



CCC-ParaSols Network Event #1

Introductions

Edited to remove some information of no use after the event on computing accounts, directions to buildings, etc.

Edinburgh: 14–16 May 2025



Science and
Technology
Facilities Council



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THE UNIVERSITY of EDINBURGH
School of Engineering



Outline



- Welcome & essential information
- What is CCC-ParaSolS and who is involved?
- Schedule for this Network Event
- Practicalities

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

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What is CCC-ParaSols?



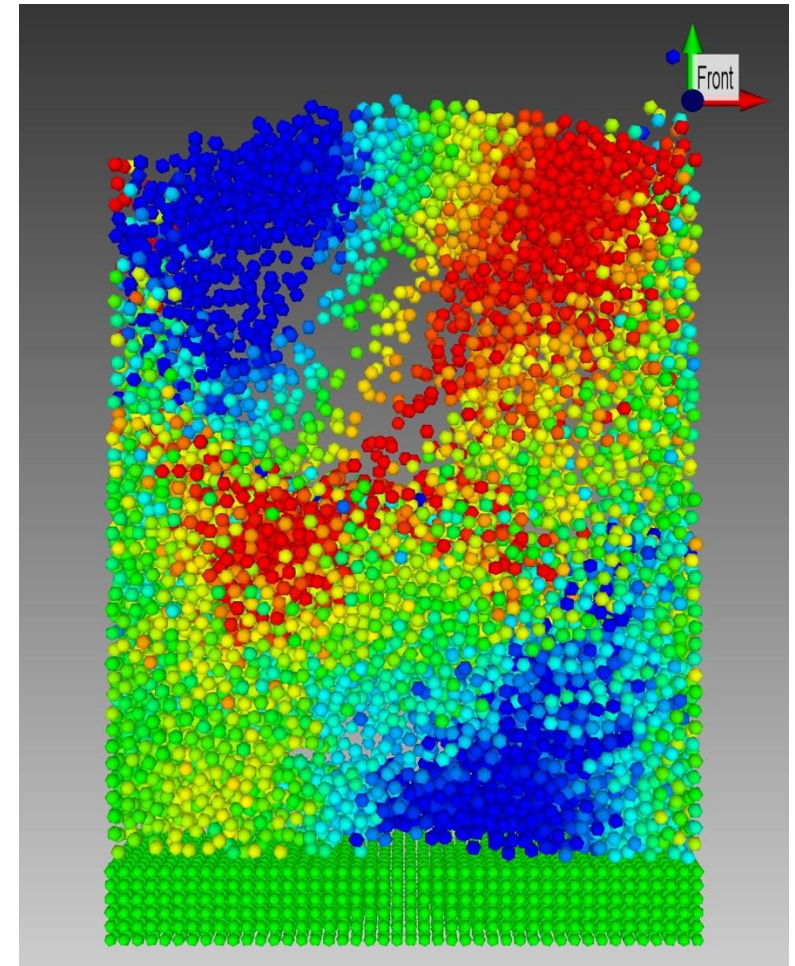
- A two-year project that started in January 2025, funded by the Science and Technology Facilities Council (STFC)
- To create a **C**ollaborative **C**omputational **C**ommunity in particulate solids simulations
- A **C**ollaborative **C**omputational **C**ommunity/**P**roject is a network of UK researchers joined together through the research software (or associated data) used.
- CCCs / CCPs have been around for a long time...

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Why is a CCC needed in this area?



- Particle-scale simulation methods such as DEM are becoming ever more popular.
- 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



