

Discrete element method simulations on national HPC facilities

15 April 2026

Dr Kevin Hanley

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- Quick overview of DEM
- DEM on HPC circa 2010
- Case study 1: triaxial tests of granular soils
- Case study 2: abrasion in particle systems
- Current drivers for adoption of HPC
- The move towards GPUs
- The CCC-ParaSolS project

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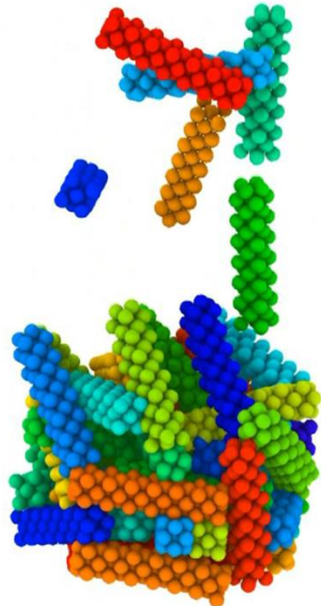
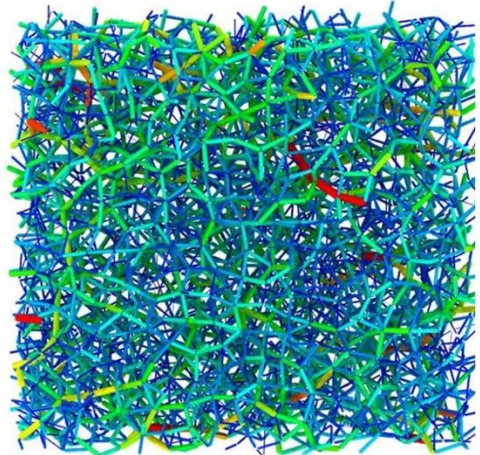
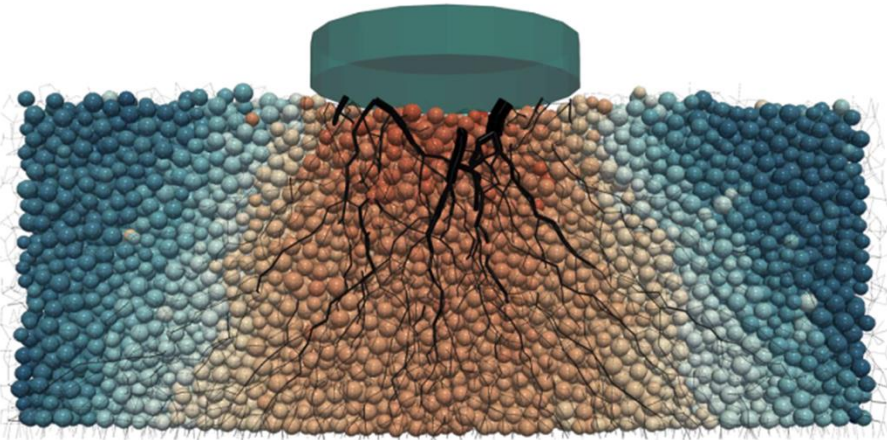
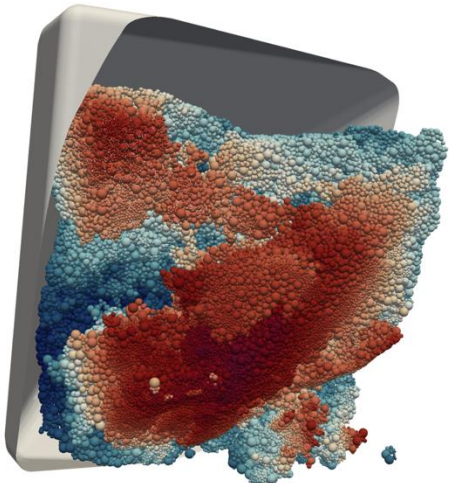
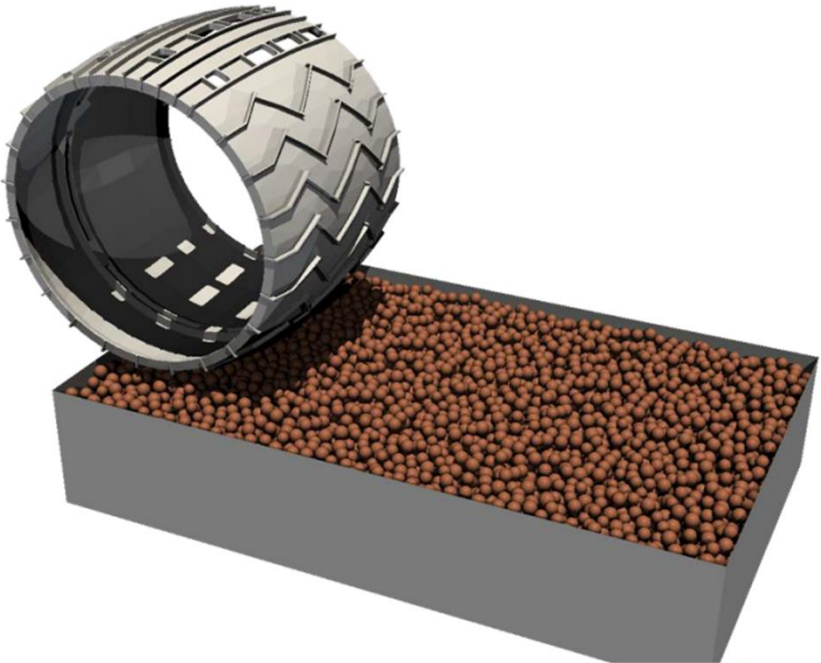
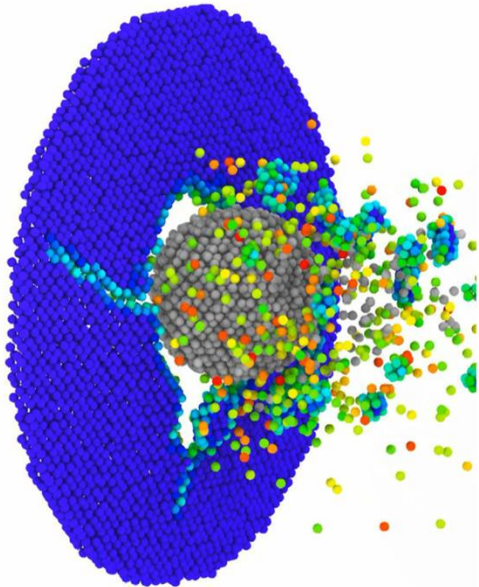
Use of the Discrete Element Method



- To simulate systems of particulate solids (granular materials)
- Particle sizes are typically larger than 1 micron



Example DEM simulations



- Defining 1979 paper →

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†

A discrete numerical model for granular assemblies

[PA Cundall](#), [ODL Strack](#)

geotechnique, 1979 · emerald.com

The distinct element method is a numerical model capable of describing the mechanical behaviour of assemblies of discs and spheres. The method is based on the use of an explicit numerical scheme in which the interaction of the particles is monitored contact by contact and the motion of the particles modelled particle by particle. The main features of the distinct element method are described. The method is validated by comparing force vector plots obtained from the computer program BALL with the corresponding plots

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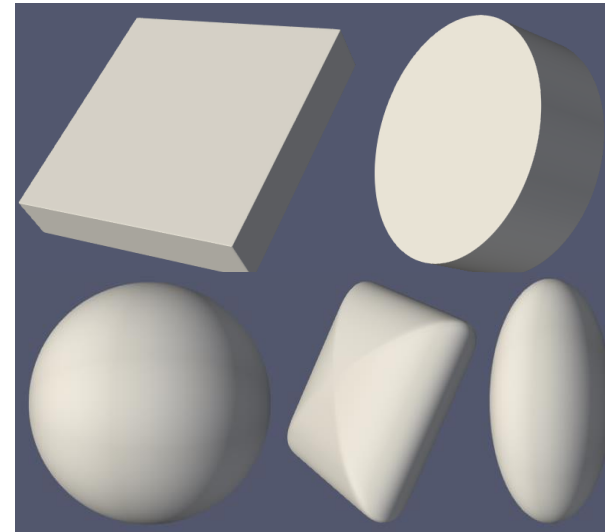
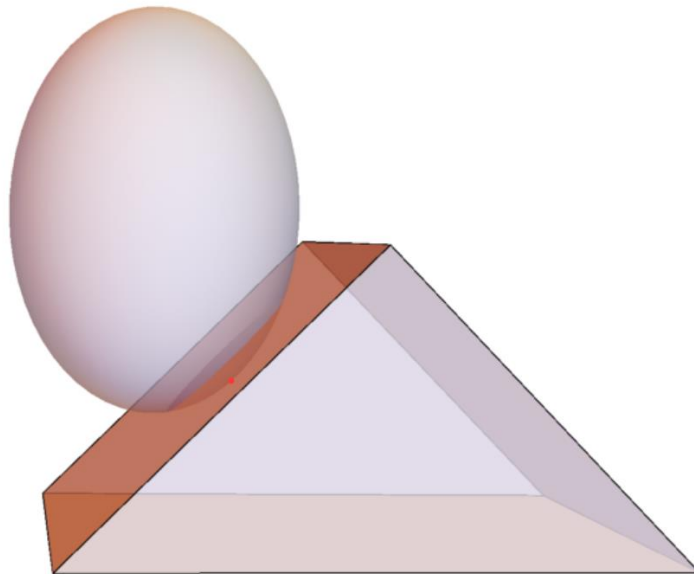
The distinct element method is a numerical model capable of describing the mechanical behaviour of assemblies of discs and spheres. The method is based on the use of an explicit numerical scheme in which the interaction of the particles is monitored contact by contact and the motion of the particles modelled particle by particle. The main features of the distinct element method are described. The method is validated by comparing force vector plots obtained from the computer program BALL with the corresponding plots obtained from a photoelastic analysis. The photoelastic analysis used for the comparison is the one applied to an assembly of discs by De Josselin de Jong and Verruijt (1969). The force vector diagrams obtained numerically closely resemble those obtained photoelastically. It is concluded from this comparison that the distinct element method and the program BALL are valid tools for research into the behaviour of granular assemblies.

La méthode des éléments distincts est un modèle numérique capable de décrire le comportement mécanique de l'assemblage de disques et de sphères. La méthode est basée sur l'utilisation d'un système numérique explicite dans lequel l'interaction des particules est contrôlée contact par contact et le mouvement des particules simulé particule par particule. Les caractéristiques principales de la méthode des éléments distincts sont décrites. La méthode est validée en comparant les tracés de vecteur de force obtenus par le programme sur ordinateur BALL avec les tracés correspondants obtenus à l'aide d'une analyse photo-élastique. L'analyse photo-élastique utilisée pour la comparaison est celle appliquée sur un assemblage de disques par De Josselin de Jong et Verruijt (1969). Les diagrammes de vecteur de force obtenus numériquement sont très voisins de ceux obtenus photo-élastiquement. Cette comparaison permet de conclure que la méthode des éléments distincts et le programme BALL sont des instruments valables pour la recherche du comportement des assemblages granulaires.

How does it work?



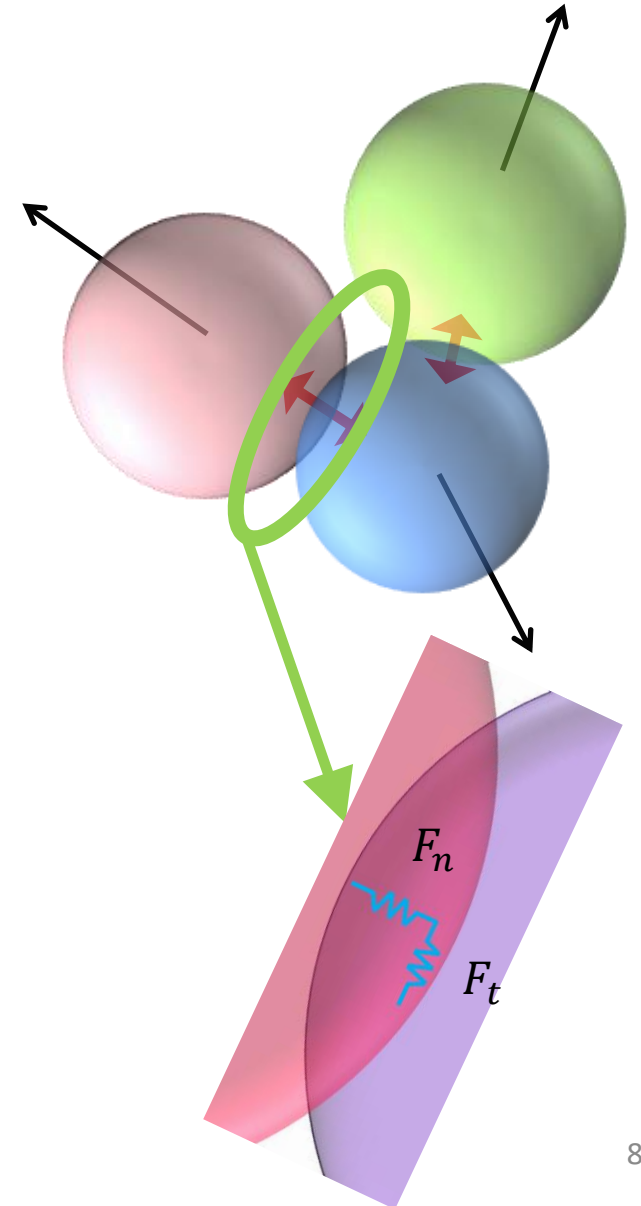
- Deterministic solution of Newton's second law of motion for each particle based on interaction forces and moments
- Explicit time integration scheme such as velocity-Verlet
- 'Standard' approach: one particle in the real system \rightarrow one simulated particle
- To reduce the computational requirements, real particles are represented by idealised rigid bodies



How does it work?



- Particles are allowed to overlap \rightarrow analogous to the deformation that occurs at real particle contacts
- Wherever there is an overlap, contact springs are inserted into the model...
- ... so that overlapping particles have a tendency to separate
- Can add conceptual dashpots to capture damping
- Coulombic friction is usually assumed: $|F_t| \leq \mu|F_n|$



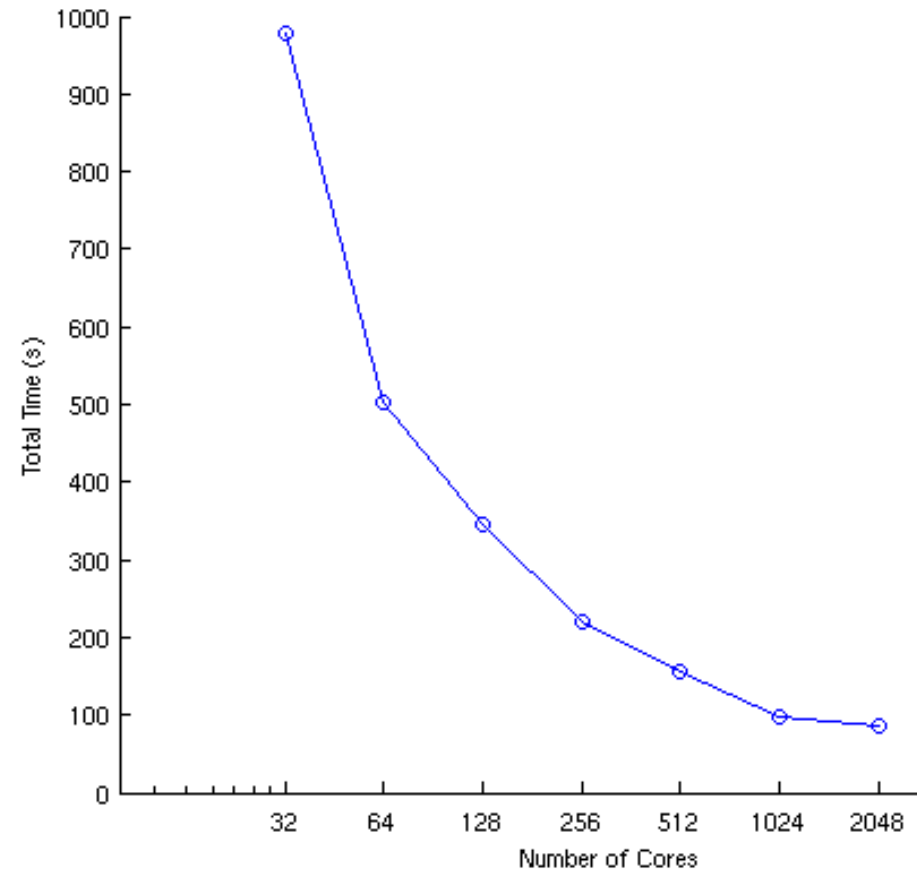
- MD and DEM are algorithmically similar → codes such as LAMMPS implement both
- Domain decomposition enabling parallelisation; similar contact detection methods
- Key differences
 - MD: for simulating atoms, molecules, ions...
 - DEM: for larger particles (~ those you can see without very expensive equipment)
 - MD: particles interact through 'potentials', e.g., Lennard-Jones
 - DEM: particles interact through 'contact laws', e.g., based on Hertzian mechanics

