UKRI Science and Technology Facilities Council

Scientific Computing

Computational Engineering Theme

David R. Emerson

Computational Engineering Theme: Objective

Introduce computational engineering research activities in the Theme and look to identify common topics for future cooperation

Computational Engineering Theme: Groups

Group 1

- Benzi John
- Zhengliang Liu
- New Recruit

Group 2

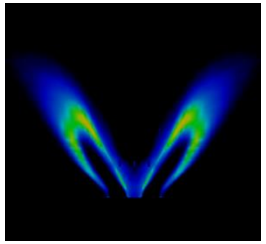
- Stephen Longshaw
- Wendi Liu
- Omar Mahfoze
- Mayank Kumar

Group 3

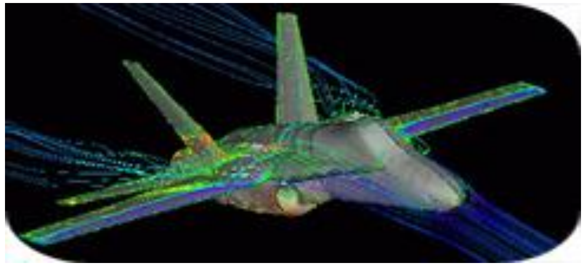
- Xiaojun Gu
- Charles Moulinec
- Stefano Rolfo
- Jian Fang
- Greg Cartland-Glover
- Wei Wang
- Chrysovalantis Tsinginos
- Bo Liu

NB: Re-Group 2, Stephen is now Director of CoSeC and temporary GL as we transition to new structure

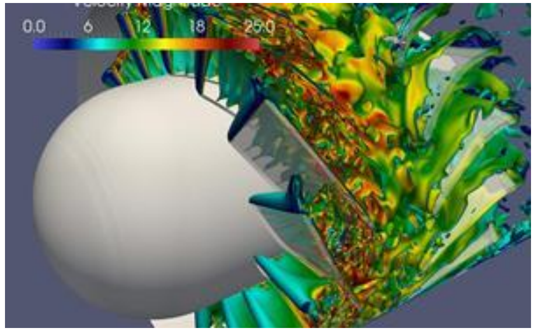
Computational Engineering Theme

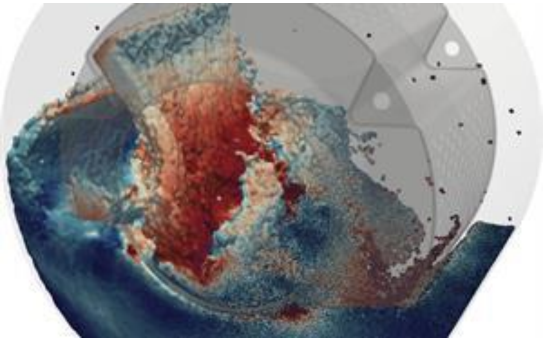


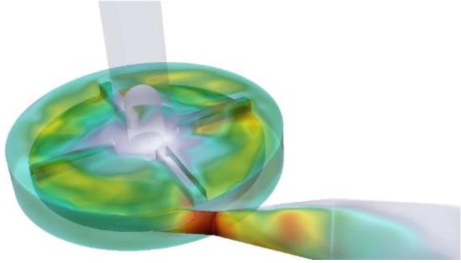
The Computational Engineering Group focuses specifically on HPC capability to model a range of fluid flows:

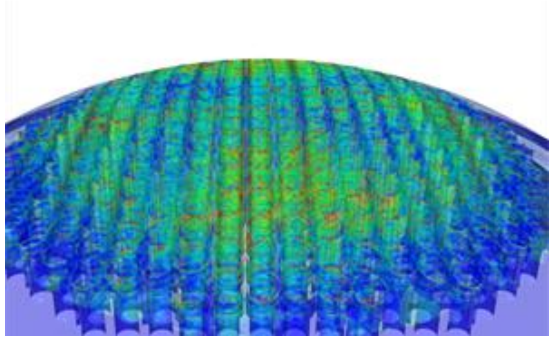


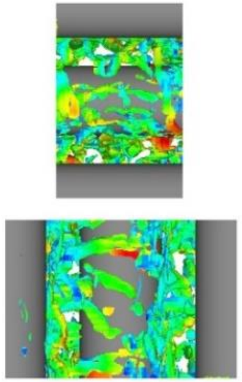
- Turbulence and combustion
- Energy (nuclear, conventional, green)
- Hypersonic Aerothermodynamics
- Micro- and nano-fluidics
- Rarefied gas dynamics
- Environmental flow modelling (e.g. urban air quality)
- Aeroacoustics (e.g. noise from turbomachinery)
- Fluid-Structure Interactions
- Multiphysics/Multiscale simulation
- Exascale software development & code coupling

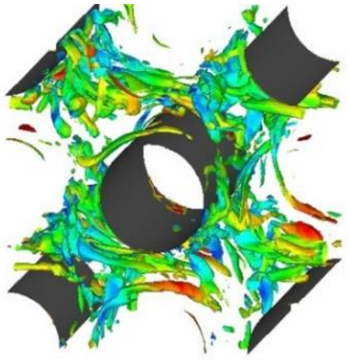












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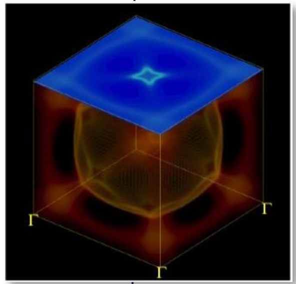
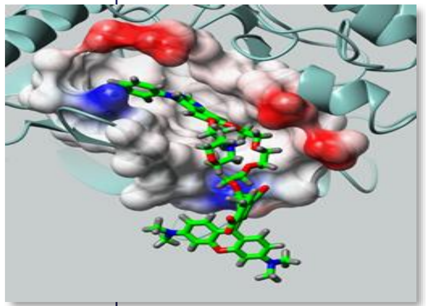
Modelling Across Scales

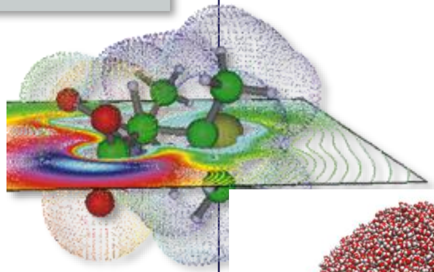
fm | pm | nm | µm | mm | m

Materials & Molecular Science

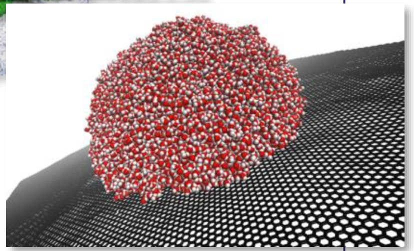


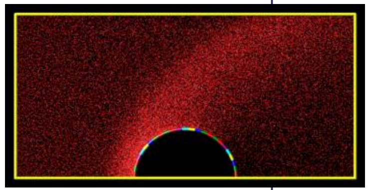


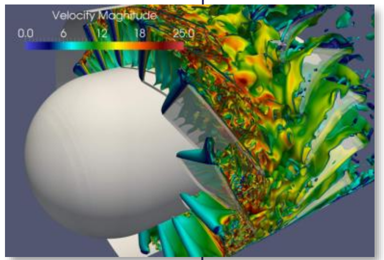
Computational Biology



Computational Engineering







Cross cutting activities:
Scientific Machine Learning (AI4Science) together with Computational Mathematics (Math Libraries for Scientific Software)

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Software Examples: General Purpose

Code_Saturne

- https://www.code-saturne.org
- Part of the EDF simulation suite
- General purpose Finite Volume CFD
- Excellent parallel scalability

OpenFOAM®

- https://www.openfoam.com
- General purpose Finite Volume CFD
- Solvers for specific physical problems built using its toolkit
- Large development and user community

Nektar++

- https://www.nektar.info
- General purpose high-order spectral/HP framework
- Based on high-order polynomial expansions

FEniCS Project

- https://fenicsproject.org
- Platform for solving PDEs
- Implements Finite Element approach

Software Examples: Dedicated CFD

- https://www.incompact3d.com
- High-order Finite Difference solvers
- Applications to incompressible flow and high-fidelity turbulence modelling
- Some work on GPU porting

Xcompact3d
in turbulence we trust

- https://github.com/weiwangstfc/CHAPSim2
- Finite Difference solvers
- Incompressible flow applications with a focus on heat transfer and nuclear applications

Direct numerical simulation of thermal stratification of supercritical water in a horizontal channel
W Wang, S He, C Moulinec, DR Emerson
Computers & Fluids, **261**, 105911, 2023

