

IMPERIAL

A subjective history of the discrete element method

CCC Parasols

Catherine O'Sullivan



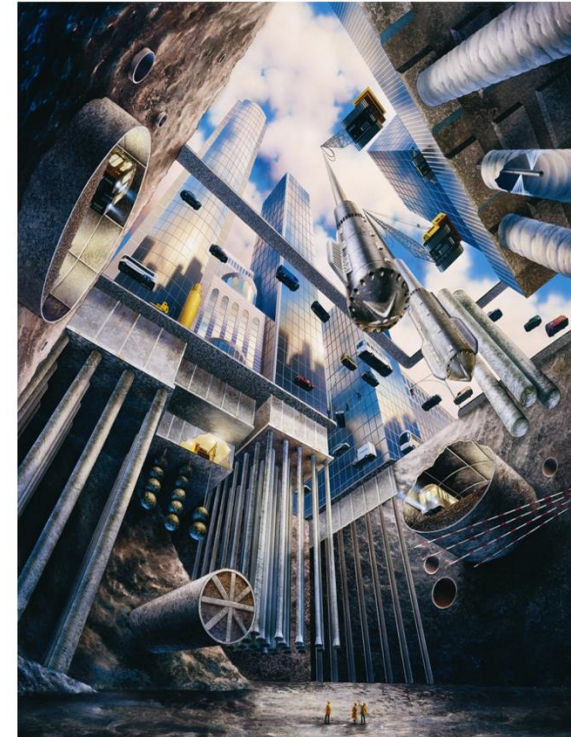
Perspective

“We must look at the lens through we see the world, as well as the world we see, and that the lens itself shapes how we interpret the world.”

Stephen R. Covey



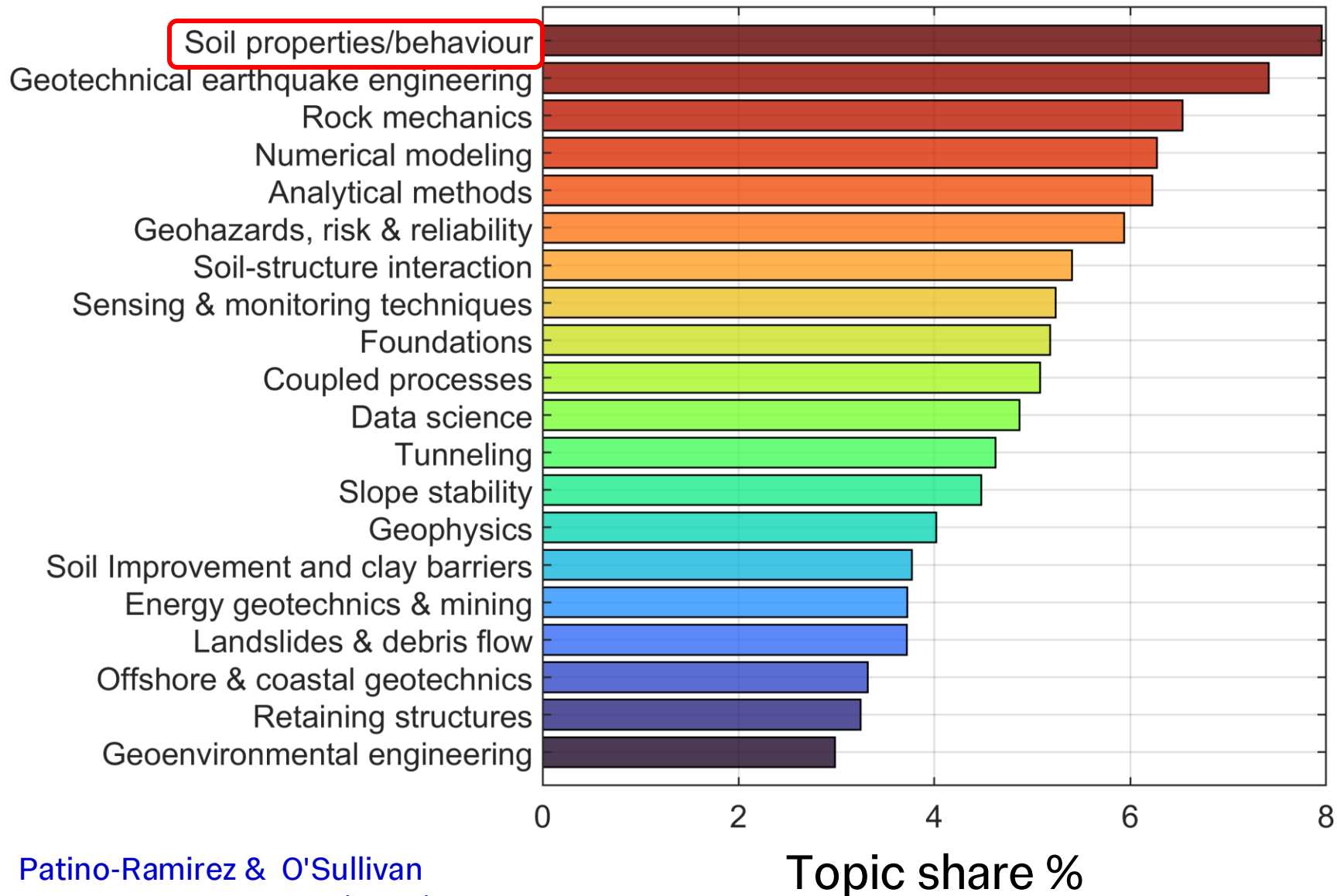
My perspective: Soil mechanics / geotechnical engineering



Keller

<https://collection.sciencemuseumgroup.org.uk/objects/>

Geotechnical Eng. research: Topic modelling



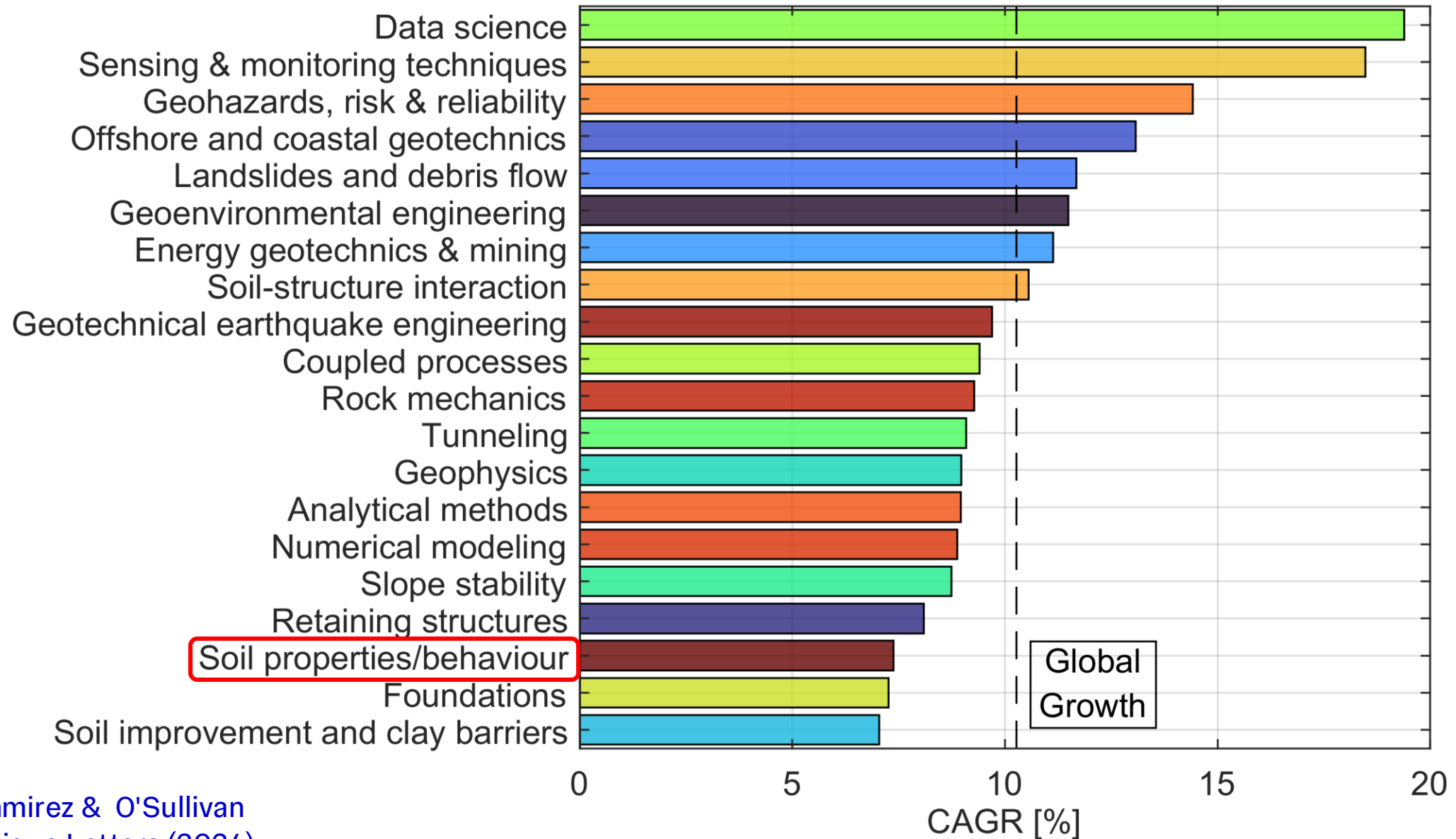
Data from 65,922
Geotechnical Engineering
journal articles (30 journals)
from 1998-2022

Title, abstract, keywords

20 prevalent topics found
using a Latent Dirichlet
Allocation (LDA) topic
model: MATLAB function
fitlda

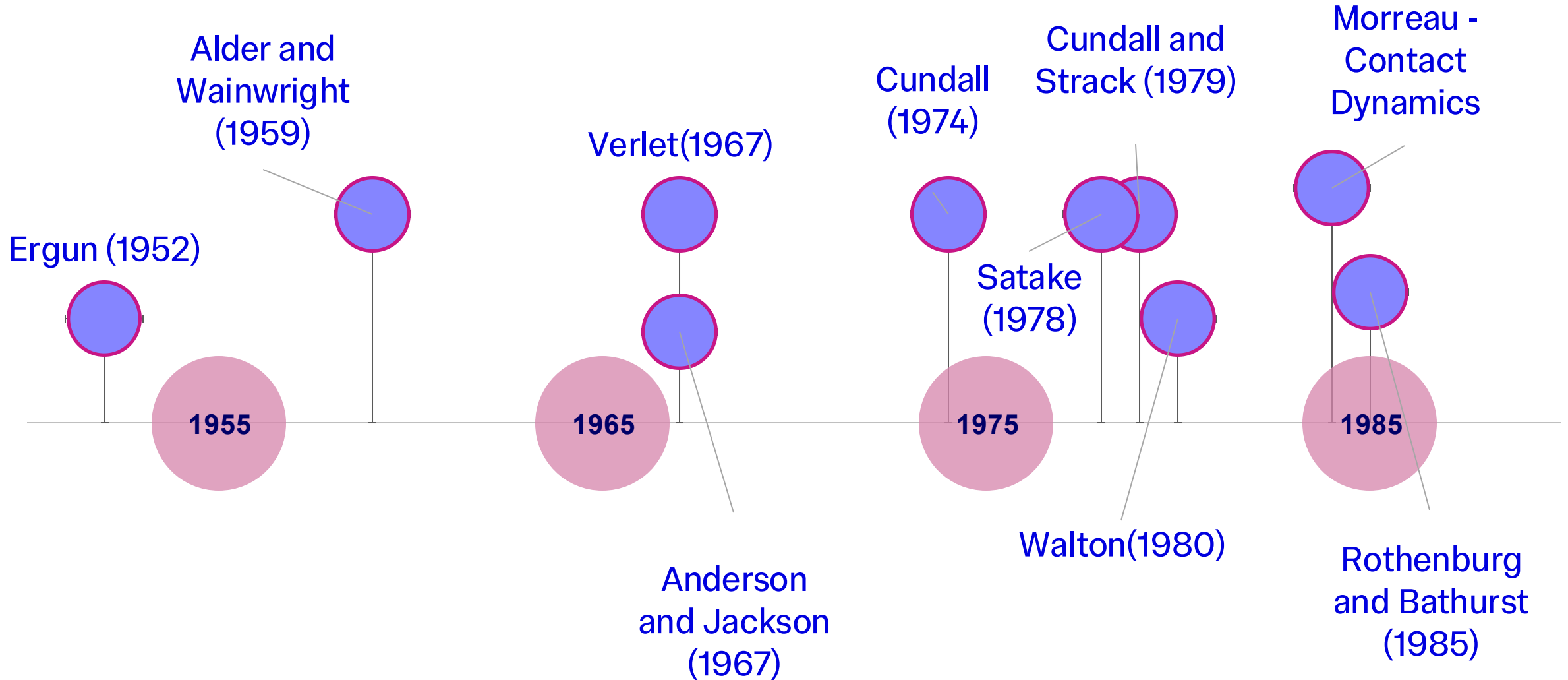
Topics named by
considering 20 word
clouds generated

Geotechnical Eng. research: Topic modelling



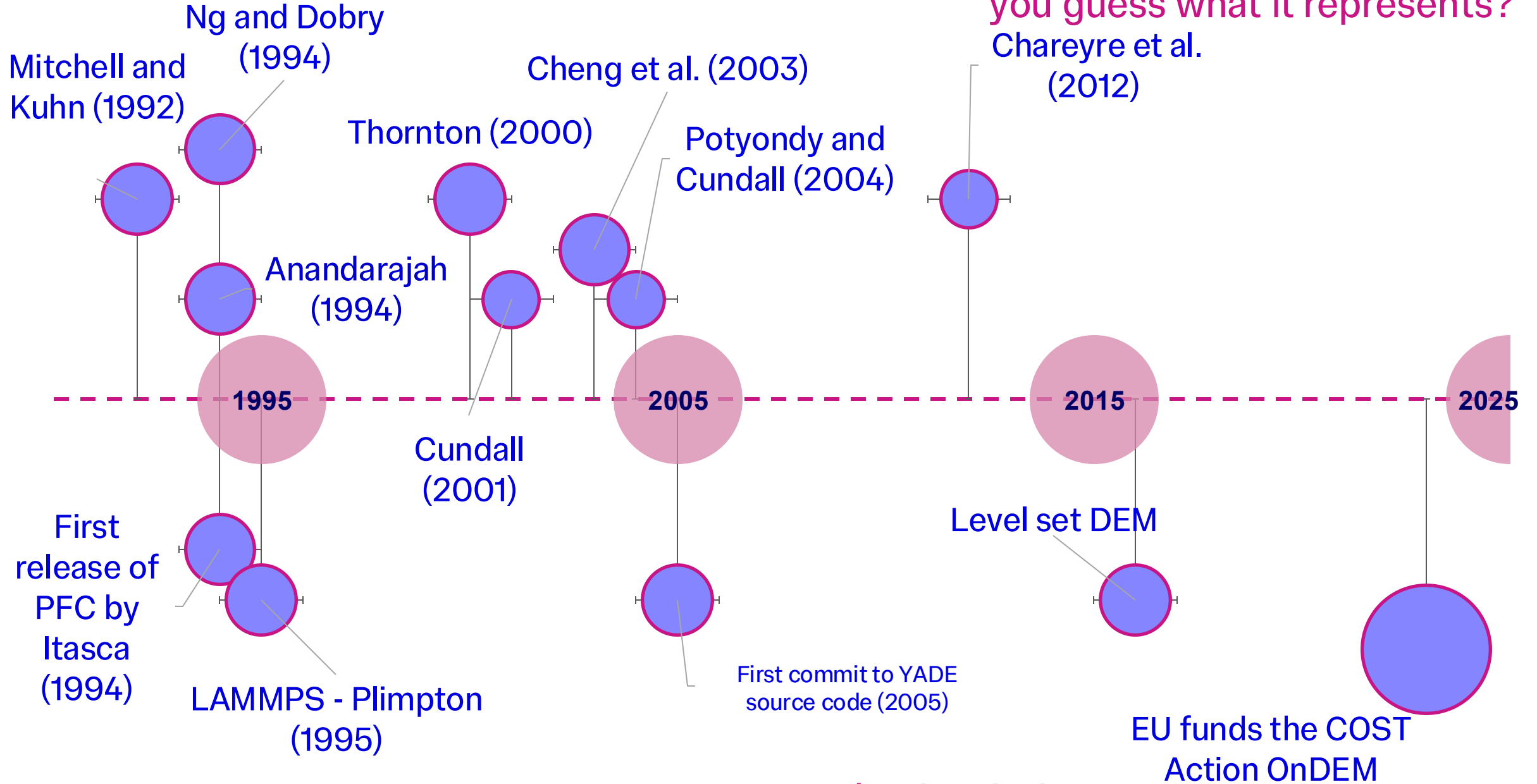
DEM Timeline 1950-1990

Each dot is a milestone – can you guess what it represents?