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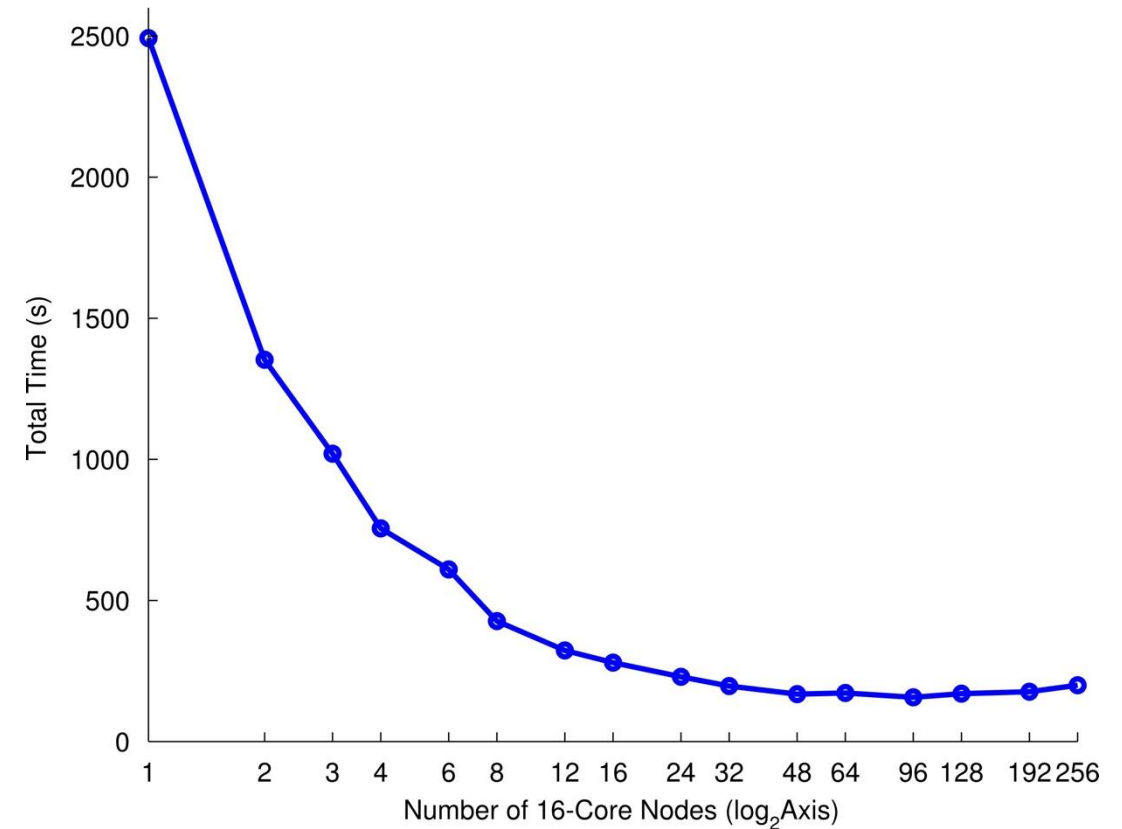
- Almost non-existent
- The norm: commercial codes, e.g., PFC or EDEM, running on workstations
- Serial DEM codes were still commonly used.
- LAMMPS had a 'GRANULAR' package though this was very limited in 2010.
- LIGGGHTS 1.0 ('LAMMPS improved for **g**eneral **g**ranular and **g**ranular **h**eat **t**ransfer simulations') was released in 2010.
- YADE, introduced in 2008, was lacking MPI support at this time.

- I joined Imperial College London in 2011 as a PDRA
 - Group of Prof. Catherine O’Sullivan
- The group decided to use LAMMPS as the basis for a DEM code capable of simulating various soil mechanics problems.
- Eventually geoLAMMPS (<https://github.com/geoLAMMPS/geoLAMMPS>) included:
 - Stress/strain control of periodically-bounded samples
 - Advanced particle–particle and particle–wall contact models
 - Energy tracing
 - Particle crushing

- The scaling of geoLAMMPS was explored on several HPC systems around this time.
- Uniaxial compression of a face-centred cubic assembly of 125,000 monosized spheres on HECToR for 100,000 timesteps →



- The scaling of geoLAMMPS was explored on several HPC systems around this time.
- Undrained triaxial compression for 100,000 timesteps of a sample of 351,248 polydisperse spheres (particle diameters from 50 μm to 1 mm) \rightarrow
- Run on CURIE (thin nodes) in 2012, accessed via PRACE

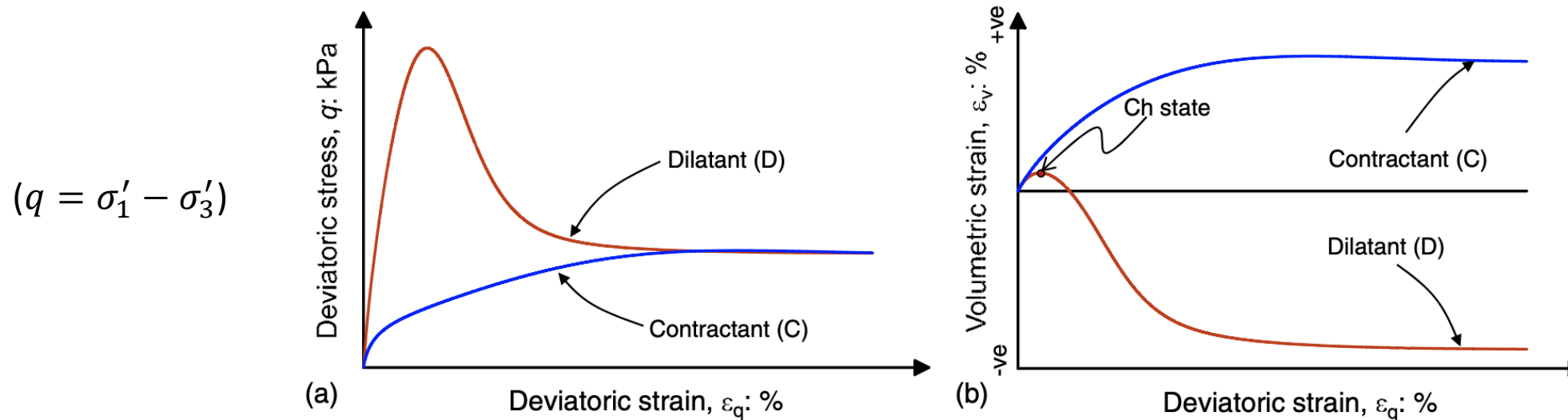


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What is a triaxial test?



- The application of some combination of stresses and strains to a granular sample to determine its shear strength.
- For the example of a drained triaxial test:



What is a triaxial test?



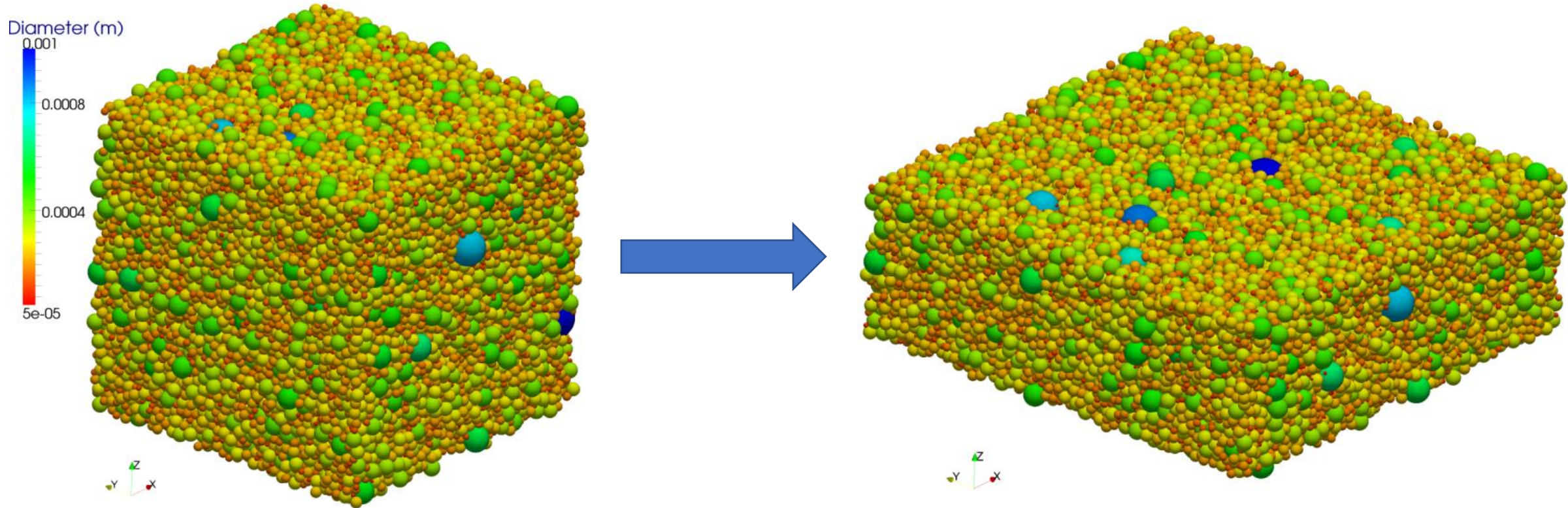
- In reality:



What is a triaxial test?



- In our DEM simulations:



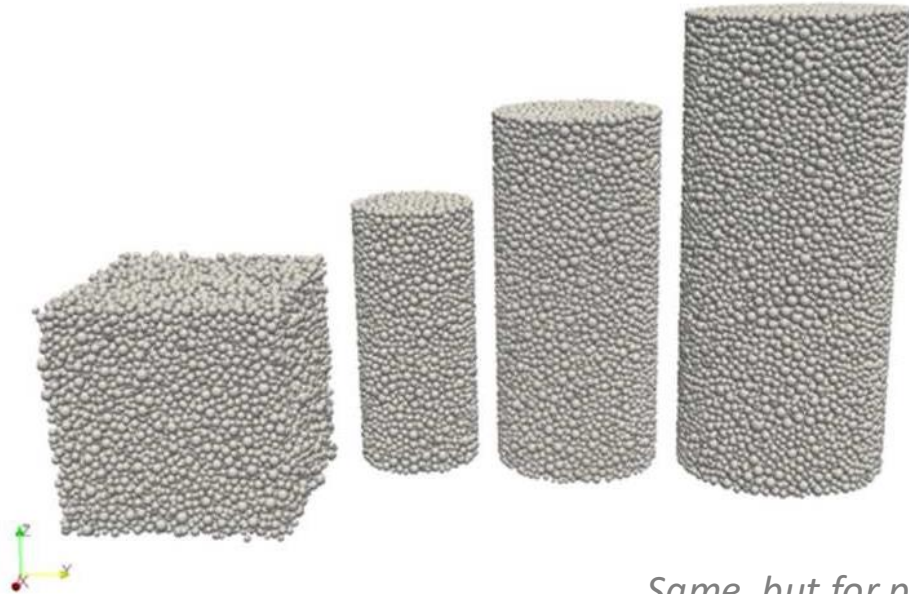
- A quick whistle-stop tour follows through some of our research on triaxial testing.
- The focus is not the research findings per se.
- Instead, note how many simulations were run, enabled by access to HPC.
- Individual simulations were seldom huge
... but they don't need to be to warrant using HPC!

Selected triaxial simulation results

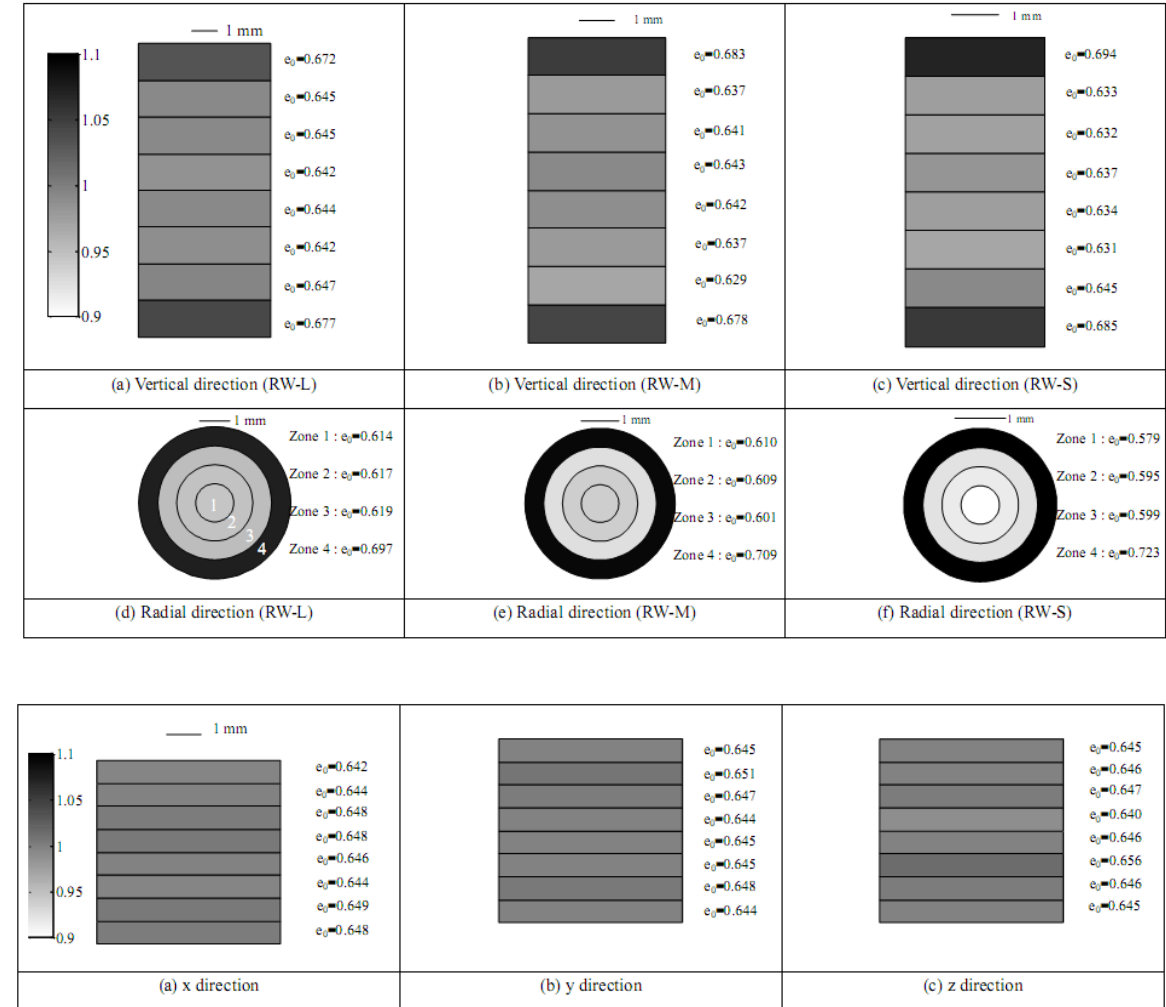


- The benefit of periodic boundary conditions

Distributions of initial void ratio of rigid-wall samples. The shading illustrates void ratios normalised by the mean value for each sample