CHAPSIM

ASTR

- https://github.com/astr-code/astr
- High-order Finite Difference solver
- Applications in compressible, supersonic, and hypersonic flows

An improved parallel compact scheme for domain-decoupled simulation of turbulence
J Fang, F Gao, C Moulinec, DR Emerson
Int Journal for Num Meth in Fluids, **90** (10), pp. 479-500, 2019

Software Examples: Enabling Libraries

Multiscale Universal Interface

- https://mxui.github.io
- General purpose code coupling
- Used to design couplings between different computational software/methods
- Designed for use in HPC environments

2DECOMP&FFT

- https://github.com/2decomp-fft
- Pencils and slabs decomposition library to support 3D structured mesh solvers
- Distributed memory 3D FFTs capabilities
- Highly scalable on hundreds/thousands of cores and supports multiple GPU partitions

Software Examples: Particle-based Methods

SPARTA

- https://sparta.github.io/
- Parallel direct simulation Monte Carlo (DSMC) method for rarefied gas dynamics from Sandia National Lab
- High-fidelity molecular-level gas dynamic solver
- Applications in space, micro/nano-fluidics & vacuum gas dynamics

PICLas

- https://github.com/piclas-framework/piclas
- Parallel 3D plasma-kinetic, particle-in-cell (PIC) code from Stuttgart
- High-fidelity rarefied (DSMC) & plasma dynamic (PIC-DSMC) solvers
- Applications in particle accelerators, thruster propulsion, vacuum devices etc.

Plasma Kinetic Code PICLas STUTTGART

dsmcFoam+

- https://github.com/MicroNanoFlows/OpenFOAM-2.4.0-MNF
- Code based on well-known OpenFOAM software
- Developed jointly with Strathclyde, Glasgow & Edinburgh
- Molecular-level gas dynamics (DSMC) solver well-suited for a range of rarefied gaseous flow applications

dsmcFoam+: an OpenFOAM based direct simulation Monte Carlo solver
C White et al., CPC **224**, pp. 22-43, 2018

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Group 1

B John, Z Liu, +1

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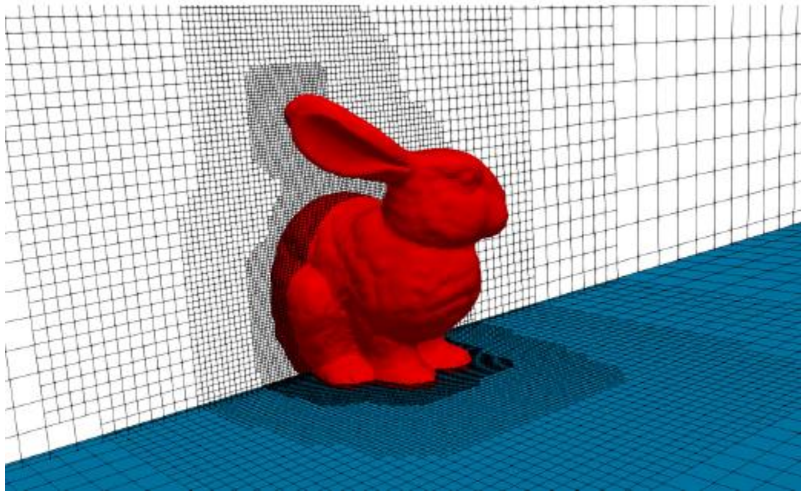
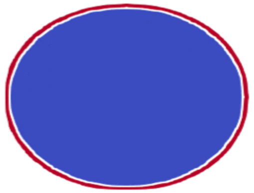
Adaptive Mesh Refinement and LBM

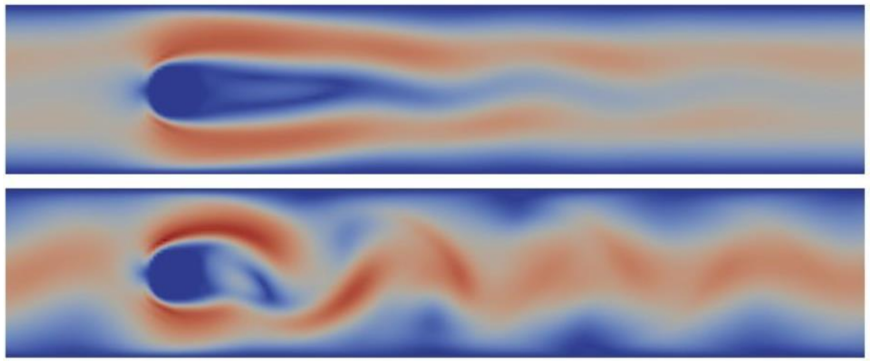
(A kinetic method for meso-scale and hydrodynamic fluid problems)



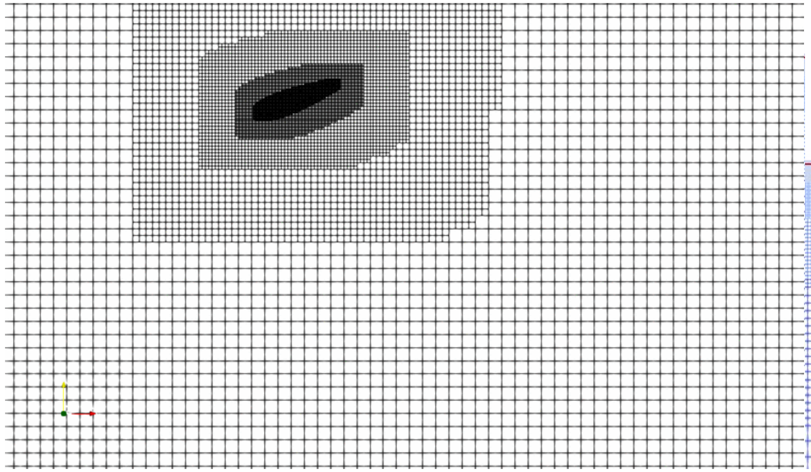
AMR mesh generation for complex geometry



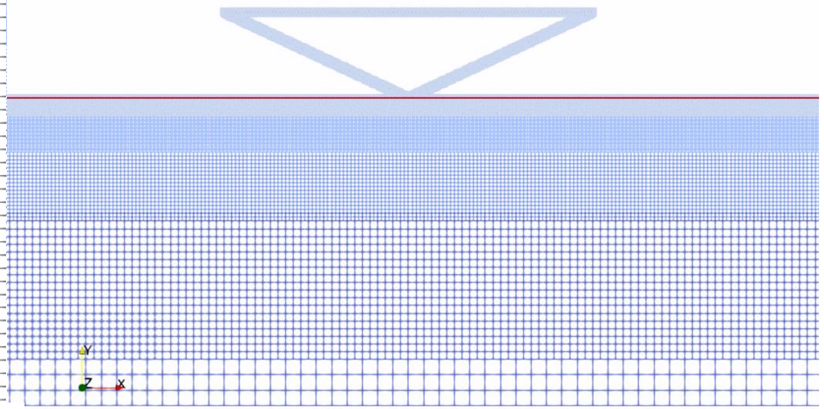
Mesh adaptation for free surface flow



LBM simulation of a cylinder using DL_MESO (uniform mesh)



Fluid-Structure interaction of a flapping foil



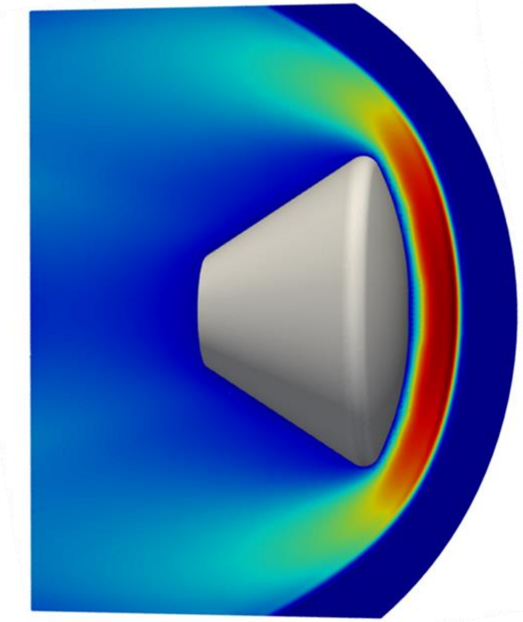
AMR-LBM simulation of a falling wedge

Future plan to incorporate AMR into DL_MESO for:

- automatically & dynamically refining and coarsening
- enhancing efficiency and accuracy
- coupling with dissipative particle dynamics (DPD)