What is missing?

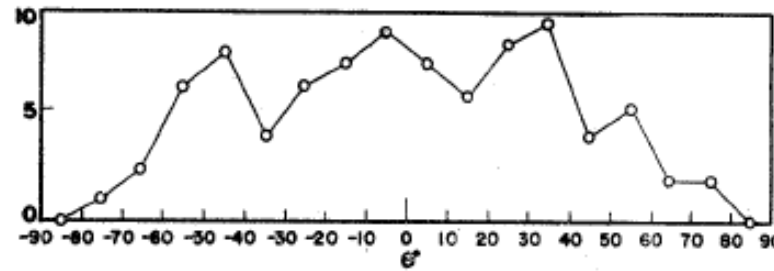
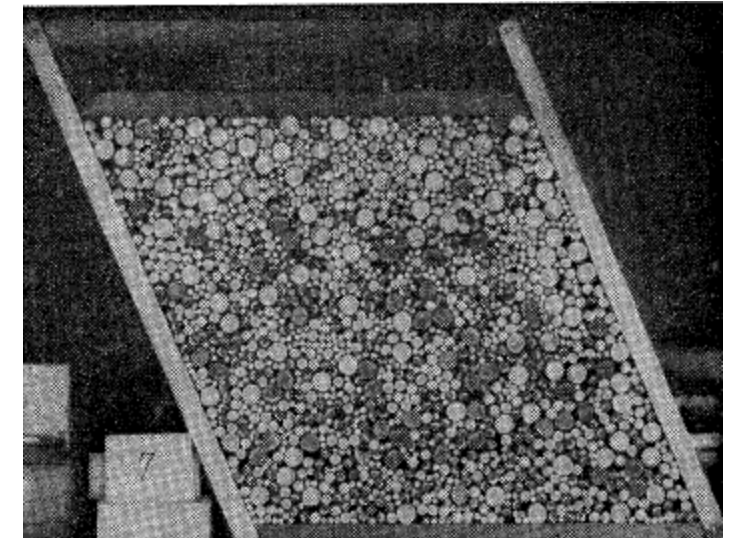
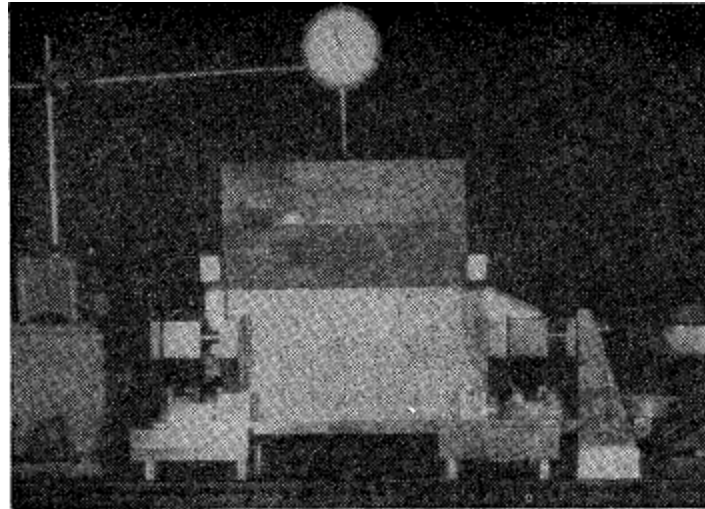
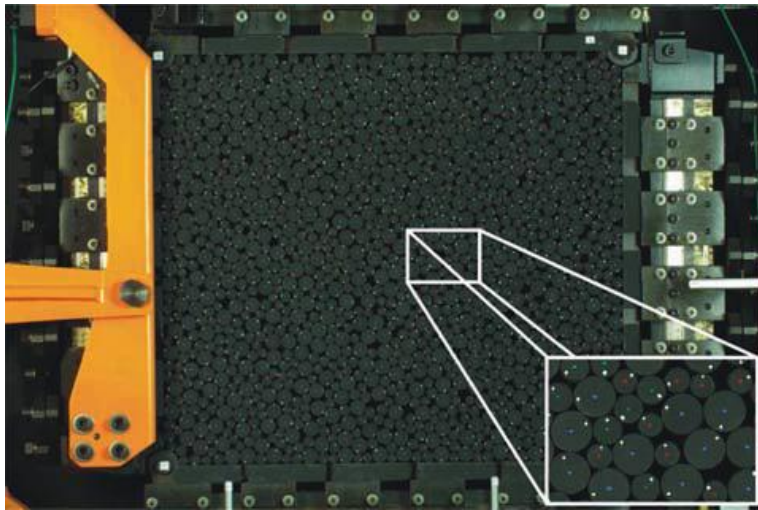
DEM Timeline 1990-2025



What is missing?

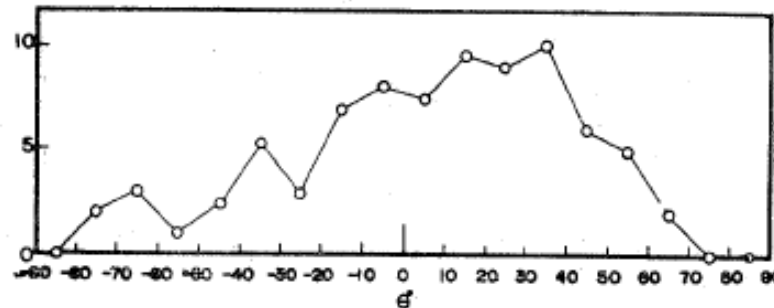
Pre-DEM – physical modelling

Schneebeli Rods



Prior to shear

Orientation of interparticle contact on shear plane

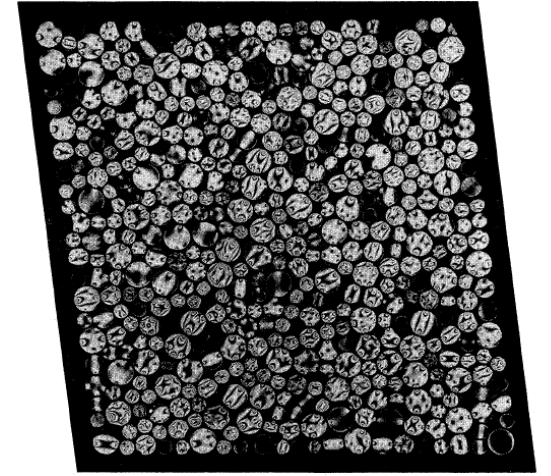
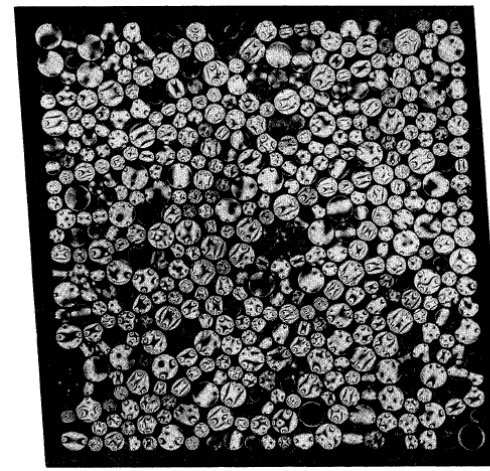
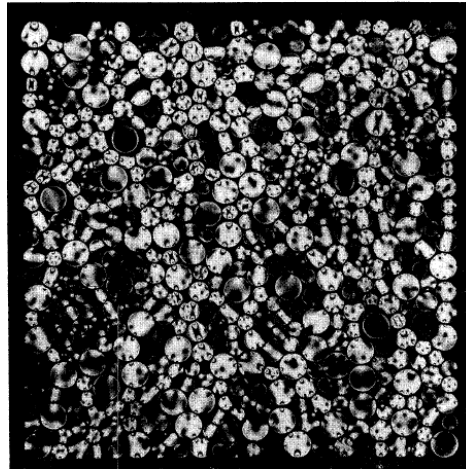
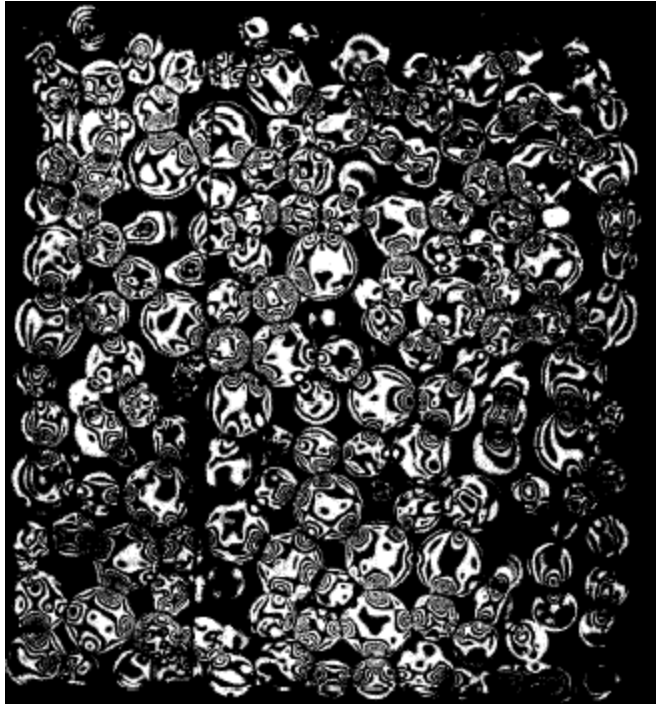
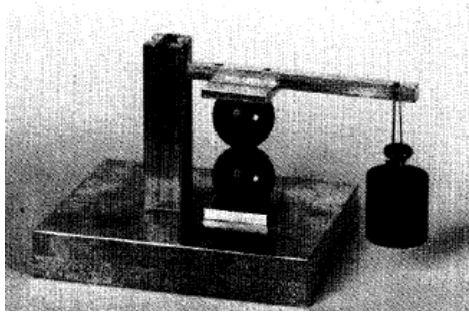
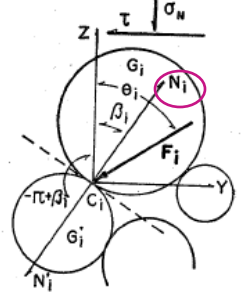


At peak

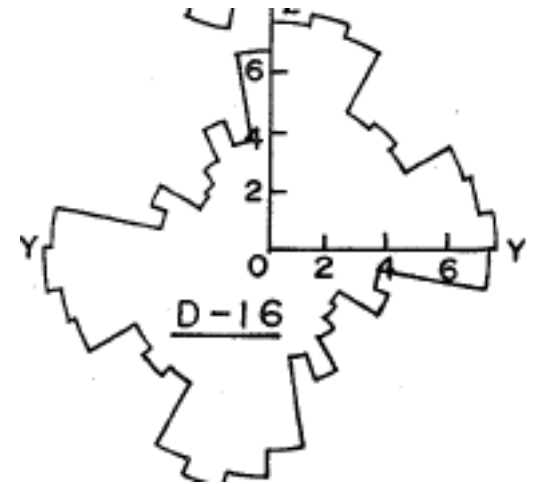
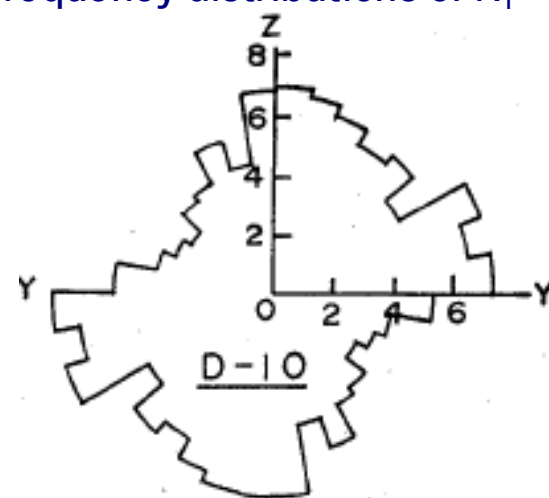
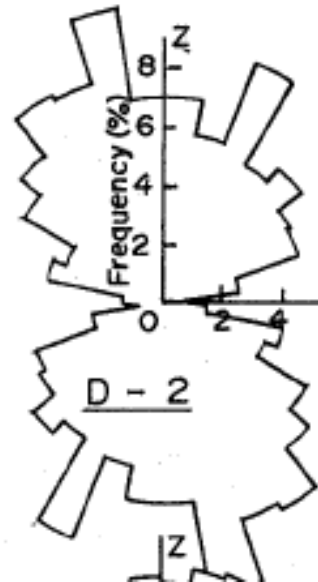
Schneebeli, G.: Une analogie mécanique pour les terres sans cohésion. C.R. Acad. Sci. 243, 125–126 (1956)

Sibille and Froiio (2007) Granular Matter

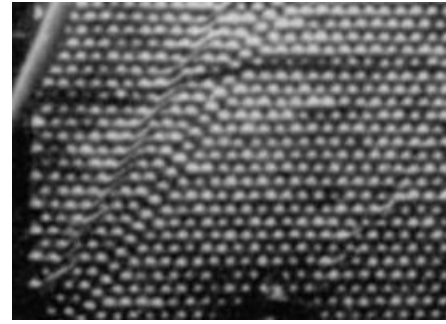
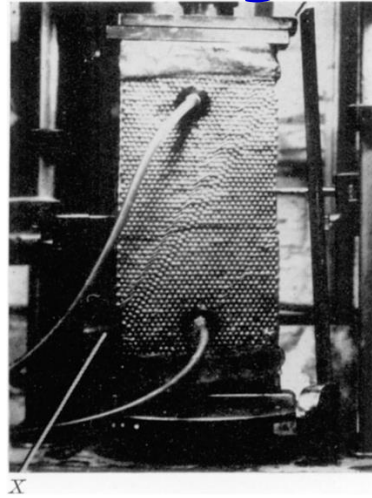
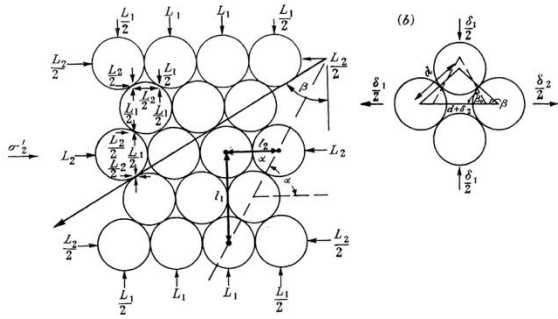
Pre-DEM – photoelasticity



