

# 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. They 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 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 HPC, in order to take advantage of the UK's DRI
- 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

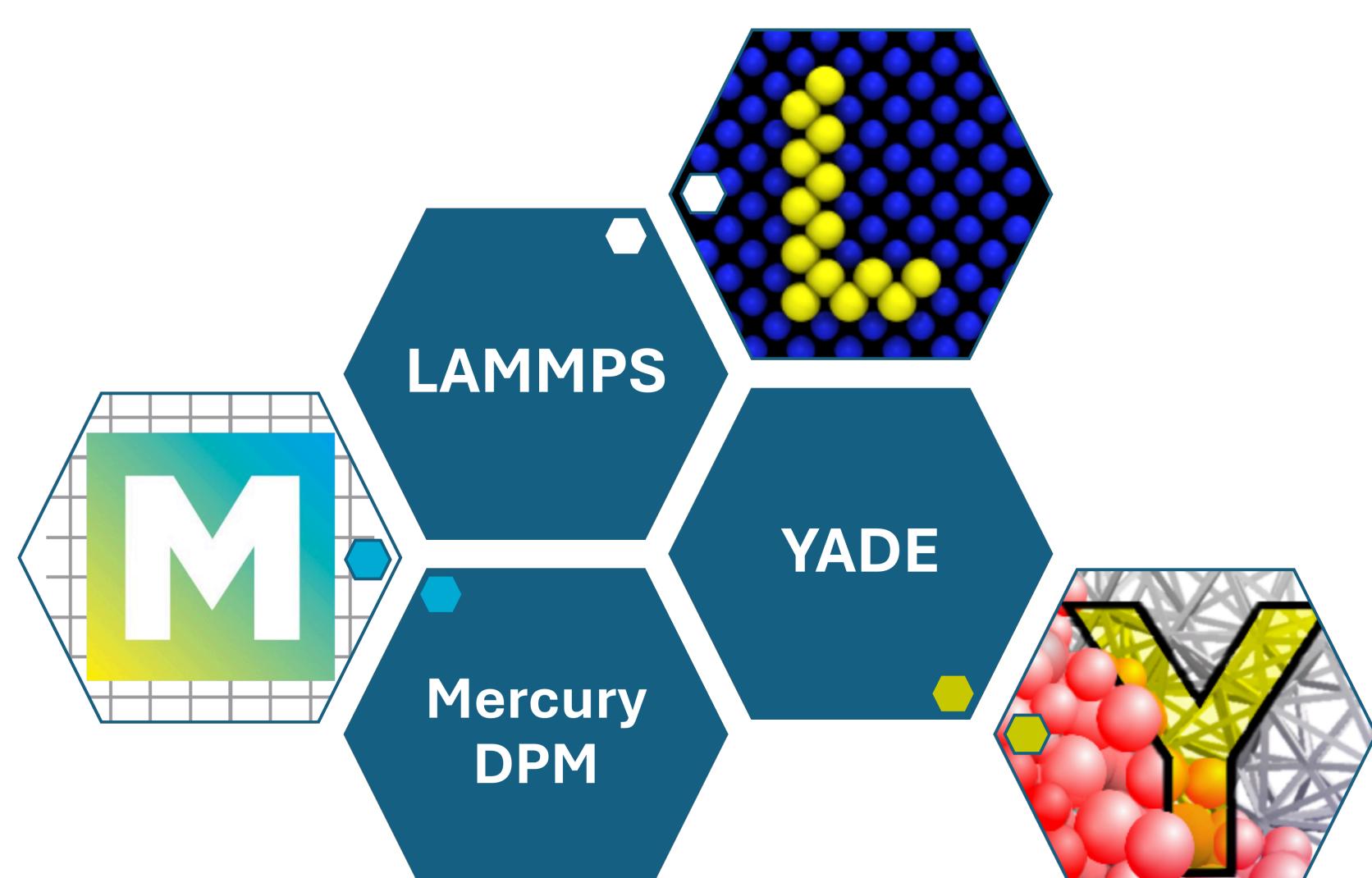
Network Event 1 took place at the University of Edinburgh from 14-16<sup>th</sup> May 2025 and Network Event 2 was held in Abingdon from 13-15<sup>th</sup> October 2025, with many attendees joining online.



Introductory training on the three DEM codes was delivered as well as training on the use of HPC via ARCHER2.

Network Events 3 & 4 are planned for 2026.

## Open-source DEM Tools



Three DEM codes have been prioritised because of their popularity and scalability: all are MPI-parallelised.

Both YADE and LAMMPS also have GPU capabilities.