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

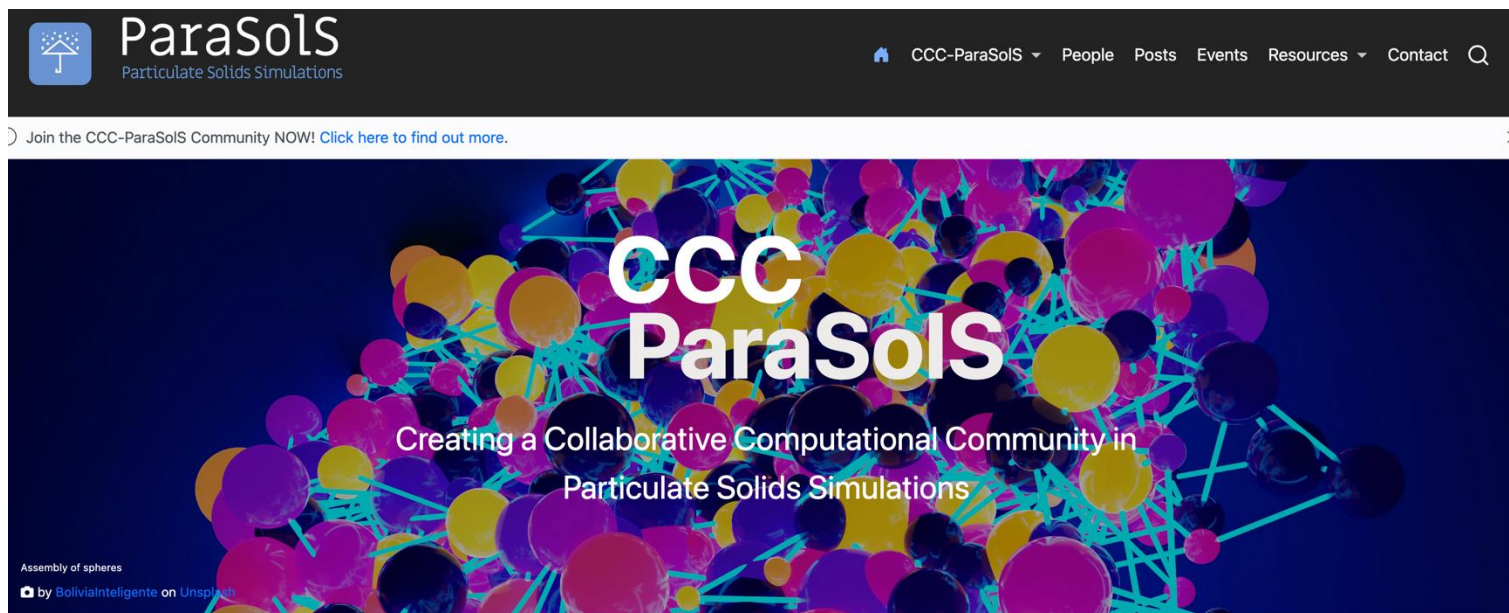
- Host physical network events at different UK locations
- Identify gaps in granular simulation capabilities via community consultation
- Undertake one or more high-priority code development projects based on this
- Produce a five-year vision for the community

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For more details



- See the website: <https://www.ccc-parasols.ed.ac.uk/>



Welcome to CCC-ParaSols

CCC-ParaSols is a two-year project — January 2025 to December 2026 — funded by the [Science and Technology Facilities Council \(STFC\)](#) to create a **Collaborative Computational Community** in particulate solids simulations.



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For more details



- Or watch the Teams webinar from the 21st of March:

<https://www.ccc-parasols.ed.ac.uk/events/past/webinar-event/>

A slide for a webinar. At the top right is a small blue square icon with a white umbrella and raindrops. The main text is in orange: "CCC-ParaSols Introductory Webinar". Below that, in blue, is "21st March 2025". A note in black italicized font says: "Note that this webinar will be recorded. The slides and recording will be made available through the event page after the webinar." At the bottom are logos for UKRI, Science and Technology Facilities Council, CoSeC, IMPERIAL, THE UNIVERSITY of EDINBURGH School of Engineering, and Gran ED.

**CCC-ParaSols
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.

UKRI Science and Technology Facilities Council CoSeC Computational Science Centre for Research Communities IMPERIAL THE UNIVERSITY of EDINBURGH School of Engineering Gran ED



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

← Core Team (entire Management Committee until recently)



David Emerson
STFC
CoSeC Member



Stefano Rolfo
STFC
CoSeC Member



Valantis Tsinginos
STFC
CoSeC Member

???