Frequency distributions of N_i



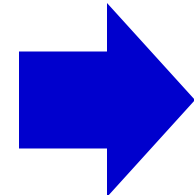
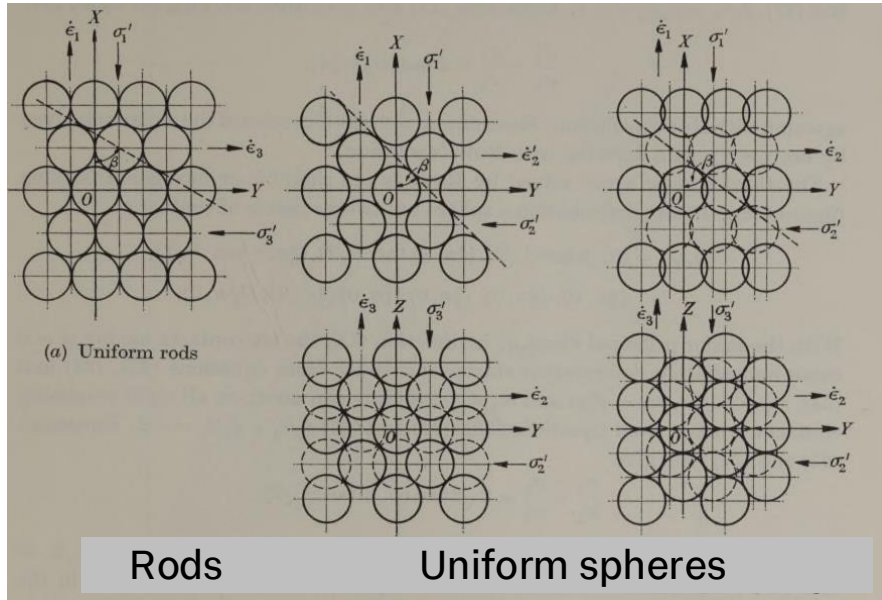
Pre-DEM – analytical models: UK in the 1960s



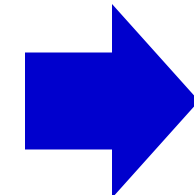
ϕ – angle of shearing resistance for soil

$\mu_{particle}$ - interparticle friction coefficient

Rowe (1962) *Proc. Royal Soc.*



Rowe's stress-dilatancy theory

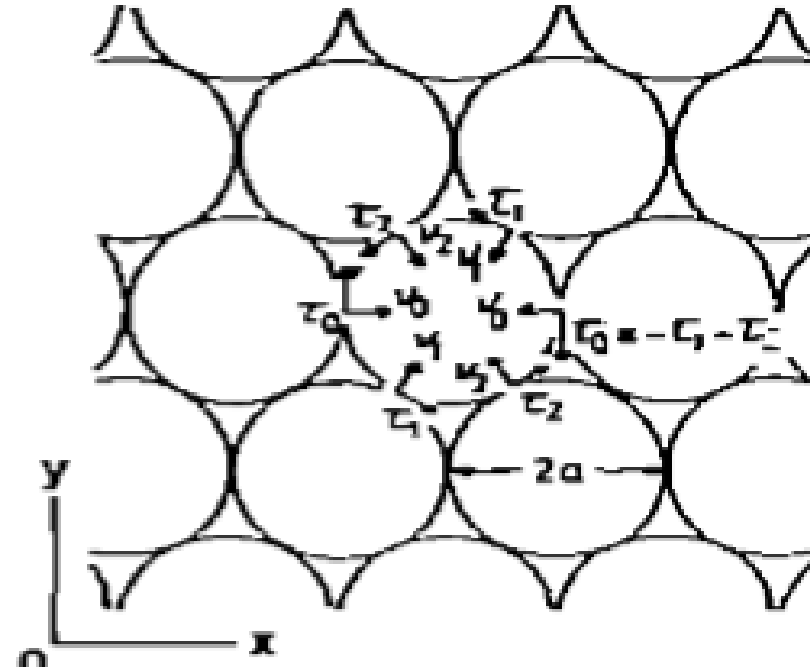
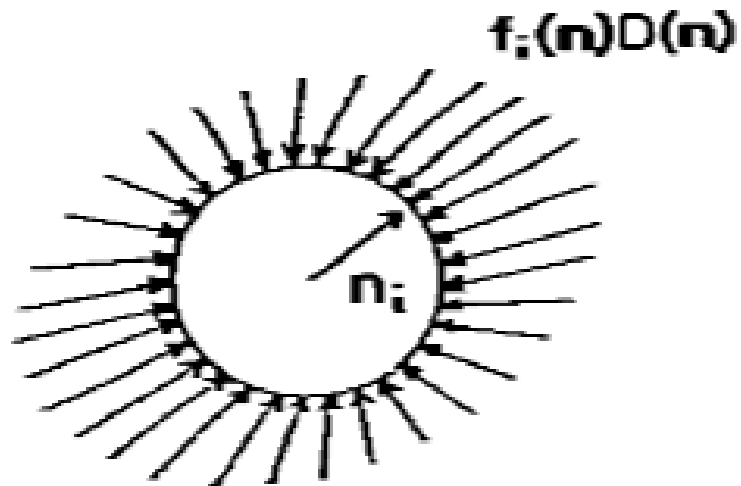


Expressions for ϕ in terms of $\mu_{particle}$

Horne (1965) *Proc. Royal Soc.*

Pre-DEM – quantifying fabric

Satake, K. (1978): *Constitution of mechanics of granular materials through graph representation*, Theoretical and Applied Mechanics, Vol. 26, 257-266



Kanatani, K. (1981) *A theory of contact force distribution in granular materials* Powder Technology 28

Pre-DEM – Molecular Dynamics

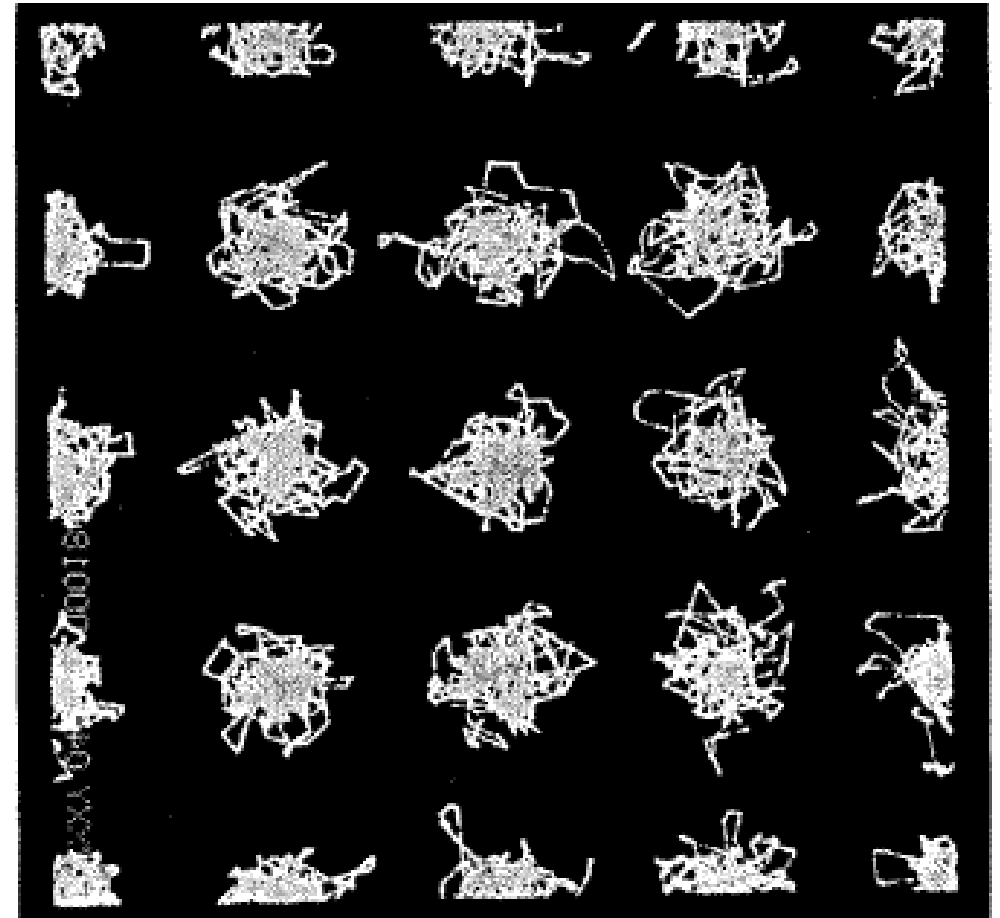
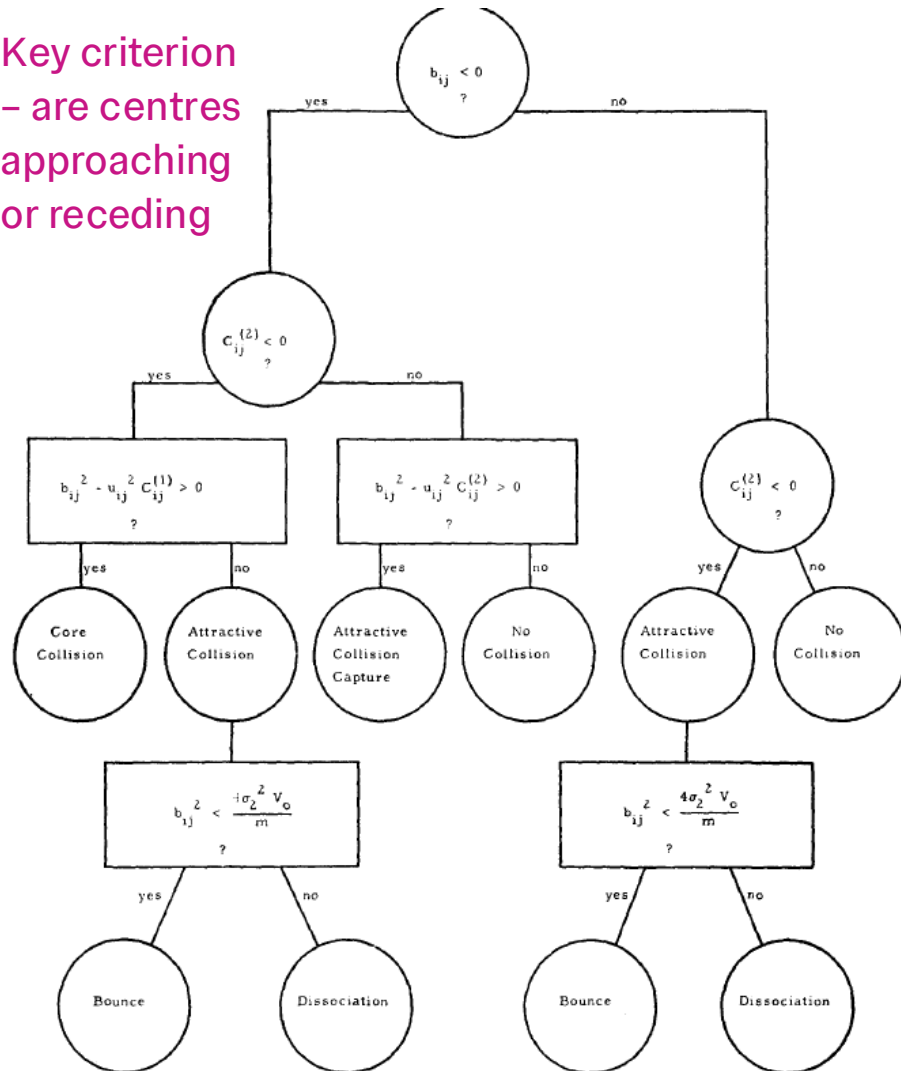
- “the nature of matter is to be found in the structure and motion of its constituent building blocks, and the dynamics is contained in the solution to the N-body problem.”
- “the N-body problem originated in the dynamics of the solar system...”
- “ a great deal of the behaviour of matter in its various states can still be understood in classical (meaning non-quantum) terms and so it is that the classical N-body problem is central to understanding matter at the microscopic level”
- The emergence of MD can be linked to the development of computers (Rapaport (2004); Ciccotti et al. (2022))

Ciccotti et al.
Eur. Phys. J. B (2022) 95:3

Pre-DEM – Molecular Dynamics

- Molecular dynamics: *B. J. Alder and T. E. Wainright, J. Chem. Phys. 27, 1207 (1957)*
 - *Simulated 32 hard spheres*

Key criterion
– are centres
approaching
or receding



Traces of 32 hard sphere particles in the periodic boundary conditions in the solid phase for about 3000 collisions

Pre-DEM – Molecular Dynamics

Basics of MD:

Spherical particles that interact with each other

Repulsion at close range – attraction over a range of separations

Lennard Jones Potential:

$$E_{LJ} = 4\epsilon \left[\underbrace{\left(\frac{\sigma}{r}\right)^{12}}_{\text{Repulsion}} - \underbrace{\left(\frac{\sigma}{r}\right)^6}_{\text{Attraction}} \right]$$

ϵ strength of interaction
 σ length scale

Outside of cutoff separation distance $E_{LJ} = 0$

\mathbf{r}_{ij} vector joining sphere centroids

$$r = |\mathbf{r}_{ij}|$$

$$\frac{dE_{LJ}}{dr} = F_{LJ} = \left(\frac{48\epsilon}{\sigma^2}\right) \left[\left(\frac{\sigma}{r}\right)^{14} - \frac{1}{2} \left(\frac{\sigma}{r}\right)^8 \right] \mathbf{r}_{ij}$$

$$m\ddot{\mathbf{r}}_i = \mathbf{f}_i = \sum_{\substack{j=1 \\ (j \neq i)}}^{N_m} \mathbf{f}_{ij}$$

Pre-DEM – Molecular Dynamics

$$v_{i_x}(t + h/2) = v_{i_x}(t - h/2) + ha_{i_x}(t) \quad (2.3.1)$$

$$r_{i_x}(t + h) = r_{i_x}(t) + hv_{i_x}(t + h/2) \quad (2.3.2)$$

Accuracy $O(h^4)$ for coordinates and $O(h^2)$ for velocities

Pre-DEM – Verlet(1967) – Argon simulation

$$m \frac{d^2 \mathbf{r}_i}{dt^2} = \sum_{j \neq i} \mathbf{f}(r_{ij}).$$

Equilibrium equation

Uses “reduced units”

$$\mathbf{r}_i(t+h) = -\mathbf{r}_i(t-h) + 2\mathbf{r}_i(t) + \sum_{j \neq i} \mathbf{f}(r_{ij}(t))h^2$$

Numerical integration

$$\mathbf{v}_i(t) = [\mathbf{r}_i(t+h) - \mathbf{r}_i(t-h)]/2h.$$

Velocity

In this kind of calculation, most of the time is spent in computing the force. If no special devices are introduced, we must, at each step, compute $\frac{1}{2}N(N-1)$ terms, most of which turn out to be zero.

We introduce the following bookkeeping device which cuts the computing time by a factor of the order of 10: Every n th step, we compute all the $\frac{1}{2}N(N-1)$ distances, and, given a particle i , we make a table of all the particles which are within a distance rm of that particle. Then, for the next $n-1$ steps in time, we take into account only the particles in the tables.

Requires $rm \ll rv$ – rv is the cutoff for a potential

Pre-DEM – coupling

A FLUID MECHANICAL DESCRIPTION OF FLUIDIZED BEDS

Equations of Motion

T. B. ANDERSON AND ROY JACKSON

University of Edinburgh, Edinburgh, Scotland

Starting from the equations of motion of a single solid particle and the Navier-Stokes equations for fluid motion, a set of equations of motion is developed for a system of fluidized particles, and the result is compared with previously proposed equations.

1967

Ergun, S. (1952) Fluid Flow through Packed Columns. Chemical Engineering Progress, 48, 89-94.

Pre-DEM – implicit methods



G. Dahlquist, P. Lotstedt (1977), Interactive Simulation of the Progressive Collapse of a House, in *Proceedings IMACS Symposium on Simulation Software and Numerical Methods for Differential Equations*, Blacksburg, Va.

