

CCC-ParaSols:

Creating a Collaborative Computational Community in Particulate Solids Simulations



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Why Particulate Solids Simulations?

Particulate solids encompass natural soil deposits, pharmaceutical powders, food ingredients (e.g., powdered milk, flour), aggregates and cement used in construction, etc. Particulate solids are often inputs to manufacturing processes or are produced as intermediate/final products and as such, **they have significant economic and societal importance**. For example, they are **fundamental to the UK chemical & pharmaceutical industry** which annually generates over £60bn of exports and directly employs more than 130,000 people across over 4,000 businesses.

Particulate solids form complex systems with material behaviours that are difficult to understand and predict. Particulate solids simulations explicitly model particles and their interactions to provide insights into granular behaviour that are difficult, or impossible, to obtain experimentally. The **most popular particle-scale simulation method is the Discrete Element Method (DEM)**, although there are many others.

Aims & Objectives

CCC-ParaSols will build the first and only overarching UK community for members from both academia and industry that exploit DEM and related methods.

It will also:

- **Promote** the use of open-source software
- **Develop** code benchmarking cases and best-practice guidelines
- **Deliver bespoke training** on using open-source codes and accessing high-performance computing (HPC), in order to take advantage of the UK's digital research infrastructure
- **Undertake one or more high-priority code development projects** based on this community needs
- Create a five-year vision for the community
- Produce a viable plan for a Collaborative Computational Project in particulate solids simulations.

Network & Training Events

The first Network Event took place at the University of Edinburgh from 14-16th May 2025.

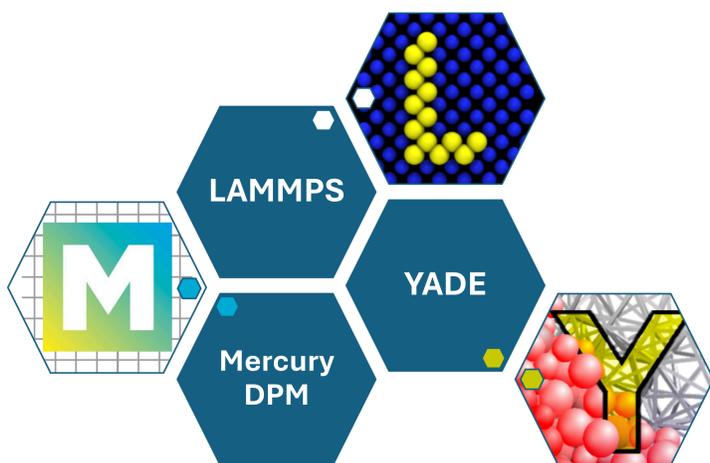


Figure 1: CCC-ParaSols members attending event 1.

More than 30 people joined the 3-day event in person, with a further 10 online. Introductory training on the three DEM codes was undertaken over two days.

Open-source DEM Tools

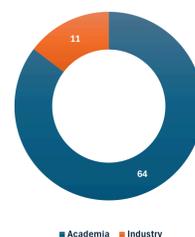
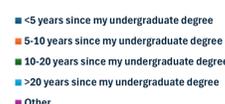
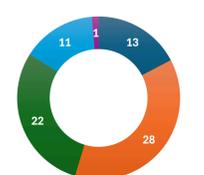
CCC-ParaSols will prioritise three open-source DEM codes: **LAMMPS**, **MercuryDPM** and **YADE**.



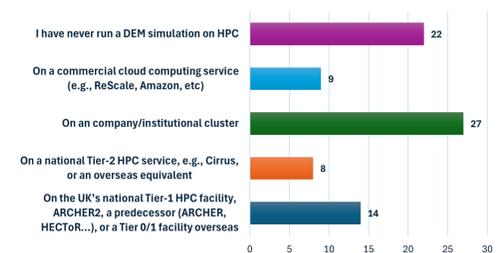
These three codes have been selected because of their **popularity** and **scalability**: all are MPI-parallelised; YADE and LAMMPS also have GPU capabilities.

Community Membership

Strong community response with 75 currently registered members from a variety of backgrounds and with varying experience.



Have you run a DEM simulation on a HPC facility?



Membership breakdown by field