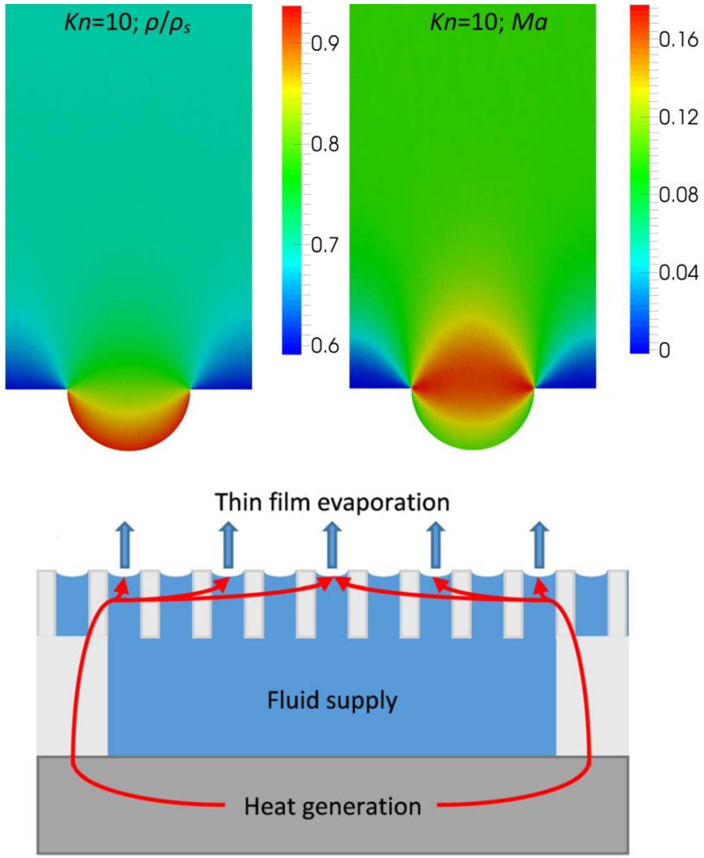
Low-density Gas Dynamics Applications

Applications range from **aerospace** to **micro/nano-scale** to **vacuum devices**. Molecular-level (DSMC) simulations carried out using SPARTA.

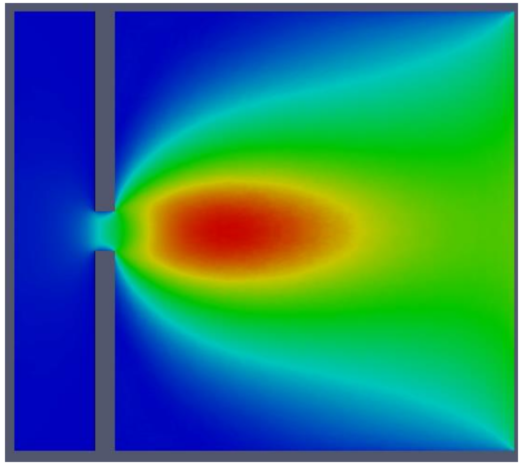


Orion capsule re-entry

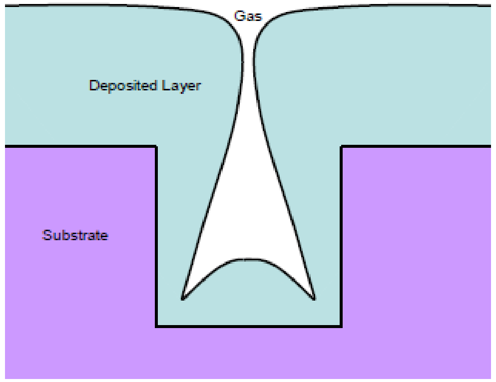
Space debris re-entry risk analysis



Nanoporous membranes for cooling in electronic devices (Nokia-Bell Labs).



Supersonic jet expansion in a vacuum device



Chemical vapour deposition (Thin film coatings)

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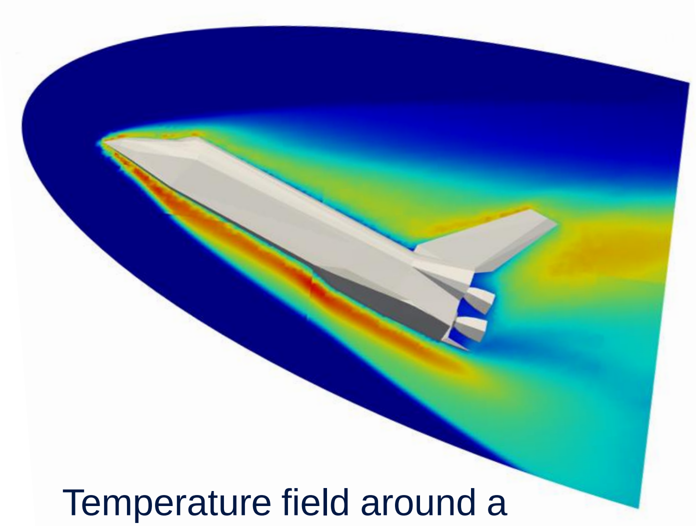
High-altitude Hypersonics (space) Applications

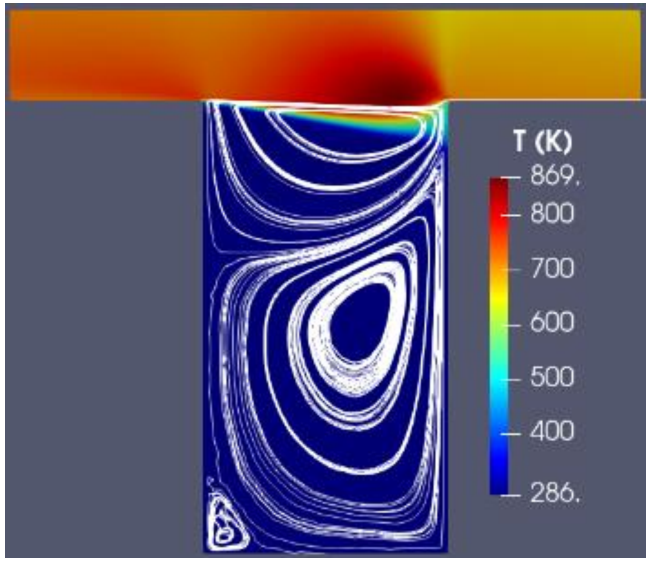
- Hypersonics is a dual-use technology, vital to UK ambitions to develop a vibrant space programme and in attaining critical defence objectives.

- Accurate modelling is challenging as gas-phase chemical reactions, ionization, radiation etc. need to be considered as gas temperature increases with Mach number, e.g. important for designing materials for thermal management (see cavity at Kn = 100) and **thermal protection systems (TPS)**.

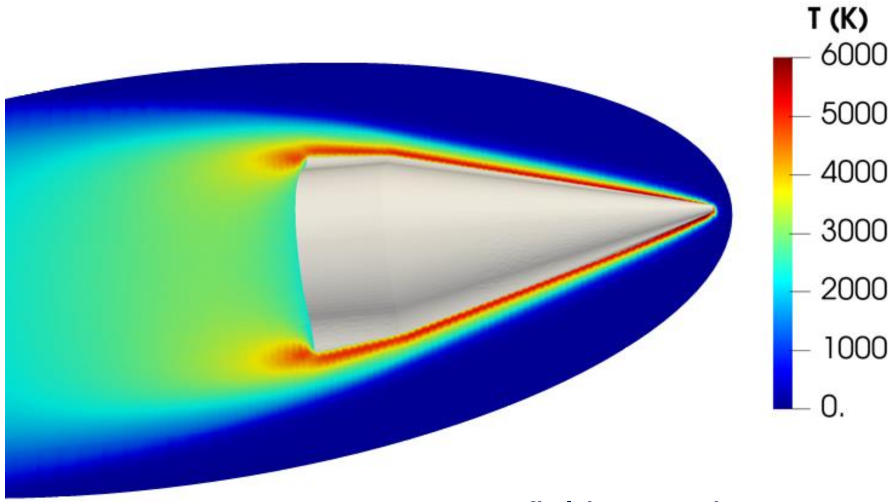
- A key example is aerothermodynamics of **re-entry** of capsules, probes, UAV etc. to planetary atmosphere. The images are our simulation results from the open-source DSMC code, SPARTA.