Same, but for periodic boundaries



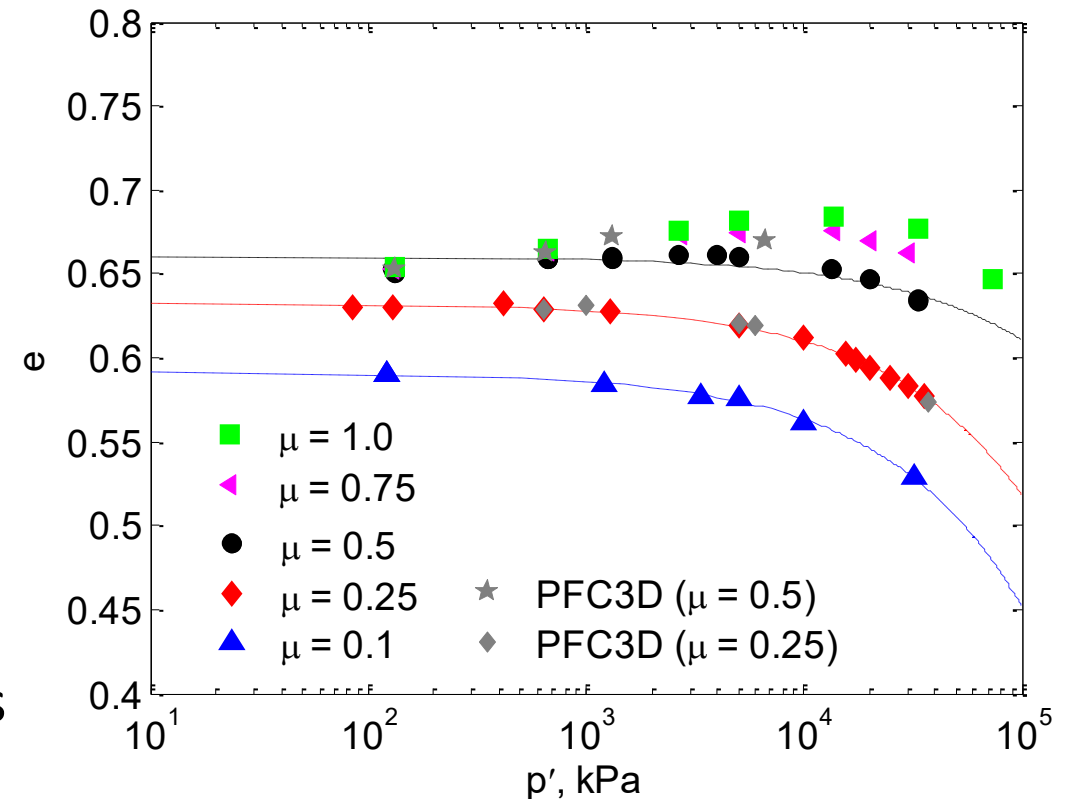
Selected triaxial simulation results



- Parametric study on the interparticle friction coefficient, μ , with 100 LAMMPS simulations

$$|F_t| \leq \mu |F_n|$$

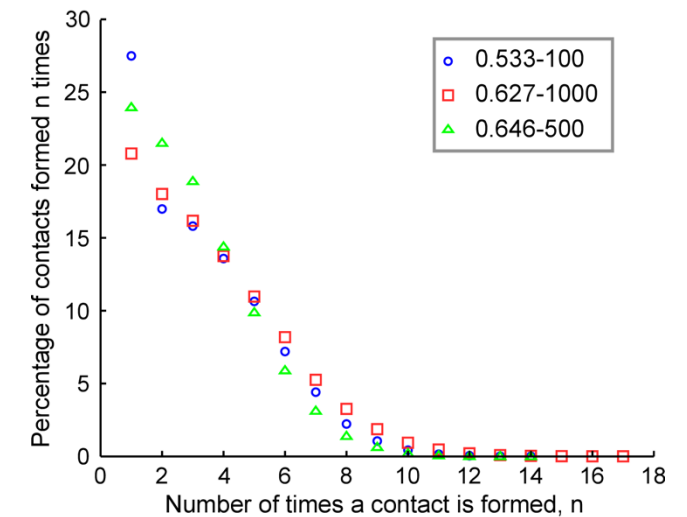
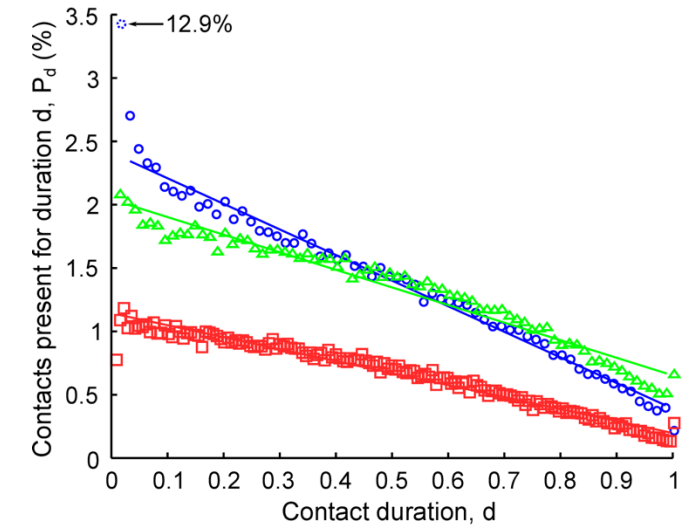
- Friction coefficients ≥ 0.5 cause the void ratio at critical state to initially increase with mean effective stress.
 - Not physically reasonable so provides an upper bound on suitable friction coefficients to use in simulations of soil



Selected triaxial simulation results



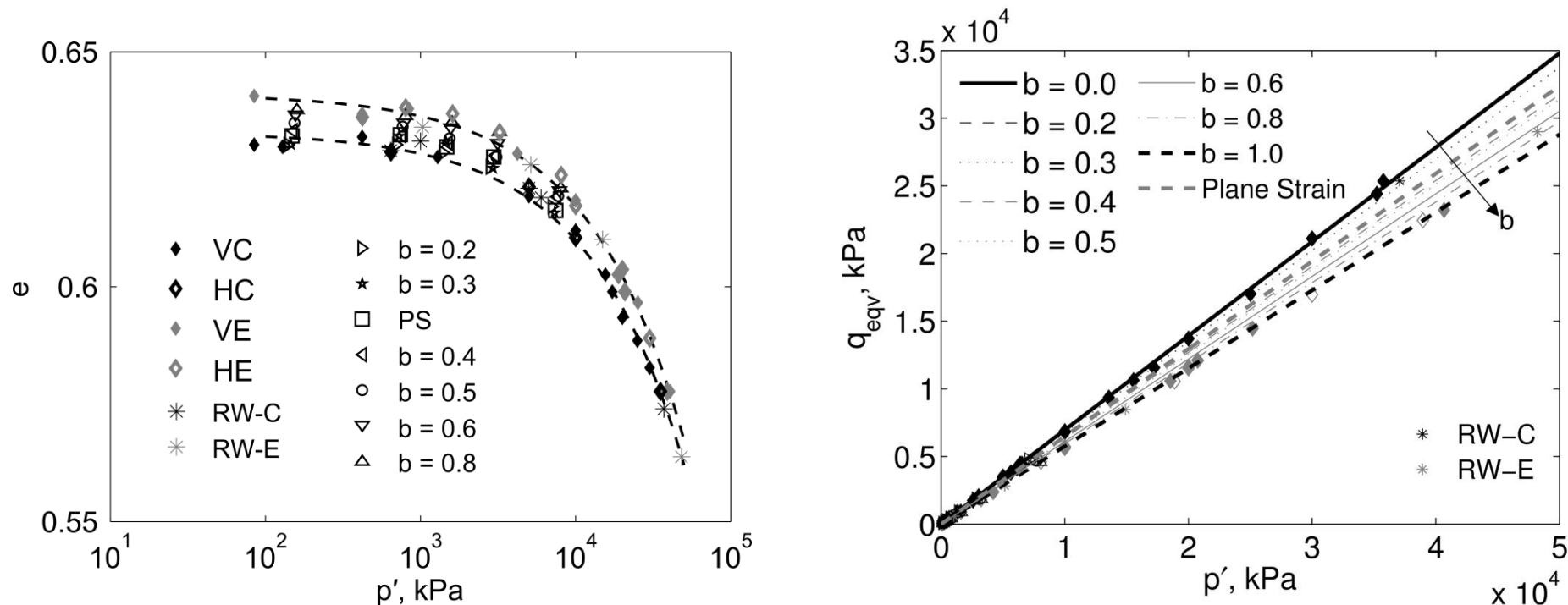
- Drained (also constant p' and undrained) triaxial simulations carried out on a numerical representation of Toyoura sand.
- Quantified duration and transitivity of contacts during the simulations
- For the drained simulations:
 - The percentage of contacts present for a given duration decreases almost linearly with duration.
 - More than 70% of contacts are created multiple times.



Selected triaxial simulation results



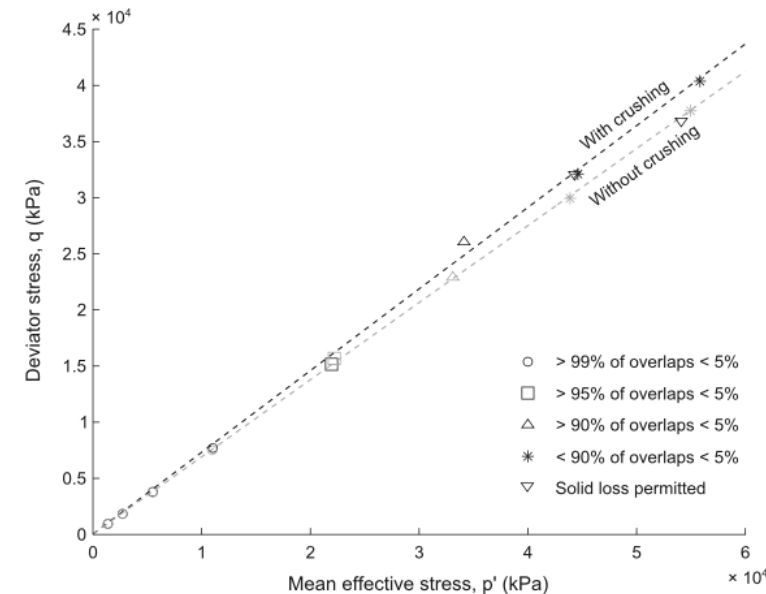
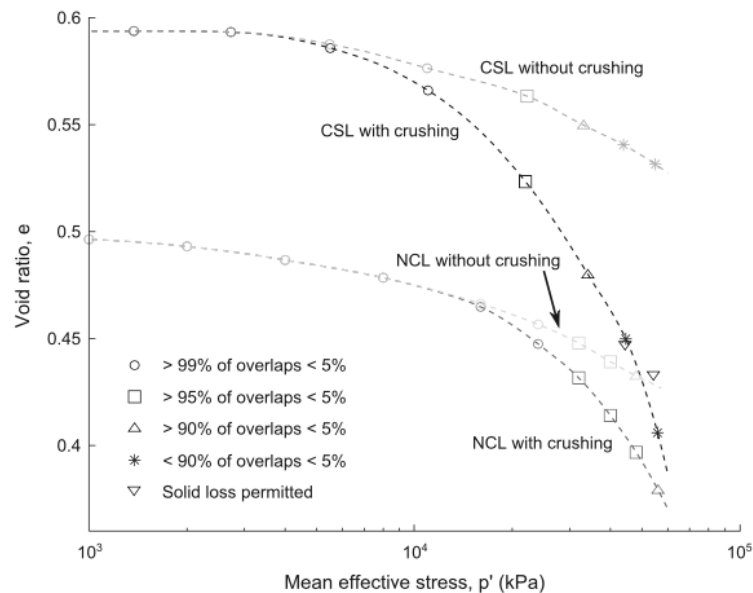
- Study of the effect of the intermediate stress ratio $b = \frac{\sigma_2' - \sigma_3'}{\sigma_1' - \sigma_3'}$ in triaxial shearing
- The position of the critical state line depends on b .



Selected triaxial simulation results

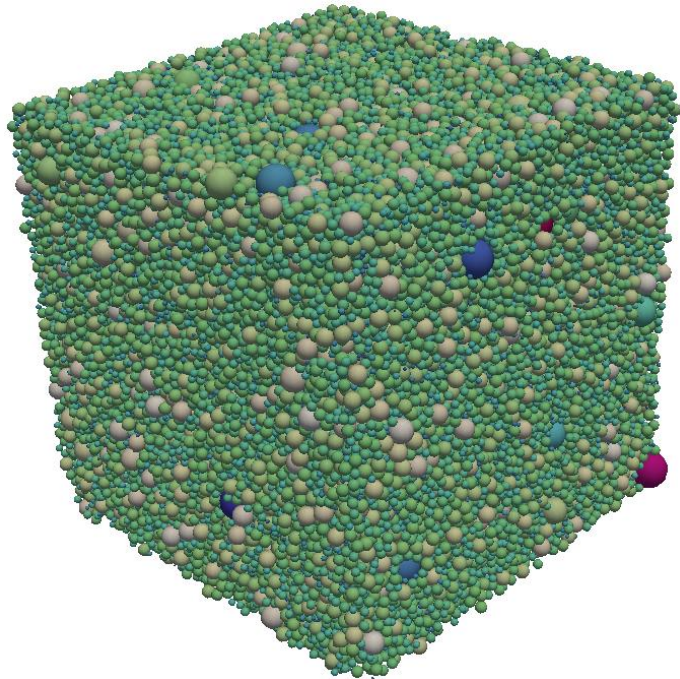


- A particle crushing model was implemented in geoLAMMPS.
- Critical state lines in e - $\log(p')$ space diverge at high stresses.

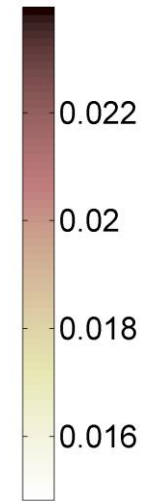
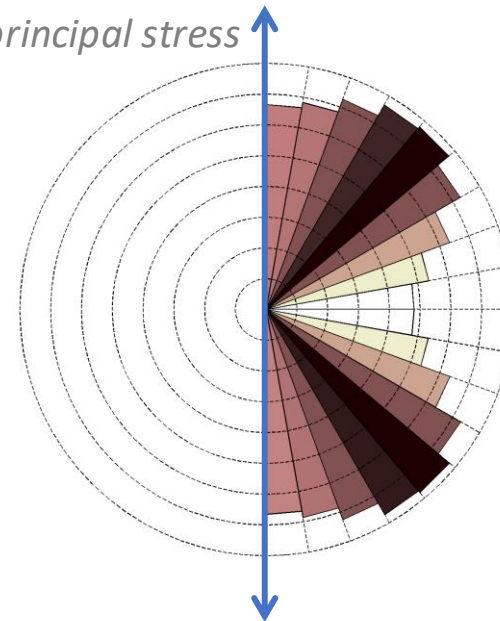


- Particle crushing continues post-critical state: a balance between particle breakage, tending to cause sample contraction, and dilation induced by particle rearrangement.

- Based on energy tracing added to geoLAMMPS
- Investigated the nature of energy dissipation during monotonic triaxial compression
- There is a preferential orientation for frictional dissipation at around 45° to the major principal stress direction.



