Implementation of multi-level contact detection in granular LAMMPS to enable efficient polydisperse DEM simulations

Tom Shire (University of Glasgow)

Kevin Hanley (University of Edinburgh)

Kevin Stratford (EPCC)

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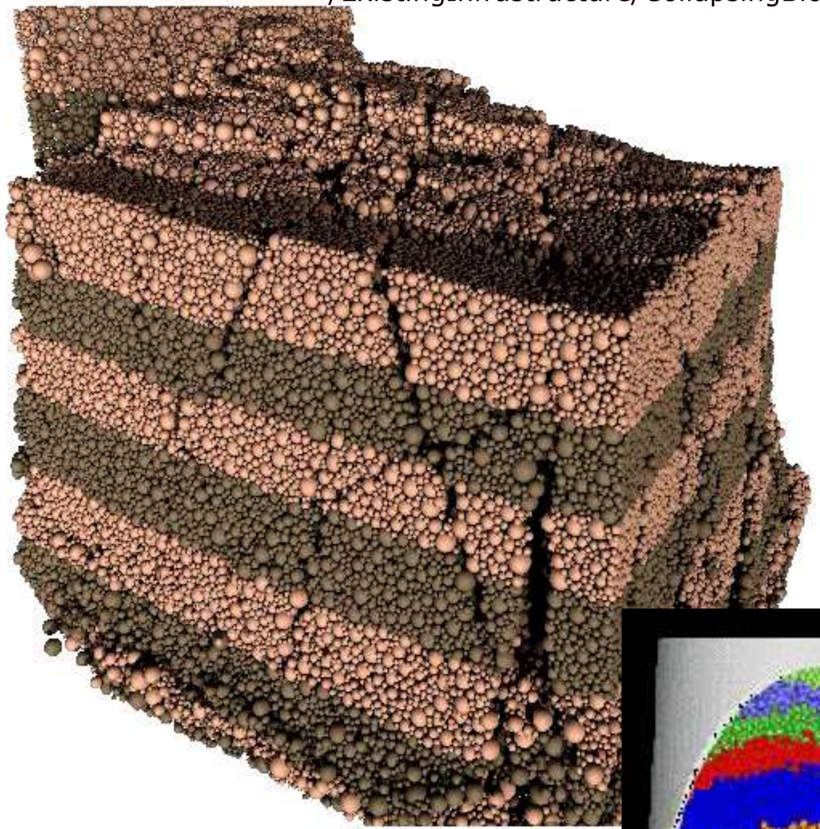
ARCHER-funded project to improve contact detection for polydisperse materials in Granular LAMMPS

- Motivation and current methods
- Improved method (Hierarchical Stencil)
- Parametric studies

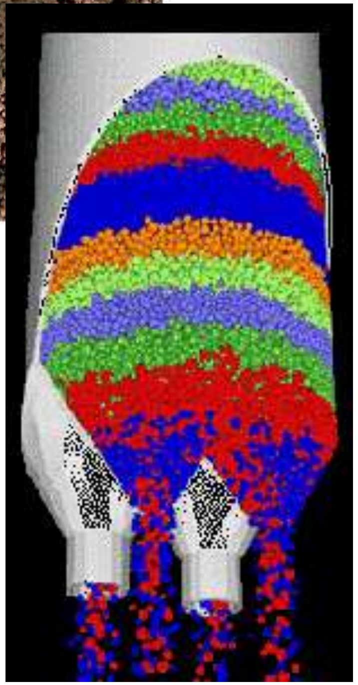
Micromechanics

https://twiki.auscope.org/wiki/pub/EarthSim/ExistingInfrastructure/CollapsingBlock3.png



DEM: Discrete Element Modelling

- Models collection of individual grains
- Developed in 1970s, but use increasing with computer power
- Allows micro-scale mechanisms to be observed

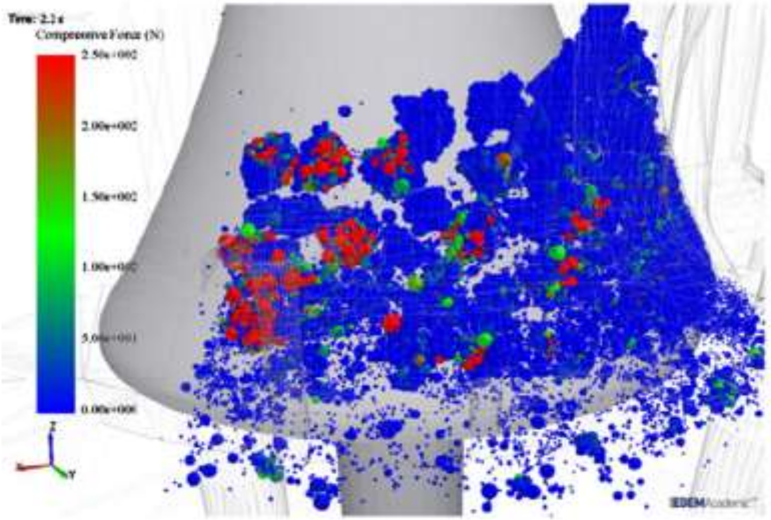


http://www.cmis.csiro.au

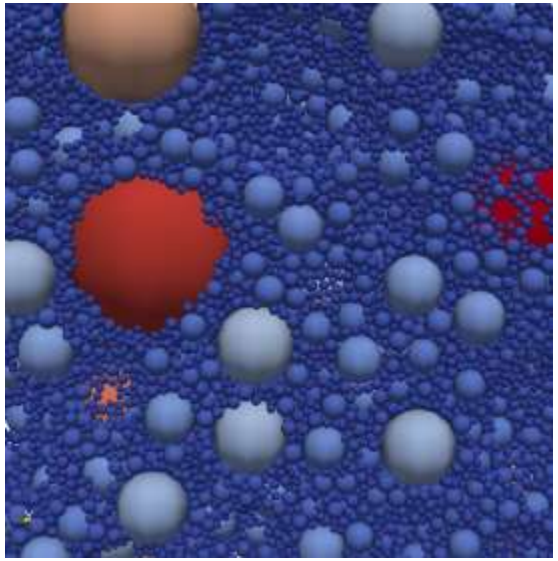
Polydisperse granular materials

Polydisperse granular materials occur in many important natural and industrial processes including:

- Geotechnical engineering
  - Natural soils with wide range of particle sizes
  - Sand particle crushing during foundation installation
- Minerals processing (crushing and segregation in grinders)
- Avalanches and landslides
- Fluidised beds



Weerasekara et al. (2013)

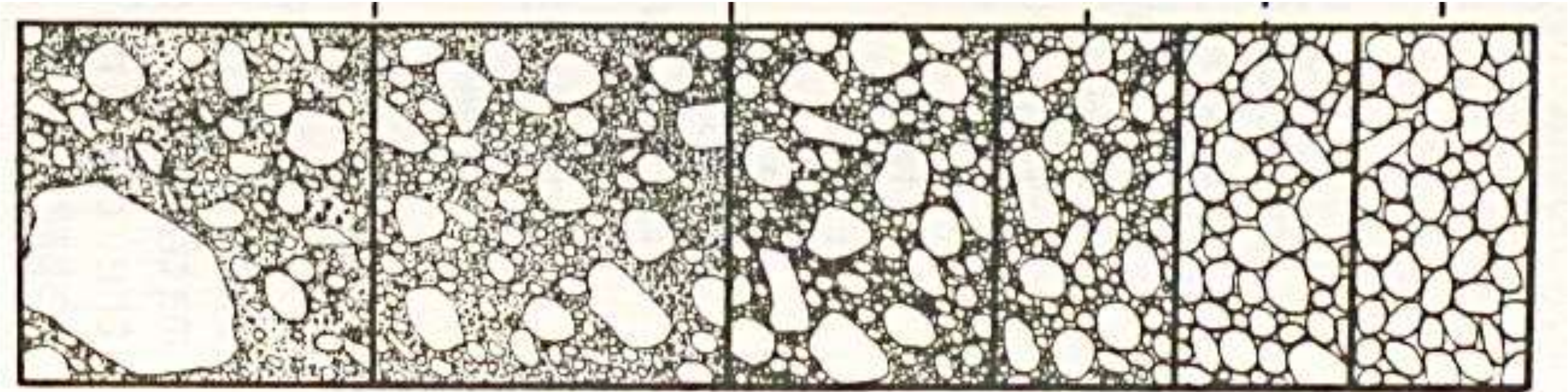


Polydisperse granular materials

Effect of polydispersity (i.e. a wide range of particle sizes) has only recently started to be considered with discrete element modelling

Polydisperse DEM – much more time consuming:

- More particles required
- Traditional contact detection much slower for polydisperse

