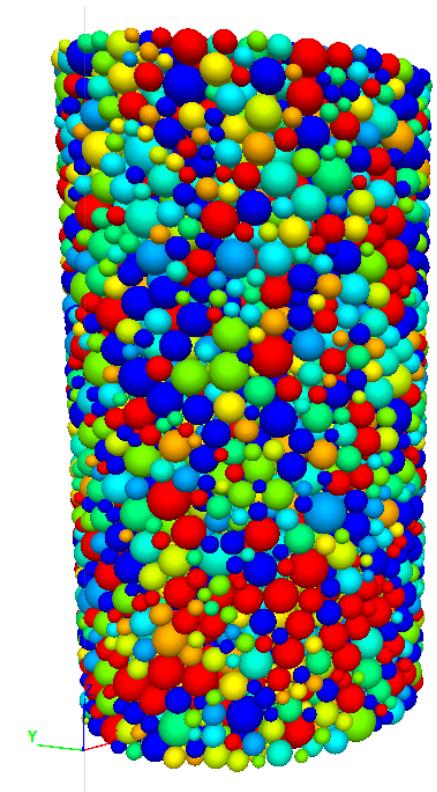
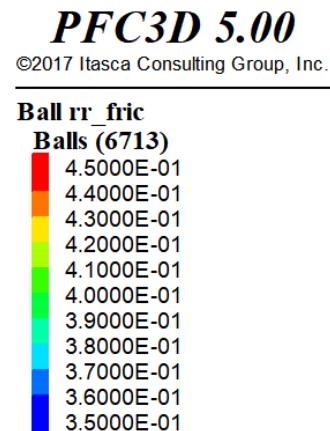
$$\mu_r = 0.1963 \psi^{-8.982}$$



Summarising:

Procedure for optimal DEM calibration using rolling resistance to mimic grain shape

- 1) Compute the *3D true sphericity* of thousands of grains from one 3D labelled image of sand (I'm sorry but you need a tomograph...)
- 2) Create the DEM initial sample replicating PSD and porosity
- 3) Apply the equation relating the *degree of true sphericity* and *rolling friction*
$$\mu_r = 0.1963 \psi^{-8.982} \text{ (for each particle)}$$
- 4) Perform the triaxial compression, calibrating the *sliding friction coefficient* by trial & error (and k_n, k_s ...)



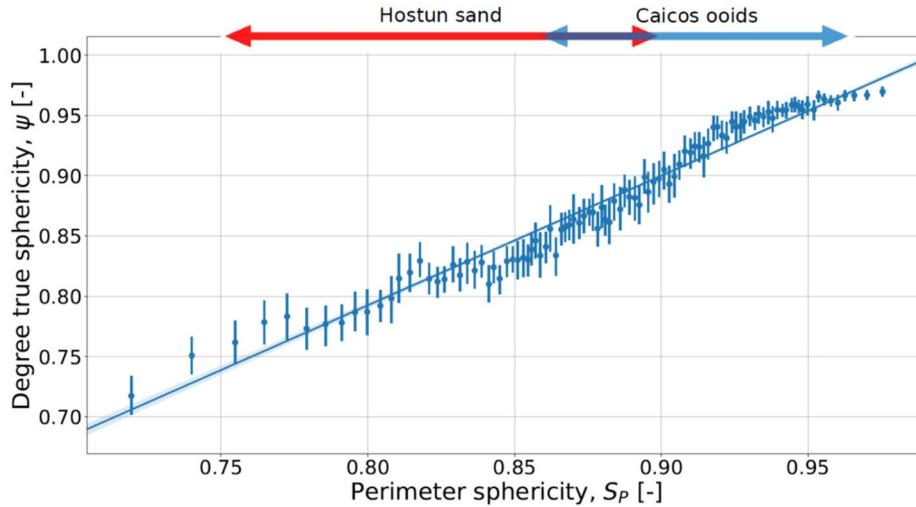
What if you don't have a tomograph?

From
projection of
grains laying
on their plane
of greatest
stability

SHAPE DESCRIPTOR	Ψ	S_A	S_D	S_C	S_P	S_{KS}
<i>True Sphericity 3D</i>	1.00	0.70	0.69	0.72	0.83	0.36
<i>Area sphericity 2D</i>	0.70	1.00	1.00	0.96	0.80	0.81
<i>Diameter sphericity 2D</i>	0.69	1.00	1.00	0.96	0.80	0.81
<i>Circle ratio sphericity 2D</i>	0.72	0.96	0.96	1.00	0.82	0.79
<i>Perimeter sphericity 2D</i>	0.83	0.80	0.80	0.82	1.00	0.45
<i>KS sphericity 2D</i>	0.36	0.81	0.81	0.79	0.45	1.00

Table 11: Correlation matrix showing 3D and 2D sphericity parameters (obtained from projections oriented along the minor principal axis). Merged data for Hostun and Caicos, 2000 grains for each one.

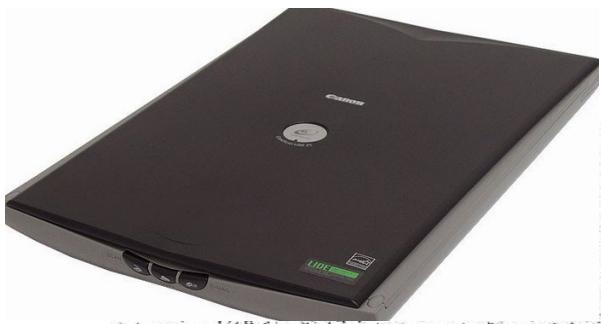
(Rorato et al.,
2019, Eng. Geo.)



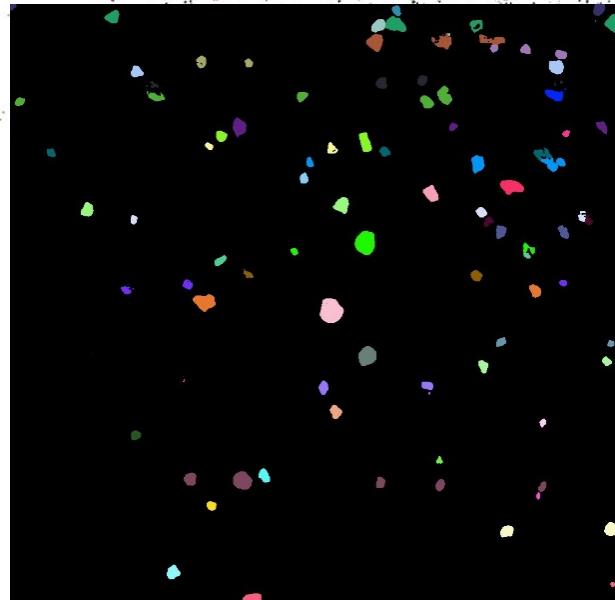
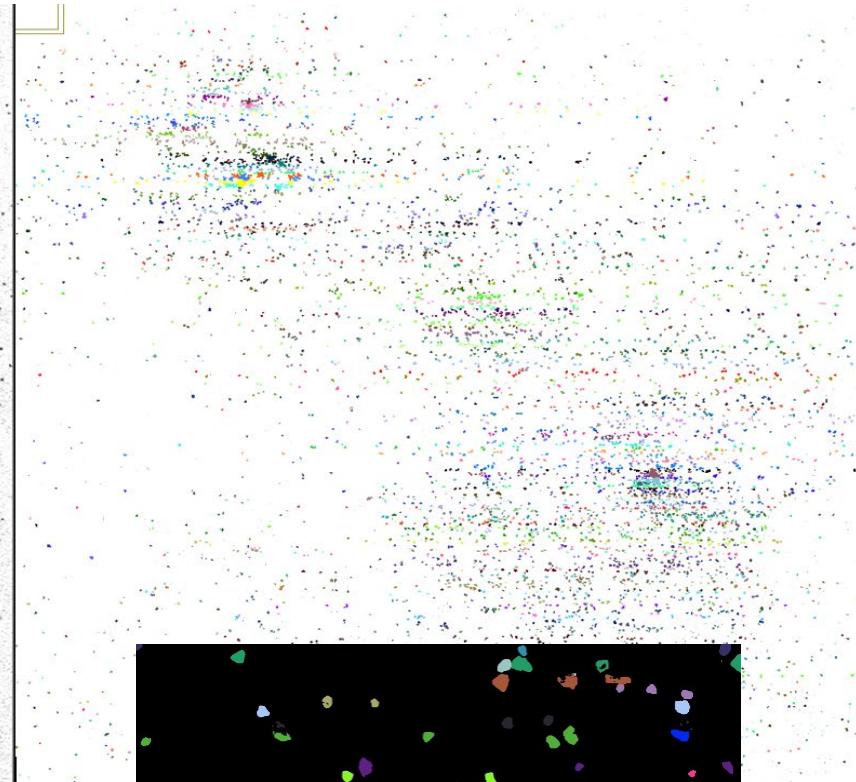
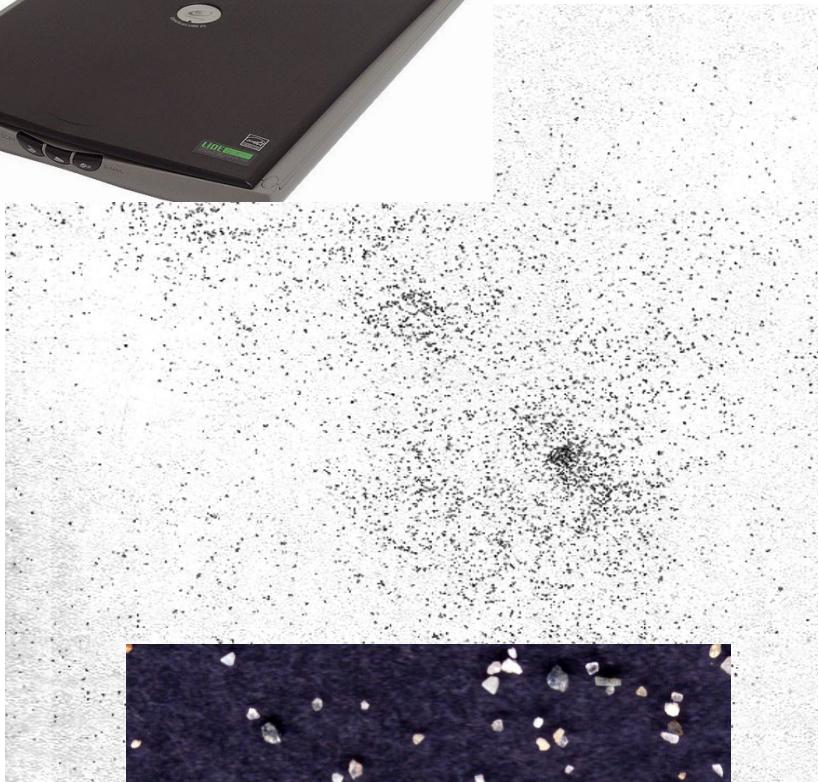
$$\psi = 1.075(S_P) - 0.067$$

[3D] [2D]

Figure 11: Linear regression line between true sphericity (3D) and perimeter sphericity (2D). The arrows show the ranges (5% and 95% percentiles) of the two sands.



Ticino sand



Summarising:

Procedure for optimal DEM calibration using
rolling resistance to mimic grain shape

- 1) Compute the *3D true sphericity* of thousands of grains from one labelled image of sand (~~I'm sorry but you need a tomograph...~~)

→ Simply scan some grains with a table scanner!

- 2) Create the DEM initial sample replicating PSD and porosity

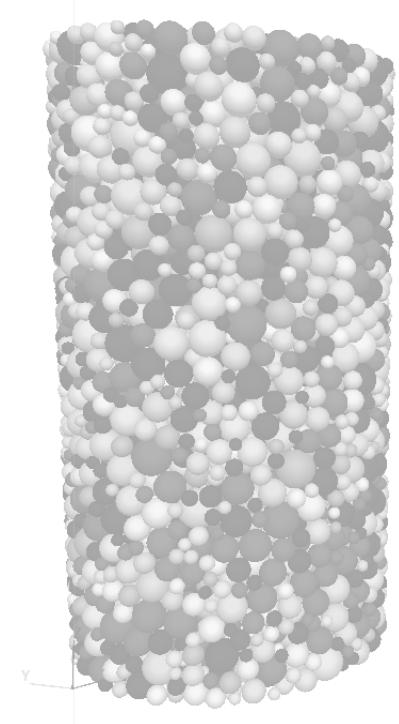
- 3) Apply the equation relating the *degree of true sphericity* and *rolling friction*

$$\mu_r = 0.1963 \psi^{-8.982} \text{ (for each particle)}$$

- 4) Perform the triaxial compression, calibrating the *sliding friction coefficient* by trial & error

PFC3D 5.00
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Ball rr_fric	Balls (6713)
4.5000E-01	
4.4000E-01	
4.3000E-01	
4.2000E-01	
4.1000E-01	
4.0000E-01	
3.9000E-01	
3.8000E-01	
3.7000E-01	
3.6000E-01	
3.5000E-01	



Conclusions

- Particle shape and shape variability are important ingredients that should be taken into account in DEM
- A novel approach to relate univocally grain shape (i.e. true sphericity) with rolling friction has been proposed. The stress-volumetric-strain responses of rounded/angular sands can be well reproduced, and the kinematics (at failure) is respected
- Doesn't matter if you don't have a tomograph, you just need perimeters sphericities...
- **The calibration coupling problem between *sliding/rolling friction coefficients* is solved, if you know the shape distribution of your sand**
- Robust model: validated for 4 different sands at 3 different confining pressures (100kPa, 200kPa and 300kPa)

Thanks for your attention

riccardo.rorato@upc.edu



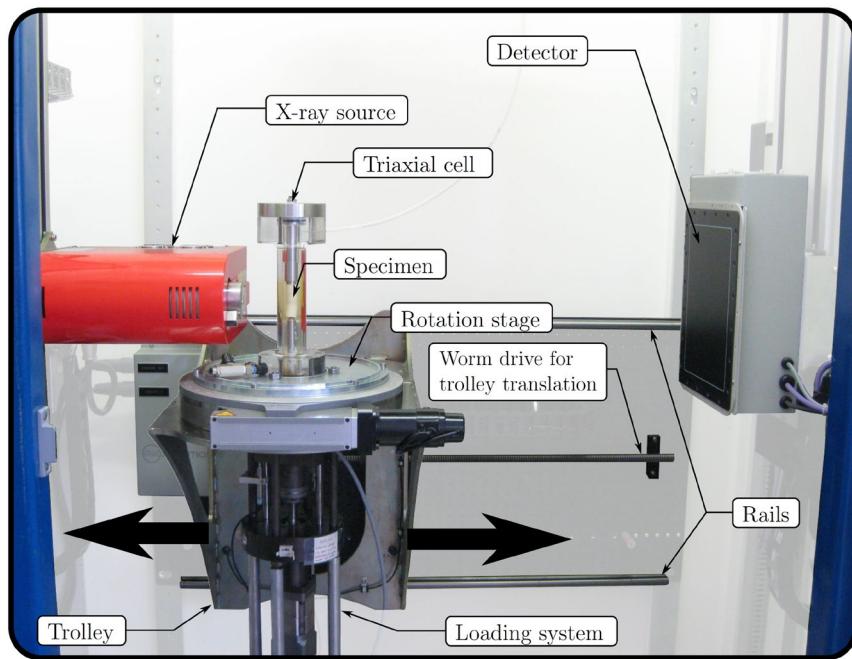
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Department of Geotechnical Engineering and Geosciences (UPC)

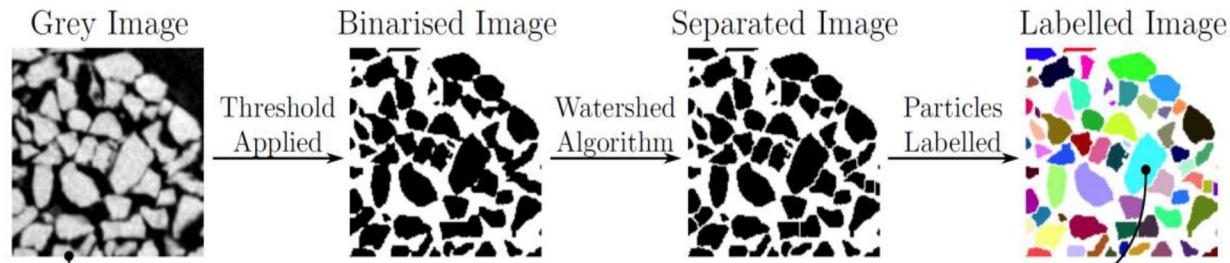
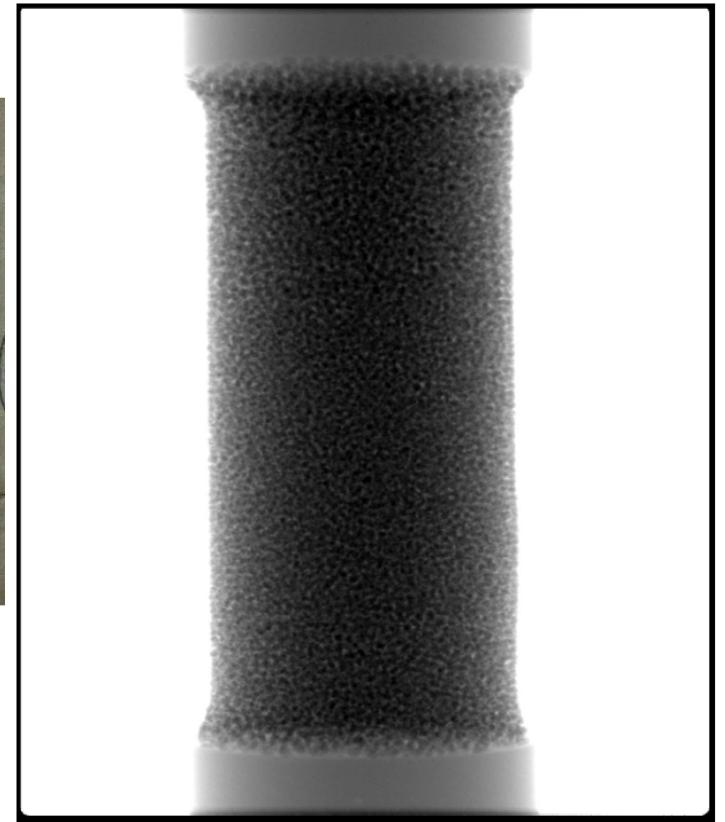
BarcelonaTech Moduli D2 Campus Nord UPC - C. Jordi Girona 1-3

Barcelona (Spain)

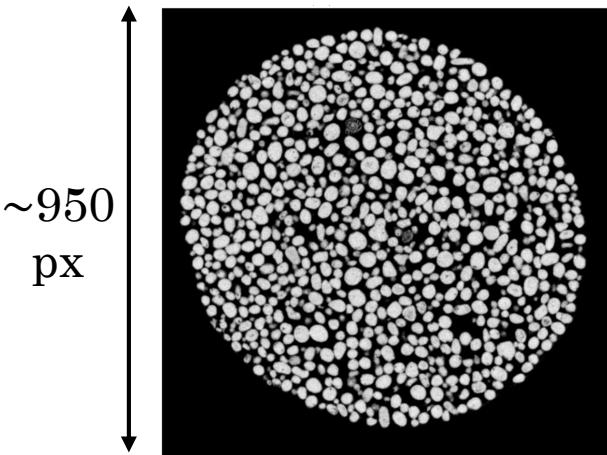
2.1) Introduction



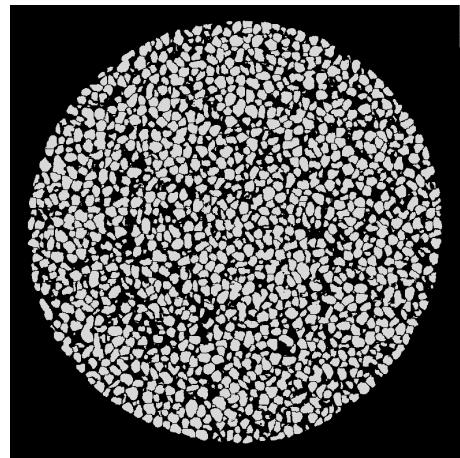
(Andò E., 2013)



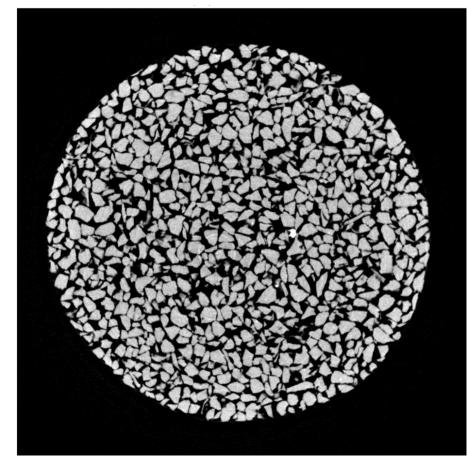
CAICOS ooids



Ottawa sand



HOSTUN sand

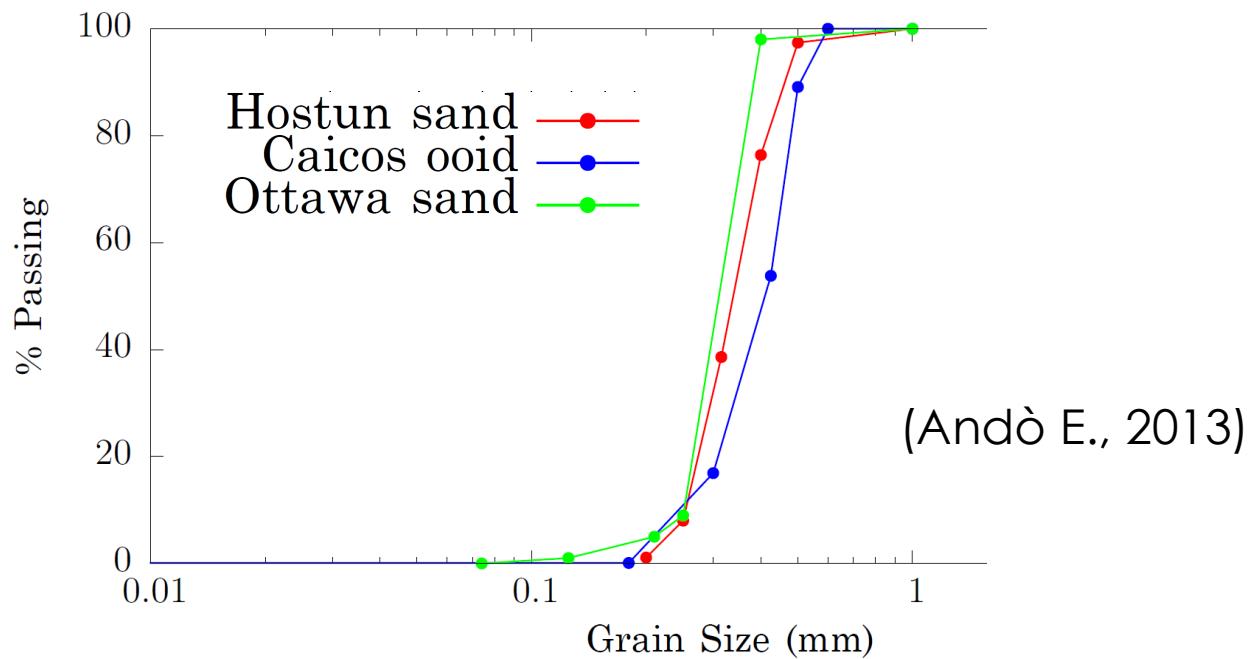


Images resolution:
 $15.56\mu m/px$

$$D_{50, ottawa} = 310\mu m$$

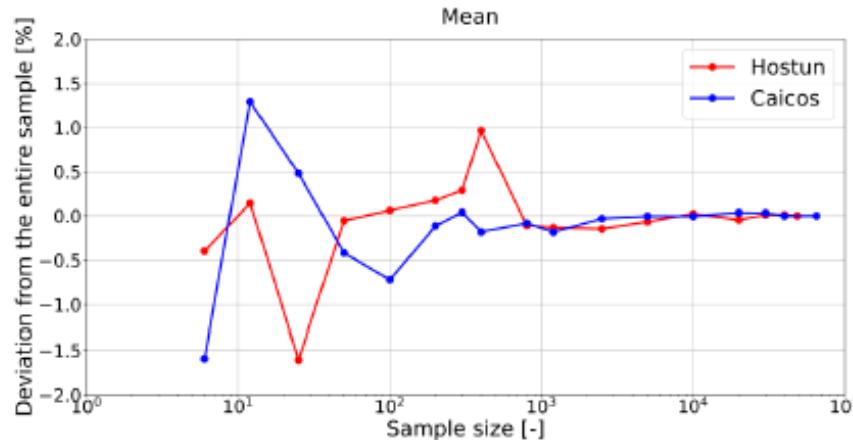
$$D_{50, Hostun} = 338\mu m$$

$$D_{50, caicos} = 420\mu m$$

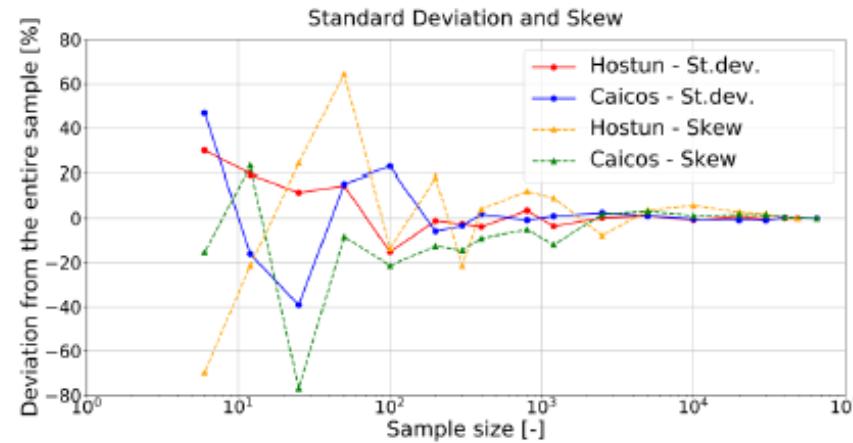


Name	Mean Hostun Caicos Ottawa	St. Dev. Hostun Caicos Ottawa	Skew Hostun Caicos Ottawa	CV Hostun Caicos Ottawa
Volume (mm³)	0.027	0.017	1.53	0.63
	0.025	0.017	2.31	0.68
	0.014	0.005	3.21	0.39
True Sphericity	0.82	0.06	-0.75	0.07
	0.94	0.04	-1.89	0.04
	0.88	0.05	-1.55	0.06
Flatness index	0.73	0.14	-0.22	0.19
	0.85	0.09	-0.65	0.11
	0.78	0.11	-0.24	0.14
Elongation index	0.76	0.12	-0.24	0.16
	0.80	0.11	-0.65	0.14
	0.79	0.11	-0.28	0.14
Intercept sphericity	0.74	0.09	-0.18	0.12
	0.81	0.08	-0.64	0.10
	0.779	0.07	-0.21	0.09
Operational Sphericity	0.58	0.07	-0.09	0.12
	0.71	0.09	-0.45	0.13
	0.64	0.06	-0.31	0.10
Convexity	0.79	0.08	-1.00	0.10
	0.92	0.06	-2.10	0.06
	0.84	0.07	-1.88	0.09
Alshibli Sphericity	2.08	1.05	2.34	0.51
	0.75	0.09	-0.18	0.12
	1.90	0.69	1.62	0.36

$\sim 10^3$ particles are enough...