Orientation of the major principal stress

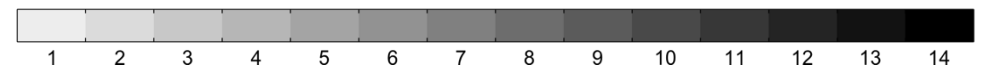
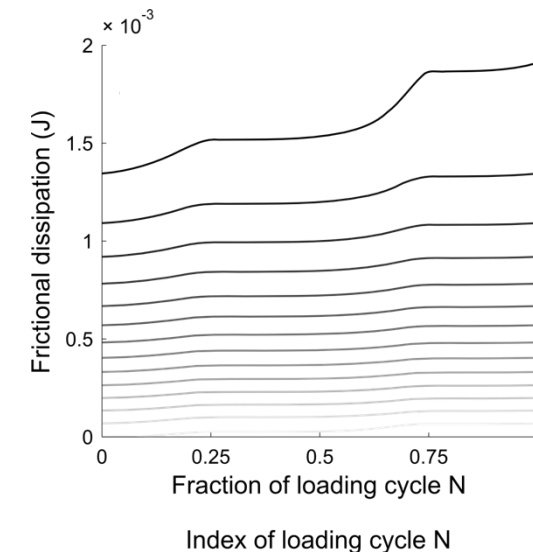
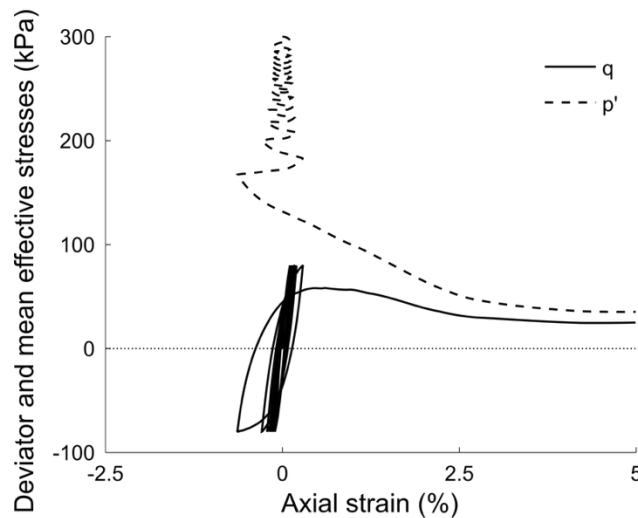
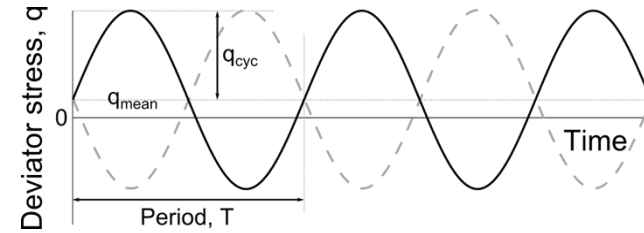


Total frictional dissipation (J) at critical state for contacts at that orientation

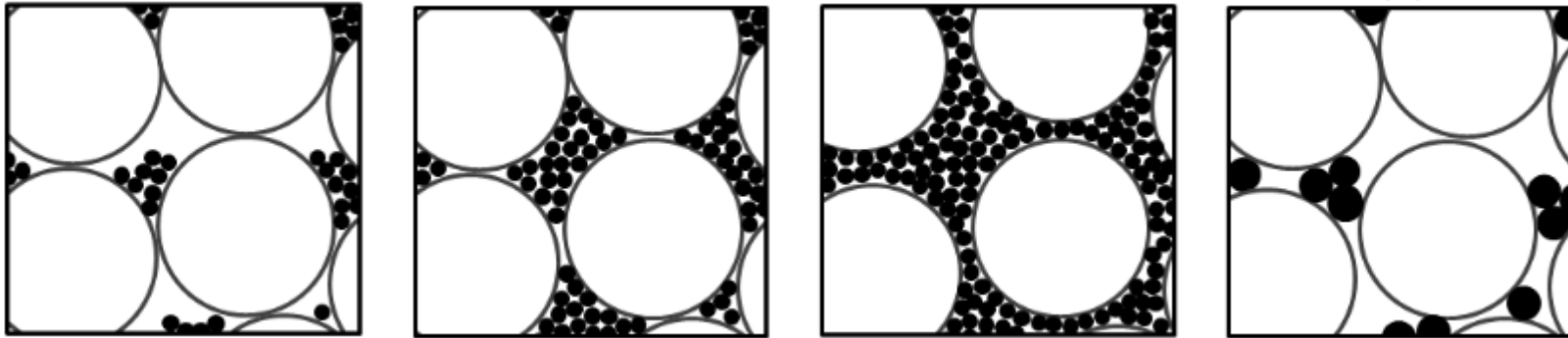
Selected triaxial simulation results



- Undrained cyclic triaxial DEM simulations:
- Following a shear reversal, there is a period of negligible frictional dissipation ($\sim 0.04\%$ axial strain in these simulations).
 - This explains, from an energy perspective, why many load cycles are needed to induce liquefaction if their amplitude is very small.



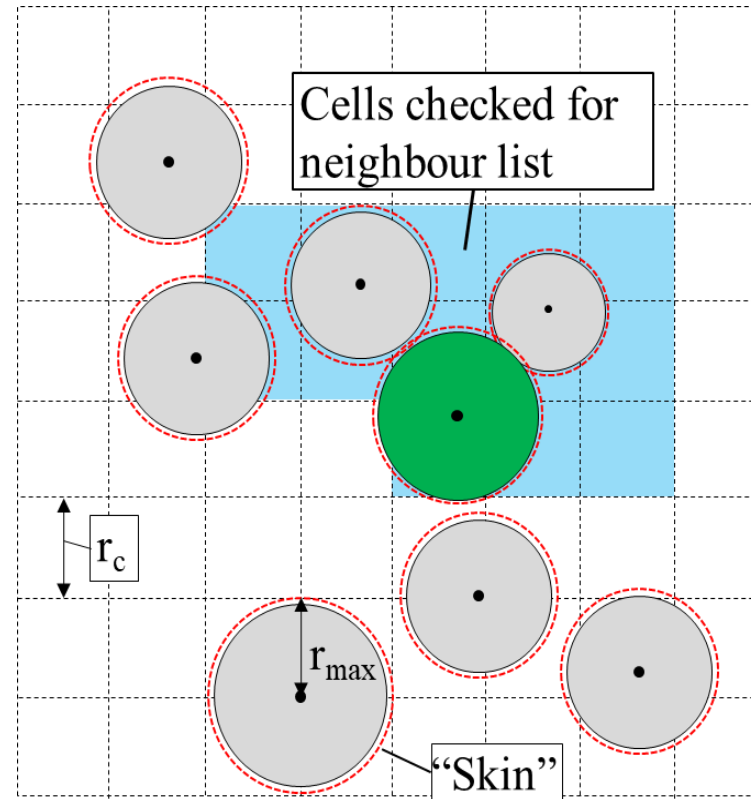
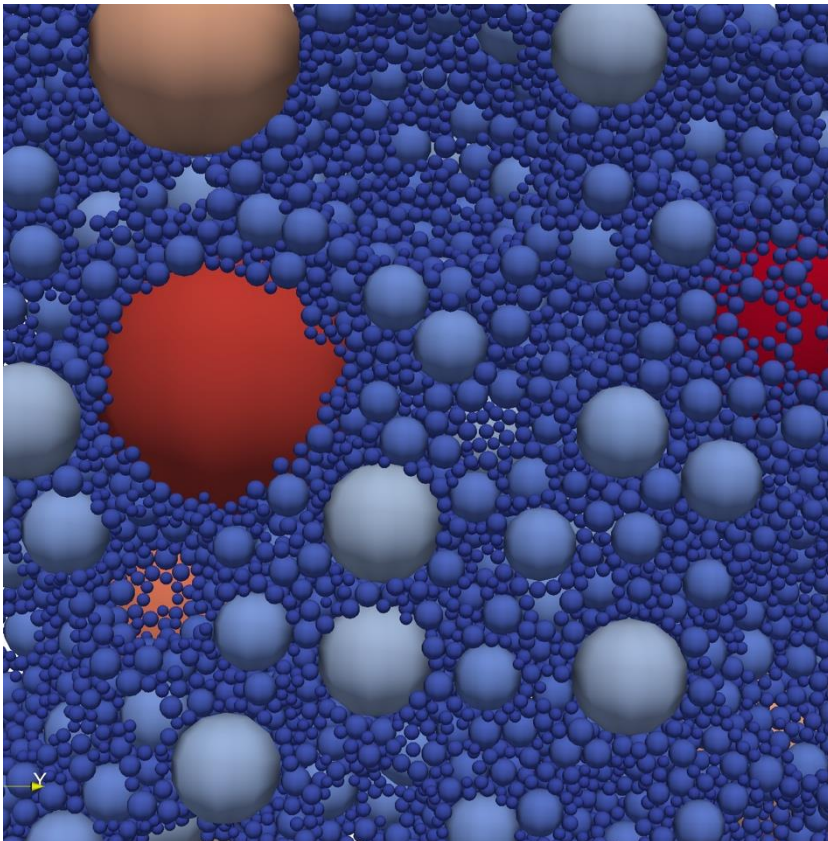
- Extensive studies on cohesionless soils with bimodal or gap-graded PSDs
- Exploring internal instability (fine particles being washed out of soil under seepage)
- Practical relevance for embankment dams and flood embankments



Schematic showing underfilled (leftmost and rightmost), filled (second from left) and overfilled soil fabric

- Even on HPC, simulations with large particle size differences create challenges.

- For simulating highly polydisperse systems where $\lambda = \frac{d_{max}}{d_{min}} \gg 1$

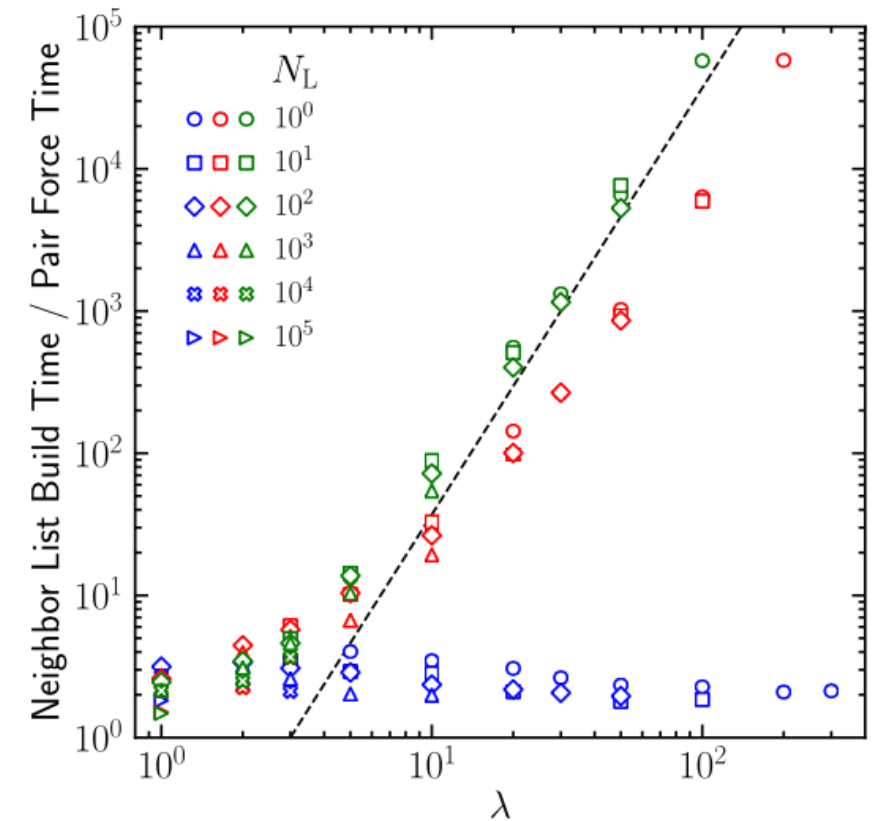


← Standard contact detection approach: Verlet neighbour list and link-cell methods. Cell size depends on the largest particle's diameter.

Code development for efficiency



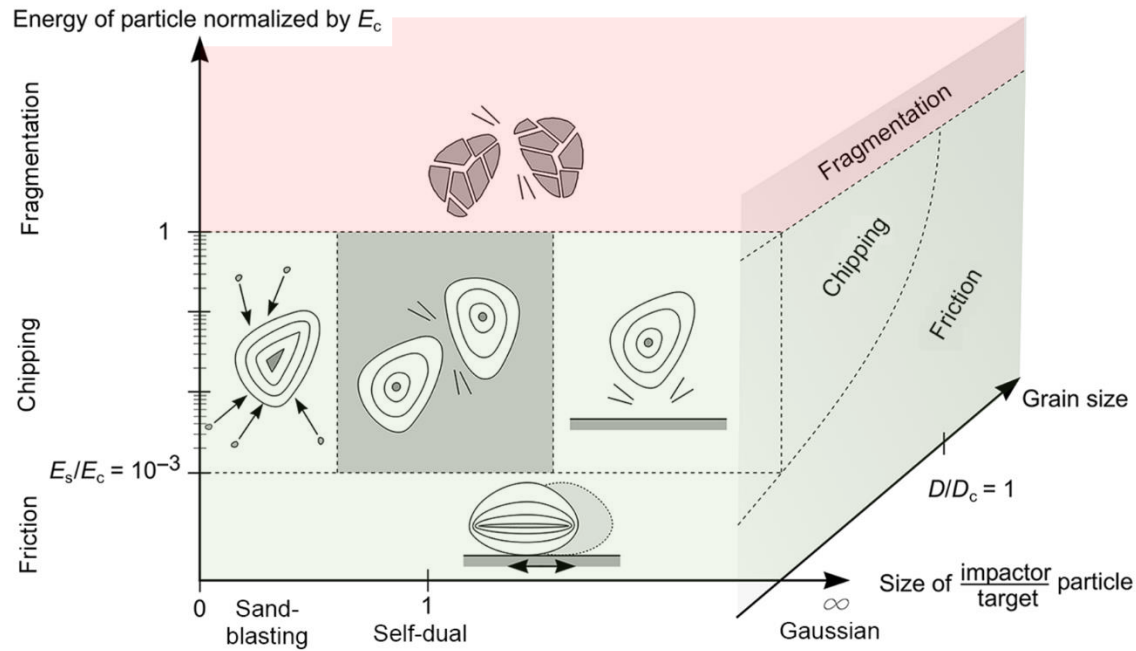
- Introduced a hierarchy of cell grids: one per particle size class. Assuming a bidisperse system...
 - A particle is binned to a 'large' or 'small' grid based on its size.
 - Identify large–large neighbours as normal.
 - Likewise small–small neighbours.
 - Small particles search the large bins for large neighbours: a one-way search
- Commensurate changes of inter-processor communication
- Available in LAMMPS as the *multi* neighbor style.



Time saving with multi (blue) compared to the standard approach (green) and a previous less effective approach to adjust bin size (red)

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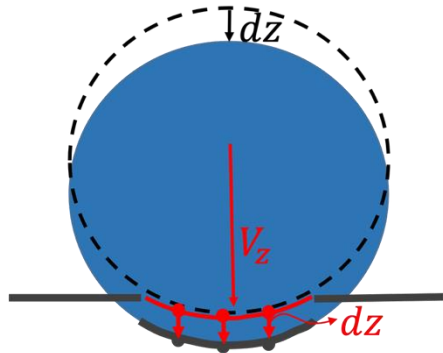
What do we mean by abrasion?



a) Particle rounding from abrasion in bed-load transport*
b) Beach pebbles in various states of wear

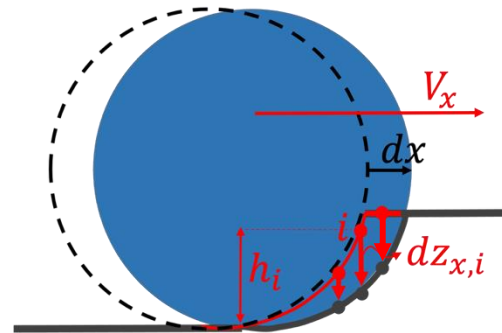
Phase space for attrition: Effect of relative size, normalised collision energy, and normalised grain size on attrition mode in bed-load transport*

