Horizons in Dry Granular Modeling: Beyond DEM

A Critical Review

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IFPRI

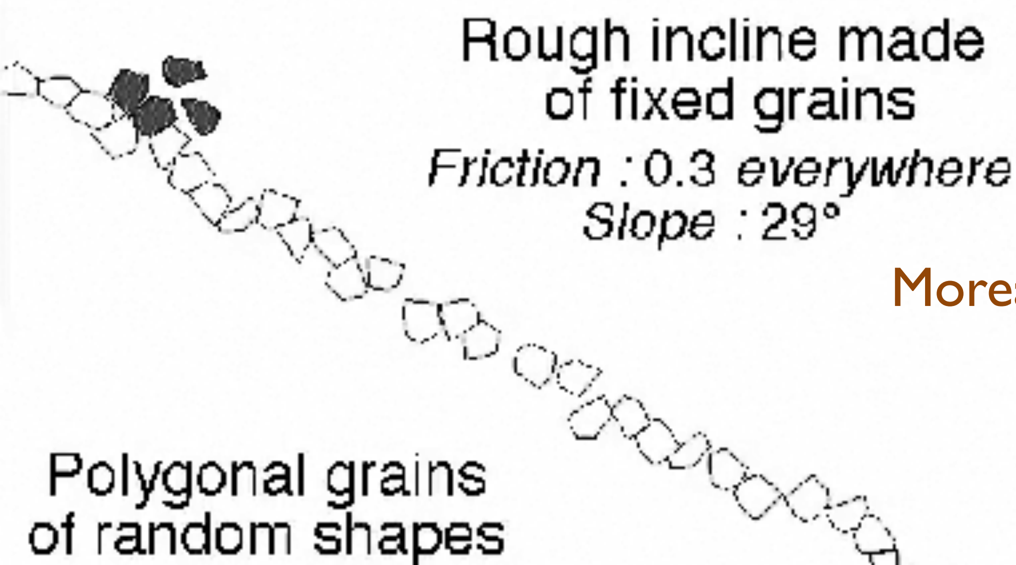
International Fine Particle Research Institute

Introduction

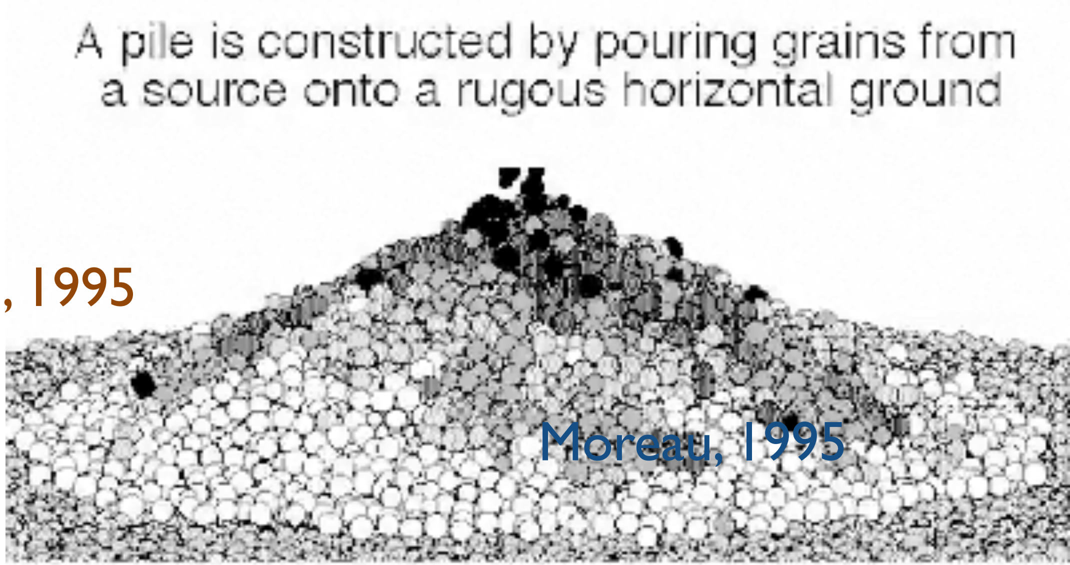
DEM = Discrete Element Method

Stepwise integration of the equations of motion (translations, rotations) for all particles by taking into account their contact interactions and external forces.

Strength: The particles are assumed to be hard (infinitely rigid) so that only rigid-body motions are considered (6 degrees of freedom per particle in 3D).



Moreau, 1995



Weakness: The contact geometry is defined in terms of small allowed overlaps and relative displacements, introducing an artificial softness of the contacts that needs to be numerically resolved.

$$\frac{\delta}{d} \ll 1$$

$$\leftrightarrow \quad \frac{p}{E} \ll 1$$

$$\leftrightarrow \quad \left(\frac{mv^2}{d^3 E}\right)^{1/2} \ll 1$$

δ	overlap
d	particle diameter
p	typical stress
E	elastic modulus
v	typical velocity
m	particle mass

$\Rightarrow$ scale separation

$\Rightarrow$ small time step + frequent contact detection (80% of cpu time)
+ fundamental issues (see below)

3 levels of computational effort

1) Basic

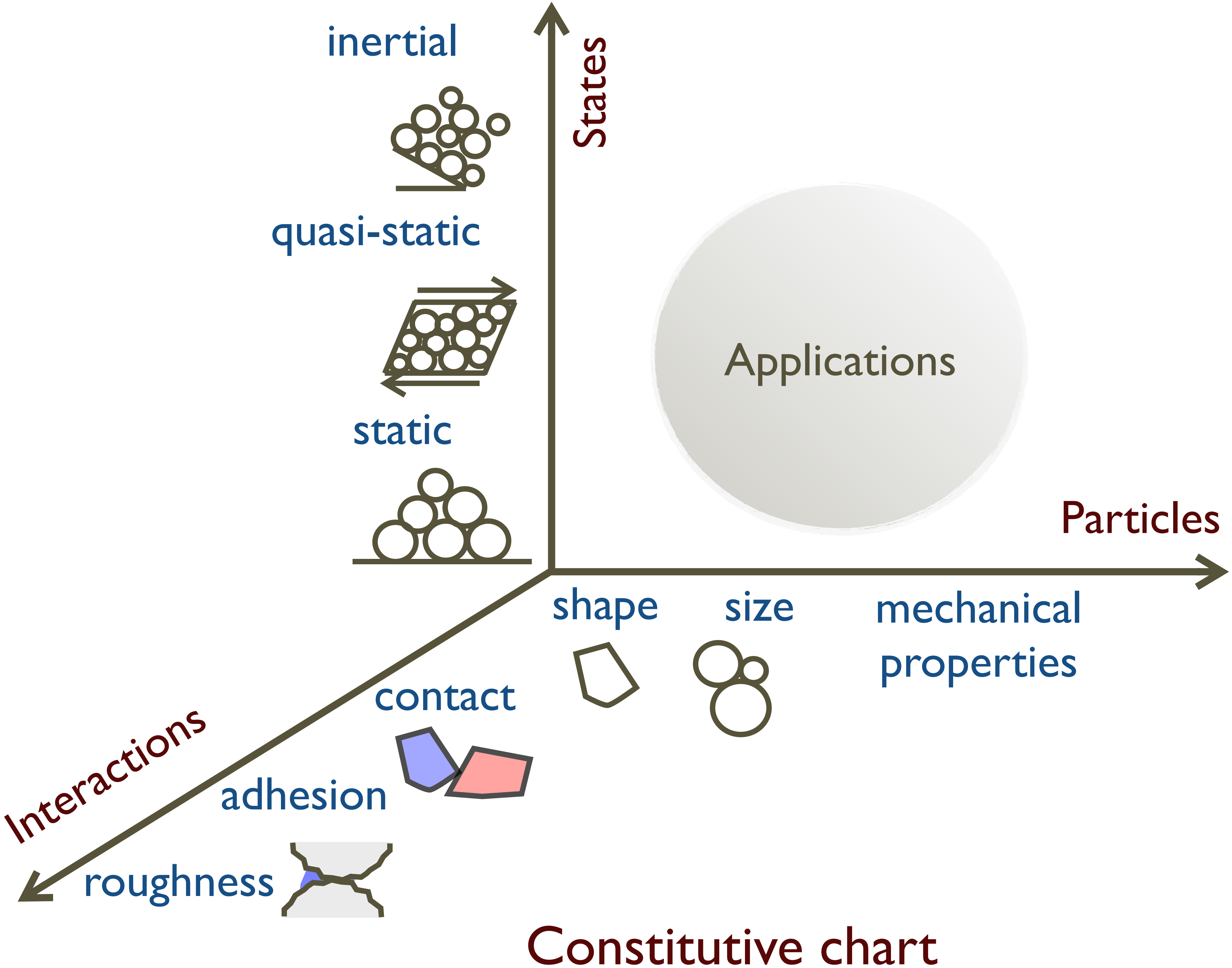
Spherical particles + frictional contact interactions

2) Extended

Particle clumps (shapes), adhesion forces (capillary, vdW, adhesion), high polydispersity, rolling friction…

3) Advanced

Aspherical particle shapes, particle fracture, fluid-grain interactions, soft (deformable) particles, hybrid methods, speedup (MPI, GPU…), validation strategy…


inertial
States
quasi-static
Applications
static
Particles
shape
size
mechanical
properties
contact
Interactions
adhesion
roughness
Constitutive chart

General trend

Increasingly realistic and numerically efficient simulations of granular systems.

We never simulate a real system, but a physical model of it.

Real system $\rightarrow$ Physical model

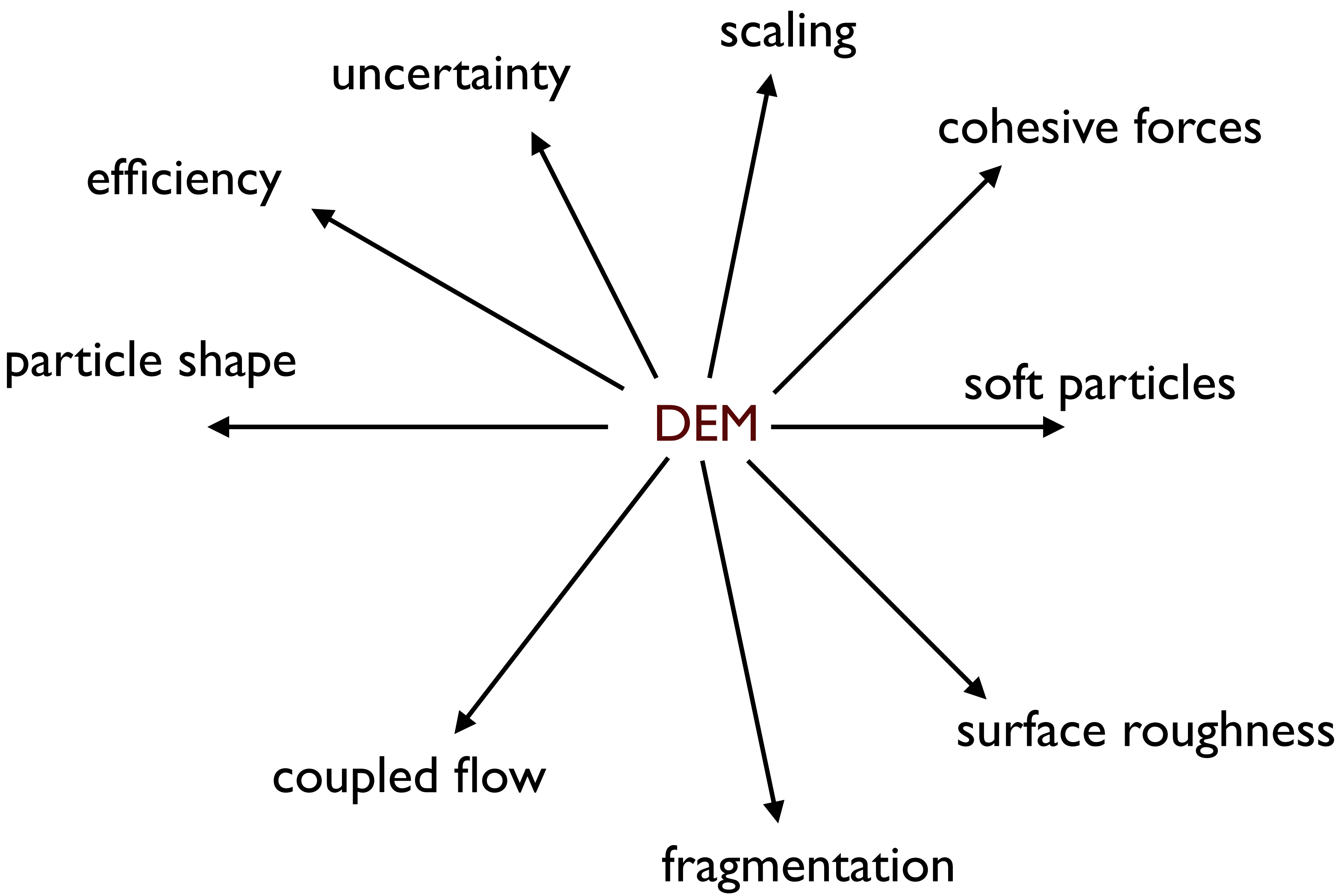
Challenge: accuracy and measurement of input parameters

Physical model $\rightarrow$ Numerical model

Challenge: precision and computational efficiency

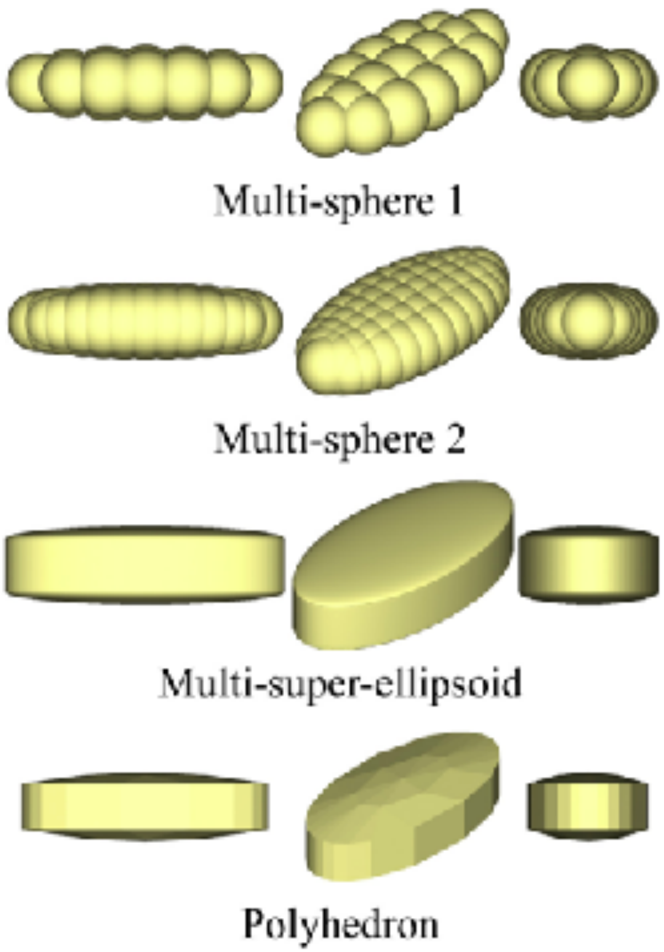
$\Rightarrow$ more realistic = higher accuracy + higher precision or better determination of uncertainty

Selected examples

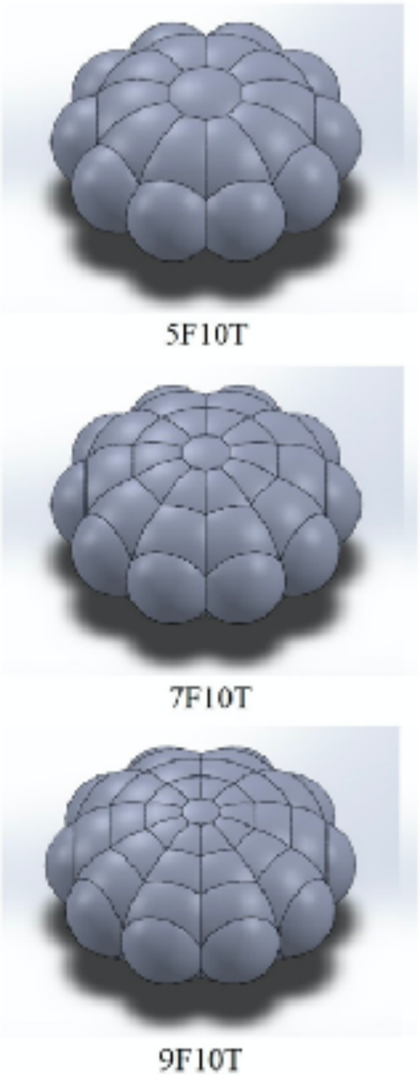


Particle shape

Clumps

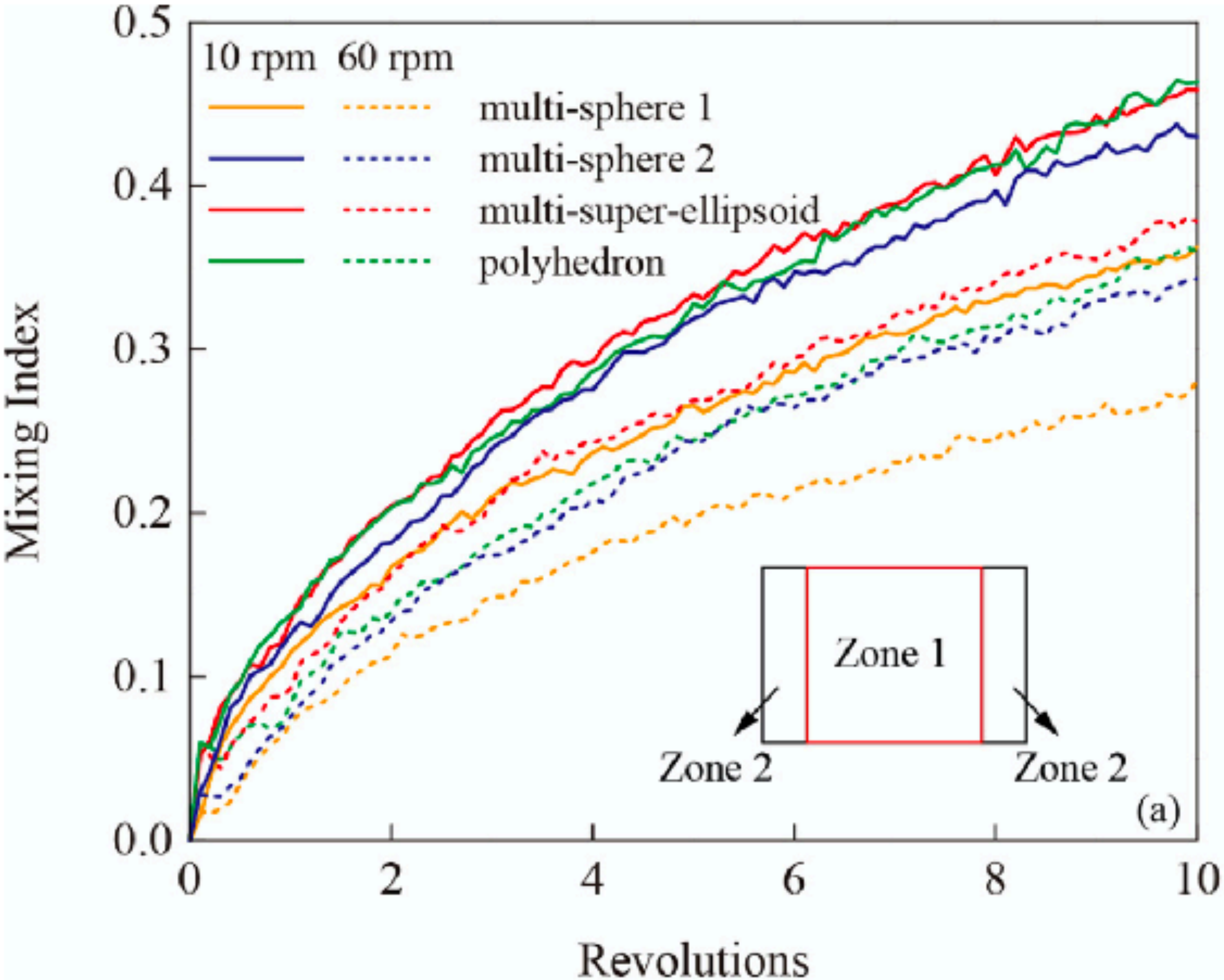


Liu, 2021



Khazeni, 2018

Ferellec, 2010



10 rpm
60 rpm
multi-sphere 1
multi-sphere 2
multi-super-ellipsoid
polyhedron
Mixing Index
0.0
0.1
0.2
0.3
0.4
0.5
0
2
4
6
8
10
Revolutions
Zone 1
Zone 2
Zone 2
(a)

