CCC-ParaSolS Network Event #2

Gap analysis of simulation capabilities & Year 2 code development projects

Abingdon: 13–15 October 2025

Science and Technology Facilities Council

CoSeC
Computational Science Centre for Research Communities

IMPERIAL

THE UNIVERSITY of EDINBURGH
School of Engineering

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Schedule for this Network Event

- **Monday 13 October — Garden Room, the Cosener's House**
  - … …
  - 12:30–14:00 Lunch
  - 14:00–15:30 Five-year vision for the community
  - 15:30–16:00 Tea/coffee break
  - 16:00–16:15 ON-DEM update (Dr Daniel Barreto)
  - **16:15–17:30 Gap analysis of simulation capabilities & Year 2 code development projects**
  - 19:00– Event dinner at Limoncello restaurant

https://www.ccc-parasols.ed.ac.uk/events/upcoming/networking-event-2/

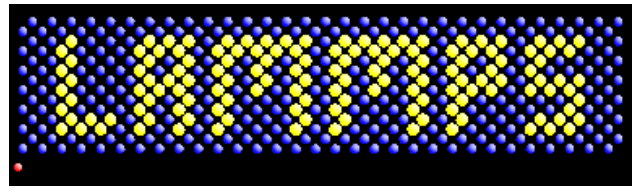
Code development in Year 2

- CCC-ParaSolS has one year of a developer's time from CoSeC for DEM code development.
- We want to use that time to achieve the highest impact among the UK DEM community, i.e., maximise the benefit.
- We went through a multi-stage process to get to the proposal presented later.

CoSeC
Computational Science Centre for Research Communities

Stage 1: Community needs analysis

- In our three prioritised codes (LAMMPS, MercuryDPM and YADE), we asked if CCC-ParaSolS members had found:

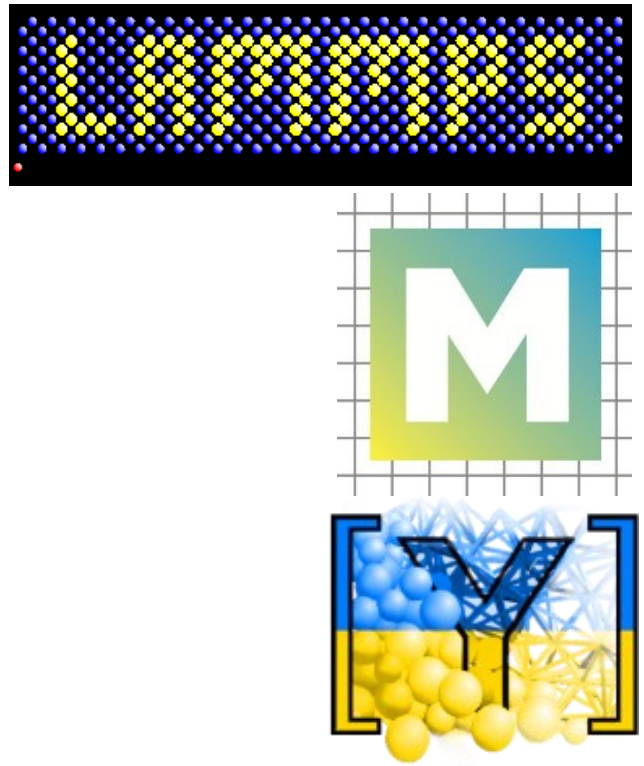


1. an architecture-related limitation of any of these codes, e.g.,
   - poor scalability on a CPU cluster
   - parts of a code not running on a GPU
   - lack of ARM64 support (e.g., to use the new Isambard 3 Grace HPC system)
   - etc.

Stage 1: Community needs analysis

…and/or…

2. a missing code feature that is preventing a scientific problem from being tackled, e.g.,
   - lack of complex geometries/particle shapes
   - missing some data interoperability features
   - missing simulation pre/post-processing tools
   - missing coupling with another simulation method
   - etc.



