CCC-ParaSoIS Introductory Webinar

21st March 2025

Note that this webinar will be recorded. The slides and recording will be made available through the event page after the webinar.

Science and Technology Facilities Council

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Outline

- What is CCC-ParaSolS?
- Who is involved?
- How can you become a member too?
- Why might you want to? (The planned activities of CCC-ParaSolS)
- CoSeC and its role in the project
- Audience questions

What is CCC-ParaSolS?

- A two-year project that started in January 2025, funded by the Science and Technology Facilities Council (STFC)
- To create a **C**ollaborative **C**omputational **C**ommunity in particulate solids simulations

Natural follow-up: what's a CCC?

- A **C**ollaborative **C**omputational **C**ommunity/**P**roject is a network of UK researchers joined together through the research software (or associated data) used.

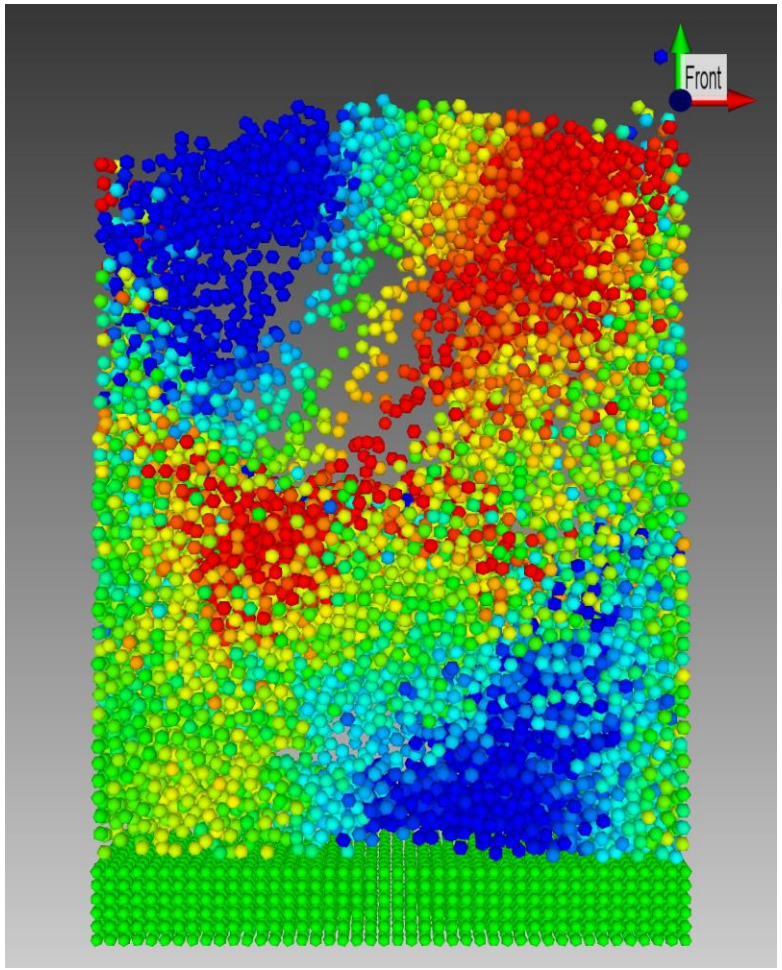
- CCC → CCP

- An established UKRI model* to ensure that research software is treated as infrastructure underpinning research outputs

* https://www.cosec.ac.uk/communities/current-ccps-and-hecs/

Why is a CCC needed in this area?

- Particle-scale simulation methods such as DEM are becoming ever more popular.
  - Scientific insights into the behaviour of particulate systems can be obtained that are challenging, or even impossible, to obtain experimentally.
  - Predictive modelling of phenomena that cannot be modelled with continuum approaches.
  - Excellent repeatability compared to physical experiments.
  - (etc…)