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



Science and
Technology
Facilities Council



A very brief history and overview of CCPs & CoSeC

David R Emerson, Stefano Rolfo, Valantis Tsinginos
STFC Scientific Computing,
Daresbury Laboratory

Towards creating the CCPs....

The 60s: Three Key Developments

Robbins Report (1963): expansion of the universities (more students entering higher education)

Flowers Report (1966): growing demand for access to computers, creation of “Regional Computer Centres” (ERCC created 1966)

Atlas Computing Laboratory (1961 - 1975): a national computing centre, in today’s terminology, a supercomputer centre

The 70s: A Concept Emerges: talks between ACL, distinguished scientists, and SRC lead to **Project 1** on “Correlations in Molecular Wave Functions” which started in **1974**

In an October **1975** meeting, a key topic was codes and their **machine dependence**. Porting s/w was important, motivated by the impact of the Flowers Report and creation of Regional Computing Centres.

The ACL closed (1975) and some key staff move to DL, with **Phil Burke** being director of the Theory and Computational Science Division. In **October 1977**, the Collaborative Computational Projects were proposed!

As a result, Project 1 was renamed as **CCP1** and others soon followed, notably CCP2 (Continuum States in Atoms and Molecules, 1978), CCP3 (Surface Science, 1978), CCP4 (Protein Crystallography, 1979), **CCP5** (Monte Carlo and Molecular Dynamics, 1979), and CCP6 (Heavy Particle Dynamics, 1979).

Engineering late to the game – started in 1990!



Scientific Computing



CoSeC and the CCPs today....

CoSeC: created in 2017 to better reflect a wider community being represented i.e. EPSRC, BBSRC, MRC

It also covered more than CCPs e.g. High End Computing (HEC) consortia

Now even broader and integral to DRI via UKRI

Enables computational research by developing software **as an infrastructure** to address complex problems requiring advanced computing

A UKRI funded Centre to deliver, enable and support collaborative computational research

Achieved through **stable long-term holistic partnerships** with researchers organised as UKRI-funded communities



CoSeC going forward....

- Through UKRI DRI STFC funds and CoSeC supports 13 CCPs as well as 6 EPSRC funded HECs
- From 2025 STFC funds and CoSeC supports 6 scoping projects to develop new communities

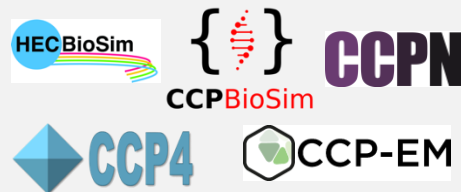
Materials

- [CCP9](#): Electronic Structure of Condensed Matter
- [CCP-NC](#): NMR Crystallography
- [CCP5](#): Simulation of Condensed Phases
- [UKCP](#): Car-Parrinello Quantum Mechanics
- [MCC](#): Material Chemistry



Biology

- [CCP4](#): Protein Crystallography
- [CCP-EM](#): Electron Cryo-microscopy
- [CCP-N](#): NMR Spectroscopy
- [CCPBioSim](#): Biomolecular Simulation
- [HECBioSim](#): HPC within Biomolecular Simulation



Imaging

- [CCPi](#): Tomographic Imaging
- [CCPSyneRBI](#): Synergistic Reconstruction for Biomedical Imaging




Engineering

- [CCP-WSI](#): Wave Structure Interaction
- [CCP-NTH](#): Nuclear Thermal Hydraulics
- [CCP-Turbulence](#): Complex Turbulence modelling
- [UKTC](#): HPC for Turbulence modelling
- [UKCOMES](#): Mesoscale Engineering
- [HEC-WSI](#): HPC for Wave Structure Interaction



New Communities

- [Particulate Solids \(Edinburgh\)](#)
- Arts, Humanities, and Culture (Durham)
- Data-driven Computational Mechanics (Imperial)
- Volume Electron Microscopy (Francis Crick)
- Numerical Relativity (King's College London)
- Theoretical and Experimental Particle Physics (Swansea)

[CCP-QC](#): Quantum Computing 



Who is involved?