Temperature field around a NASA **Space Shuttle** (Mach 25)



Thermal Management Mach 6.9 temperature/velocity field in deep cavity to reduce surface heating



Temperature field around an HGV model (at 90 km altitude and AoA 20^0)

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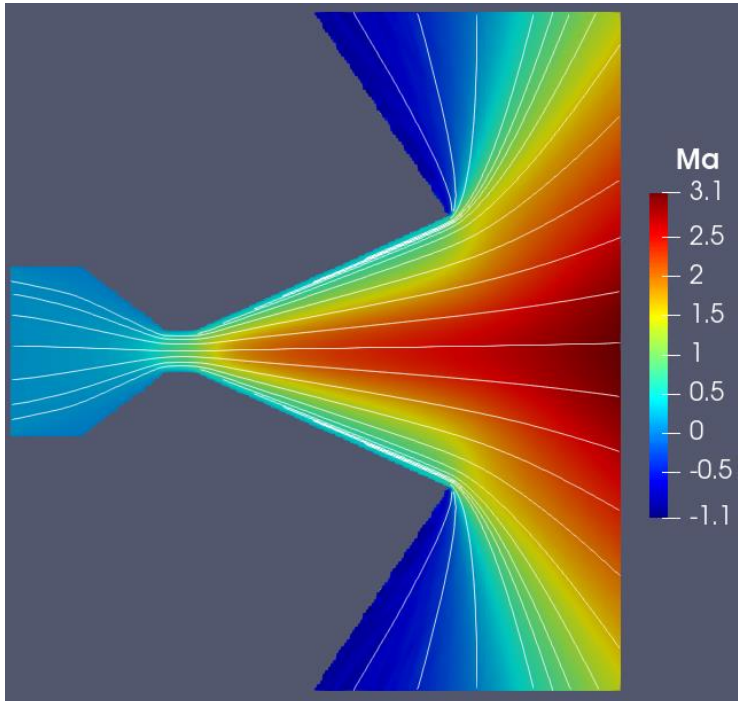
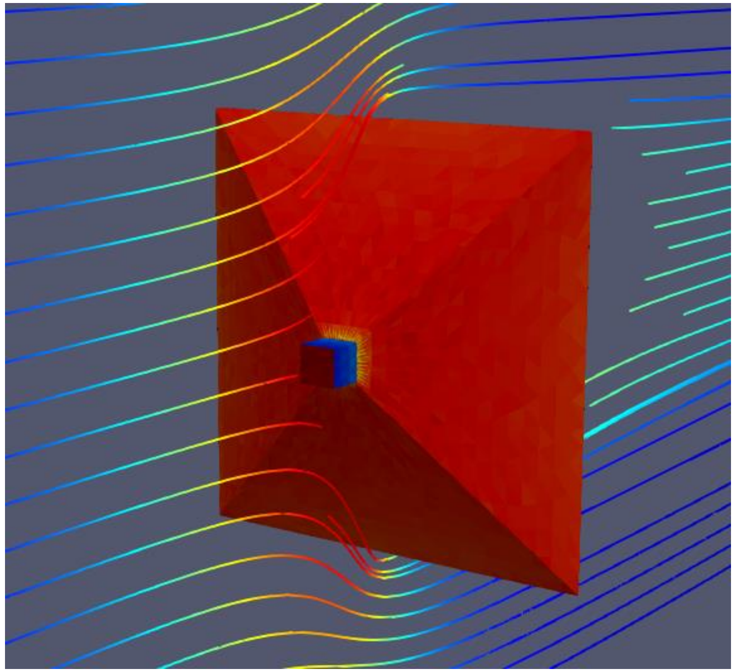
Modelling and Simulation for Satellite Applications - Thruster Propulsion and Satellite Aerodynamics

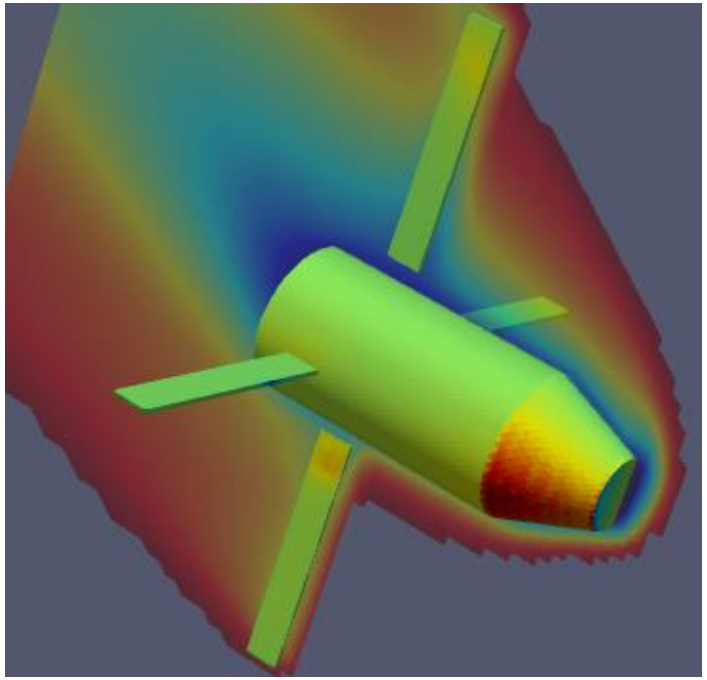
We have expertise in rarefied gas dynamics, particle-in-cell (PIC) methods for neutral, reactive and low-density plasma flow and multi-scale code-coupling techniques.



Thruster propulsion and Nozzle plume expansion



Flow-field & thermal load on a **CubeSat De-orbit Sail** satellite (at H=125 km)



Flow-field & forces on a descending satellite (**ESA satellite debris** test case)

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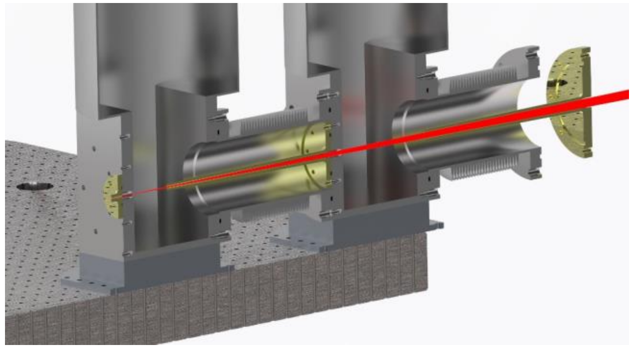
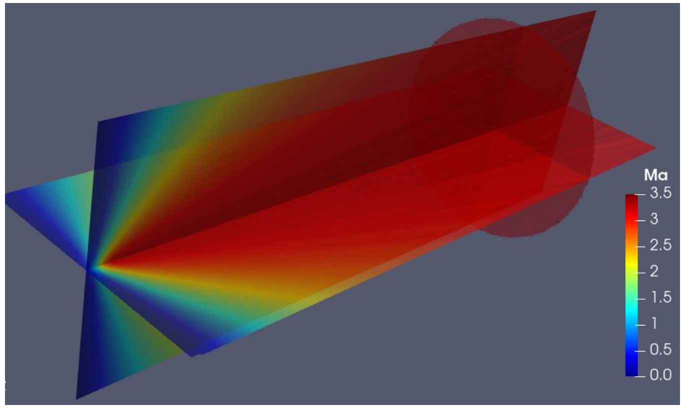
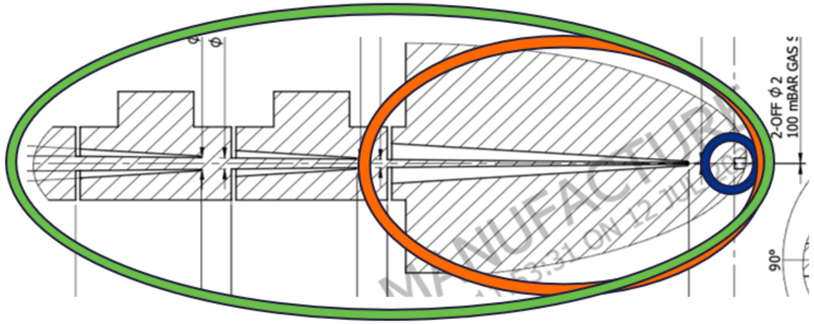
EPAC Laser-Wakefield Accelerator Modelling: (Gas Cell & Vacuum Regions)

- Laser-driven plasma wakefield accelerators (LWFA) capable of generating high quality electron beams up to a few GeV over cm scales.
- Optimising the gas cell density profile and gas expansion into the low-density vacuum drift regions are important for the generation of high-quality electron beams and the overall vacuum design.