Normal Impact



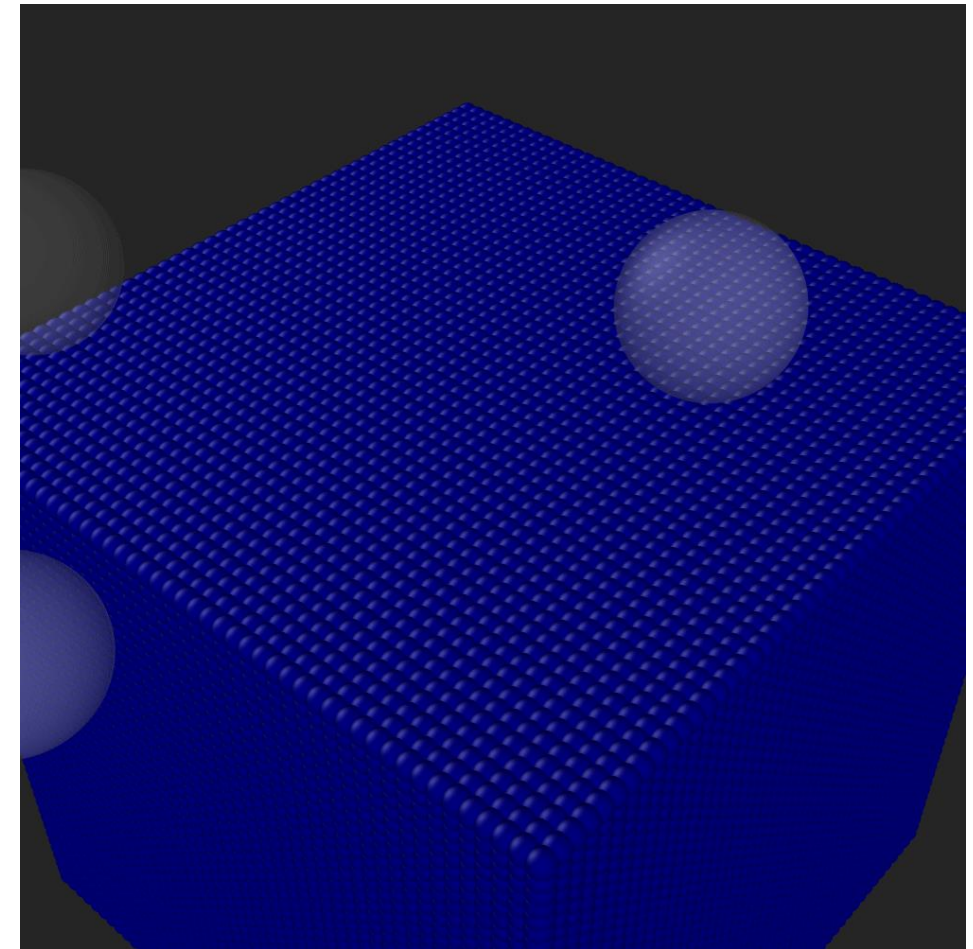
$P_z > H \rightarrow$ indentation

Lateral Impact



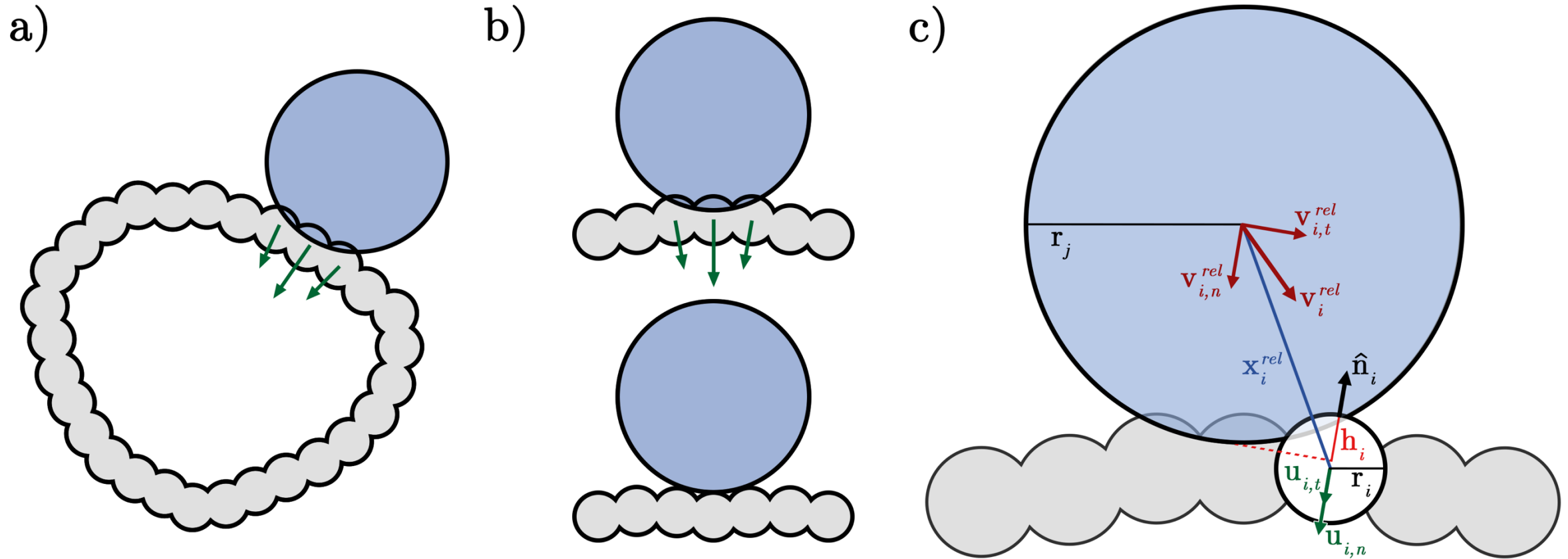
$P_x > \mu_a H \rightarrow$ scratch

Deformation of a flat surface through indentation and scratching

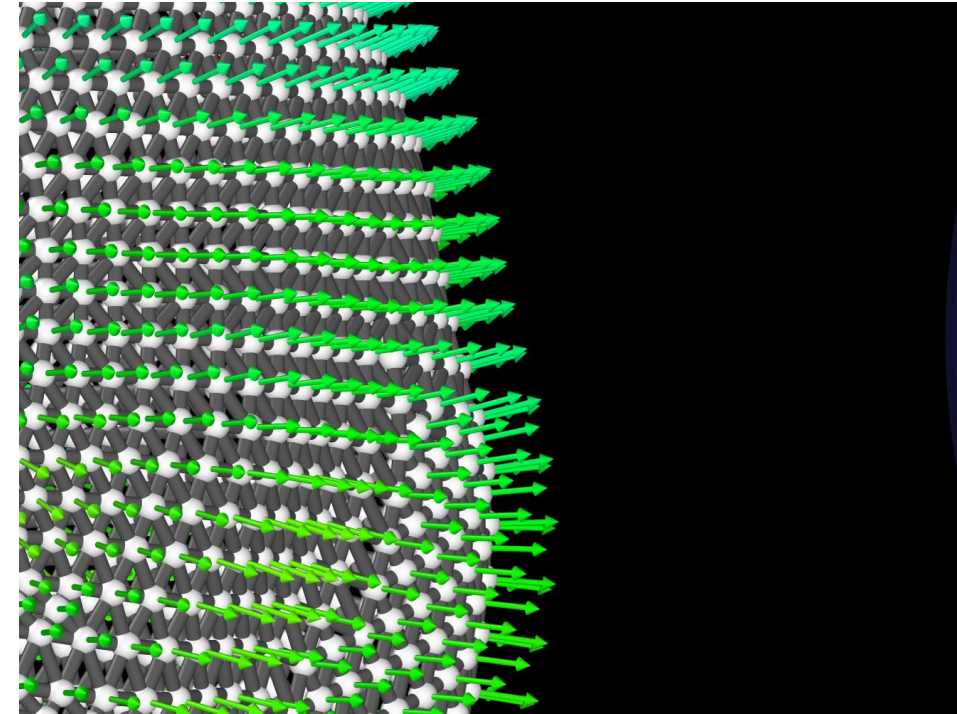
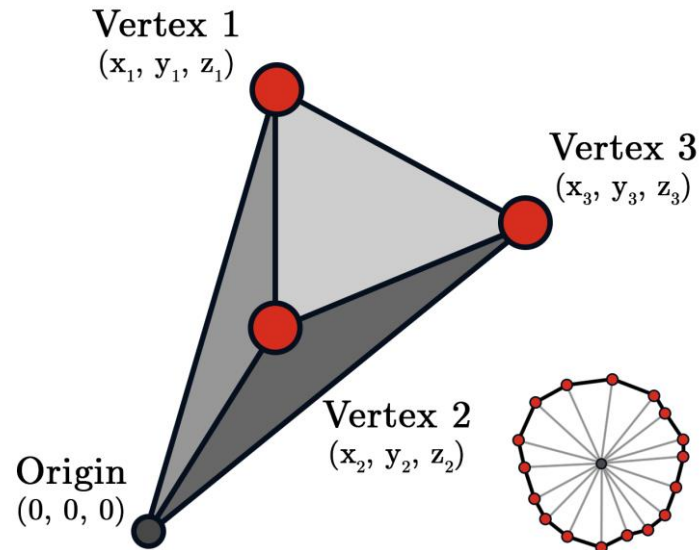
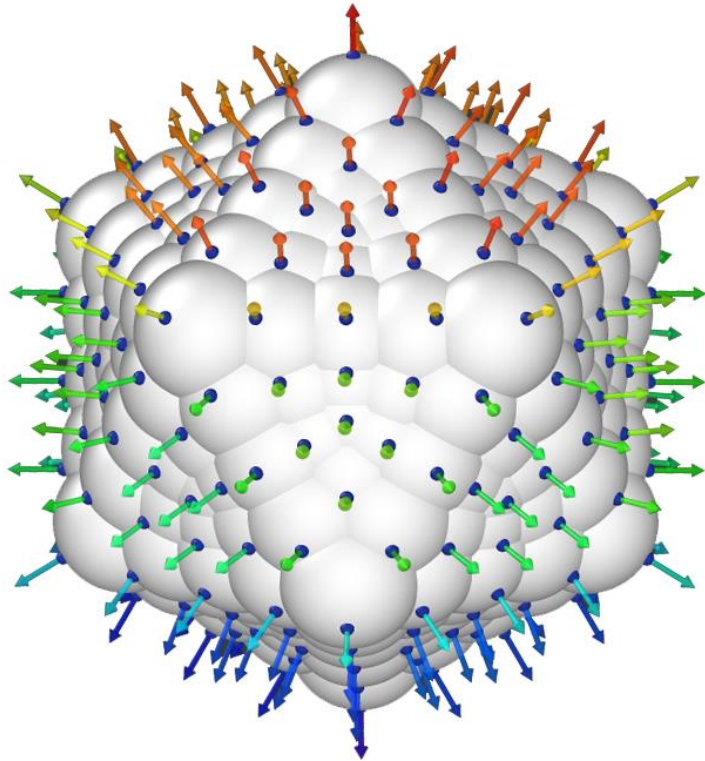


Abrasion of a flat surface under scratching, normal and oblique impacts. Surface atoms are colour-coded by their total displacements.