Liu, 2021

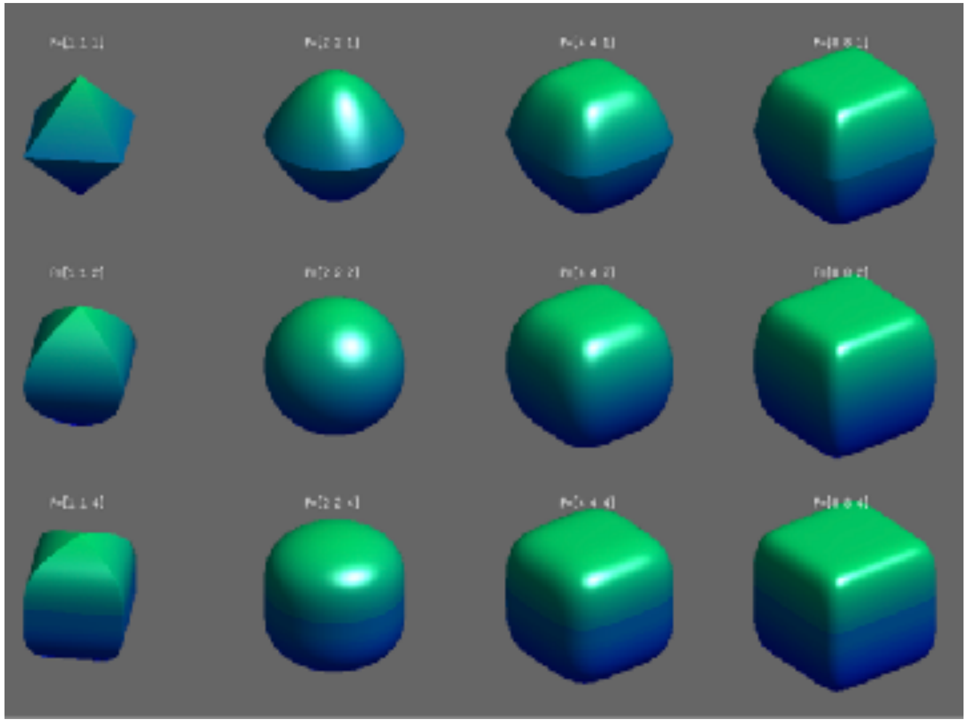
Analytic smooth shapes: ellipsoids, super-quadrics…

super-quadrics

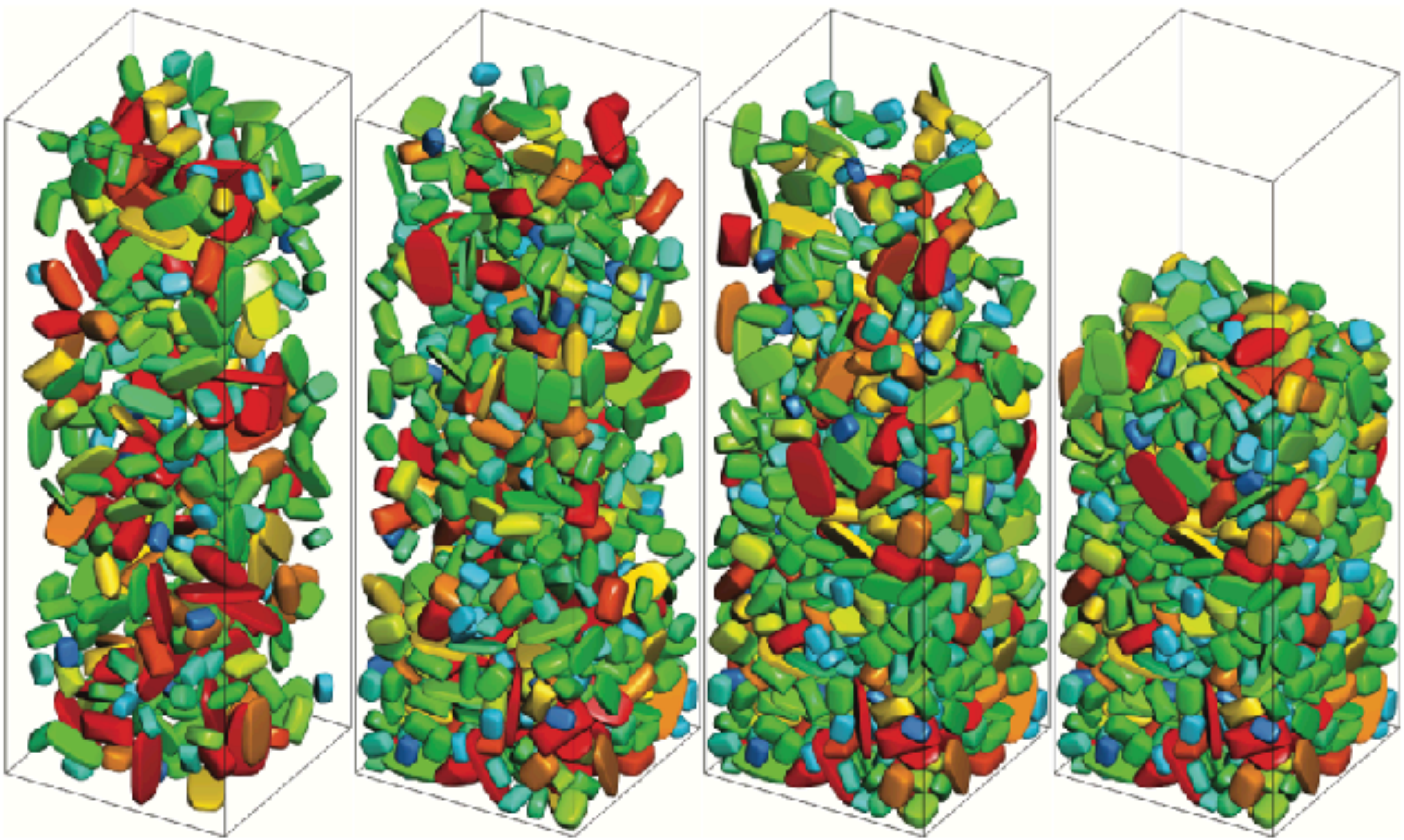
$$\left|\frac{x}{A}\right|^r + \left|\frac{y}{B}\right|^s + \left|\frac{z}{C}\right|^t = 1$$

exponents $\rightarrow$ blockiness

scales $\rightarrow$ aspect ratio



Feng, 2021

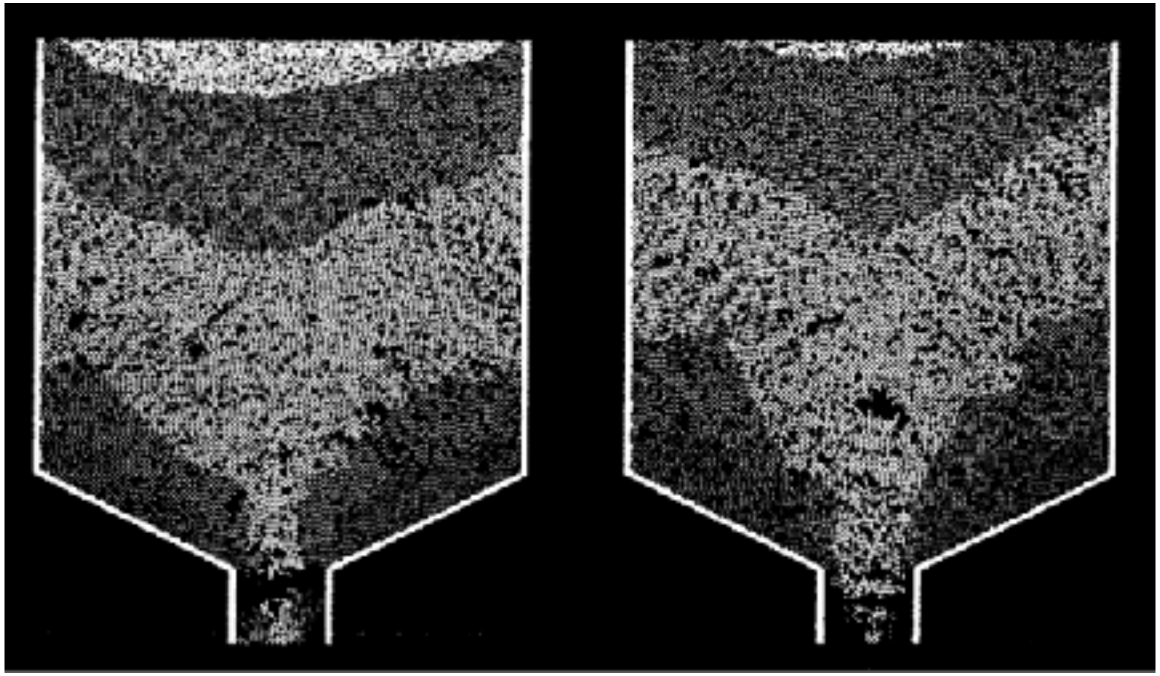


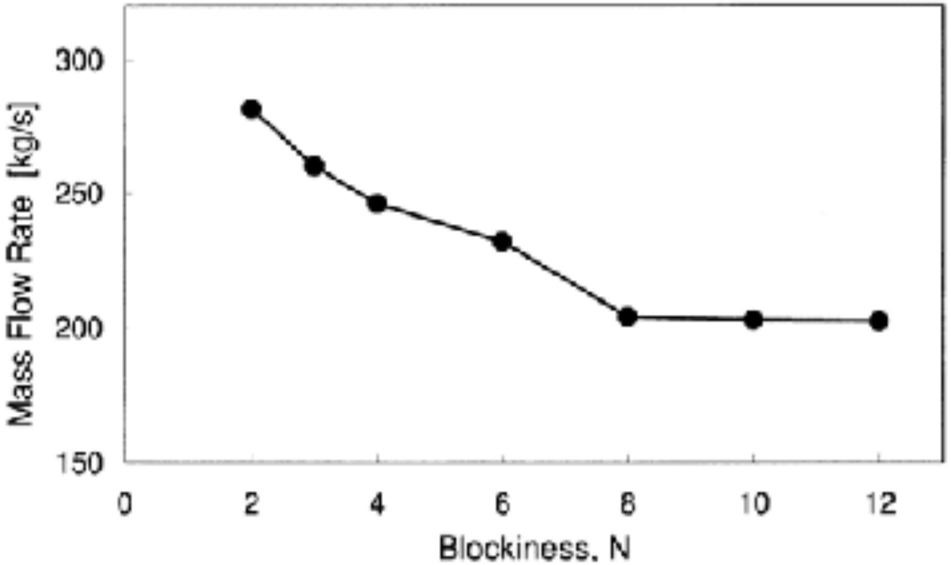
(A) t = 0.25s (B) t = 1.25s (C) t = 2.50s (D) t = 5.0s