Gas expansion (Mach number field) in the first vacuum region



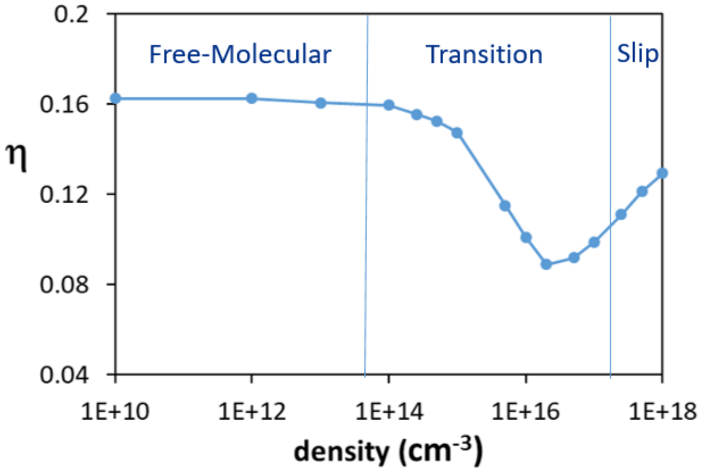
ASTeC

Overall vacuum design

SCD Gas cell region

SCD First accelerator vacuum region

Gas dynamics and transmission probability characteristics in the first low-density region of a laser wakefield accelerator using DSMC.



Transmission probability for various operating conditions

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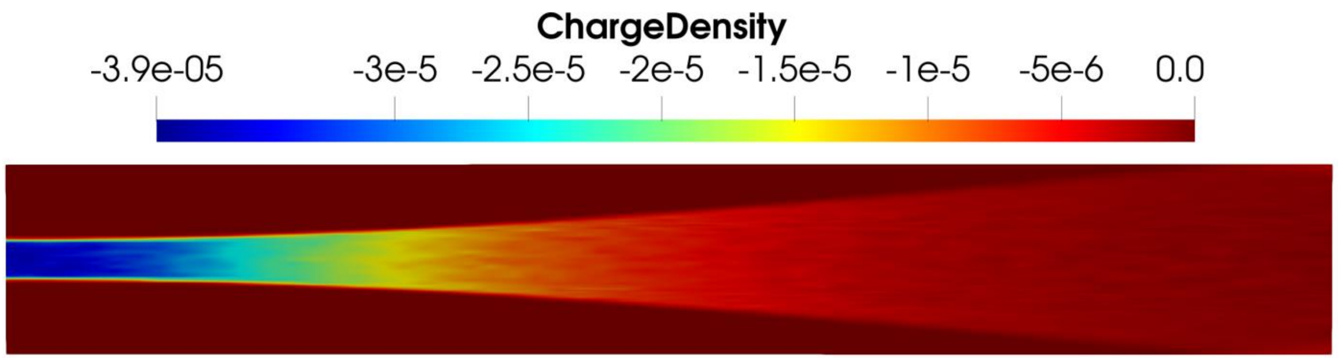
Benzi John, Keith Middleman, Oleg B. Malyshev, Xiaojun Gu, Daniel R. Symes & David R. Emerson, “Numerical investigation of transmission probability characteristics in the first low-density region of a laser wakefield accelerator”, *Microfuidics and Nanofuidics* (2023) 27:52.

Space Charge Compensation for ISIS RF Ion Sources

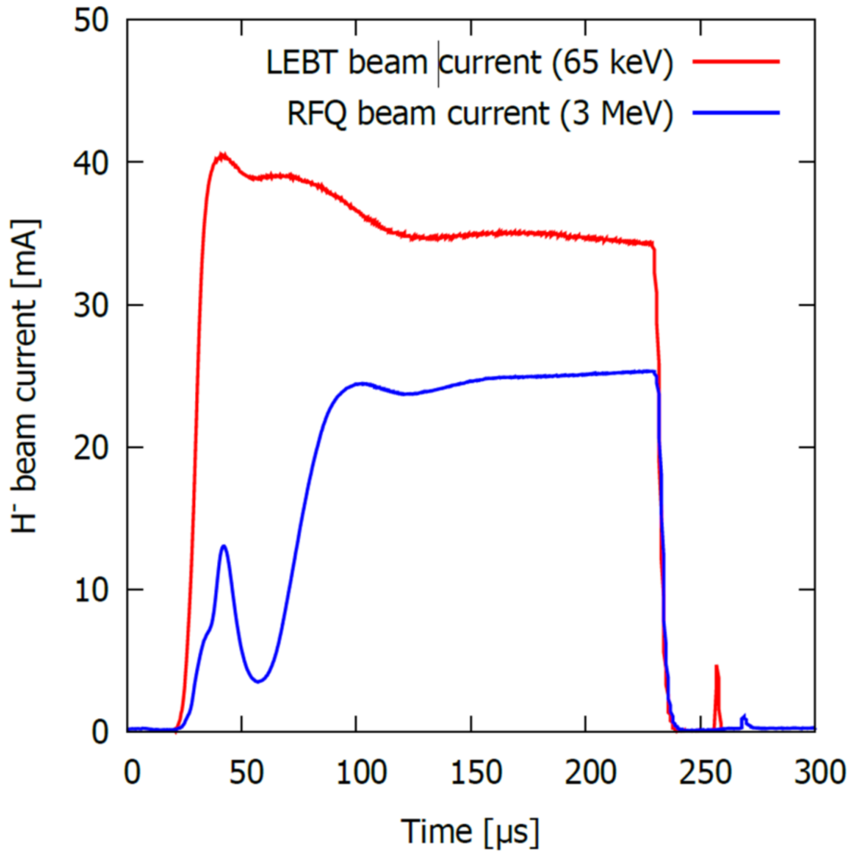
- Space charge compensation (SCC) is crucial to overcome the transport limits of high intensity ion beams in the low-energy beam transport (LEBT) region of particle accelerators.

- For an ISIS RF **H^- ion** beamline, the ensemble of H^- ions create a repulsive force causing ion beam instabilities.

- Understanding and optimisation of the SCC process is relevant to the design phase of ISIS II and, in general, for particle accelerators & beam neutralisation in fusion facilities.



PIC simulation showing beam divergence for an uncompensated ion beam due to space charge effects.



Beam pulse showing losses due to poor transport efficiency and large beam emittance.

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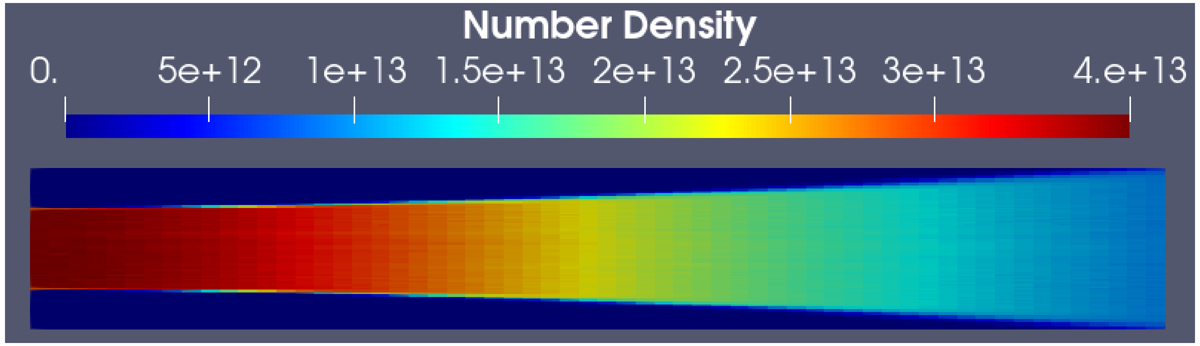
ISIS Colleagues: Olli Tarvainen & Dan Faircloth (LEB group)