- Recently expanded the Management Committee:

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Vasileios Angelidakis
Queen's University Belfast,
UK



Wonjun Cha
University of Birmingham,
UK



Liang Cui
University of Surrey, UK



Charley Wu
University of Surrey, UK



Sina Haeri
HR Wallingford, UK



Dariel Hernández-Delfin
Imperial College London,
UK



Marv Khala
AstraZeneca, UK

Who is involved?



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

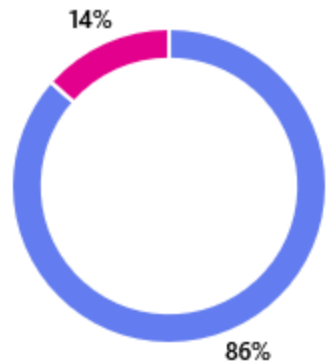
- Comprised of academic and industrial representatives
- The open-source DEM code trainers at this Network Event are on one of these Committees.

Who is involved?

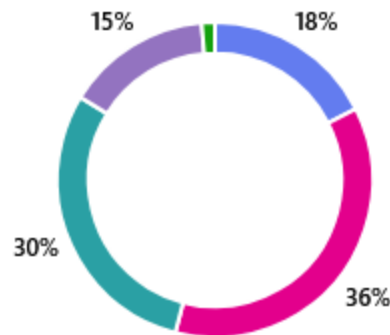


- Most importantly, members have been joining the community:

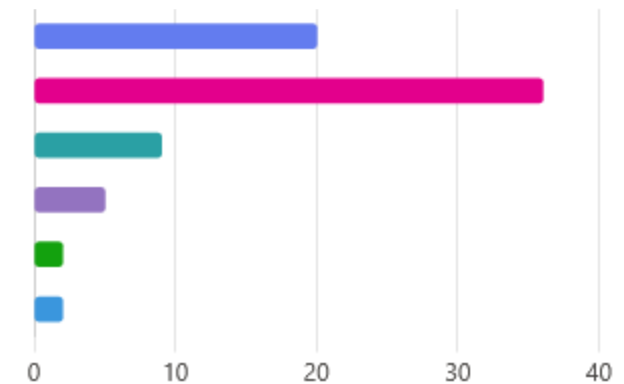
- Academia 64
- Industry 10



- < 5 years since my undergraduate degree 13
- 5-10 years since my undergraduate degree 27
- 10-20 years since my undergraduate degree 22
- >20 years since my undergraduate degree 11
- Other 1



- Chemical/process engineering 20
- Civil or geotechnical engineering 36
- Mechanical engineering 9
- Physics 5
- Pure or applied mathematics 2
- Other 2



Schedule for this Network Event



• Wednesday 14 May — G.26 Charlotte Murchison Lecture Theatre

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- 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
- 15:00–15:30 Tea/coffee break
- 15:30–17:00 Facilitated workshop on actions the CCC-ParaSolS community should take, and major foreseeable changes in DEM
- 17:00–17:30 Management Committee meeting (open to MC members only)
- 19:00– Event dinner at Scotts Kitchen

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

Showcase of experiences with DEM



- **Wednesday 14 May — G.26 Charlotte Murchison Lecture Theatre**
 - 14:00–15:00 Showcase of experiences with DEM
 - *Contributions of up to 5 minutes per person on some/all of the following:*
 - Why did you start to use DEM?
 - What challenges have you encountered?
 - What lessons have you learned from your experience with DEM?
 - Joys & frustrations
 - Why did you pick your favoured DEM code?

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Facilitated workshop



- **Wednesday 14 May — G.26 Charlotte Murchison Lecture Theatre**
 - 15:30–17:00 Facilitated workshop on actions the CCC-ParaSolS community should take, and major foreseeable changes in DEM
 - *Breakout groups to address these questions:*
 1. What actions should the community take in the remainder of CCC-ParaSolS and beyond to facilitate and encourage the adoption of open-source DEM codes?
 2. What actions should the community take to improve its diversity?
 3. What DEM code developments would be of greatest benefit to advance science in the UK?
 4. What major changes do we foresee in DEM in the next five years?