Stage 1: Community needs analysis

- E-mail on 12 August:

Identification of potential code development projects

CCC-ParaSolS will undertake one or more high-priority code development projects in year 2 which are of greatest benefit to the community. CCC-ParaSolS has one year of developer time at CoSeC for this purpose. These developments will be in one or more of the three open-source codes we have prioritised: LAMMPS, MercuryDPM and/or YADE.

These potential code developments are in two categories:

1. to enable new scientific problems to be tackled that cannot be at present due to missing code features
2. to enable modern hybrid computing architectures to be exploited, or exploited more efficiently

Please complete this form to suggest potential code development(s):

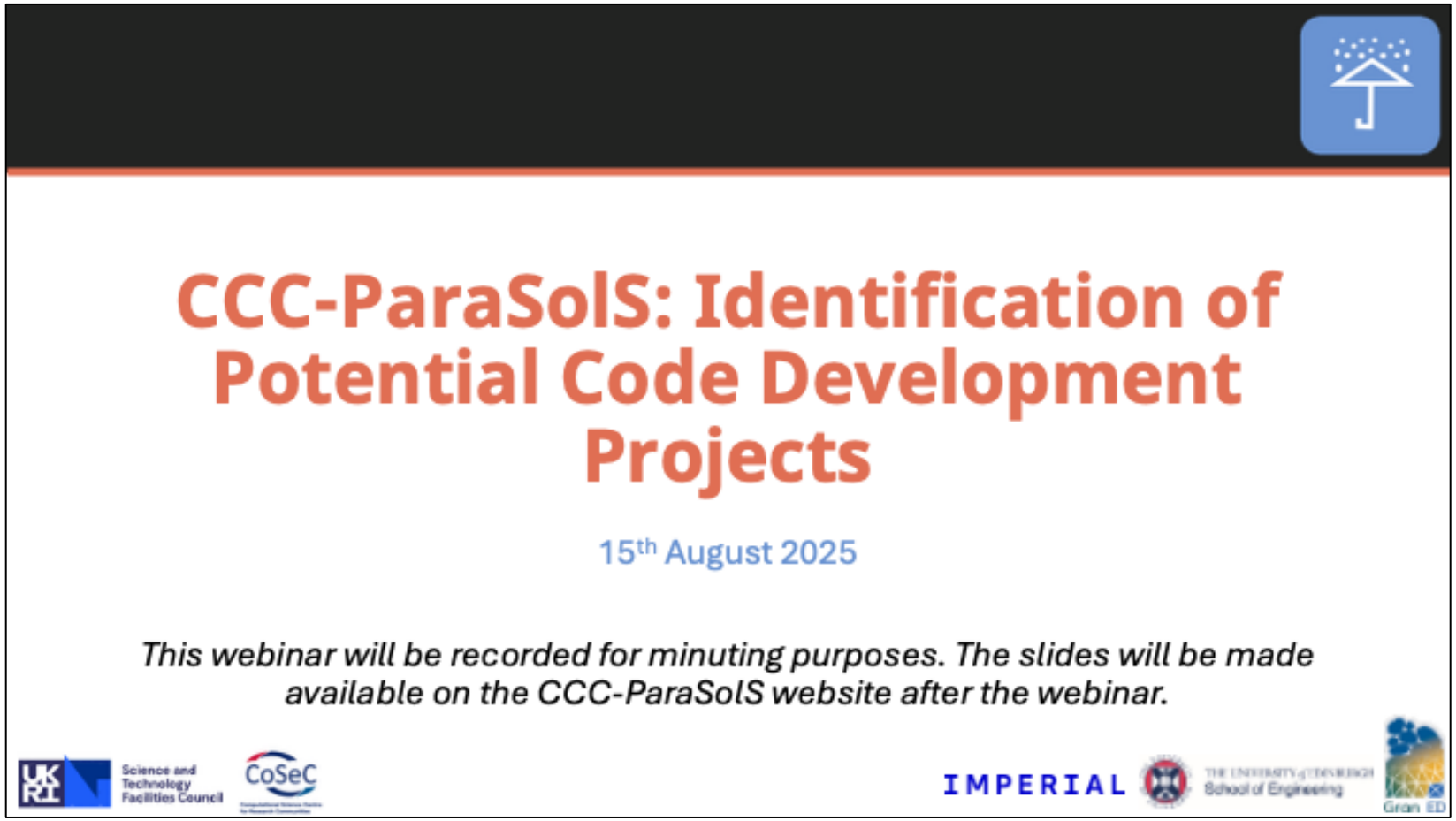
https://forms.office.com/e/LgxAPCc6rR

This form will close on 29 August. Please bear in mind that we are seeking projects that will have a high impact among the UK community, i.e., are of widespread benefit, not only of benefit to your own research.

Any suggestions submitted will be reviewed and shortlisted by the Management Committee in early September. The relevant code developers and CoSeC will also be consulted to ensure feasibility of implementation within the 12-month timeframe. Following this process, a proposal for the code development projects will be presented for discussion at Network Event 2 in October.

Stage 1: Community needs analysis

- Supported by an explanatory webinar on 15 August:



What we are seeking for suggestion α

Slide taken from webinar on 15 August

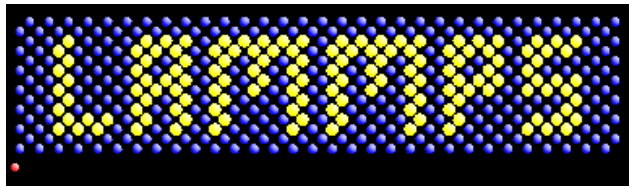
- **Impact**
  - α should be of substantial and widespread benefit, not only for your research alone
  - For overcoming architecture-related limitations, we will favour architectures likely to become increasingly important for large-scale simulations
  - Development projects should strengthen a possible future application for a follow-on *Collaborative Computational Project*
- **Novelty**
  - For new features, α would preferably not be available in *any* open-source code