(a)



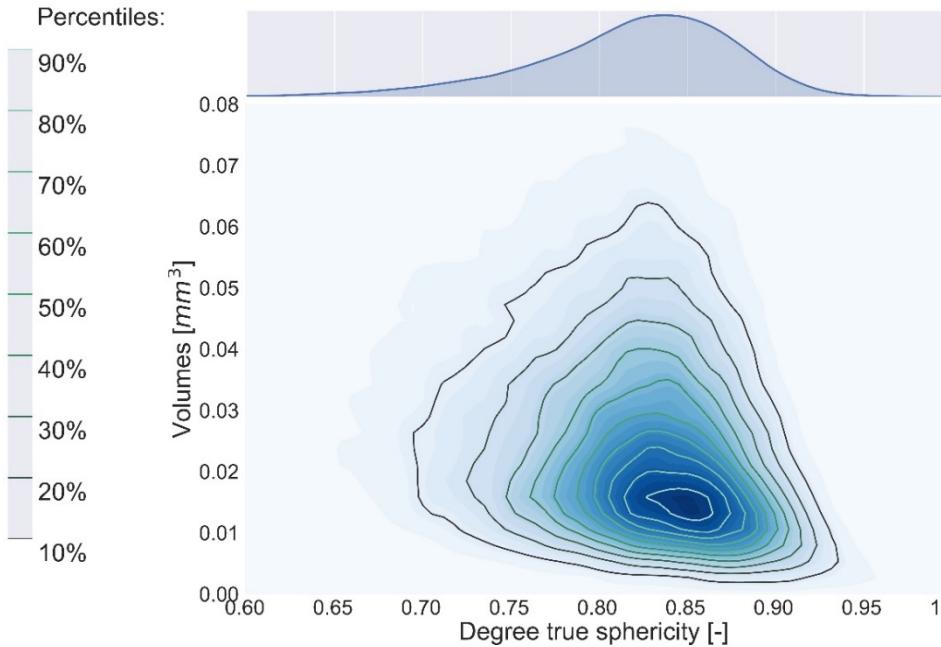
(b)

Figure 6.32: Evolution of the first three sample moments (mean, standard deviation, skew) of true sphericity with sample size

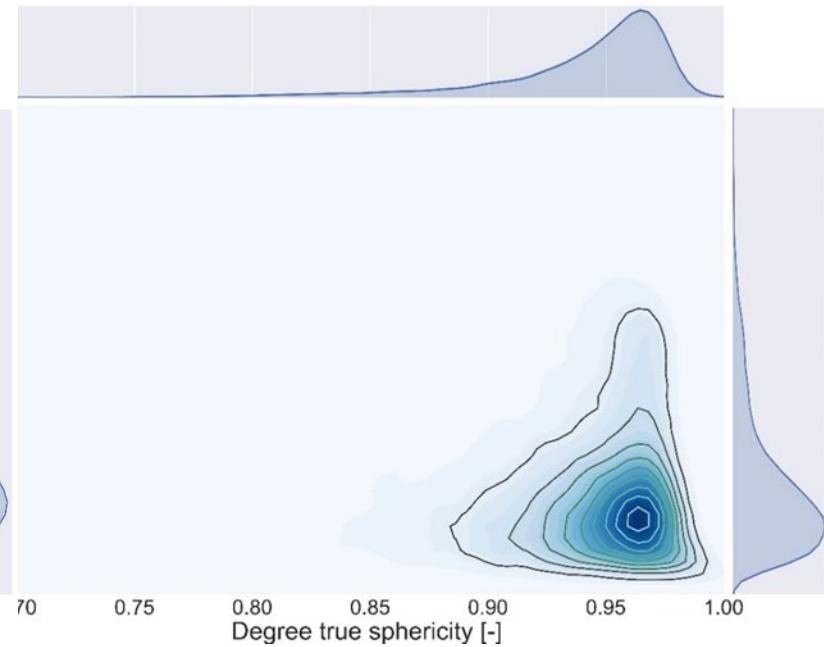
2.4) 3D shape descriptors: correlations

e.g., *degree of true sphericity VS particle volume*

HOSTUN sand



CAICOS ooids



HOSTUN sand

<i>SHAPE DESCRIPTOR</i>	<i>V</i>	<i>Ψ</i>	<i>FI</i>	<i>EI</i>	<i>Ψ_{int}</i>	<i>Ψ_{op}</i>	<i>Co</i>	<i>Ψ_{al}</i>
<i>Grain volume</i>	1.00	-0.26	0.13	0.09	0.16	0.03	-0.39	-0.20
<i>True Sphericity</i>	-0.26	1.00	0.37	0.26	0.47	0.62	0.84	-0.31
<i>Flatness index</i>	0.13	0.37	1.00	-0.21	0.36	0.34	0.05	-0.80
<i>Elongation index</i>	0.09	0.26	-0.21	1.00	0.83	0.32	0.10	-0.17
<i>Intercept sphericity</i>	0.16	0.47	0.36	0.83	1.00	0.51	0.12	-0.62
<i>Operational sphericity</i>	0.03	0.62	0.34	0.32	0.51	1.00	0.43	-0.33
<i>Convexity</i>	-0.39	0.84	0.05	0.10	0.12	0.43	1.00	0.11
<i>Alshibli Sphericity</i>	-0.20	-0.31	-0.80	-0.17	-0.62	-0.33	0.11	1.00

48612 grains

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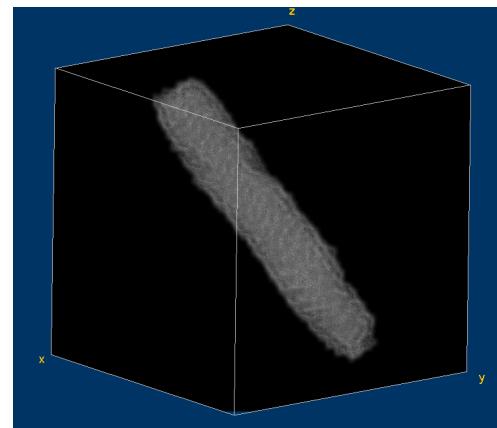
<i>SHAPE DESCRIPTOR</i>	<i>V</i>	<i>Ψ</i>	<i>FI</i>	<i>EI</i>	<i>Ψ_{int}</i>	<i>Ψ_{op}</i>	<i>Co</i>	<i>Ψ_{al}</i>
<i>Grain volume</i>	1.00	-0.07	0.08	0.07	0.10	0.13	-0.28	-0.11
<i>True Sphericity</i>	-0.07	1.00	0.30	0.46	0.59	0.70	0.86	0.32
<i>Flatness index</i>	0.08	0.30	1.00	-0.22	0.17	0.25	0.15	-0.69
<i>Elongation index</i>	0.07	0.46	-0.22	1.00	0.92	0.56	0.18	-0.37
<i>Intercept sphericity</i>	0.10	0.59	0.17	0.92	1.00	0.67	0.24	-0.65
<i>Operational sphericity</i>	0.13	0.70	0.25	0.56	0.67	1.00	0.48	-0.39
<i>Convexity</i>	-0.28	0.86	0.15	0.18	0.24	0.48	1.00	0.04
<i>Alshibli Sphericity</i>	-0.11	-0.32	-0.69	-0.37	-0.65	-0.39	0.04	1.00

65056 grains

2.4) Projected (2D) measures of shape

See Table 2.1 (p. 13) of the Thesis for reference

Random oriented projection

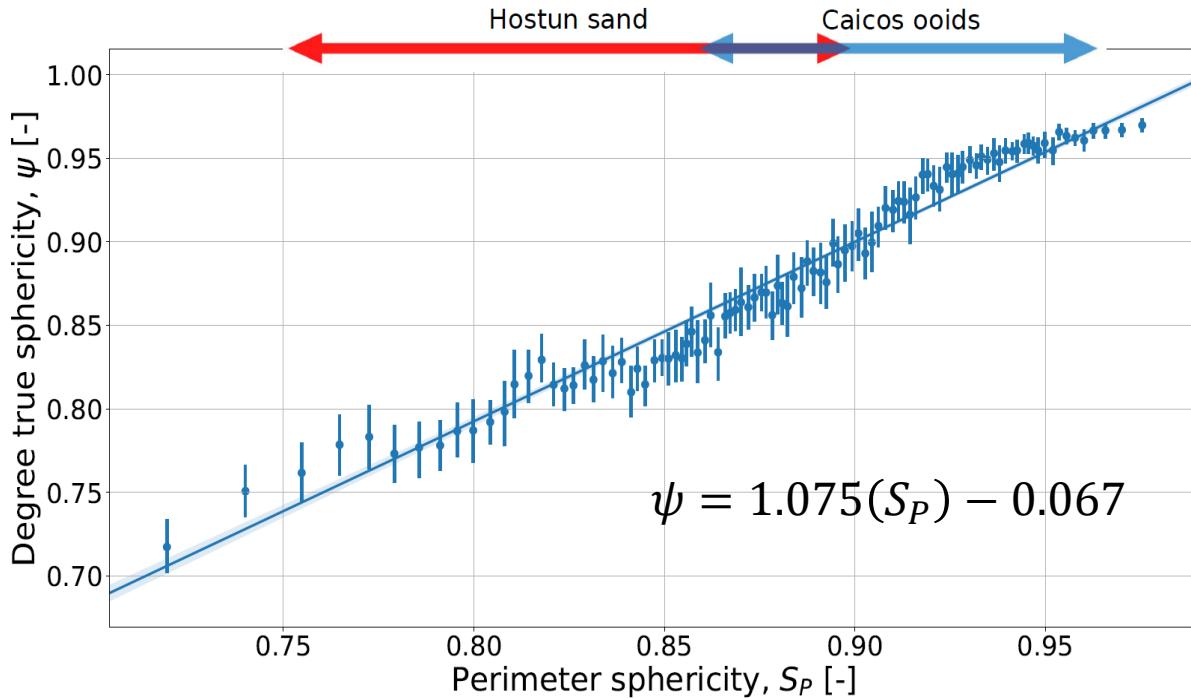


Oriented projection
(along the minor principal axis)



SHAPE DESCRIPTOR	Ψ	S_A	S_D	S_C	S_P	S_{KS}
<i>True Sphericity</i> <i>3D</i>	1.00	0.58	0.61	0.66	0.55	0.49
<i>Area sphericity</i> <i>2D</i>	0.58	1.00	0.99	0.95	0.72	0.81
<i>Diameter sphericity</i> <i>2D</i>	0.61	0.99	1.00	0.93	0.65	0.80
<i>Circle ratio sphericity</i> <i>2D</i>	0.66	0.95	0.93	1.00	0.71	0.77
<i>Perimeter sphericity</i> <i>2D</i>	0.55	0.72	0.65	0.71	1.00	0.34
<i>KS sphericity</i> <i>2D</i>	0.49	0.81	0.80	0.77	0.34	1.00

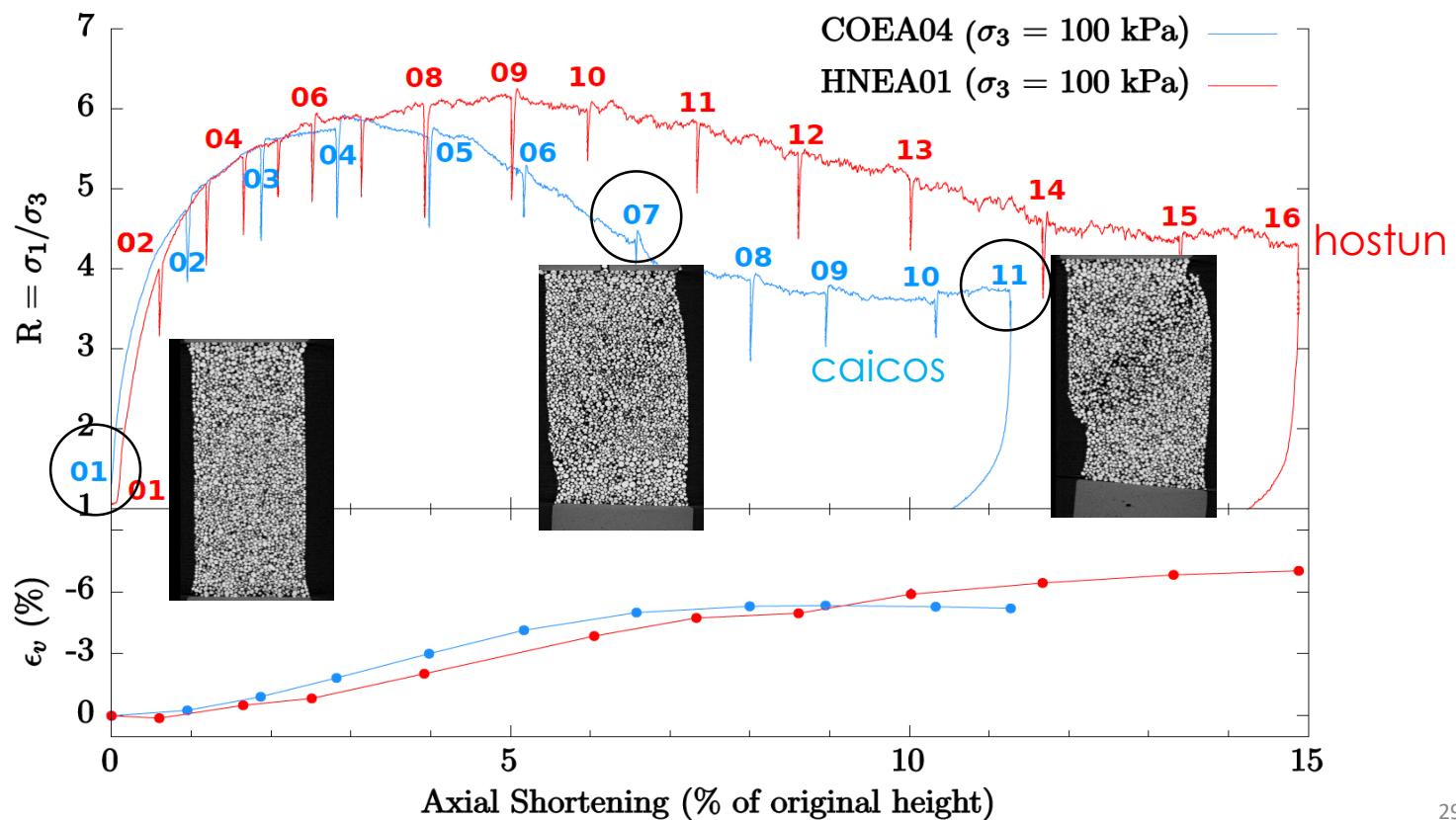
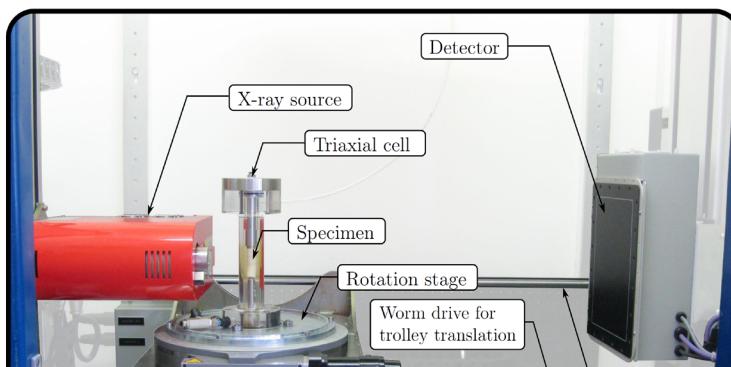
SHAPE DESCRIPTOR	Ψ	S_A	S_D	S_C	S_P	S_{KS}
<i>True Sphericity</i> <i>3D</i>	1.00	0.70	0.69	0.72	0.83	0.36
<i>Area sphericity</i> <i>2D</i>	0.70	1.00	1.00	0.96	0.80	0.81
<i>Diameter sphericity</i> <i>2D</i>	0.69	1.00	1.00	0.96	0.80	0.81
<i>Circle ratio sphericity</i> <i>2D</i>	0.72	0.96	0.96	1.00	0.82	0.79
<i>Perimeter sphericity</i> <i>2D</i>	0.83	0.80	0.80	0.82	1.00	0.45
<i>KS sphericity</i> <i>2D</i>	0.36	0.81	0.81	0.79	0.45	1.00



$$\psi = \frac{S_n}{S} = \frac{\text{Surface area of the equivalent sphere}}{\text{Surface area of the grain}}$$

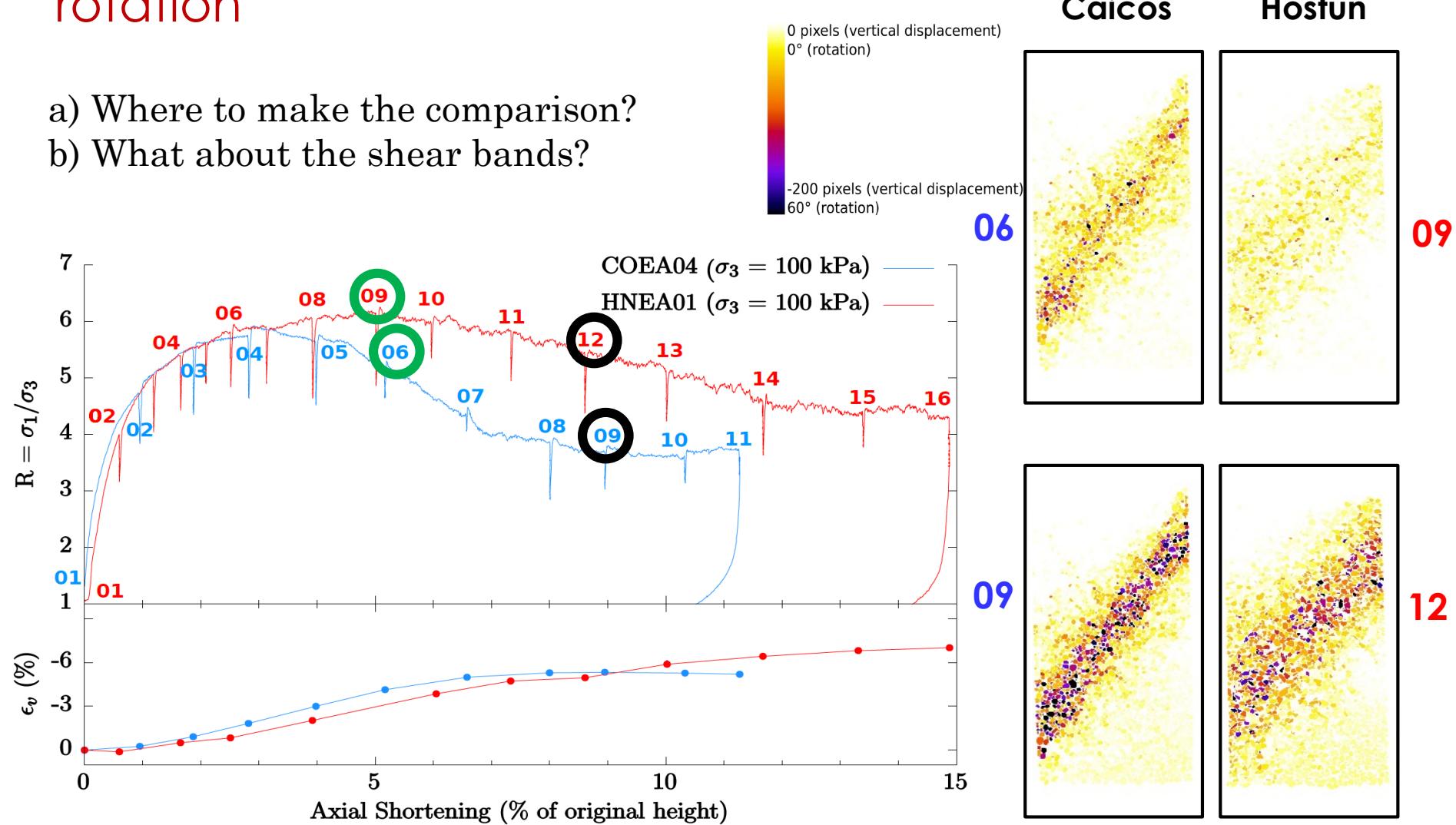
$$S_P = \frac{p_n}{p} = \frac{\text{Perimeter of the equivalent circle}}{\text{Perimeter of the grain}}$$

3.1) Triaxial tests scanned by x-rays



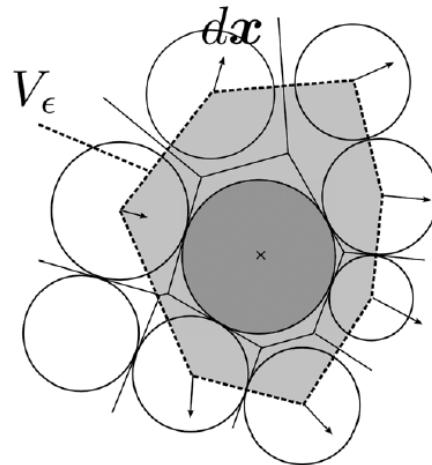
Relationship between grain shape and magnitude of rotation

- a) Where to make the comparison?
- b) What about the shear bands?



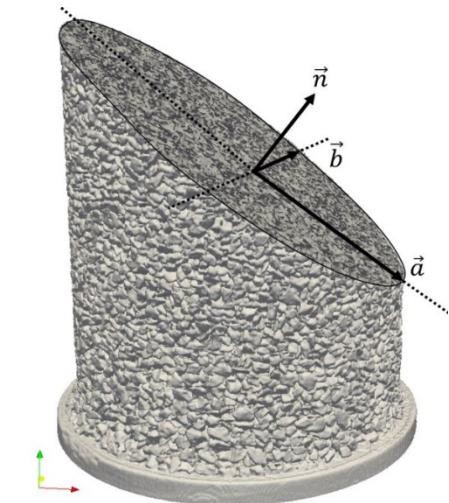
Necessary to separate the study inside/outside the shear band

3.4) Shear bands identification

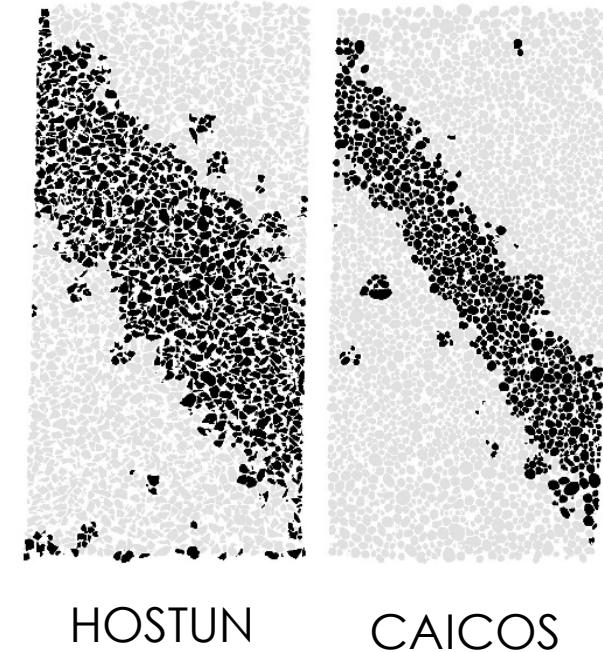
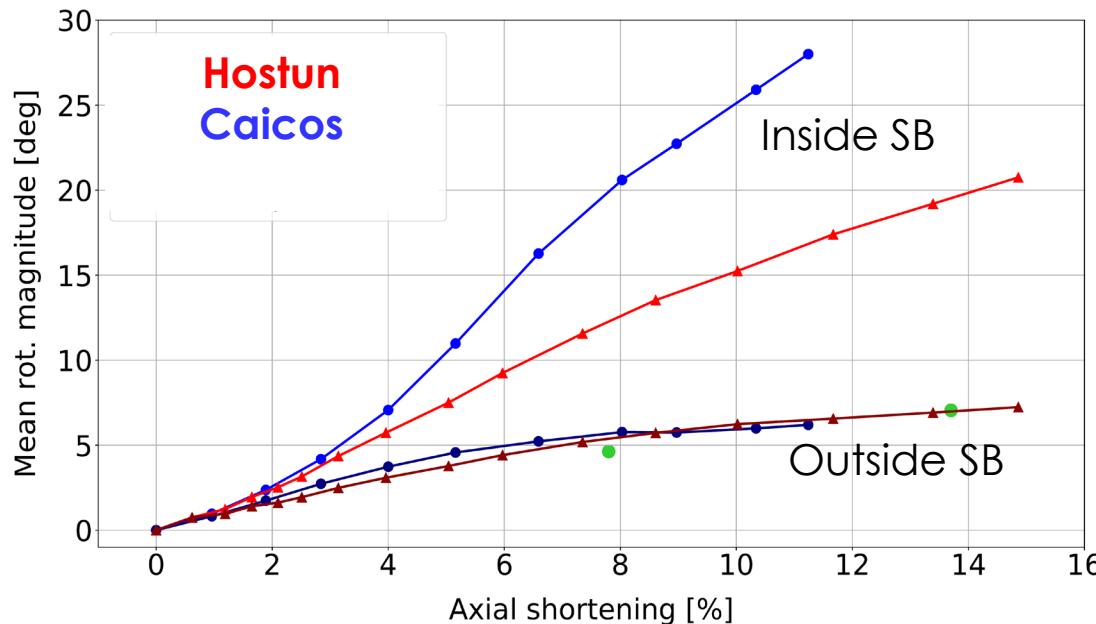


YADE TesselationWrapper
(Catalano et al., 2014)

$$\bar{\boldsymbol{\varepsilon}} = \frac{1}{2} (\langle \nabla \mathbf{d}\mathbf{x} \rangle + \langle \nabla \mathbf{d}\mathbf{x} \rangle^T)$$

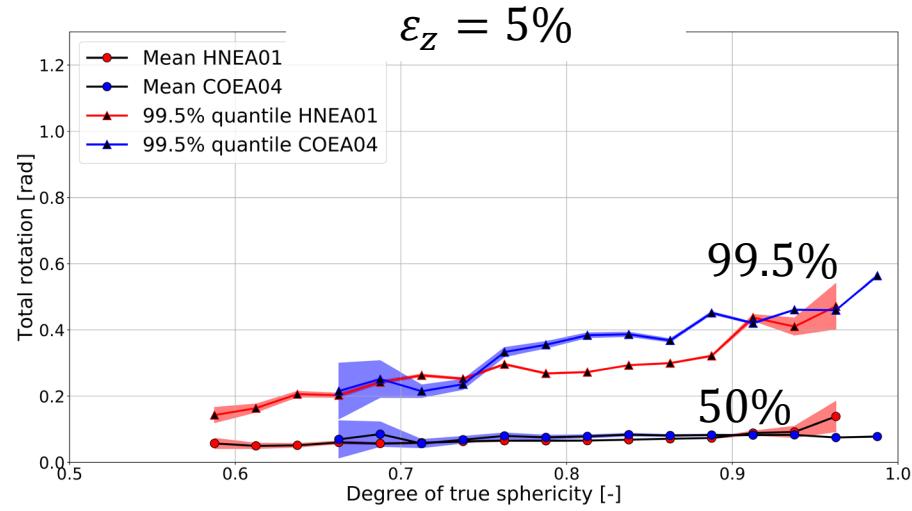


History of mean grain rotations

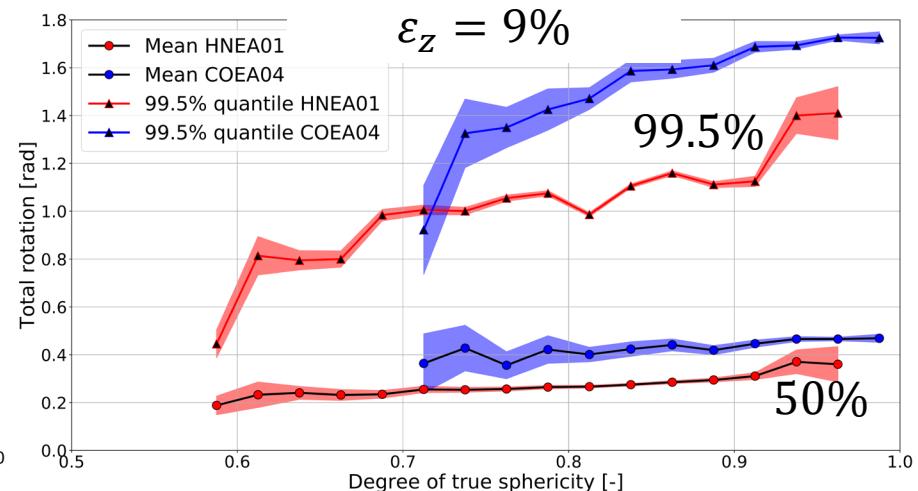
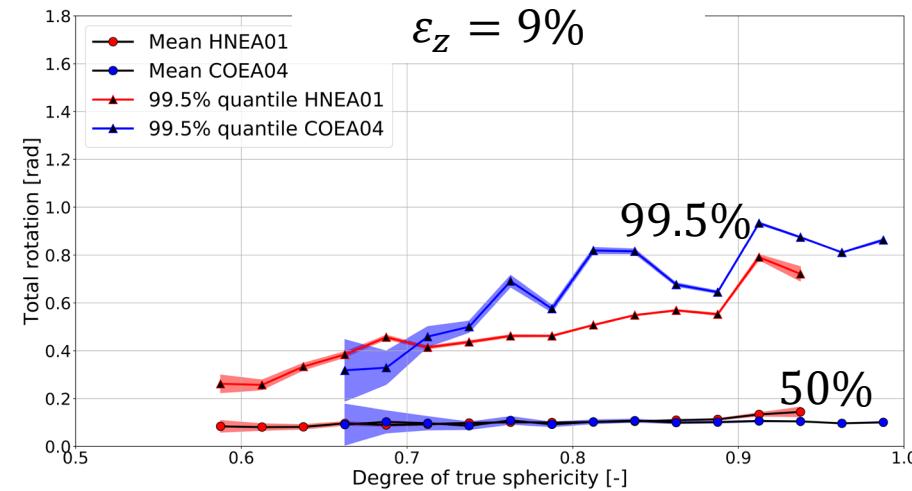
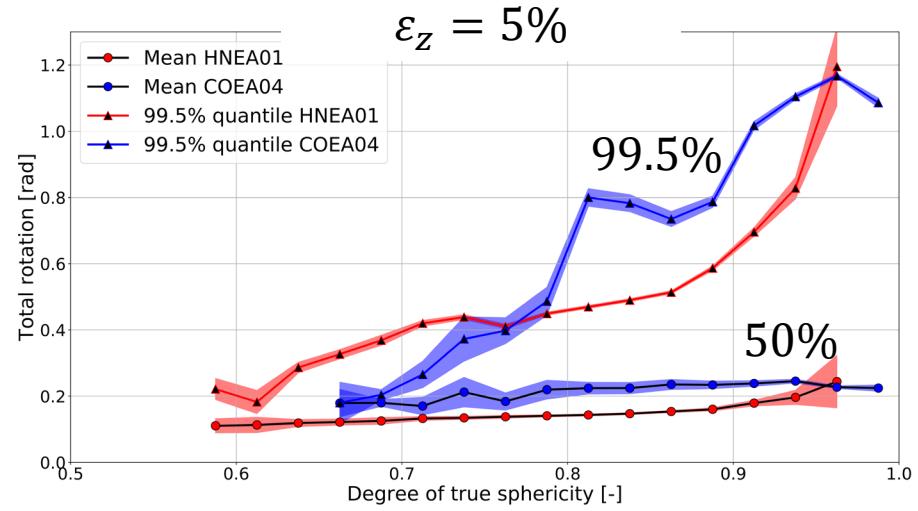