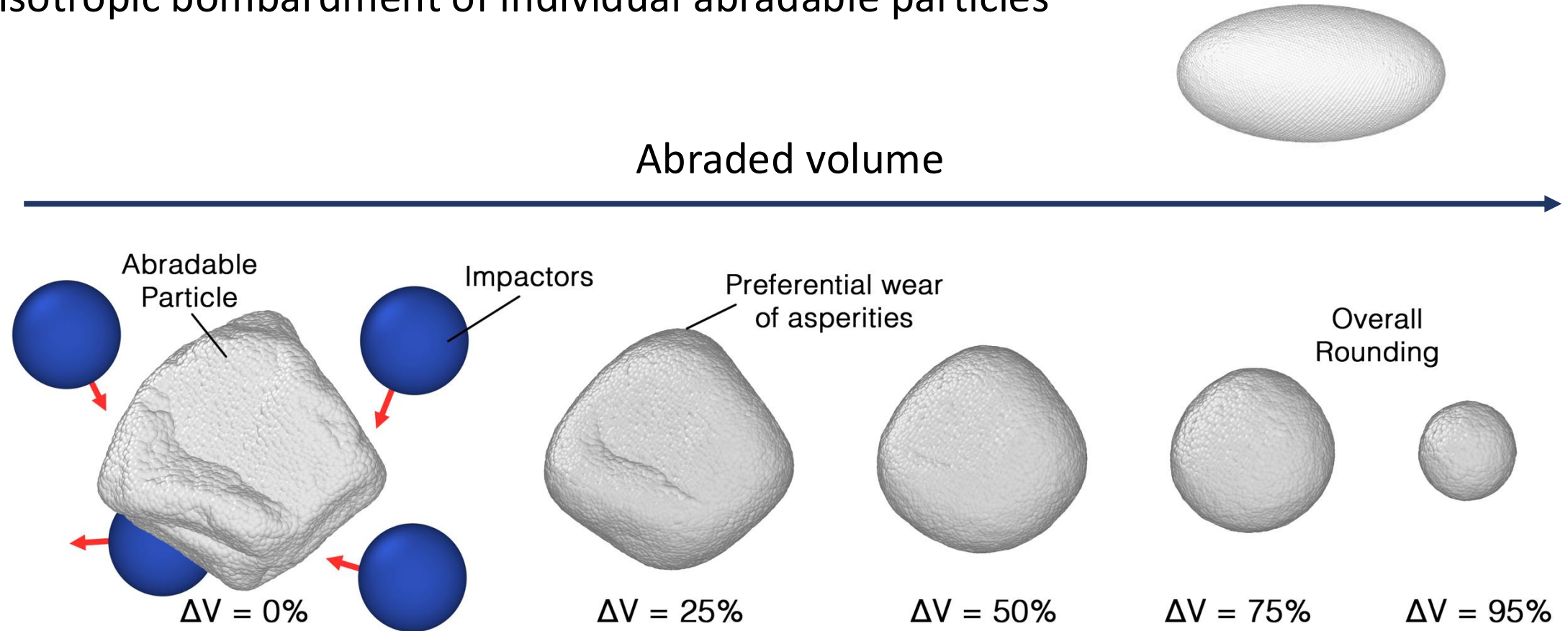
Particle representation



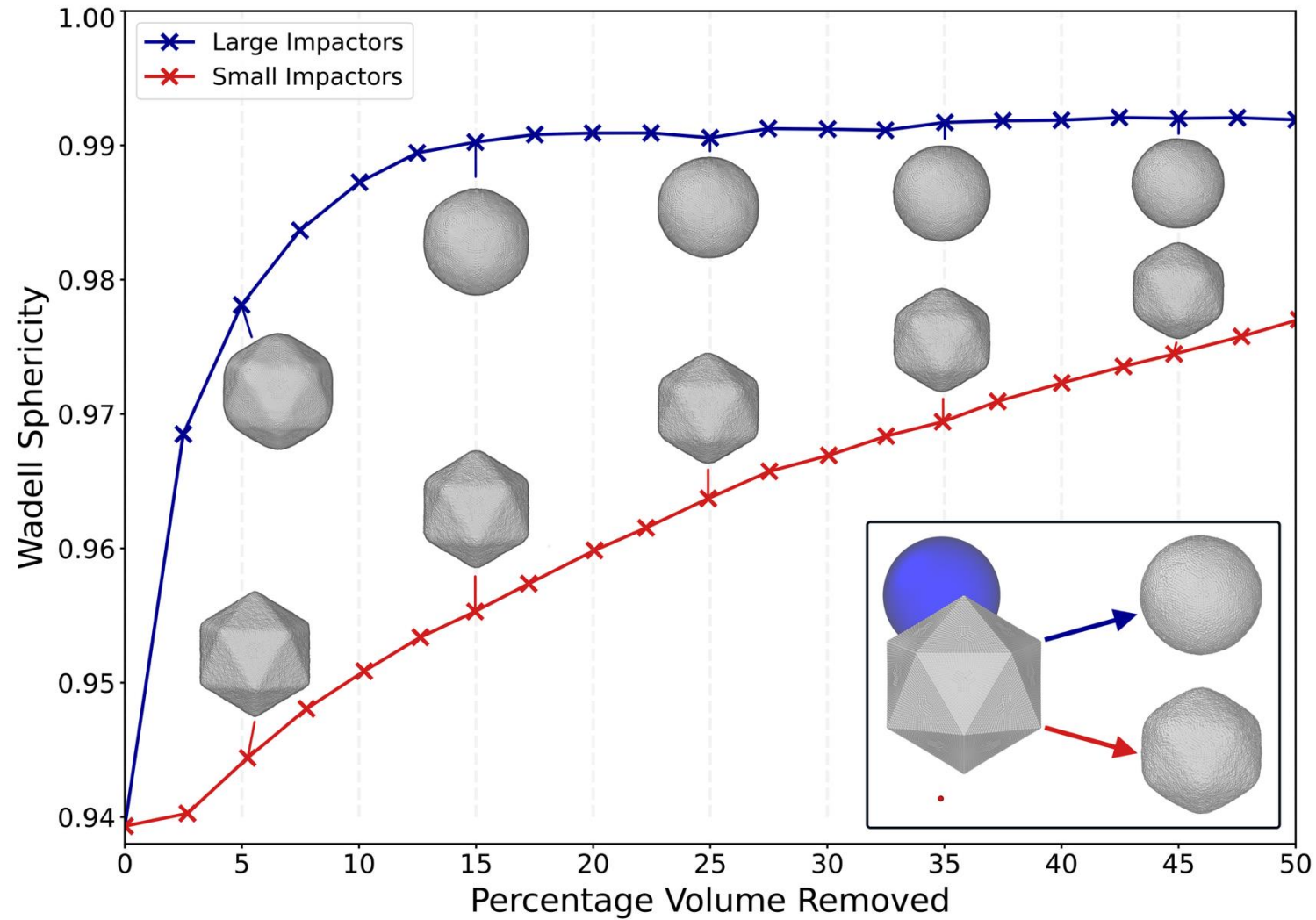
Particle representation

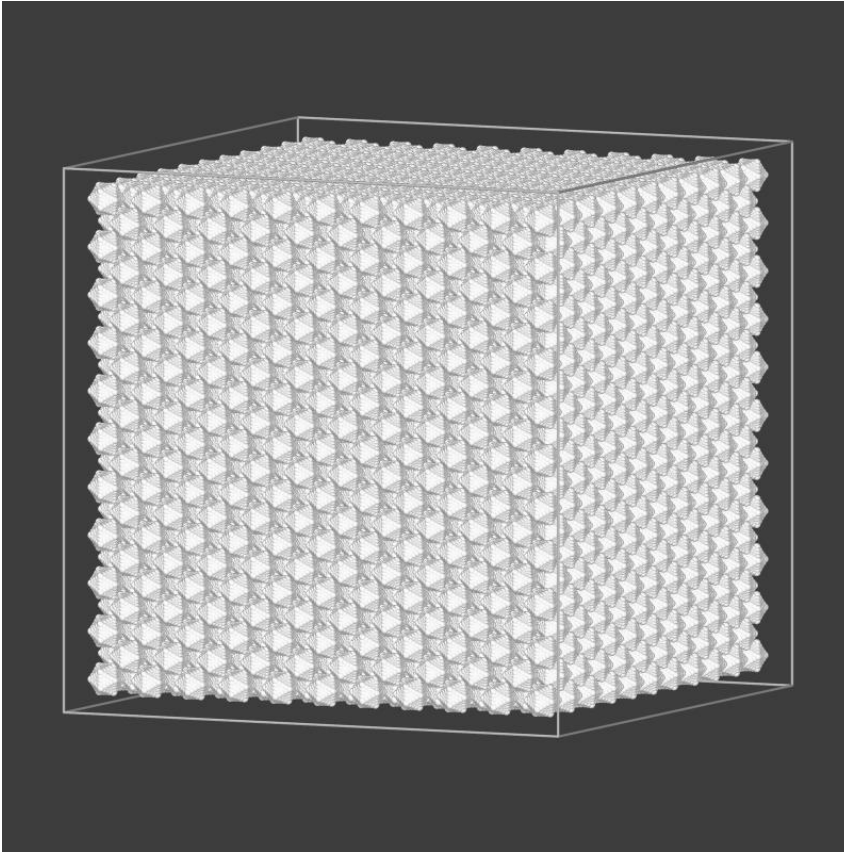


- Isotropic bombardment of individual abradable particles

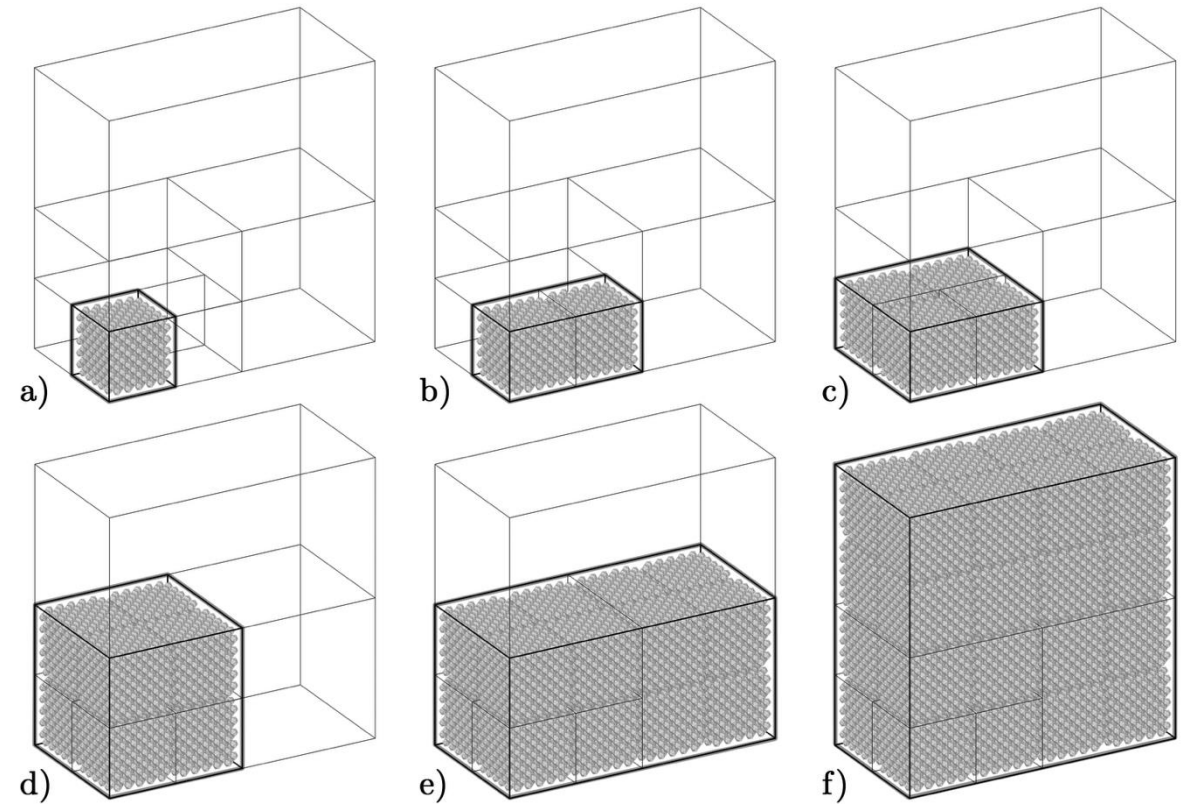


Isotropic bombardment



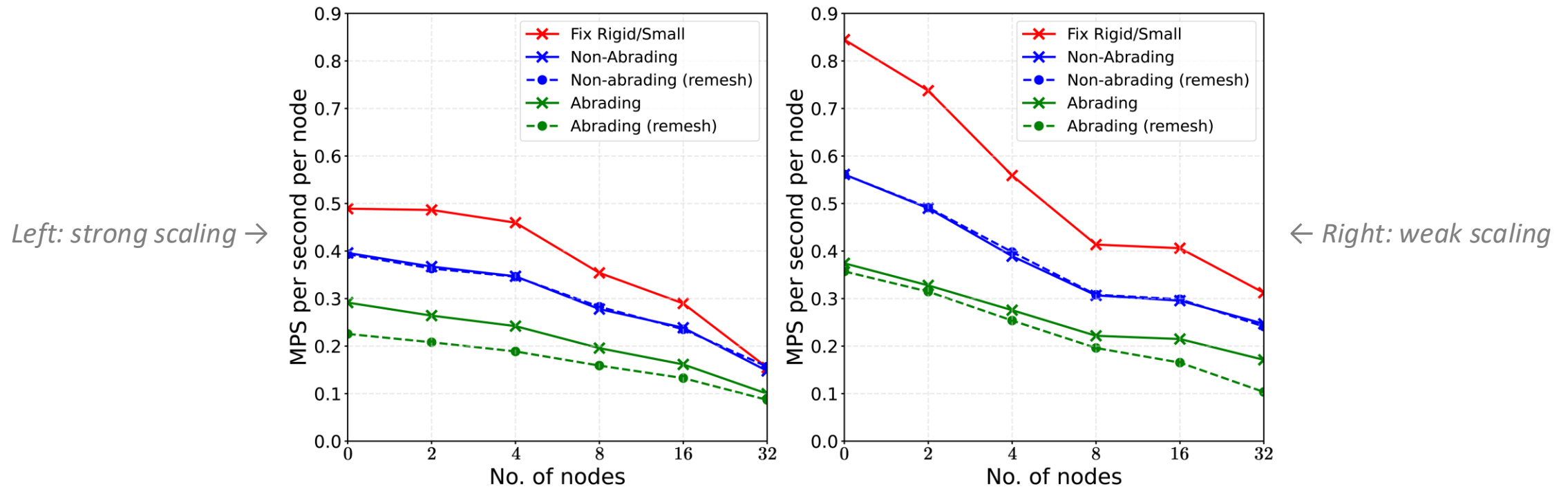


Strong scaling simulation setup: 4,631 bodies comprising 1,125,333 spheres abrading in a periodic cell under a Langevin thermostat



Weak scaling simulation setups ranging from 665 bodies (161,595 spheres) to 21,280 bodies (5,171,040 spheres)

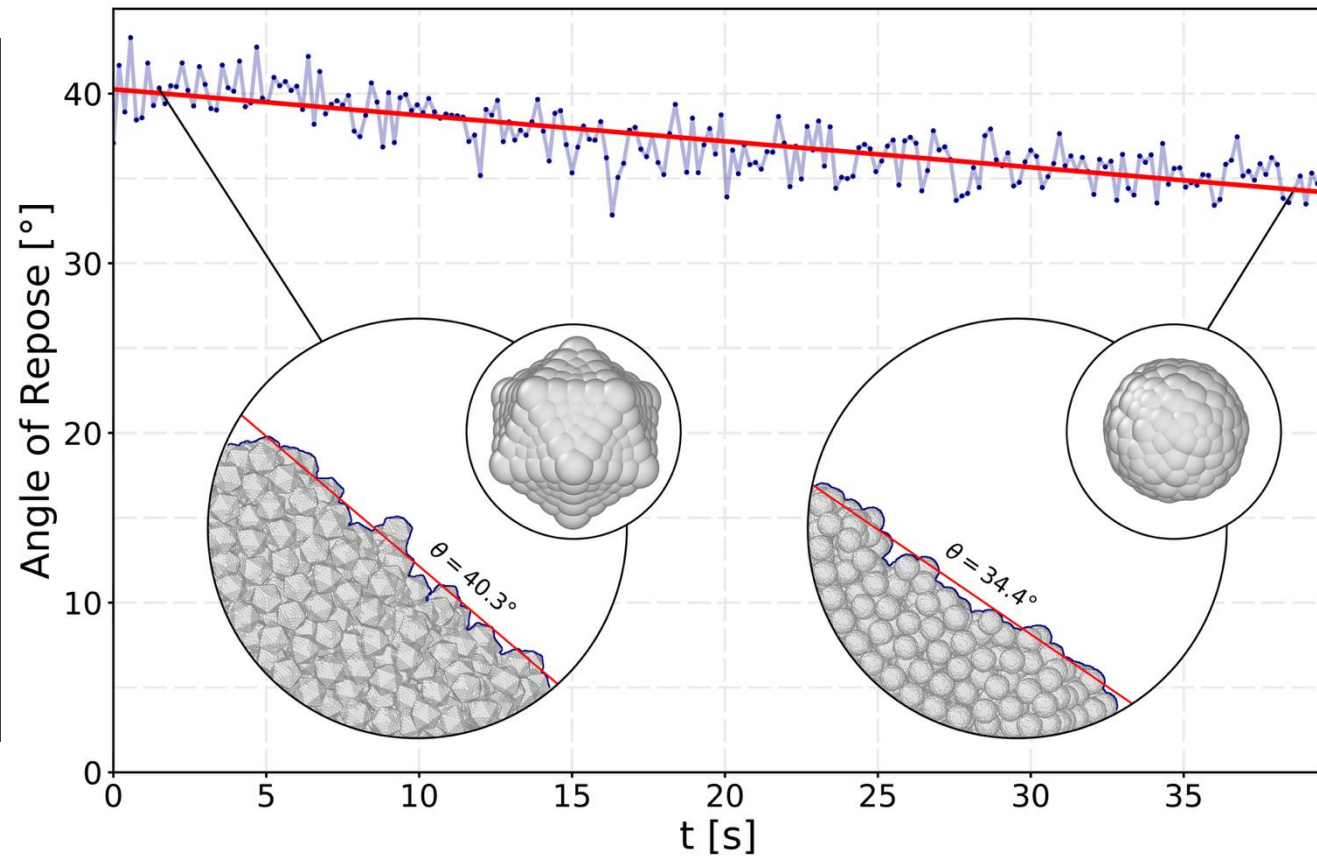
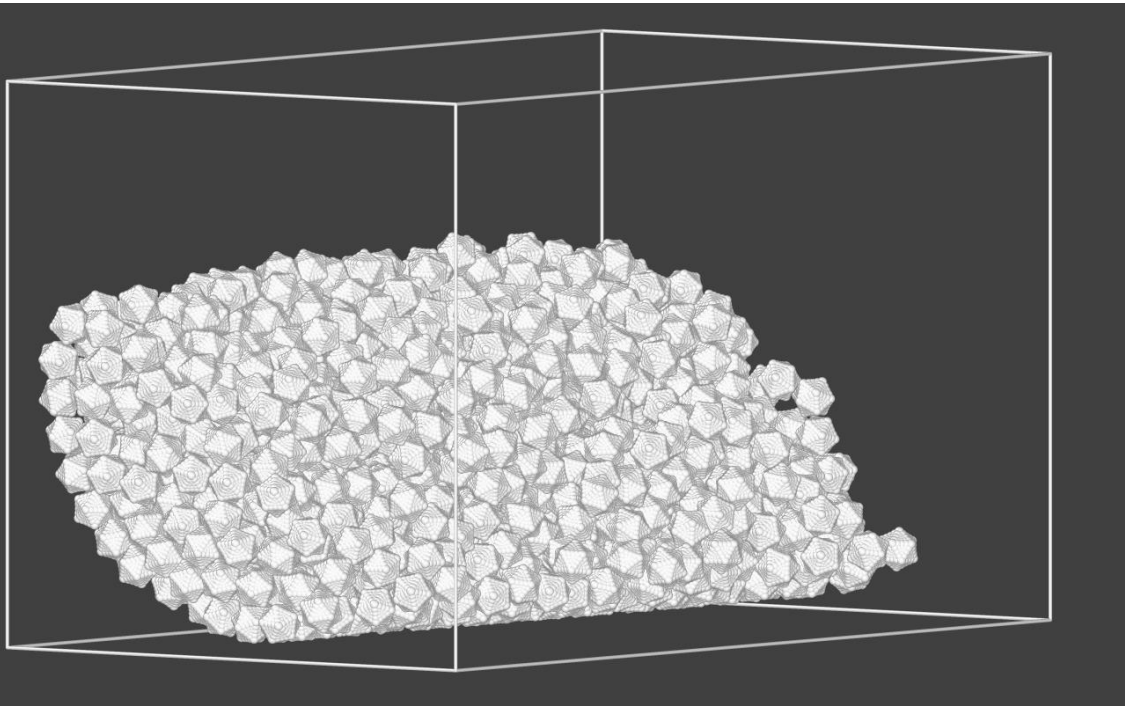
- Scaling data from CIRRUS (SGI ICE XA System) using 36 MPI tasks per node
- The y-axes represent millions of particle-timesteps (MPS) per second per node, with ideal scaling represented by the horizontal.



A larger, dynamic system



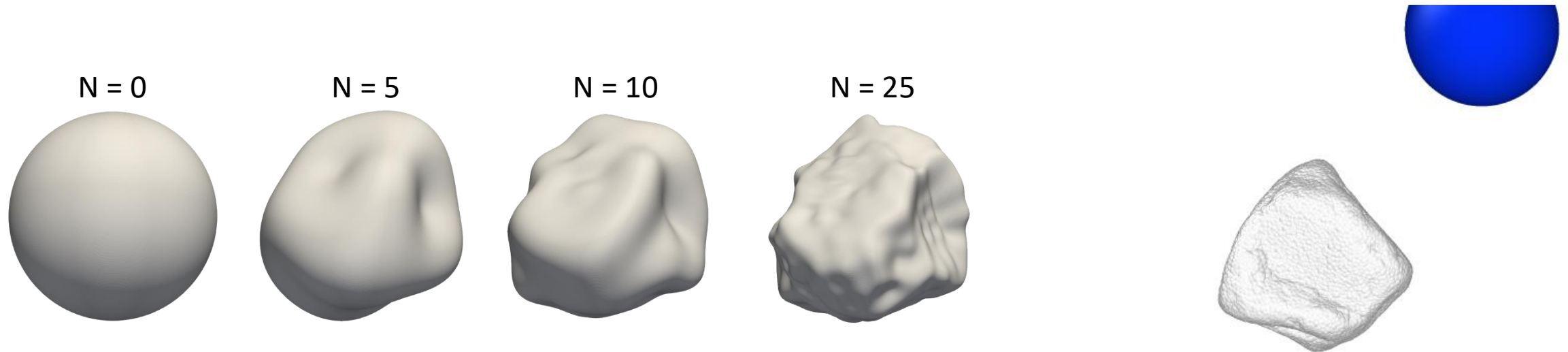
- 1,276 icosahedra comprising 310,068 spheres abrading in a rotating drum



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1. Real granular systems contain enormous numbers of particles.
 - More than 1 billion (10^9) sand grains per cubic metre!
 - We often reduce the simulated system size
 - e.g., by simulating a slice from a larger system
 - and/or increase the particle size for tractability
 - “meso-scale” particles.
 - However, these strategies cannot always be applied and can be detrimental to the quality of the simulation output.

