Grand Challenges

UK Consortium on Mesoscale Engineering Sciences (UKCOMES)

Over the next 5-10 years UKCOMES will continue investigations into the challenging environments of porous media using the Lattice Boltzmann method and taking advantage of emerging computing hardware such as GPUs, Quantum computers and AI.

The Community

www.ucl.ac.uk/mesoscale-modelling-consortium/

The United Kingdom Consortium on Mesoscale Engineering Sciences (UKCOMES) is a group of researchers across the UK who develop and apply mesoscopic modelling techniques to explore systems of scientific and industrial interest at scales between atomistic and continuum levels. The consortium applies and studies several modelling techniques, predominately Dissipative Particle Dynamics (DPD) – a particle-based method similar to atomistic molecular dynamics (MD) – and the Lattice Boltzmann Equation (LBE) method, capable of modelling fluid flows with complex geometries and interactions between multiple fluids and phases. Its core support focuses on developing the consortium's community codes for DPD and LBE simulations, DL_MESO and HemeLB: adding new functionalities, optimising for various computing architectures (including the UK's national supercomputer ARCHER2) and improving interoperability with other codes and libraries.

The Challenge

To characterise and model porous media using numerical simulation

Porous media are central to many natural and engineered systems, playing a critical role in renewable energy and sustainable technology developments. Technologies such as fuel cells, batteries, electrolysers, oil recovery, energy storage and even biological systems (blood vessels, tissues) rely on transport through complex poor networks. Highly coupled multiphysics processes – fluid flow, mass and heat transfer, phase change, and chemical reactions – occur within interconnected pores and strongly influence efficiency, capacity, safety and degradation. Understanding and predicting porous systems often requires quantitative information at the pore scale, where these fundamental mechanisms originate.

Despite their importance, porous media remain challenging to characterise and model due to heterogeneity, hierarchical structure, and dynamic phase interactions. Experimental imaging methods – e.g. X-ray microtomography, focused-ion-beam scanning electron microscopy (FIB-SEM), transmission electron microscopy (TEM) – enable direct visualisation of microstructure and transient processes, but are limited by spatial resolution, imaging speed, and extreme operating conditions. Analytical approaches work only for idealized geometries, typically neglecting real-world non-linearities. Numerical simulation has thus become essential for investigating pore-scale physics, uncovering underlying mechanisms, and guiding the design of advanced porous materials for energy, environmental and health applications.

The Solution

Using the Lattice Boltzmann method to simulate multiphysics flow in complex porous media

The Lattice Boltzmann Equation (LBE) method has become a versatile and powerful framework for simulating multiphysics flows in complex porous media. Originating from kinetic theory, LBE recovers macroscopic conservation laws – those solved directly by computational fluid dynamics (CFD) methods – while retaining mesoscopic information on particle collisions and momentum exchange. This allows it to capture microstructural effects, interface dynamics and non-equilibrium transport, and to couple hydrodynamics and with thermal, mass transport and chemical fields (reactions). Its local, explicit and highly parallelisable algorithm is well suited to high-performance computing (HPC) platforms, including GPUs and exascale architectures, and naturally handles complex geometries – enabling direct simulation of porous structures derived from micro-CT or FIB-SEM images without generating meshes or transforming coordinates.

Since real porous systems span nano- to macroscale regimes, LBE has been integrated with complementary multiscale techniques, including molecular dynamics (LBE-MD) for nanoconfined gases, pore network methods (LBE-PNM) for multiphase flow and evaporation, discrete element methods (LBE-DEM) for flows in deformable porous media, and finite-volume methods (LBE-FVM) for heat-transfer problems. Recent integration of machine learning (ML) and data-driven models has opened new possibilities, e.g. using large datasets generated from high-fidelity pore-scale LBE simulations to train neural networks and surrogate models to predict permeability, effective diffusivity and interfacial transport. These hybrid LBE-ML approaches greatly reduce computational cost while maintaining physical accuracy, enabling predictive digital twins for porous materials and renewable energy devices.

The Outcome

Using Lattice Boltzmann on emerging computing hardware such as GPUs and Quantum computers and integrating with AI workflows

The UK aims to lead globally in net-zero and health technologies. Understanding, predicting and optimising porous media in these fields is crucial to these ambitions. LBE is highly-suited to porous media simulation, exploiting emerging computing hardware (GPUs, quantum architectures) and integrating seamlessly with AIdriven workflows for accelerated modelling and optimization. As porous media span nano- to macro-scales, increased computational power will enable higher resolution and more reliable predictions.

Key application areas include:

- Next-generation batteries (metal-air, solid-state)
- Hydrogen production and storage (metal-organic frameworks, geological reservoirs)
- Real-time simulation of fluid circulation in human bodies

These systems are notoriously difficult to model using traditional MD or CFD. LBE's flexibility and HPC efficiency enable it to tackle these challenges and make advances ranging from hydrogen-storage design to clinical diagnostics. Future LBE software tools will feature advanced multiphysics solvers (fluid dynamics, heat transfer, phase-change phenomena), and multiscale models linking pore-scale physics to system-level behaviour.

ML techniques will further reduce computational costs, enabling faster insights without sacrificing physical fidelity. This capability is essential for designing and licensing next-generation fission systems, including high temperature gas-cooled reactors and molten salt reactors, priorities within the UK's advanced modular reactor programme and energy security agenda. An AI-enhanced thermal hydraulics framework, validated against international (OECD/NEA) benchmarks, will significantly cut simulation costs, speed up design cycles, provide near real-time operational insights and support digital-twin deployment across reactor types, including Small Modular Reactors and emerging fusion demonstrators.

Building on the UK's strong expertise in high-temperature, high-pressure gas-cooled reactor technologies, a UK-led international validation consortium pool experimental data and develop robust AI/ML frameworks specifically for high-temperature and high-pressure gas-cooled reactor systems.

This roadmap strengthens the UK's ambitions for clean, resilient, sovereign nuclear energy – reinforcing international regulatory leadership, attracting industrial investment, and developing a workforce skilled in multiphysics and AI integration.

More Information

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