Total rotation magnitude VS 3D true sphericity: 50% and 99.5% quantiles

Outside SB



Inside SB

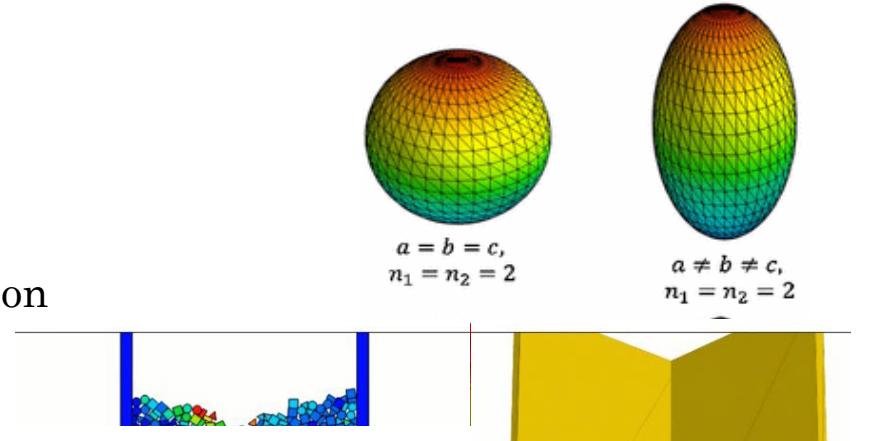


Outline of the presentation

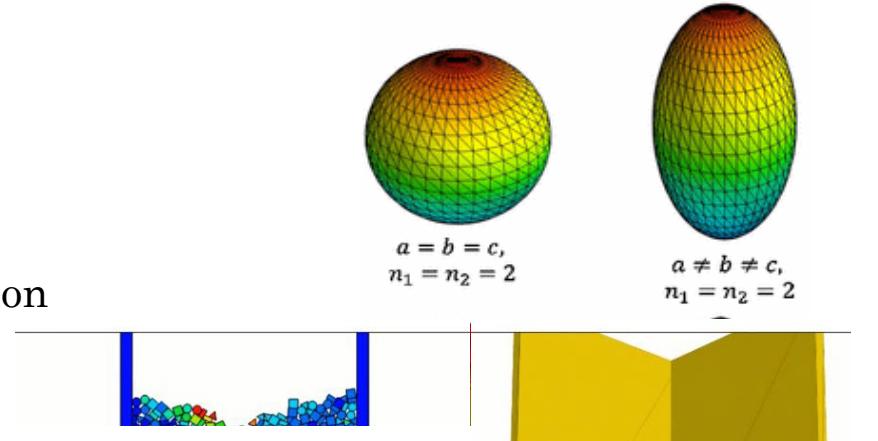
1. Research motivation
2. X-rays micro-tomography for geomaterials
3. Study of grain kinematics during triaxial tests
4. **A DEM rolling resistance contact model accounting for Particle Shape**
5. Cone Penetration Test on a Virtual Calibration Chamber (VCC) using DEM
6. Conclusions

4.2) Particle shape in DEM

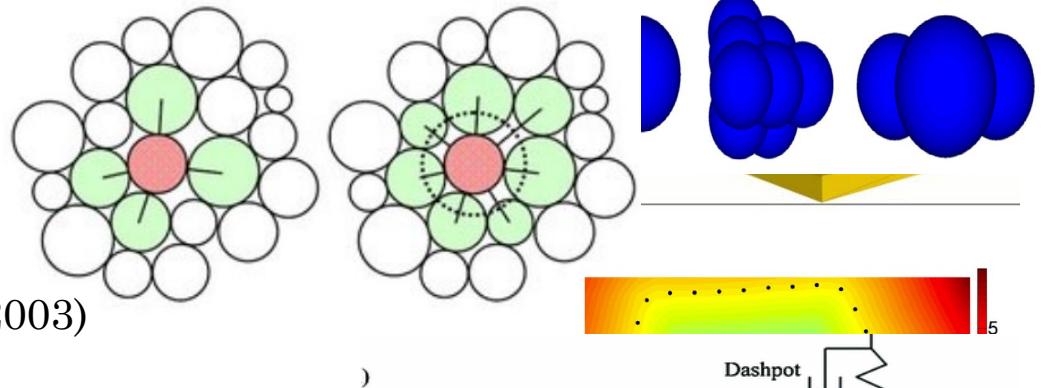
- Continuous analytical particle shape description



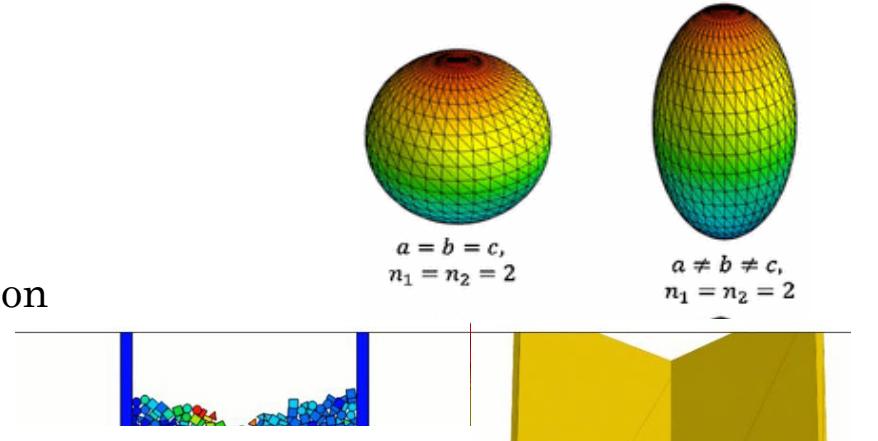
- Polyhedral particles



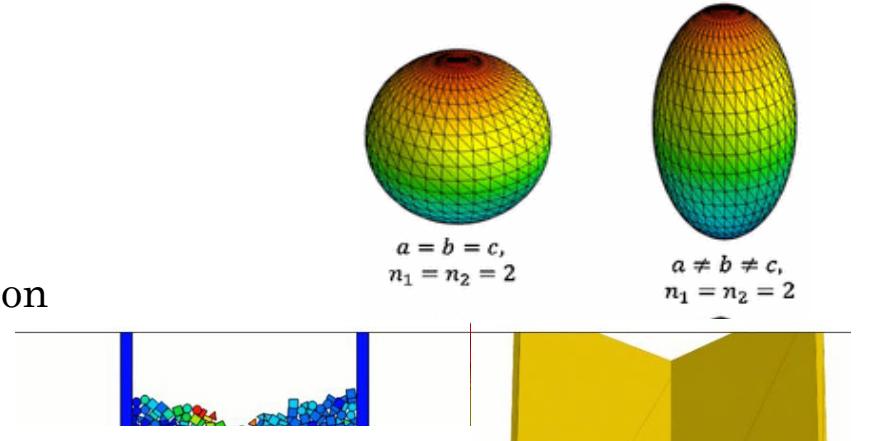
- Aggregates of spheres (clumps)



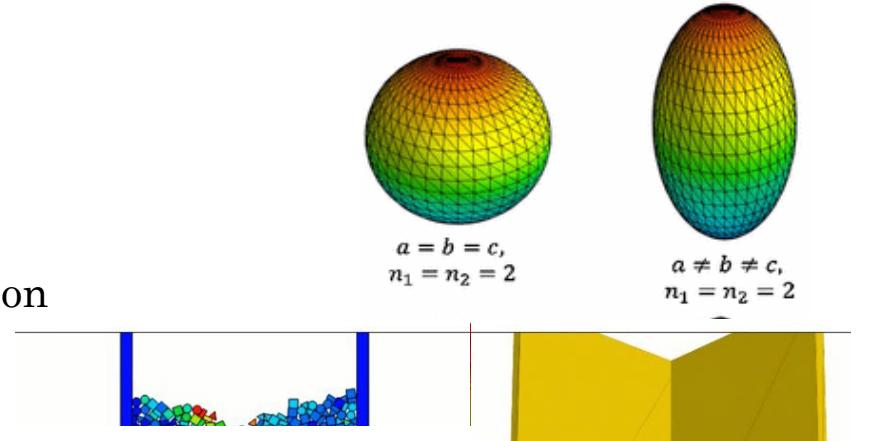
- Contact at distance (Hentz, 2004)



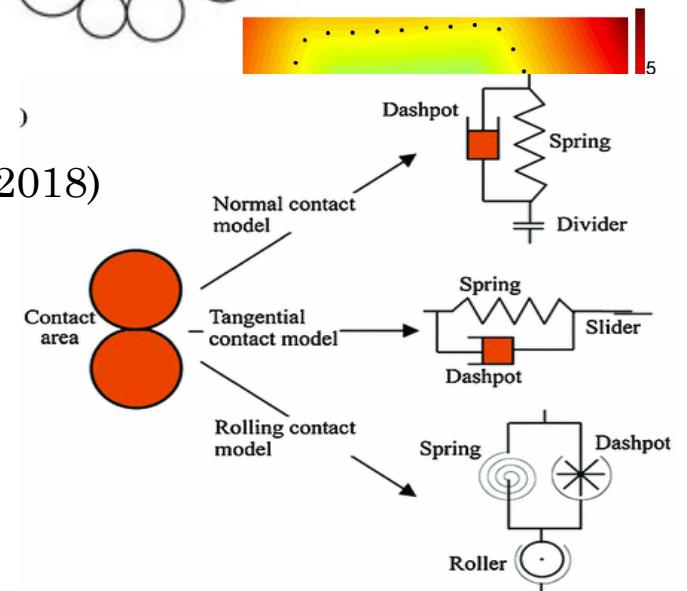
- Inhibit particles rotations (Calvetti, 2003)



- Level-set description (Jerves 2016, Nadimi & Fonseca 2018)



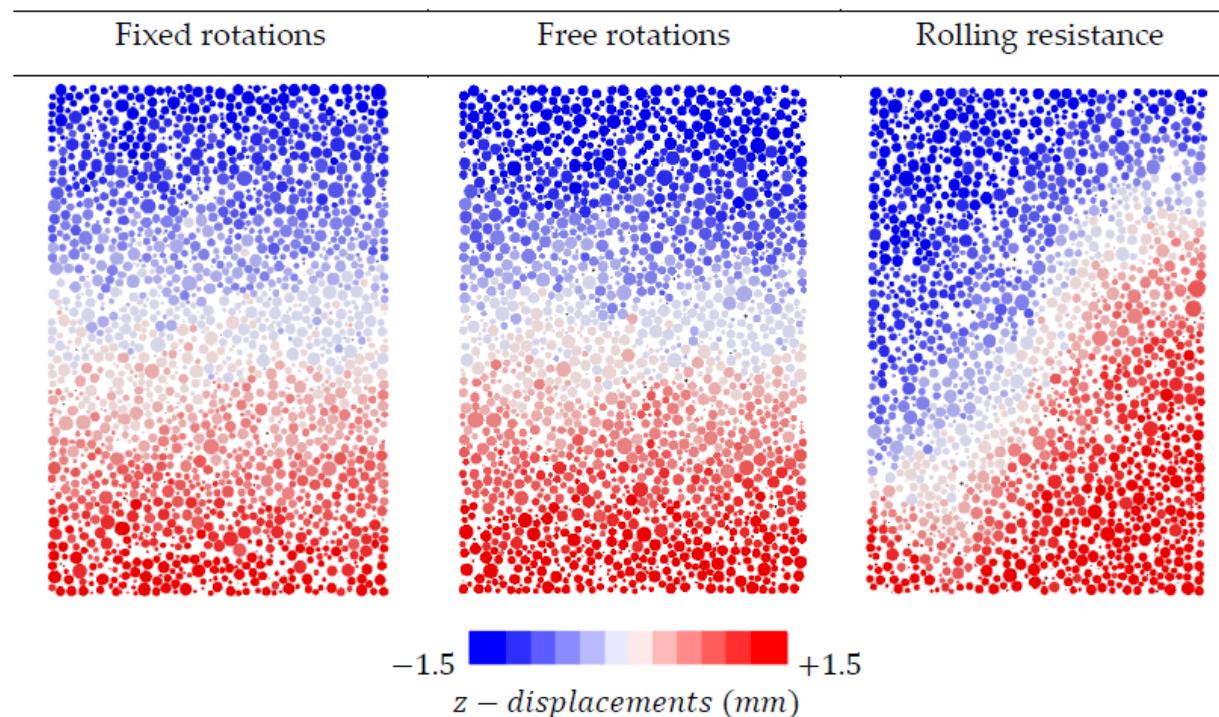
- **Rolling resistance contact models**



- Well-established technique to mimic particle shape effects
- The contact detection remains efficient
- It allows the localisation of failure in shear bands

e.g., end of a DEM Triaxial Test using:

- Freely rotating spheres
- Fixed rotating spheres
- Spheres with rolling resistance



2) Isotropic compression at 100kPa confining pressure (with rigid-walls and servo-controlled mechanism)

3) Triaxial compression:

- Change the contact model to the Linear Rolling Resistance CM (*Iwashita & Oda, 1998*) with $\mu_r = \alpha \psi^b$
- Shearing at low strain rate (“*Inertial number*”): 0.05m/s each platen

$$I = \frac{\dot{\gamma}d}{\sqrt{P/\rho}},$$

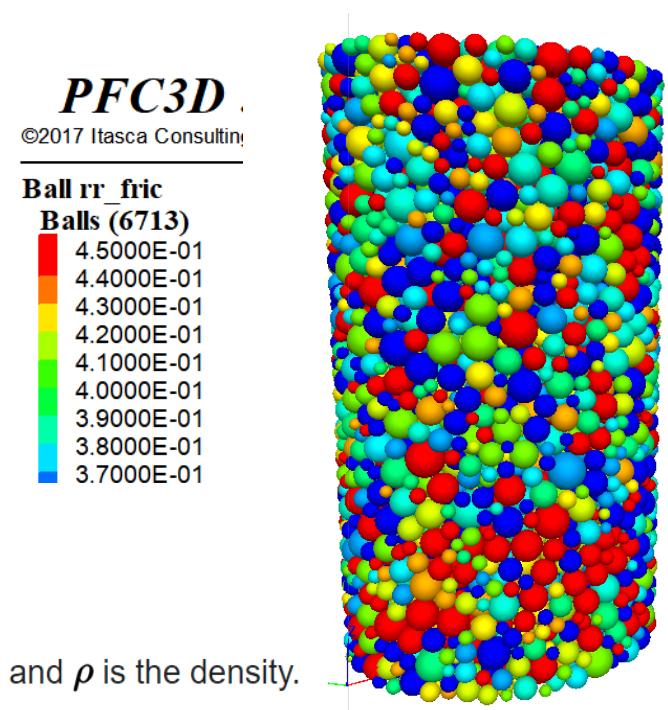
where $\dot{\gamma}$ is the shear rate, d the average particle diameter, P is the pressure and ρ is the density.

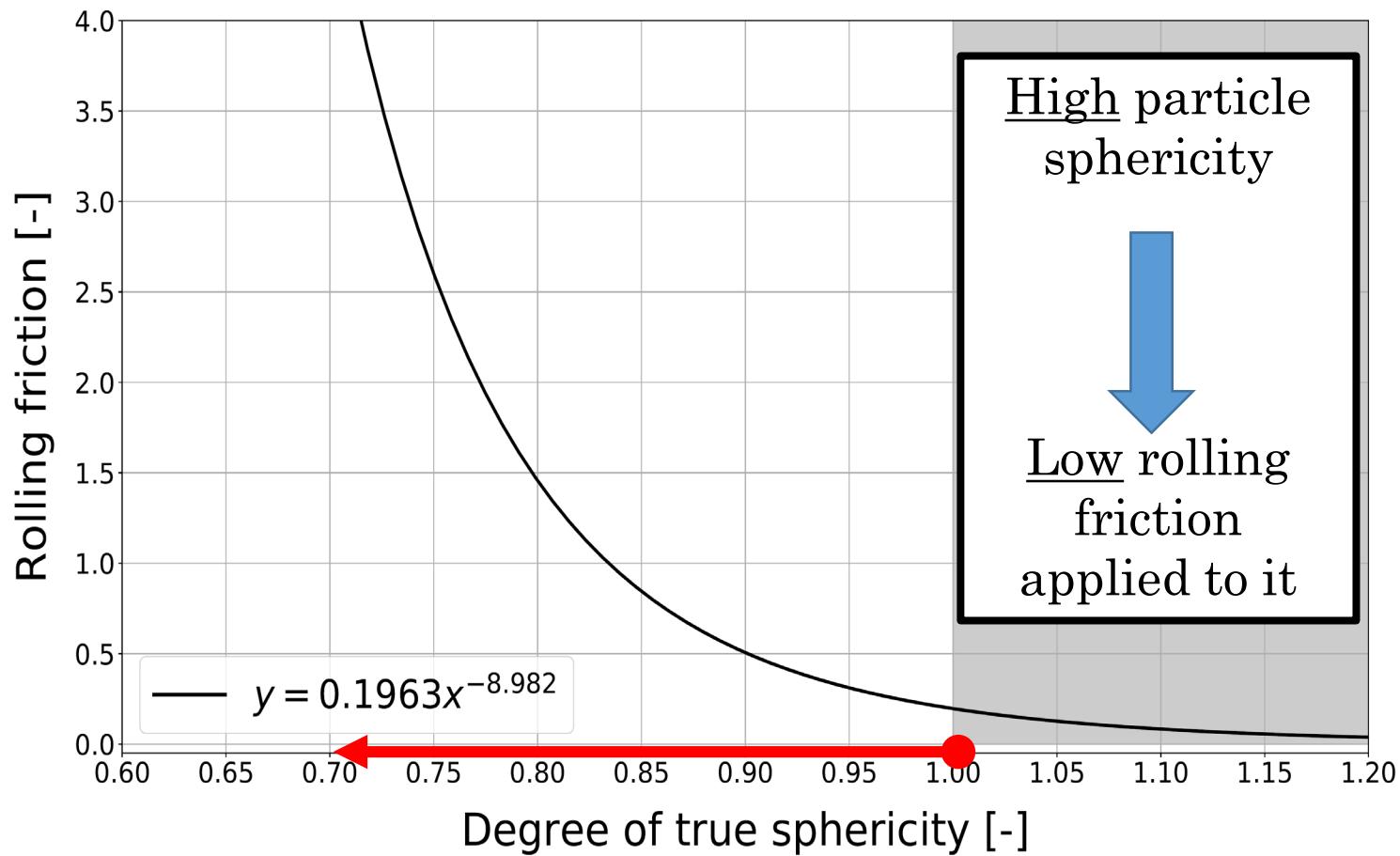
Generally three regimes are distinguished:

- $I < 10^{-3}$: quasi static flow
- $10^{-3} < I < 10^{-1}$: dense flow
- $I > 10^{-1}$: collisional flow

$I \cong 4.74 \cdot 10^{-4}$ (*Hostun PSD*)
 $I \cong 4.00 \cdot 10^{-4}$ (*Caicos PSD*)

- Calibrate the contact stiffness (k_n, k_s) by fitting the initial elastic part of the stress-strain response.



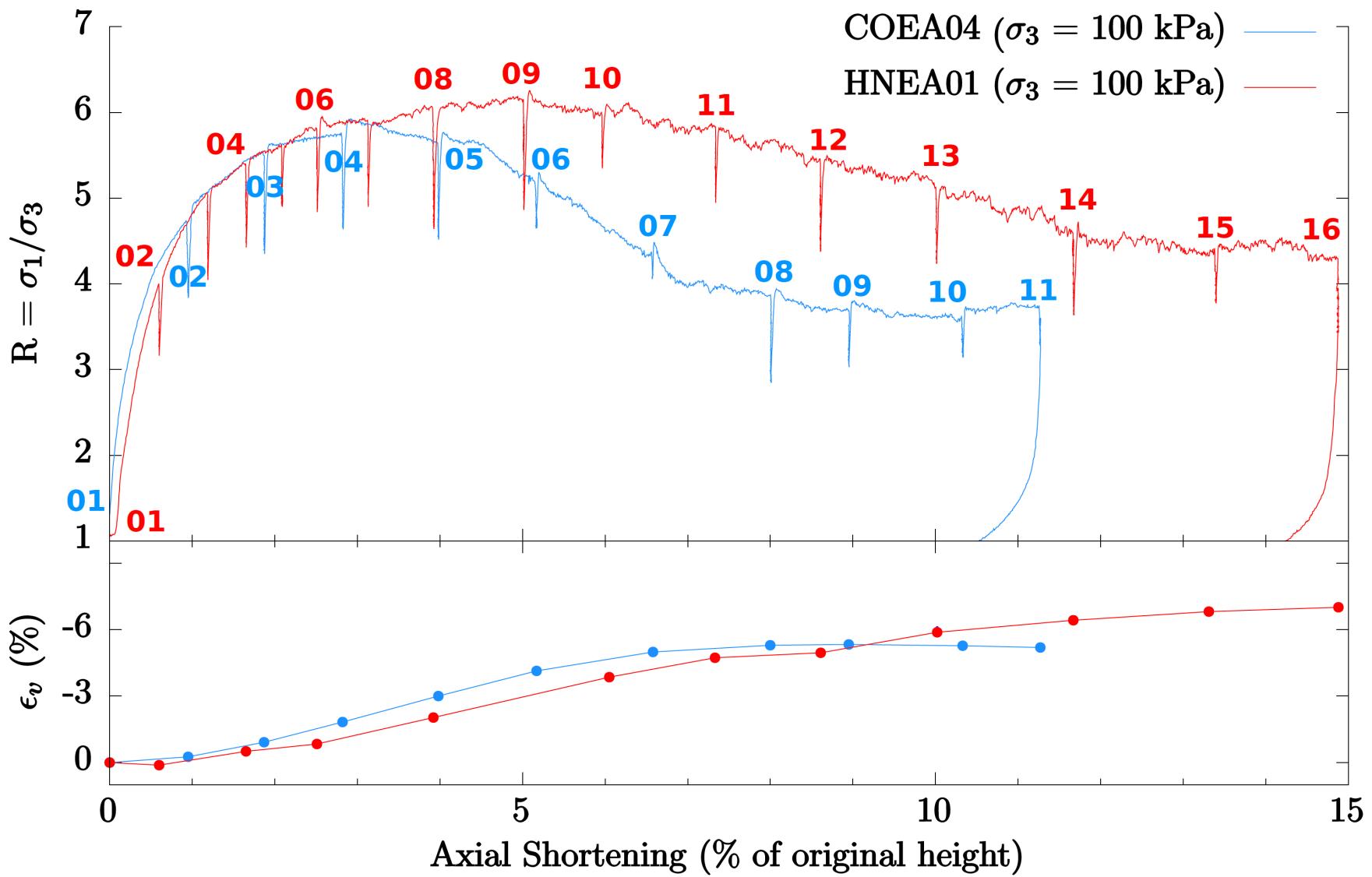


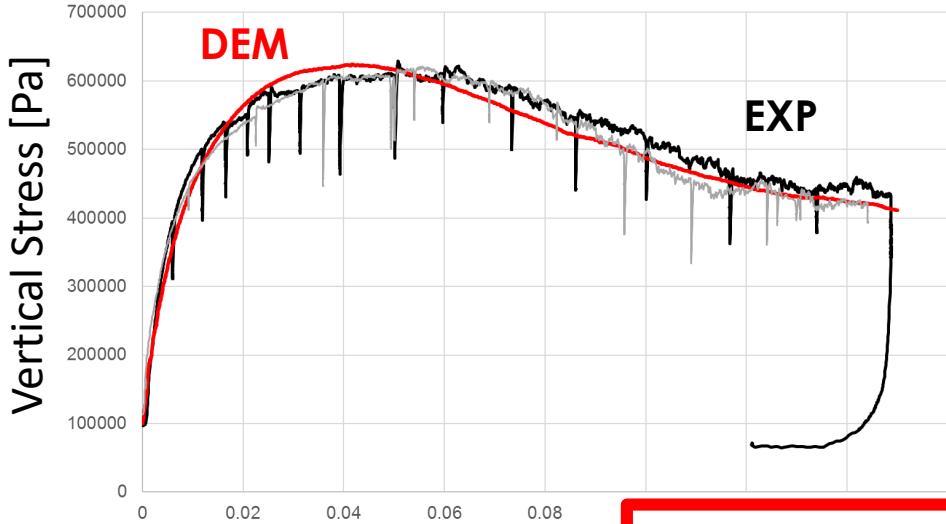
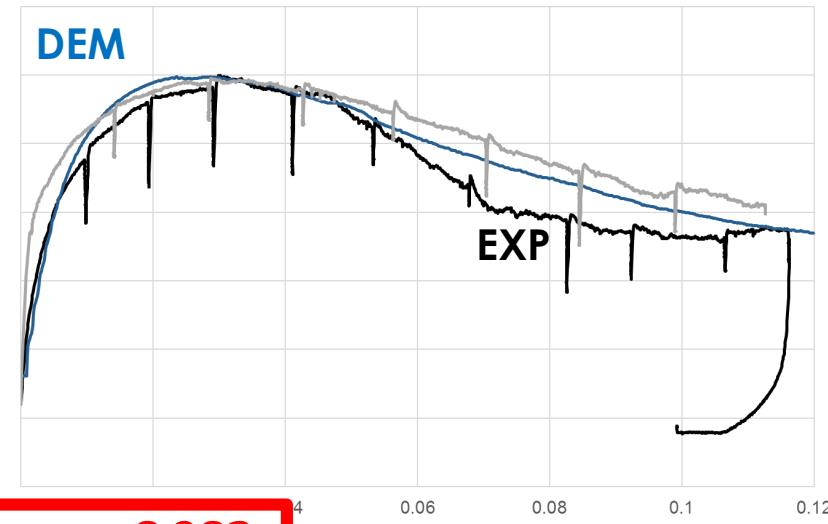
$$\mu_r = 0.1963 \psi^{-8.982}$$

Calibrated for two sands but meant to be “universal”!