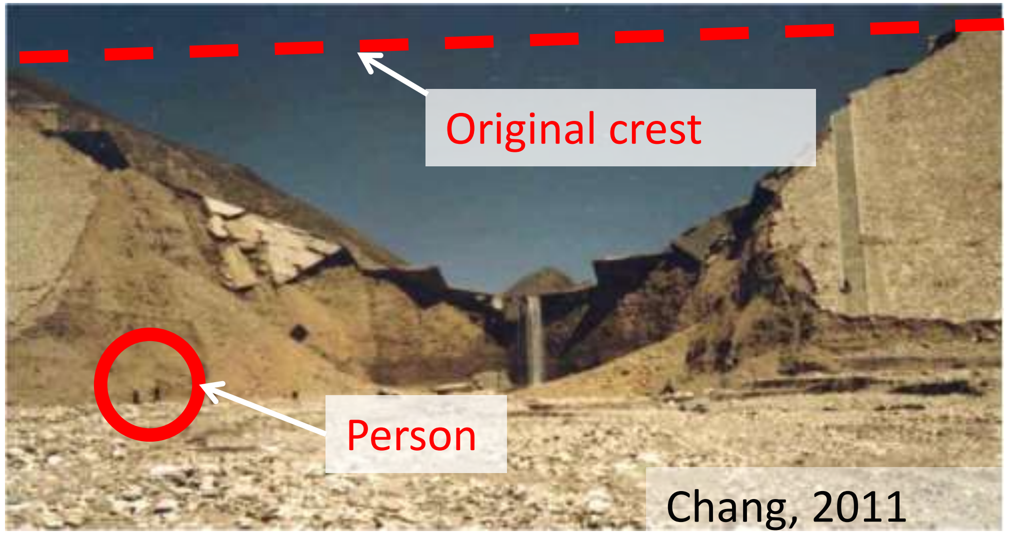


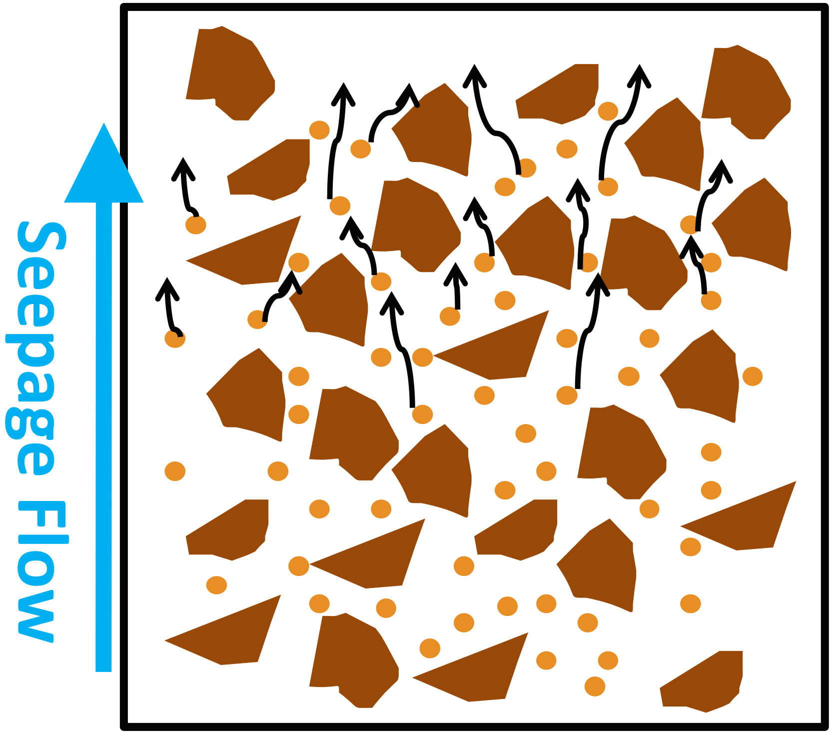
Context: Suffusion

Form of erosion in gap graded soils

Fine fraction eroded by seepage;
Coarse fraction stays in place

Erosion of fines at **low hydraulic gradients (*i = Δh/L*)**





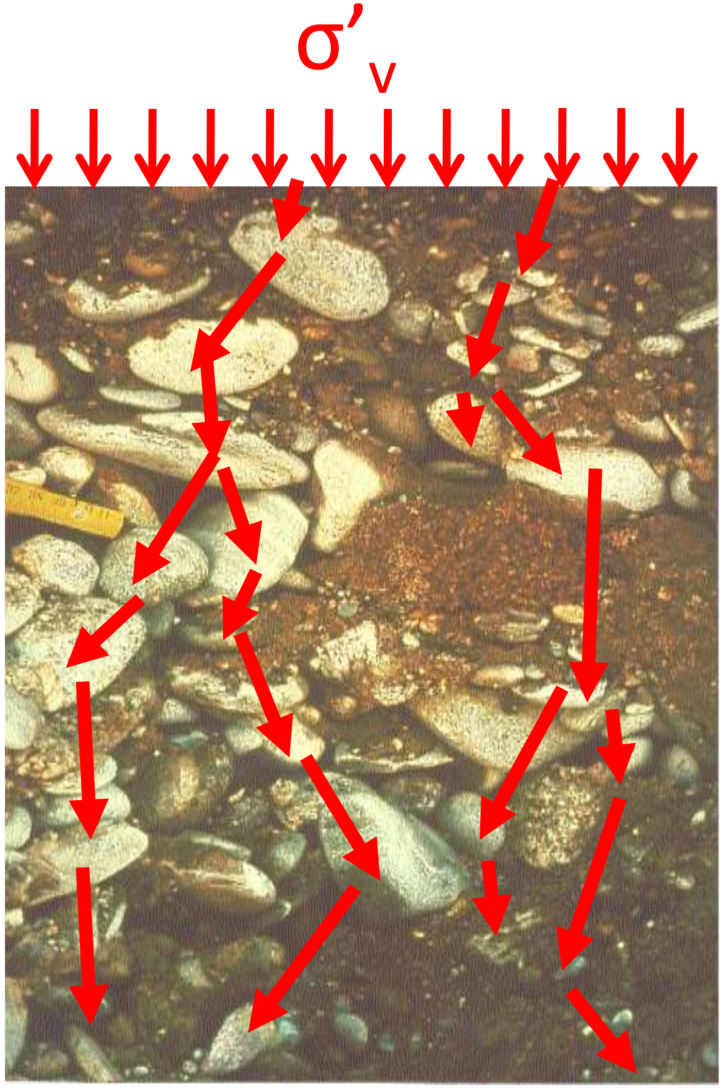
Gouhou Dam, China (1993):

71m High; 300 Deaths

Context: Suffusion

Coarse particles transfer stress, fines loose and under reduced stress

- DEM used to analyse stress in coarser and finer fraction (effect of fabric)
- DEM-CFD used to model initiation of suffusion
- Such soils are highly polydisperse: real rockfill dam materials can be $R_{max}/R_{min} \approx 10000+$



