

CCC-ParaSols: 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 method is the Discrete Element Method (DEM)**, although there are many others.

Aims & Objectives

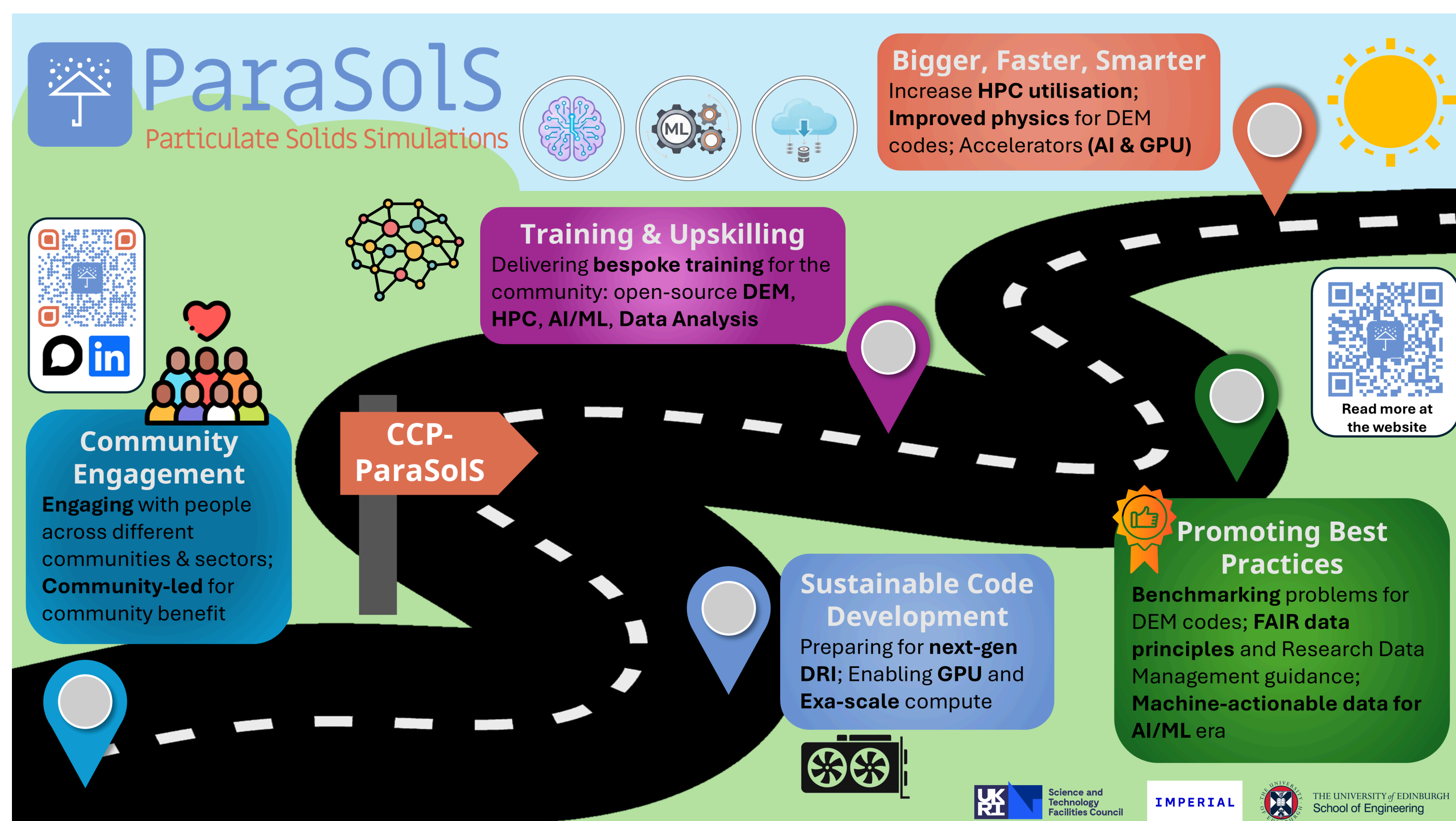
CCC-ParaSols is building an overarching UK community for members from both academia and industry that exploit DEM and related methods.