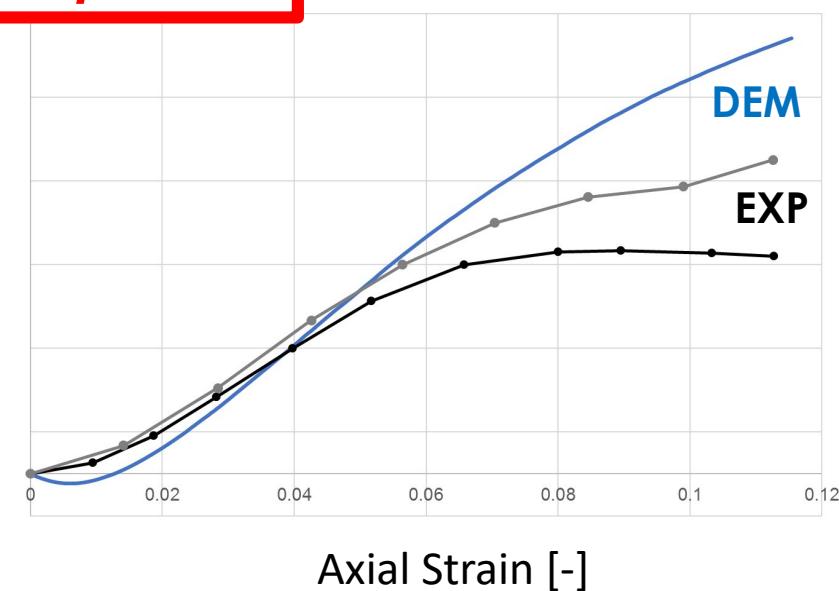
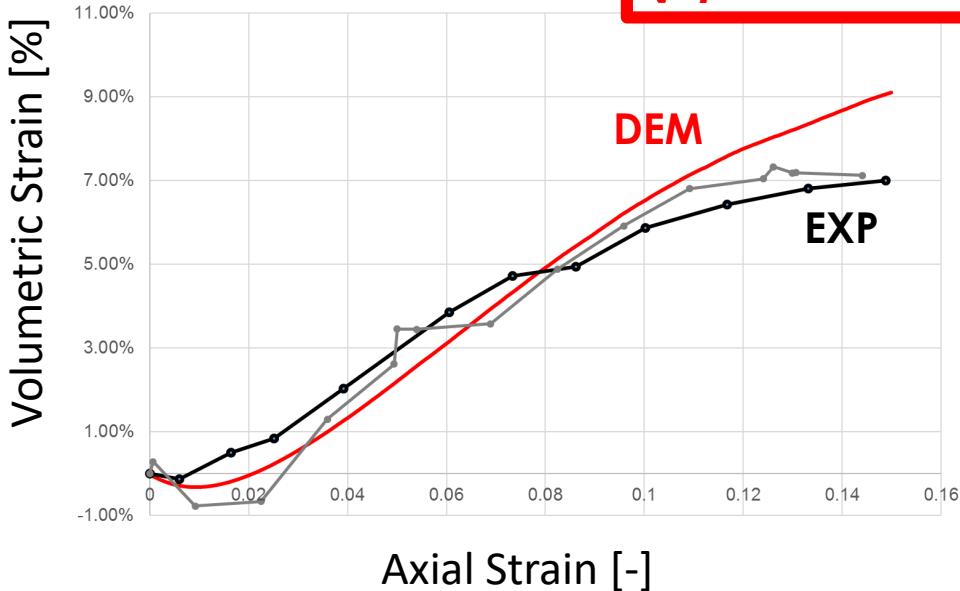
Stress-Volumetric-Strain + Kinematics Responses

(Linear CM + RR , 100kPa)



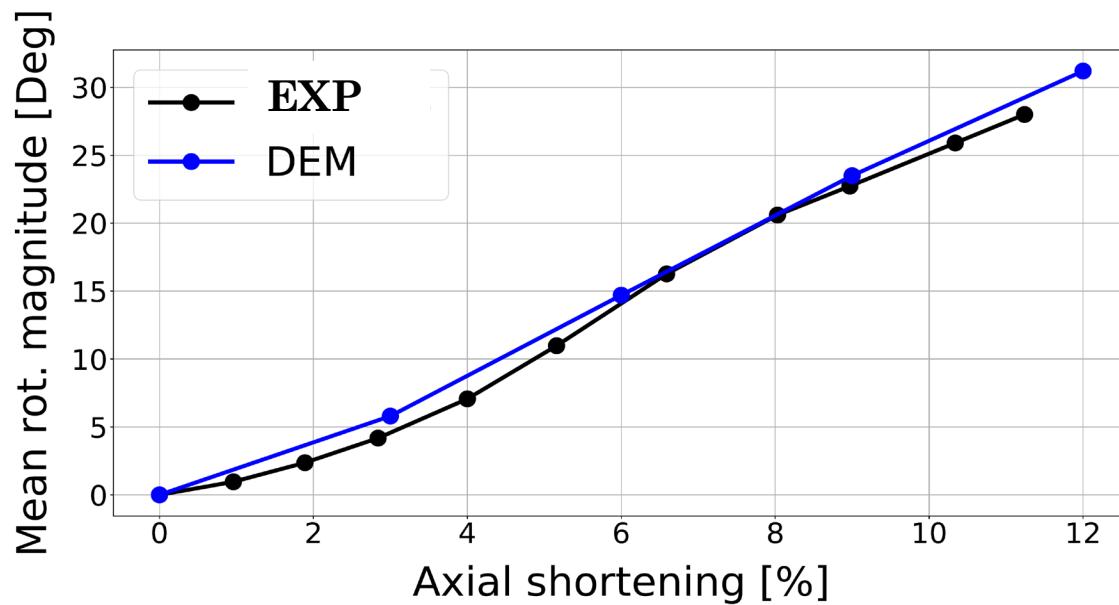
HOSTUN sand $\mu = 0.575$ **CAICOS ooids** $\mu = 0.575$ 

$$\mu_r = 0.1963 \psi^{-8.982}$$

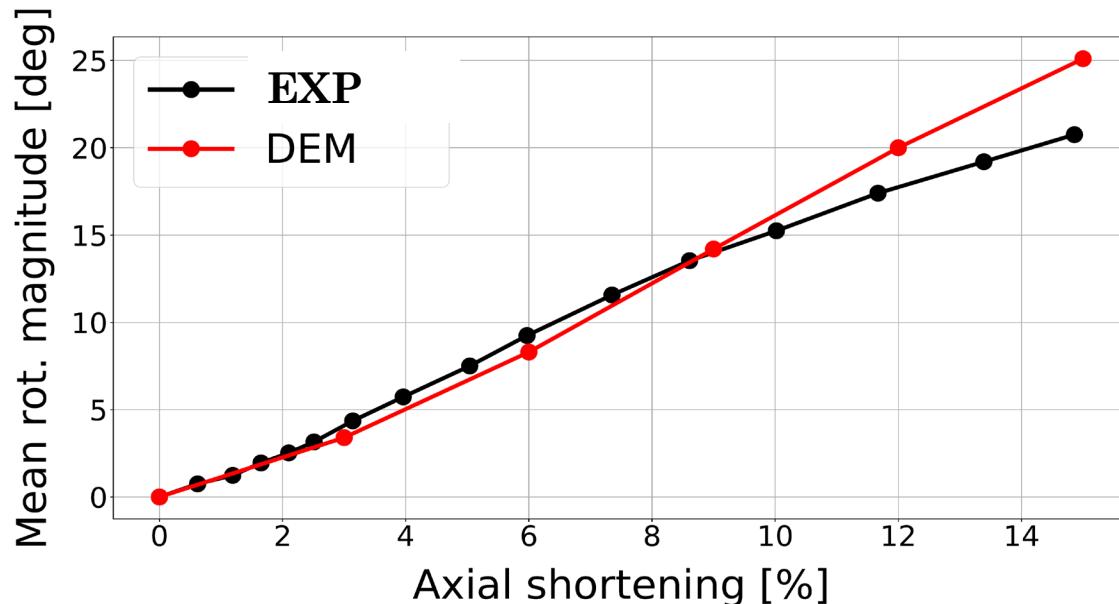


Histories of Mean Rotations (EXP vs DEM) inside the shear band

CAICOS ooids

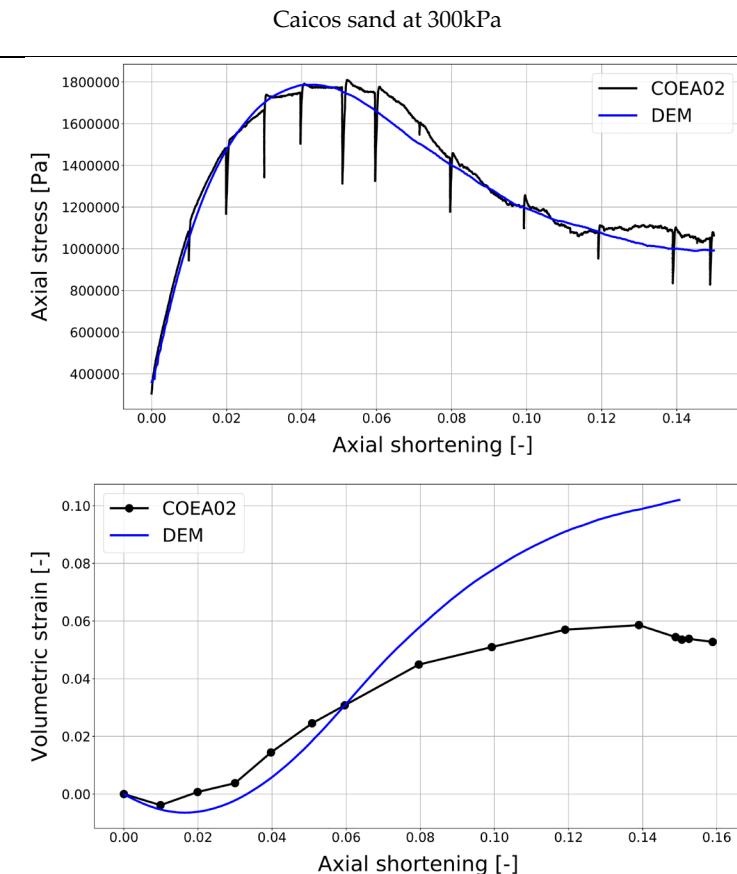
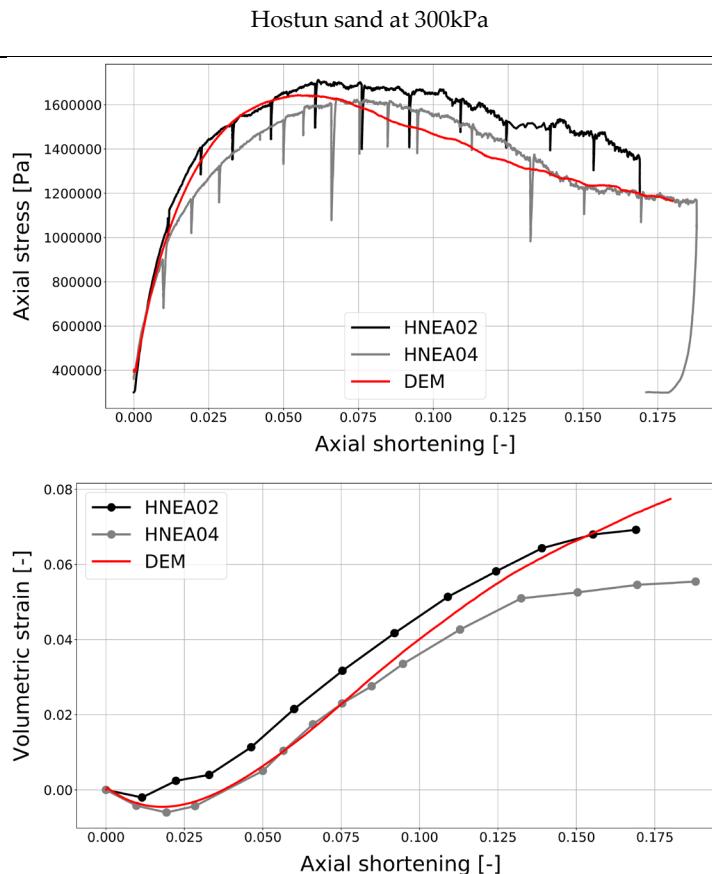


HOSTUN sand



4.6) Validation 1: Hostun/Caicos sands at 300kPa

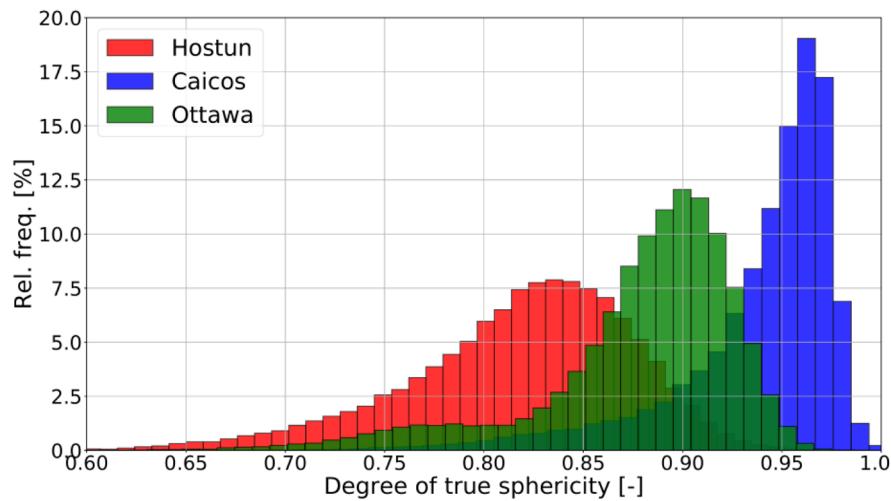
Sands for which all the DEM parameters are known and for which we calibrated the equation $\mu_r = 0.1963 \psi^{-8.982}$



4.7) Validation 2: Ottawa sand (we have tomographic images)

Procedure:

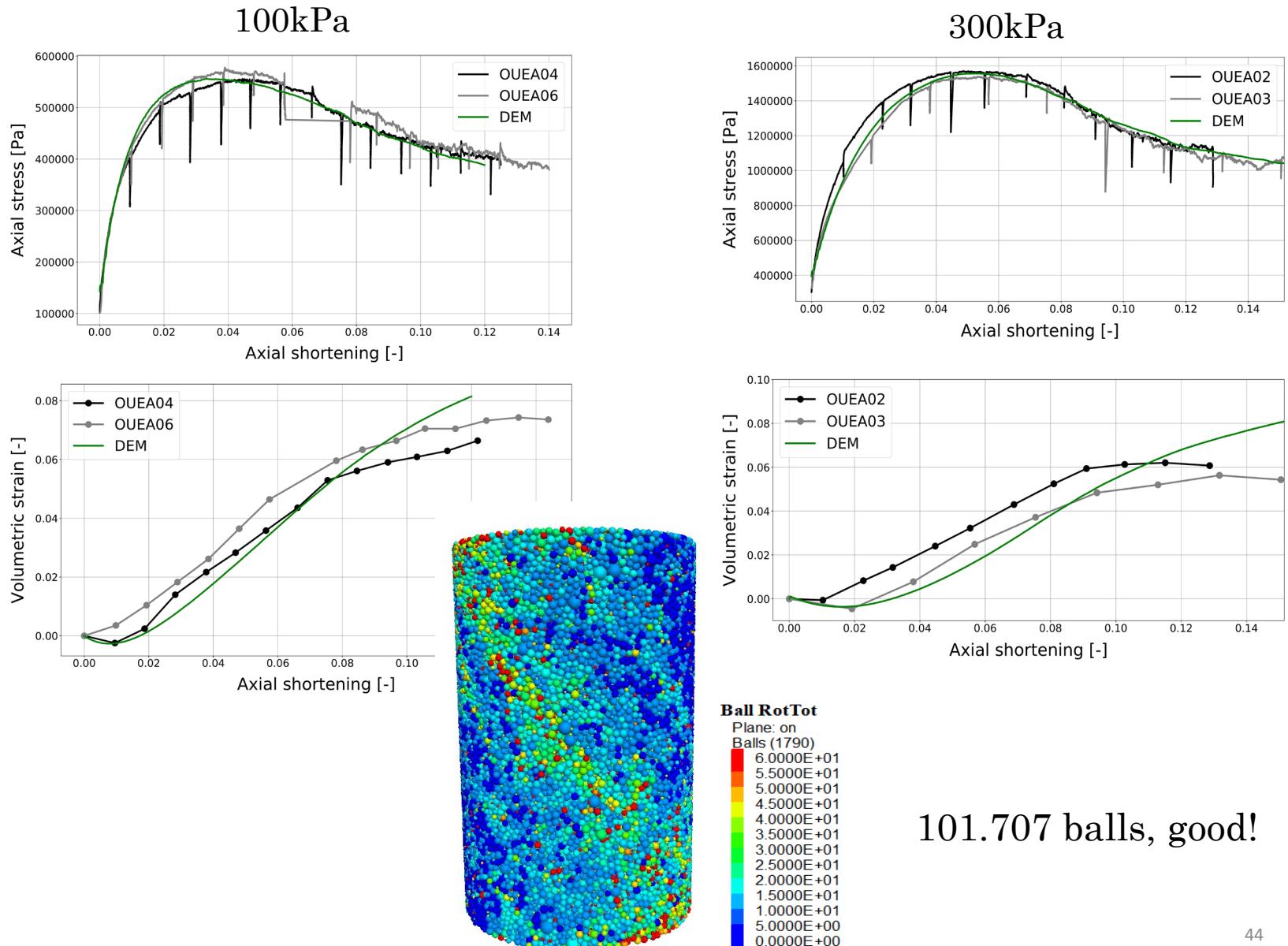
- 1) Create the DEM initial sample replicating PSD and porosity.
- 2) Apply the proposed equation relating the *degree of true sphericity* and *rolling friction*



$$\mu_r = 0.1963 \psi^{-8.982} \quad (\sim 113.000 \text{ values})$$

- 3) Perform the triaxial compression at low shear rate, with
 $\mu = 0.45$

Macroscopic responses – Ottawa sand



4.8) Validation 3: Ticino sand (new sand)

- 1) Compute the *3D true sphericity* of thousands of grains from one 3D labelled image of sand (I'm sorry but you need a tomograph...)
- 2) Create the DEM initial sample replicating PSD and porosity
- 3) Apply the equation relating the *degree of true sphericity* and *rolling friction*
$$\mu_r = 0.1963 \psi^{-8.982} \quad (\text{for each particle})$$
- 4) Perform the triaxial compression, calibrating the *sliding friction coefficient* by trial & error

What if you don't have a tomograph?

From projection of grains
laying on their plane of
greatest stability

$$\psi = 1.075(S_P) - 0.067$$

4.8) Validation 3: Ticino sand (3D shape is not known)

1) Compute the *3D true sphericity* of thousands of grains from one 3D labelled image of sand (~~I'm sorry but you need a tomograph...~~)

2) Create the DEM initial sample replicating PSD and porosity

3) Apply the equation relating the *degree of true sphericity* and *rolling friction*

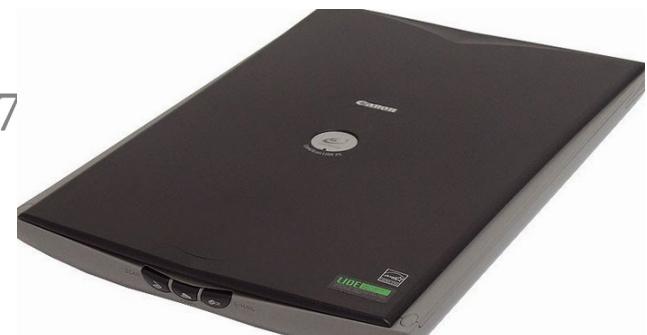
$$\mu_r = 0.1963 \psi^{-8.982} \text{ (for each particle)}$$

4) Perform the triaxial compression, calibrating the *sliding friction coefficient* by trial & error

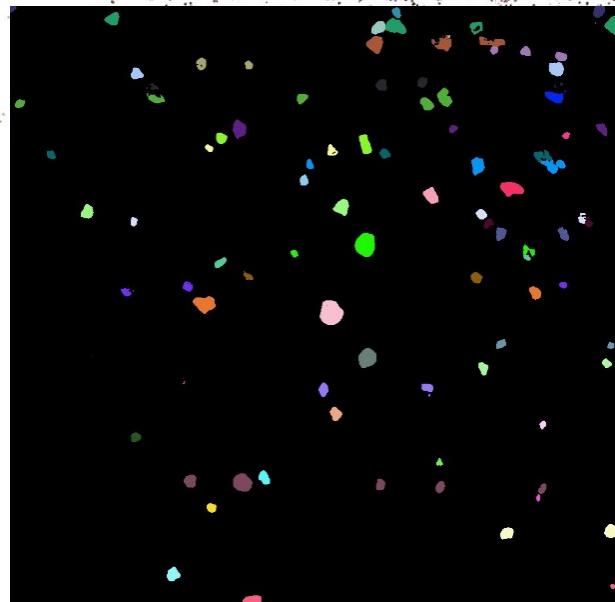
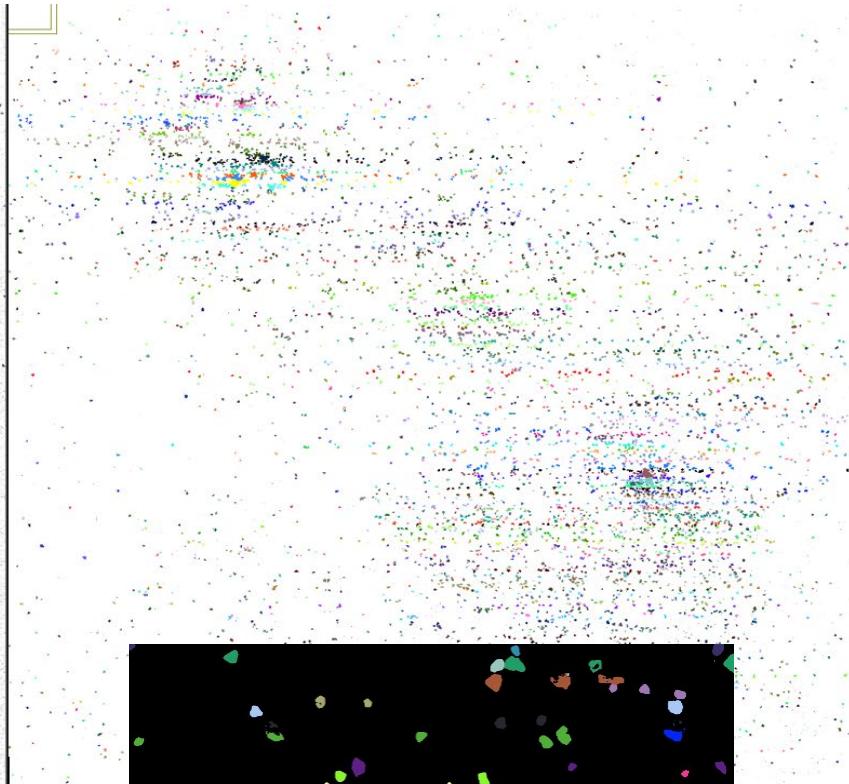
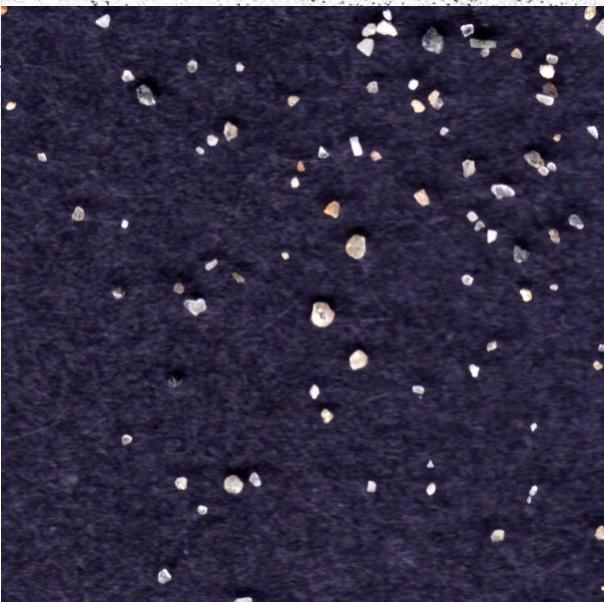
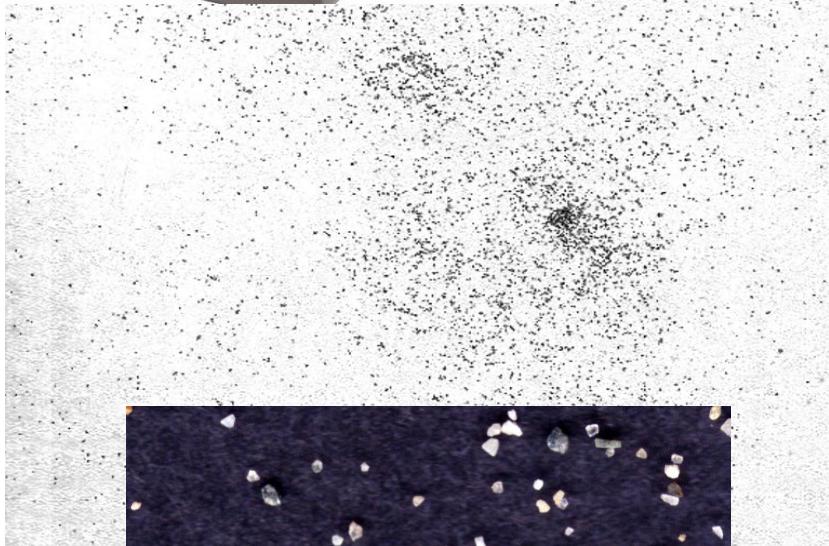
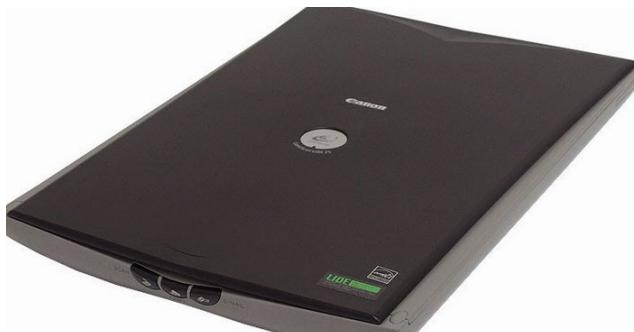
What if you don't have a tomograph?

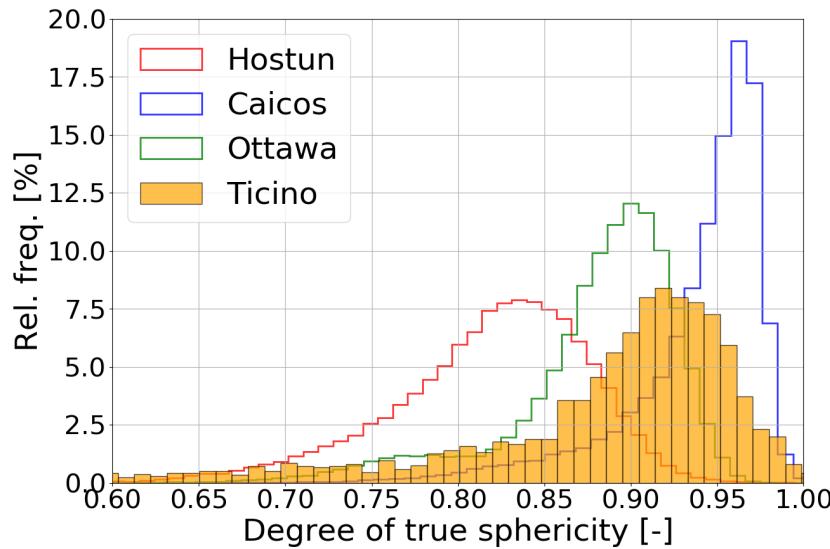
From projection of grains
laying on their plane of
greatest stability

$$\psi = 1.075(S_P) - 0.067$$



You do not need a tomograph anymore!