- Matrix solution to Lagrange's equation of motion in generalized coordinates.
- Time is advanced in small steps until a constraint change (contact change) is noted and then the matrix must be resolved.
- Explicit time integration → large time steps unless there are a large number of collisions
- If a given block has more than one sliding contact with friction no unique solution exists
- Walton concludes that explicit methods might be less efficient but more “surely soluble”

Cundall's path to Trubal

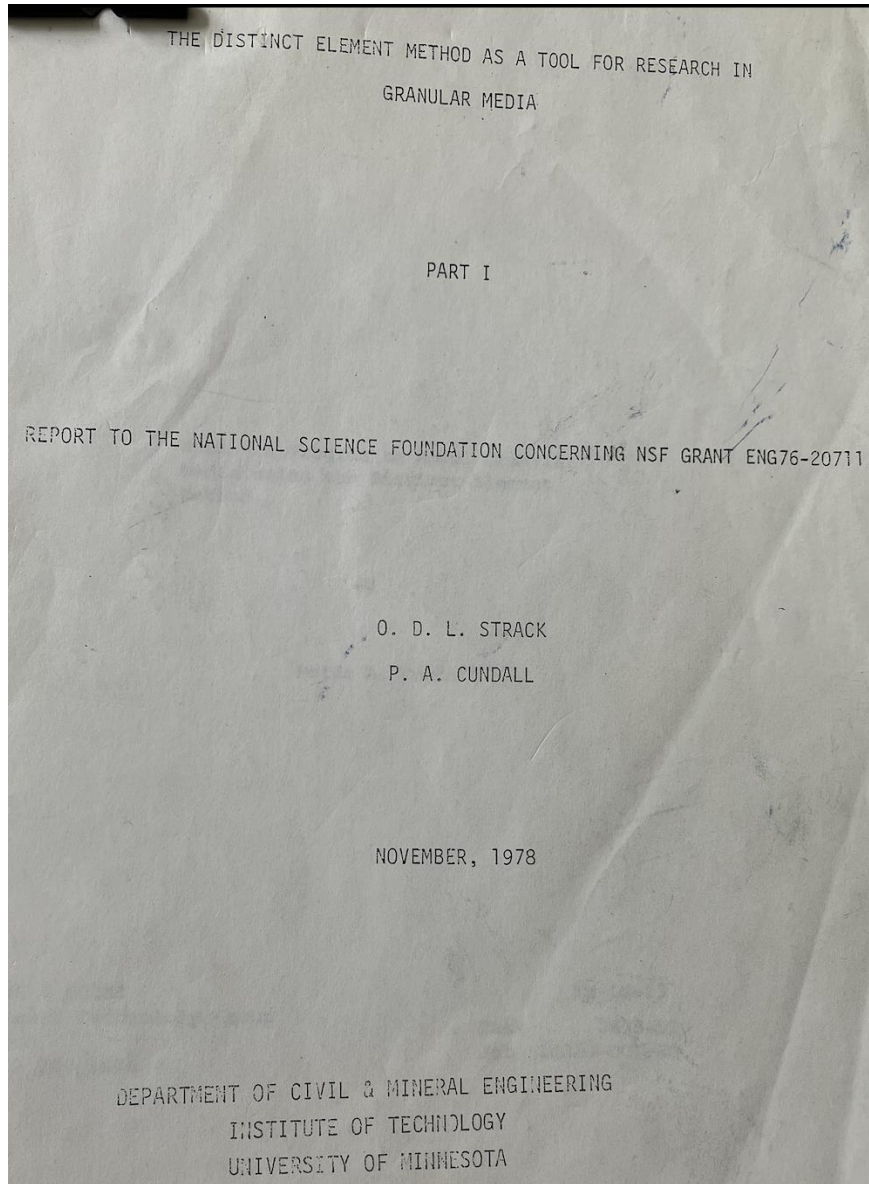
P. Cundall (1971), A Computer Model for Simulating Progressive Large Scale Movements in Blocky Rock Systems, *Proc. Symp. Rock Fracture (ISRM)*, Nancy, paper 11-8.

Cundall's path to Trubal

P. A. Cundall (1974), *Rational design of tunnel supports: A computer model for rock mass behavior using interactive graphics for the input and output of geometrical data*, U.S. Army Corps of Engineers Technical Report MRD-2-74.

- Used a small NOVA mini-computer (16 bit)
- Wrote in assembly language
- Considered motion of a system of polygonal blocks
- The force between two contacting polygons was chosen to be proportional to the depth of penetration of the corner of one polygon into the side of another.
- Linked data structures were used for efficient use of memory.
- Small calculation cells were used to narrow the limits of searches for corners near a given polygon side.

Cundall and Strack 1978- 1979



The distinct element method as a tool for research in granular media

Part I

Report to the National Science Foundation Concerning NSR Grant ENG76-20711

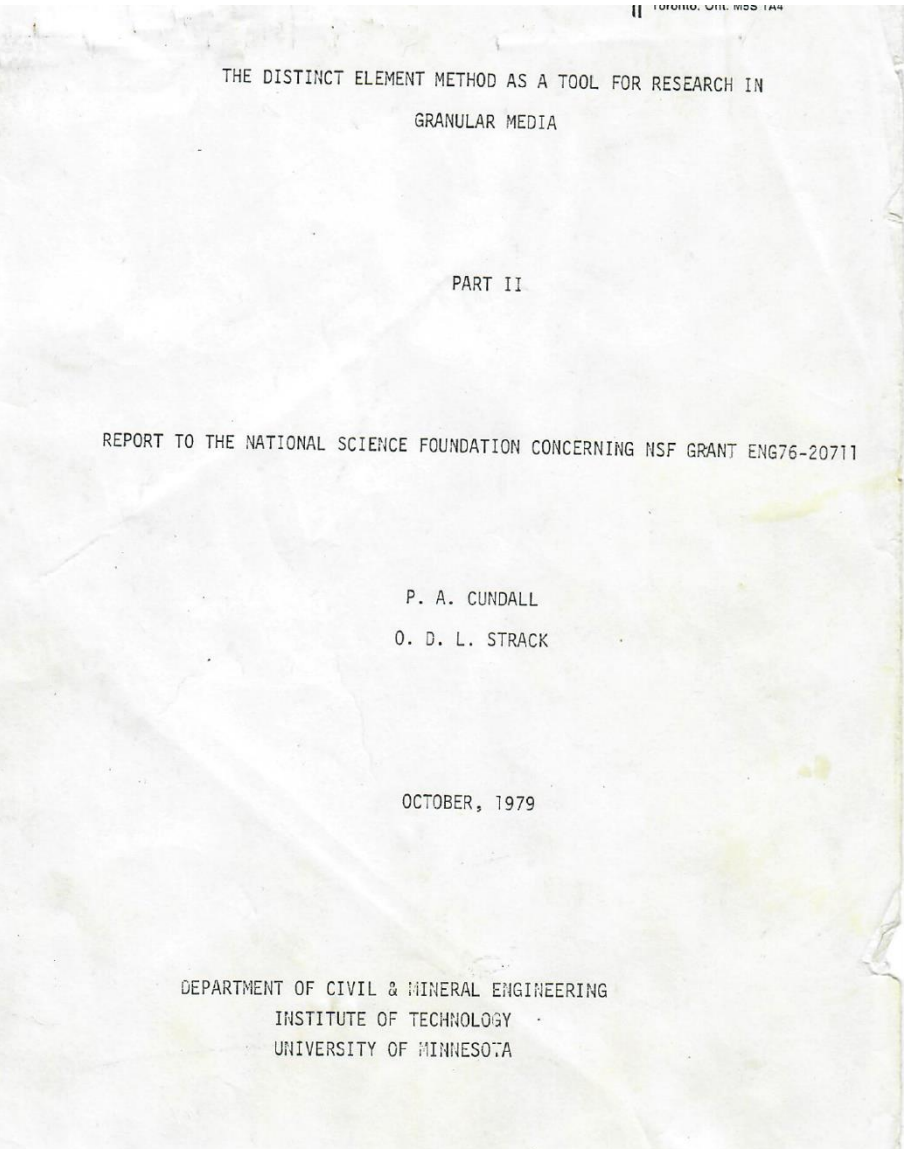
ODL Strack

PA Cundall

November 1978

Department of Civil and Mineral Engineering
Institute of Technology
University of Minnesota

Cundall and Strack 1978- 1979



The distinct element method as a tool for research in granular media

Part II

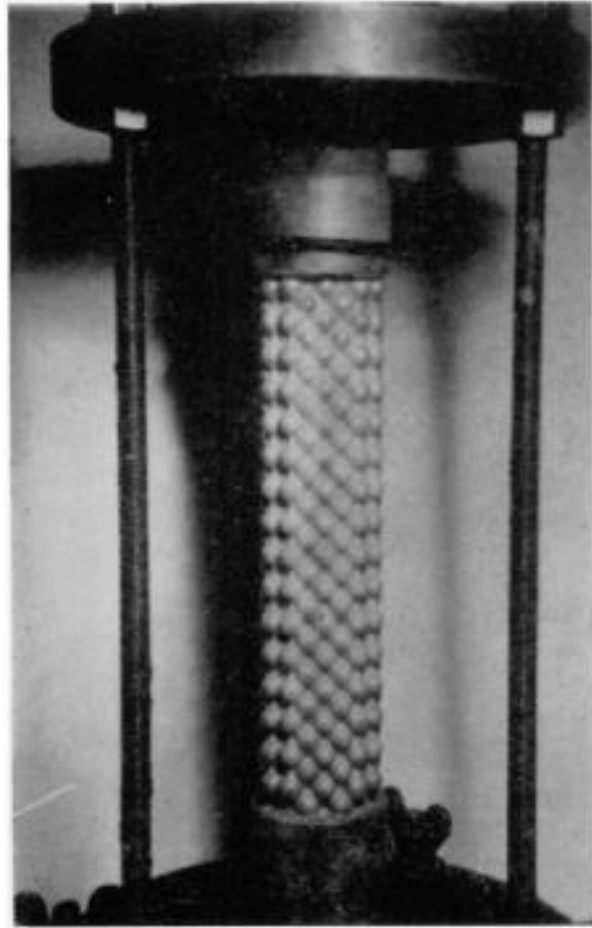
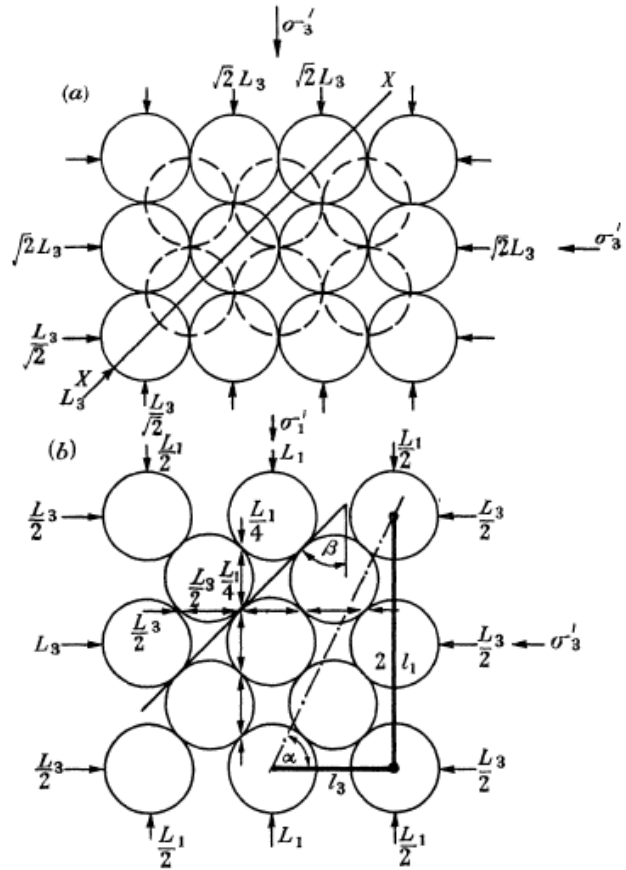
Report to the National Science Foundation Concerning NSR Grant ENG76-20711

PA Cundall
ODL Strack

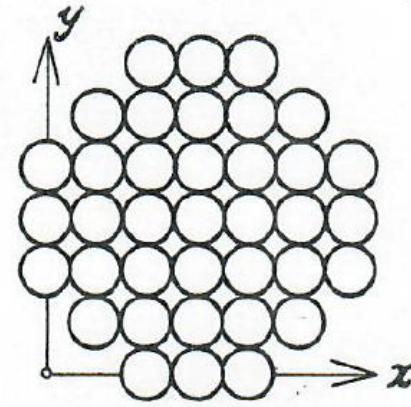
October 1979

Department of Civil and Mineral Engineering
Institute of Technology
University of Minnesota

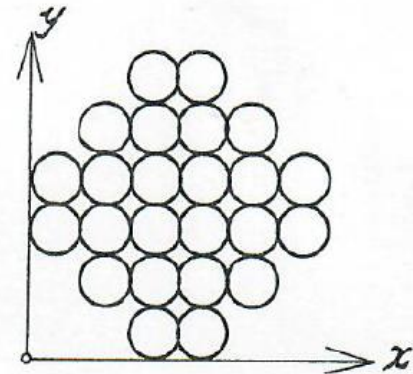
Cundall & Strack NSF Report 1979 – page 165