  - Either someone isn't already implementing α **or** CCC-ParaSolS could usefully contribute to the ongoing implementation of α
- **Feasibility**
  - α must be possible to implement and verify/validate in the 12-month timeframe

Stage 2: MC review and shortlisting

- Suggestions were anonymised, reviewed and shortlisted by the Management Committee on 2 September.

- Only 5 suggestions were received:
  - 4 architecture-related limitations
  - 1 missing code feature

- Number of mentions:



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Stage 2: MC review and shortlisting

- Only one (near-)duplicate: a DEM code that can properly exploit GPUs

- Summary of other suggestions:
  - Triangulated boundary walls in LAMMPS
  - A mature MPI implementation in YADE for all particle types
  - Coupled CFD–DEM simulations, done properly

- Some of these could be time-consuming — but we don't necessarily need to have finished development in 12 months as long as there is a useful output from the 12 months of effort.

Stage 2: MC shortlisting outcome

- ‘Triangulated boundary walls in LAMMPS’
  - This development is already well underway by the LAMMPS developers: https://github.com/lammps/lammps/pull/4213

- ‘A mature MPI implementation in YADE for all particle types’
  - The direction of travel for HPC is away from CPU clusters and towards hybrid architectures.
  - Hence, this may not make such a compelling case in a future *Collaborative Computational Project* application.

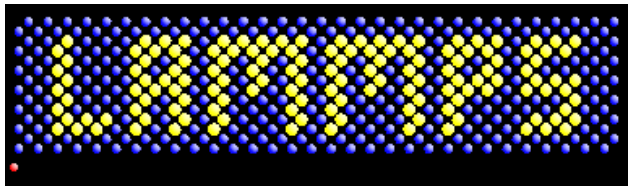
Stage 2: MC shortlisting outcome

- ‘A DEM code that can properly exploit GPUs’
  - Being able to use GPUs and hybrid HPCs effectively will be essential to exploit the UK’s future Tier-1/2 HPCs.
  - Would greatly strengthen a *Collaborative Computational Project* application (green/energy-efficient computing, etc.)
  - The suggestion favoured by the Management Committee

- ‘Coupled CFD–DEM simulations, done properly’
  - Would be valuable to many, but GPU capability would be needed to efficiently run coupled simulations as well.
  - This would be better as a subsequent code development, after the GPU implementation.