Space Charge Compensation for H^- ion beams

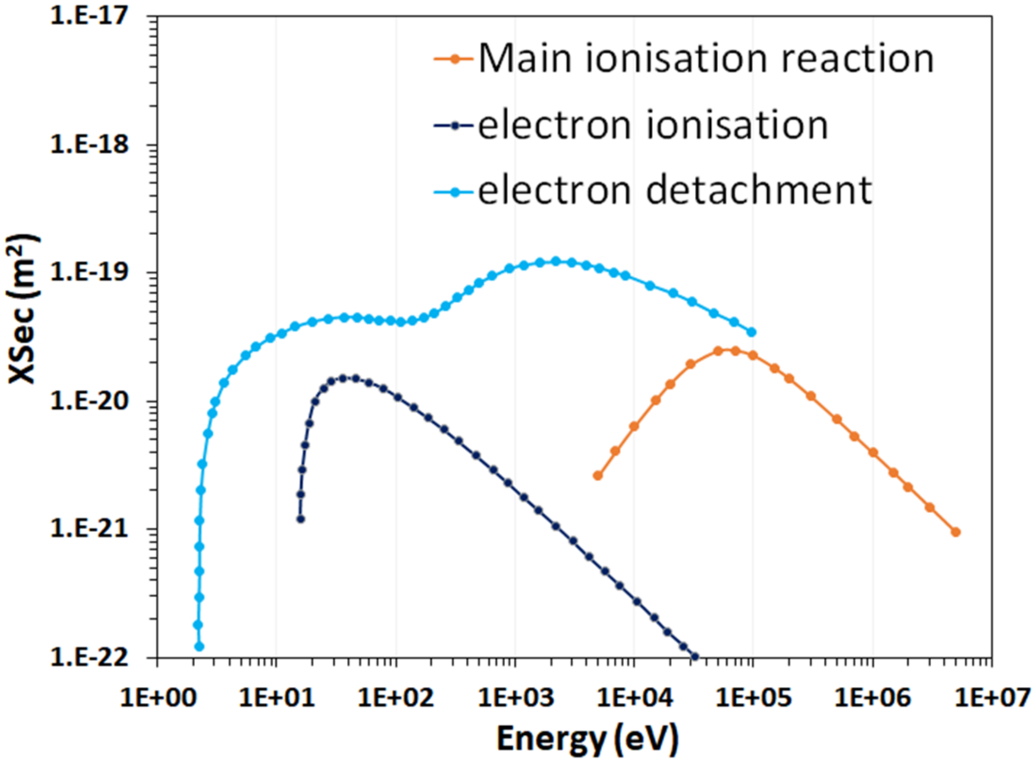
- SCC enabled through the ionisation of a background H_2 gas, producing oppositely charged H_2^+ ions.
- Customising a plasma-kinetic PIC code (PICLas) for the SCC problem by implementing reactions, corresponding cross-sections, and species energy distributions.

$$H^- + H_2 \rightarrow H^- + H_2^+ + e^-$$
$$e^- + H_2 \rightarrow H_2^+ + 2e^-$$
$$H^- + H_2 \rightarrow H + H_2 + e^-$$



SCC through H^- beam interaction with H_2 gas

Uncompensated (top) & space charge compensated beam (bottom)

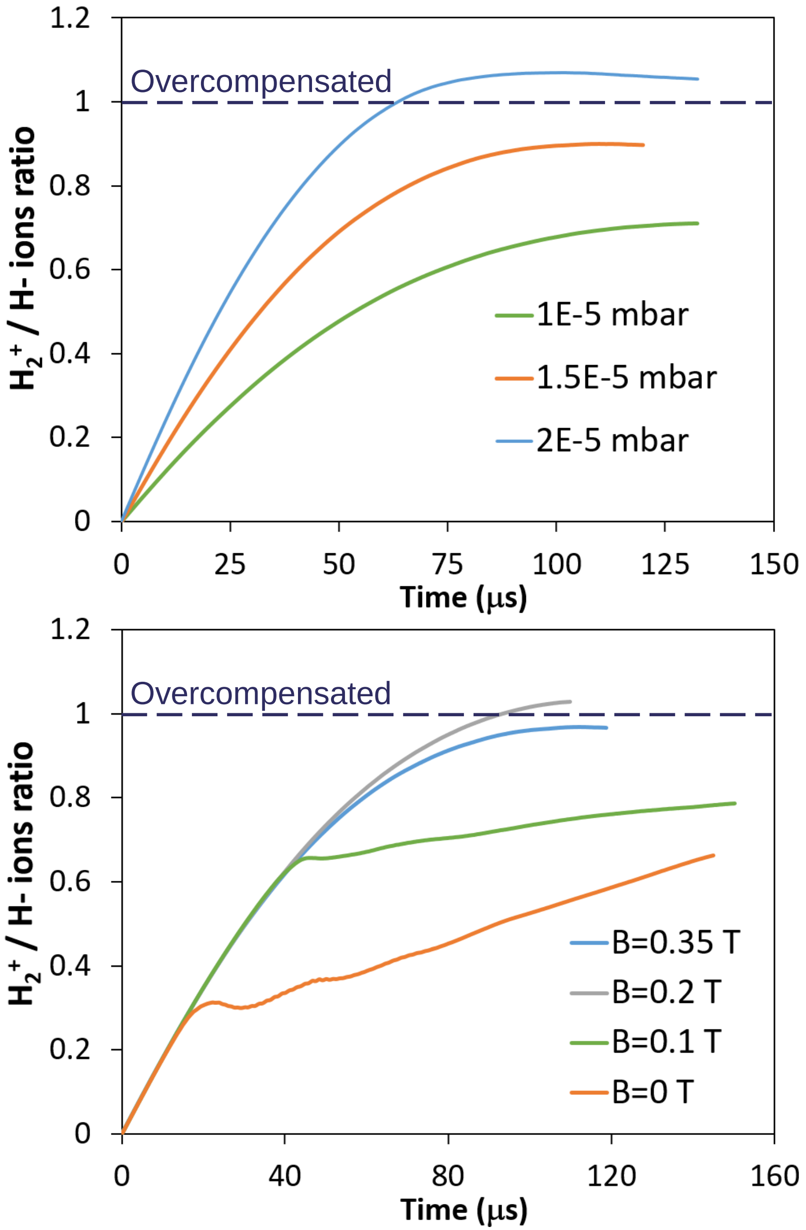


Future plasma simulation priority areas

- Main goal will be to develop strategies to achieve a high SCC degree in a short time. Key parameters being studied include the impact of magnetic field, background gas, the role of electrons in the SCC acceleration process, beam induced light emission process etc.

- SCC work with ISIS has broadened, as it is now part of the **STFC-DAE (India) project** studying SCC of pulsed high-current negative (H^-) and positive (H^+) ion beams.
  - 36 keV (ISIS), 65 keV (FETS, ISIS) H^- ion & 50 keV (LEHIPA, India) H^+ ion sources.

- **Long term plan**: Work together with STFC facilities to build a plasma simulation capability in areas that can support the design of next-generation particle accelerators, for e.g., involving laser-plasma interactions, wakefield acceleration, and XFEL.



Effect of gas pressure & magnetic field on SCC.

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Group 2

S. Longshaw, O. Mahfoze, M. Kumar, W. Liu

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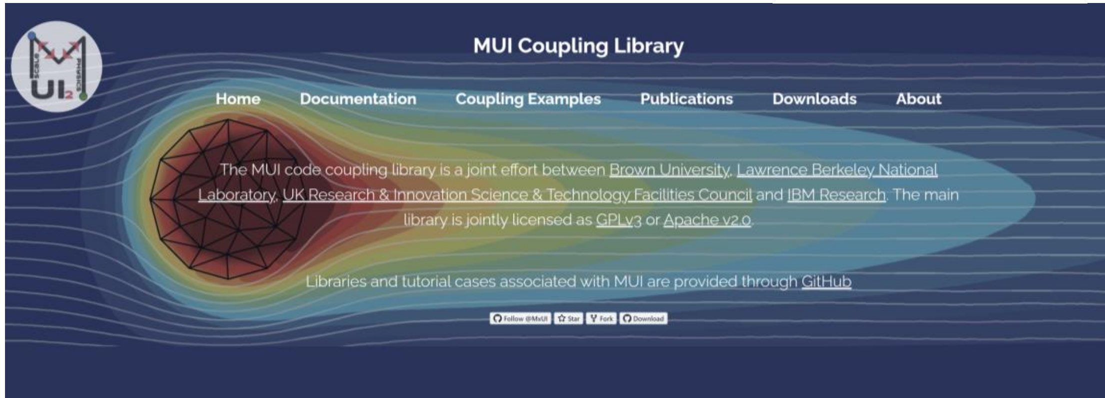
Multi-physics and Multi-scale Modelling

Motivation: Many practical applications involve multiple physical aspects (e.g. structural mechanics and fluid dynamics) and/or involve multiple length or time scales (e.g. macroscopic fluids and microscopic protein folding). Our focus has been developing a partitioned capability to perform high-fidelity multi-physics and multi-scale modelling at scale!