## Code Development

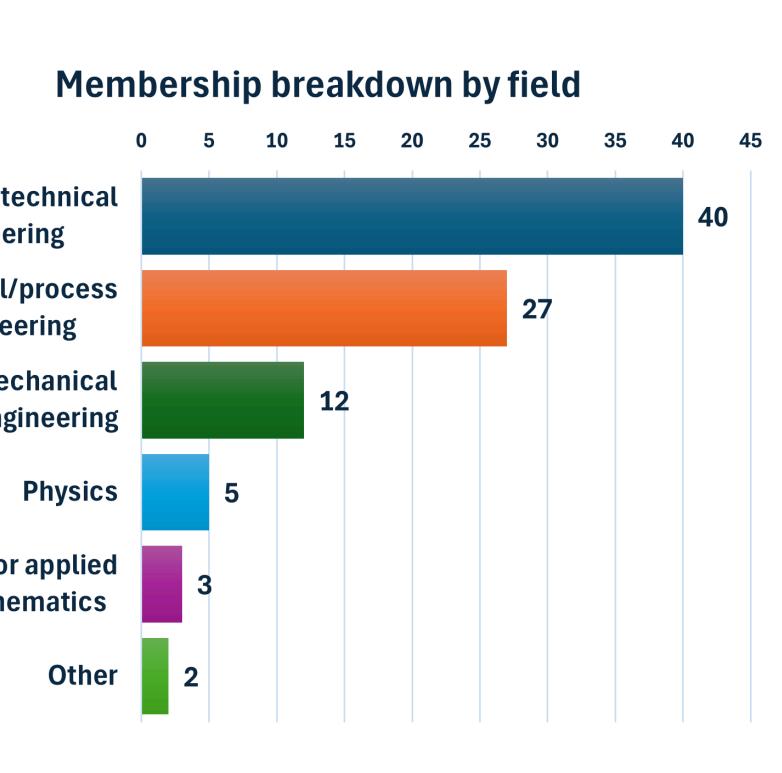
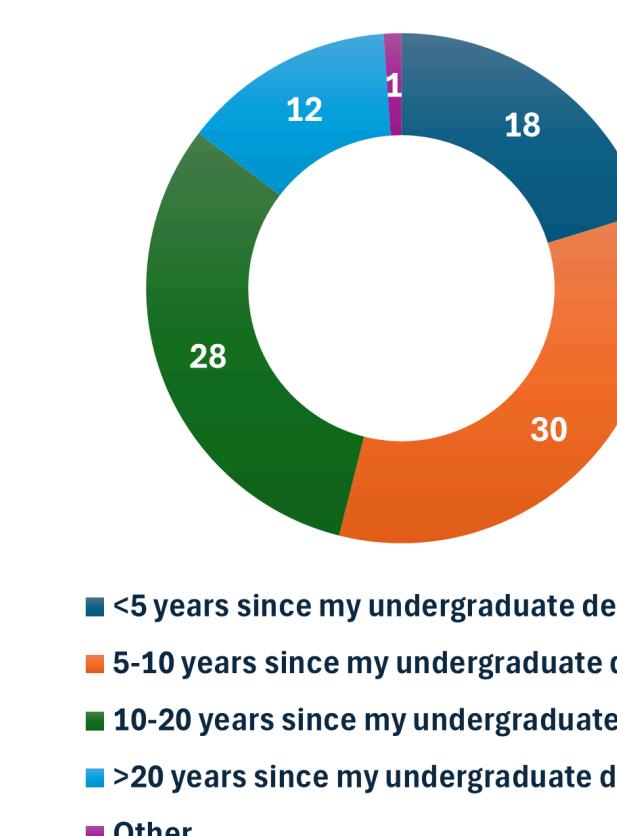
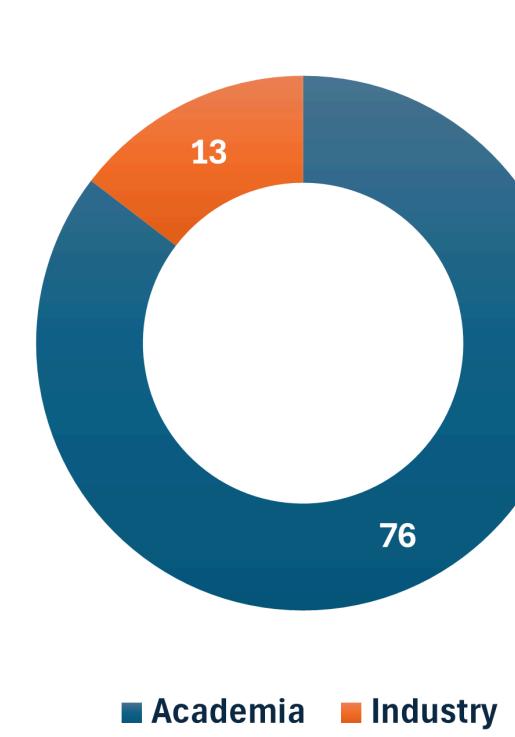
CCC-ParaSolS has one year of a developer's time from CoSeC for DEM code development. The community has been engaged and multi-step process has been followed to identify the priority code developments.

Based on the gathered feedback, the addition of GPU capabilities to MercuryDPM will be pursued.



## Community Membership

Strong community response with ~90 currently registered members from a variety of backgrounds and with varying experience.



## Five-Year Vision

Our main goal is to develop a suite of high-performance, validated and scalable open-source codes for particulate solids simulations, and democratise adoption of these codes for economic and societal benefit in the UK.

These benefits include increased sustainability through:

- reducing waste and increasing process efficiency within numerous sectors of industry
- pre-empting natural disasters caused by climate change