Grand Challenges

The Collaborative Computational Community in Particulate Solids Simulations (CCC-ParaSolS)

CCC-ParaSolS aims to develop cutting-edge software and deliver specialised training to enable the realistic modelling of particulate materials, which are essential to UK industries including chemical, pharmaceutical and construction. Our goal is to provide the particulate community with accurate and efficient frameworks for their modelling needs.

The Community

ParaSolS Particulate Solids Simulations www.ccc-parasols.ed.ac.uk

CCC-ParaSolS aims to unite scientists and engineers from academia and industry with a common interest in modelling particulate solids for a variety of applications. Building on existing discipline-specific networks, the community will embed diversity and inclusiveness in its composition, governance, and activities. The community will also promote the use of open-source software and best practices in validation, benchmarking, and research data management. Bespoke training on discrete element methods (DEM), high performance computing (HPC), reproducible research, and FAIR data principles will be delivered by code developers, EPCC, and CoSeC. A training programme will be designed to be inclusive of historically underrepresented groups. Through community consultation, CCC-ParaSolS will identify gaps and barriers in the current modelling capabilities that are inhibiting high-impact scientific discoveries and slowing the transition from workstations to HPC, and from CPUs to GPUs, to improve energy efficiency and performance.

The Challenge

To develop and enable the use of simulation codes at industrially relevant scales for the particulate solids simulation community

Particulate solids are a large and diverse category of materials that include natural soil deposits, mineral ores, pharmaceutical powders and food ingredients. These have significant economic and societal importance. Numerical modelling provides a means to improve efficiency and safety in the vast number of applications that involve particulate solids, by providing insights into the behaviour of these complex granular systems. To enable the modelling of particulate solids at very large scales desired by industry, code developments are essential to effectively exploit modern hybrid computing architectures and derive performance gains from the integration of mechanistic solvers with physics-informed AI. The physical models underpinning simulation codes require additional development to capture the complexity of real-

Grand Challenges

world particulate processes quantitatively and reliably for all applications. Simulation codes need rigorous verification, validation, and benchmarking for which high-quality data from physical experiments are essential. These data are sometimes lacking and are often not in the public domain. The particulate solids simulation community has historically favoured commercial codes run on workstations, limiting the scale of the problem that can be simulated and not taking advantage of the UK's Digital Research Infrastructure (DRI).

The Solution

To promote and accelerate the development of open-source software for particulate solids simulations

CCC-ParaSolS will promote and accelerate the development of open-source software for particulate solids simulations, which is future-proofed by being deployable on all current and emerging computing architectures found within the UK's DRI, and capable of efficiently utilising computational resources at exascale and beyond. Targeted developments will improve the physical models underpinning simulation codes and integrate multiscale and multiphase modelling capabilities, bringing the community ever closer to capturing the detail and complexity of real particulate solids systems in a virtual environment.

The software suite, including codes for DEM simulations, multi-scale and multi-physics coupling frameworks, visualisation and data analysis, will be comprehensively validated with openly shared data, built on FAIR principles, with AI integrated where advantageous. These technical contributions will ensure that the UK continues to lead in the development and exploitation of particle-scale methods.

The Outcome

A suite of codes for particulate solids simulations available for use for economic and societal benefit in the UK

A suite of high-performance, validated and scalable open-source codes for the numerical modelling of particulate solids will be developed, that democratises the adoption of these codes for economic and societal benefit in the UK. These benefits include reducing waste and increasing process efficiency within numerous sectors of industry, and pre-empting natural disasters caused by climate change. This main goal and the roadmap for CCC-ParaSolS supports UK goals to achieve net zero by 2050 and adapt to the risks posed by climate change without sacrificing economic prosperity. CCC-ParaSolS will be a diverse and inclusive community in accordance with both UKRI's EDI principles and broader goals to create a more equitable society.

More Information

CoSeC
www.CoSeC.ac.uk
CoSeC@stfc.ac.uk

CCC-ParaSolS
www.ccc-parasols.ed.ac.uk
ParaSolS@ed.ac.uk