Event dinner at Scotts Kitchen



- **Wednesday 14 May**
 - 19:00– Event dinner at **Scotts Kitchen**
 - [4-6 Victoria Terrace, Edinburgh, EH1 2JL](#)
 - w3w: [///salon.define.librarian](https://salon.define.librarian)

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

Schedule for this Network Event



• Thursday 15 May — TLG, Fleeming Jenkin Building

- 09:00–12:30 Training on MercuryDPM
- 12:30–14:00 Lunch (CR4, Hudson Beare Building)
- 14:00–17:30 Training on LAMMPS
- 19:00– Event dinner at Amber Restaurant @ The Scotch Whisky Experience



Anthony Thornton
University of Twente,
Netherlands



Dan Bolintineanu
Sandia National
Laboratories

Each code training session will include a tea/coffee break: same place as lunch

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

Event dinner at Amber Restaurant



- **Thursday 15 May**
 - 19:00– Event dinner at **Amber Restaurant** @ The Scotch Whisky Experience
 - 354 Castlehill, The Royal Mile, Edinburgh, EH1 2NE
 - w3w: [///often.chin.bared](https://www.often.chin.bared)



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

Schedule for this Network Event



- **Friday 16 May — TLG, Fleeming Jenkin Building**

- 09:00–12:30 Training on Yade
- 12:30–13:30 Lunch (CR4, Hudson Beare Building)

- **Friday 16 May — CR2, Sanderson Building**

- 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
- 15:30–16:30 Career development workshop for women



Vasileios Angelidakis
Queen’s University
Belfast, UK

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

'Ask the experts' panel session



- **Friday 16 May — CR2, Sanderson Building**

- 13:30–15:00 'Ask the experts' panel session on code capabilities for attendees' specific applications

- The panel will comprise:

- Vasileios Angelidakis
 - Dan Bolintineanu
 - Anthony Thornton
 - Stefano Rolfo (STFC)
- } three code trainers

- If you have questions about DEM codes, their capabilities or broader questions about particulate solids simulations, CCCs/CCPs/CoSeC, or the UK's digital research infrastructure, this is an excellent opportunity to ask!

'Ask the experts' panel session



- **Friday 16 May — CR2, Sanderson Building**

- 13:30–15:00 'Ask the experts' panel session on code capabilities for attendees' specific applications


- You can ask questions during the session, of course.
- Alternatively, submit your questions in advance via a MS form:

[link & QR code removed post-event]

- We will place printed copies of this QR code around the rooms we are in.

Practicalities: expense reimbursement




- If eligible for expense reimbursement, you will have received an e-mail with this expenses claim form attached  [form removed post-event]
- Once you have completed and signed the form, send it and copies of your receipts to ParaSolS@ed.ac.uk within three months of the expense being incurred.

<https://www.ccc-parasols.ed.ac.uk/events/reimbursement-of-expenses.html>

Practicalities: computing accounts



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- The code training tomorrow and Friday morning will take place in a computing lab.
 - If you have brought a laptop, you can use that if you wish. Only a web browser and wi-fi are needed.
 - If you haven't brought a laptop, no problem. You can use a computer in the computing lab — but you will need to [UoE guest account image removed post-event] set up a temporary guest account. 
- eduroam should work for most. If you need wi-fi guest access, ask Kevin or JP.

Practicalities: cloud platform



[link to access the cloud platform removed post-event]

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From e-mail
on Tuesday



CCC-ParaSoLS Training (CPU Only) Sign Up

Course Details

Name	CCC-ParaSoLS Training (CPU Only)
Purpose of Training	Training event for the CCC-ParaSoLS a new community supported by CoSeC (additional CPU only)
Start Date	2025-05-14
End Date	2025-05-16

Name

Email

SIGN UP

I have read and accept the terms and conditions.

Terms and Conditions

For general help with this site, find the  in the top right (these pages have specific information for each area of our site).

Questions?



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ParaSols

Particulate Solids Simulations

parasols@ed.ac.uk

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



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