Key library: The Multiscale Universal Interface (MUI) code coupling library

- Collaboration between STFC Daresbury Lab, Brown University; Lawrence-Berkeley National Lab and IBM Research UK
- Written in C++11 (with wrappers for C, Fortran and Python)
- Header-only design
- Creates a peer-to-peer MPI based interface between two or more codes
- Open-source, licensed as either GPLv3 or Apache 2.0
- Website: https://mxui.github.io/
- Library: https://github.com/MxUI/MUI
- Demos: https://github.com/MxUI/MUI-demo



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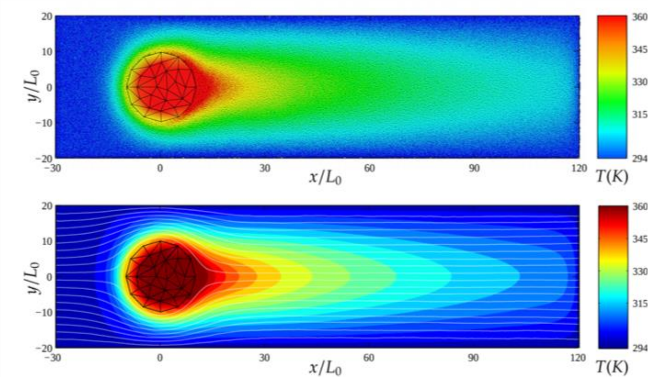
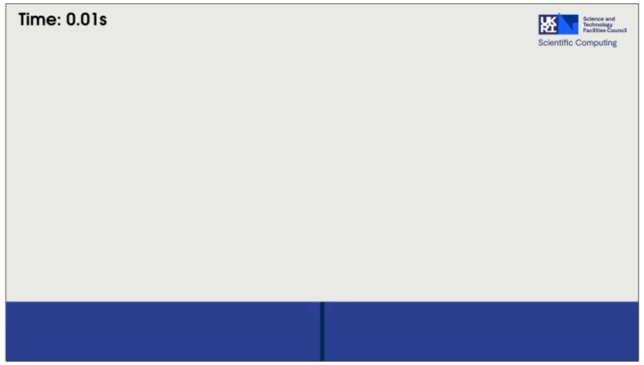
Tang Y.-H., Kudo, S., Bian, X., Li, Z., & Karniadakis, G. E. **Multiscale Universal Interface: A Concurrent Framework for Coupling Heterogeneous Solvers**, *Journal of Computational Physics*, 2015, 297.15, 13-31. https://doi.org/10.1016/j.jcp.2015.05.004

Multi-physics Modelling Examples

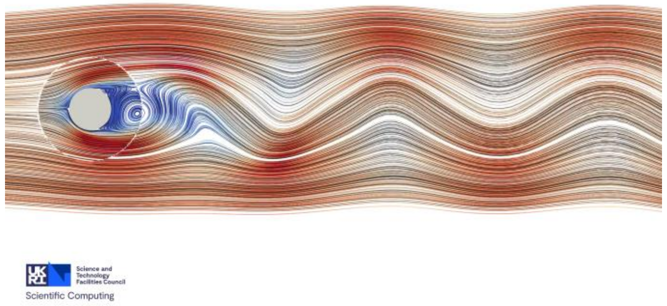
Energy conservative dissipative particle dynamics (eDPD) & Finite Element

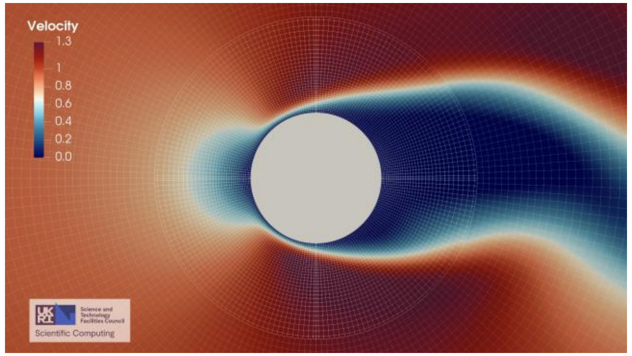


CFD & Structural Mechanics (FSI)

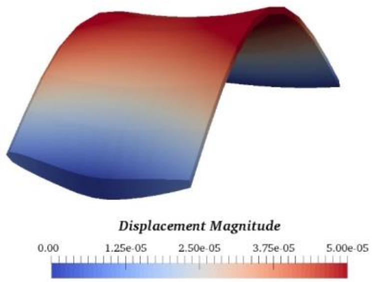


Fluid & Fluid coupling for optimising the performance and functionality

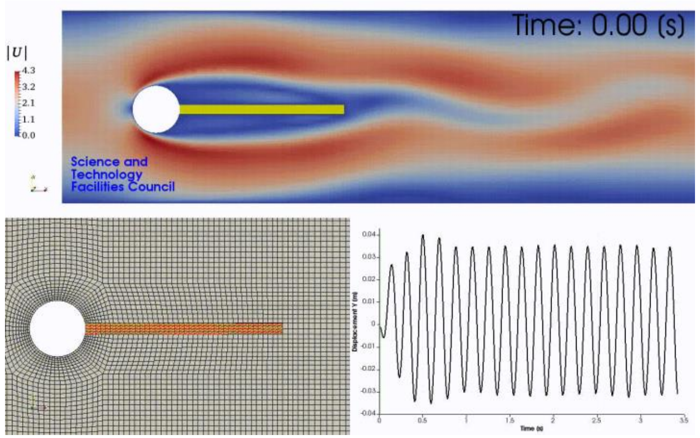




Vortex-induced vibration of the trailing edge of a hydrofoil



2-D Flow Past Elastic Plate Behind a Rigid Cylinder



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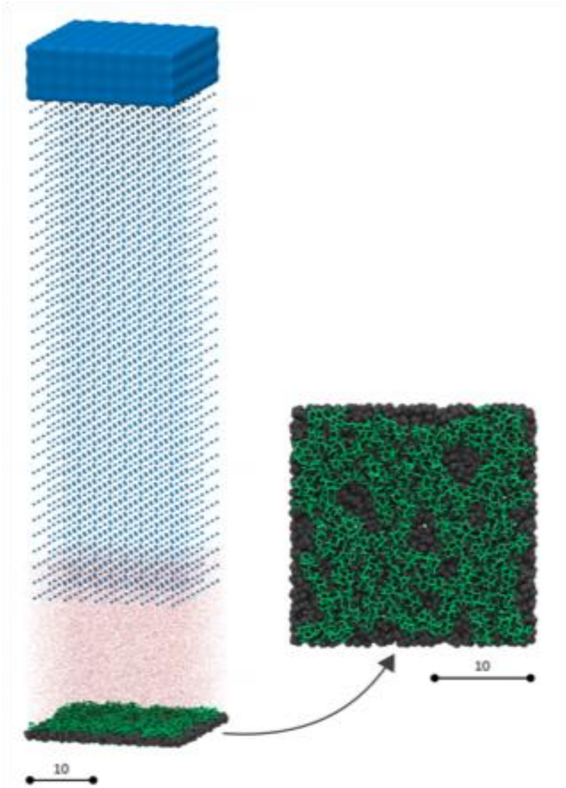
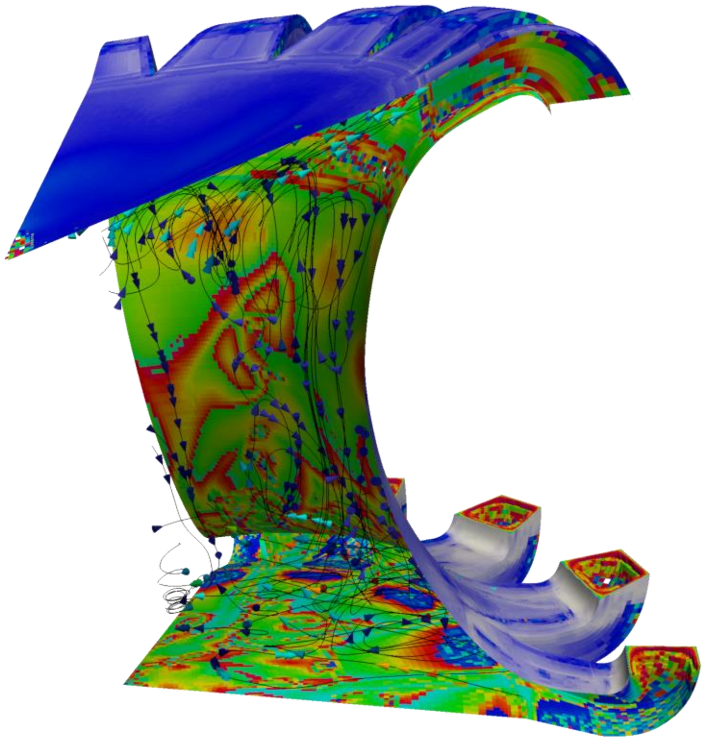
Multi-scale Modelling Example