DEM

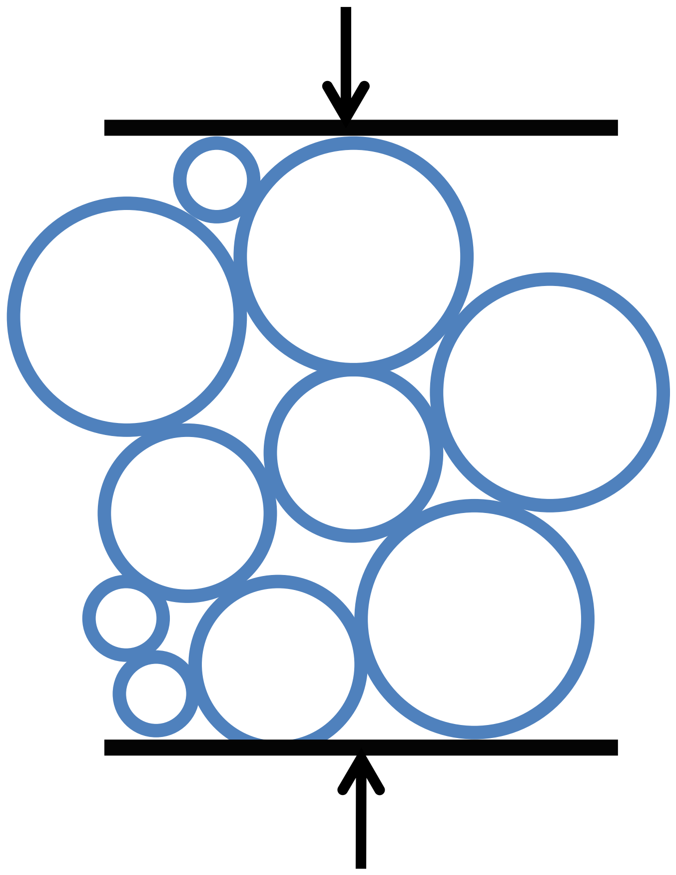
- Most geomechanics codes based on Distinct Element Method: Cundall and Strack (1979)

- Consider only coarse particles (>100μm):
  - Body forces dominate

- LAMMPS contains a popular DEM package for use with HPC systems
  - Highly efficient for massively parallel simulations

DEM – Calculations in a Timestep

Initial information:
- Particle geometry, density
- Other geometry e.g. walls
- Contact model



DEM – Calculations in a Timestep

Initial information:
- Particle geometry, density
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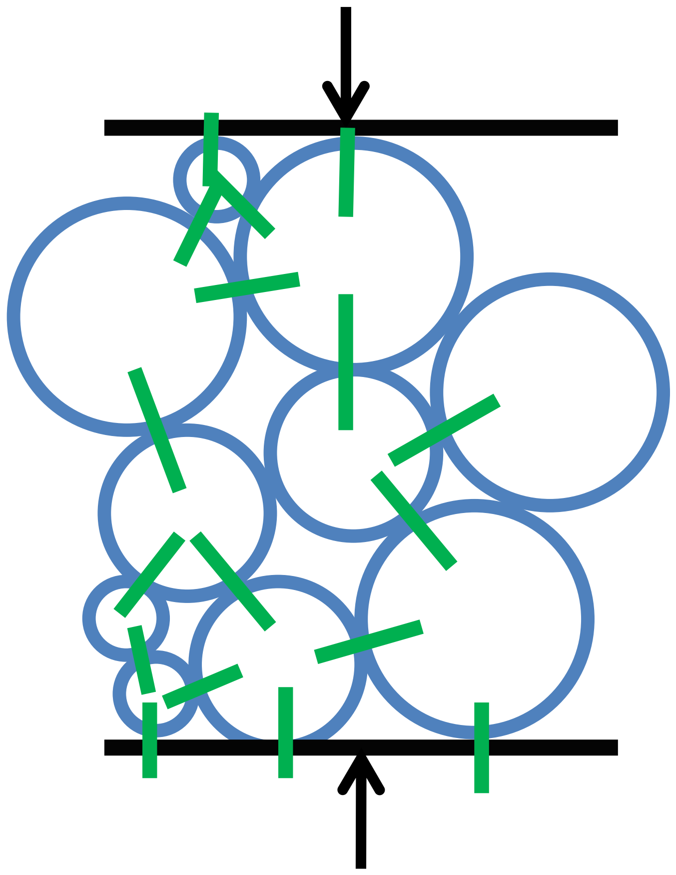
- Contact model

Time = t
•Identify particles in contact
•Calculate contact force
(proportional to overlap)



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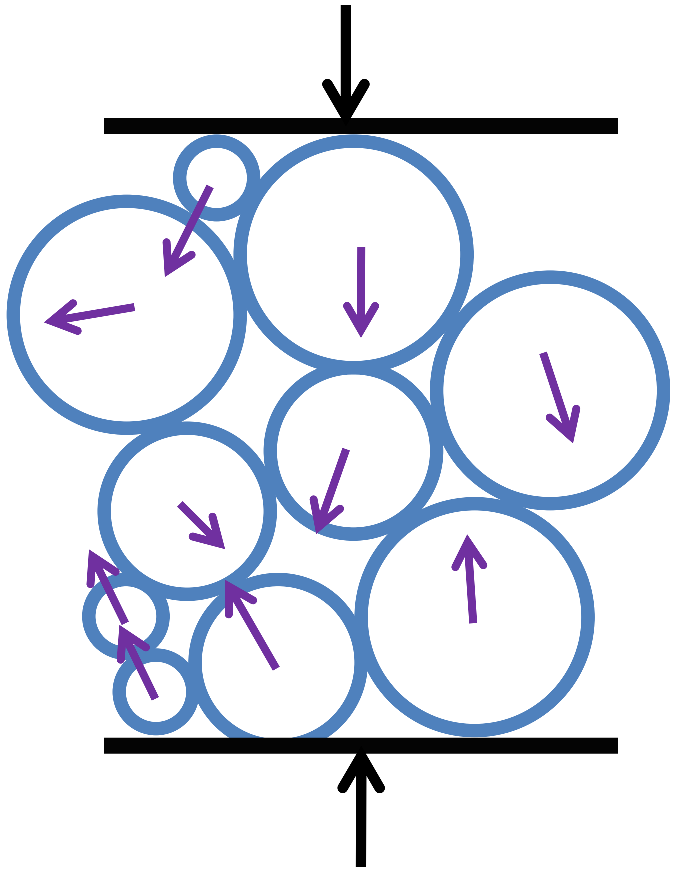
↓