Stage 2: MC shortlisting outcome

- Which code?



  - UKRI would prefer to have a strong codebase in the UK.
  - One of the community suggestions was specifically to add GPU capabilities to MercuryDPM.

- MercuryDPM was favoured; it is now UK-led (Prof. Anthony Thornton, University of Manchester).

Targeting different systems

- Diversity in HPC systems (Top500: Nvidia 117 and AMD 23)

- Re-coding for different architectures
- Use of different proprietary models (e.g., CUDA, HIP, ROCm)
- Different optimisations may be required

Tackling the bottleneck

- **Open standards (e.g. OpenMP)**
  - Support different types of GPUs
  - Easy to use
- **Domain Specific language** (DSL) or **High-Level abstraction** (HLA) libraries
  - Portability across architectures
  - Performance optimisation
  - Abstraction of complexity

Examples of such libraries

- **OPS**: Part of the OP-DSL project (https://op-dsl.github.io/)
- **Kokkos**: (https://github.com/kokkos/kokkos)

DSL: Programming language designed for a given problem

HLA: Design approach that provides simplified interfaces hiding complexity

MercuryDPM & GPU

- **MercuryDPM–GPU**:
  - Based on OpenMP directives ⇒ **Targeting portability**
  - Development at a very early stage
- **Current Status** (Based on repository commits)
  - Functions for matrix–vector multiplications based on OpenMP
  - Develop CMake
  - Some work on structure of arrays to minimise memory throughput issues
- **OpenMP** can target both **NVIDIA** & **AMD** GPUs **BUT** performance **NOT** optimal (no fine tuning of available resources, no availability of streams/events, limited control of memory management).
- No proper support of STL containers in GPUs

OPS vs Kokkos

OPS

- Domain-specific language for structured grids & particle/grid interactions

Features

- Automatic memory management
- Built-in MPI support
- Functions for handling iterations
- Performance is tuned
- Automatic support of multiple GPUs
- Performance updates can benefit the whole community