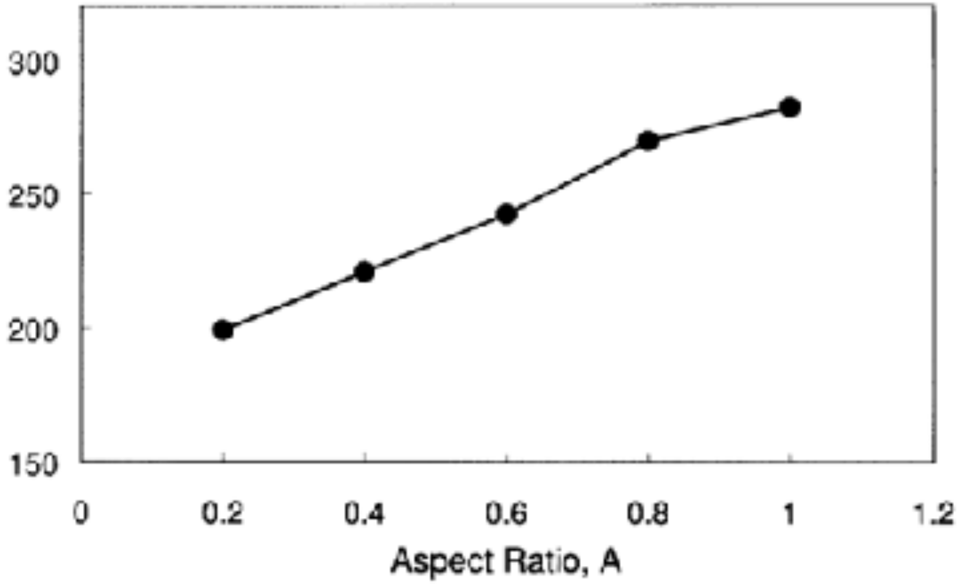
2D version

Hopper flow

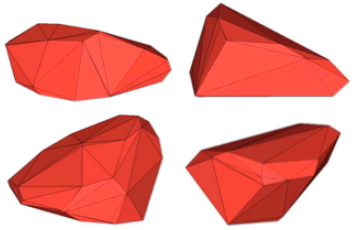
Cleary, 2002

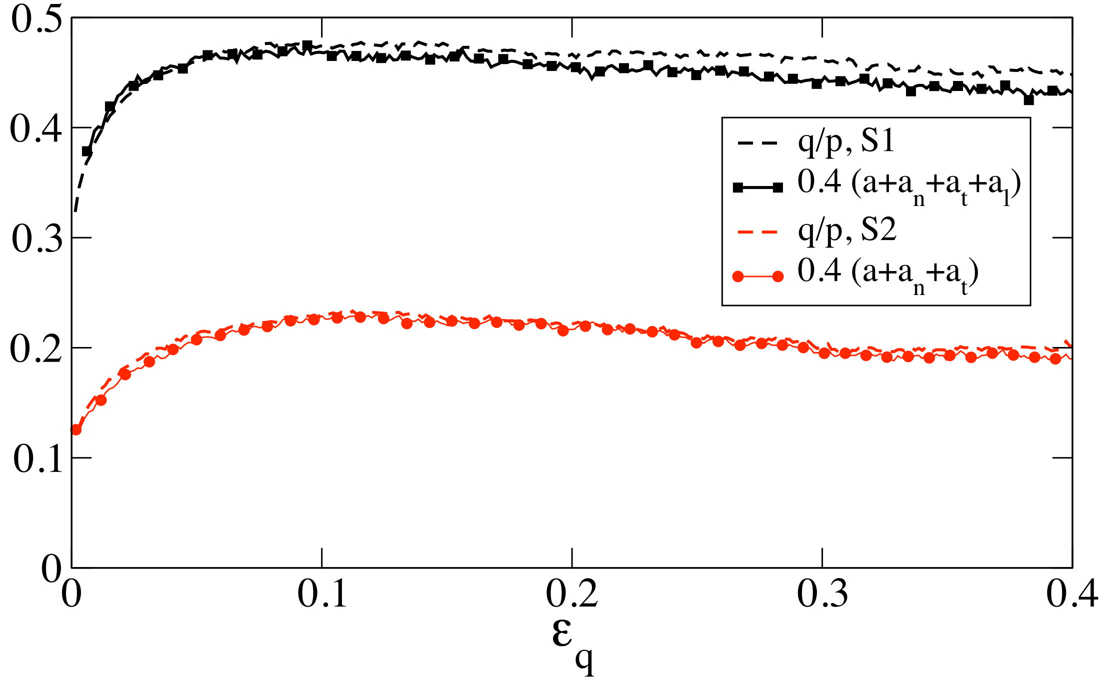




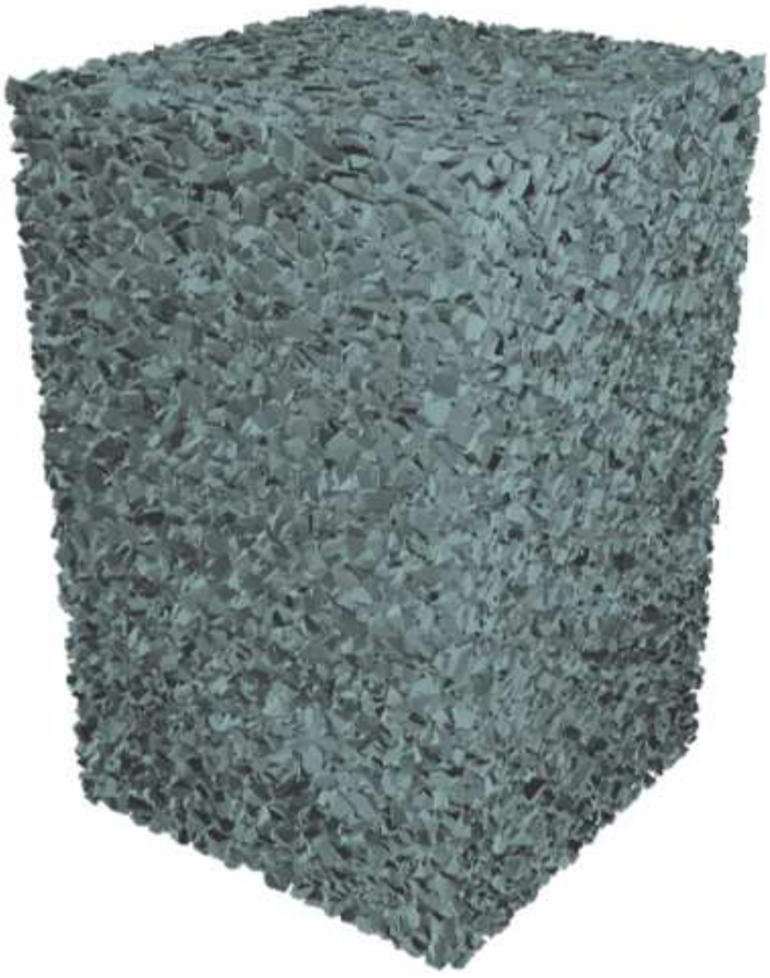


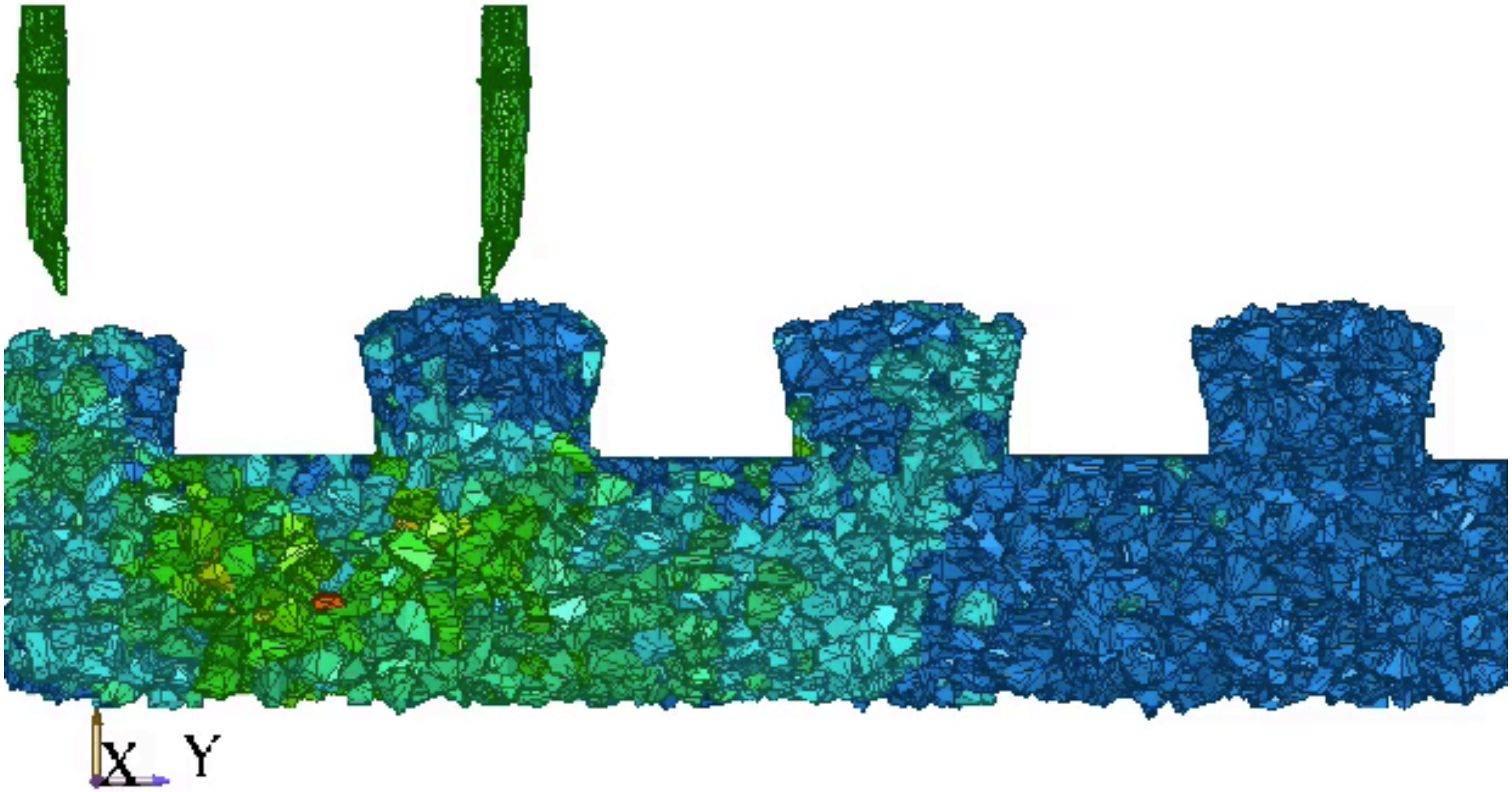
Facetted shapes





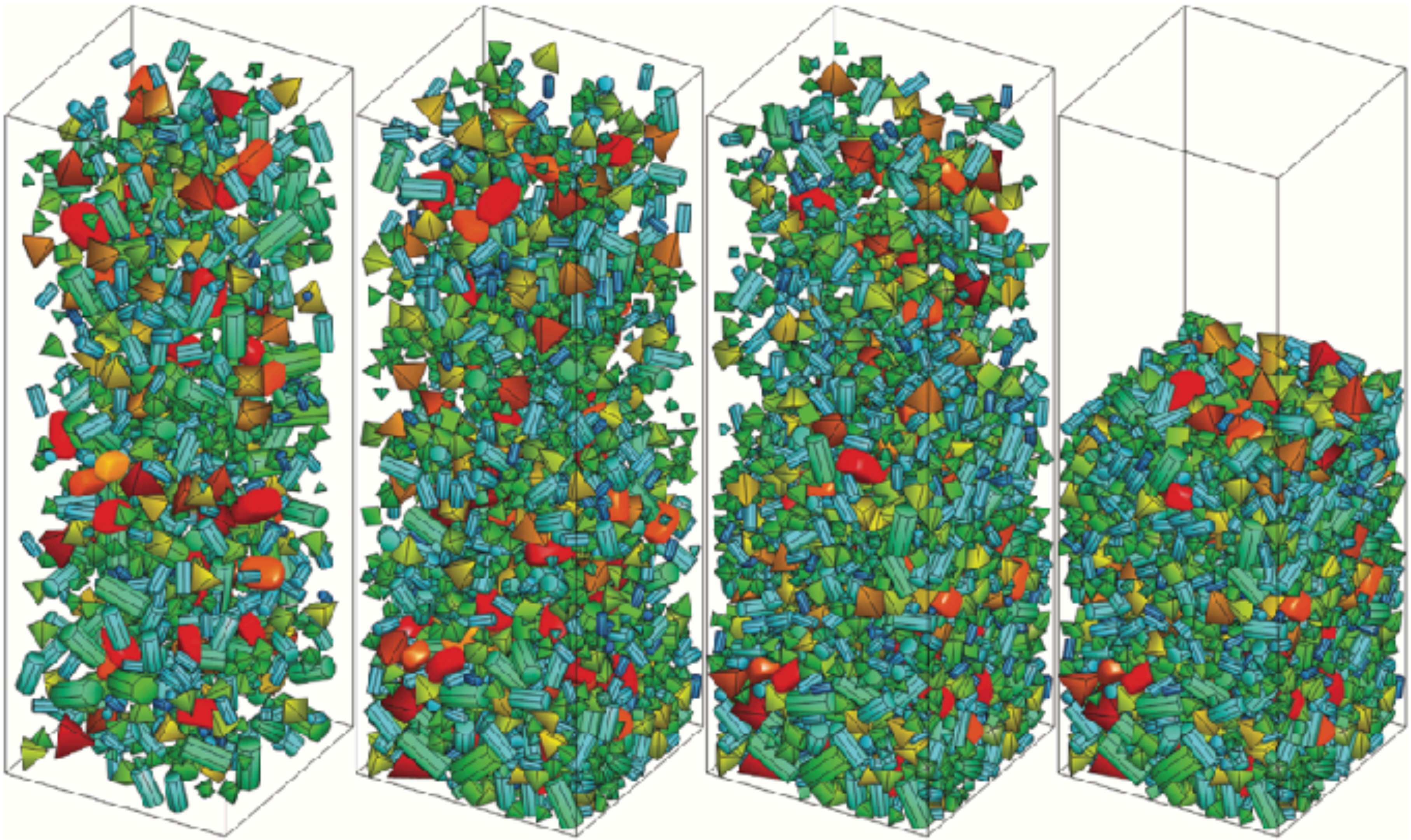
Azéma, 2009



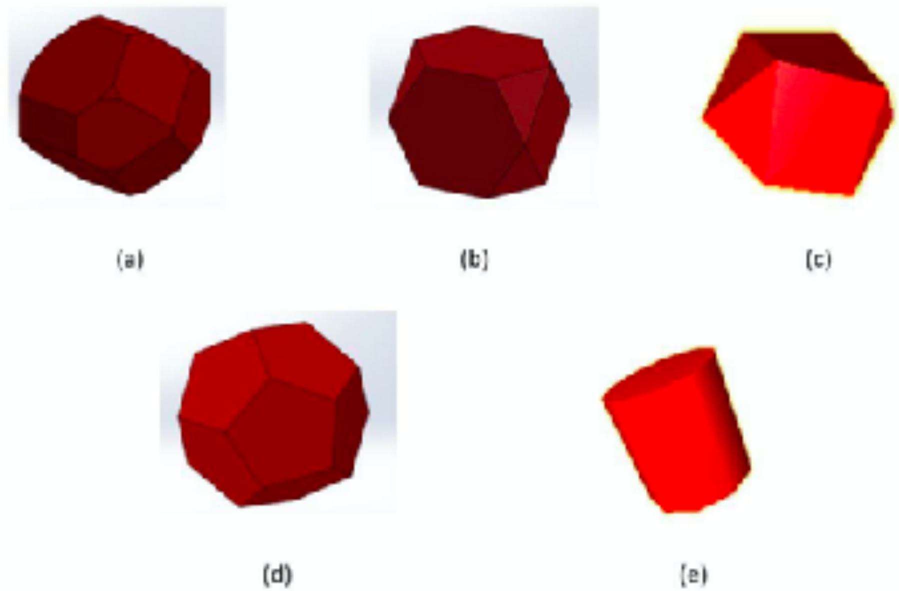


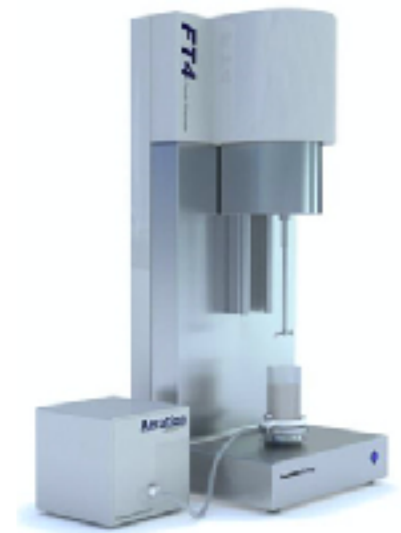
Perales, 2011

Feng, 2021

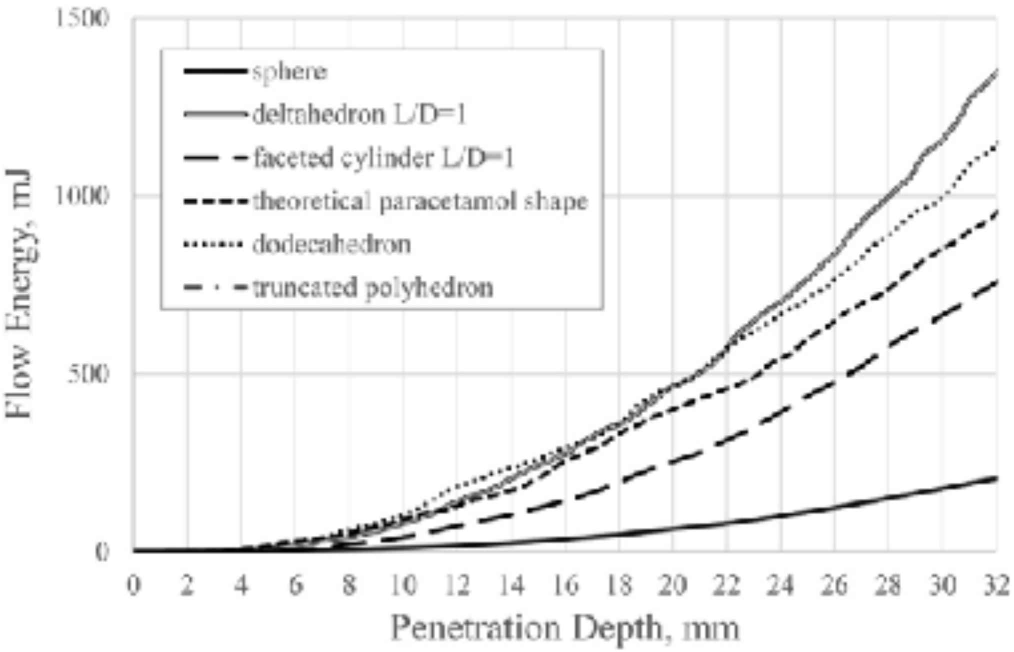


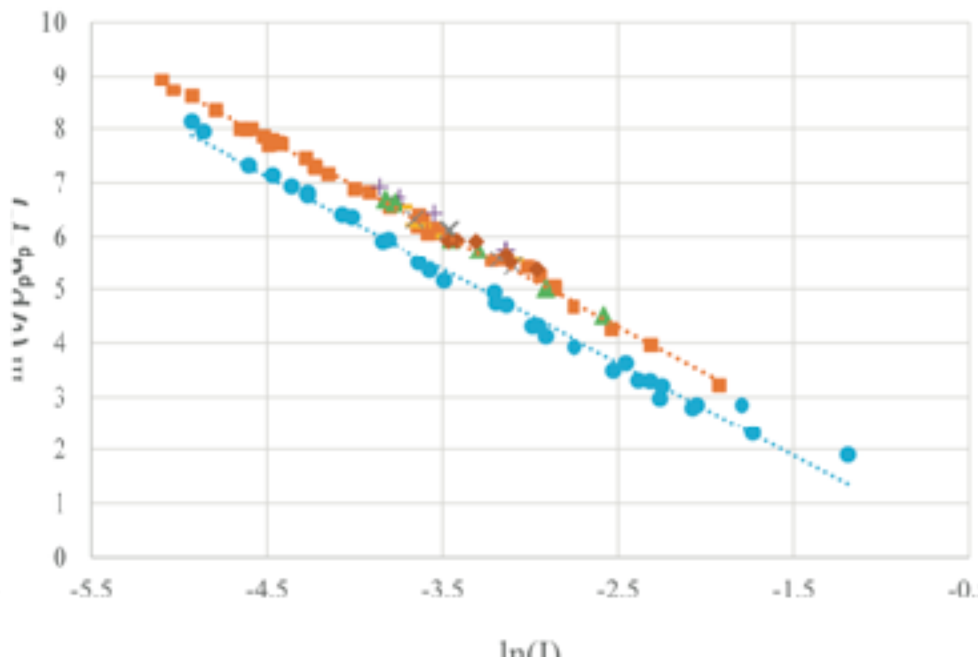
(A) t = 0.25s (B) t= 1.25s (C) t = 2.5s (D) t = 5.0s





