Simulating Flow Through Rocks at Unprecedented Scale on ARCHER2

THE UNIVERSITY of EDINBURGH

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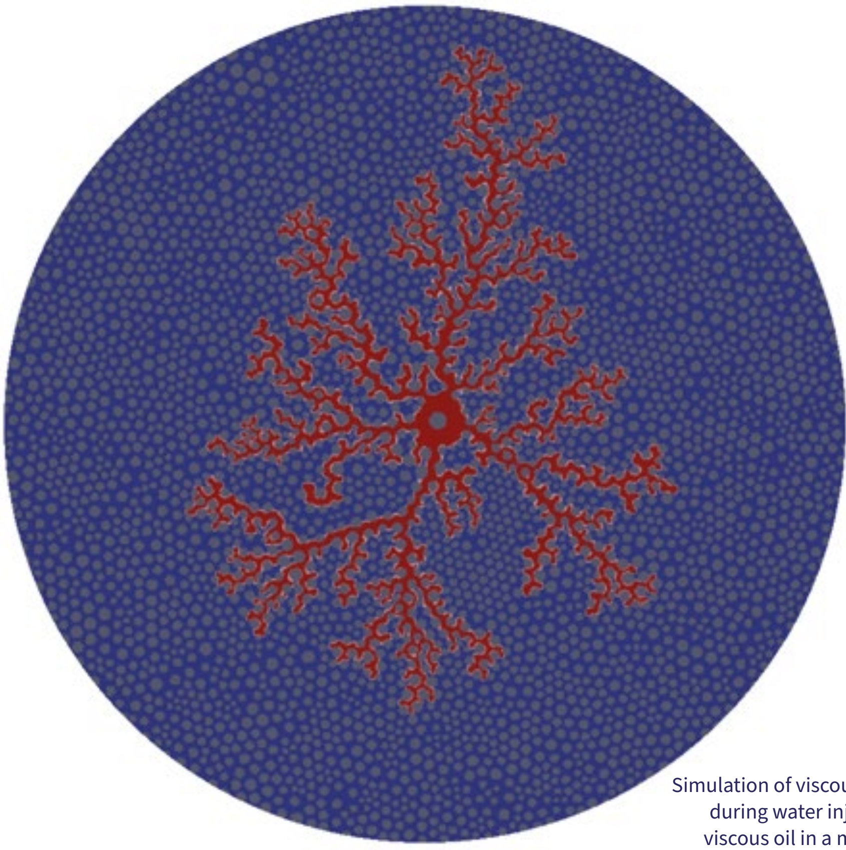
Understanding how fluids and chemicals flow through porous materials is essential for many areas of research. However, to simulate this in any detail requires vast amounts of computing power. Researchers at Heriot-Watt University and the University of Edinburgh have enhanced the GeoChemFoam modelling code to allow it to fully exploit the computational power of ARCHER2. As a result, the code can now run more precise simulations in greater detail, with a quicker turnaround time.



Simulation of viscous fingering during water injection into viscous oil in a micromodel

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Challenge

Porous materials are ubiquitous in science and engineering – spanning geological formations, soils, construction materials, catalysts, and biological tissues. Understanding how fluids and chemicals move through these complex pore networks is critical for applications from groundwater remediation and carbon storage to improving building materials and biomedical implants. Researchers increasingly use 3D X-ray micro-CT scans to capture a material's pore structure at micron-scale resolution, then simulate flow and reactions directly on these images for predictive insights. However, the *scale and detail* of such images pose a formidable challenge: even a single sample can contain billions of voxels (3D pixels), making it extremely data intensive.

Converting these massive images into computational meshes and solving fluid equations at the pore-scale pushes beyond the current limits of standard computing and software tools. Compounding the issue, many traditional computational tools for mesh generation and processing run in *serial* on a single compute core and are constrained by the memory of one machine. This means that previously scientists had to analyse small sub-volumes of a sample or use coarser models, creating the risk of introducing large errors when extrapolating to the whole material. For example, in digital rock studies, analysis based on a small sub-region of a heterogeneous rock can lead to a drastic misestimation of properties such as permeability.