It is also:

- **Promoting** the use of open-source software
- **Developing** code benchmarking cases and best-practice guidelines
- **Delivering bespoke training** on using open-source codes and accessing HPC, in order to take advantage of the UK's DRI
- **Undertaking high-priority code development projects**
- **Producing a viable plan for a Collaborative Computational Project in particulate solids simulations.**

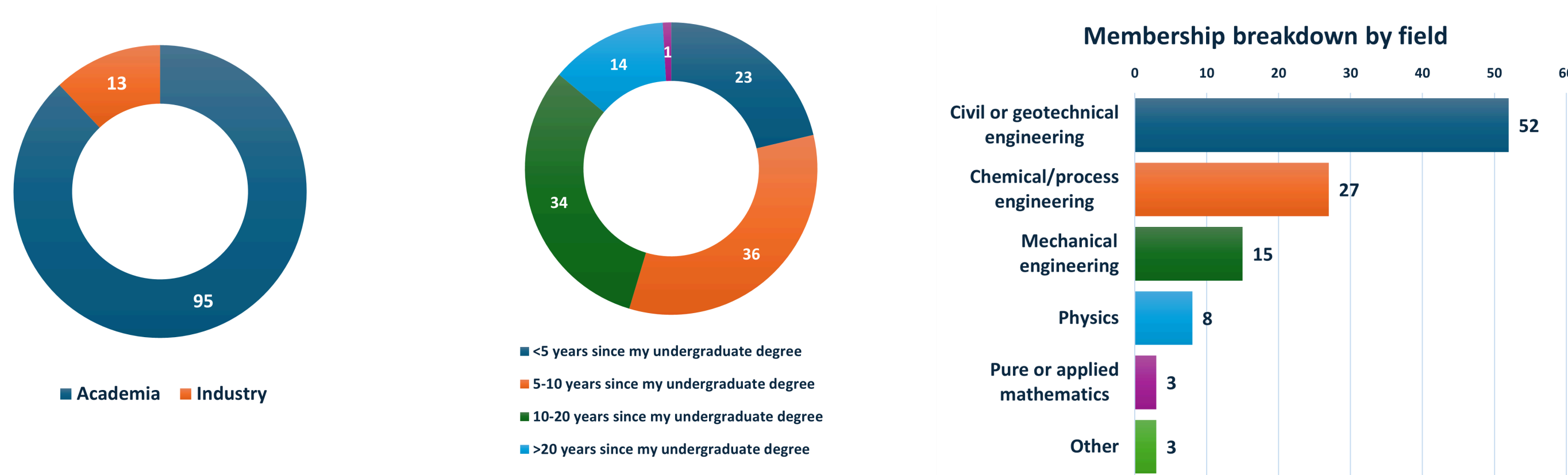
Five-Year Vision

Main goal: **develop a suite of high-performance, validated and scalable open-source codes** for particulate solids simulations, and **democratise adoption** of these codes for UK economic and societal benefit.