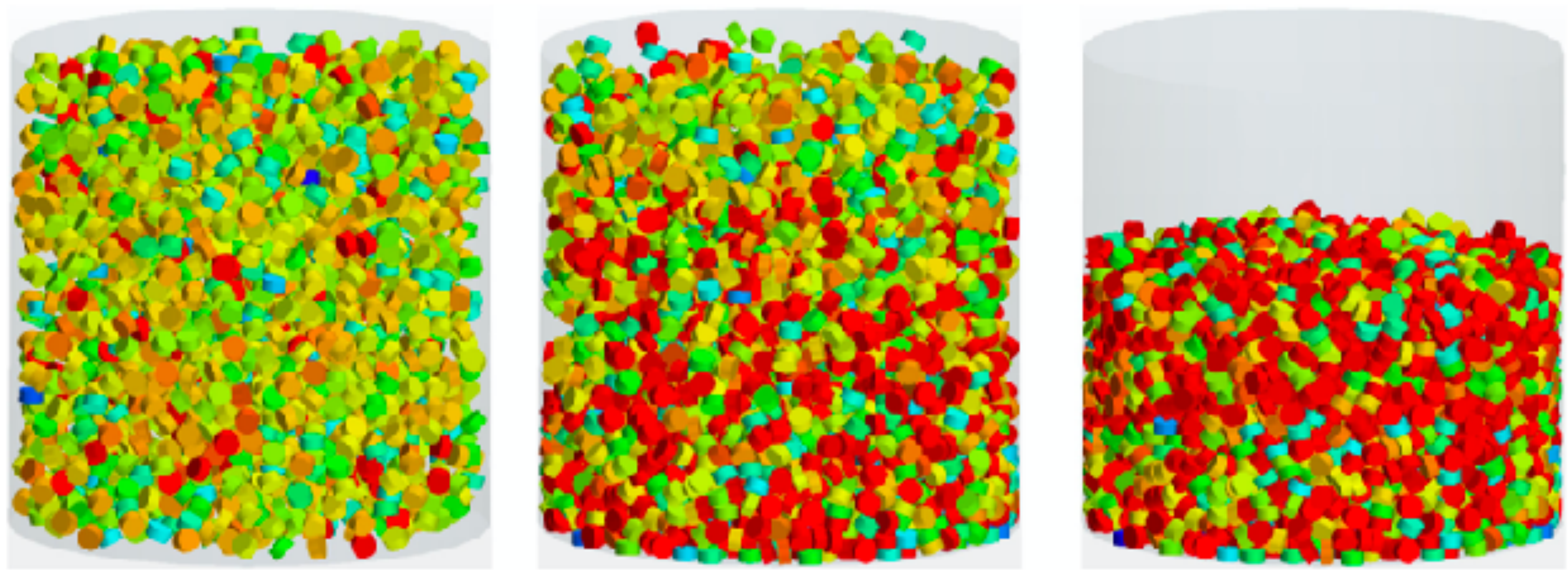
Vivacqua, 2019



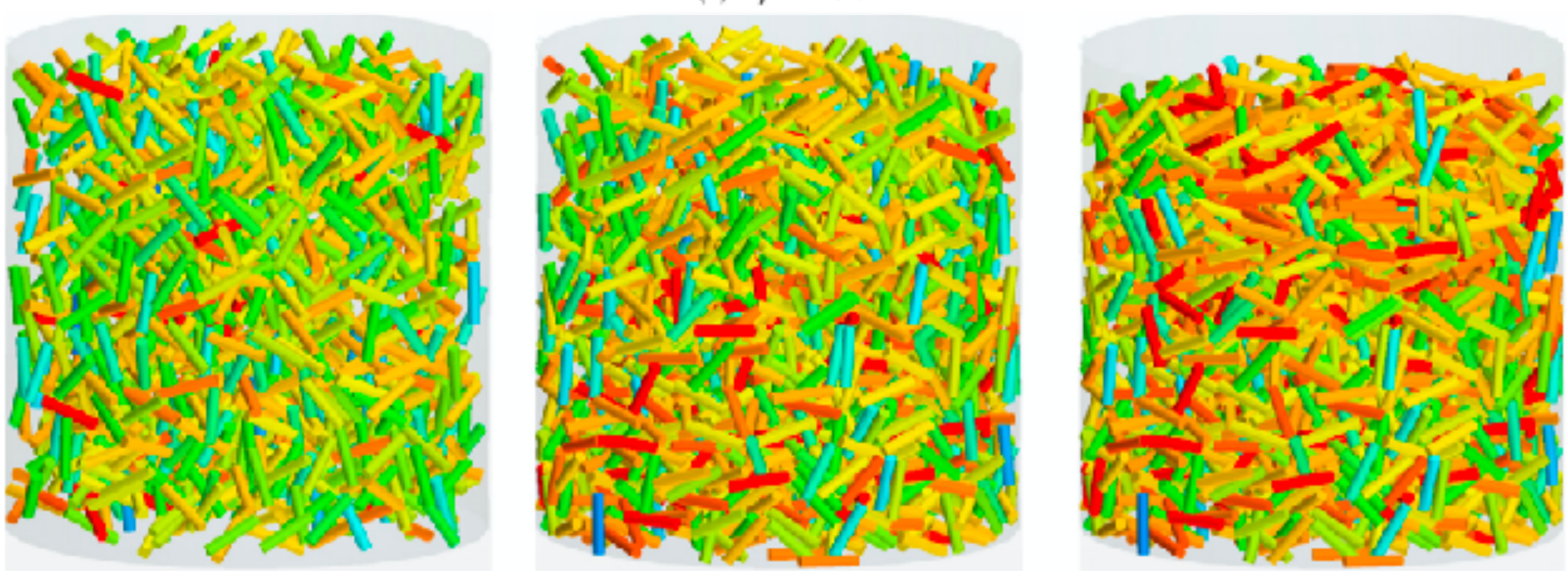


Cylinders

Feng, 2017



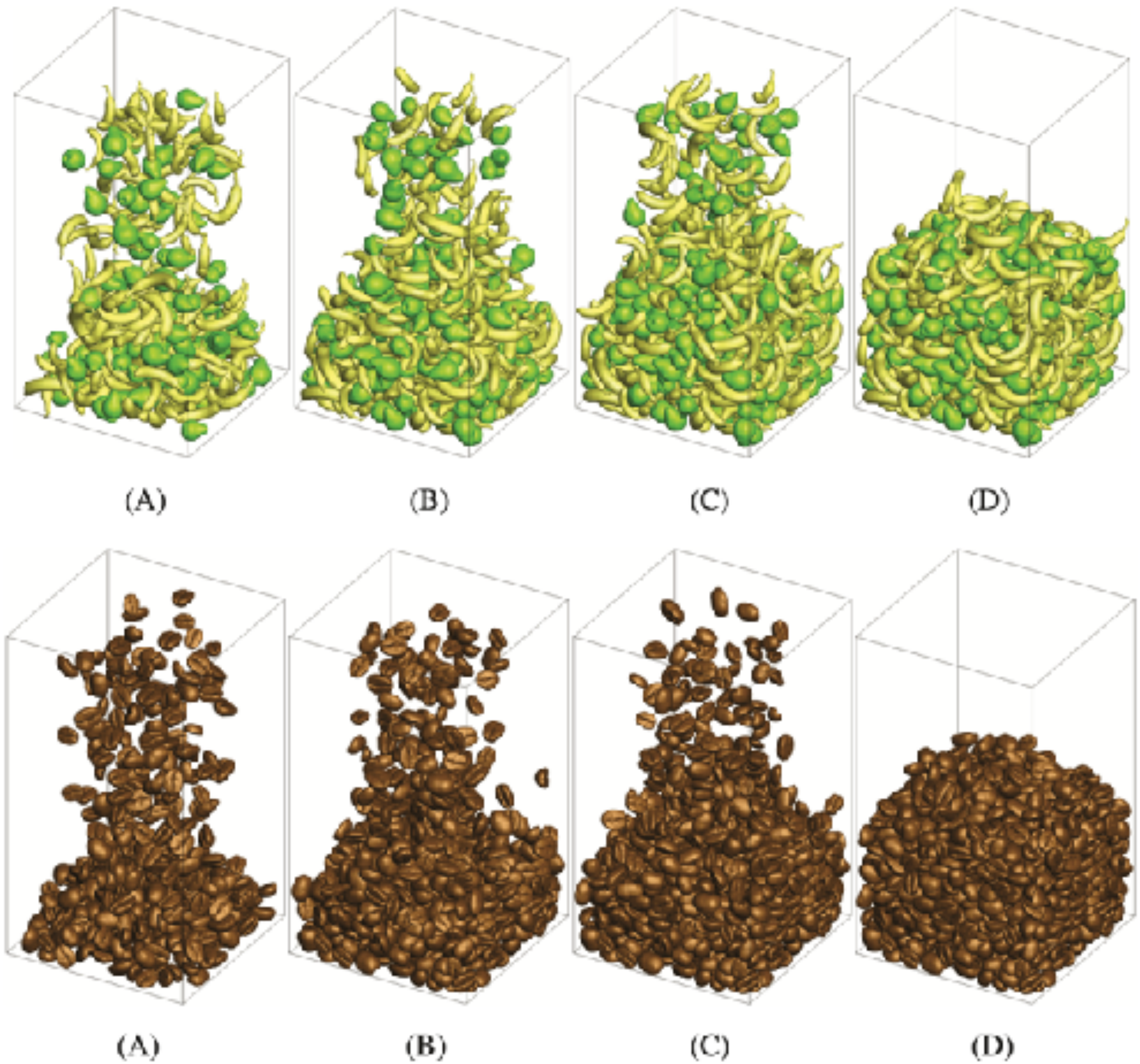
(b) $H/D = 0.5$.



(a) $H/D = 5$.

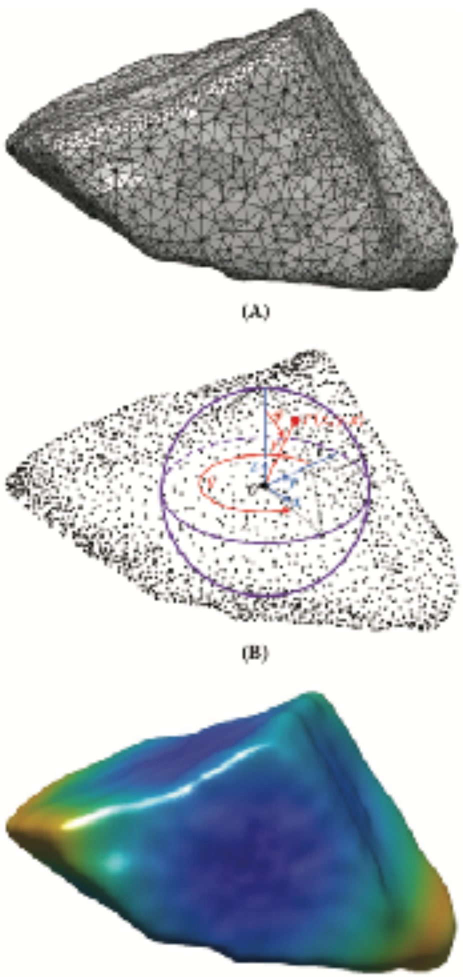
Triangulated surfaces

Feng, 2020



Representation using spherical harmonics

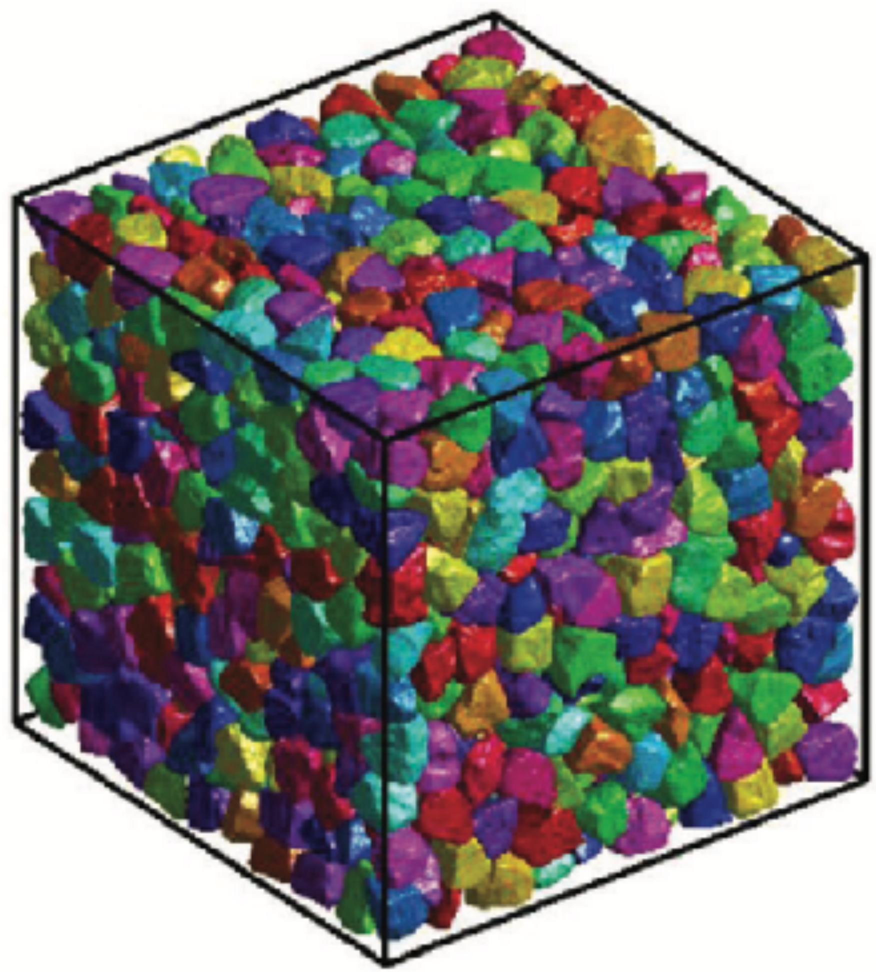
$$r(\theta, \varphi) = \sum_{n=0}^{N} \sum_{m=-n}^{n} a_n^m Y_n^m(\theta, \varphi)$$



(A)

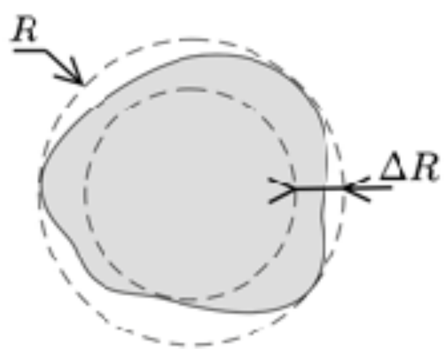
(B)

(C)



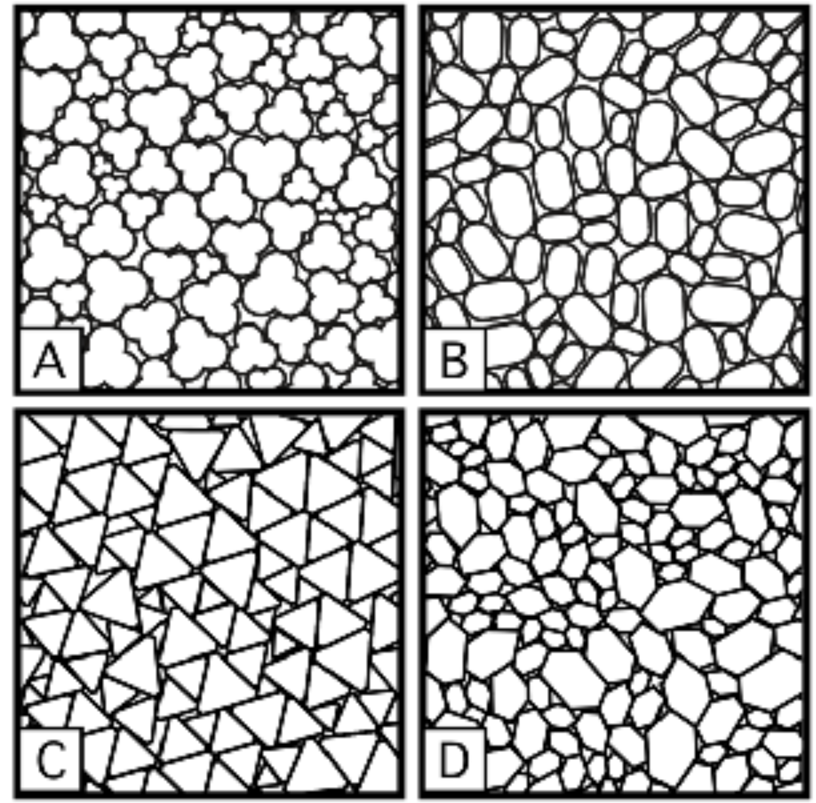
Wang, 2021

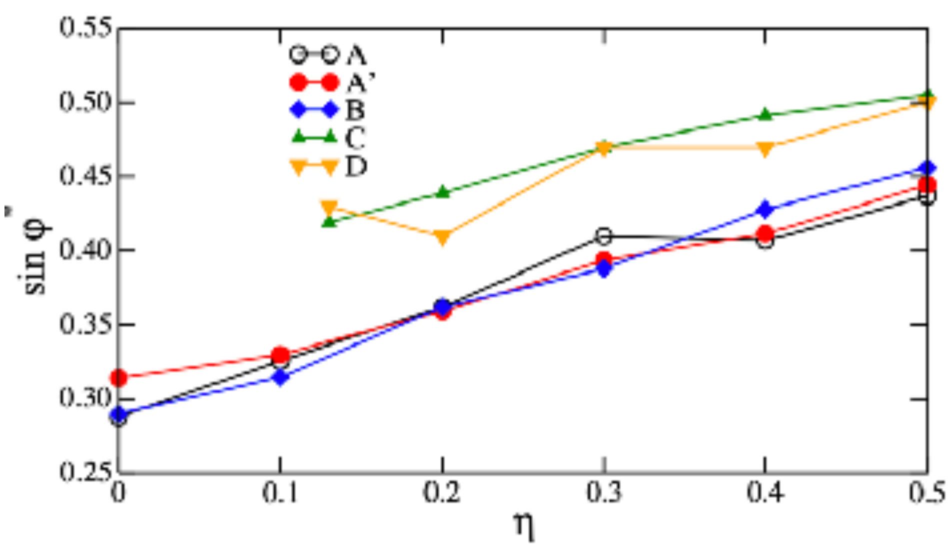
2D shapes

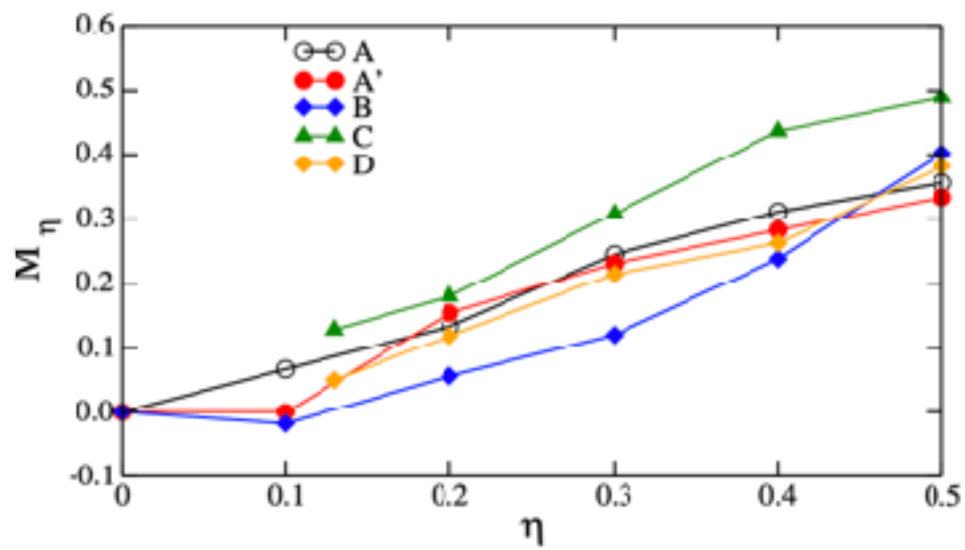


$$\eta = \frac{\Delta R}{R}$$

Saint-Cyr, 2012



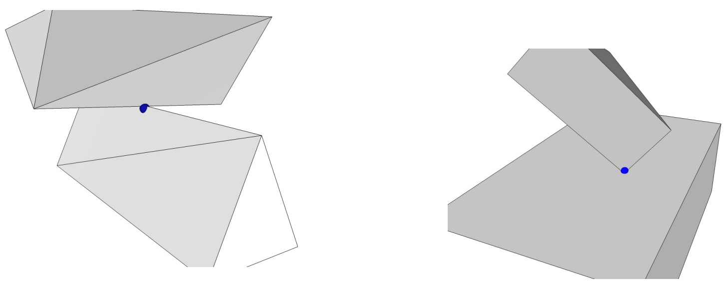




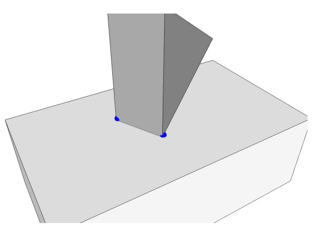
Multiple contacts

Point contacts between two smooth particle surfaces can be treated as Hertz contacts independently of particle shapes. But facetted contacts need to be represented by multiple point contacts.

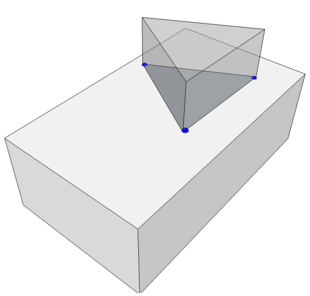
Since the particles are rigid, an edge-face contact should be represented by at least two point contacts (i.e. two geometrical constraints), and a face-face contact by at least three point contacts.