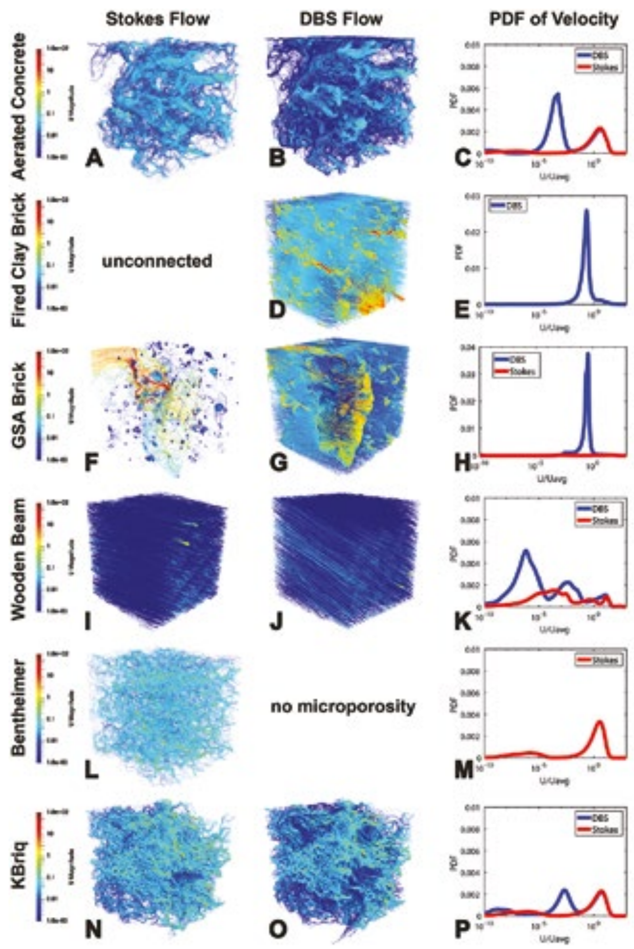
The challenge addressed by the ARCHER2 eCSE10-2 project[1] was to enable *truly high-resolution, pore-scale simulations* on much larger computational domains than before. Crucially, while the project's initial demonstrations used micro-CT data from rock, the techniques developed are applicable to *any* porous material. Whether the goal is to model water flow in soil aggregates, chemical diffusion in catalyst pellets, or nutrient transport in bone scaffolds, researchers needed a general, scalable solution to handle ultra-large 3D images and harness the power of High Performance Computing (HPC) for pore-scale modelling.

Solution

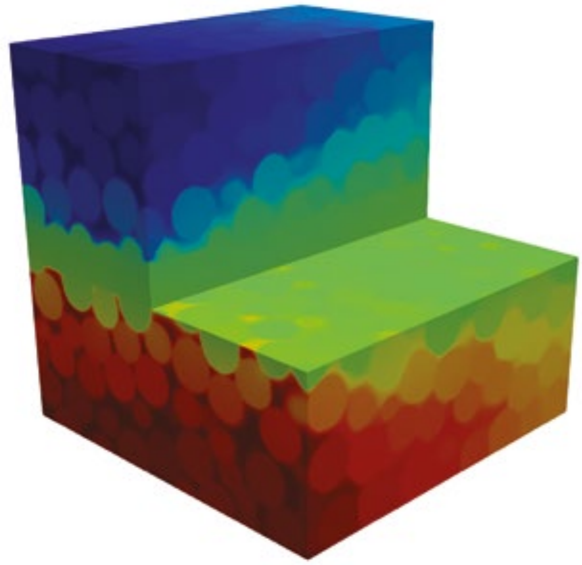
To overcome these limitations, this project optimised the GeoChemFoam code – an open source code for pore-scale simulation – to run on ARCHER2, the UK National Supercomputing Service. The team created a Python-based tool, capable of slicing the input micro-CT data and distributing the workload across many processors. Running across multiple compute nodes simultaneously allows the code to effectively tap into hundreds of terabytes of aggregate memory. Key software on ARCHER2 was also upgraded in the course of this project. The high-memory nodes and powerful CPUs of the ARCHER2 system can now be leveraged to full effect.

Importantly, these solutions were implemented in a general way: nothing is hard-coded to rocks or geoscience. Any volumetric dataset of a porous material can be simulated, opening the door for cross-disciplinary use. The success of the project demonstrates how investing effort in HPC software development can generalise to benefit a broad range of scientific domains, rather than solving a one-off problem.

1. https://www.archer2.ac.uk/ecse/reports/eCSE10-02/



Modelling air flow through a range of building materials



Modelling temperature distribution in a porous-medium heat exchanger

Impact

This work has significantly improved the computational efficiency of GeoChemFoam. These improvements not only reduce turnaround time for researchers but also enable more accurate and representative simulations, potentially saving weeks of experimental work and thousands of pounds in lab costs.