•Calculate resultant force for each particle



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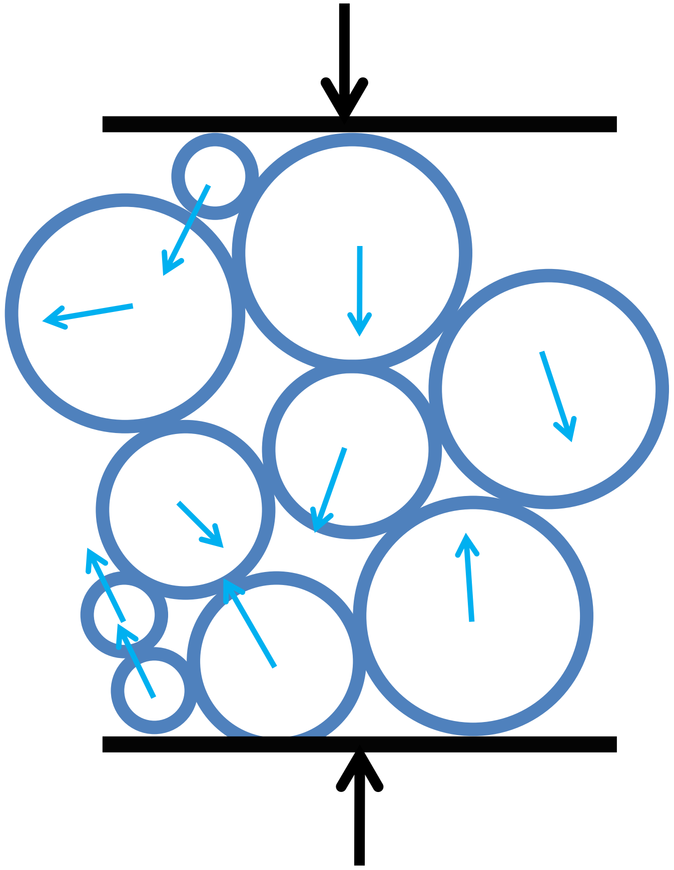
•Calculate accelerations (F = ma)
•Integrate for velocities



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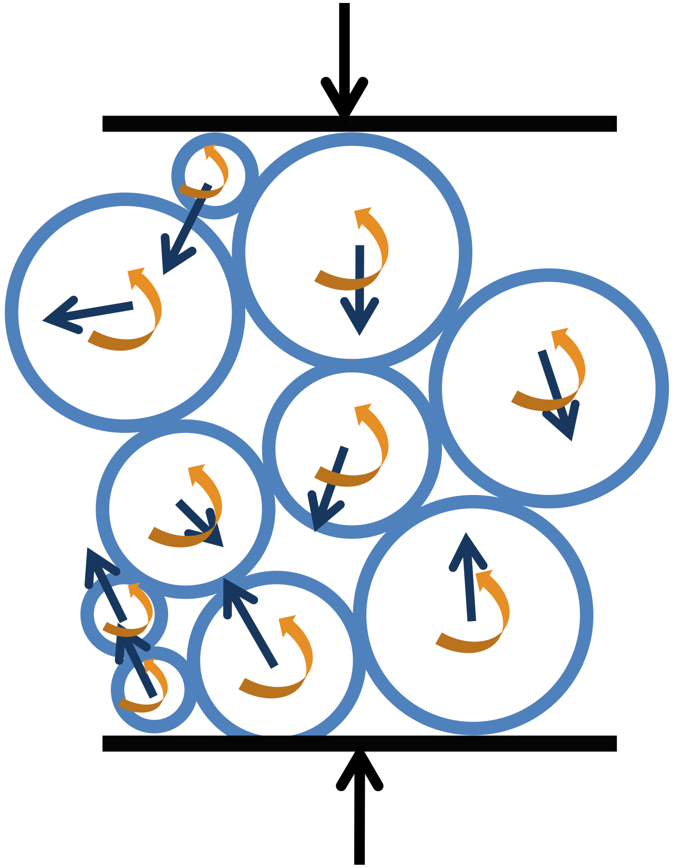
•Calculate displacements and rotations
•Update particle positions at end of timestep



DEM – Calculations in a Timestep

Initial information:
- Particle geometry, density
- Other geometry e.g. walls
- Contact model

Move forward one timestep

Time = t + Δt
- Identify particles in contact
- Calculate contact force (proportional to overlap)