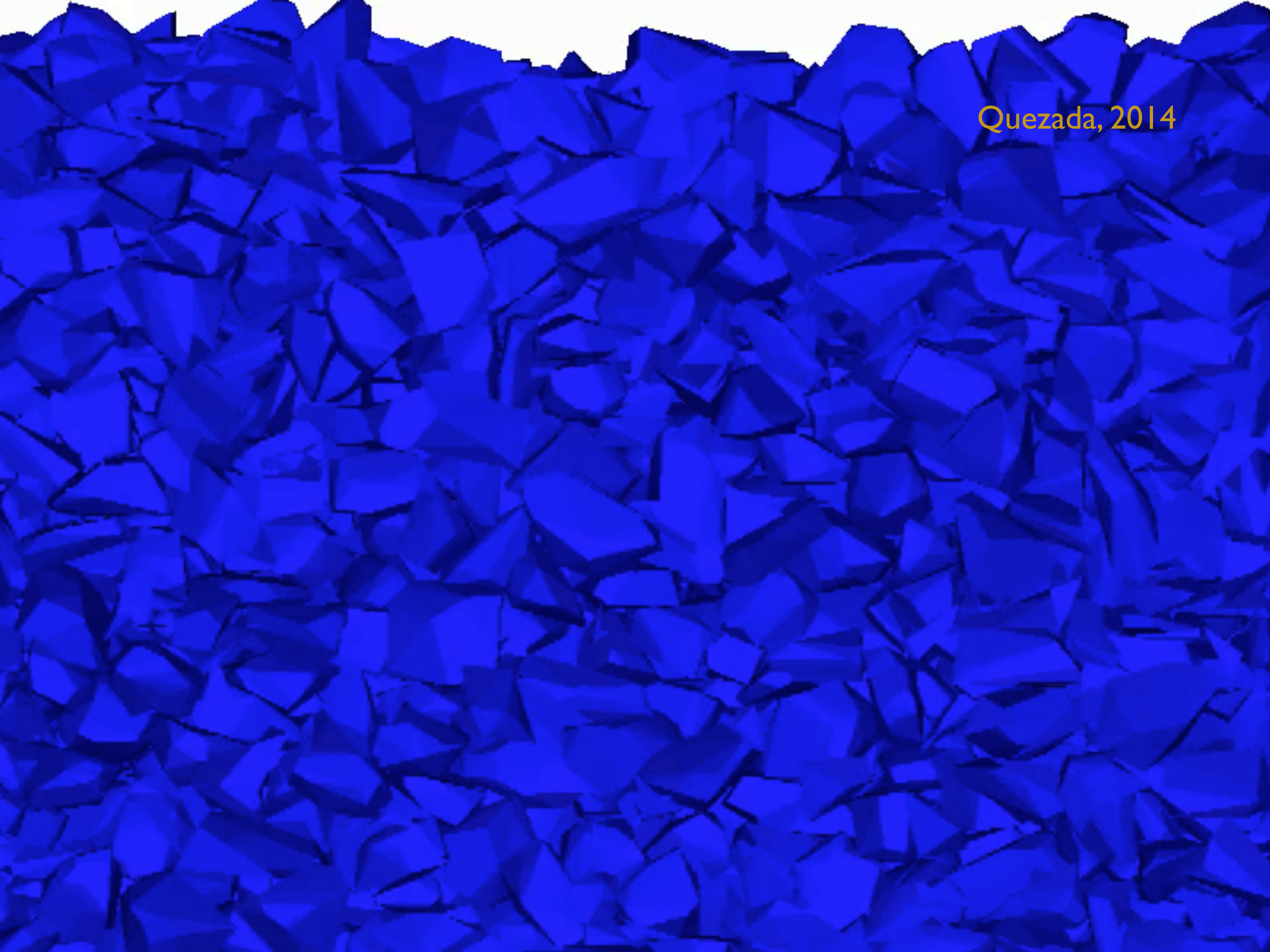
Simple contact

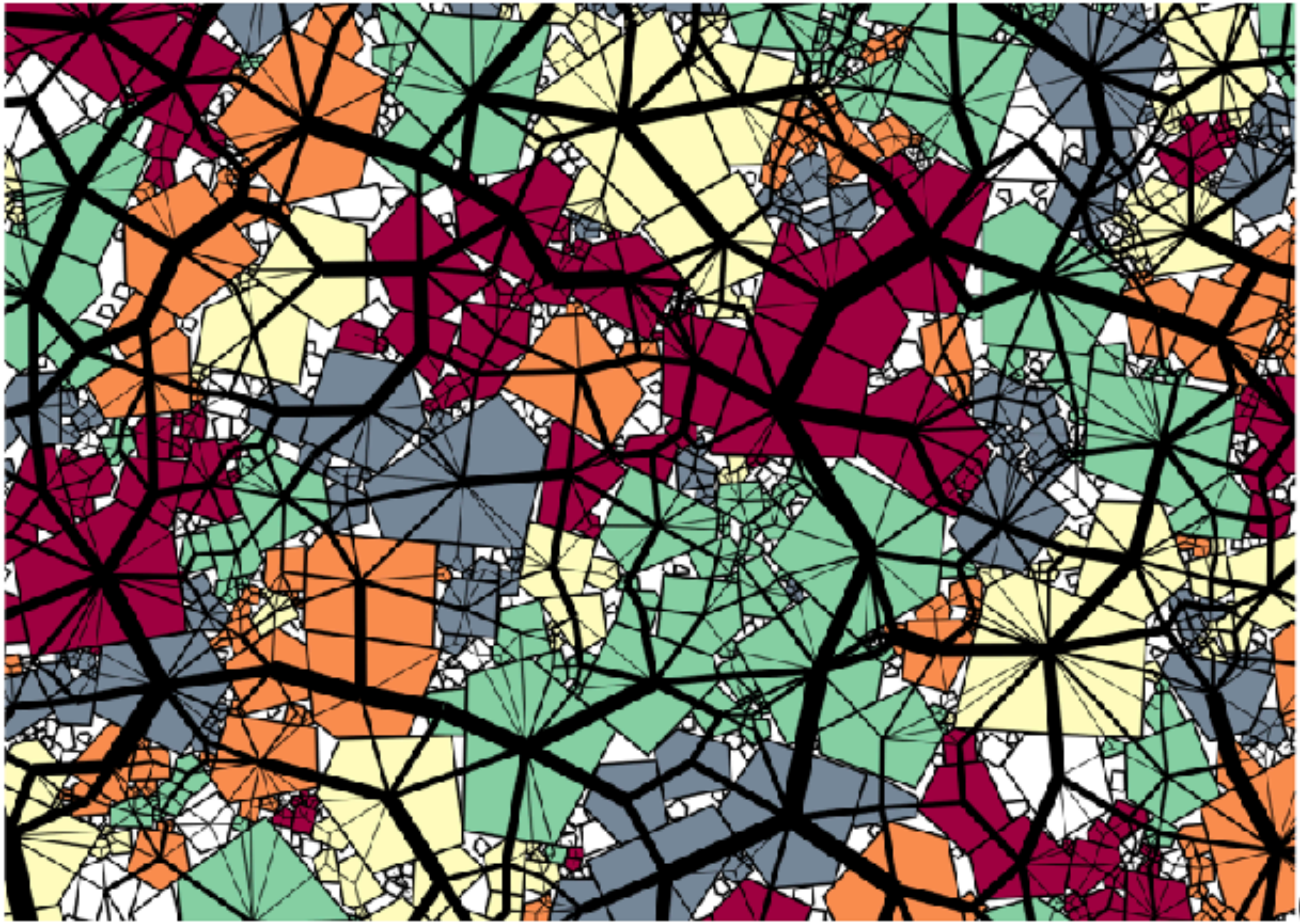


Double contact



Triple contact


Quezada, 2014



Size polydispersity vs. shape polydispersity

Nguyen, 2015

Force laws

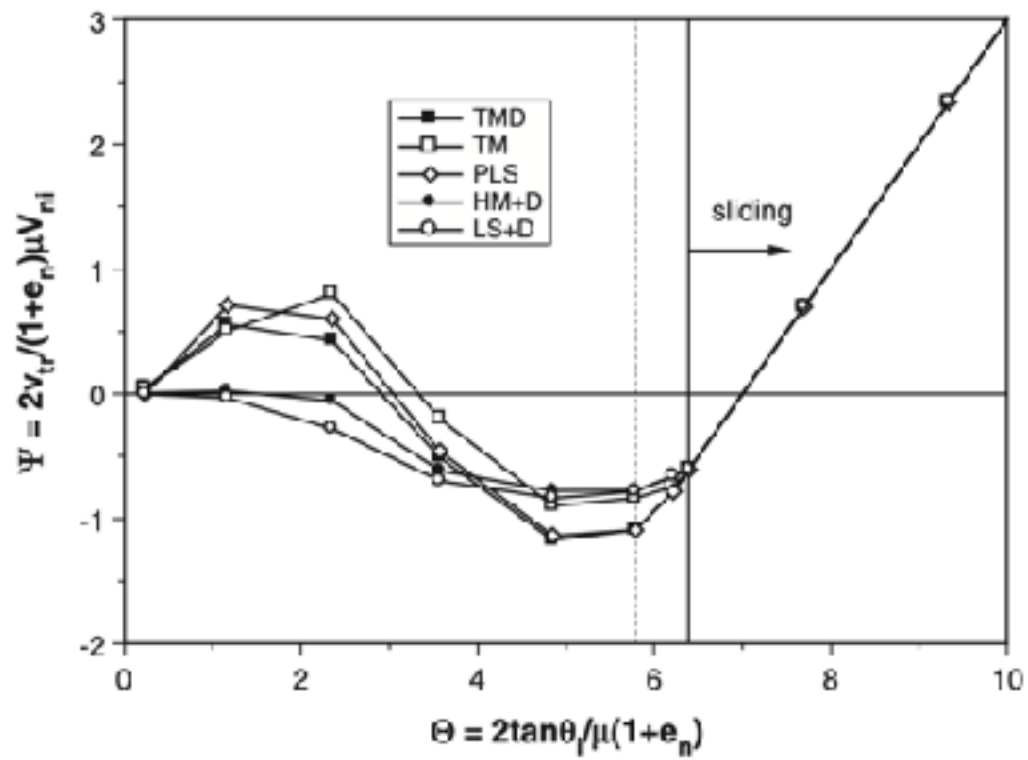
Rigorous contact detection algorithms have been developed. However, the contact force laws are still often based on ad-hoc formulations.

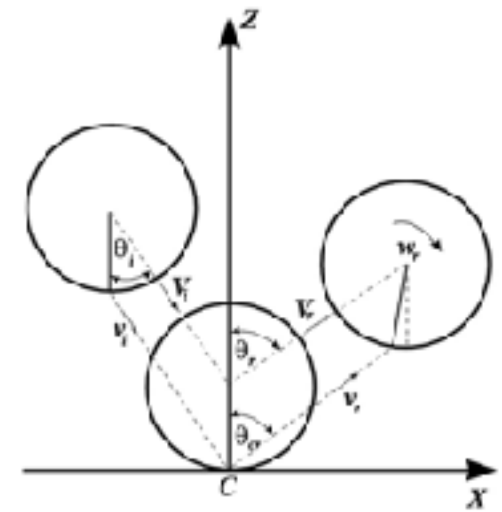
Even the most elementary force laws are presently revisited to cope with problems arising from particle shape, cohesive interactions, dissipation for plastic deformations…

Viscous damping $F_d = C(\delta)\dot{\delta}$ Kacianauskas, 2015

Dimensional analysis to obtain generic shapes of the damping function

Tangential collisions with plastic and visco-elastic laws



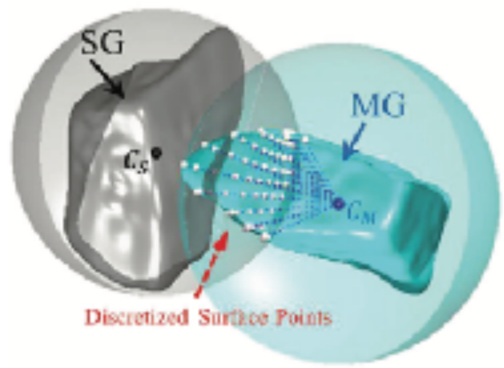


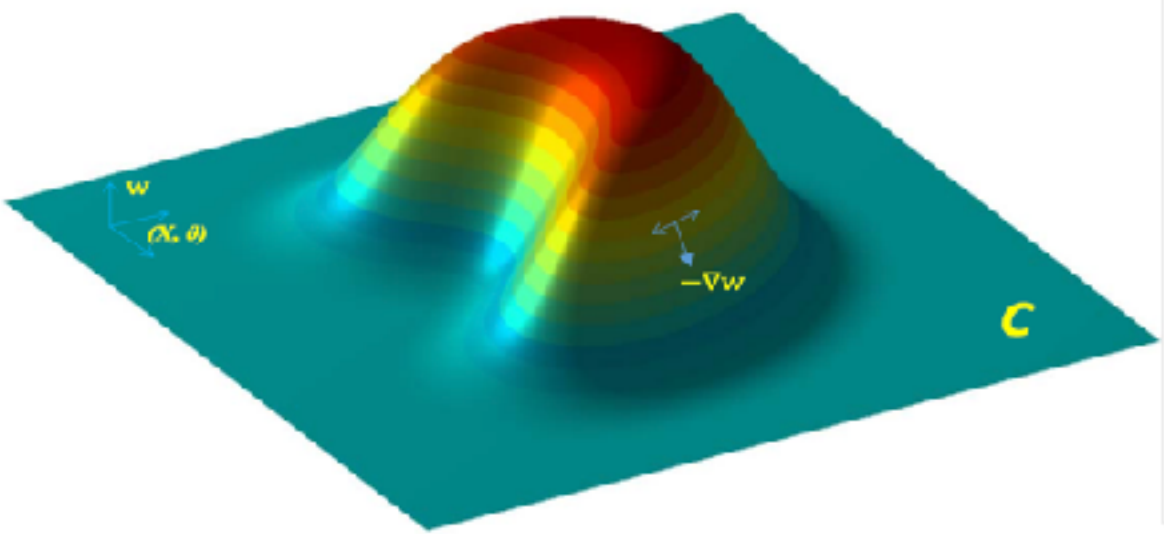
Thornton, 2013

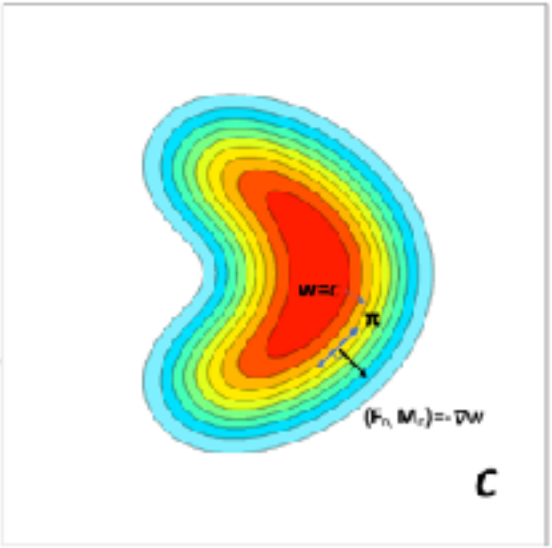
« It is currently unclear what significance the choice of contact force model has on the resulting flow or its properties. »

Energy-conserving contact theory Feng, 2012

Energy considerations may suggest a more rigorous choice of the force laws: Derivation of contact laws from a potential energy function.