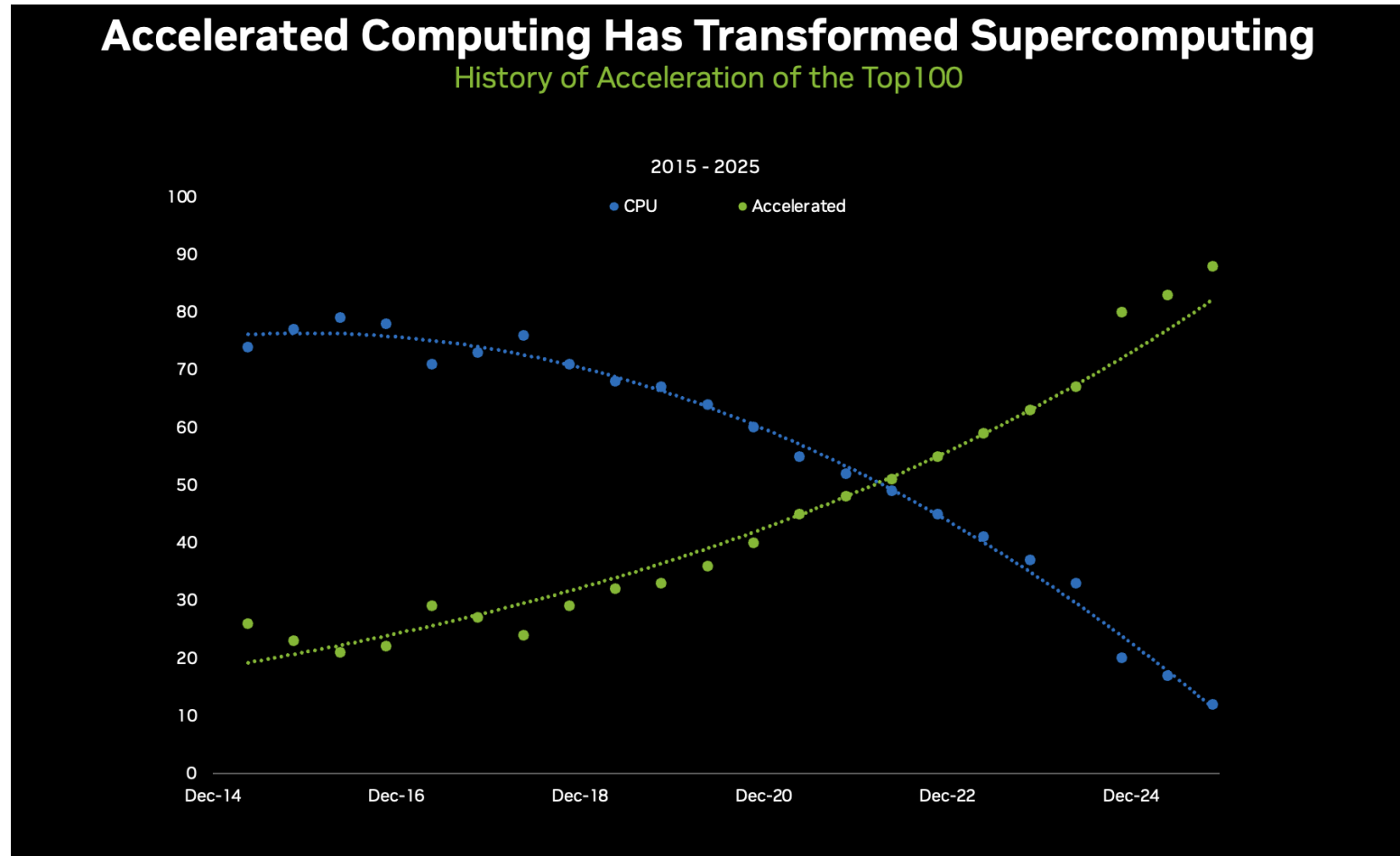
- Individual particles are being increasingly simulated at higher fidelity, e.g., LS-DEM, SH-DEM, or high-resolution polyhedra/multi-sphere clumps.



An arbitrarily shaped particle represented at different degrees of expansion ($N = 0, 5, 10, 25$) of the spherical harmonic representation

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The move towards GPUs



The move towards GPUs



Green500 Data

Rank	TOP500 Rank	System	Cores	Rmax (PFlop/s)	Power (kW)	Energy Efficiency (GFlops/watts)
1	420	KAIROS - BullSequana XH3000, GH Superchip 72C 3GHz, NVIDIA GH200 Superchip, Quad-Rail NVIDIA InfiniBand NDR200, RedHat Enterprise Linux, EVIDEN CALMIP / University of Toulouse - CNRS France	13,056	3.05	46	73.282
2	171	ROMEO-2025 - BullSequana XH3000, Grace Hopper Superchip 72C 3GHz, NVIDIA GH200 Superchip, Quad-Rail NVIDIA InfiniBand NDR200, Red Hat Enterprise Linux, EVIDEN ROMEO HPC Center - Champagne-Ardenne France	47,328	9.86	160	70.912
3	225	Levante GPU extension - BullSequana XH3000, GH Superchip 72C 3GHz, NVIDIA GH200 Superchip, Quad-Rail NVIDIA InfiniBand NDR200, RedHat Enterprise Linux, EVIDEN DKRZ - Deutsches Klimarechenzentrum Germany	35,904	6.75	110	69.426
4	213	Isambard-AI phase 1 - HPE Cray EX254n, NVIDIA Grace 72C 3.1GHz, NVIDIA GH200 Superchip, Slingshot-11, HPE University of Bristol United Kingdom	34,272	7.42	117	68.835

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What is CCC-ParaSols?



- A two-year project that started in January 2025, funded by the STFC

47

- To create a **C**ollaborative **C**omputational **C**ommunity in particulate solids simulations

Hopefully a precursor to a long-term
Collaborative **C**omputational **P**roject
(A CCP is a specialised, researcher-led network funded by UKRI to develop, distribute and maintain scientific software)

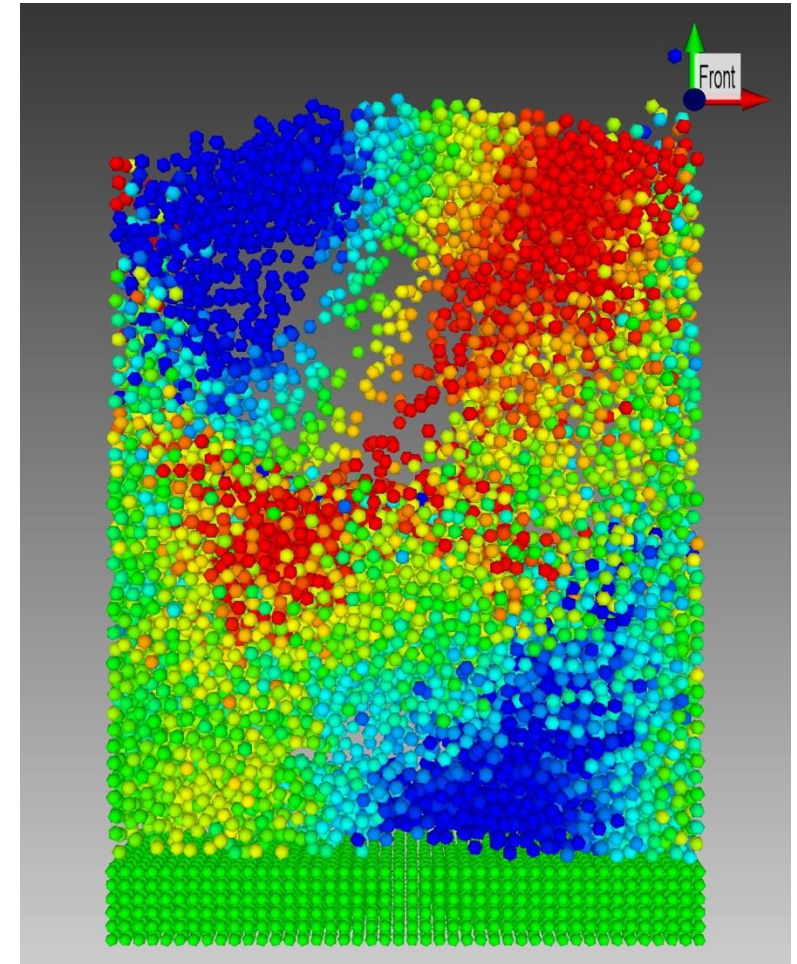
Intended to be:

- Cross-disciplinary
- Diverse
- Inclusive of everyone with an interest in this category of simulation methods

Why is a CCC needed in this area?



- DEM and other particle-scale simulation methods are becoming ever more popular.
- Developments of simulation methods happen in discipline silos.
- How to overcome this?
 - **CCC-ParaSolS**, as an overarching UK community that embeds diversity and inclusiveness in all activities



48

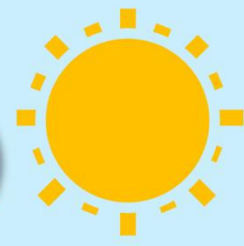


ParaSols

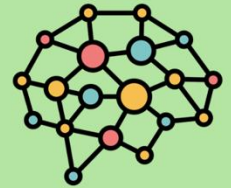
Particulate Solids Simulations



Bigger, Faster, Smarter
Increase **HPC** utilisation;
Improved physics for DEM codes; Accelerators (**AI & GPU**)



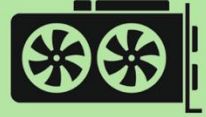
Community Engagement
Engaging with people across different communities & sectors;
Community-led for community benefit



Training & Upskilling
Delivering **bespoke training** for the community: open-source **DEM**, **HPC**, **AI/ML**, **Data Analysis**

CCP-ParaSols

Sustainable Code Development
Preparing for **next-gen DRI**; Enabling **GPU** and **Exa-scale** compute



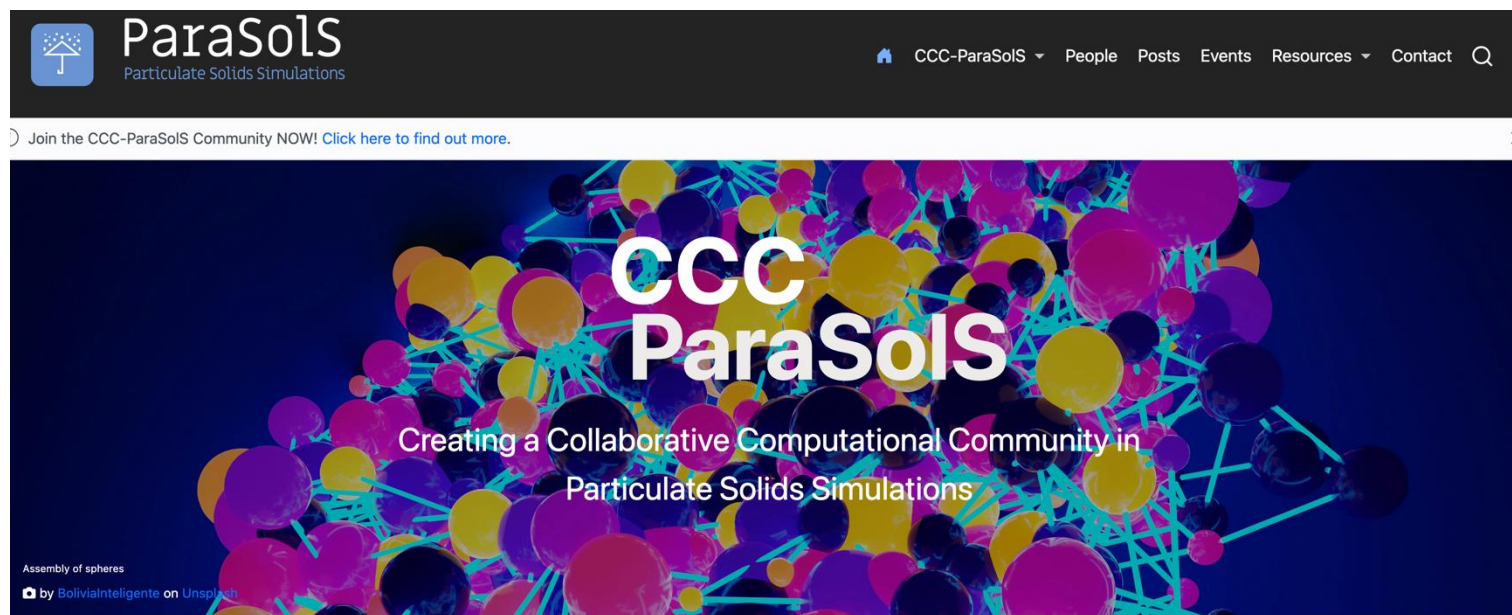
Promoting Best Practices
Benchmarking problems for DEM codes; **FAIR data principles** and Research Data Management guidance;
Machine-actionable data for AI/ML era



For more details of the project



- <https://www.ccc-parasols.ed.ac.uk/>



Welcome to CCC-ParaSoLS

CCC-ParaSoLS is a two-year project — January 2025 to December 2026 — funded by the [Science and Technology Facilities Council \(STFC\)](#) to create a **Collaborative Computational Community** in particulate solids simulations.



Science and Technology Facilities Council



IMPERIAL



THE UNIVERSITY of EDINBURGH
School of Engineering



Management Committee



Kevin Hanley
University of Edinburgh
Project Lead



Catherine O'Sullivan
Imperial College London
Project Co-Lead



J.P. Morrissey
University of Edinburgh
Researcher Co-Lead



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Imperial College London,
UK



Marv Khala
AstraZeneca, UK

<https://www.ccc-parasols.ed.ac.uk/people/>

Advisory Committee



Daniel Barreto
Edinburgh Napier
University, UK



Dan Bolintineanu
Sandia National
Laboratories



Chris Johnson
University of Manchester,
UK



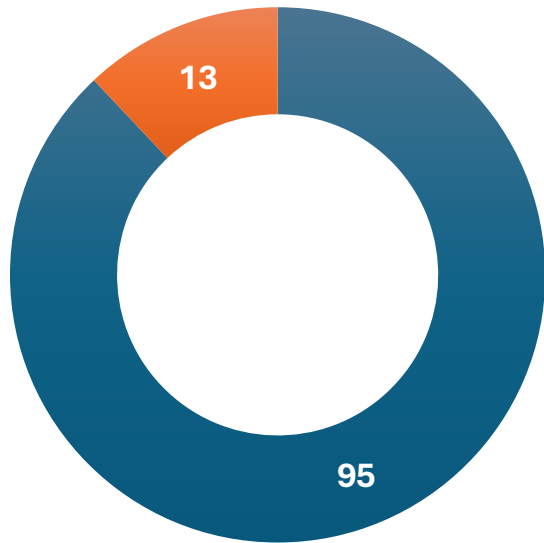
Marina Sousani
Astec Industries



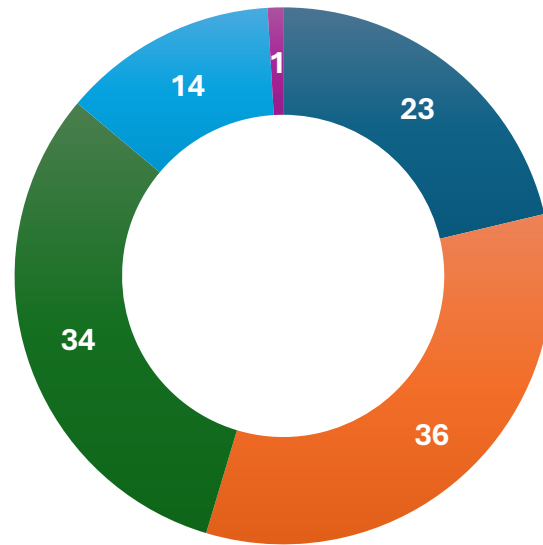
Anthony Thornton
University of Manchester

- Comprised of academic and industrial representatives
- Both the full Management Committee and the Advisory Committee meet quarterly.