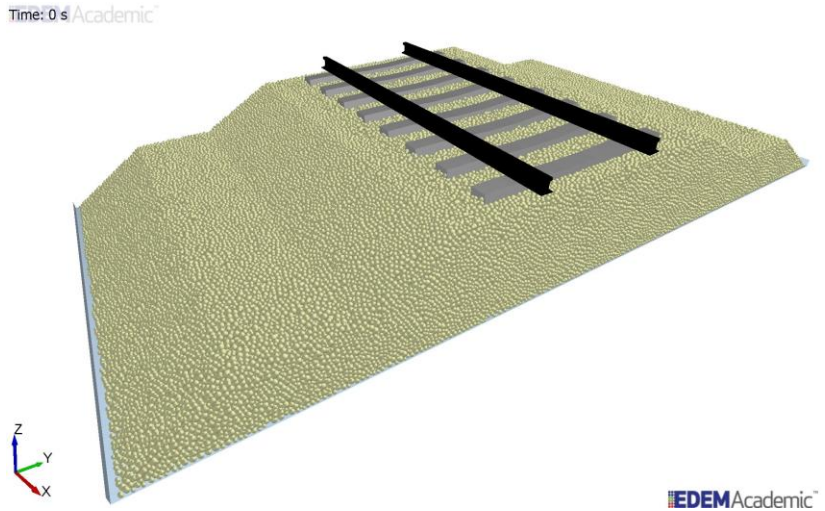


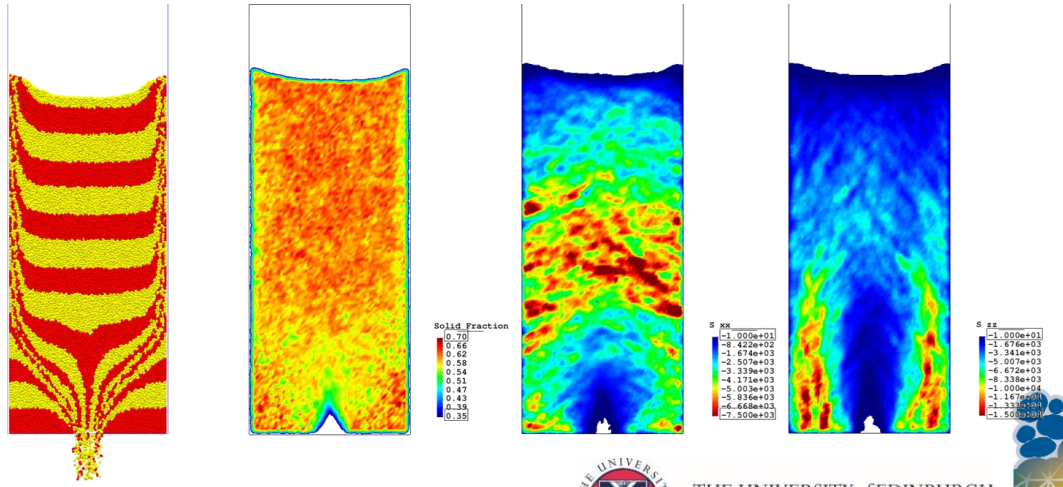
Why is a CCC needed in this area?

- Developments of simulation methods happen in discipline silos.

- How to overcome this?

➢ **CCC-ParaSolS**, as an overarching UK community that embeds diversity and inclusiveness in all activities.





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Who is involved?

Kevin Hanley
University of Edinburgh
Project Lead

Catherine O'Sullivan
Imperial College London
Project Co-Lead

J.P. Morrissey
University of Edinburgh
Researcher Co-Lead

David Emerson
STFC
CoSeC Member

Stefano Rolfo
STFC
CoSeC Member

Valantis Tsinginos
STFC
CoSeC Member

← Current Management Committee (your presenters today)

https://www.ccc-parasols.ed.ac.uk/people/

Who is involved?

- This Management Committee will be expanded by appointing 6 members from the community with the following constraints:
  - at least 1 early-career representative
  - at least 1 industry representative
  - at least 1 member representing NERC-remit research
  - at least 2 of the 6 will be women
- If you would like to be part of the Management Committee, we will be announcing a call for self-nominations to all community members next week.

Who is involved?