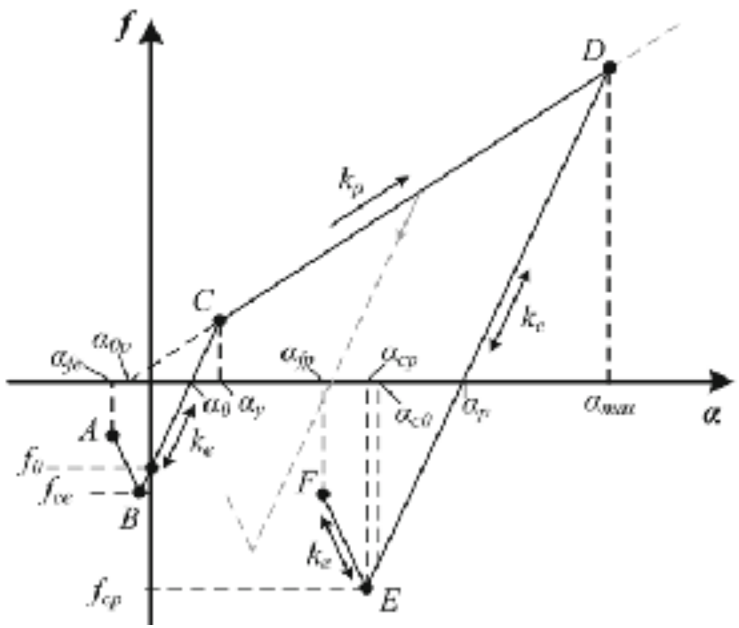


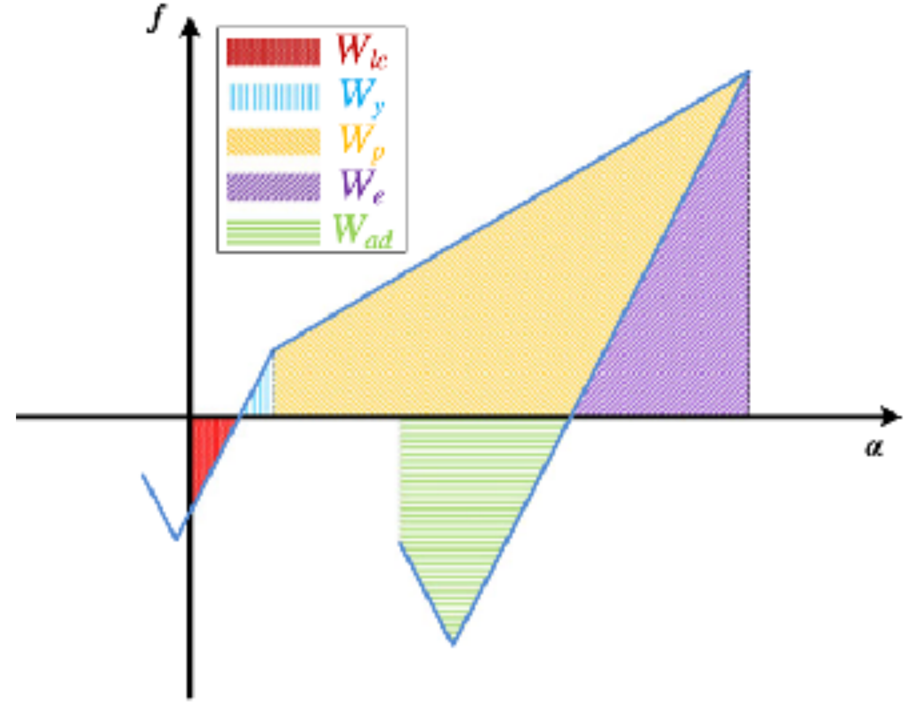


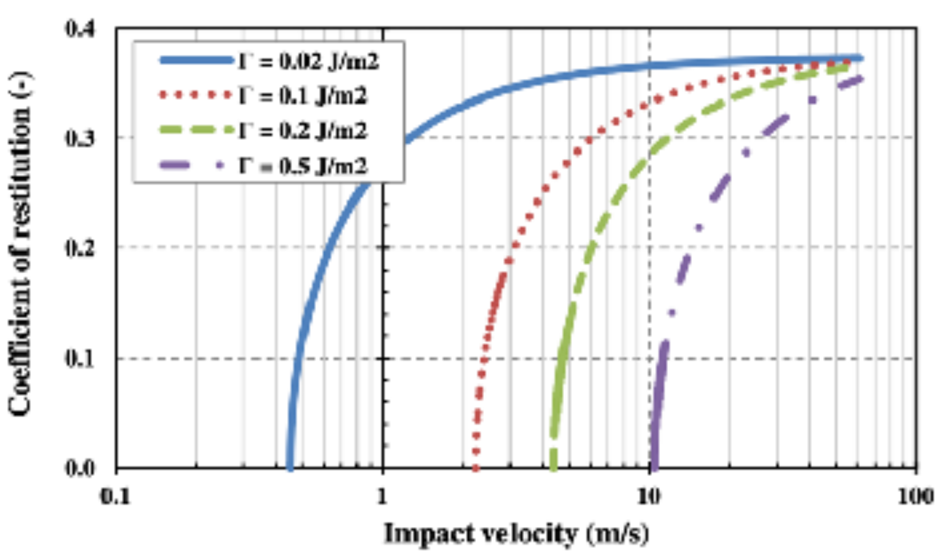


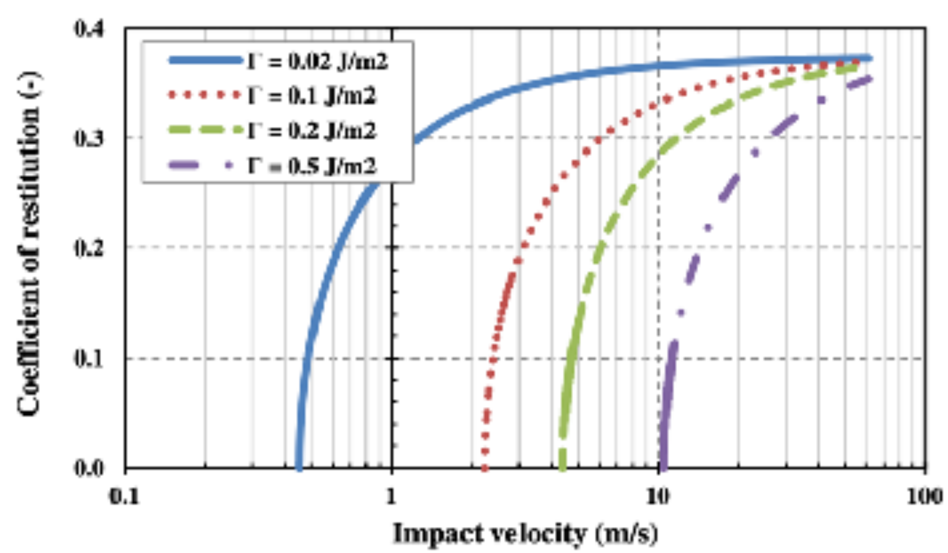
Elasto-plastic and adhesive force law

Pasha, 2014





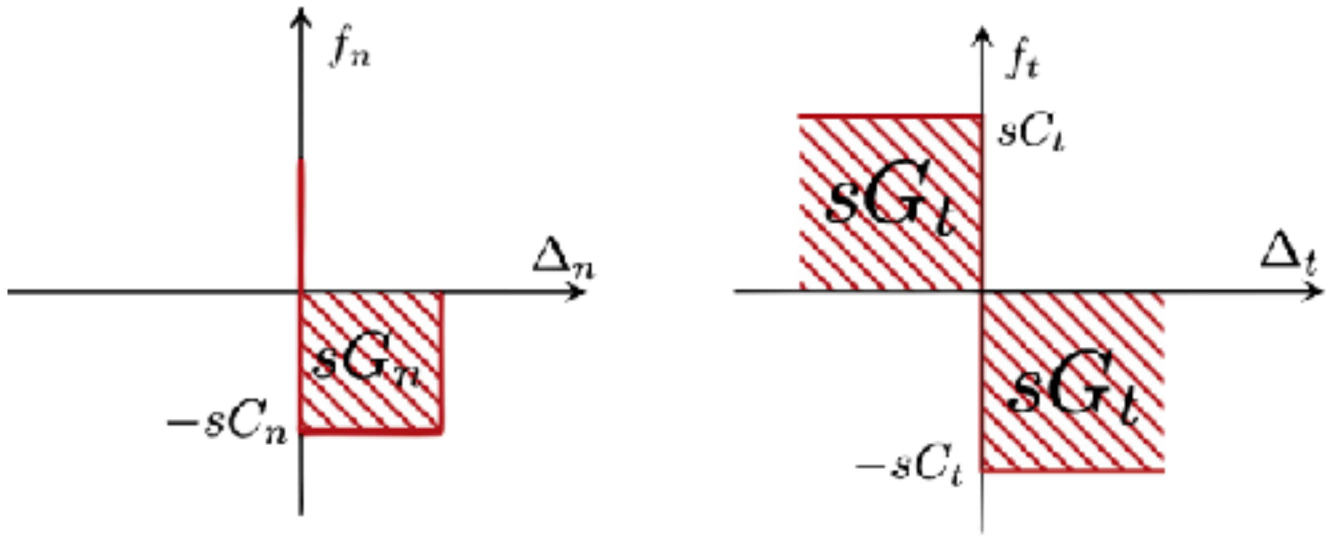


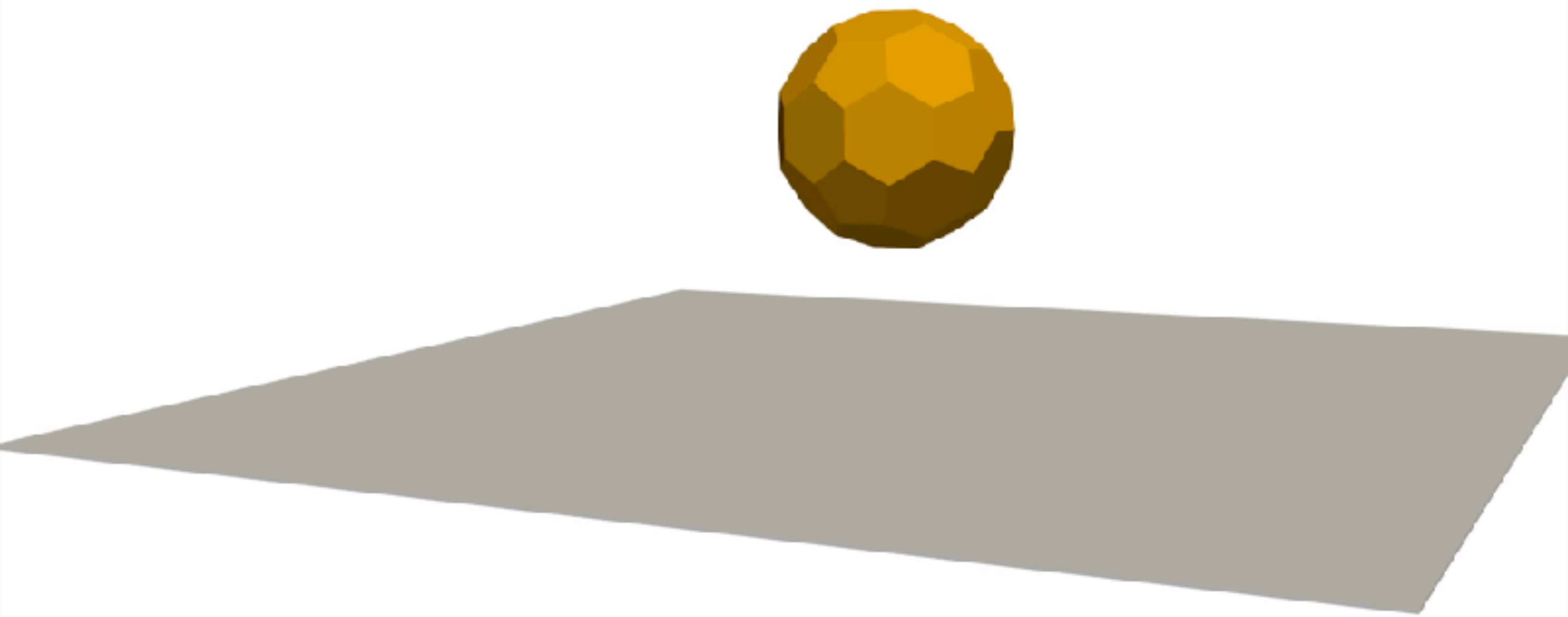


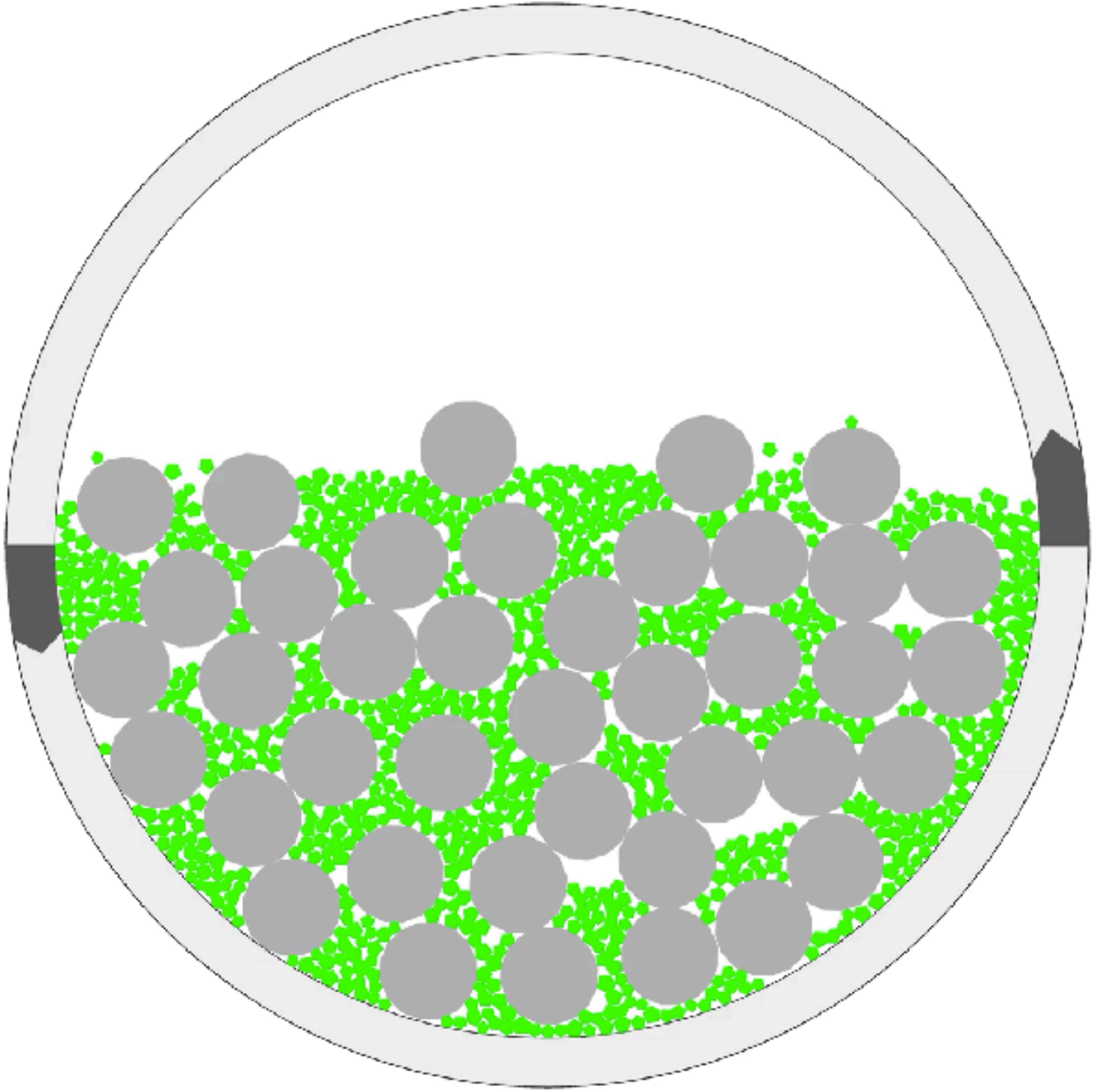
Cohesive law based on fracture mechanics

Orozco, 2019

A contact breaks only when a force threshold is reached (cracking) and the amount of energy consumed by the contact is equal to the fracture energy. The behavior becomes independent of other contact parameters.







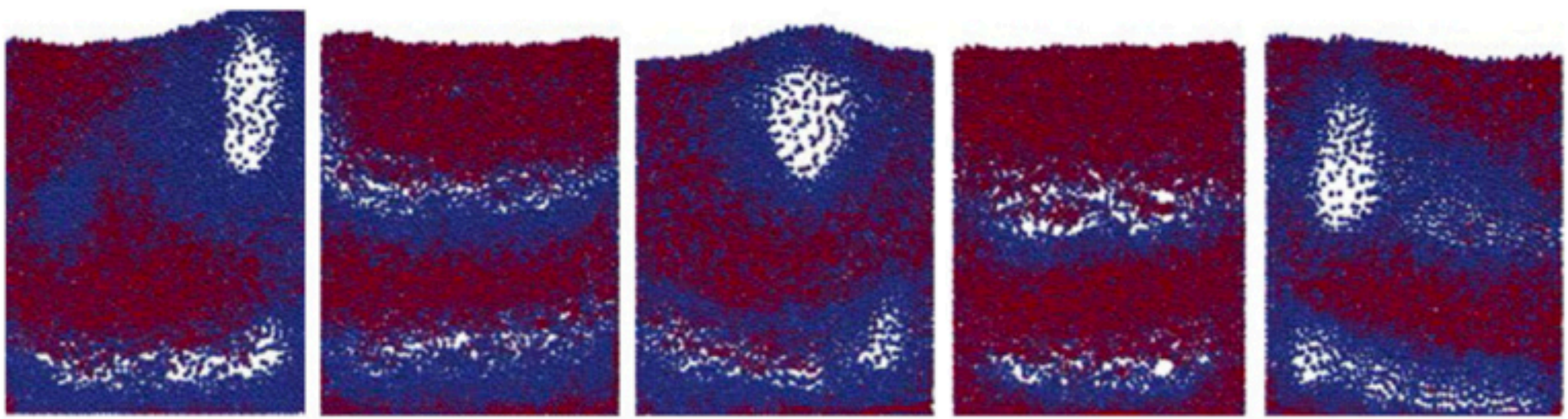
Adhesion and stiffness

The flow behavior of cohesionless granular materials is insensitive to contact stiffness. When adhesion is added, the latter should be rescaled with stiffness.