↓

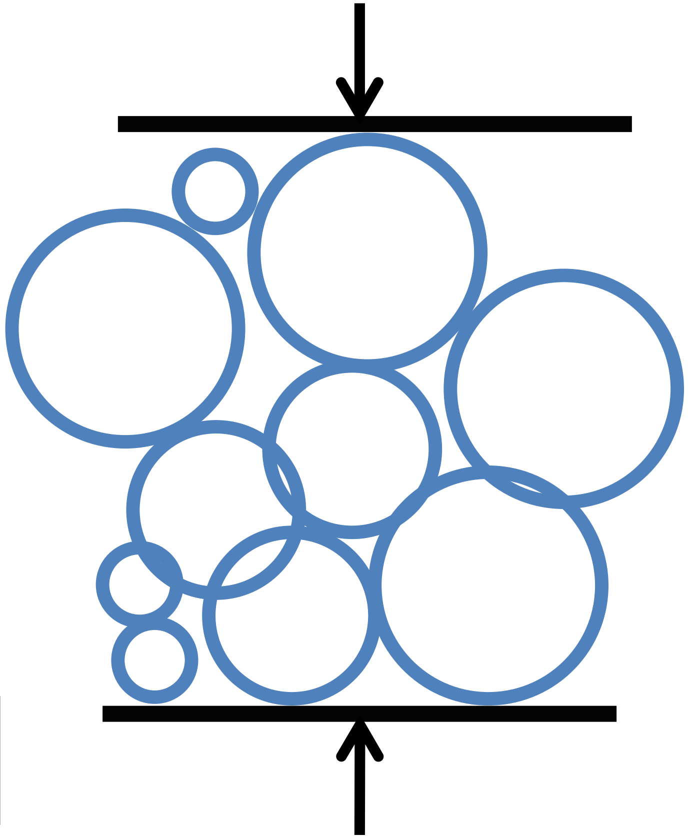
- Calculate resultant force for each particle

↓

- Calculate accelerations (F = ma)
- Integrate for velocities

↓

- Calculate displacements and rotations
- Update particle positions at end of timestep



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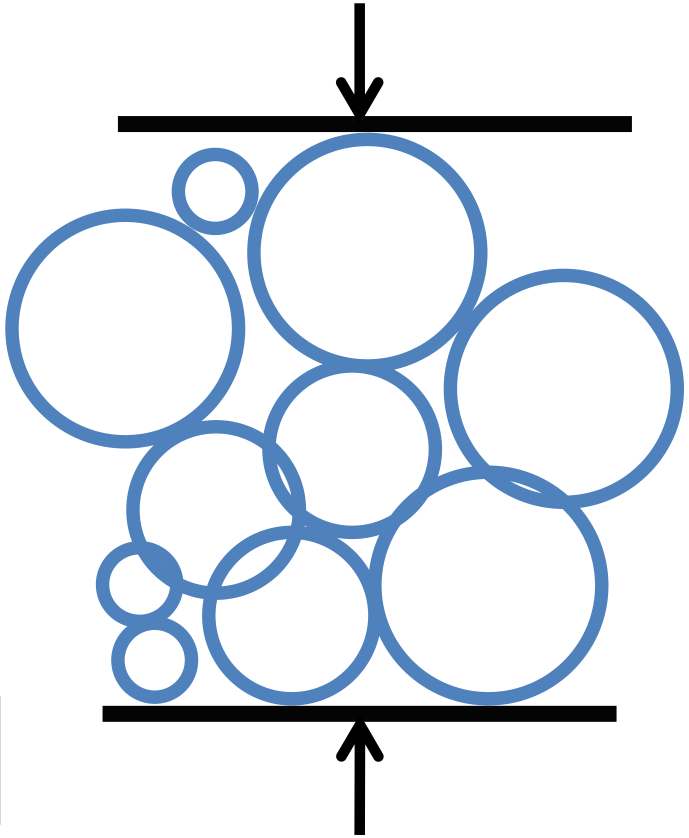


Contact detection

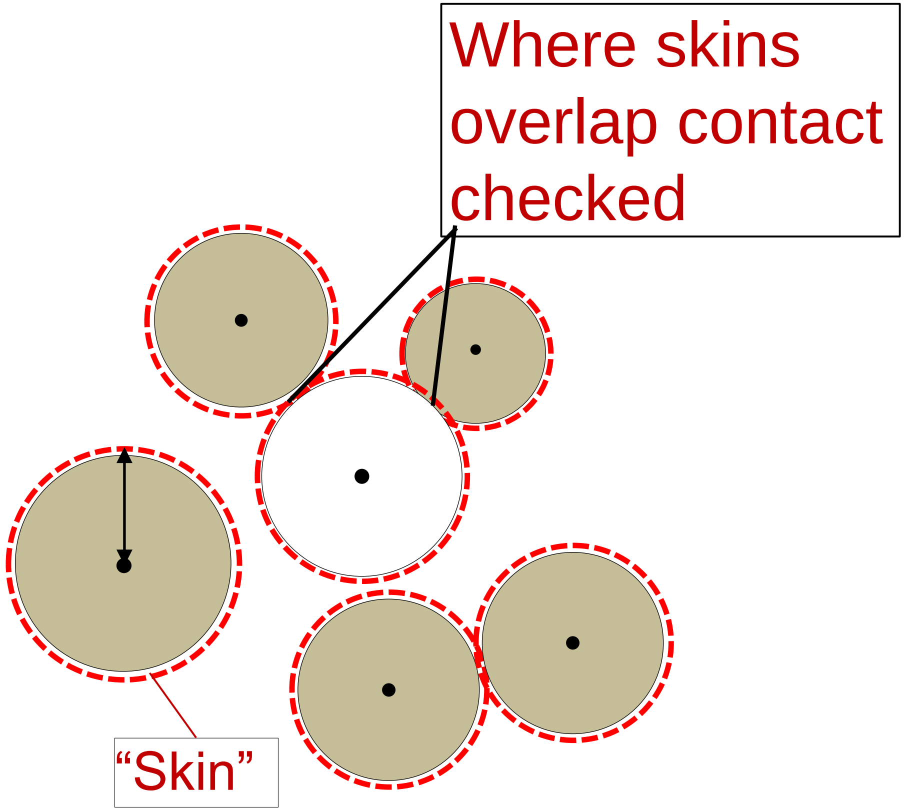
Neighbour lists

Each particle has a surrounding “***skin***” (perhaps ~ 10% of diameter)