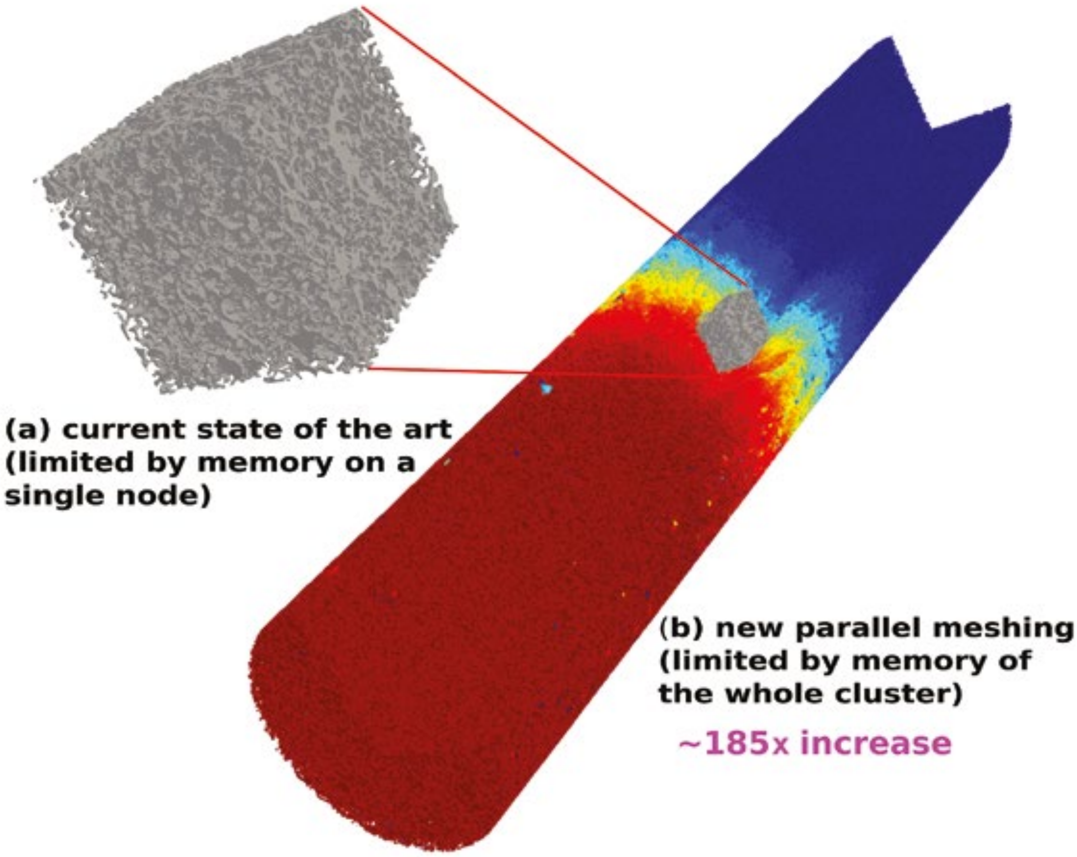
The project has delivered tools and techniques that extend well beyond a single case study in geoscience. By enabling ultra-large pore-scale simulations on ARCHER2, the work has laid a foundation for breakthroughs across multiple disciplines. Researchers in energy and environmental science can now model processes such as CO_2 sequestration, hydrogen storage, and contaminant transport at previously unattainable resolution. For example, subsurface engineers could simulate groundwater flow in soil pores or the effectiveness of carbon capture in reservoir rock with new levels of confidence in the results.