Current membership

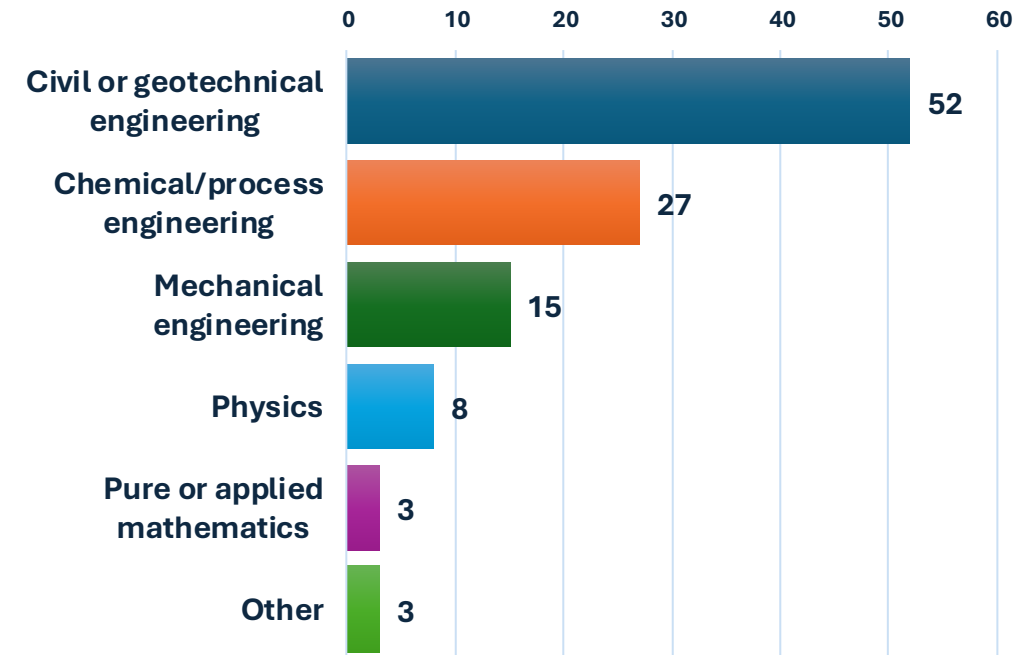


■ Academia ■ Industry



■ <5 years since my undergraduate degree
 ■ 5-10 years since my undergraduate degree
 ■ 10-20 years since my undergraduate degree
 ■ >20 years since my undergraduate degree
 ■ Other

Membership breakdown by field



Network events (NEs)



NE1: Edinburgh, May 2025



NE2: Abingdon, October 2025



NE3: Manchester, January 2026



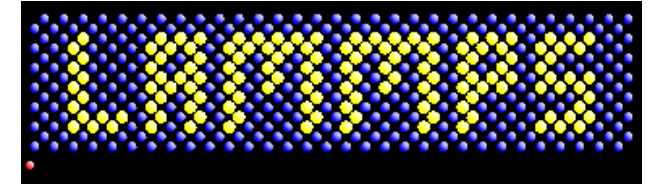
NE4: Belfast, March 2026



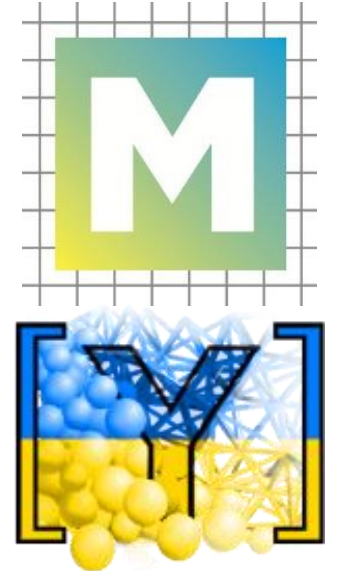
Training provision at NEs



- **NE1:** Using open-source DEM codes: LAMMPS, MercuryDPM & YADE
- **NE2:** Using HPC (ARCHER2) & running LAMMPS simulations on HPC
- **NE3:** Getting started with AI/ML for DEM users
- **NE4:** Data analysis & visualisation, running LAMMPS on GPU and advanced AI/ML



55



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Code benchmarking & development



- We are developing code benchmarking cases for all three codes and best-practice guidelines.
- In 2026, CCC-ParaSolS began a two-stage code development project:
 1. Adding particle capabilities to the Oxford Parallel library for Structured mesh solvers (OPS)
 2. Adding GPU capabilities to MercuryDPM through the OPS-Particle DSL

56

Discourse discussion forum



Category

- General**
Create topics here that don't fit into any other existing category.
- DEM Discussions**
A place for questions and discussions on DEM. Subcategories for specific DEM codes.
 - LAMMPS
 - MercuryDPM
 - YADE
 - LIGGGHTS
 - MFIX
 - Other
- Domain Specific Discussion**
 - GPU Computing
 - Geotechnical
 - Foods
 - HPC
 - Pharmaceutical
 - Physics
 - Geology
- Data**
 - Data Management
 - Data Processing
 - Analysis
- Community**
Non-technical topics of the ParaSoLS community, including announcements, upcoming events, new publications or other resources, advertisements, etc.
 - Announcements
 - Events
 - Teaching & Outreach
 - Diversity & Inclusion
 - Introductions
- ON-DEM**
A discussion forum for ON-DEM
 - General
 - WG1
 - WG2
 - WG3
 - WG4
 - WG5
 - WG6
- Visualisation Corner**
A place to show off your latest simulation or analysis. Or to ask questions on how to visualise complex data.
 - Paraview
 - Ovito
 - Python
- Jobs Board**
Welcome to the ParaSoLS Job board!
- Off-topic**
Topics that are not about CCC-ParaSoLS, DEM or do not fit in any other category.

CCC-ParaSoLS Network Event 4 — Belfast, 24th–26th March 2026 Events		2	18	4d
18th BGA Young Geotechnical Engineers Symposium Events networking, conference		0	10	4d
EPSRC fellowships - just announced Jobs Board		0	6	4d
Alert Geomaterials - Good source for job ads Jobs Board		0	6	4d
CUDA PINN Demo code GPU Computing gpu, ml		0	9	5d
Engaging the Community / Webinar Series Teaching & Outreach ccc-parasols, webinar		0	17	5d
Ray tracing and cpus for DEM GPU Computing		1	13	5d
Datasets for Data Analysis & Visualisation Session at NE4 Visualisation Corner ccc-parasols, data-analysis, paraview, vtk		2	24	6d
Prescribed angular and linear velocity LAMMPS		4	19	10d
(Re-)Creating mercury data files for running coarse graining with MercuryCG MercuryDPM data-analysis, mercurycg		5	21	11d
CCC-ParaSoLS Network Event 3 - Manchester, January 7th-8th, 2026 Events		5	61	13 Feb
Past, Present and Future of Particle Technology Conference — Leeds, 30 March–1 April 2026 Events		0	4	13 Feb



<https://parasols.discourse.group/>

How to become a member too?



<https://www.ccc-parasols.ed.ac.uk/about/join.html>



I would like to
join CCC-ParaSols



ParaSols
Particulate Solids Simulations

Join the CCC-ParaSols Community

Become a member of the community

Enter your First Name*

Enter your Last Name*

Enter your Affiliation*

Please provide the main organisation you are affiliated with

Enter your email address to subscribe*

EMAIL

Provide your email address to subscribe. For e.g abc@xyz.com

I agree to receive your newsletters and accept the data privacy statement.

You may unsubscribe at any time using the link on our website.

SUBSCRIBE

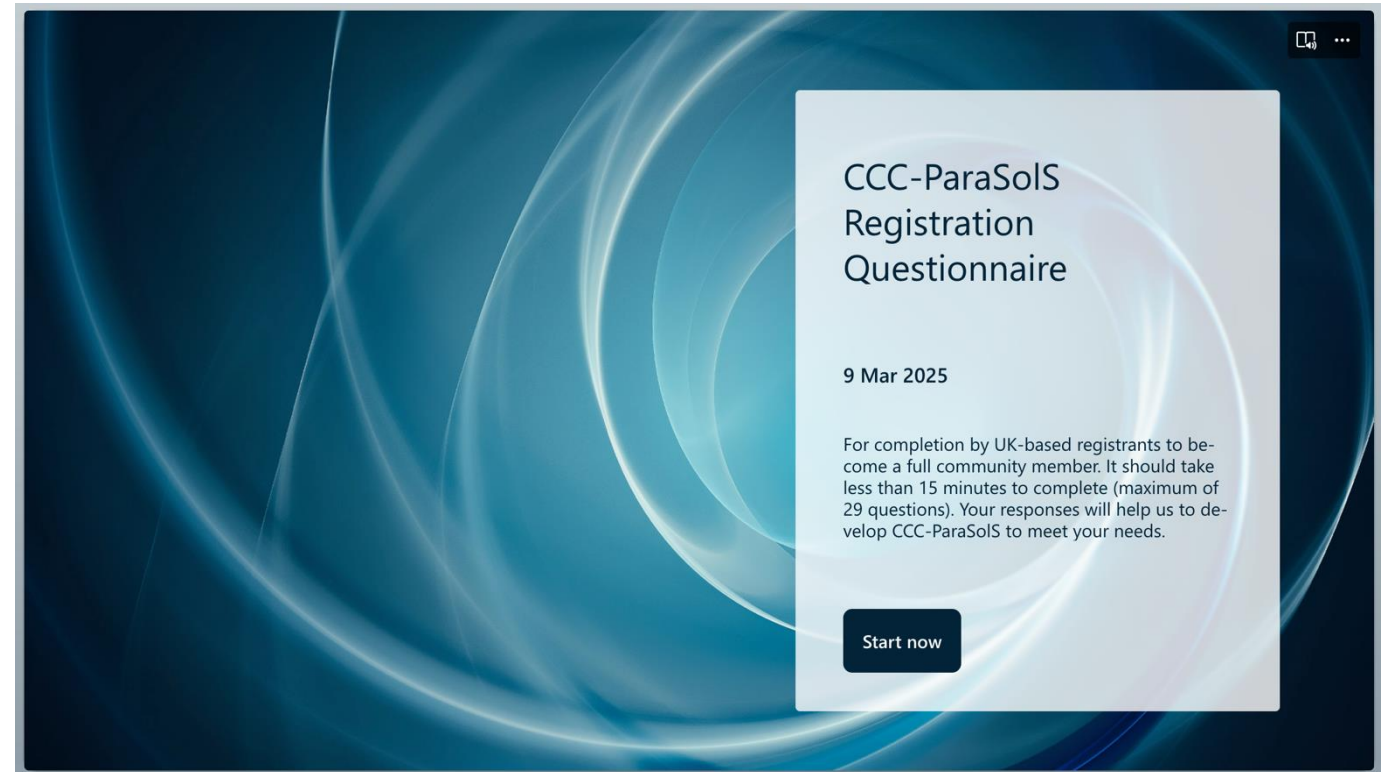
We use Brevo as our marketing platform. By submitting this form you agree that the personal data you provided will be transferred to Brevo for processing in accordance with [Brevo's Privacy Policy](#).

How to become a member too?



59

- You will then be e-mailed a link to a registration questionnaire.
- This must be completed to become a full community member.
 - Should take < 15 minutes to complete



Get in touch



ParaSols

Particulate Solids Simulations

parasols@ed.ac.uk

<https://www.ccc-parasols.ed.ac.uk/>



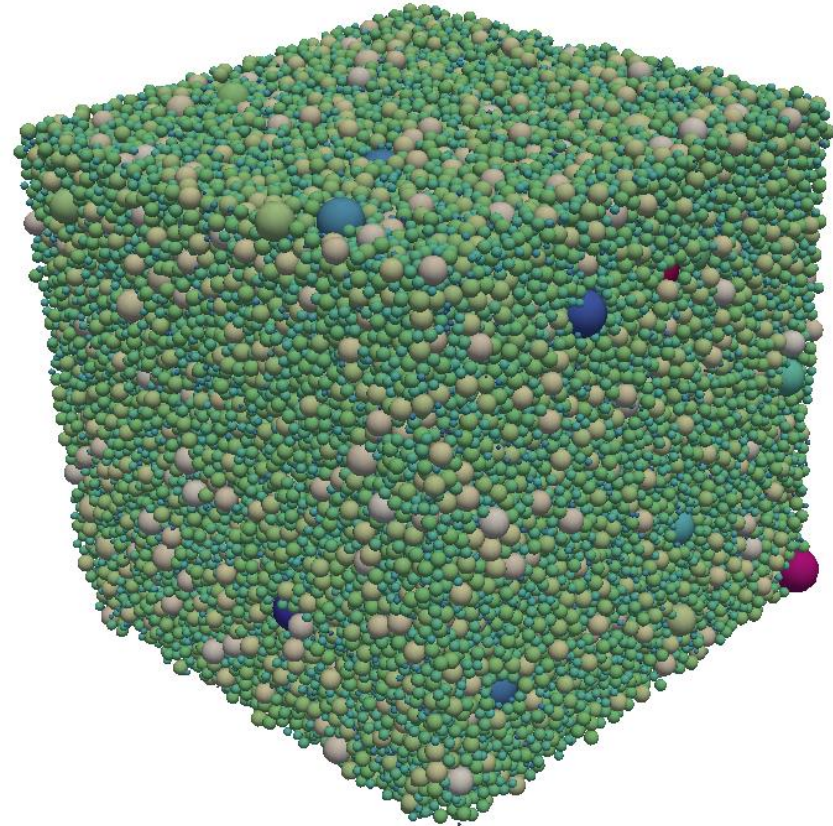
<https://parasols.discourse.group/>



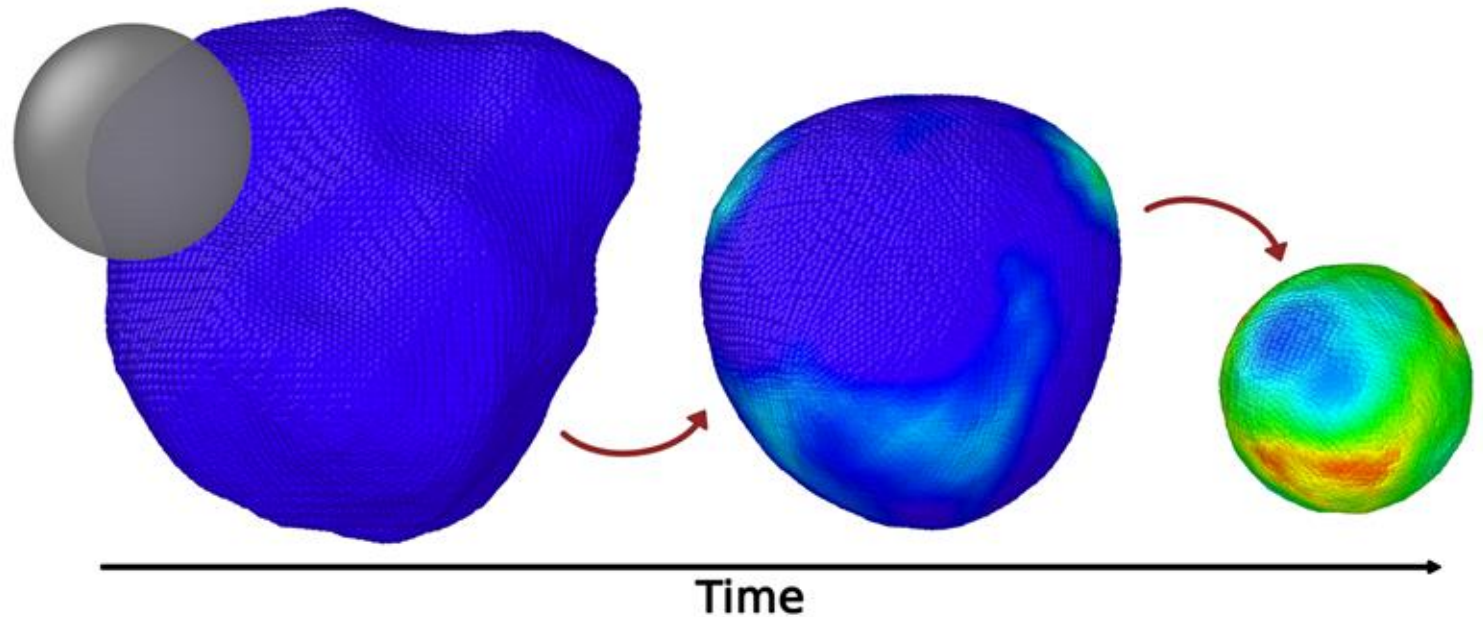
<https://www.linkedin.com/company/ccc-parasols/>

- HPC has been essential for my research and that of my collaborators.
- The DEM community should be making greater use of HPC.
 - Often many variations of a baseline DEM simulation are run — even small simulations could be bundled together to make effective use of HPC.
- CCC-ParaSols is helping to lower the barriers to using open-source codes and to accessing HPC.
- The changes of computing architectures within the UK's Digital Research Infrastructure (DRI) necessitate code developments.

- Enormous thanks to the research collaborators on the research presented herein:
- For ‘Case study 1: triaxial tests of granular soils’
 - Jonathan Fannin
 - Xin Huang
 - Joel Keishing
 - Fiona Kwok
 - Catherine O’Sullivan
 - Tom Shire
 - Kevin Stratford
 - Ahmer Wadee



- Enormous thanks to the research collaborators on the research presented herein:
- For ‘Case study 2: abrasion in particle systems’
 - Rosario (Enzo) Capozza
 - Haydn Rogan
 - David Scott
 - Kevin Stratford
 - James Young



- The Core Team behind the CCC-ParaSols project also comprises
 - David Emerson
 - John (JP) Morrissey
 - Catherine O'Sullivan
 - Stefano Rolfo
 - Chrysovalantis Tsinginos



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 - EPSRC EP/R005877/1 for the abradable DEM research
 - UKRI/ST/B000493/1 for CCC-ParaSolS
- And for access to HPC resources:
 - CURIE (Tier-0)
 - HECToR / ARCHER / ARCHER2 (Tier-1)
 - Cirrus (Tier-2)
 - Institutional clusters (cx1 @ Imperial & Eddie @ Edinburgh)



Engineering and
Physical Sciences
Research Council



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