Neighbour list stores list of pairs whose skins overlap

At each timestep: check contacts between listed neighbour pairs

Intermittently ***rebuild neighbour list*** as particles move

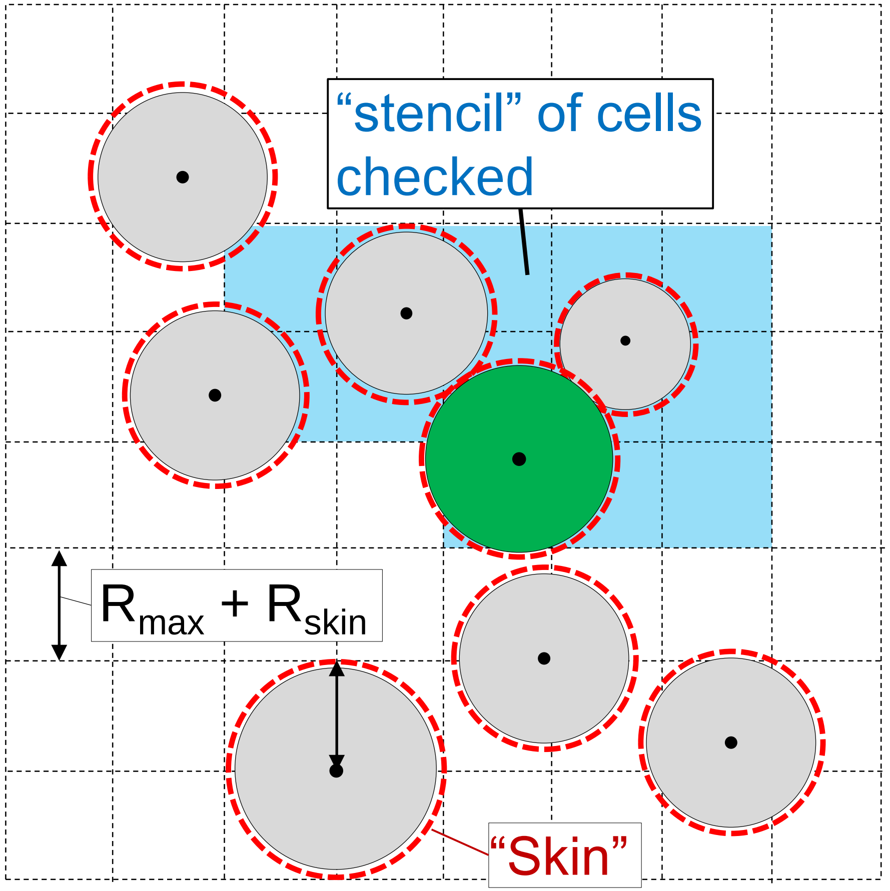


Contact detection : link-cell method

Building the neighbour list:

Link-cell method used to avoid checking all particle pairs:

1. Link-cells overlain on DEM domain
   - Cell length ~max particle radius
2. For a given particle:
   - Check for skin overlaps in “home cell” and surrounding cells
   - Where skins overlap pair added to neighbour list