Kokkos

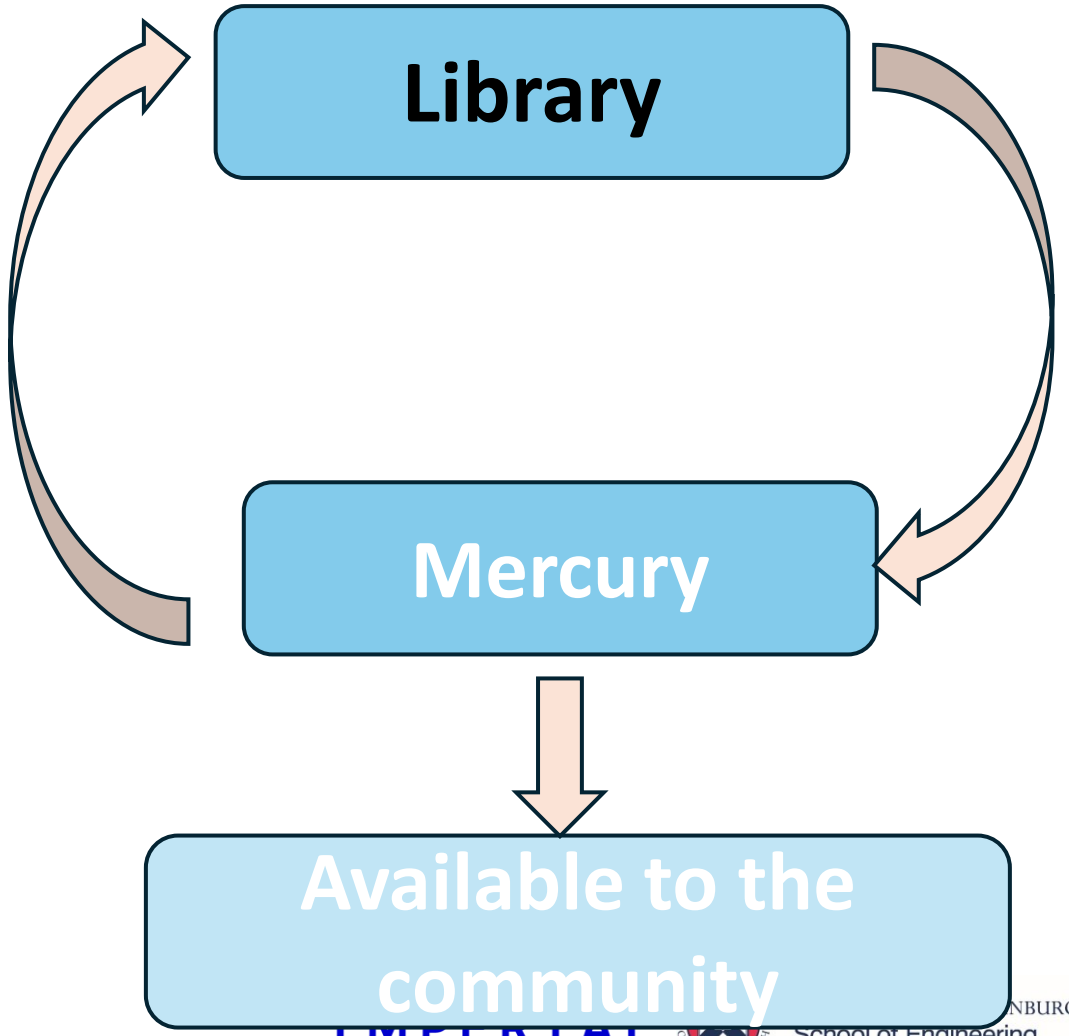
- **Higher level abstraction** (Programming modeling that enables performance portability)

Features

- User-defined memory layout
- No built-in MPI support; user must provide MPI support
- Parallel patterns ("directives") to handle iterations
- User can tune parallel performance
- Multiple GPUs not automatically supported (??).
- Performance updates may not be passed to the whole community

Plan for code developments

- Optimisation of the library for DEM simulations (5m)
- Developing the MercuryDPM-library version (3m)
- Testing & further optimisation of CPU and GPU versions of MercuryDPM ⇒ Addition to library templates (if necessary) ⇒ Developments become available to community and beyond (3m)
- Public release of Mercury-library & writing final report (1m)



Discussion time!

1. Based on our choice, can we satisfy more than one goal?
2. How do all codes benefit from current developments?
3. Any suggestions on the best way to achieve our goal?

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Event dinner at Limoncello

- **Monday 13 October**
  - 19:00– Event dinner at Limoncello
  - 13 Ock St, Abingdon OX14 5AL
  - w3w: ///pine.level.fries

https://www.ccc-parasols.ed.ac.uk/events/upcoming/networking-event-2/

Event dinner at Limoncello

from The Cosener's House, 15-16 Abbey Cl, Abin...
to Limoncello, 13 Ock St, Abingdon OX14 5AL

7 min (0.3 mile)

via Abbey Cl and A415

Mostly flat

Use caution – walking directions may not always reflect real-world conditions

The Cosener's House
15-16 Abbey Cl, Abingdon OX14 3JD

- Walk west towards Abbey Cl
  23 ft
- Slight left onto Abbey Cl
  476 ft
- Turn left onto Market Pl
  220 ft
- Turn right onto High St/A415
  Continue to follow A415
  0.2 mi

Limoncello
13 Ock St, Abingdon OX14 5AL