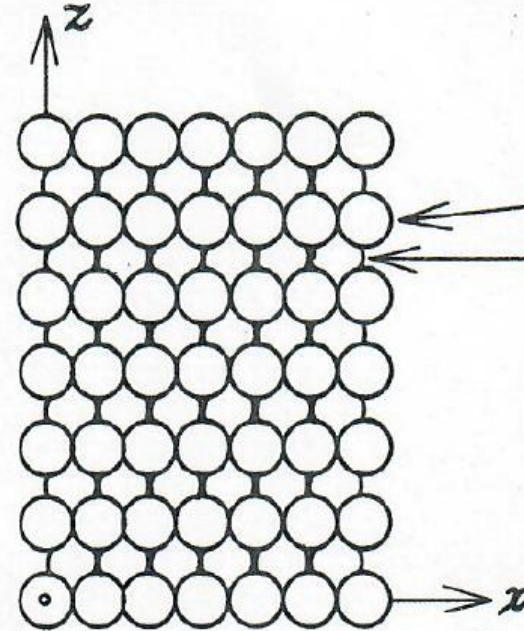
Rowe (1962) *Proc. Royal Soc.*



large layer



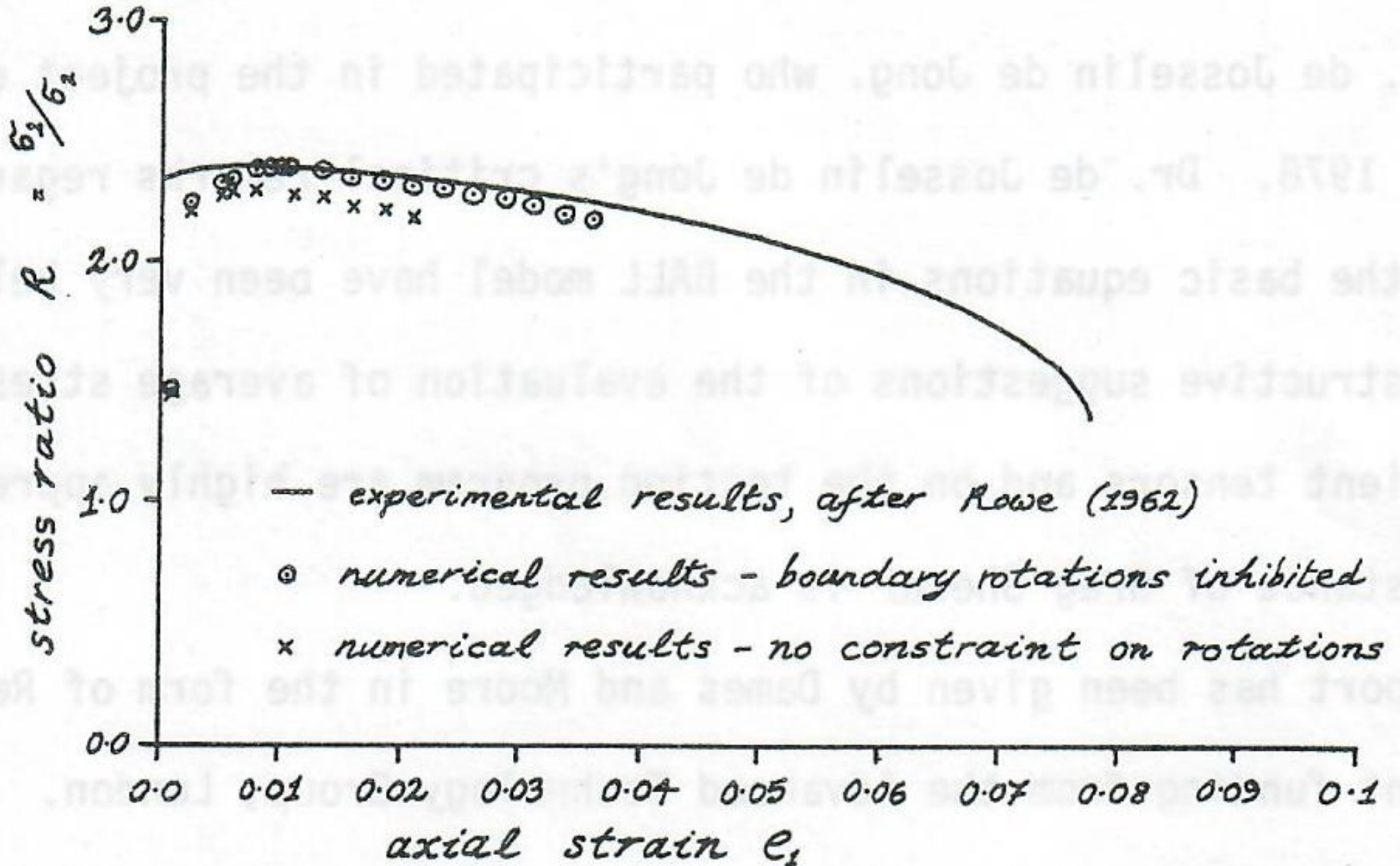
small layer



large layer

small layer

Cundall & Strack NSF Report 1979 – page 173



Cundall and Strack 1978- 1979

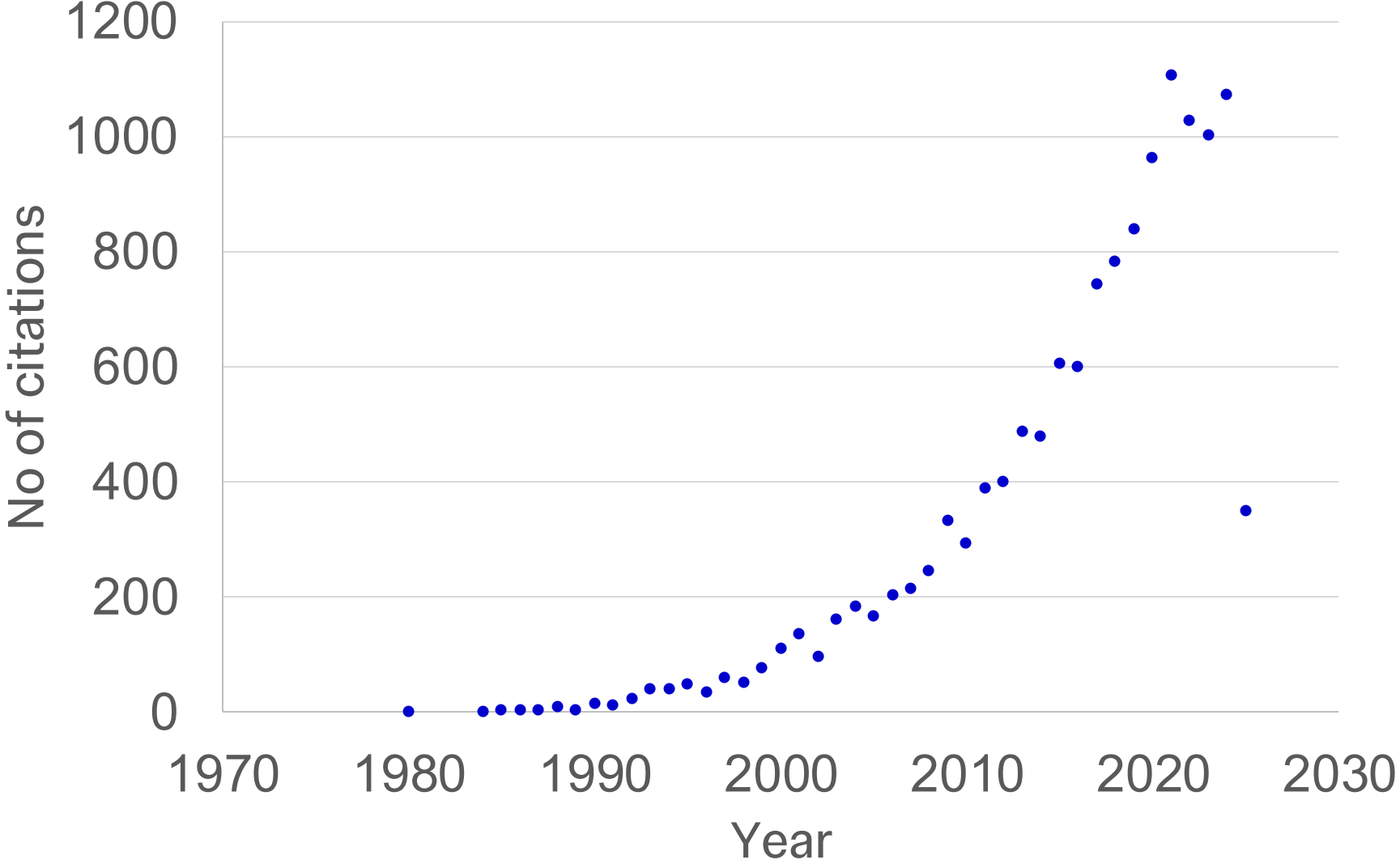
CUNDALL, P. A. & STRACK, O. D. L. (1979). *Géotechnique* **29**, No. 1, 47–65

A discrete numerical model for granular assemblies

P. A. CUNDALL* and O. D. L. STRACK†

Cundall and Strack 1978-1979

9th May 2025 - 13,413 citations



- Cundall, P. A. (1971). A computer model for simulating progressive, large-scale movements in blocky rock systems. *Proc. Symp. Int. Soc. Rock Mech., Nancy 2*, No. 8.
- Cundall, P. A. (1974). *A computer model for rock-mass behavior using interactive graphics for the input and output of geometrical data*. Report MRD-2-74 prepared at the University of Minnesota under Contract number DACW 45-74-C-006, for the Missouri River Division, US Army Corps of Engineers, available from National Technical Information Service—report number AD/A-001 602.
- Cundall, P. A. (1978). *BALL—A program to model granular media using the distinct element method*. Technical Note, Advanced Technology Group, Dames & Moore, London.
- Dantu, P. (1957). Contribution à l'étude mécanique et géométrique des milieux pulvérulents. *Proc. 4th Int. Conf. Soil Mech. Fdn Engng, London 1*, pp. 144.
- De Josselin de Jong, G. & Verruijt, A. (1969). Etude photo-élastique d'un empilement de disques. *Cah. Grpe fr. Etud. Rhéol. 2*, 73-86.
- Deresiewicz, H. (1958). Mechanics of granular material. *Advd. appl. Mech. 5*, 233-306.
- Drescher, A. & De Josselin de Jong, G. (1972). Photoelastic verification of a mechanical model for the flow of a granular material. *J. Mech. Phys. Solids 20*, 337-351.
- Mindlin, R. D. (1949). Compliance of elastic bodies in contact. *J. appl. Mech. 71*, No. 3, 259-268.
- Mindlin, R. D. & Deresiewicz, H. (1953). Elastic spheres in contact under varying oblique forces. *J. Appl. Mech. 20*, 327-344.
- Nayak, P. R. (1972). Surface roughness effects in rolling contact. *Trans. Am. Soc. mech. Engrs Series E, J. Appl. Mech. 39*, No. 2, 456-460.
- Rodriguez-Ortiz, J. M. (1974). Estudio del comportamiento de medios granulares heterogéneos mediante modelos discontinuos analógicos y matemáticos. PhD thesis, Universidad Politécnica de Madrid.
- Serrano, A. A. & Rodriguez-Ortiz, J. M. (1973). A contribution to the mechanics of heterogeneous granular media. *Proc. Symp. Plasticity and Soil Mech., Cambridge*.
- Strack, O. D. L. & Cundall, P. A. (1978). *The distinct element method as a tool for research in granular media*. Report to National Science Foundation from Department of Civil and Mineral Engineering, University of Minnesota, USA.
- Wakabayashi, T. (1957). Photoelastic method for determination of stress in powdered mass. *Proc. 7th Jap. Nat. Congr. Appl. Mech.* 153-192.

Initial DEM codes – Ng and Dobry 1994

“Researchers have

- either used the codes made available by Cundall [BALL (Cundall and Strack 1979) and TRUBAL (Strack and Cundall 1984)],
- have modified these programs to fit their needs [Thornton (1988), CONBAL (Ng 1989), and DISC (Ting et al.1989)],
- or have developed their own codes [DIBS (Walton 1982; Kuhn 1989), and GLUE (Bathurst and Rothenburg 1989)].”

Linking DEM and MD – Walton(1980) thesis



LAWRENCE LIVERMORE LABORATORY

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UCRL 52915

Particle-Dynamics Modeling

of

Geological Materials

Otis R. Walton

March 25, 1980

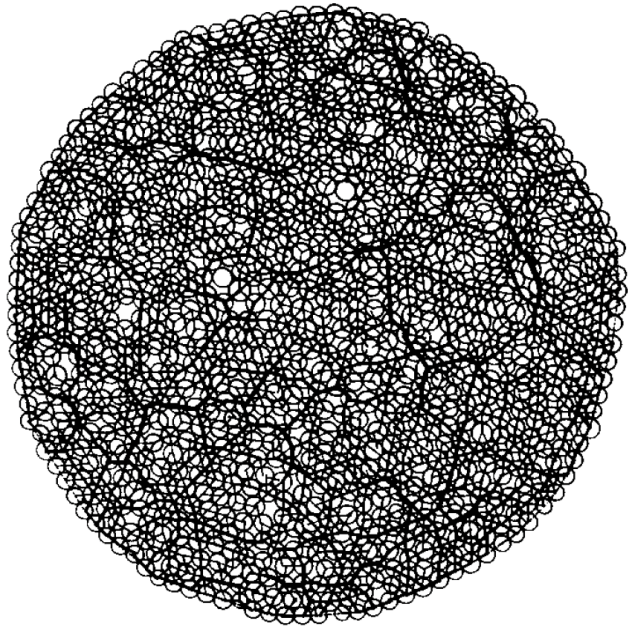
Explicit reference to key MD contributions including Wainwright and Alder 1958

Explicit reference to the potential of using quaternions to look at asymmetric particles.

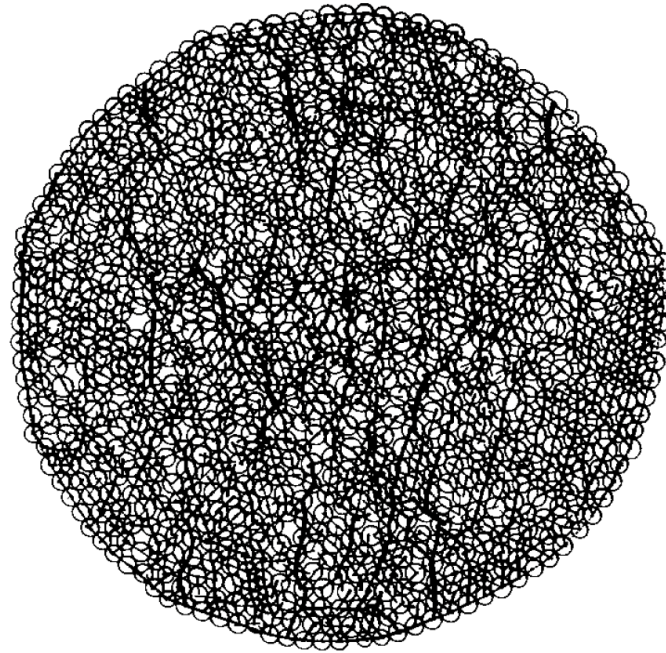
Stress – force - fabric

Rothenburg, L. & Bathurst, R. J. (1989). *Géotechnique* **39**, No. 4, 601–614

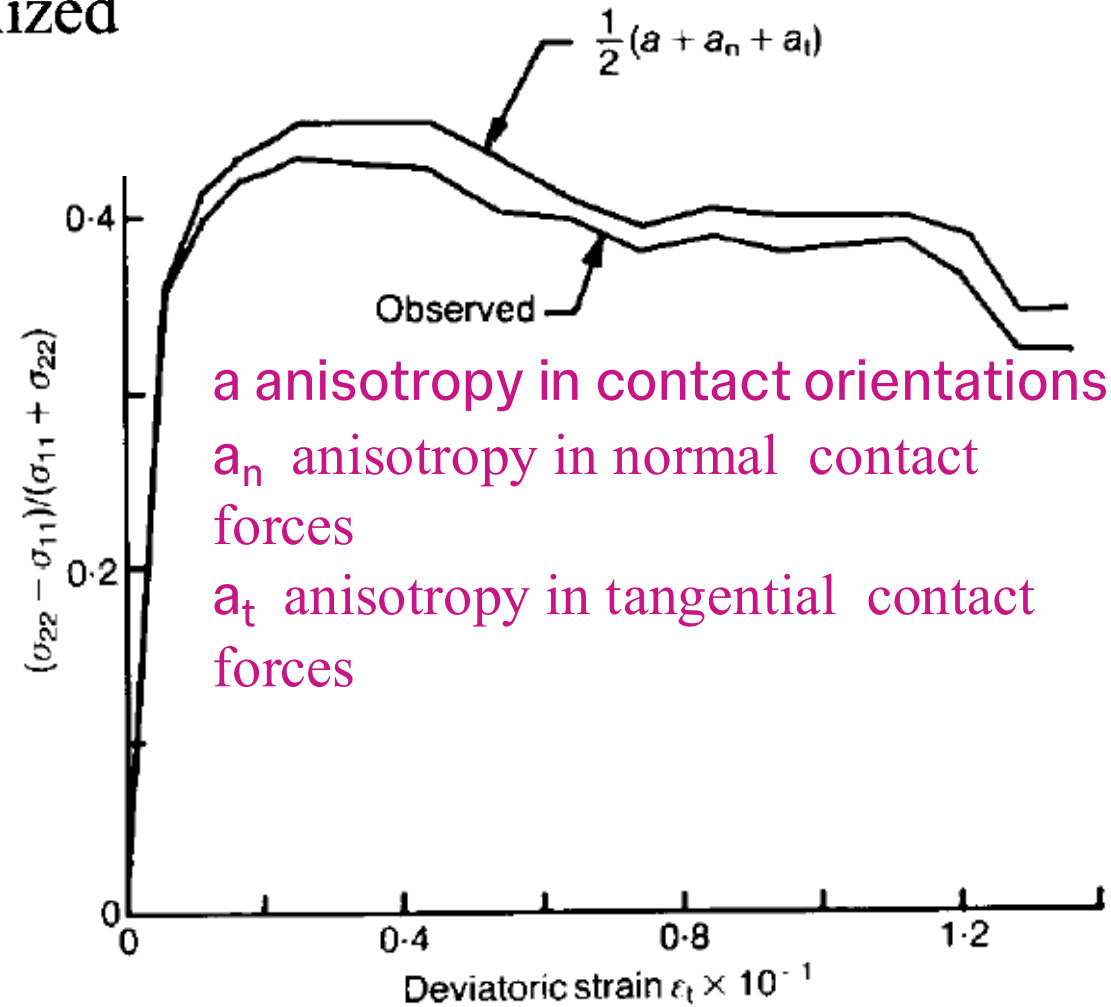
Analytical study of induced anisotropy in idealized granular materials