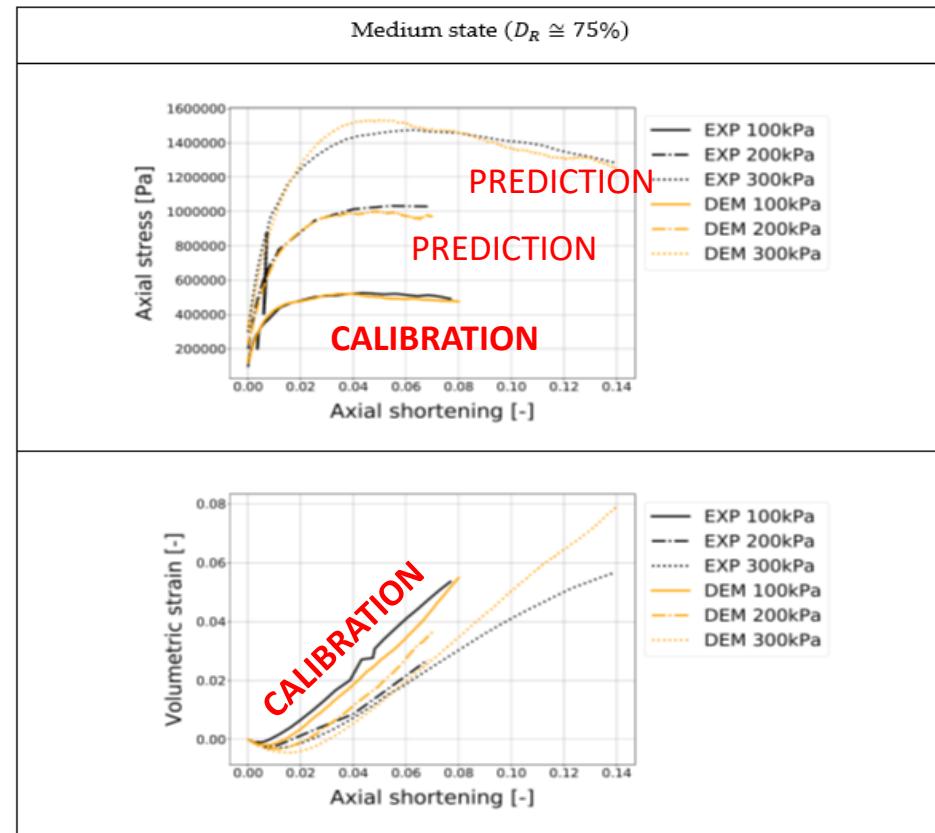


1 calibration ($100kPa, D_R = 75\%$)

$$Emod = 4e8 \text{ Pa}, Kr = 2.0 \\ \mu = 0.60$$

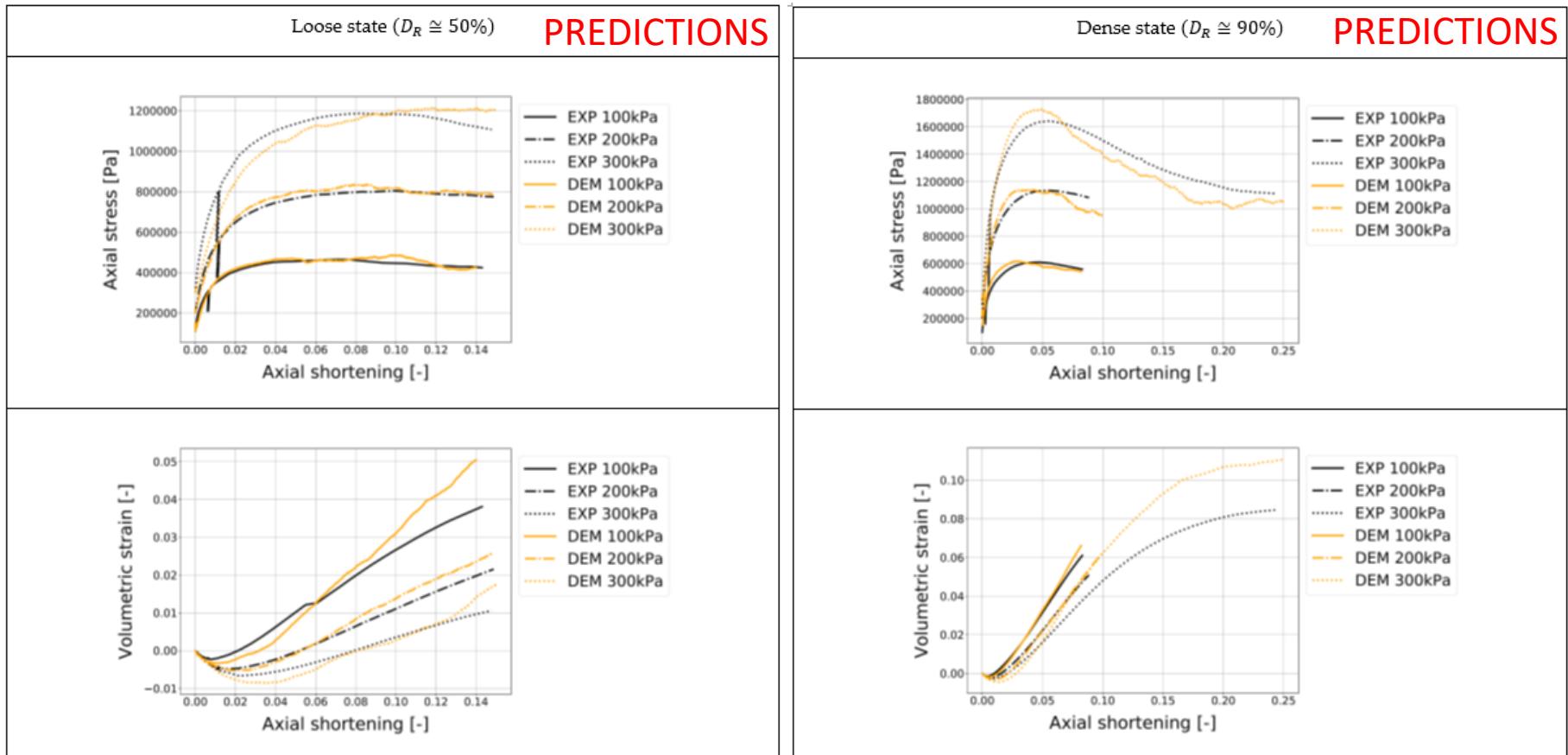
8 predictions

Using:
 $\mu_r = 0.1963 \psi^{-8.982}$



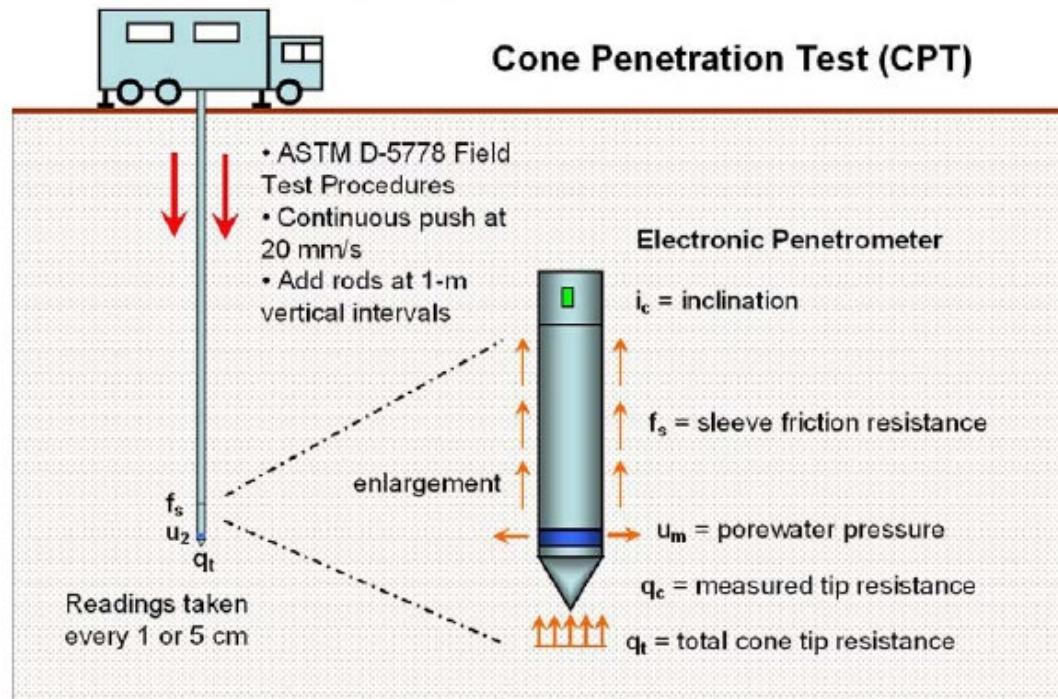
$$\mu_r = 0.1963 \psi^{-8.982}$$

$\mu = 0.60$



5.1) CPT Test and Calibration Chambers

Cone rig with hydraulic pushing system



Cone Penetration Test (CPT)



(Mayne, 2009)

Basic geotechnical investigation tool

CPT advantages:

- Fast, reliable, sensitive
- Versatile: onshore & offshore
- Modular: shear wave, resistivity...

CPT difficulties in analysis:

- Drained case (sands)
- Hard to model
- Hard to interpret

Calibration Chambers

CPT in controlled conditions (stress, density)

Pros: reliable & simple empirical relations

Cons: Expensive & time-consuming

One of the largest CC CPT testing campaigns ever performed was that carried out at the geotechnical laboratories of ENEL-CRIS, Milan and ISMES, Bergamo, Italy



ISMES Calibration Chamber:

1,2 x 1,5 m

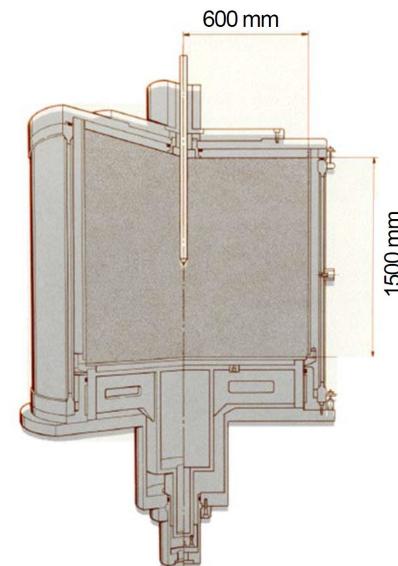
4 types BC

5 types of sand (**Ticino**, Toyoura, Hokksund, Quoiu and Kenya)

Most of the tests were performed on Ticino sand

	Top and bottom boundary		Lateral boundary	
BC Name	Stress	Strain	Stress	Strain
BC1	const.	-	const.	-
BC2	-	0	-	0
BC3	const.	-	-	0
BC4	-	0	const.	-

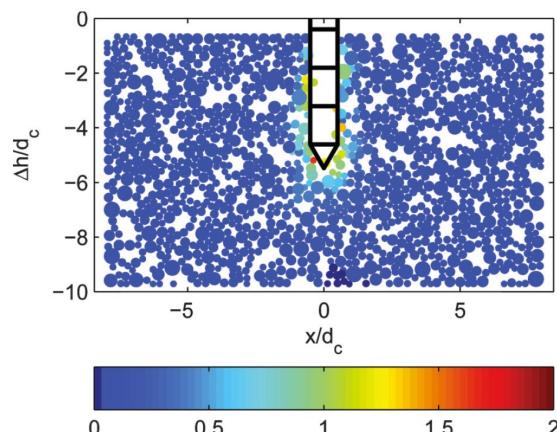
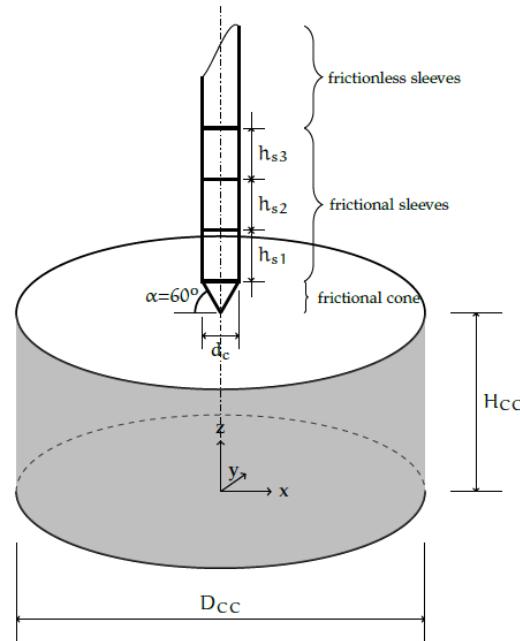
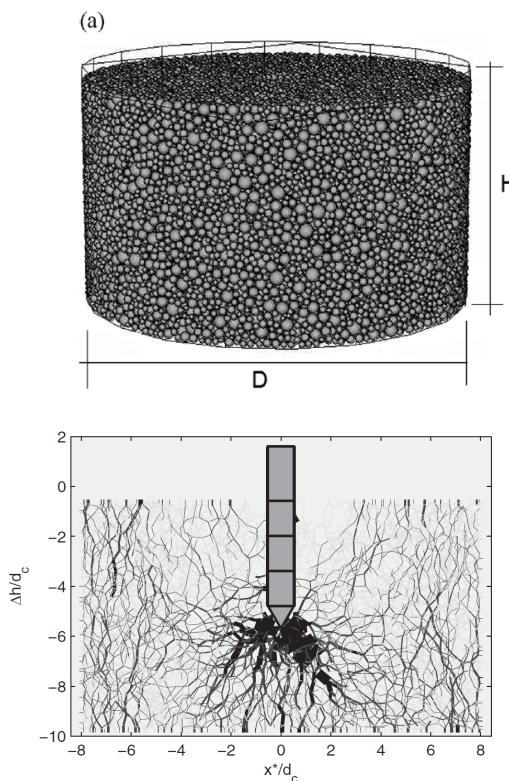
Sand gradation	D _{min}	D _{max}	D ₅₀	γ _{min}	γ _{max}	e _{min}	e _{max}	R
	[mm]	[mm]	[mm]	[kN/m ³]	[kN/cm ³]	[-]	[-]	[-]
TS4	0.3	0.9	0.53	13.64	17.24	0.578	0.924	0.40



5.2) Previous work at UPC on CPT-VCC (Enel-Ismes CC) using DEM

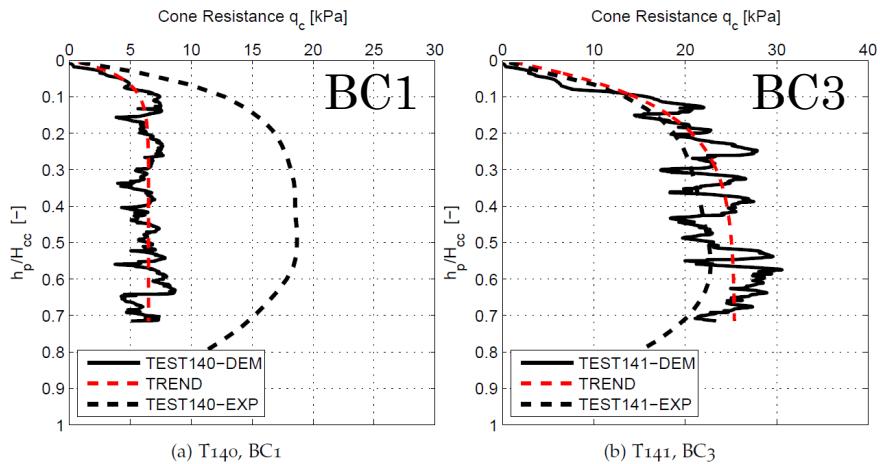


Joanna
Butlanska
PhD (2014)



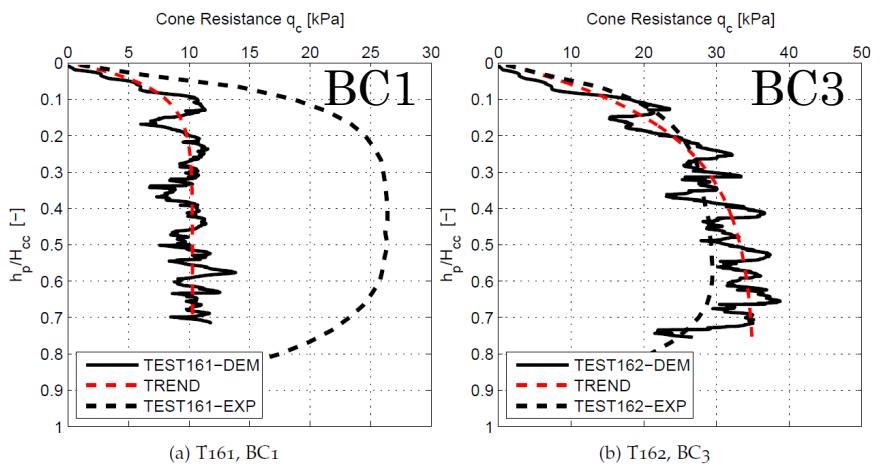
$$\sigma_v = 122 \text{ kPa}$$

$$\sigma_h = 54 \text{ kPa}$$



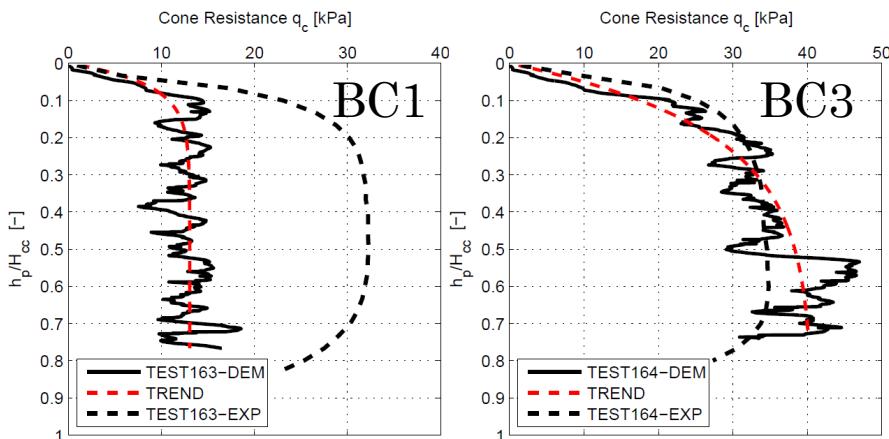
$$\sigma_v = 212 \text{ kPa}$$

$$\sigma_h = 88 \text{ kPa}$$



$$\sigma_v = 313 \text{ kPa}$$

$$\sigma_h = 133 \text{ kPa}$$



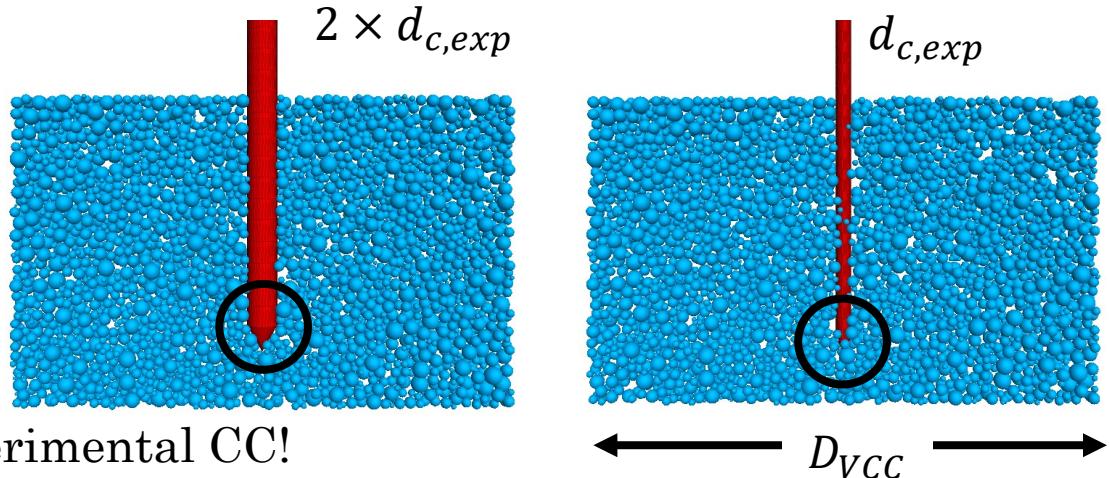
Parameter	Value or relationship
Chamber sizes (height, diameter)	70cm, 120cm
Normal contact stiffness	$300 \text{ MN/m} \cdot 2.0 \frac{D_1 D_2}{D_1 + D_2}$
Shear contact stiffness	$0.25 k_n$
Inter-particle friction coefficient	0.35 (19.3°)
Ball rotation	Inhibited
Local damping	0.1
Ball density	2500 kg/m ³
Ball size	GSD × 50
Boundary conditions	BC1 - BC3
Cone size	$d_{c,EXP} \times 2 = 71.2 \text{ mm}$
Penetration velocity	$v_{c,EXP} \times 5 = 10 \text{ cm/s}$
Cone tip	$\mu_{c,t} = \mu_b = 0.35$
Frictional cone sleeves (<100cm)	$\mu_{c,s} = \mu_b = 0.35$
Frictionless cone sleeves (>100cm)	$\mu_{c,s} = 0$

BC1

BC3

The R_d ratio :

$$R_d = \frac{D_{VCC}}{d_c}$$



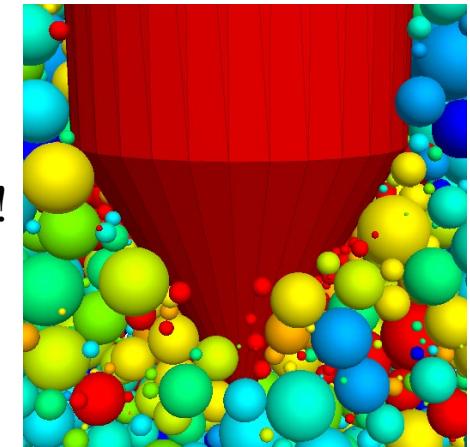
was **half** compared to the experimental CC!

It is important not to change the R_d ratio.

However, if $R_{d,exp} = R_{d,num}$, we need to halve particle size to have ~ 10 contacts “cone tip/particles” $\rightarrow 1.74 \times 10^6$ particles!

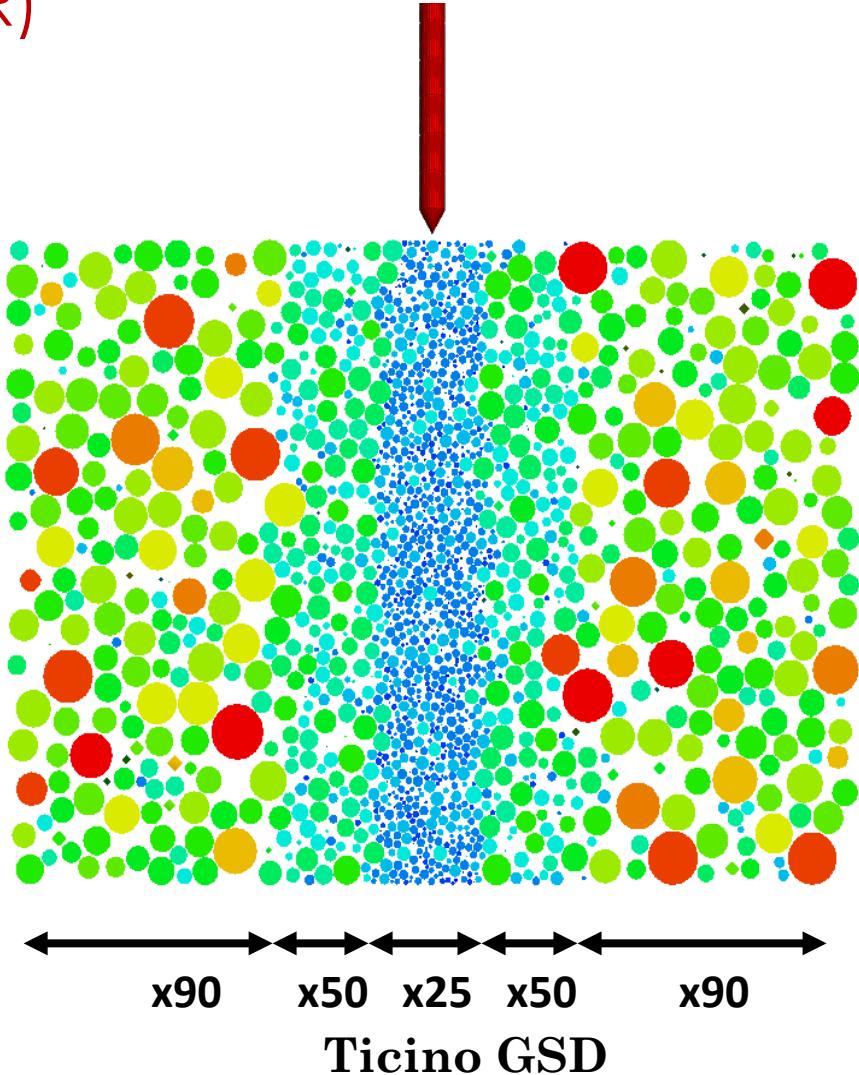
So, how to:

- 1) Maintain R_d ratio equal to the physical experiments?
- 2) Guarantee a minimum number of contacts cone/particles of 10?
- 3) Have a reasonable number of particles?



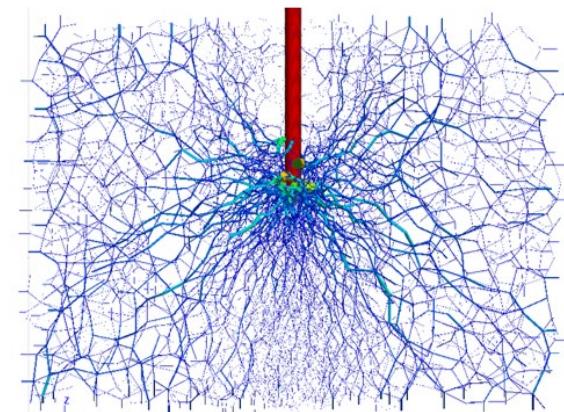
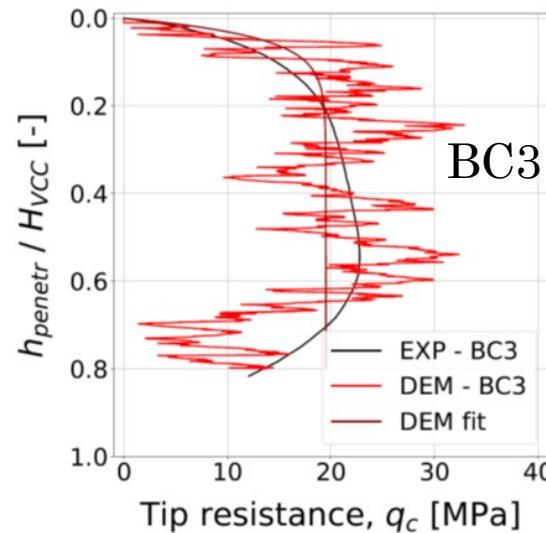
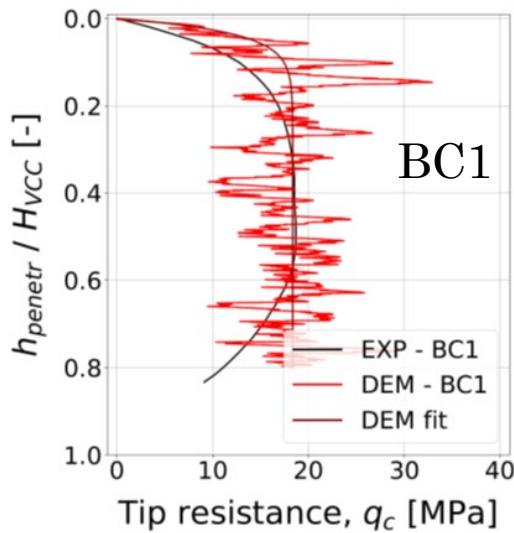
Multi-scaling technique!