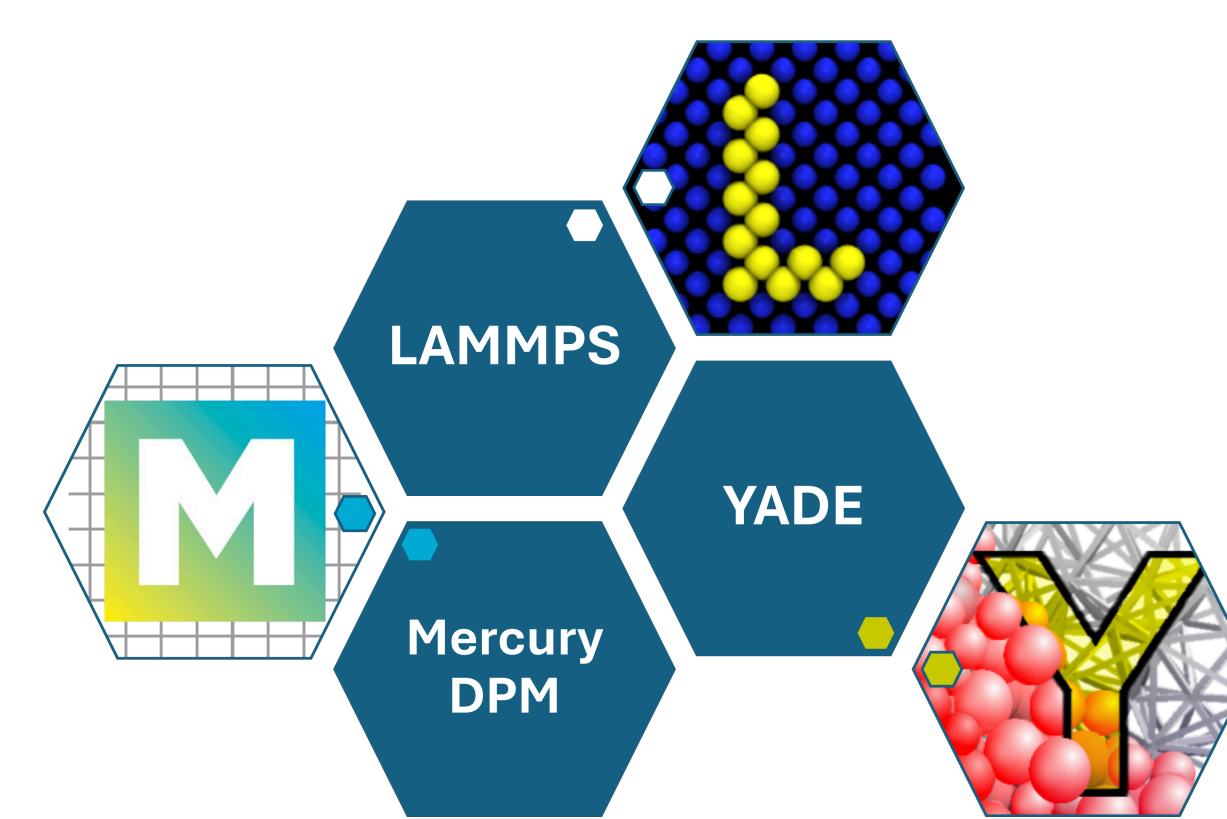


Community Membership

Strong community response with ~110 currently registered members from a variety of backgrounds and with varying experience.



Open-source DEM Tools



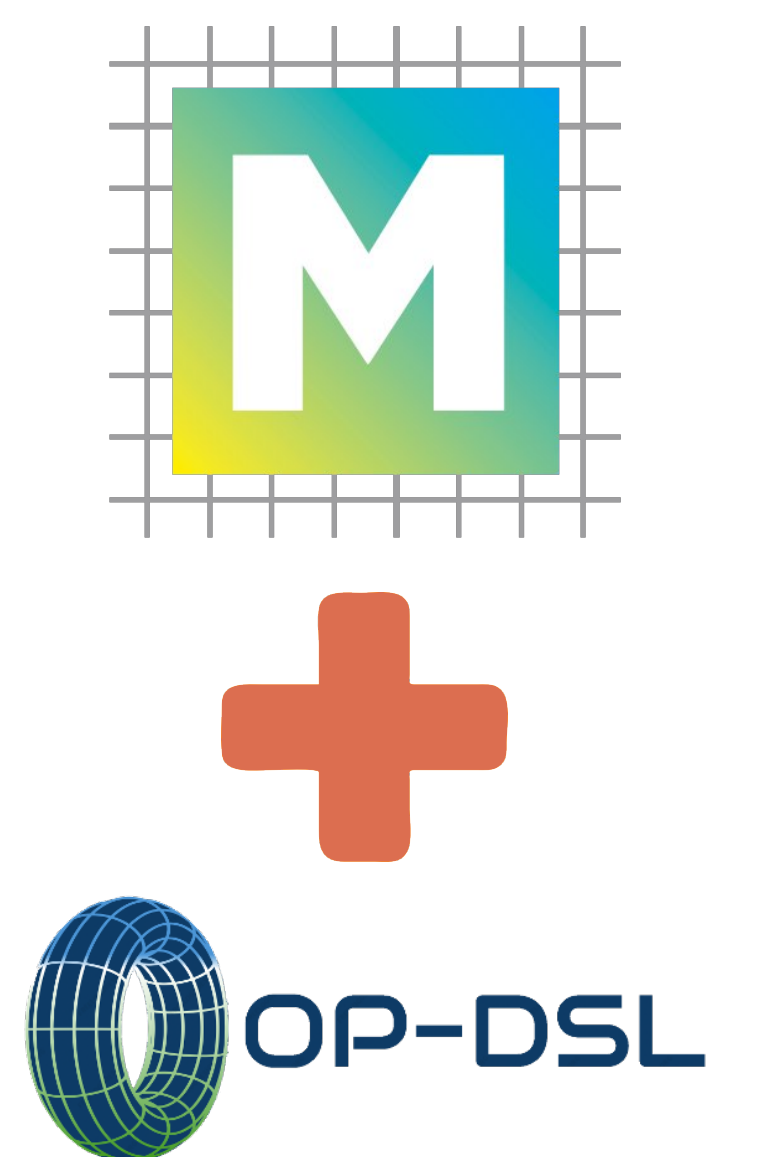
Three DEM codes have been prioritised because of their **popularity** and **scalability**: all are **MPI-parallelised**.

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 based on community feedback, the **addition of GPU capabilities to MercuryDPM** will be pursued.

This is to be accomplished through the use of the Oxford Parallel suite and **development of OPS-Particle** is well underway.



Network & Training Events

Across four events to date, training has been delivered on using the **three DEM codes**, using HPC via ARCHER2, and introducing AI/ML, **data analysis & visualisation** and GPU computing.



Network Events 1-4: University of Edinburgh, May 2025; Abingdon, October 2025; University of Manchester, January 2026; Queen's University Belfast, March 2026.



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