Isotropic



Peak stress

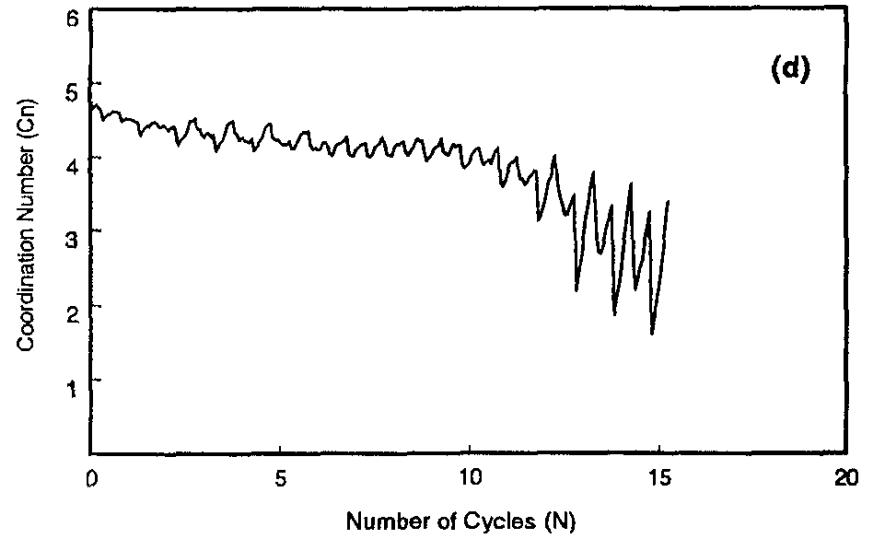
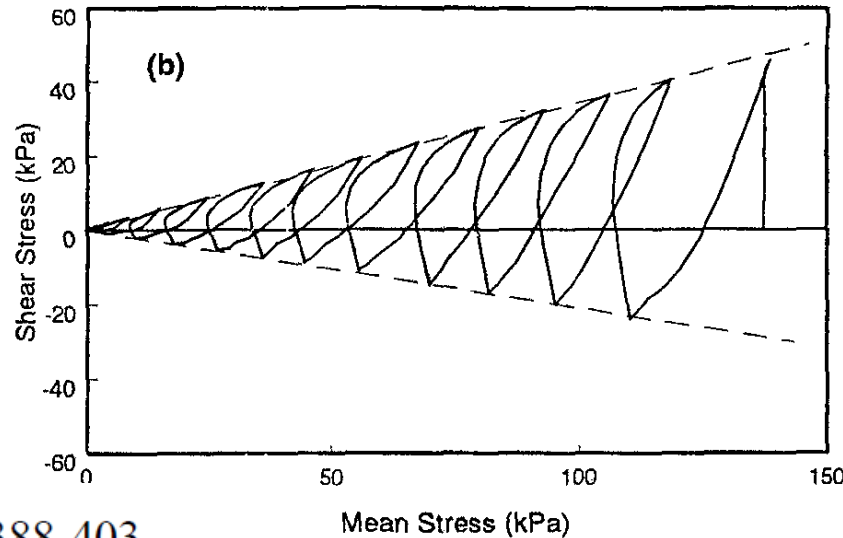
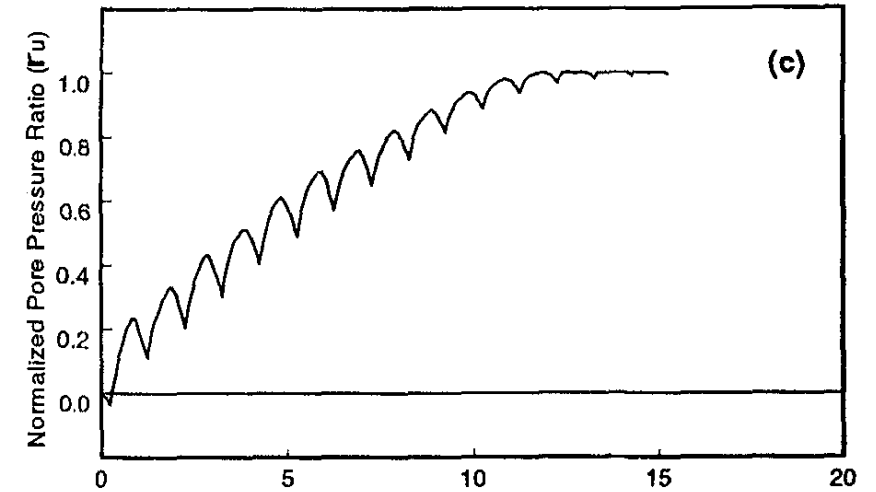
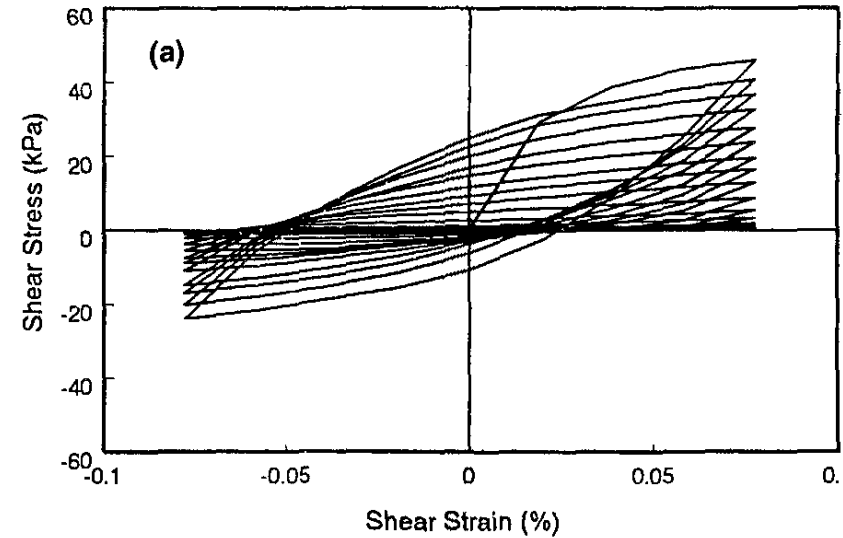


Liquefaction

NUMERICAL SIMULATIONS OF MONOTONIC AND CYCLIC LOADING OF GRANULAR SOIL

By Tang-Tat Ng,¹ Associate Member, ASCE, and
Ricardo Dobry,² Member, ASCE

3D specimen



Coupling – Coarse Grained

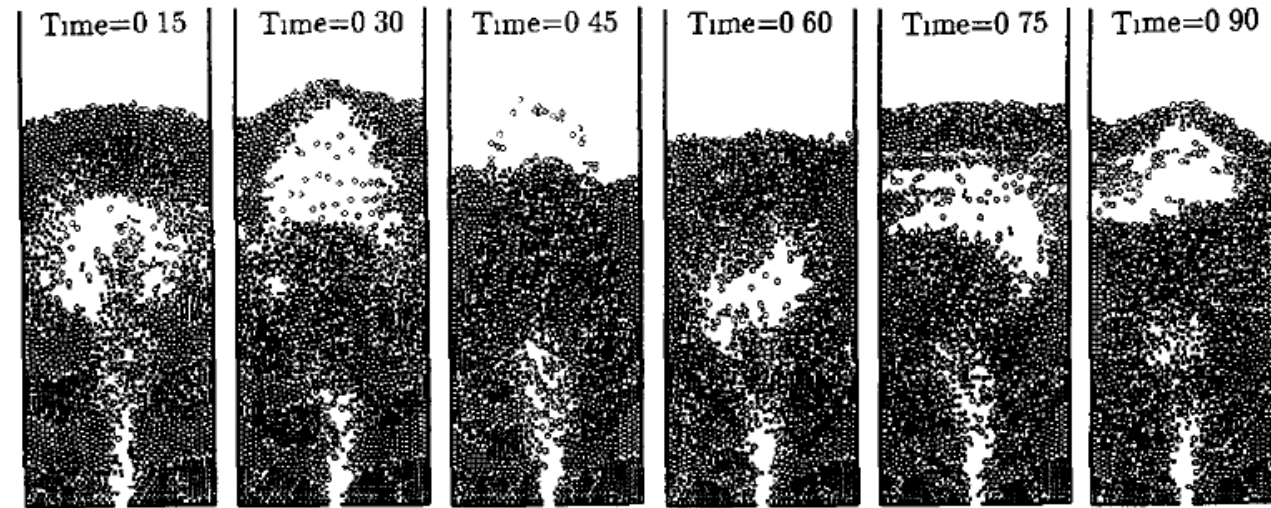
Powder Technology 1993

Discrete particle simulation of two-dimensional fluidized bed

Y. Tsuji, T. Kawaguchi and T. Tanaka

Department of Mechanical Engineering, Osaka University, Suita, Osaka 565 (Japan)

(Received December 1, 1992; in revised form April 19, 1993)



Chem. Eng. Science 1997

Numerical simulation of the gas–solid flow in a fluidized bed by combining discrete particle method with computational fluid dynamics

B. H. Xu and A. B. Yu

School of Materials Science and Engineering, The University of New South Wales, Sydney 2052, Australia

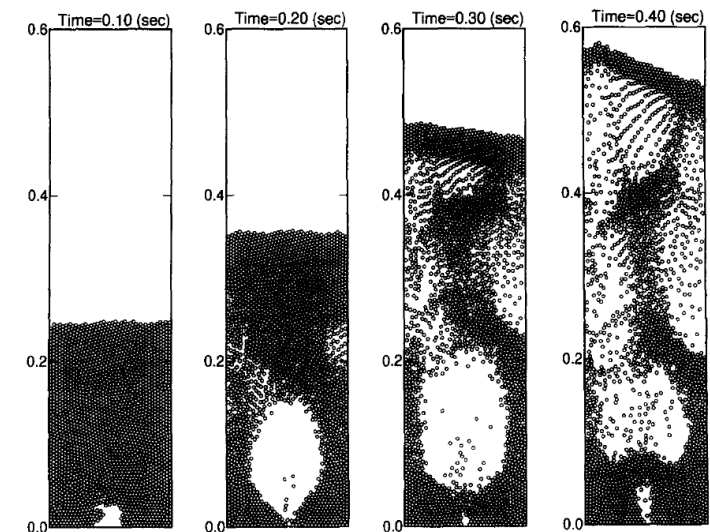
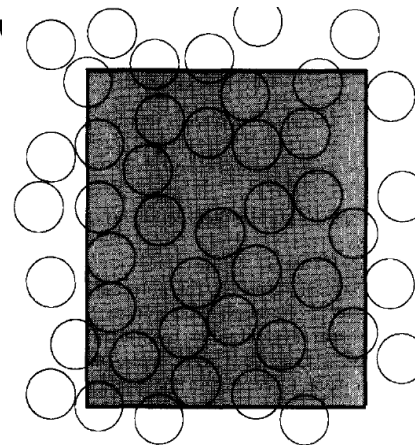
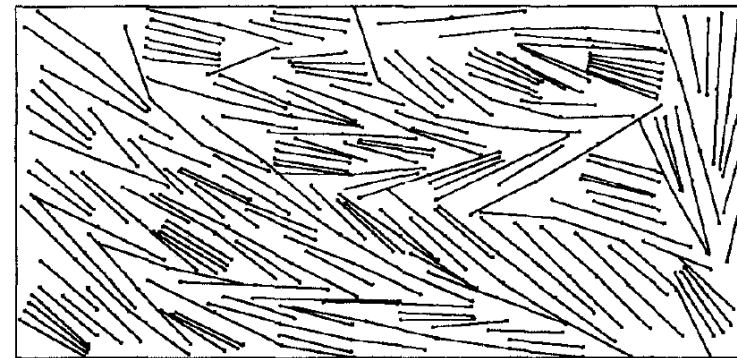
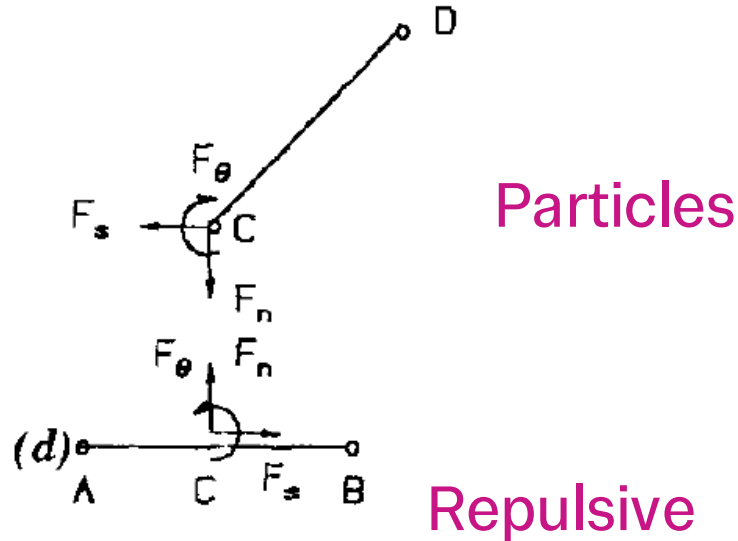


Fig. 3. Schematic illustration of the particles in a computational cell (shaded area).

Clay

DISCRETE-ELEMENT METHOD FOR SIMULATING BEHAVIOR OF COHESIVE SOIL

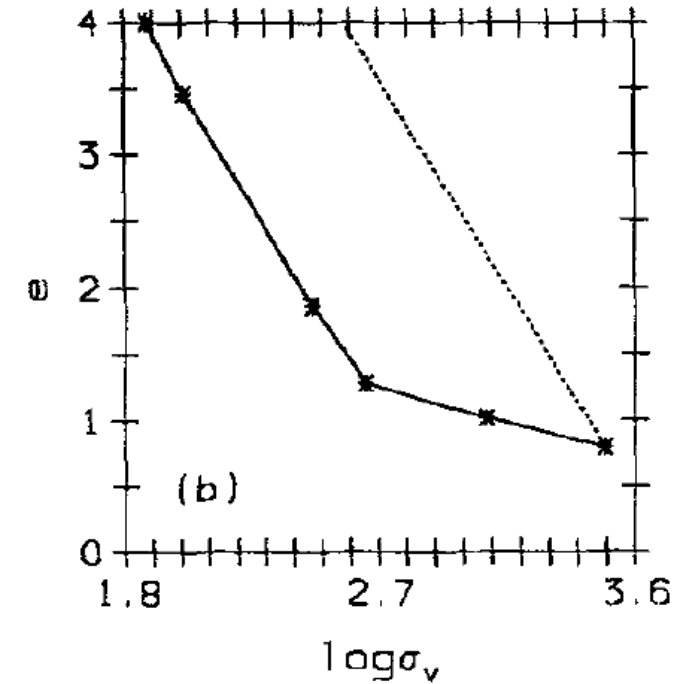
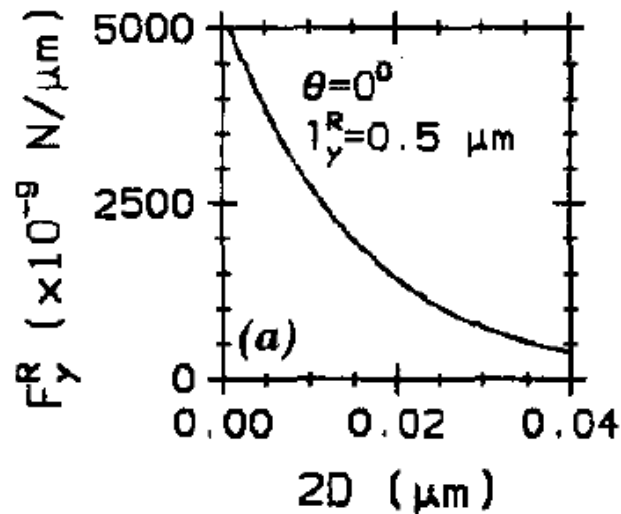
By A. Anandarajah¹



$e=1.868$



$e=0.800$



J. Geotech. Engrg., 1994, 120(9): 1593-1613

Review Article

Modeling granular media on the computer

H. J. Herrmann and S. Luding

Institute for Computer Applications 1, Pfaffenwaldring 27, D-70569 Stuttgart, Germany

Received December 19, 1997

- Recognize that modelling has been carried out for 2 decades
- Classify models as hard sphere (Event Driven) or soft sphere (MD) (describe both algorithms)
- Also refer to stochastic approaches and lattice models

21st Century

A discontinuous future for numerical modelling in geomechanics?