5.3) DEM simulations of CPT tests in the ENEL-ISMES calibration chamber (with RR)

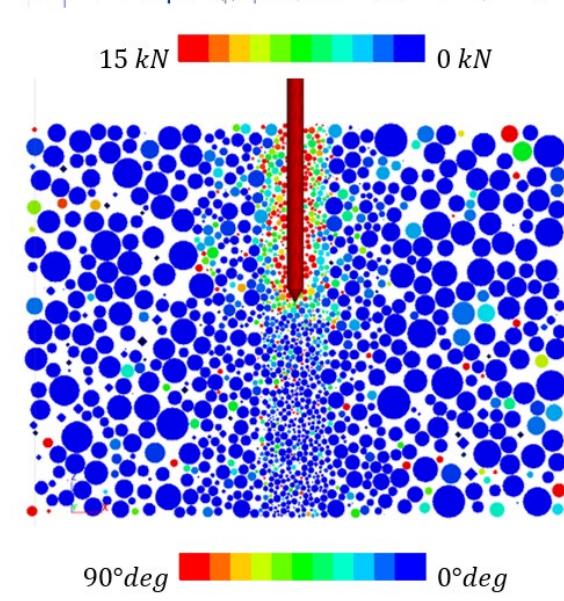
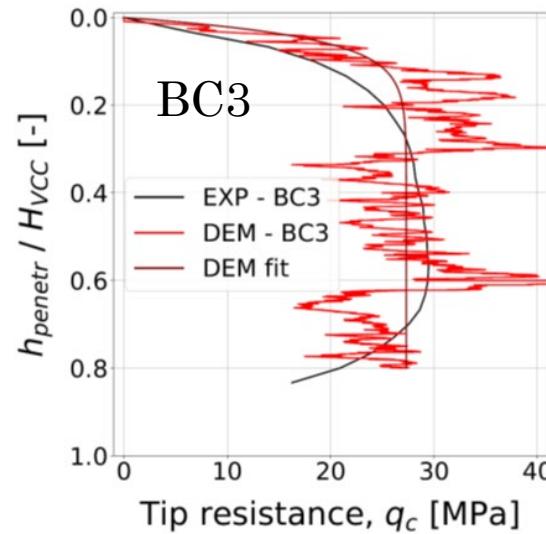
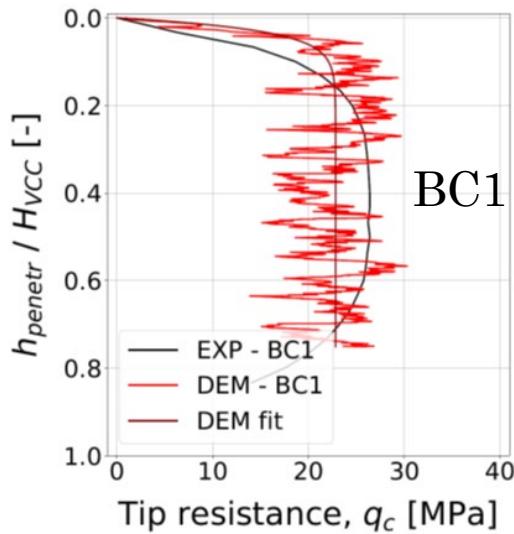


Parameter	Symbol	Value or relationship
Chamber sizes (height, diameter)	H_{VCC}, D_{VCC}	100cm, 120cm
Effective normal contact stiffness	E_{mod}	$4.0 \cdot 10^8$ Pa
Normal-to-shear stiffness ratio	k_{ratio}	2.0
Inter-particle friction coefficient	μ_b	0.60 (calibrated)
Wall friction	μ_w	0.0 (frictionless)
Degree of true sphericity	ψ	Distributions known from 2D scans
Rolling friction coefficients	μ_r	$\mu_r = 0.1963(\psi)^{-8.982}$ (Eq. 8.6)
Rolling stiffness	k_r	$k_s R$ (Eq. 8.1)
Local damping		0.7
Ball density	ρ	2500 kg/m ³
Ball size (GSD of Ticino sand)	GSD	$GSD \times 90$ (coarse, far from the cone) $GSD \times 50$ (in between coarse/fine) $GSD \times 25$ (fine, near the cone)
Boundary conditions	BC	BC1 - BC3
Confining pressures	σ_v, σ_h	<ul style="list-style-type: none"> $\sigma_v = 122kPa - \sigma_h = 54kPa$ $\sigma_v = 212kPa - \sigma_h = 88kPa$
Initial relative density (initial porosity, DEM)	D_R (n_0)	$D_R \cong 90\%$ $(n_0 = 0.375)$
Cone size	d_c	$d_{c,EXP} \times 1 = 35.6mm$
Cone stiffness	k_n, k_s	$k_n = k_s = 3 \cdot 10^6 N/m$
Penetration velocity	v_c	$v_{c,EXP} \times 5 = 10cm/s$
Cone tip friction coefficient	$\mu_{c,t}$	$\mu_{c,t} = \mu_b = 0.60$

$$\sigma_v = 122 \text{ kPa} - \sigma_h = 54 \text{ kPa}$$



$$\sigma_v = 212 \text{ kPa} - \sigma_h = 88 \text{ kPa}$$



BC1



BC3

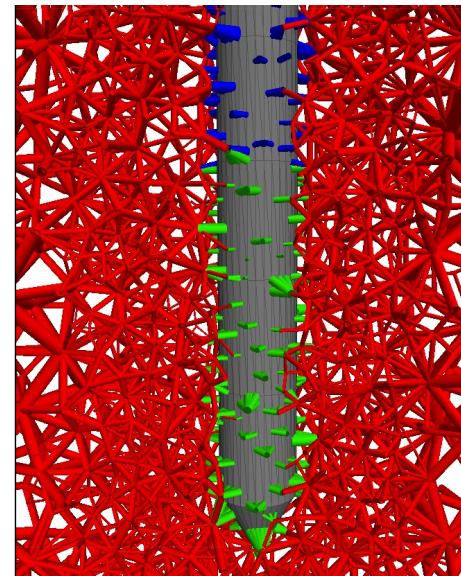


5.4) Effect of particle shape on penetration resistance: parametric study (BC1)

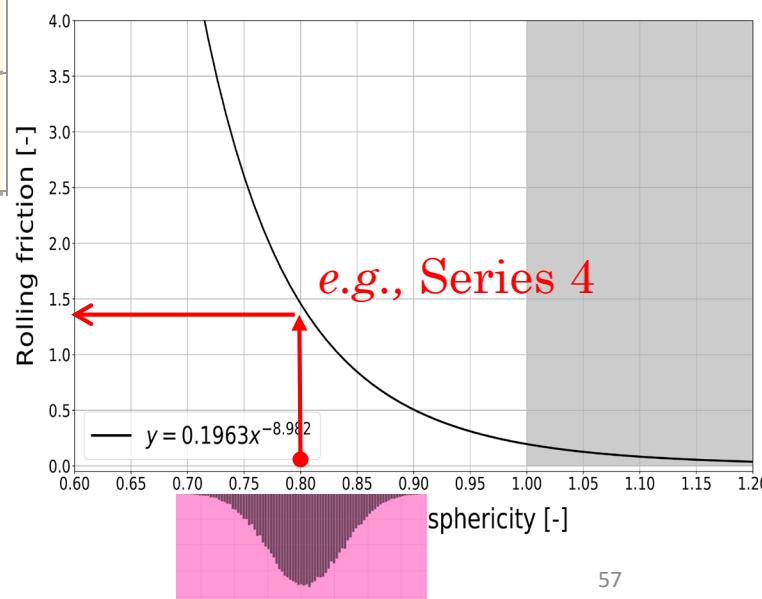
- Artificial sand with variable μ_s and shape ($\sim \mu_r$)

Friction coefficient	Case A	Case B	Case C
μ_b (ball-ball)	0.60	0.30	0.60
$\mu_{c,t}$ (ball-cone tip)	0.60	0.30	0.30

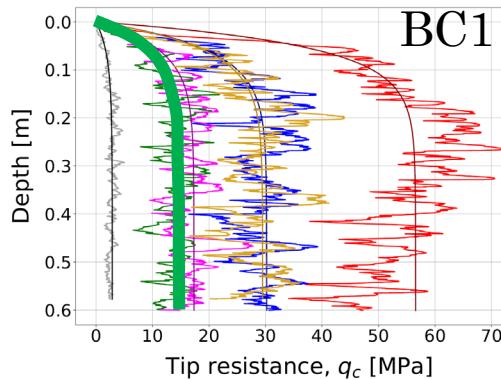
█ = μ_s
█ = $\mu_{shaft} = 0.0$
█



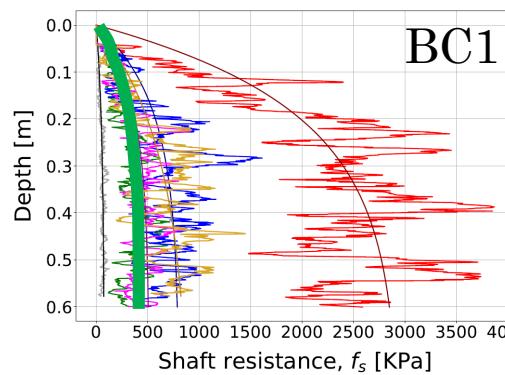
Series	Friction case	Particle shape	Rolling condition at contacts
1	A – B – C	Perfect smooth spheres	Free rotations, $\mu_r = 0.0$
2	A – B – C	Iper-angular	Fixed rotations, $\mu_r = \infty$



Tip resistance



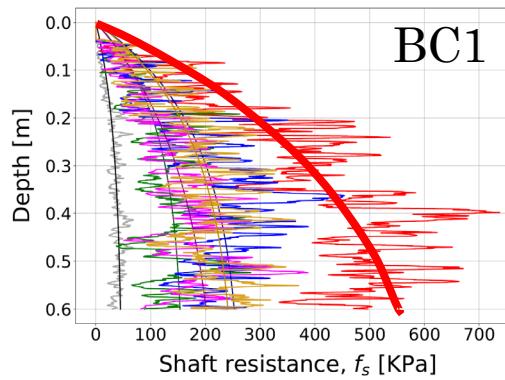
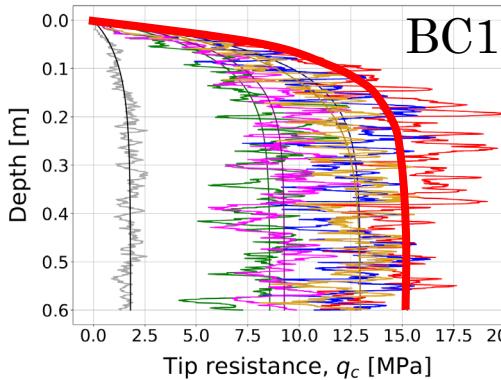
Shaft resistance



Case
A

$$\begin{aligned}\mu_{balls} &= 0.60 \\ \mu_{cone} &= 0.60\end{aligned}$$

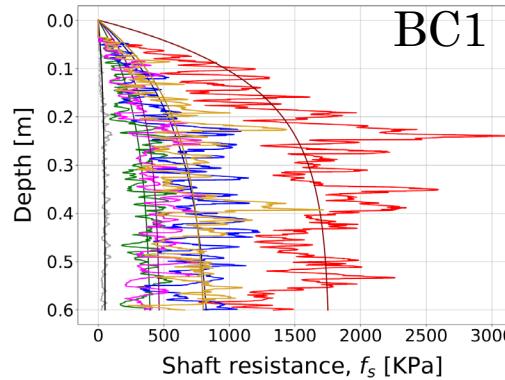
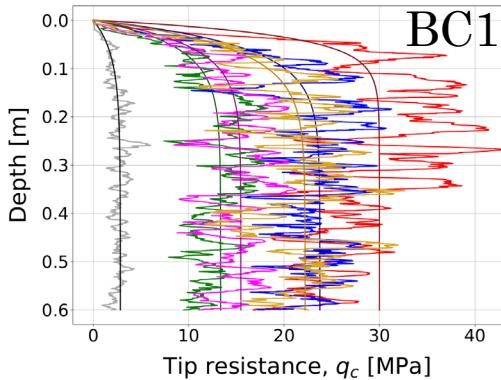
- free rotations
- fix rotations
- RR low - single
- RR high - single
- RR low - variable
- RR high - variable



Case
B

$$\begin{aligned}\mu_{balls} &= 0.30 \\ \mu_{cone} &= 0.30\end{aligned}$$

- free rotations
- fix rotations
- RR low - single
- RR high - single
- RR low - variable
- RR high - variable



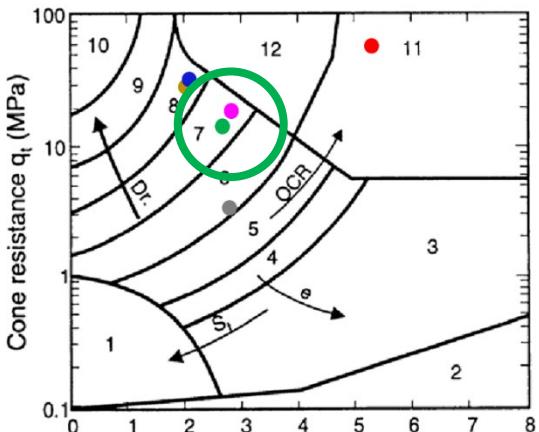
Case
C

$$\begin{aligned}\mu_{balls} &= 0.60 \\ \mu_{cone} &= 0.30\end{aligned}$$

Robertson & Campanella charts (Robertson, 1986-1990)

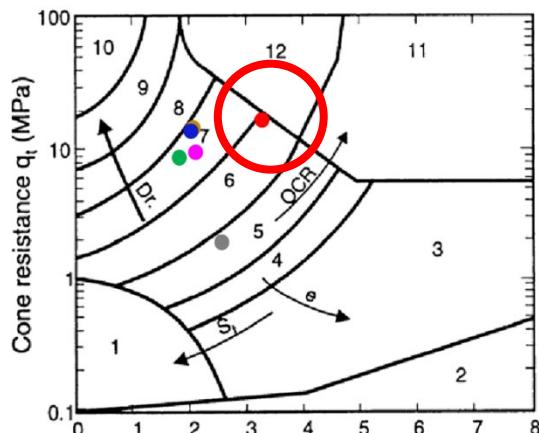
Case A

$$\mu_{\text{balls}} = \mu_{\text{cone}} = 0.60$$



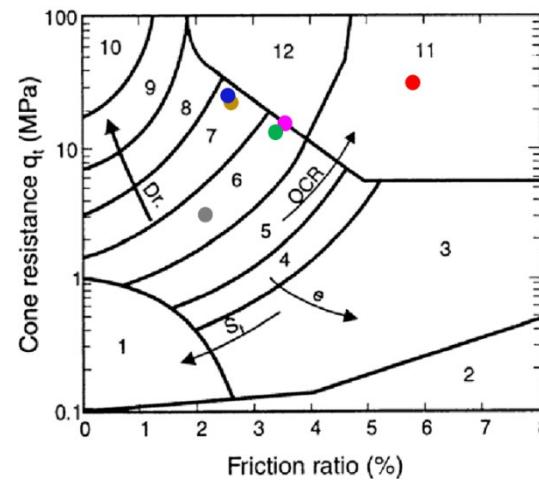
Case B

$$\mu_{\text{balls}} = \mu_{\text{cone}} = 0.30$$



Case C

$$\mu_{\text{balls}} = 0.60 \\ \mu_{\text{cone}} = 0.30$$



Zone	Soil Behavior Type
1	Sensitive fine grained
2	Organic material
3	Clay
4	Silty Clay to clay
5	Clayey silt to silty clay
6	Sandy silt to clayey silt
7	Silty sand to sandy silt
8	Sand to silty sand
9	Sand
10	Gravelly sand to sand
11	Very stiff fine grained*
12	Sand to clayey sand*

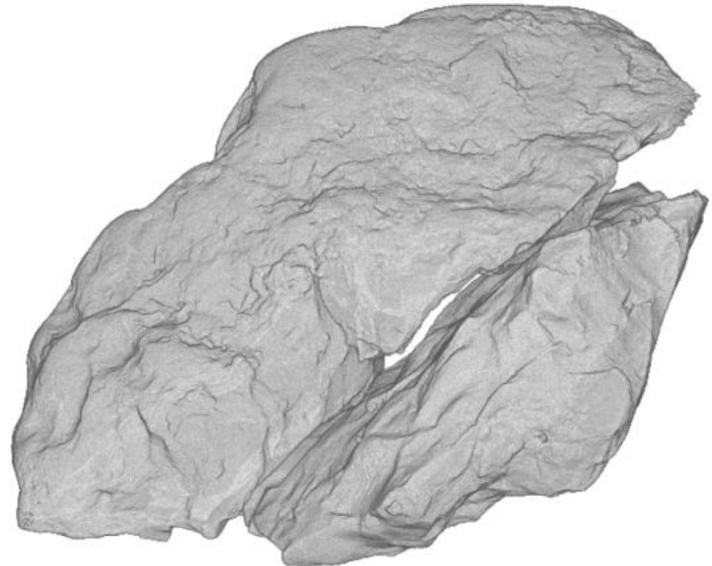
* Overconsolidated or cemented

- free rotations
- fix rotations
- RR low - single
- RR high - single
- RR low - variable
- RR high - variable

6.2) Perspectives

Particle shape

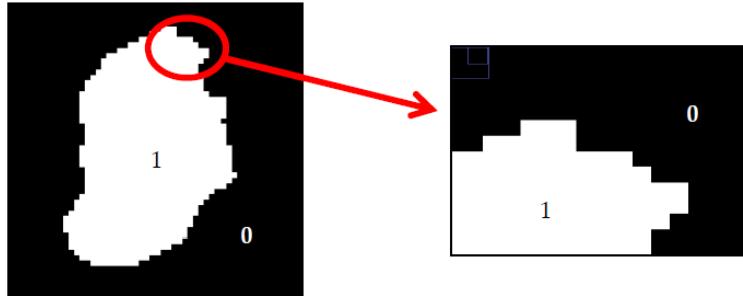
- Exploit higher resolutions scans now available
- Investigate the effect of particle Roundness



(Wiebicke, 2017)

Numerical simulations

- Include particle crushing in our DEM simulations (Ciantia crushing model)
- Model the lateral membrane in the TX-DEM tests to better reproduce the shear bands
- Simulate other laboratory tests with the proposed CM
- Simulate other Boundary Value problems



Marching Cubes algorithm

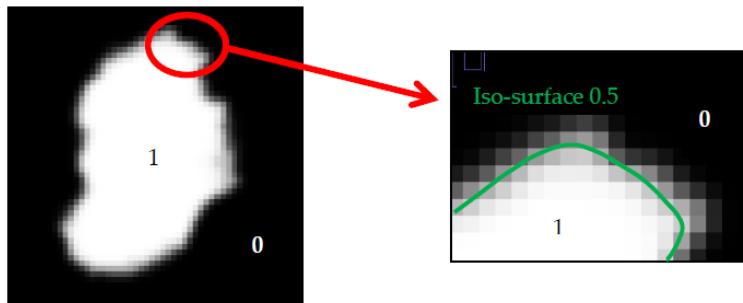


Figure 6.15: Visualisation of the Gaussian filter applied to grain number 46972



Figure 6.17: On the left, slice of the initial binarised sphere. On the right, the same sphere after the Gaussian filter is applied

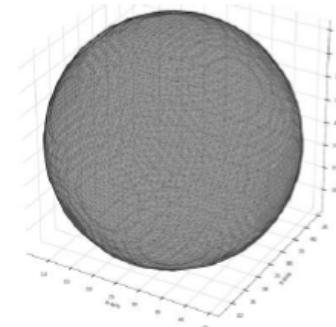


Figure 6.18: Surface mesh visualisation after application of the MC-algorithm

PCA vs Inertia axis for grain lengths

plained in the previous section. The two approaches to obtain the grains lengths (PCA and inertia tensor) are equivalent. Indeed the inertia tensor reported in Eq. (6.2) can be rewritten as:

$$\begin{aligned} I &= \sum_n m_n \cdot [(x_n \cdot x_n) I_3 - (x_n \cdot x_n^T)] = \sum_n m_n \cdot (x_n \cdot x_n) I_3 - \sum_n m_n \cdot x_n \cdot x_n^T = \\ &= I_3 \cdot \text{tr}(C) \cdot C \end{aligned} \quad (6.5)$$

where C is the mass-weighted variance-covariance matrix defined as

$$C = \sum_n m_n x_n \cdot x_n^T \quad (6.6)$$

The variance-covariance matrix C is symmetric, and therefore it can be diagonalised (obtaining the matrix D) by the matrix R (*i.e.*, the rotation matrix), as

$$C = RDR^{-1} = RDR^T. \quad (6.7)$$

It is now possible to rewrite the inertia tensor I as:

$$I = I_3 \cdot \text{tr}(C) \cdot C = RR^T \cdot \text{tr}(C) \cdot RDR^T = R[\text{tr}(C)I_3 \cdot D]R^T \quad (6.8)$$

and since the matrix $[\text{tr}(C)I_3 \cdot D]$ is diagonal, it follows both the I and C are diagonalised by the same rotation matrix R . Therefore the eigenvectors, which are the body orientation in space, are the same for both approaches: PCA and inertia tensor. This has also been verified numerically, comparing both techniques in the validation that follows, obtaining exactly the same results.

Shape VS rotation

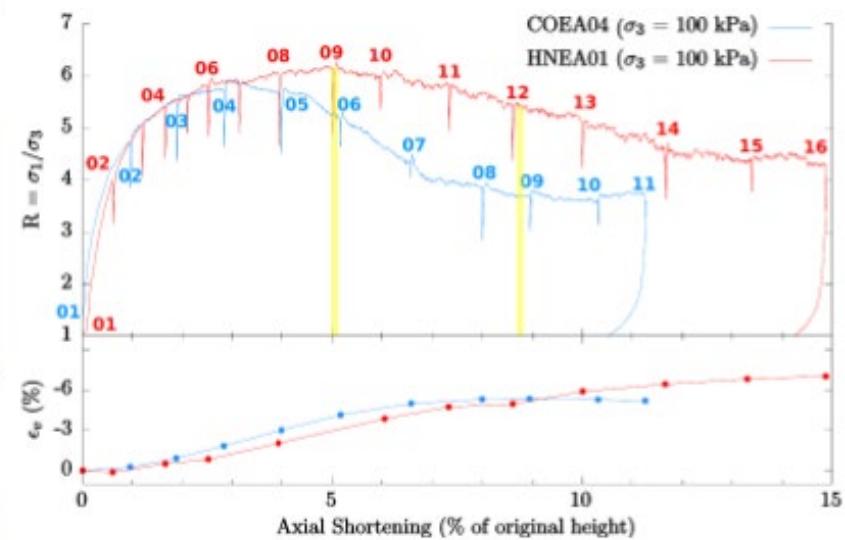
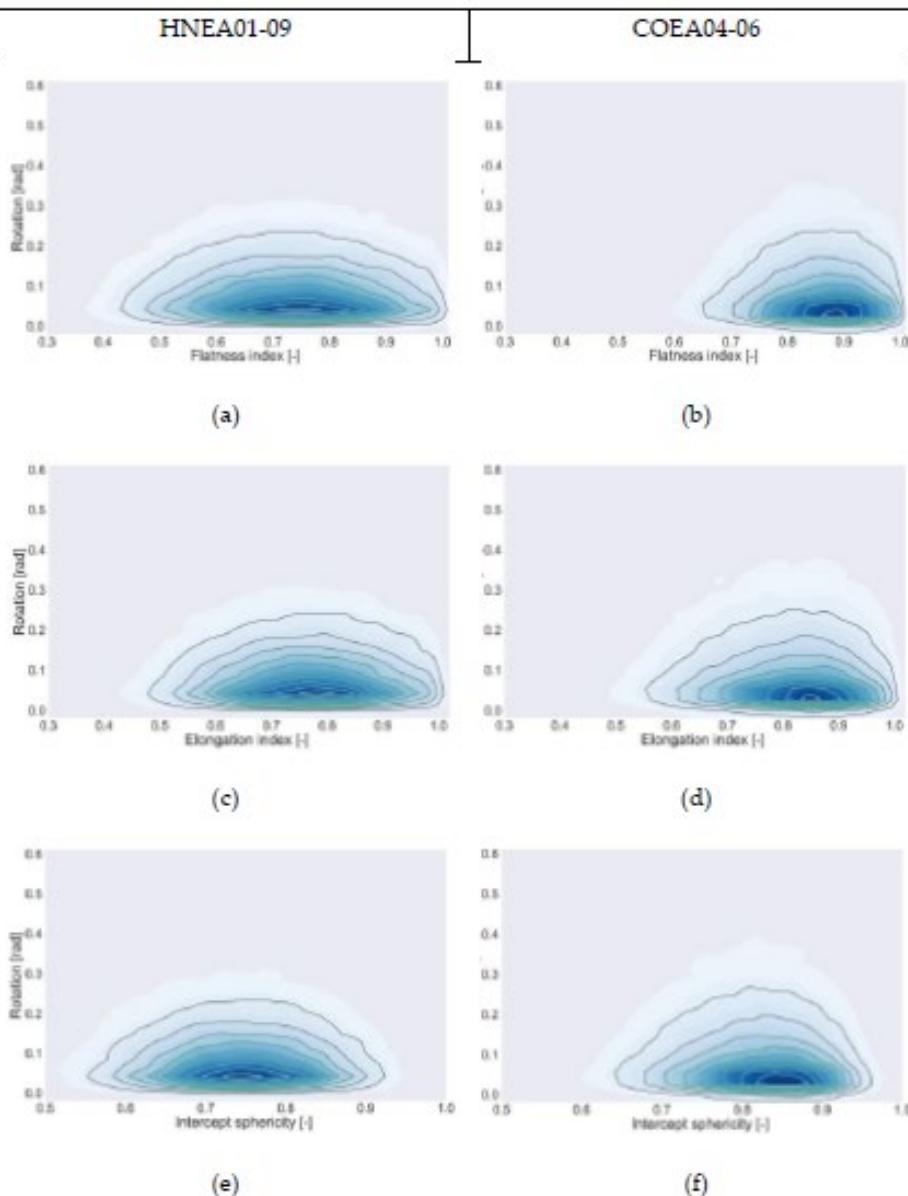


Figure 7.17: Normalised bivariate frequency density plots of form descriptors versus cumulative grain rotation magnitude at 5% shortening (loading stages HNEA01-09 and COEA04-06, respectively 48.612 and 65.056 grains). The contours colour bar is shown in Figure 7.5c.

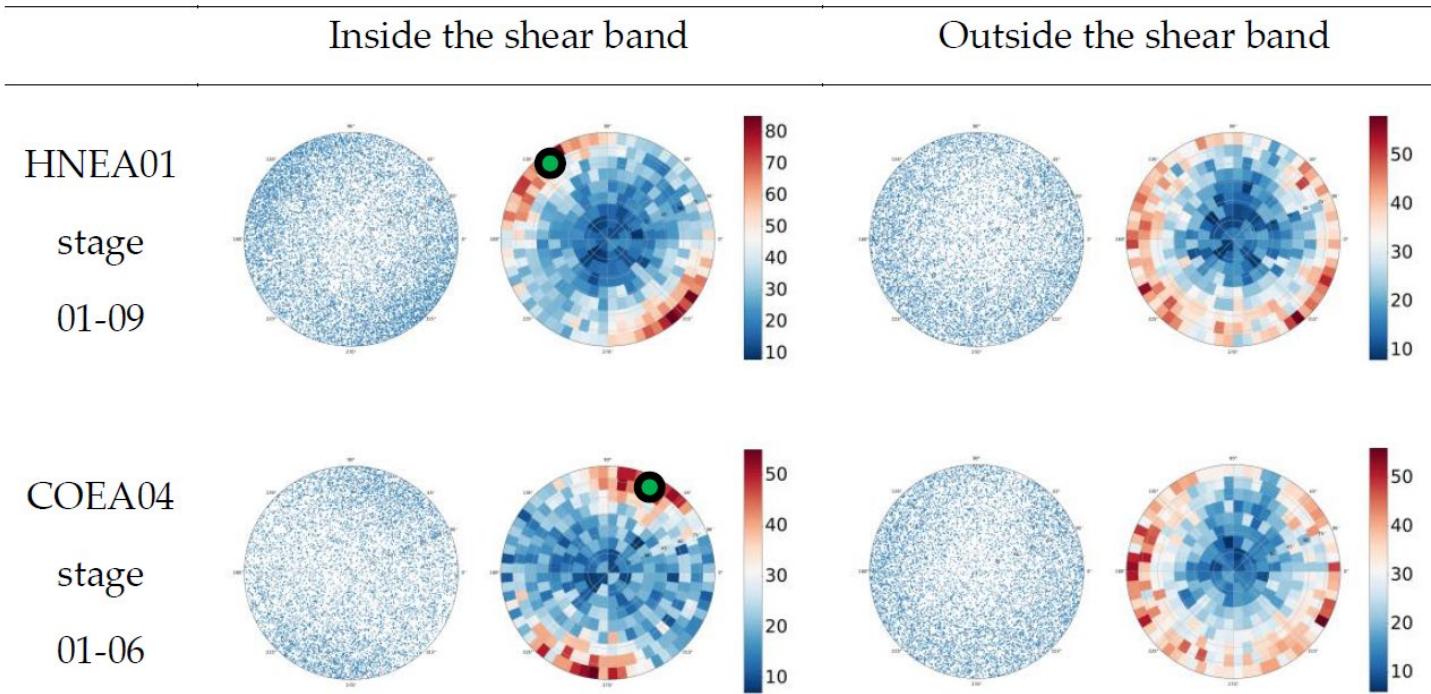
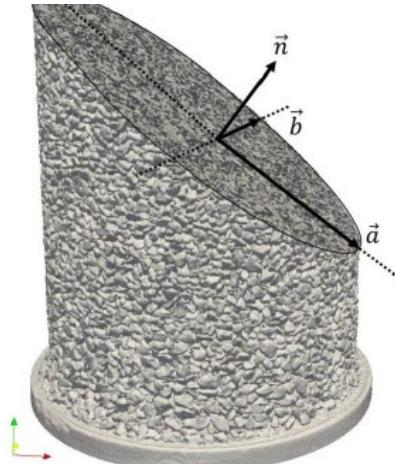
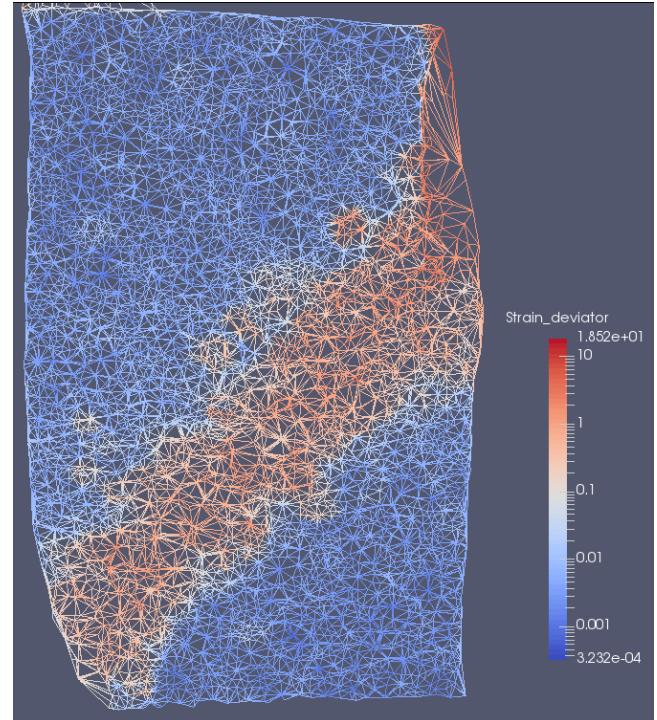
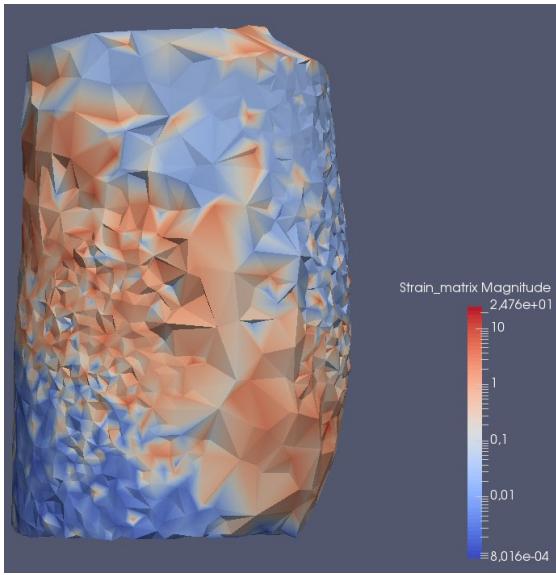
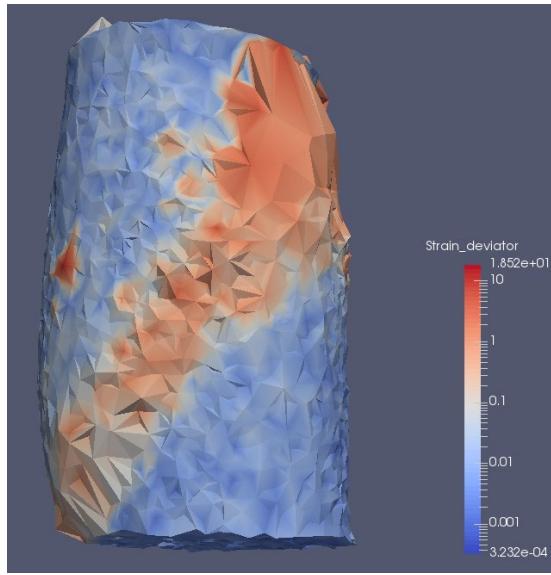


Figure 7.15: Stereoplots showing the rotation verson directions at 5% shortening. The green dots indicate the orientation of vector \vec{b} (see Figure 7.7) belonging to the shear bands of Hostun and Caicos sands. The stereoplot angles markers are not shown for readability, see Figure 7.5b for reference.