Vasileios Angelidakis
Queen's University Belfast, UK

Daniel Barreto
Edinburgh Napier University, UK

Dan Bolintineanu
Sandia National Laboratories

Chris Johnson
University of Manchester, UK

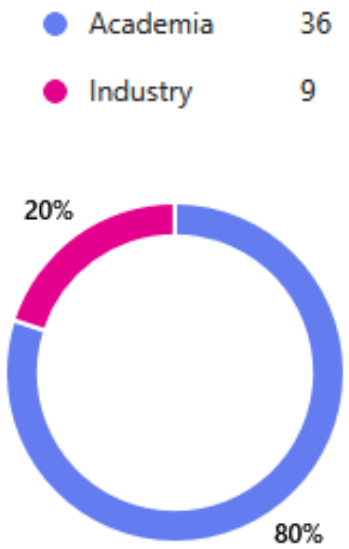
Marina Sousani
Astec Industries

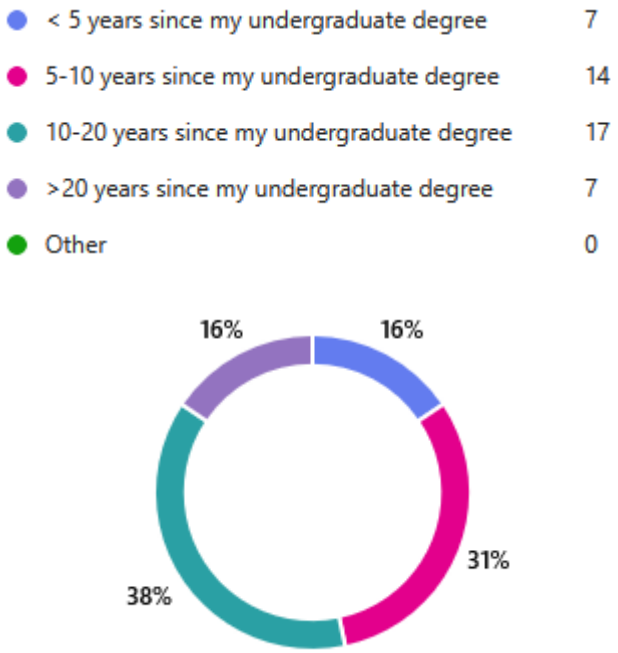
Anthony Thornton
University of Twente, Netherlands

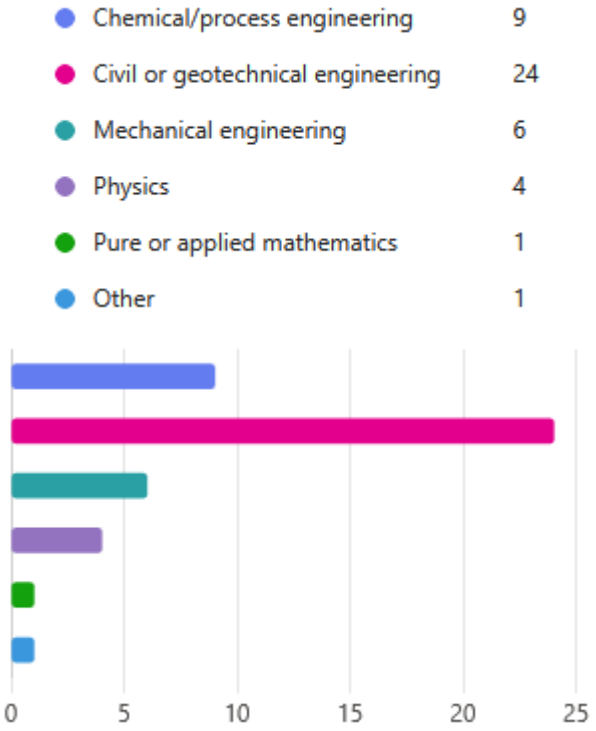
- Advisory Committee
  - Comprised of academic and industrial representatives
  - Representatives of the three open-source DEM codes prioritised by CCC-ParaSolS

Who is involved?

- Most importantly, members have been joining the community:



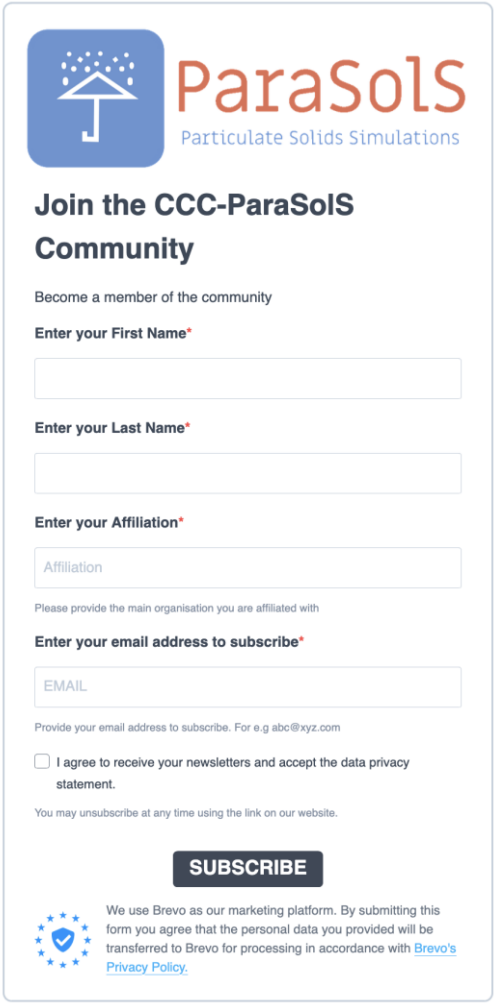




How to become a member too?