Proceedings of the Institution of
Civil Engineers
Geotechnical Engineering 149
January 2001 Issue 1
Pages 41–47

Paper 12211

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Accepted 25/05/2000

Keywords:

design methods & aids/mathemati-
cal modelling/stress analysis



Peter A. Cundall

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Cundall's list of phenomena captured

- (a) Continuously non-linear stress-strain response, with ultimate failure, followed by softening or hardening.
- (b) Behaviour that changes in character, according to stress state-for example, the crack patterns in rock are quite different in the tensile, unconfined and confined regimes.
- (c) Memory of previous stress or strain excursions, commonly expressed in terms of yield surfaces-the memory may be modified or erased (e.g. kinematic or isotropic hardening).
- (d) Spontaneous localisation-for example, shear bands and crack patterns.
- (e) Dilatancy that depends on history, mean stress and initial state.
- (f) Hysteresis at all levels of cyclic loading/unloading; cyclic energy dissipation is strongly dependent on cyclic load amplitude.
- (g) Transition from brittle behaviour at low mean stress to ductile behaviour at high mean stress.
- (h) A non-linear envelope of strength as a function of mean stress and of relative magnitude of principal stresses.
- (i) Non-linear dependence of 'elastic' stiffness on confining stress and its history.
- (j) Induced anisotropy of stiffness and strength, strongly influenced by stress or strain path.
- (k) Spontaneous emission of acoustic energy.

21st Century

Chemical Engineering Science 62 (2007) 3378–3396

Discrete particle simulation of particulate systems: Theoretical developments

H.P. Zhu, Z.Y. Zhou, R.Y. Yang, A.B. Yu*

Chemical Engineering Science 63 (2008) 5728–5770

Discrete particle simulation of particulate systems: A review of major applications and findings

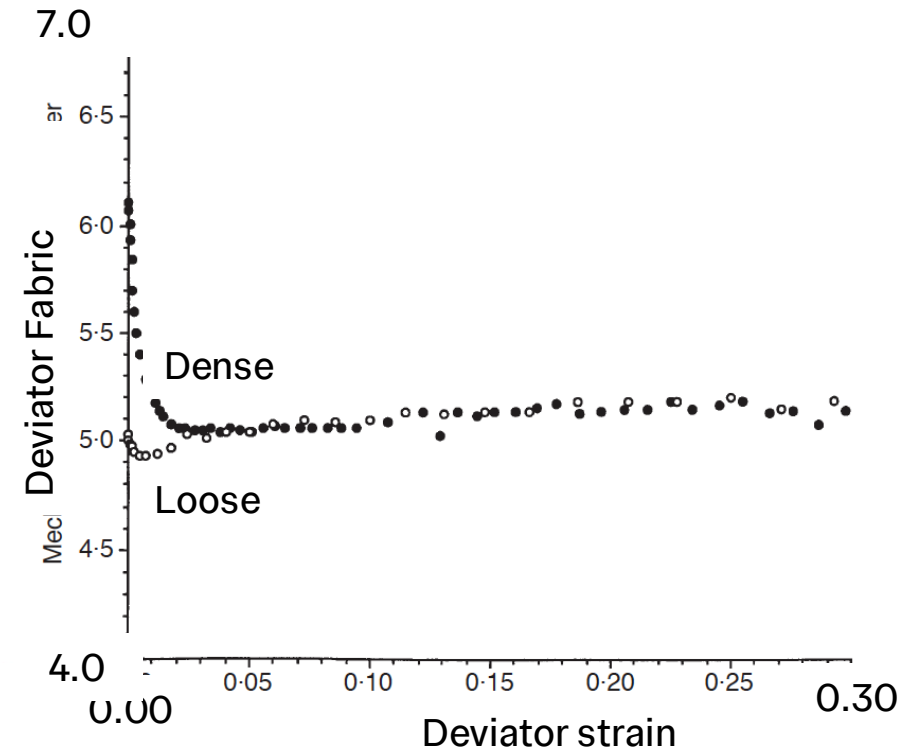
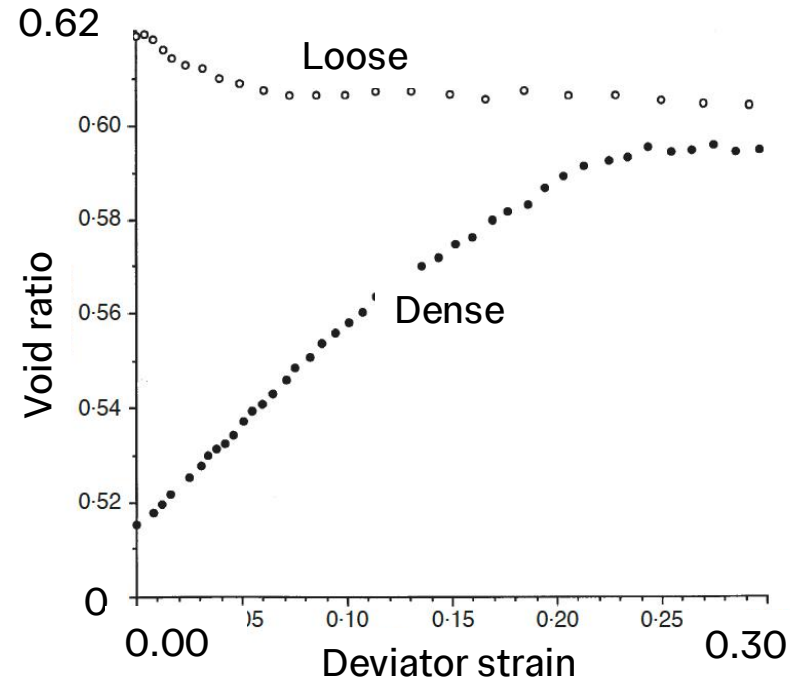
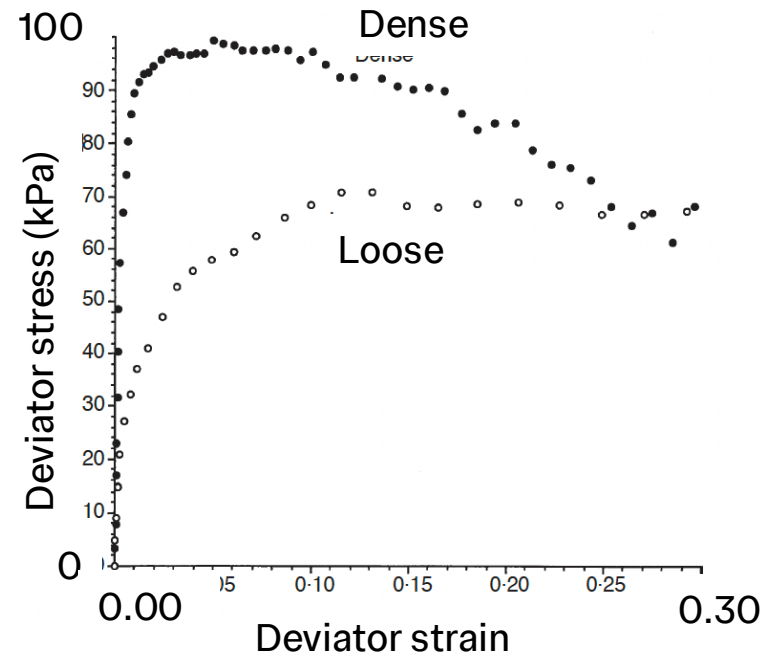
H.P. Zhu, Z.Y. Zhou, R.Y. Yang, A.B. Yu*

Thornton (2000)

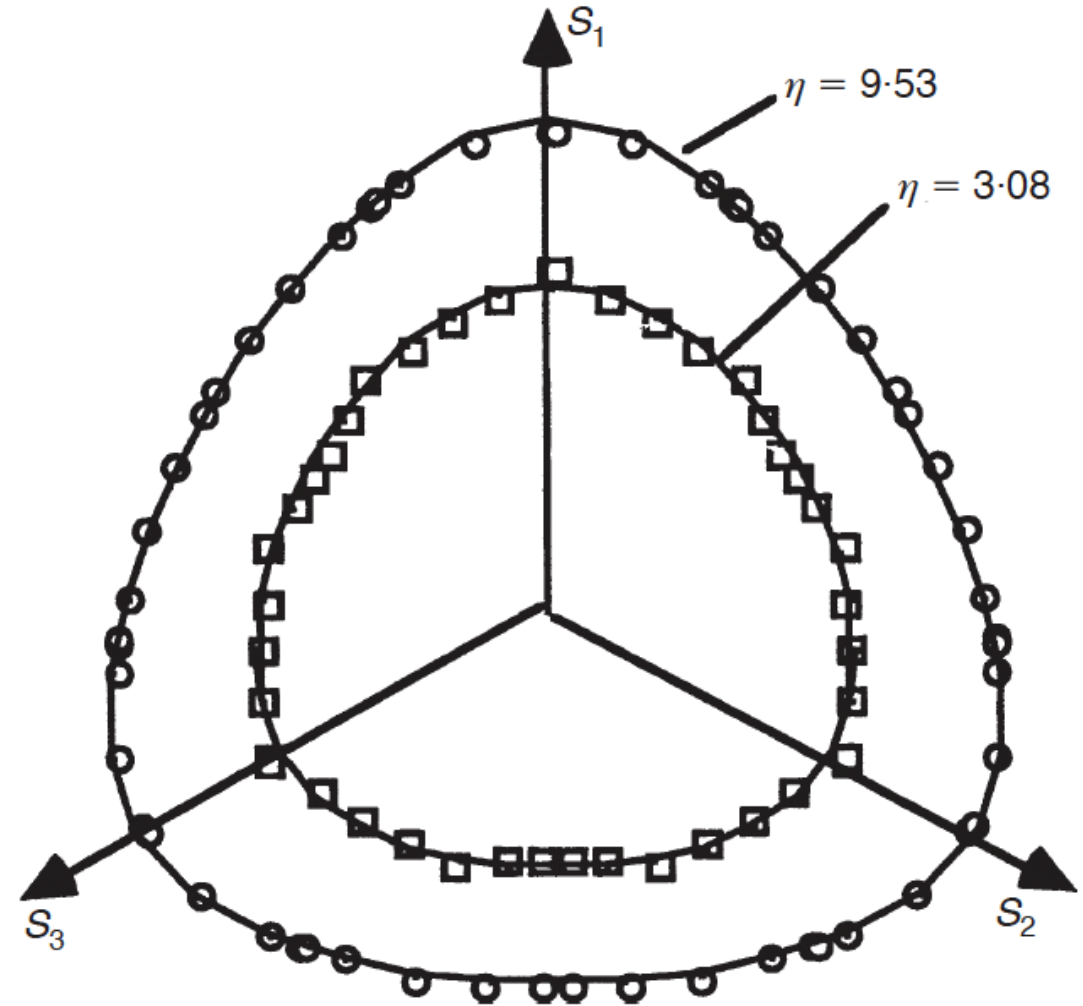
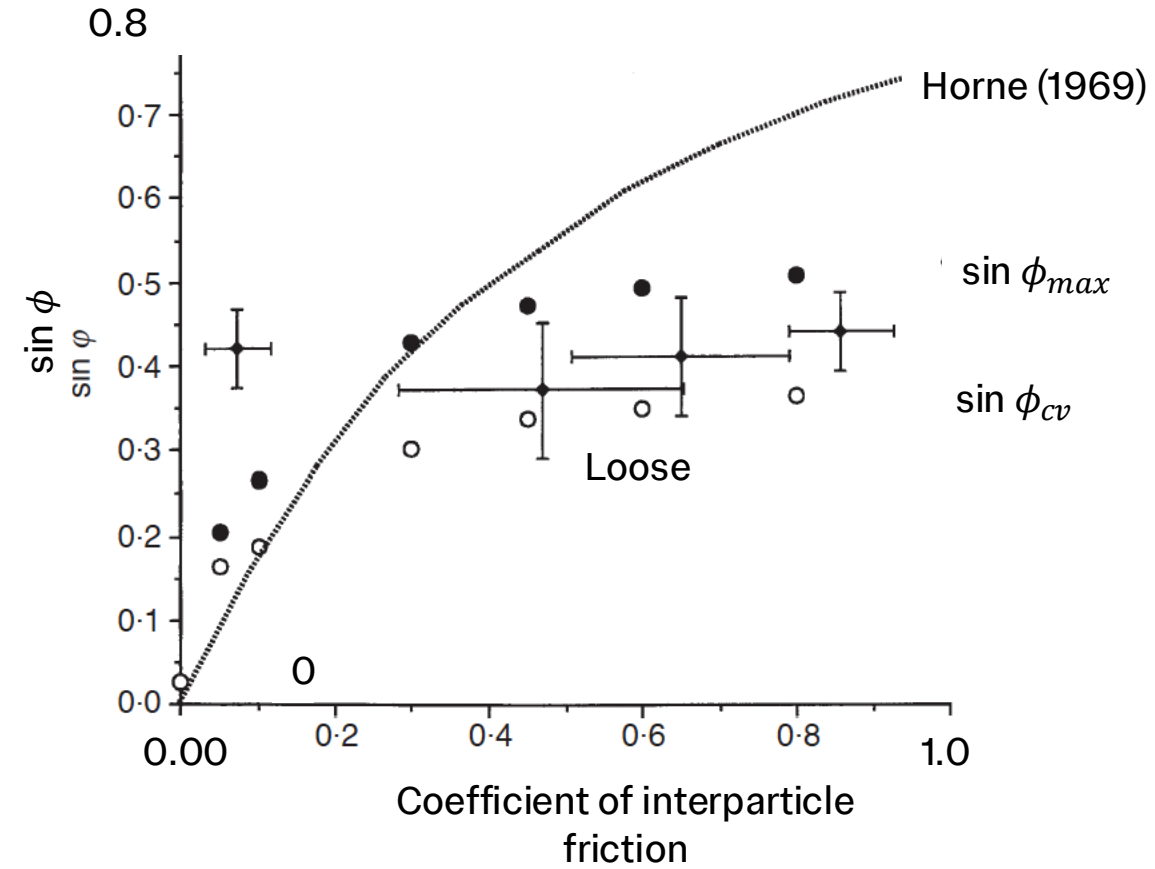
Thornton, C. (2000). *Géotechnique* 50, No. 1, 43–53