Direction of rotation



- Triangulating the grains centres of masses and calculating the deviatoric strain → YADE (Grain-based deviatoric strain)



Choose a threshold: **0.10**

- $> 0.10 \rightarrow$ Inside shear band
- $< 0.10 \rightarrow$ Outside the shear band

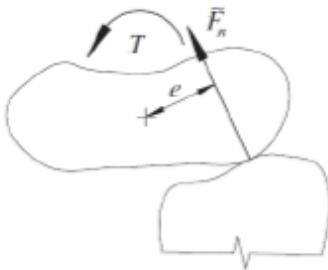


Figure 4.16: Non-spherical particles in contact. The contact normal forces shows an eccentricity that induces a torque (Wensrich and Katterfeld, 2012)

It is evident that the contact normal force does not pass through the particles centres of mass, therefore the eccentricity 'e' creates a rolling moment of magnitude

$$|M| = e \cdot |F_n| \quad (4.37)$$

That should be comparable to any value of rolling resistance torque provided by the mentioned contact models. A comparison between Eq. (4.36) and (4.37) inspires the following relationship:

$$\langle e \rangle \cong \eta R_r \rightarrow \eta \cong \frac{\langle e \rangle}{R_r}$$

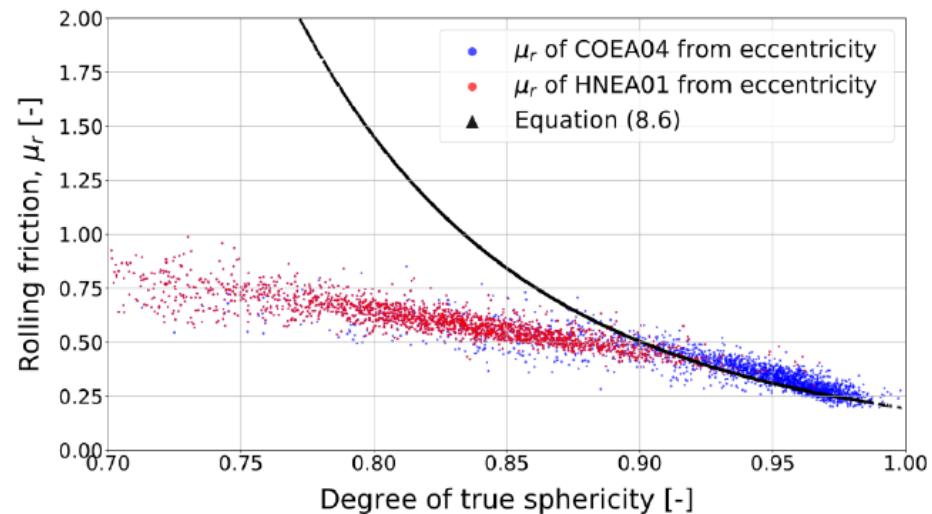


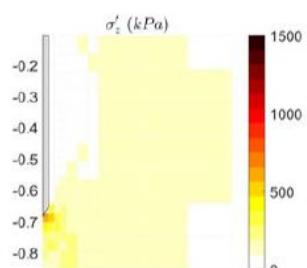
Figure 8.13: Rolling frictions of all particles involved in the simulation obtained from both eccentricity calculation and Equation 8.6. For high values of particle sphericity (i.e., $\psi > 0.90$) the two approaches provide similar values.

Vertical and radials stress distributions induced by the cone penetration

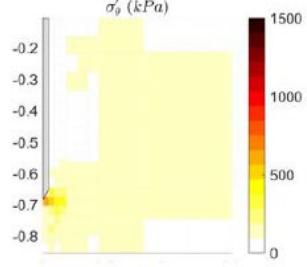
**Case
A**

$$\mu_{balls} = \mu_{cone} = 0.60$$

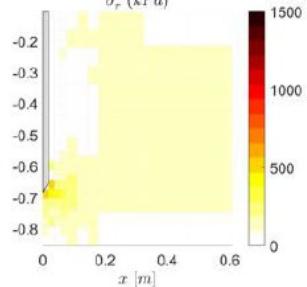
Vertical



Radial



Radial

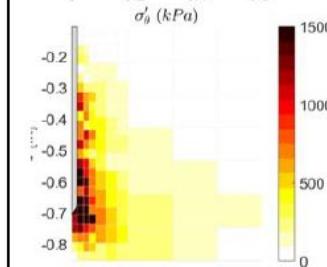
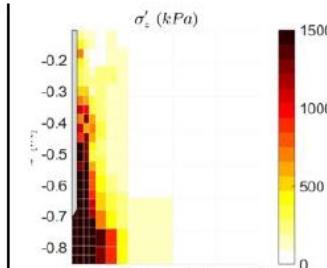
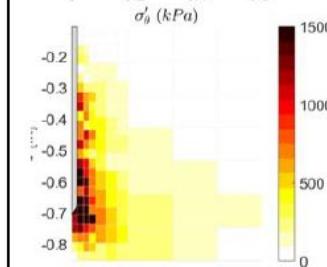
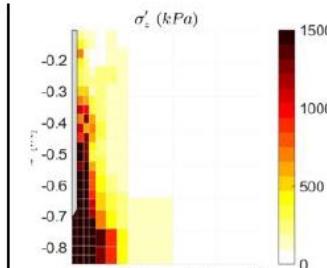
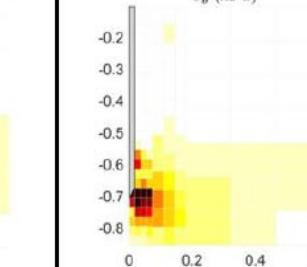
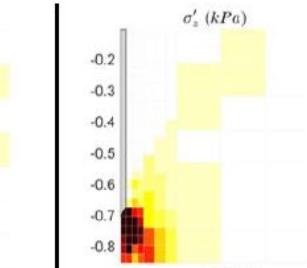
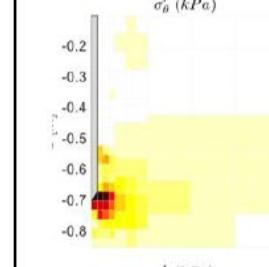
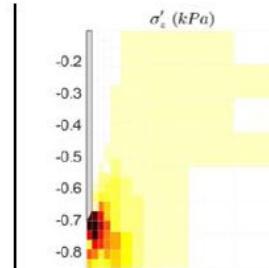


Free
rotations

RR low
(single)

RR high
(single)

Fixed
rotations

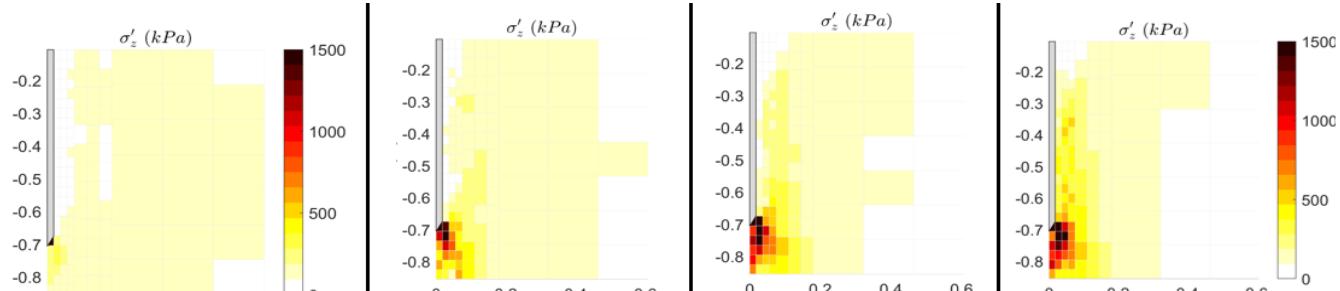


Vertical and radials stress distributions induced by the cone penetration

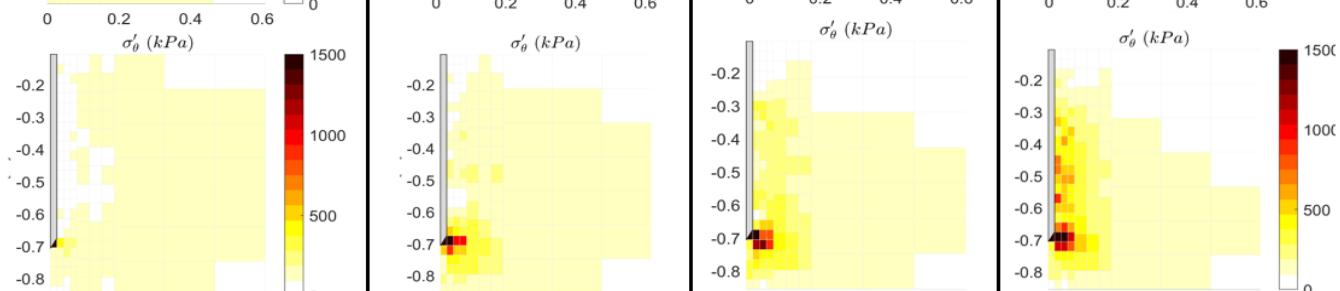
**Case
B**

$$\mu_{balls} = \mu_{cone} = 0.30$$

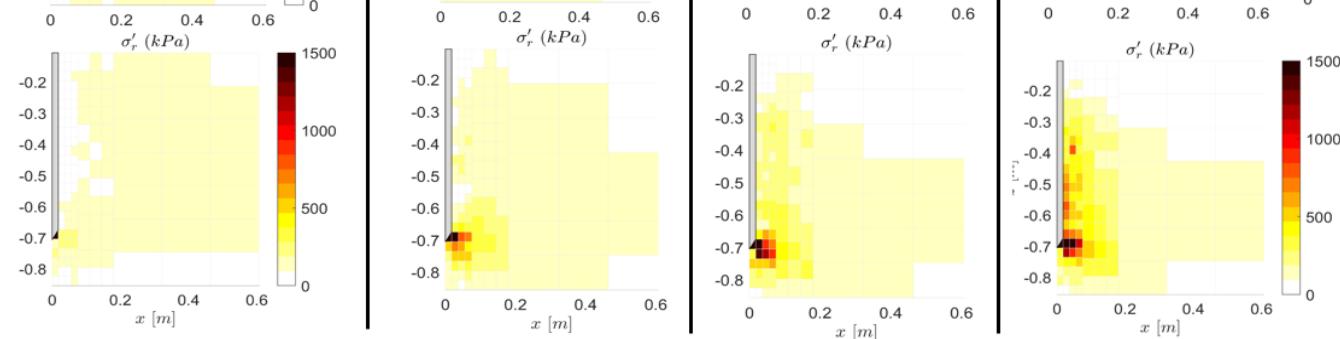
Vertical



Radial



Radial



Free
rotations

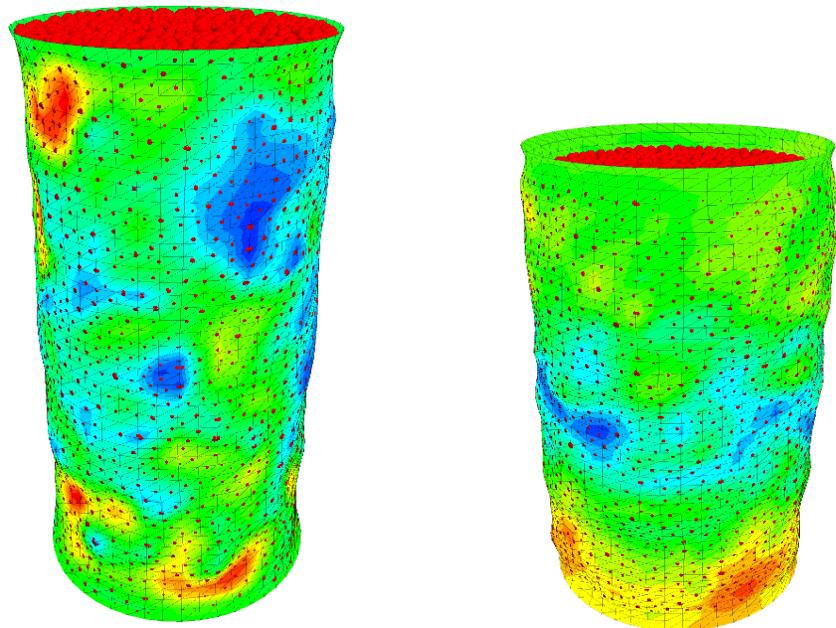
RR low
(single)

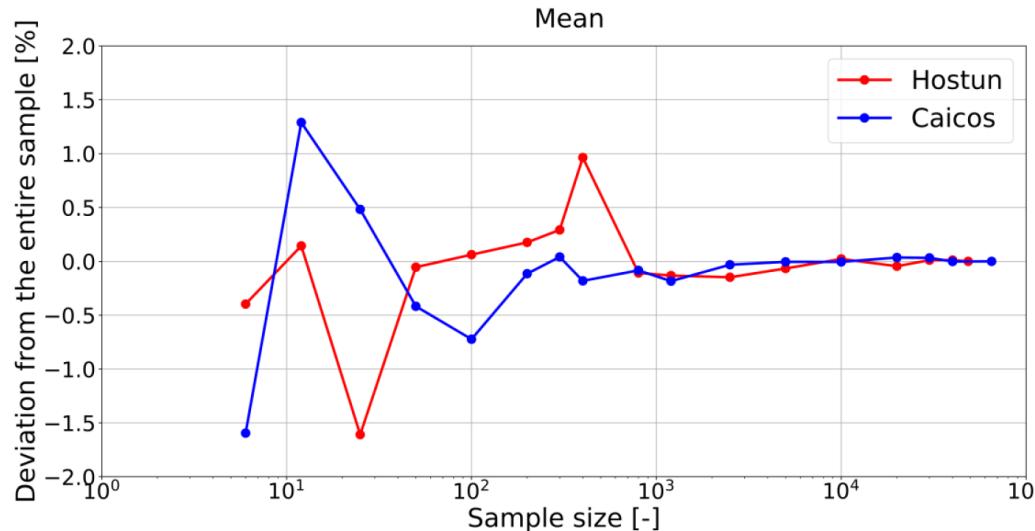
RR high
(single)

Fixed
rotations

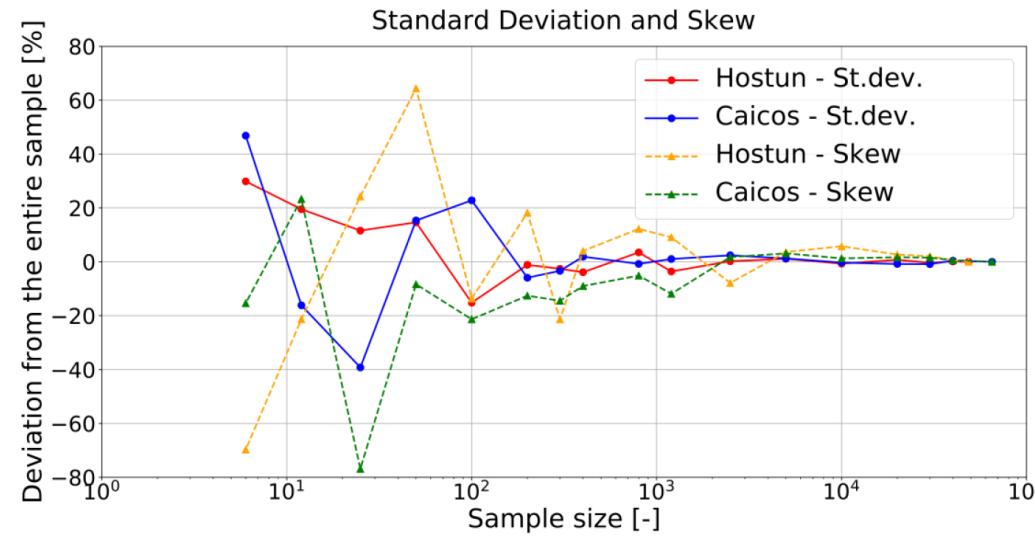
Implement the rolling resistance contact model with Hertzian formulation (ready) and test it (TX test on 3 sands, at 100kPa and 300kPa confining pressure)

Model the cylindrical external wall as a flexible elastic membrane with finite elements (FLAC3D “shell” element) to facilitate the localisation of shear failure





(a)

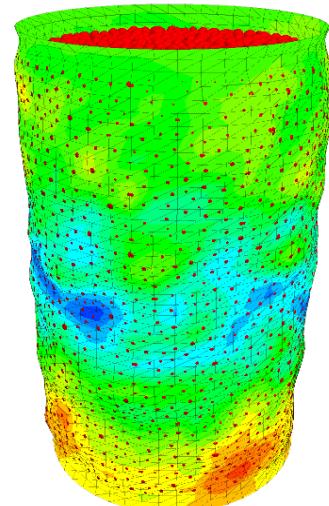
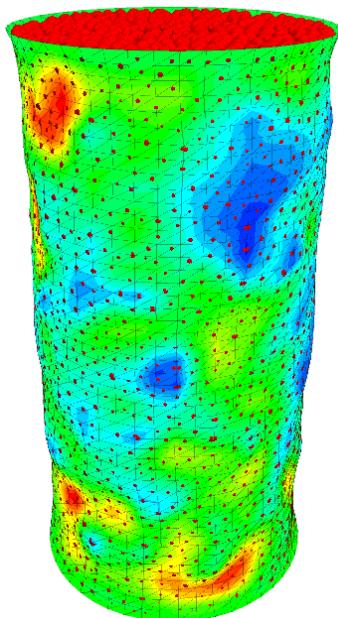


(b)

Figure 12: Evolution of the first three sample moments (mean, standard deviation, skew) of true sphericity with sample size

Looking forward...

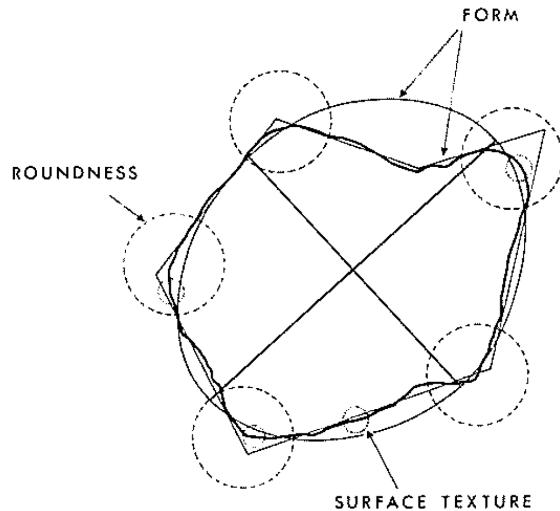
- 1) Implement the rolling resistance contact model with Hertzian formulation (ready) and test it (TX test on 3 sands, at 100kPa and 300kPa confining pressure)
- 2) Exploit the proposed approach relating ψ and "*B*" using the more ~~complicated~~/complete contact model incorporating twisting resistance (*Jiang, 2015*) instead of the basic model (*Iwashita, 1998*).
- 3) Model the cylindrical external wall as a flexible elastic membrane with finite elements (FLAC3D "shell" element) to facilitate the localisation of shear failure



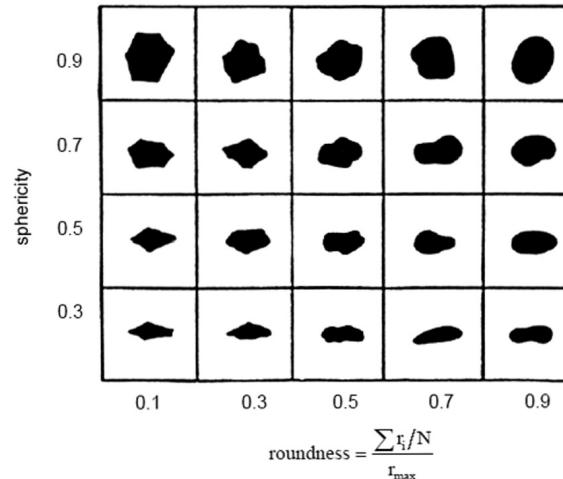
- 4) Perform DEM simulations of engineering problems at large scale (e.g. CPT in VCC)

Particle shape description in literature

Three independent aspects of shape (Barrett, 1980)



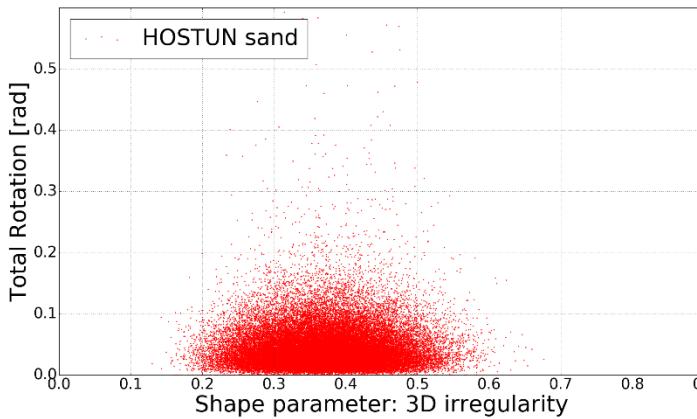
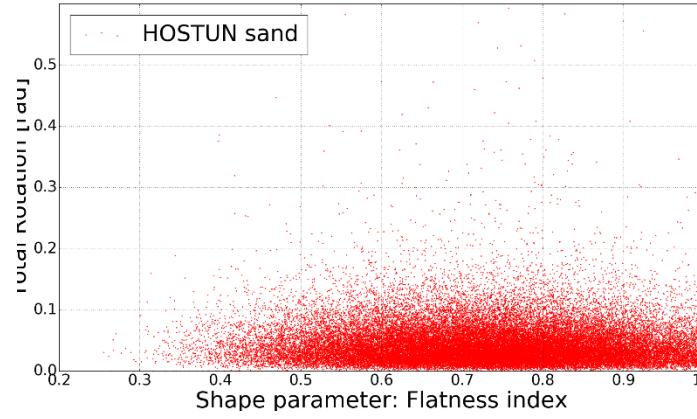
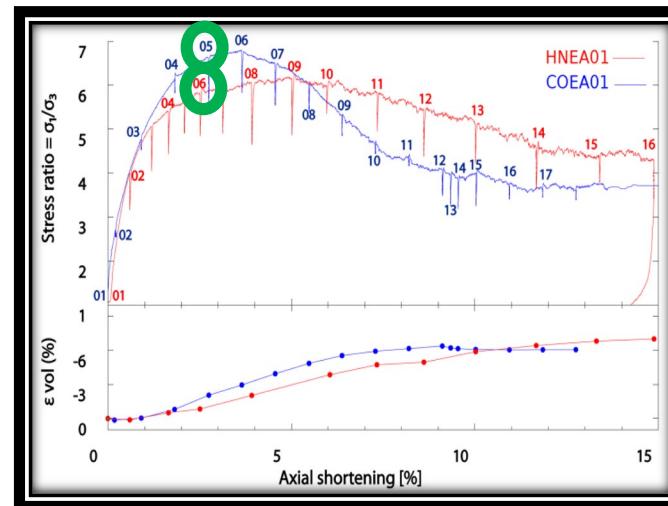
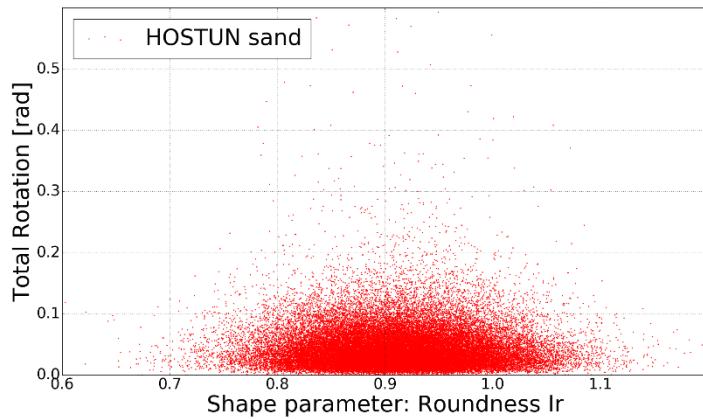
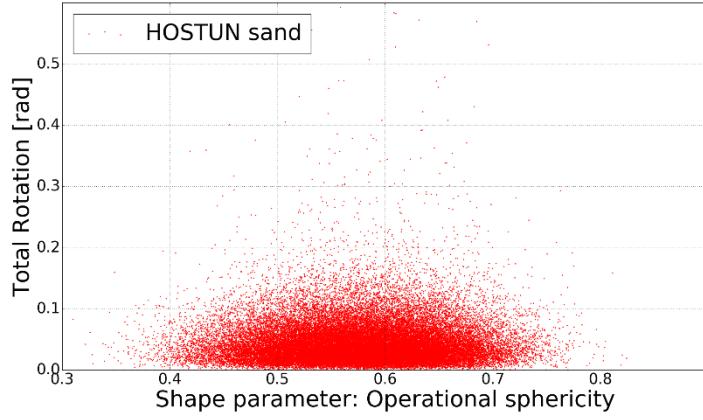
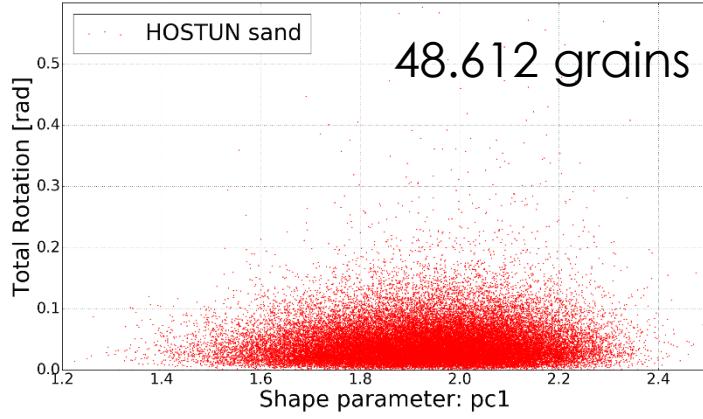
Krumbein & Sloss visual chart (1963)



At least 25-30 different definitions of Sphericity, Roundness and Roughness exist in literature (most in 2D!)