$$A^S = A^R (Y_S/Y_R)^{2/5}. \qquad A^S = A^R (k_S/k_R)^{1/2}.$$

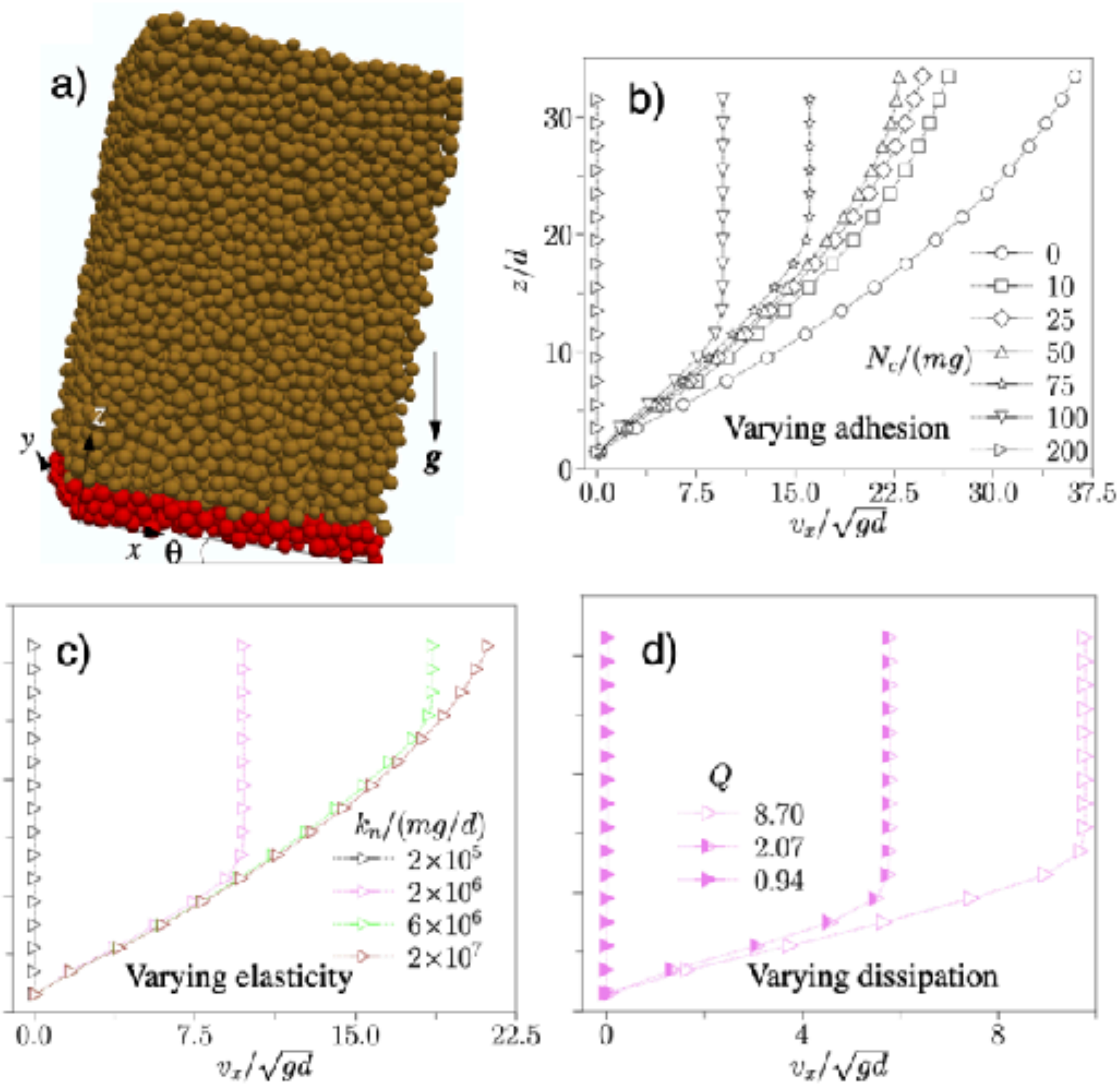
Moreno-Atanasio, 2007 Liu, 2016

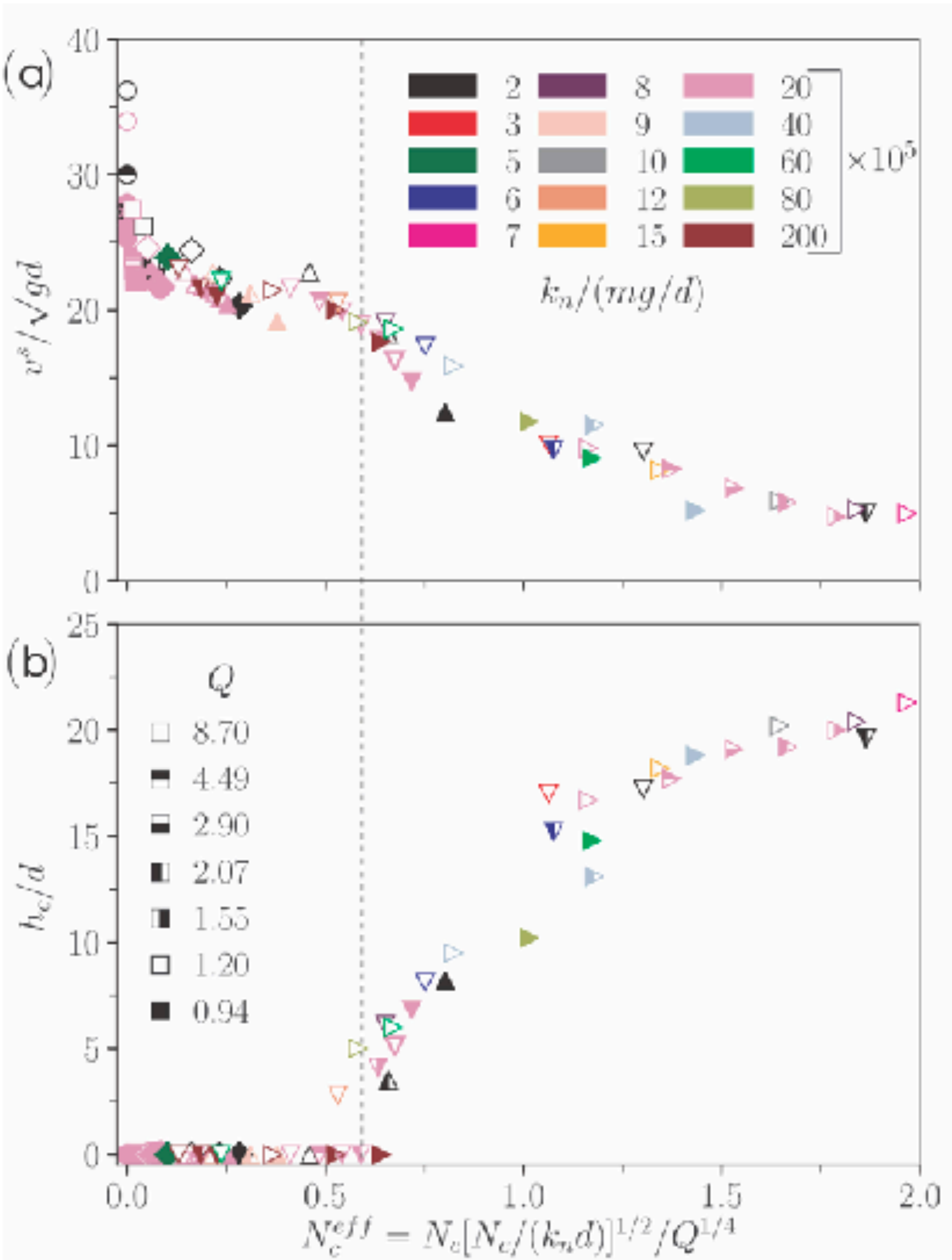
Kobayashi, 2013 Gu, 2016



$Y = 7 \times 10^{10}\ Pa$ Original model; $Y = 10^8\ Pa$ Original model; $Y = 10^8\ Pa$ Modified model; $Y = 10^6\ Pa$ Original model; $Y = 10^6\ Pa$ Modified model

Mandal, 2019


a)
z
y
x
θ
g
b)
Varying adhesion
$N_c/(mg)$
0
10
25
50
75
100
200
z/d
0
10
20
30
0.0
7.5
15.0
22.5
30.0
37.5
$v_x/\sqrt{gd}$
c)
Varying elasticity
$k_n/(mg/d)$
2×10^5
2×10^6
6×10^6
2×10^7
0.0
7.5
15.0
22.5
$v_x/\sqrt{gd}$
d)
Varying dissipation
Q
8.70
2.07
0.94
0
4
8
$v_x/\sqrt{gd}$



effecive cohesion force

$$N_c^{eff} = N_c\left[\left(\frac{N_c}{k_n d}\right)^a \frac{1}{Q^b}\right]$$

$$\frac{\delta_c}{d}$$

$$a \simeq \frac{1}{2} \qquad b \simeq \frac{1}{4}$$

Soft particles

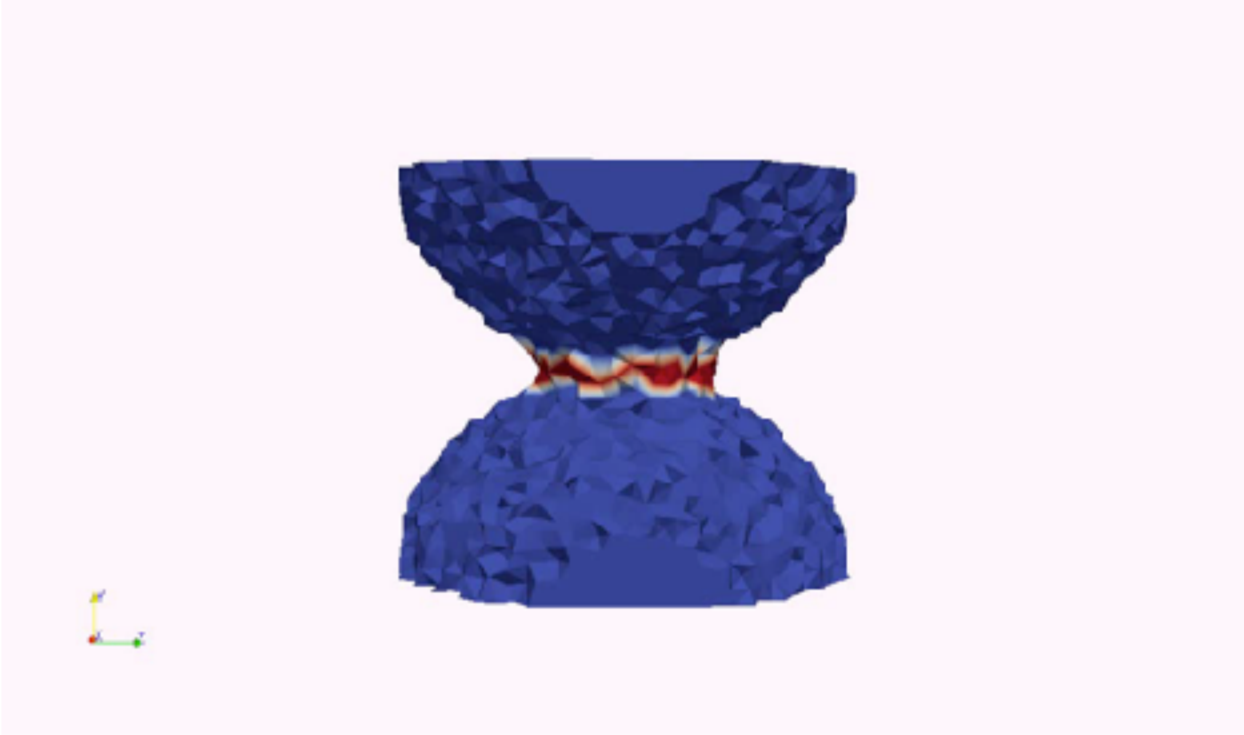
Soft (deformable) particles can be modeled by introducing internal degrees of freedom.

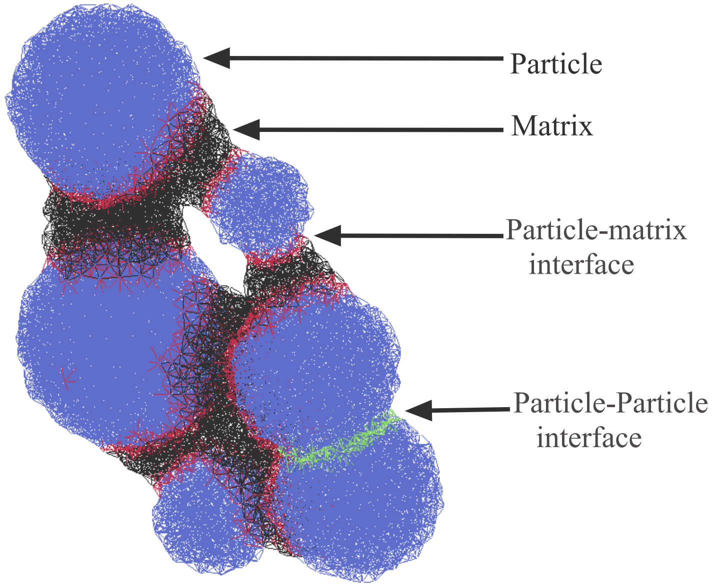
Lampoh, 2014

Lattice Element Method (LEM)

The particle is replaced by a network of linear or nonlinear springs.

Affes, 2012

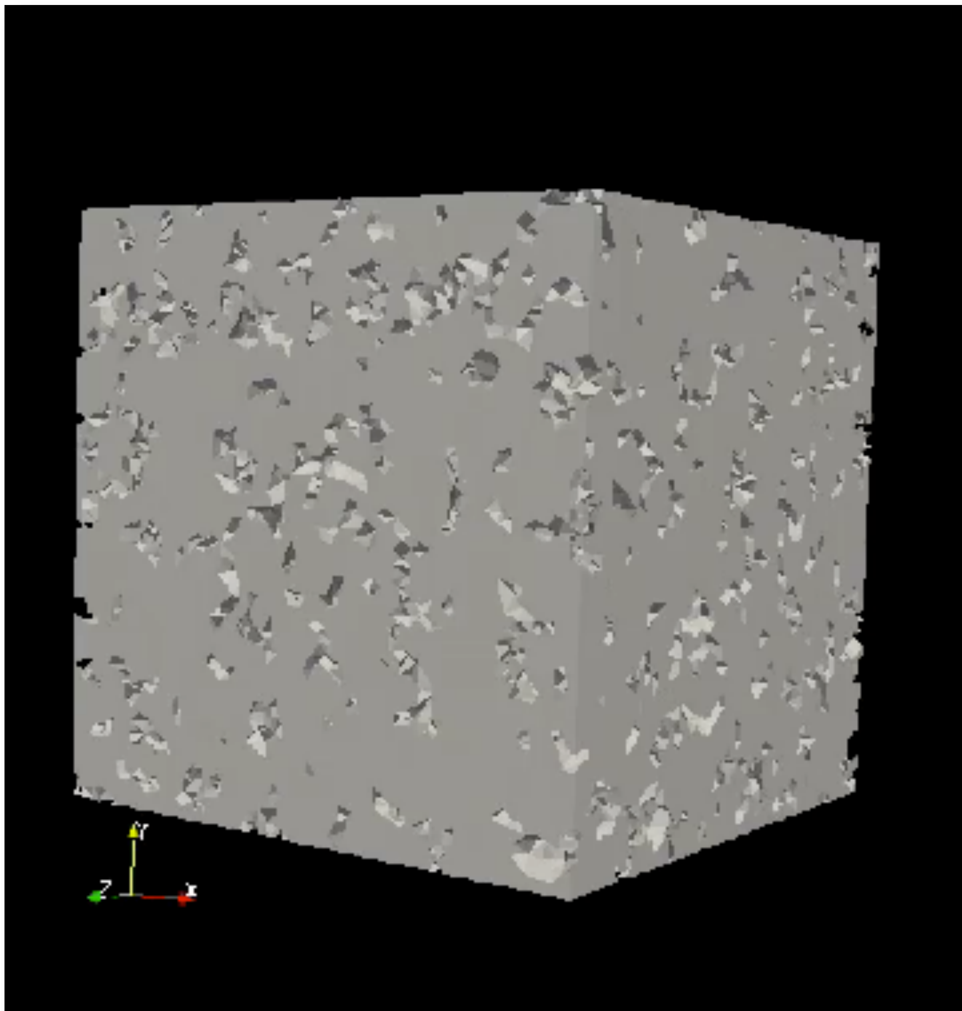


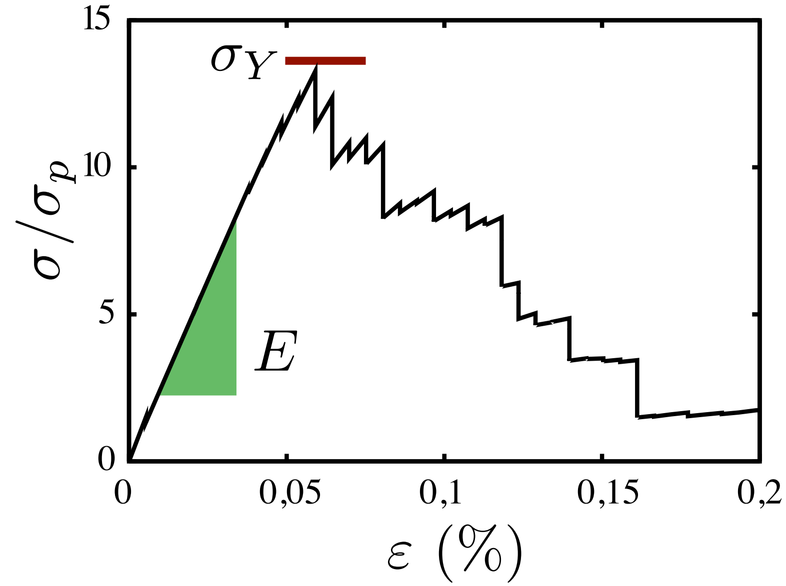


Benefits:

1) A solid matrix can be introduced
2) The bonds can be broken

Application to cemented granular materials.



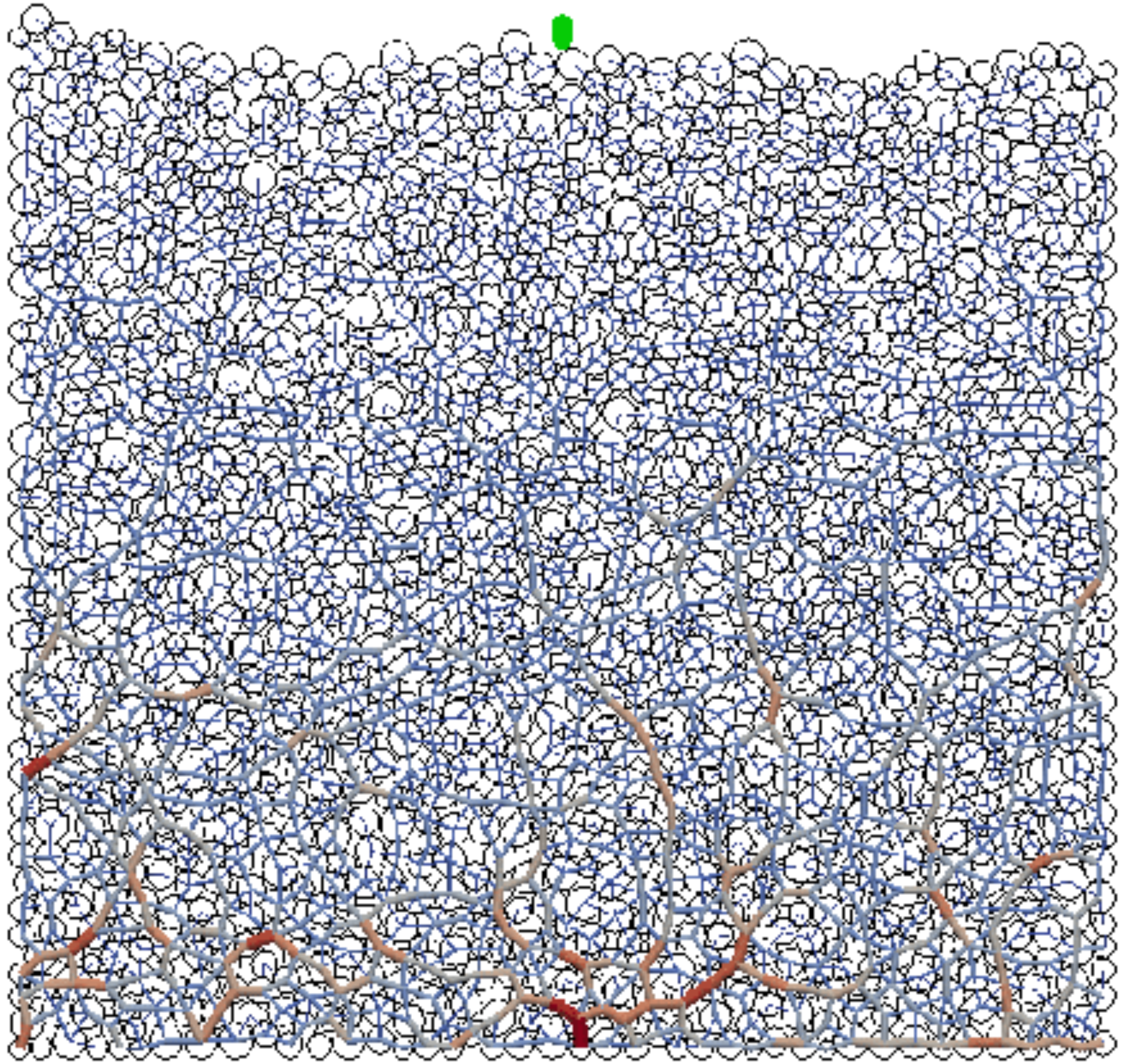


Elastic-brittle behavior

Affes, 2012

Application to root growth

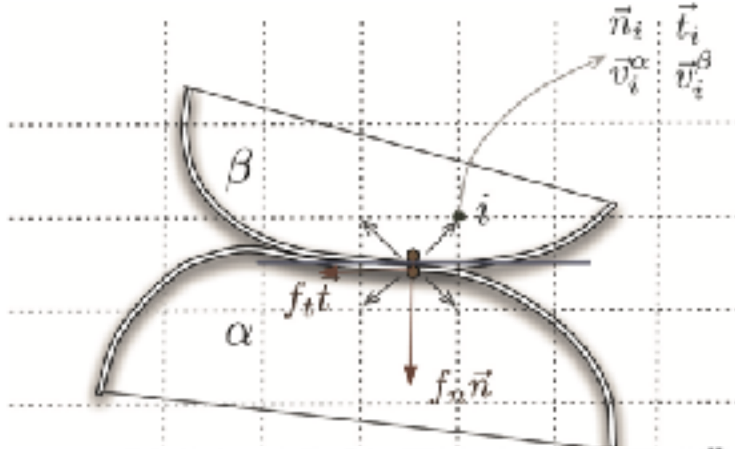
Fakih, 2018

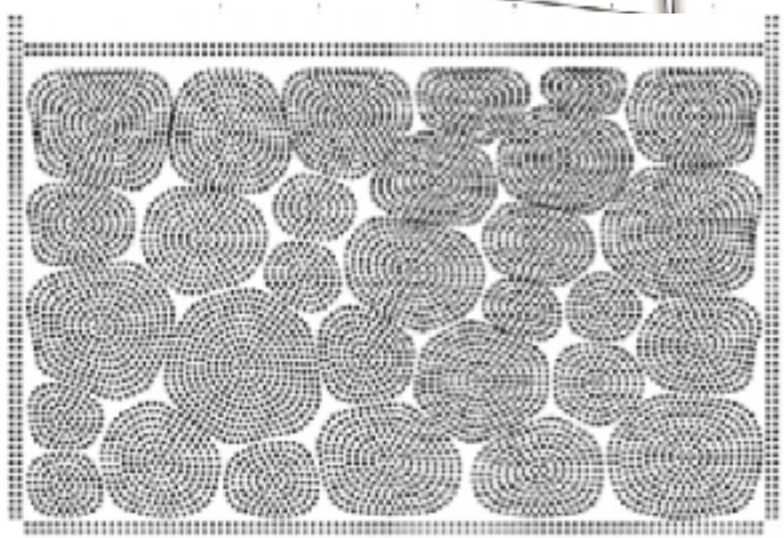


Material Point Method (MPM)