Numerical simulations of deviatoric shear deformation of granular media

C. THORNTON



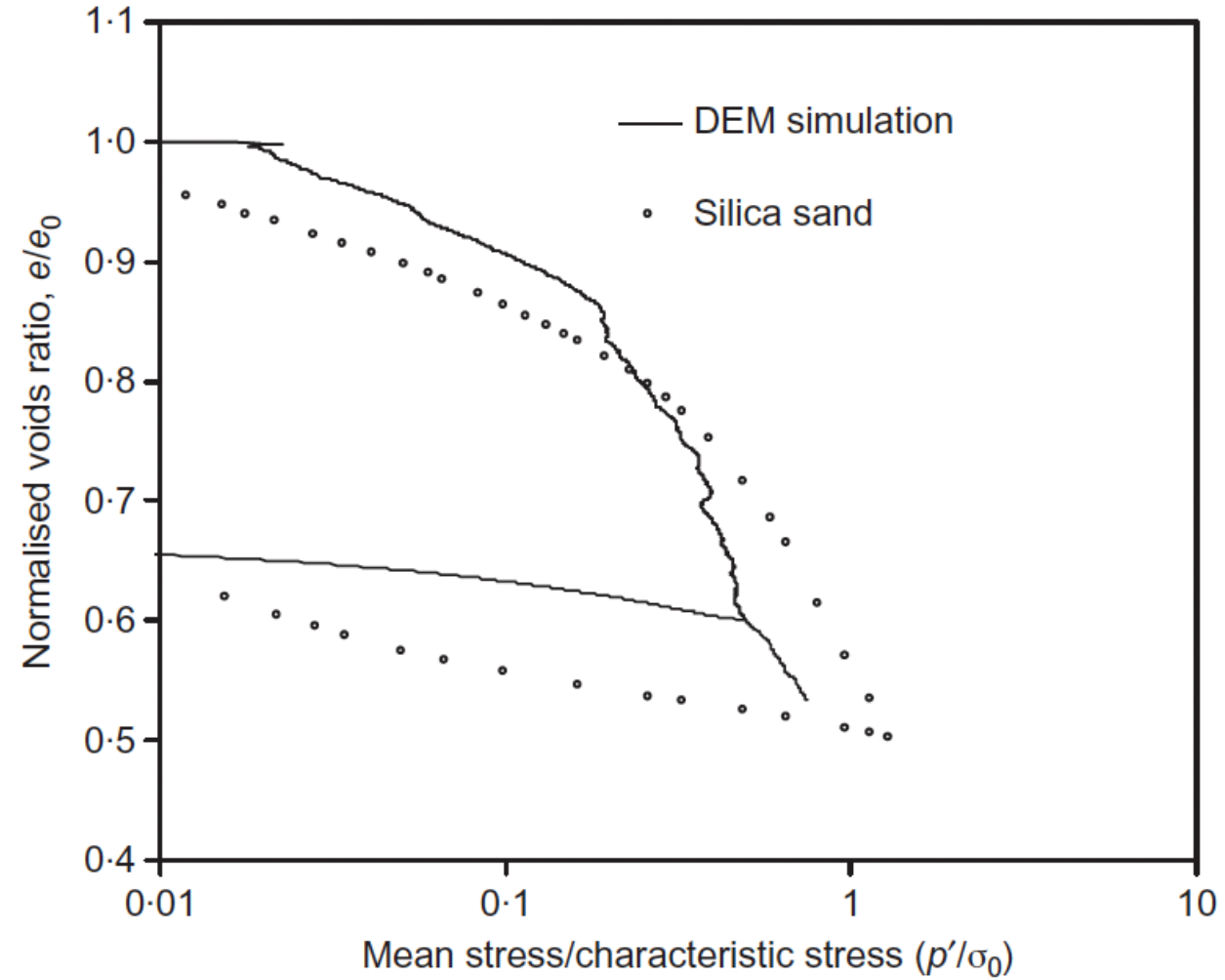
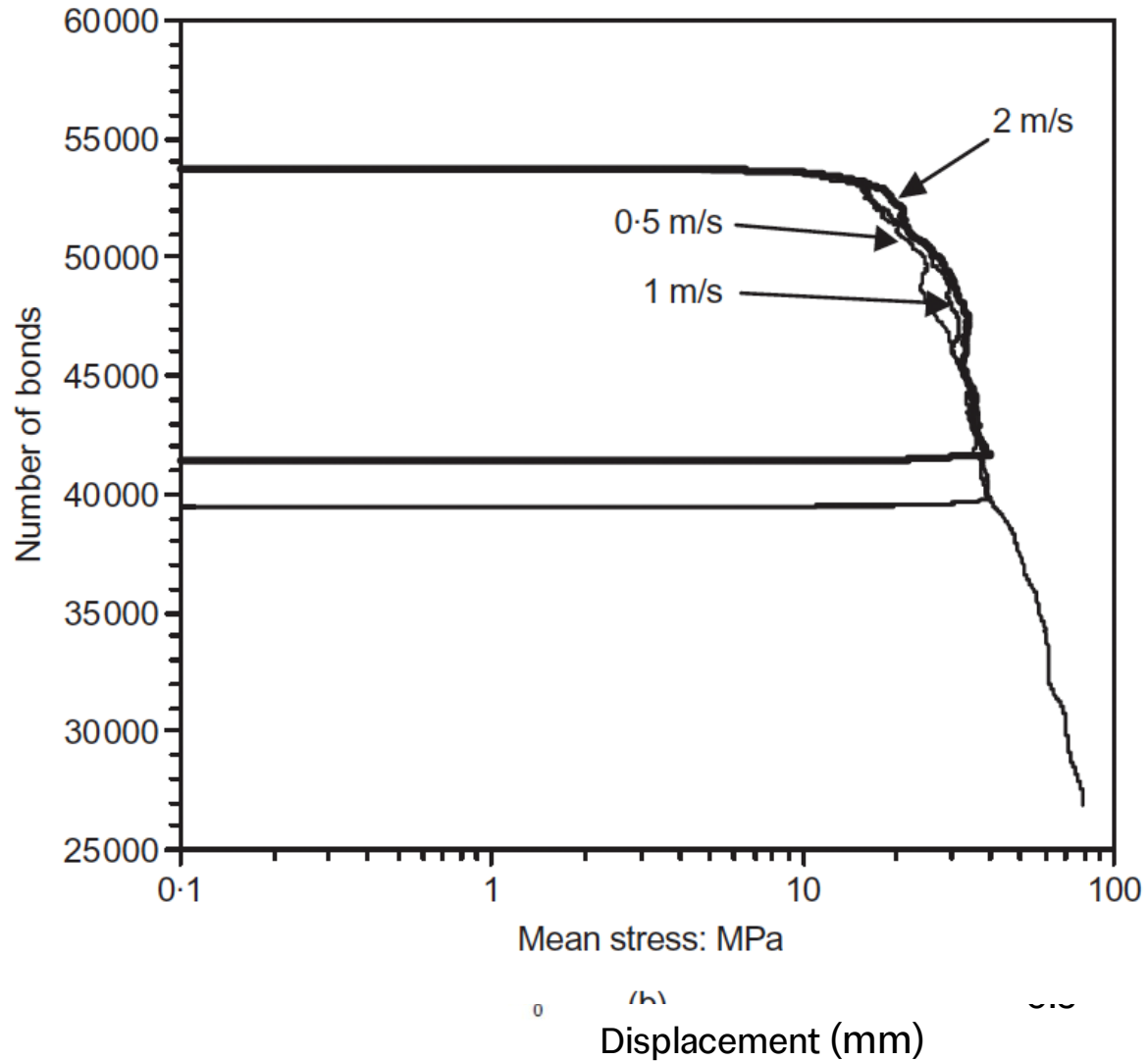
Thornton (2000)



Radial deviatoric loading + Lade's failure states

Particle crushing

(a)

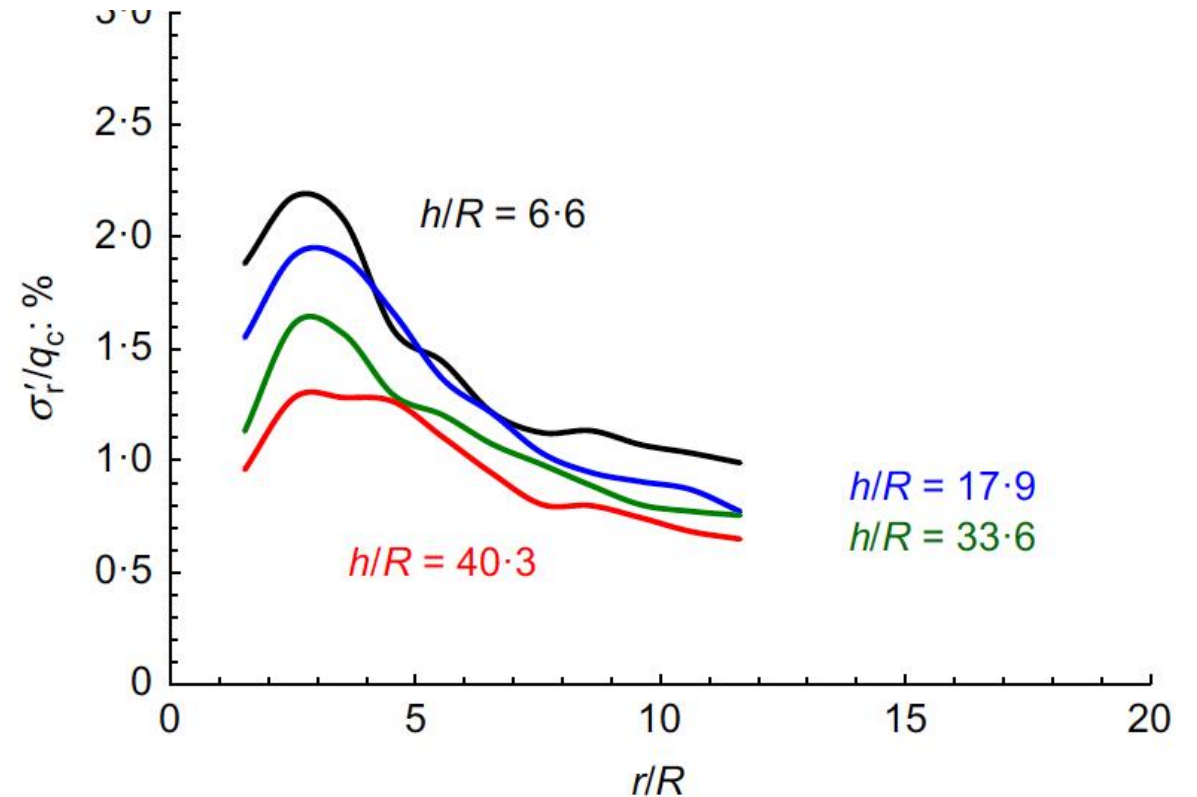


Post 2020: DEM becomes mainstream?

Jardine (2020) 56th Rankine lecture

Effective stresses predicted by DEM modelling with crushable grain model for sand mass of calibration chamber during mini-ICP installation, normalised by q_c values and plotted against radius r/R : (a) radial stresses

Simulations by Matteo Ciantia



Hight De Mello Lecture - 2024

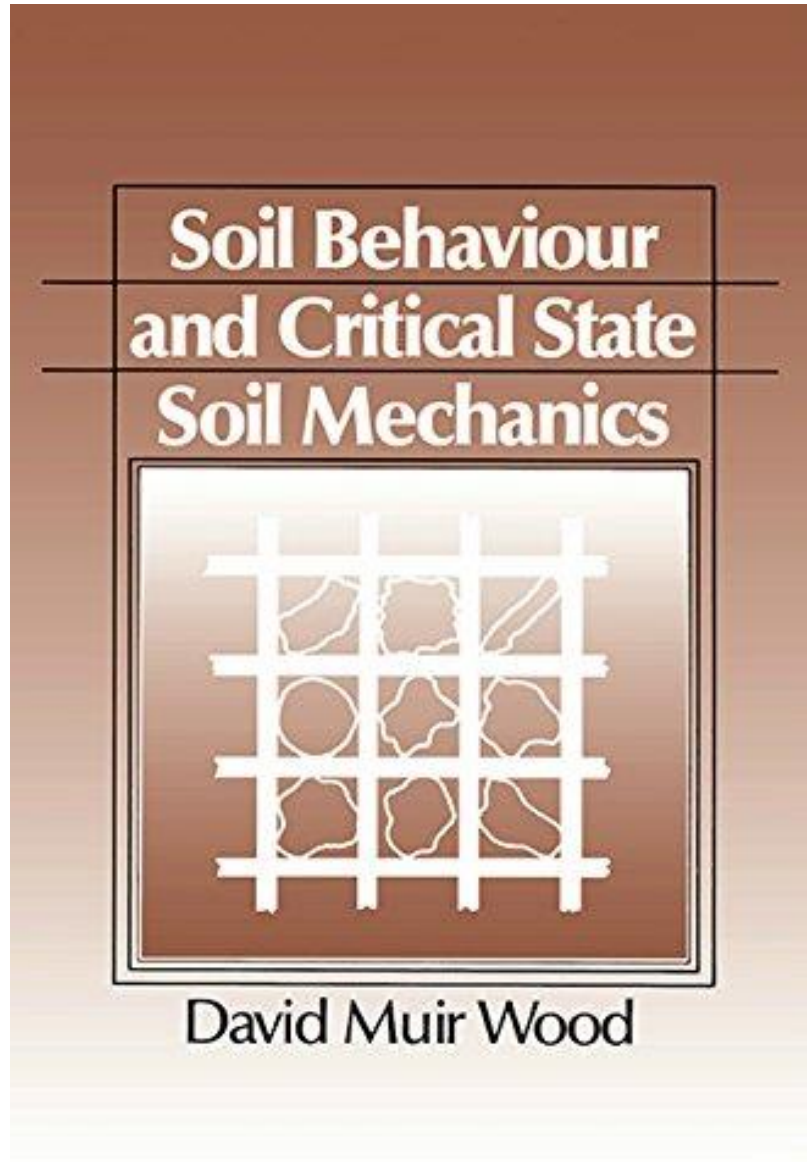
uses insights from Discrete Element Modelling and Microcomputed Tomography to speculate on reasons for the difference in behaviour observed between moist tamped and sedimented sands at the same global void ratio and stress state.

Perspectives

Rapaport (2004): “Understanding is achieved once a plausible model is able to reproduce and predict experimental observation”.....”there is no inherent value to an excessively complex model if there is no way of establishing that all its features are essential for the desired results” “the practical consequence of this is that features should be added gradually”

From The Art of Molecular Dynamics

Muir Wood (1990)



1

Introduction: models and soil mechanics

1.1 Use of models in engineering

Scientific understanding proceeds by way of constructing and analysing models of the segments or aspects of reality under study. The purpose of these models is not to give a mirror image of reality, not to include all its elements in their exact sizes and proportions, but rather to single out and make available for intensive investigation those elements which are decisive. We abstract from non-essentials, we blot out the unimportant to get an unobstructed view of the important, we magnify in order to improve the range and accuracy of our observation. A model is, and must be, unrealistic in the sense in which the word is most commonly used. Nevertheless, and in a sense, paradoxically, if it is a good model it provides the key to understanding reality. (Baran and Sweezy, 1968)

Engineering is concerned with understanding, analysing, and predicting the way in which real devices, structures, and pieces of equipment will behave in use. It is rarely possible to perform an analysis in which full knowledge of the object being analysed permits a complete and accurate description of the object to be incorporated in the analysis. This is particularly true for geotechnical engineering. The soil conditions under a foundation or embankment can be discovered only at discrete locations by retrieving samples of soil from boreholes or performing in situ tests; soil conditions between such discrete locations can be deduced only by informed interpolation. (This is a major difference between geotechnical engineering and structural or mechanical engineering, in which it is feasible to specify and control the properties of the steel, concrete, or other material from which a structural member or mechanical component is to be manufactured.)

Not only is it rarely possible to perform such an analysis, it is rarely desirable. Understanding of the behaviour of real objects is improved if intelligent simplifications of reality are made and analyses are performed

Key points in introduction (Muir Wood, 1990)

1

- Scientific understanding proceeds by way of constructing and analysing models of the segments or aspects of reality under study (*quote from Baran and Sweezy, 1968*)

Soil Mechanics

- It is rarely possible to perform an analysis in which full knowledge of the object being analysed permits a complete and accurate description of the object to be incorporated in the analysis (*DMW*)

a sense, paradoxically, if it is a good model it provides the key to understanding reality. (Baran and Sweezy, 1968)
Engineering is concerned with understanding, analysing, and predicting

- Understanding of the behaviour of real objects is improved if intelligent simplifications of reality are made and analyses are performed using simplified models of the real objects (*DMW*)

to specify and control the properties of the steel, concrete, or other material from which a structural member or mechanical component is to be

- ..conceptual models..focus attention on the important features of a problem and leave aside features which are irrelevant. The choice of model depends on the application (*DMW*)

~~Perspectives~~ Practical reality?

- As engineers – is understanding sufficient?
- Is predictive simulation to inform engineering design a form of understanding?