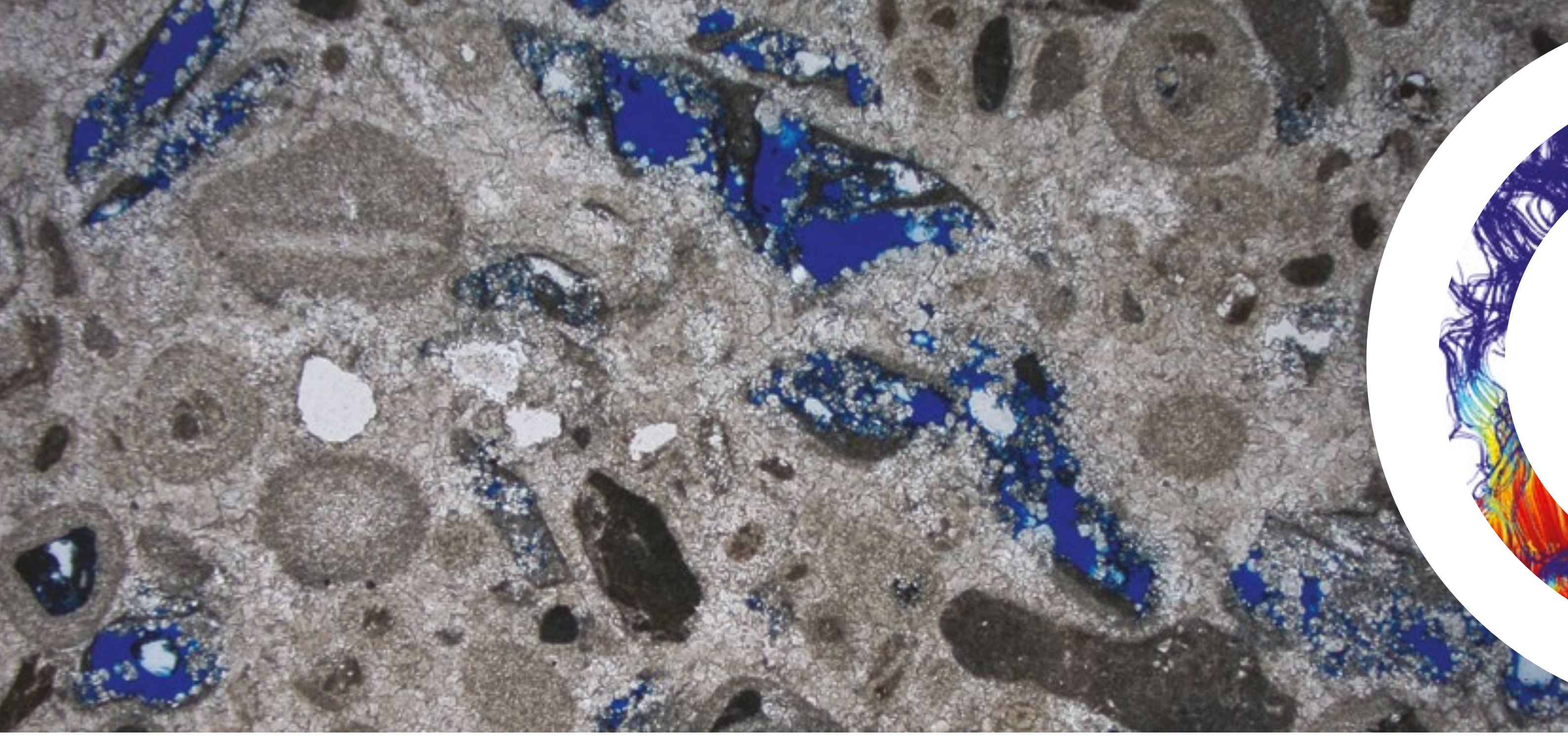
In materials science and engineering, the same capabilities allow detailed analysis of building materials (such as concrete or historical stone) to predict durability and weathering by tracking moisture or chemical ingress through micro-cracks and pores. Chemical manufacturers and petrochemical researchers can apply the tools to porous catalysts and filters, using simulations to optimise designs for better flow distribution and reaction efficiency. Even the biomedical field stands to benefit: the methods make it feasible to simulate fluid and nutrient perfusion in complex tissue scaffolds and biomaterials, aiding the design of implants that promote cell growth.

Beyond academic research, the broader industrial and societal relevance is clear. Many industries deal with porous media – oil and gas companies characterising digital rocks, environmental agencies examining soil contamination, construction firms assessing concrete longevity, or medical device companies testing biomaterial implants. The HPC-enabled tools from this project can accelerate innovation in these sectors by replacing months of physical testing with faster computational experiments.

Moreover, the case study exemplifies how investment in national HPC infrastructure and software development yields widely applicable benefits: not only advancing fundamental science, but also providing practical capabilities that align with national priorities (such as clean energy and healthcare technology). By democratising access to high-fidelity pore-scale simulation, ARCHER2 is helping the UK research community stay at the cutting edge of solving complex multi-scale problems.

This successful project demonstrates a compelling return on investment for HPC – empowering researchers across domains to tackle grand challenges in energy, environment, and materials using the same powerful computational tools. The impact will continue to grow as more users adopt these methods for their own porous materials, driving new discoveries and informing policy and industry with better predictive models enabled by ARCHER2.





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https://github.com/GeoChemFoam

References:
Multi-Billion Voxel Micro-CT Images of Porous Materials Using OpenFOAM on ARCHER2, Julien Maes, Gavin J. Pringle, Hannah P. Menke, pre-print available at **https://arxiv.org/abs/2512.08438**

ARCHER2-eCSE10-2 Technical Report: **https://zenodo.org/records/18174111**

About ARCHER2
ARCHER2 is the UK's National Supercomputing Service, a world class advanced computing resource for UK researchers. ARCHER2 is provided by UKRI, EPCC, HPE and the University of Edinburgh. ARCHER2 is the latest in a series of National Supercomputing Services provided to UK researchers.

More ARCHER2 case studies can be found at:
https://www.archer2.ac.uk/research/case-studies/

The eCSE Programme
The Embedded CSE (eCSE) programme provides funding to the ARCHER2 user community to develop software in a sustainable manner to run on ARCHER2. Funding enables the employment of a researcher or code developer to work specifically on the relevant software to enable new features or improve the performance of the code.

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