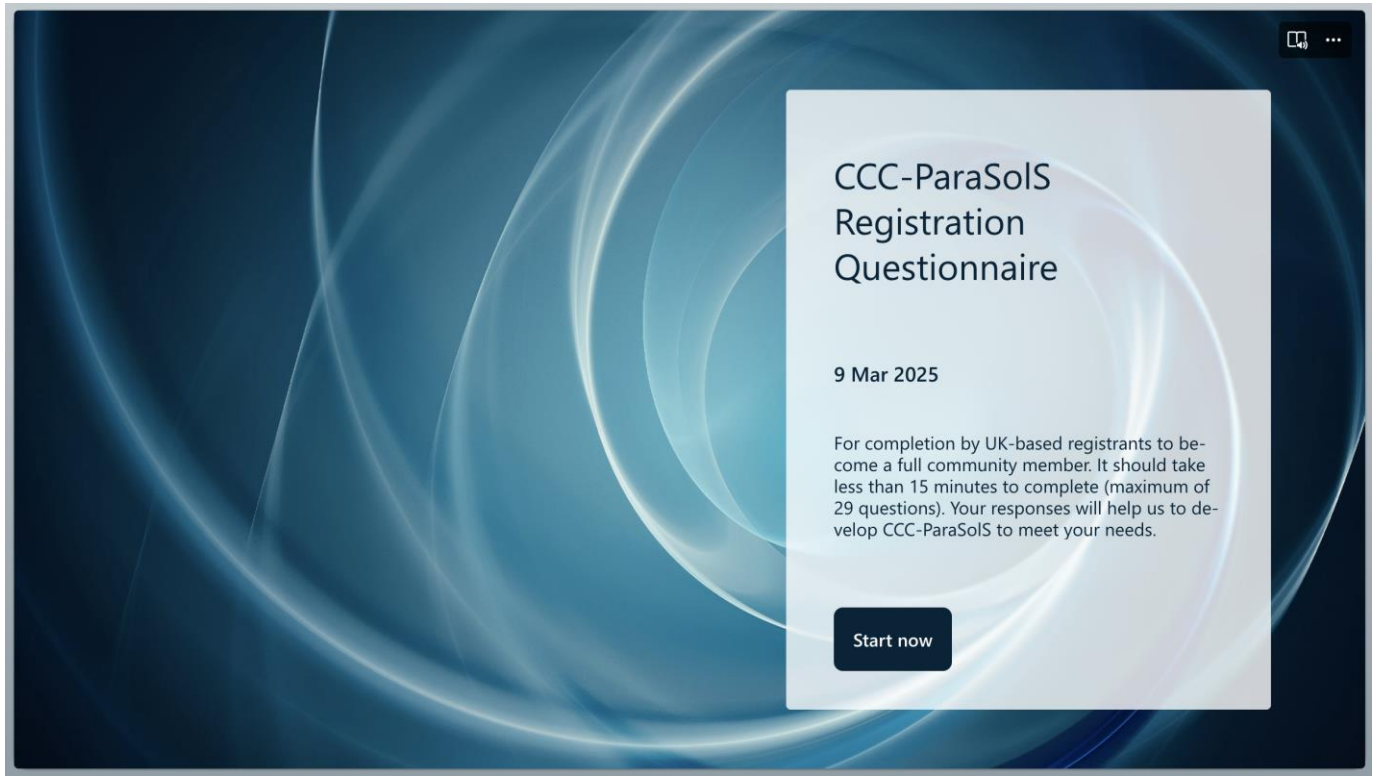
- If you are based in the UK and interested in simulating particulate solids, we encourage you to join:
  - https://www.ccc-parasols.ed.ac.uk/about/join.html

I would like to **join CCC-ParaSolS**



How to become a member too?

- You will then be e-mailed a link to a registration questionnaire.
- This must be completed to become a full community member.
  - Should take < 15 minutes to complete



Initial community feedback

What do you think are the major barriers to DEM use?

What do you think CCC-ParaSolS should deliver?

Why are you interested in joining CCC-ParaSolS?