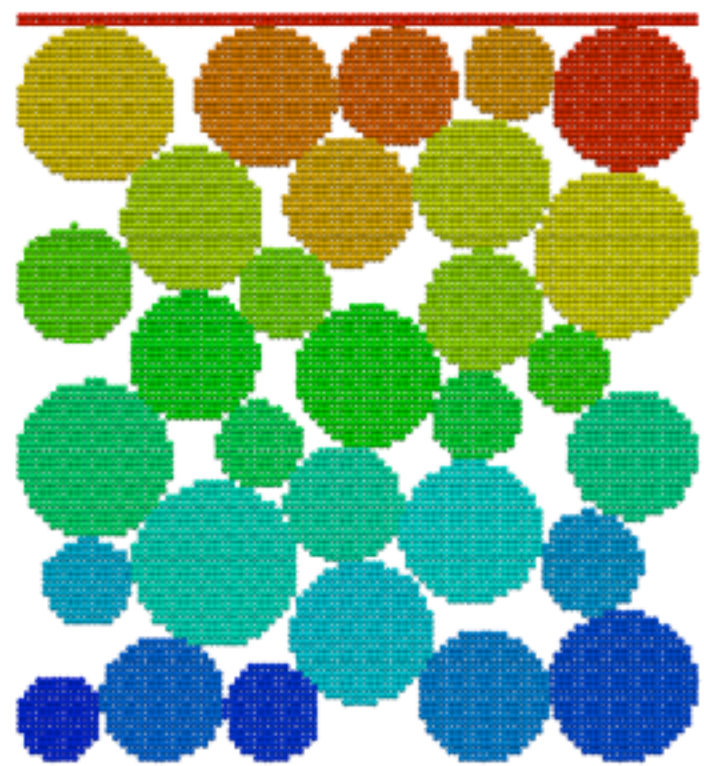
Benefits:

1) The particles can have arbitrary constitutive behavior
2) Large elastic or plastic deformations can be reached
3) The contacts do not need to be soft





Nezamabadi, 2015



Validation

The accuracy of the physical model can be evaluated by direct or indirect comparison with measurements on the real system. But it needs:

1) An estimation of the uncertainties in the values of simulation input parameters

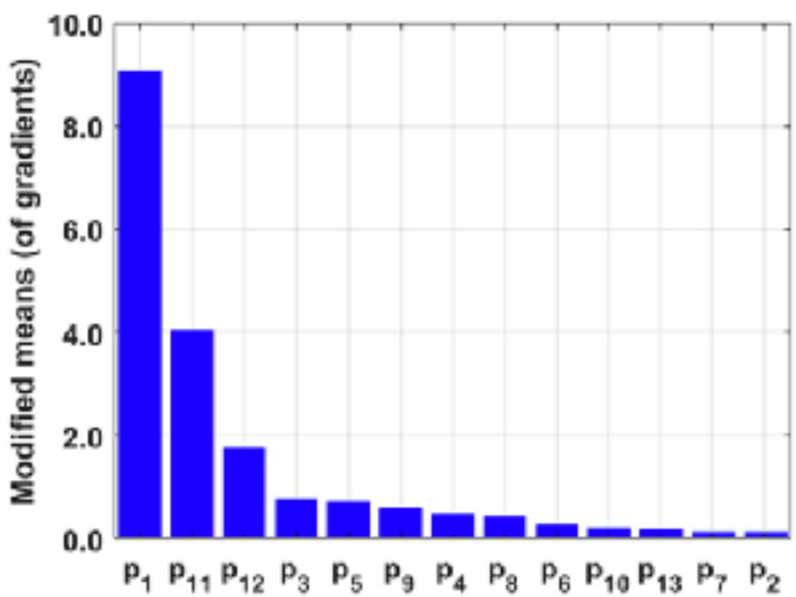
2) A quantitative assessment of their impact on the simulated behavior (micro-scale or macro-scale variables of interest)

3) An estimation of finite size effects

4) An evaluation of uncertainties in the initial state (crucial for transients)

Sensitivity analysis of CFD-DEM on fluidized beds — Bakshi, 2018

Label	Model parameter			Range		
	Physical representation	Symbol	Units	Nominal	Min.	Max.
P_1	normal spring stiffness p-p (10^{P_1})	k_n	[N/m]	2.00	1.00	3.00
P_2	normal spring stiffness p-w (10^{P_2})	k_{nw}	[N/m]	2.00	1.00	3.00
P_3	friction coefficient p-p	μ	–	0.30	0.05	0.90
P_4	friction coefficient p-w	μ_w	–	0.30	0.05	0.90
P_5	normal restitution p-p	e_n	–	0.90	0.50	0.98
P_6	normal restitution p-w	e_{nw}	–	0.90	0.50	0.98
P_7	tangential-normal stiffness ratio p-p	k_t/k_n	–	0.29	0.10	0.90
P_8	tangential-normal stiffness ratio p-w	k_{tw}/k_{nw}	–	0.29	0.10	0.90
P_9	tangential-normal damping ratio p-p	η_t/η_n	–	0.50	0.10	0.90
P_{10}	tangential-normal damping ratio p-w	η_{tw}/η_{nw}	–	0.50	0.10	0.90
P_{11}	collision-DEM time-step ratio	τ_{col}/τ_{dem}	–	50	20	50
P_{12}	fluid equations tolerance ($10^{P_{12}}$)		–	−4.00	−6.00	−3.00
P_{13}	DEM-fluid grid interpolation width		$[d_p]$	2.00	1.00	2.50

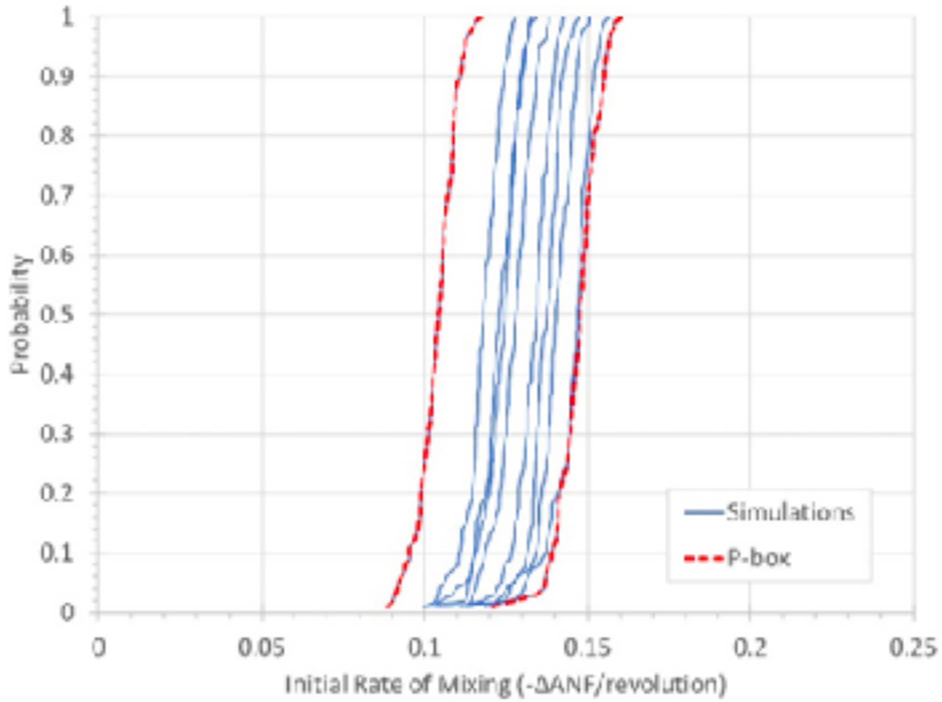


Uncertainty quantification in simulation of mixing

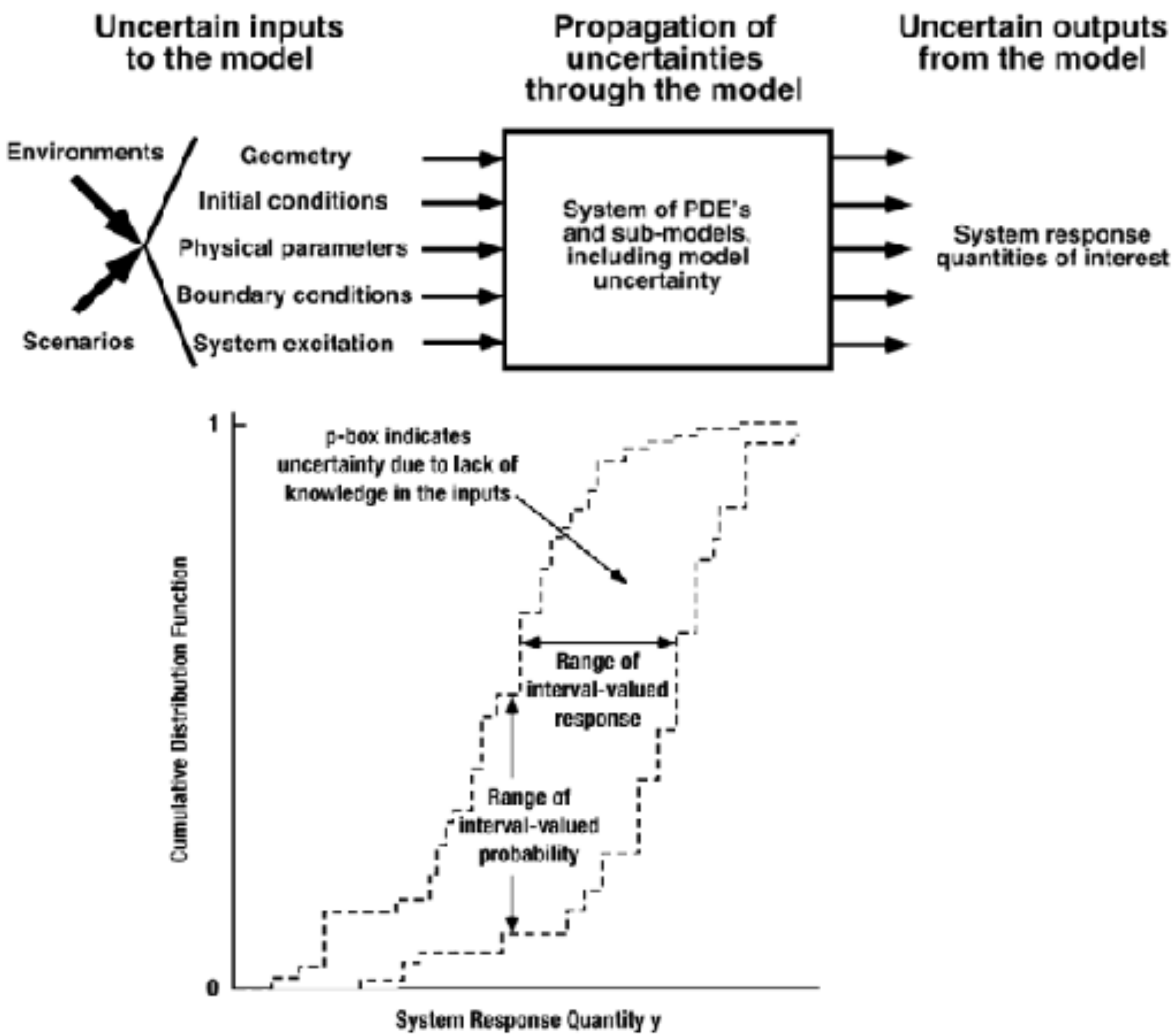
Dahl, 2022

Tumbler system: uncertain input parameters.

Parameter	Lower bound	Base case	Upper bound	Type
Rotation rate (rev/min)	29	30	31	epistemic
Glass diameter (cm)	0.270057	0.310134	0.340163	aleatory
Glass density (g/cm^3)	2.2835	2.513	2.85	epistemic
Glass-glass coeff of restitution	0.926186	0.969565	0.993185	aleatory
Glass-wall coeff of restitution	0.629237	0.954934	0.989071	aleatory
Particle-particle coeff of friction	0.131000	0.273370	0.414350	aleatory
Particle-wall coeff of friction	0.057700	0.251369	0.382600	aleatory

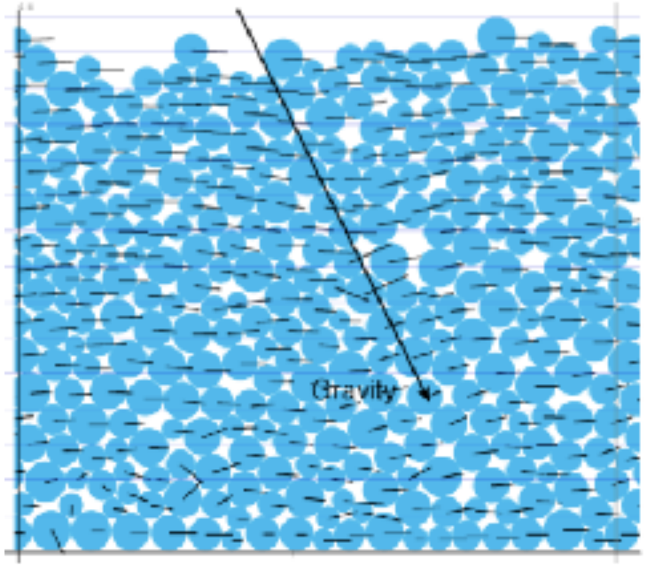


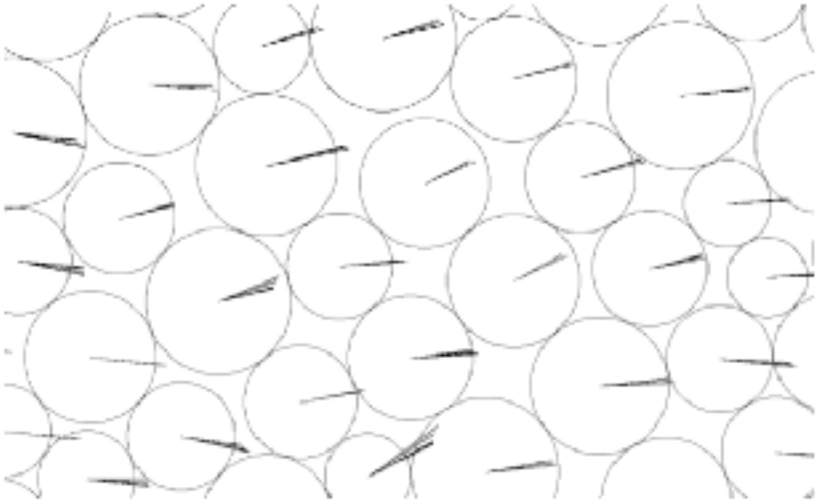
General mathematical method Roy & Oberkampf, 2011



In DEM, the material parameters generally have unique values for all particles or contacts. Real particles show broad property distributions (material polydispersity). No investigations have been so far reported on the simulation of granular materials with distributed parameter values (friction coefficients, restitution coefficients…). How such distributions are upscaled is an interesting issue in itself.

No methodology has been so far developed for the preparation of initial samples with specified characteristics for DEM simulations. For transient flows, the memory of the initial state is probably the most influent source of error.



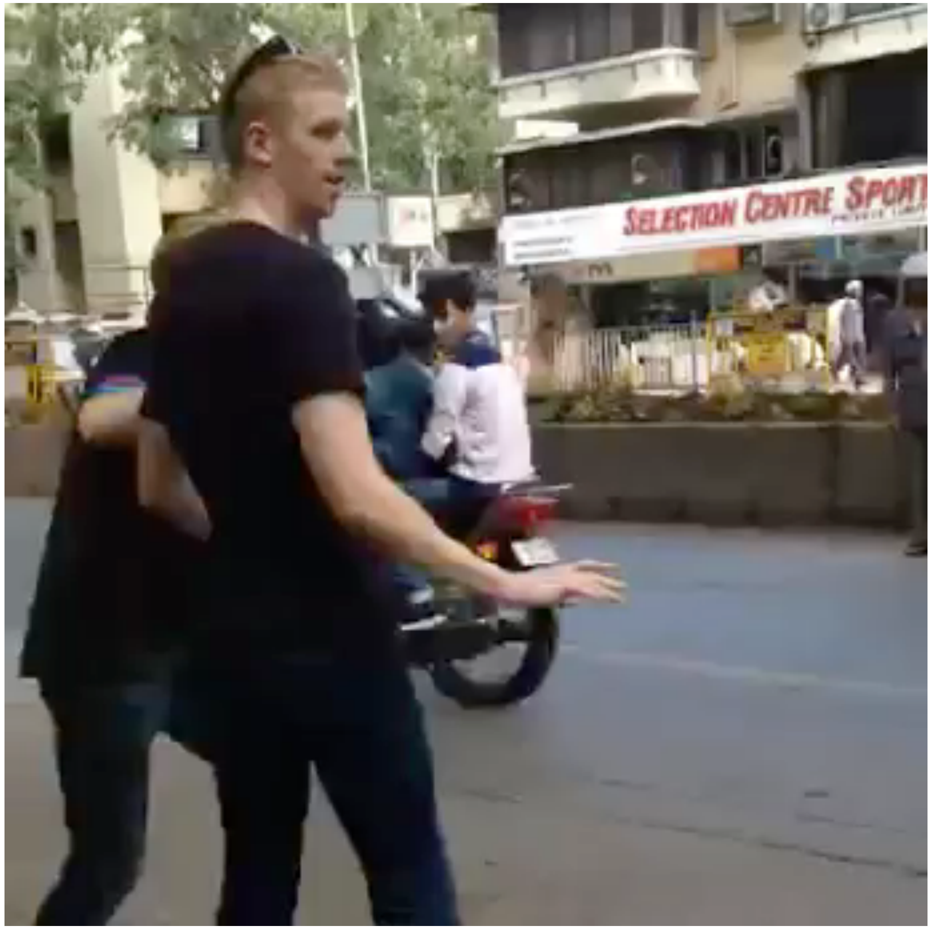


Concluding remarks

For a decade, the DEM has considerably evolved in maturity. But there are vast scopes for its development by:

- Working out consistent approaches incorporating progress in different aspects: shape+force law, cohesion+roughness, shape+roughness, softness+fracture…
- Validating the contact laws (including damping terms and cohesive effects)
- Defining a framework for sensitivity analysis in different systems
- By extending the DEM to include internal degrees of freedom. On the long term, consider the « soft particle + hard contact » model as an alternative for the « hard particle + soft contact » model (made possible by speedup strategies).

DEM is a paradigm or framework for elaborating physical models of various systems composed of « particles » (in the general sense). It can be used not only as a predictive tool, but also as a lab to create new materials and processes.



This is not just a technique!