

# 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

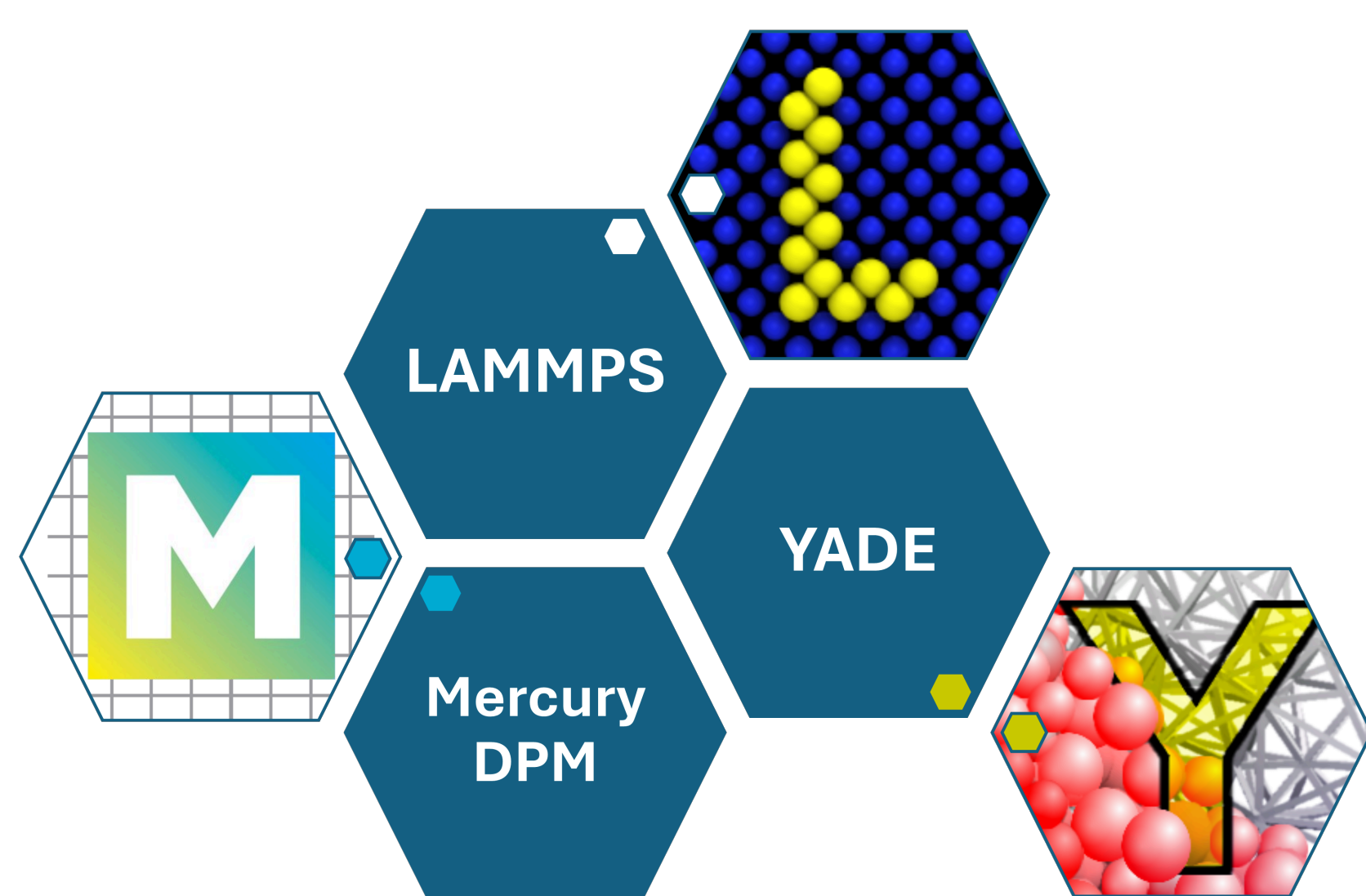
**Network Event 1** took place at the *University of Edinburgh* from 14-16<sup>th</sup> May 2025 and **Network Event 2** was held in *Abingdon* from 13-15<sup>th</sup> October 2025, with many attendees joining online.



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

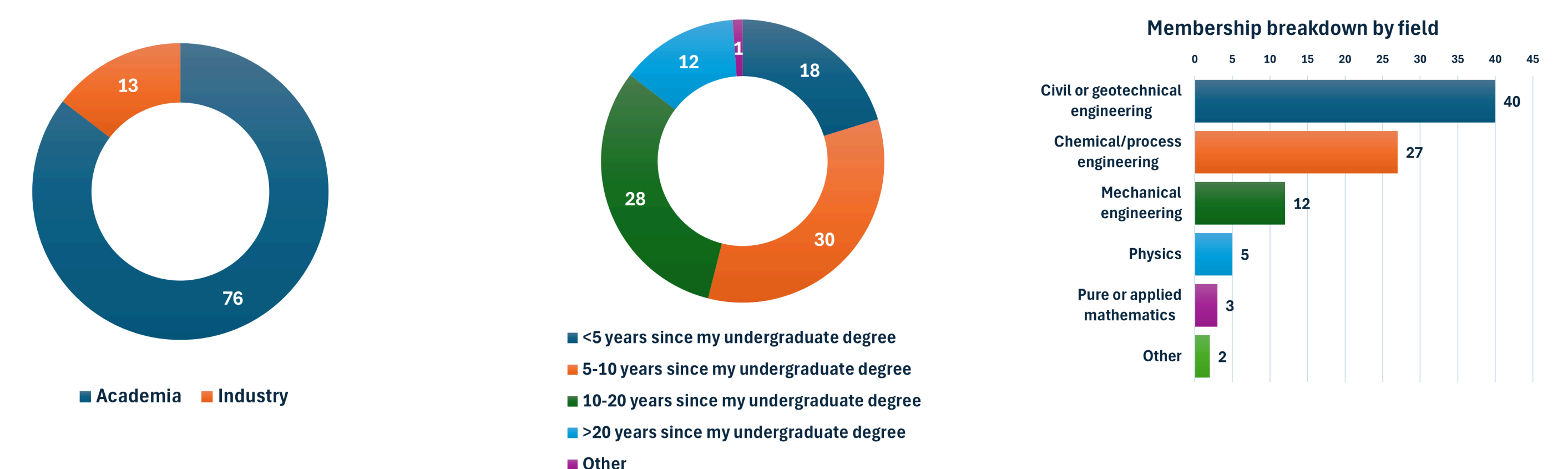


Three DEM codes have been prioritised because of their **popularity** and **scalability**: all are **MPI-parallelised**.

Both YADE and LAMMPS also have **GPU capabilities**.

## Community Membership

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



## 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.



## 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