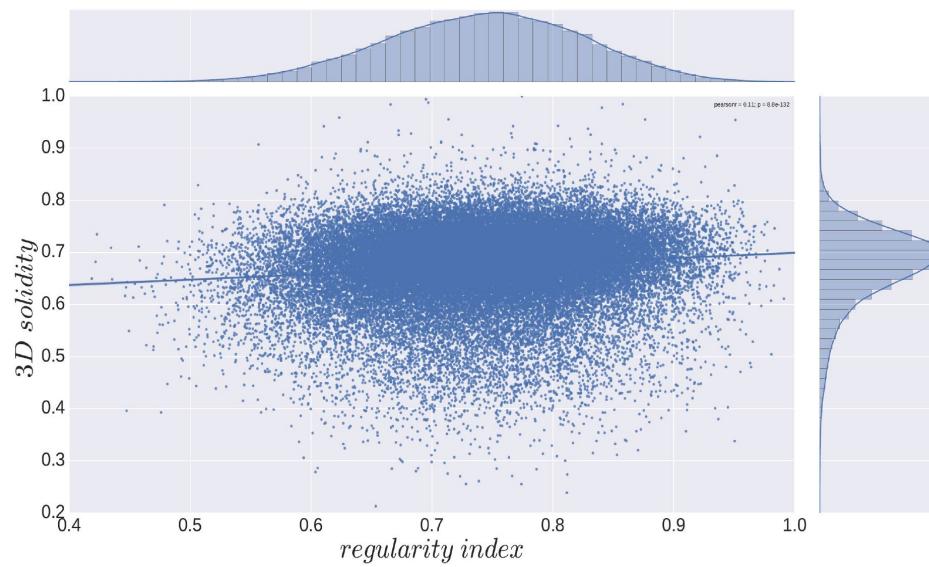
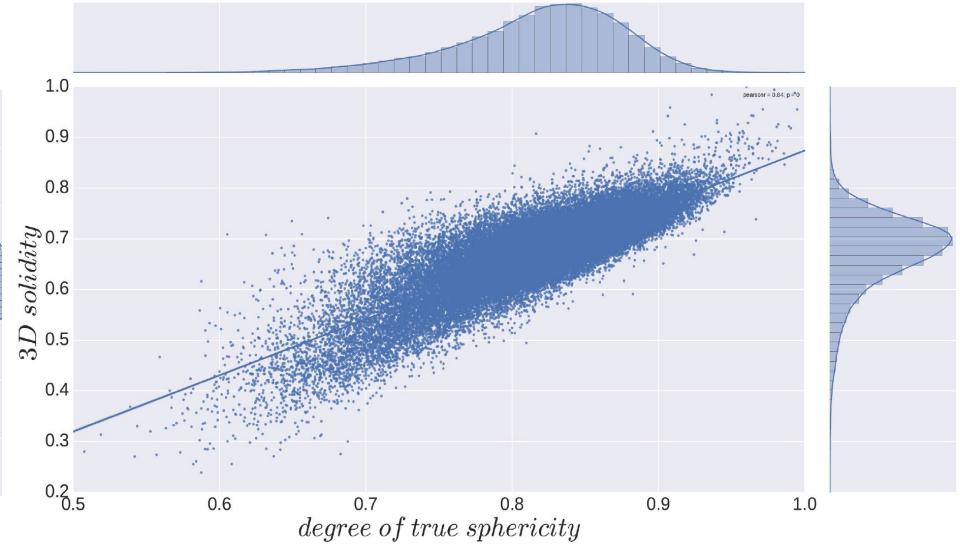
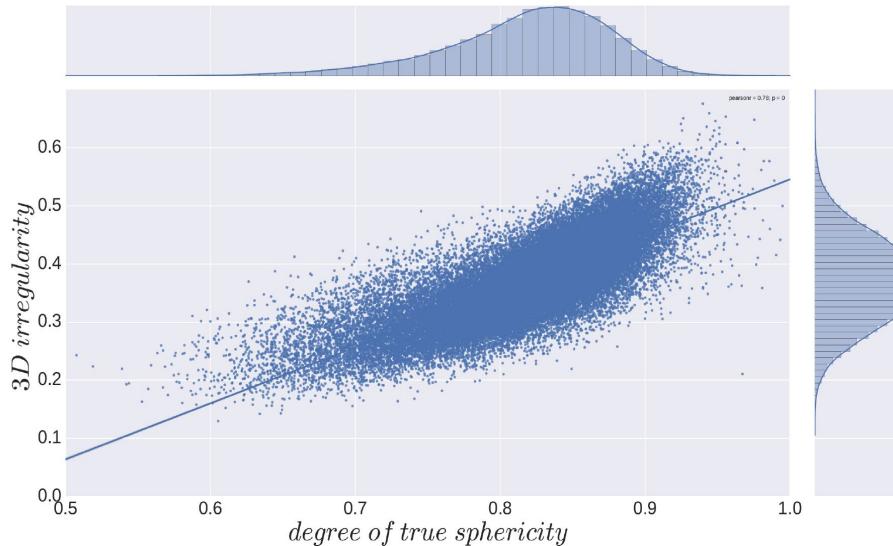
Effect of shape on geotechnical properties:

- Packing (Holubec & D'Appollonia, 1973 – Cho & Santamarina, 2006)
- Grain Size Distribution from sieving (Arasan et al., 2011 – Mora, 1998)
- Shear strength (Holubec & D'Appollonia, 1973 – Rousé, 2008)
- Grains stiffness (Santamarina, 2004)
- Liquefaction potential (Ashmawy, 2003)
- Cone penetration resistance in CPT (Liu & Lehane, 2013)



It seems there is no relevant relationship between grains rotation and many shape descriptors...

... but some are correlated!

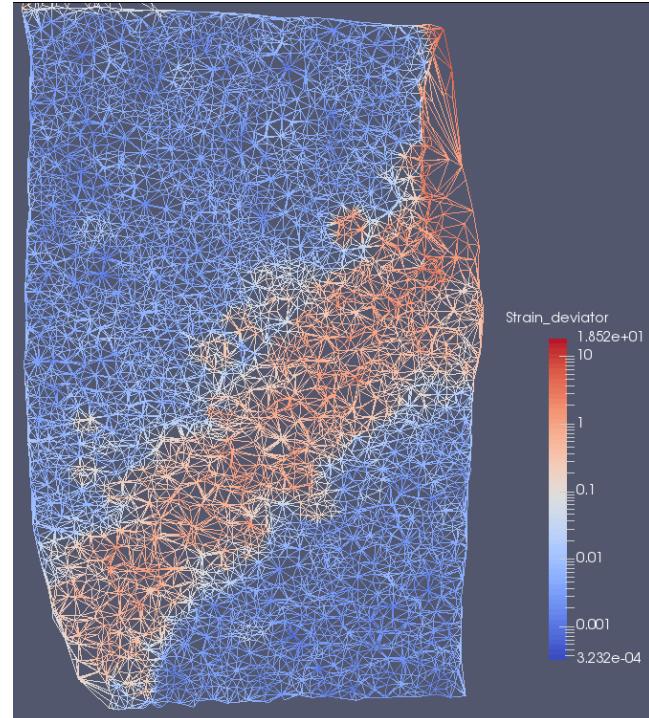
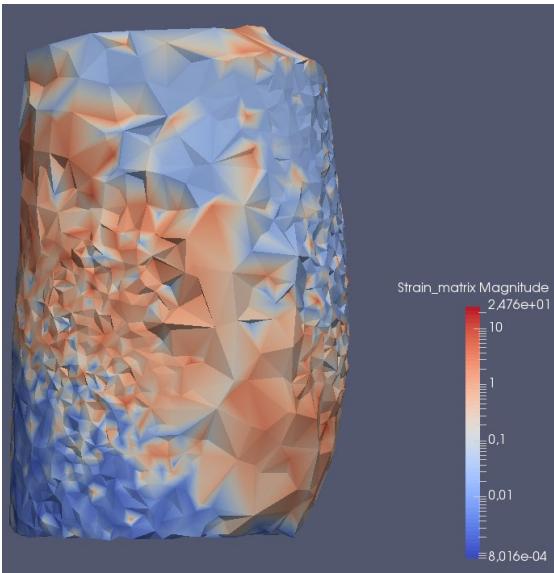
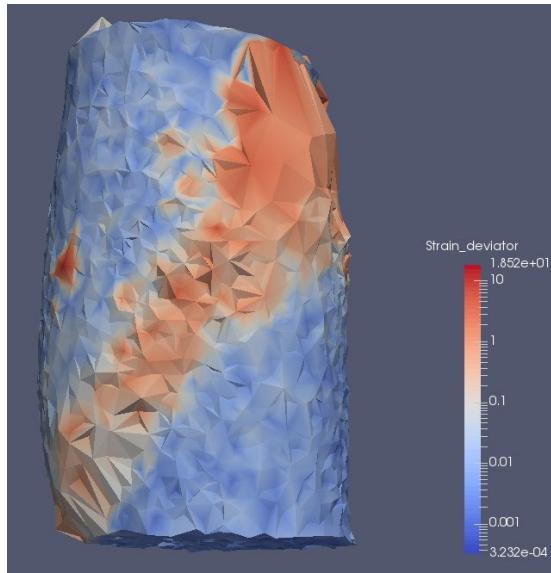


SHAPE DESCRIPT.	Degree true Sphericity	Operational sphericity	3D Irregularity	Flatness index	Elongation index	Regularity index	3D-Form Factor	Roundness X_s	Roundness I_R	3D Solidity
Degree true Sphericity	1.00	0.84	0.89	0.57	0.38	0.70	1.00	0.97	0.61	0.92
Operational sphericity	0.84	1.00	0.95	0.52	0.46	0.72	0.84	0.83	0.64	0.73
3D Irregularity	0.89	0.95	1.00	0.61	0.46	0.79	0.90	0.87	0.60	0.76
Flatness index	0.57	0.52	0.61	1.00	-0.07	0.72	0.57	0.51	0.35	0.39
Elongation index	0.38	0.46	0.46	-0.07	1.00	0.65	0.38	0.31	0.24	0.24
Regularity index	0.70	0.72	0.79	0.72	0.65	1.00	0.70	0.61	0.43	0.47
3D-Form Factor	1.00	0.84	0.90	0.57	0.38	0.70	1.00	0.97	0.62	0.92
Roundness X_s	0.97	0.83	0.87	0.51	0.31	0.61	0.97	1.00	0.75	0.94
Roundness I_R	0.61	0.64	0.60	0.35	0.24	0.43	0.62	0.75	1.00	0.60
3D Solidity	0.92	0.73	0.76	0.39	0.24	0.47	0.92	0.94	0.60	1.00

Table 7.5: Correlation matrix of the shape parameters for the two sands together (101.270 grains). See Table 7.1 for all the references. The shading colours depend on the correlation coefficient: **Green=high correlation ($r > 0.75$)**, **red=bad correlation ($r < 0.50$)**

2) Separate the grains inside/outside the shear band → Done

- Triangulating the grains centres of masses and calculating the deviatoric strain → Done in YADE (it was already programmed...)

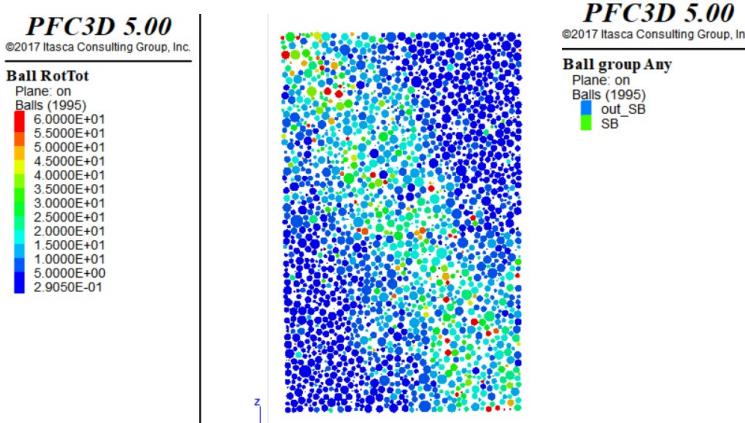


Choose a limit: **0.10**

- $> 0.10 \rightarrow$ Inside shear band
- $< 0.10 \rightarrow$ Outside the shear band

How to separate the grains inside/outside the shear band?

- 1) Visually (easy but not automated, must be done singularly by hand after each simulation. And it's not very accurate)



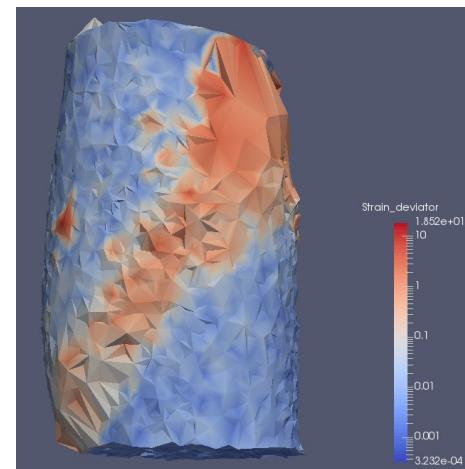
At $\varepsilon_z = 12\%$:

- Hostun: MeanRot_SB = 17.0°
- Caicos: MeanRot_SB = 34.5°

- 2) Triangulating the “grains” centres of masses and calculating the deviatoric strain → in YADE (as I did in the EXP)

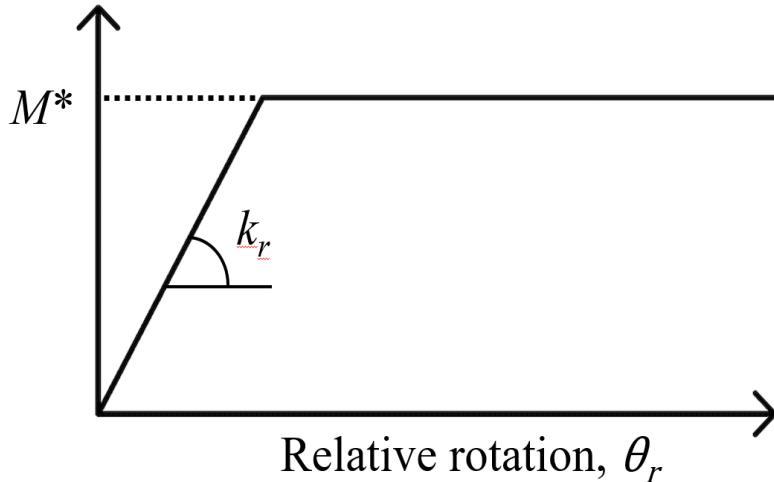
Choose a limit: **0.10**

- $> 0.10 \rightarrow$ Inside shear band
- $< 0.10 \rightarrow$ Outside the shear band



Rolling Resistance linear Contact Model

Rolling Resistance, M_r



$$k_r = k_s \bar{R}^2 \quad (\text{Rolling Stiffness})$$

$$\frac{1}{\bar{R}} = \frac{1}{R^{(1)}} + \frac{1}{R^{(2)}} \quad (\text{Rolling Radius})$$

$$M^* = \mu_r \bar{R} F_n^l$$

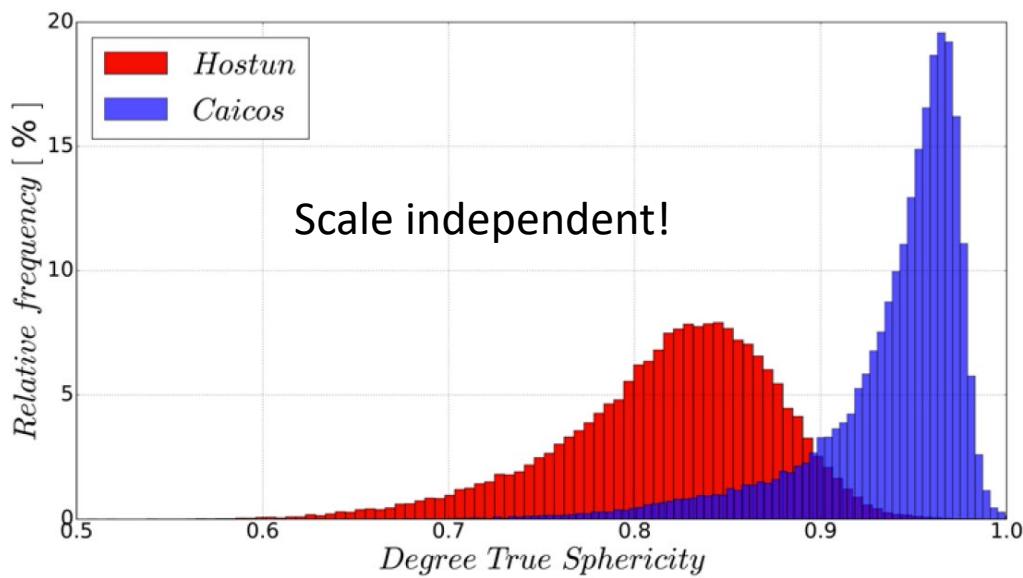
Rolling Friction

These are ALL CONTACT PROPERTIES...
NOT “GRAINS” properties!

So, how to relate shape (particle property) to
rolling resistance (contact property)?
→ “Inheritance”: The contacts properties are
inherited from balls properties

Objective: Relate the grain shape to a “Rolling Resistance Torque”

From the experiments, we know the “*degree of true sphericity*” is the shape parameter that most affects the particles rotations

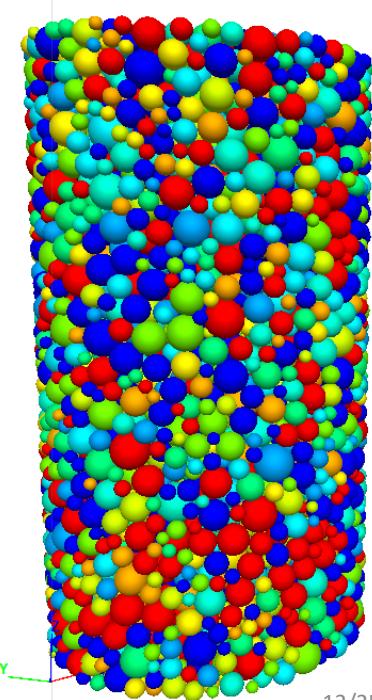
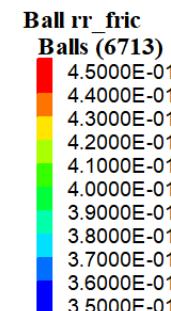


$$M^r = \begin{cases} M^r, & \|M^r\| \leq M^* \\ M^* (M^r / \|M^r\|), & \end{cases}$$

$$M^* = \mu_r \bar{R} F_n^l$$

$$\mu_r = \min(\mu_{r(i)}, \mu_{r(j)})$$

PFC3D 5.00
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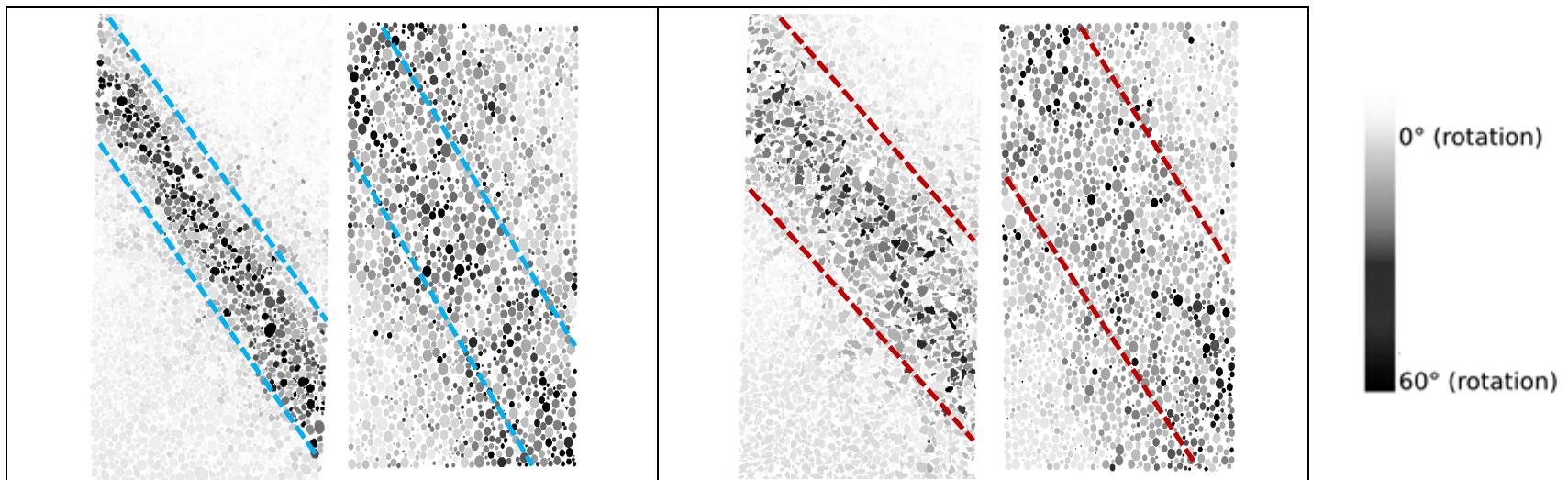
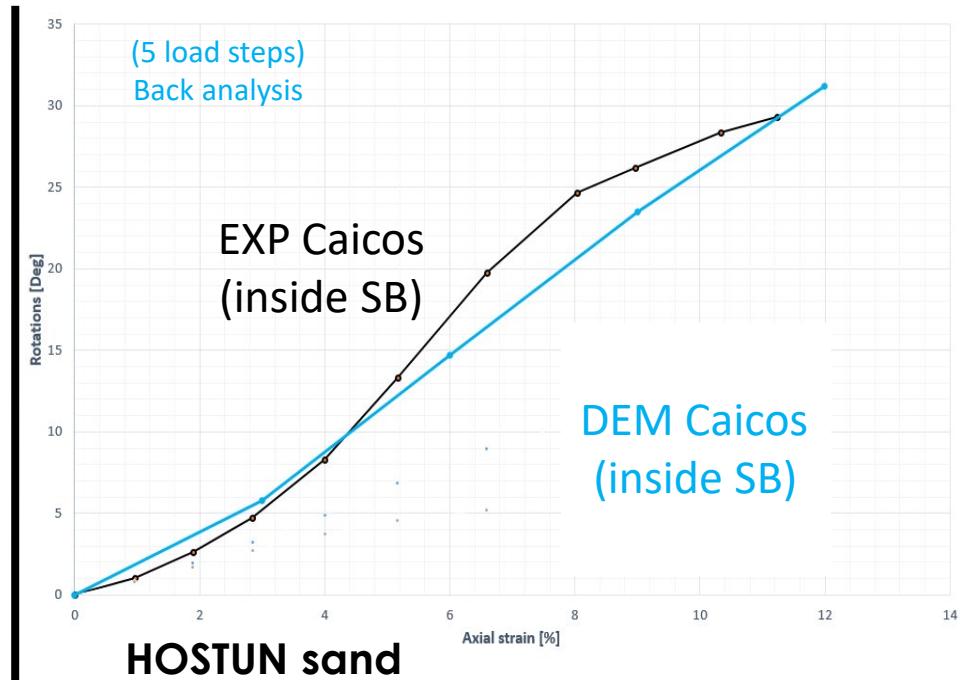
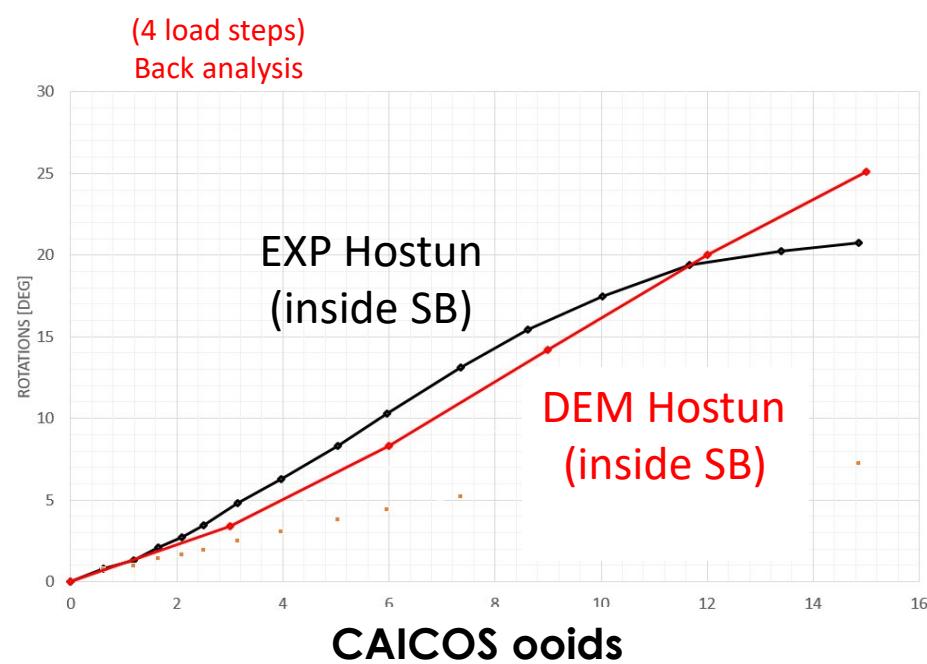


Power law:

$$\mu_r = a(\psi)^b$$

(Sphere: $\mu_r = a$)

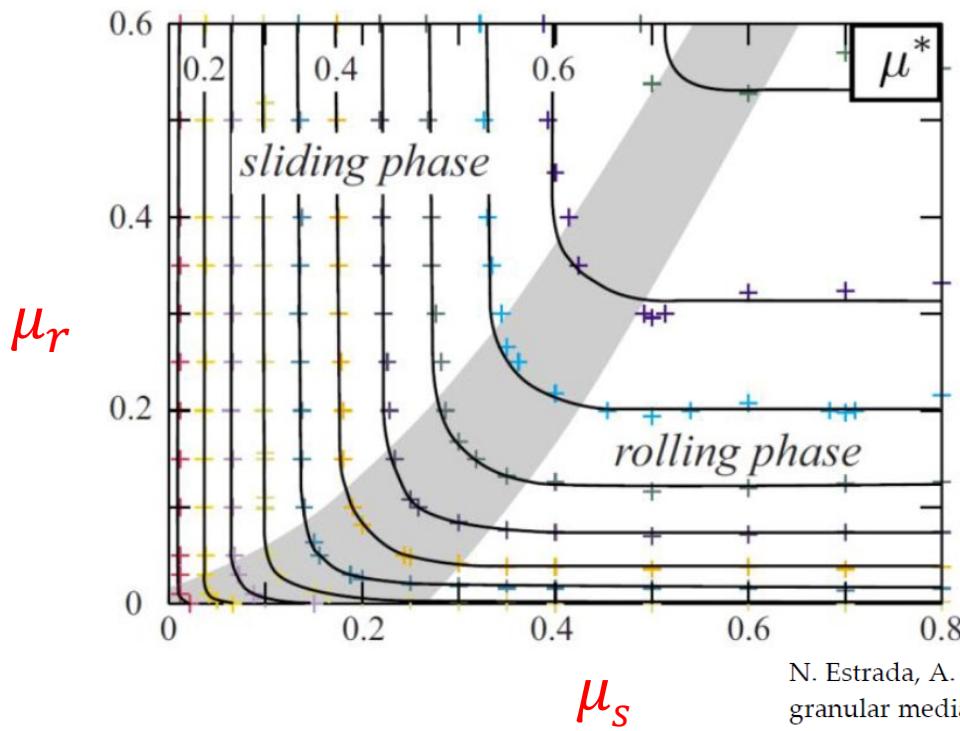
Histories of Mean Rotations (EXP vs DEM) inside the shear band



DVC Software Tomowarp2 – Discrete approach (Tudisco *et al.* 2017)

Try to find the set of parameters (a , b and fric , by trial & error) that best match the triaxial responses of HNEA01/COEA04 (in order of importance):

- 1) Stress-strain response
- 2) Rotations inside shear band**
- 3) Volumetric response
- 4) Thickness of shear band



The same mechanical response can be obtained by using several sets of parameters, but the rotation information (from EXP) provides a UNIQUE solution

N. Estrada, A. Taboada, and F. Radjaï, "Shear strength and force transmission in granular media with rolling resistance," *Phys. Rev. E - Stat. Nonlinear, Soft Matter Phys.*, vol. 78, no. 2, pp. 1–11, 2008.

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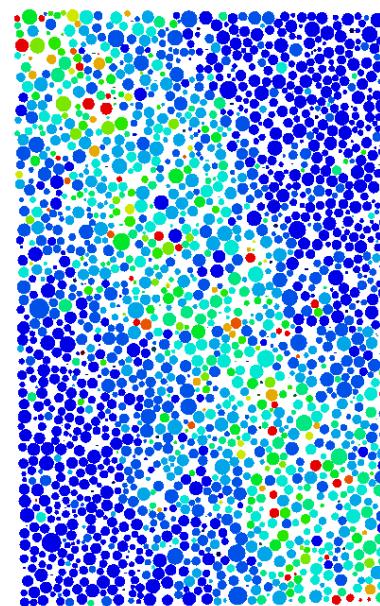
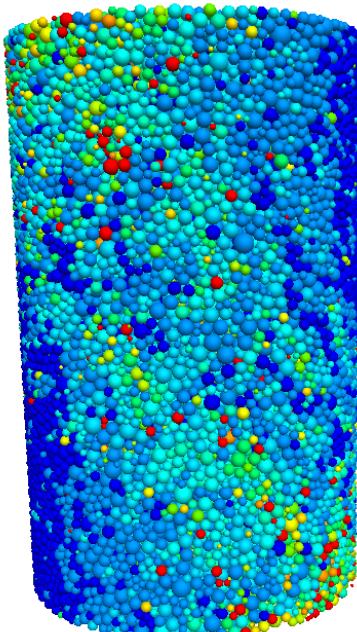
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HOSTUN
SAND

Ball RotTot

Balls (57784)

6.0000E+01
5.5000E+01
5.0000E+01
4.5000E+01
4.0000E+01
3.5000E+01
3.0000E+01
2.5000E+01
2.0000E+01
1.5000E+01
1.0000E+01
5.0000E+00
0.0000E+00



PFC3D 5.00

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CAICOS
SAND

Ball RotTot

Balls (51679)

6.0000E+01
5.5000E+01
5.0000E+01
4.5000E+01
4.0000E+01
3.5000E+01
3.0000E+01
2.5000E+01
2.0000E+01
1.5000E+01
1.0000E+01
5.0000E+00
0.0000E+00