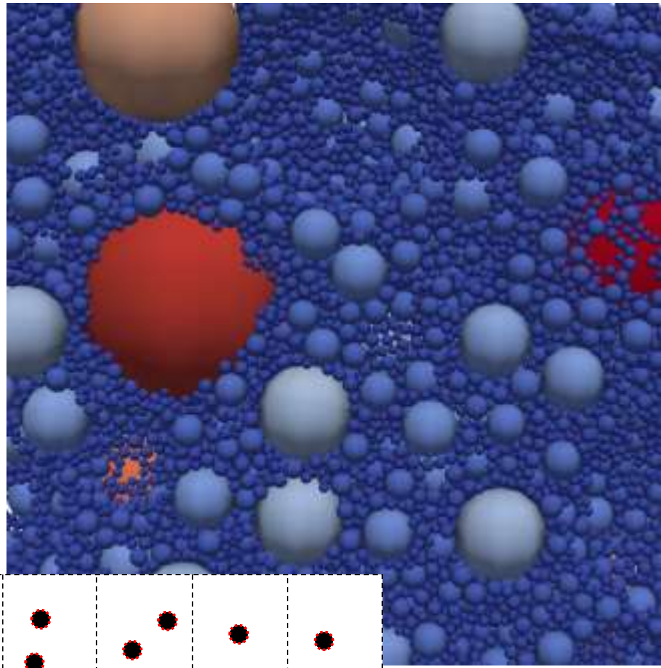


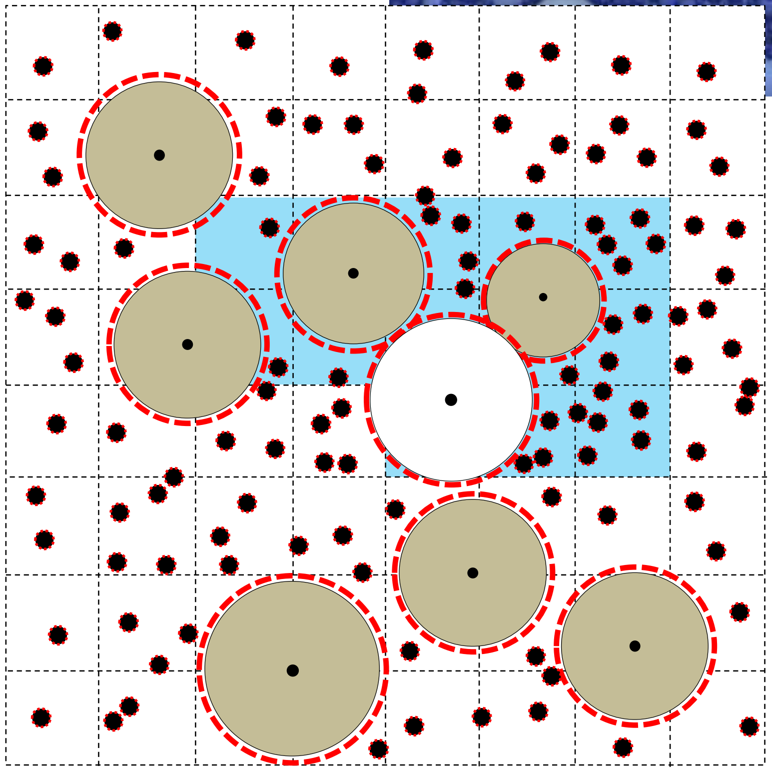
Drawbacks

Link-cells are efficient for monodisperse DEM

But when for polydisperse DEM neighbour list building becomes prohibitive

Cell size based on R_{max} means huge numbers of small particles in each cell





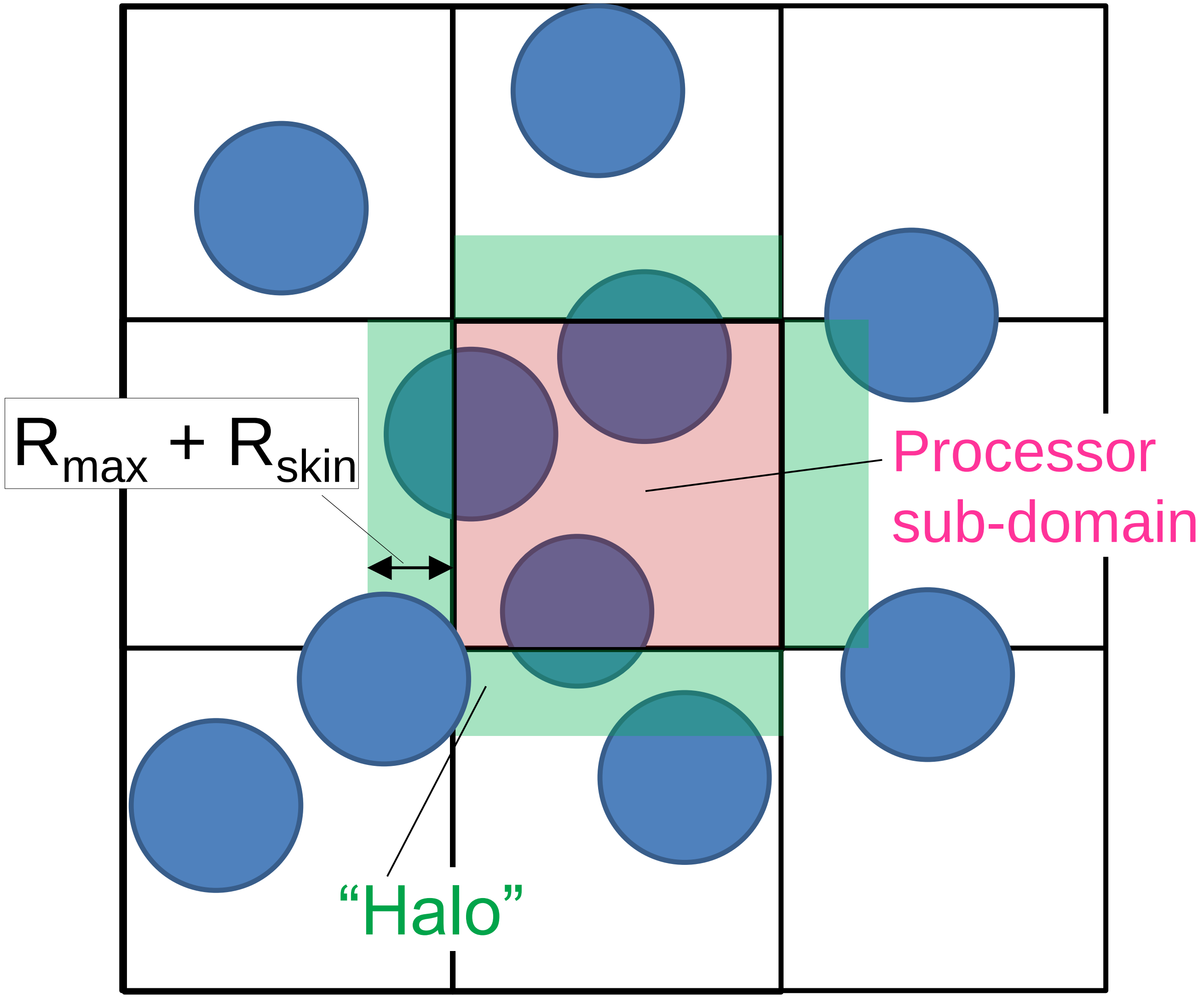
Inter-processor communication

Spatial decomposition for parallel processing

Communicate particle information across processor sub-domain boundaries

“Halo” across which comm occurs related to R_{max}

Similar drawbacks to link-cells



Archer project

Aims:

1. Extend existing contact detection scheme for MD part of LAMMPS (in ‘t Veld et al, 2008) to work for DEM part
2. Demonstrate effectiveness and scaling for large DEM simulations of polydisperse particles on ARCHER
3. Release a well-documented version of the implementation into the main version of the open-source LAMMPS code