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What CCC-ParaSolS will do

Enable Use of DEM/HPC/GPU

- Deliver bespoke training on using open-source DEM & high-performance computing (HPC)
- Develop code benchmarking cases and best-practice guidelines
- Promote the use of open-source software for granular simulations
- Promote best practices in validation, benchmarking, and research data management

Develop a Community

- Host physical network events at different UK locations
- Identify gaps in granular simulation capabilities via community consultation
- Undertake one or more high-priority code development projects based on this
- Produce a five-year vision for the community

Network events

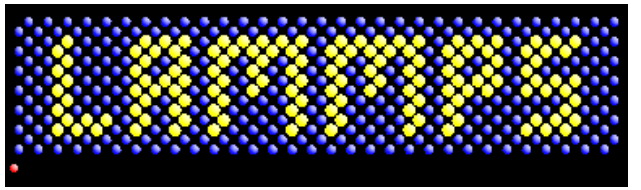
- 3 physical events at different UK locations
  - facilitated workshops
  - networking
  - research dissemination
  - training
- + virtual events

1. *to expand the community in the UK using open-source DEM codes*
2. *to support new users of HPC and GPUs for DEM*
3. *to identify and fill gaps in simulation capabilities*
4. *to co-create a five-year vision for the community*

- More on the events later in this presentation!

Training provision

1. Open-source DEM codes: LAMMPS, MercuryDPM & YADE (delivered by developers)



2. HPC using ARCHER2 and running LAMMPS simulations on HPC (EPCC*)

3. [Subject to change based on community input] Handling and post-processing of large data volumes, reproducible research and FAIR data principles (partly CoSeC)

Code benchmarking & development

- We will develop code benchmarking cases for all three codes and best-practice guidelines on:
  - reproducible research
  - how to use the three target codes effectively
  - setting initial conditions, boundary conditions and dealing with static and dynamic simulations

- We will undertake one or more high-priority code development projects, based on community consultation.
  - 12 months of developer time from CoSeC for this purpose

Physical event #1: Edinburgh

- At the University of Edinburgh, 14–16 May 2025
- UK-based members of CCC-ParaSolS are invited to register their interest in attending now:

https://www.ccc-parasols.ed.ac.uk/events/upcoming/networking-event-1/

Physical event #1: Edinburgh

- Registration of interest closes on **22 April**
- We will inform you whether you have been selected to attend, with reimbursement of expenses if required, by 25 April.

https://www.ccc-parasols.ed.ac.uk/events/upcoming/networking-event-1/

Provisional plan for this event

- **Wednesday 14 May**
  - 11:30–13:00 Arrival & lunch
  - 13:00–13:30 Introductions (project & people)
  - 13:30–14:00 A historical perspective on simulating particles
  - 14:00–15:00 Showcase of experiences with DEM

    Hear from a diverse range of speakers at all career stages: why they started to use DEM, challenges they encountered, non-technical lessons learned from experience, joys & frustrations, why they chose their favoured code…
  - 15:00–15:30 Tea/coffee break
  - 15:30–17:00 Facilitated workshop to introduce open-source DEM codes, and use of HPC and GPUs for DEM simulations
  - Evening Dinner

https://www.ccc-parasols.ed.ac.uk/events/upcoming/networking-event-1/

Provisional plan for this event

- **Thursday 15 May**
  - 09:00–12:30 Training on MercuryDPM
  - 12:30–14:00 Lunch
  - 14:00–17:30 Training on LAMMPS
  - Evening Dinner

Each code training session will include a tea/coffee break

https://www.ccc-parasols.ed.ac.uk/events/upcoming/networking-event-1/

Provisional plan for this event

- **Friday 16 May**
  - 09:00–12:30 Training on Yade
  - 12:30–13:30 Lunch
  - 13:30–15:00 '*Ask the experts*' panel session on code capabilities for attendees' specific applications
  - 15:00–15:30 Closing remarks and tea/coffee
  - 15:30–17:30 Career development workshop for women

https://www.ccc-parasols.ed.ac.uk/events/upcoming/networking-event-1/

Subsequent physical events

- #2 somewhere in England, tentatively in October 2025
  - Will include a training course on introducing HPC using ARCHER2, and running LAMMPS simulations on HPC
- #3 tentatively in Northern Ireland in March 2026
  - May be a joint event with the ON-DEM COST Action

- For all events, CCC-ParaSolS will be able to reimburse the travel, accommodation and subsistence expenses of some attendees.
- An online joining option will be available to facilitate those who cannot attend in person.

CoSeC and its role in CCC-ParaSolS

CoSeC

Computational Science Centre
for Research Communities

CCC-ParaSolS workplan in summary

https://www.ccc-parasols.ed.ac.uk/about/

Questions?

- **Thank you for your attention!**
- Q&A time. If any questions occur to you after this webinar, e-mail

parasols@ed.ac.uk

and we will get back to you.

ParaSolS
Particulate Solids Simulations

https://www.ccc-parasols.ed.ac.uk/

https://www.linkedin.com/company/ccc-parasols/