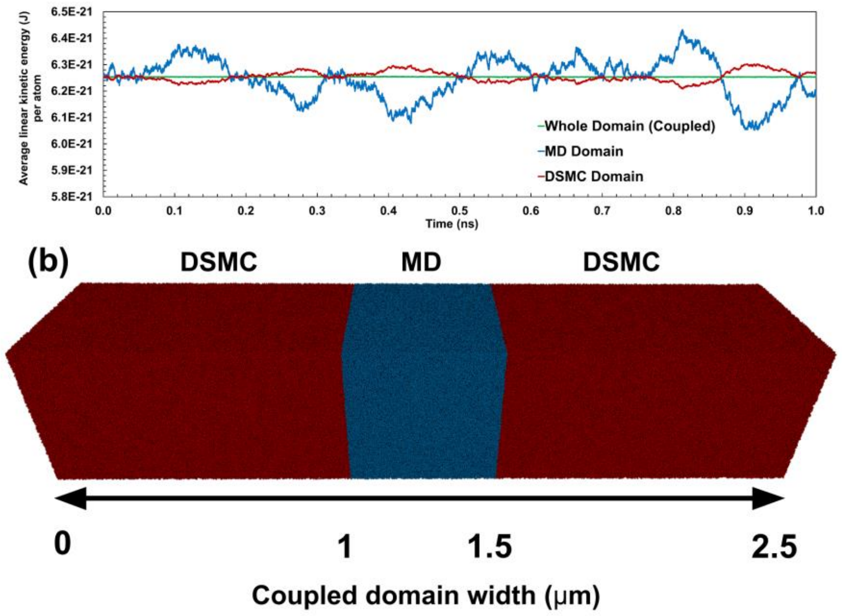
Particle CFD (SPH) & DPD



CFD with Neutronics



Molecular Dynamics (MD) & direct simulation Monte Carlo (DSMC)

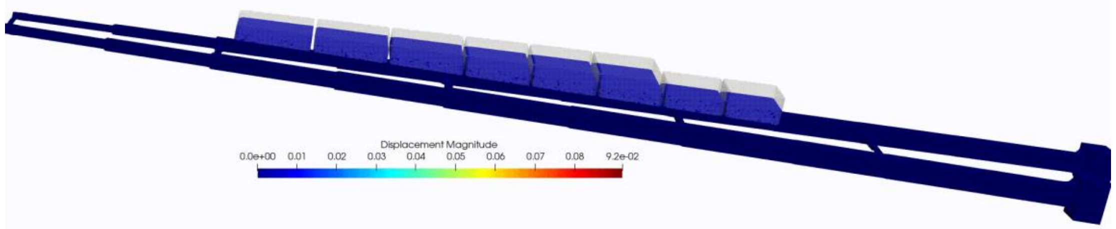


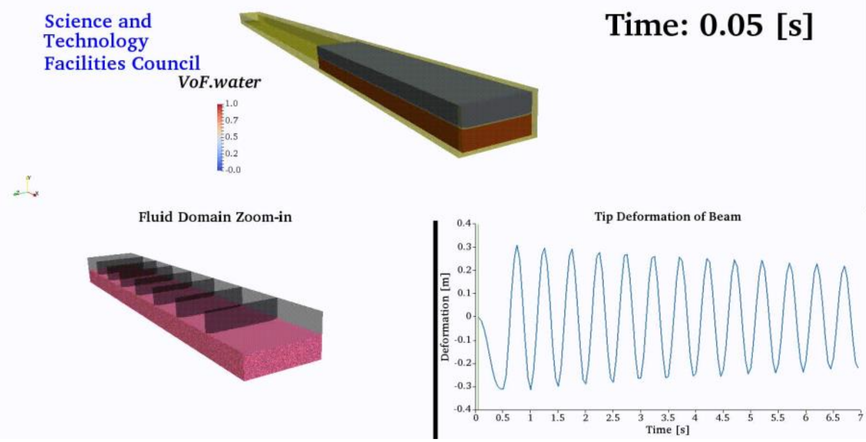
Coupling Molecular Dynamics and Direct Simulation Monte Carlo using a general and high-performance code coupling library
SM Longshaw, R Pillai, L Gibelli, DR Emerson, DA Lockerby
Computers & Fluids, **213**, 104726, 2020

Sloshing Wing Dynamics (SLOWD)

Project studied wing dynamics and damping to investigate the effect of sloshing on the dynamics of flexible wing–like structures carrying fuel. Involves the development of experimental, numerical (STFC) and analytical methods.

- Partners: Airbus + 8 others across Europe
- STFC work package leader for WP5 – coupled fluid structure interaction (FSI) modelling
- Understanding the precise dynamics of fuel sloshing on wing with a focus on the Wing of Tomorrow prototype and damping characteristics, resulting in numerous physical experimental rigs in the UK and across Europe and verified FSI frameworks plus model using commercially viable software





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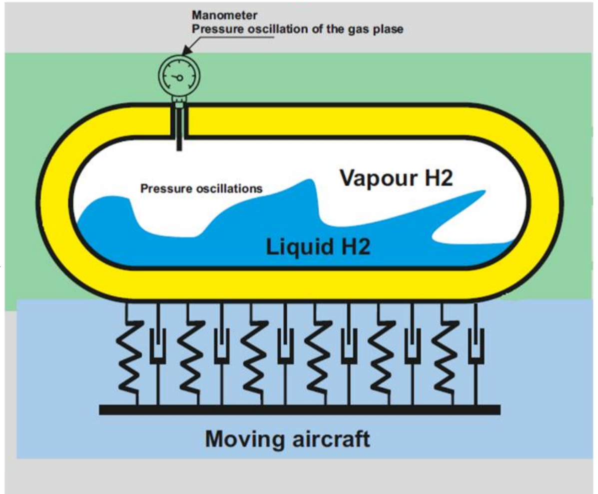
Hydrogen Aircraft Sloshing Tank Advancement

A direct follow on from the completed sloshing wing dynamics project. Project will develop an advanced high fidelity numerical tool able to design the first generation of cryogenic liquid hydrogen (LH2) tanks when sloshing effects are present.

- Partners: 15 participant organisations across Europe and South Africa , including Airbus UK, Airbus GMBH, ArianeGroup (Germany)
- Delivering coupled thermal fluid structure interaction (TFSI) modelling capability for the consortium
- Utilising software and modelling outputs of the sloshing wing dynamics project (SLOWD) and modifying to understanding sloshing and fluid dynamics of LH2 storage tanks for use in aviation applications



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Collaborative Computational Project in Wave Structure Interaction

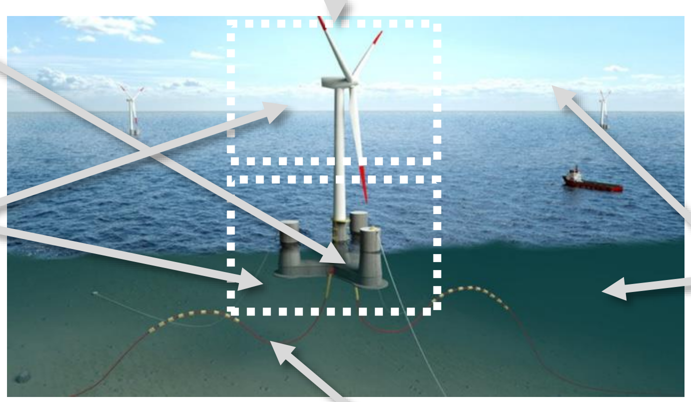
This project funded by EPSRC, brings together two computational communities – fluid dynamics and structural mechanics. There are 10 participant organisations across the UK. In this project, STFC will deliver:

- A fully coupled floating offshore wind turbine simulation framework for the community.
- Parallelisation and performance optimisation

Flexible Structure

Rigid Floating Body

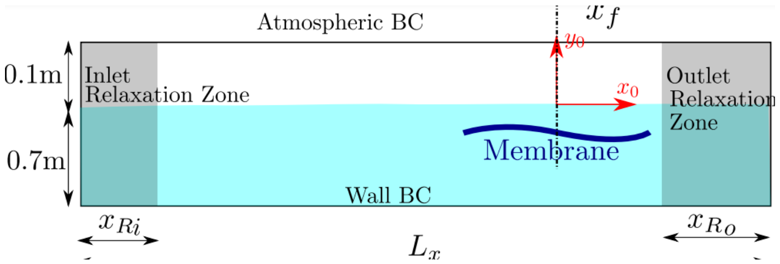
Near-field: multi-phase fluid dynamics and single phase aerodynamics



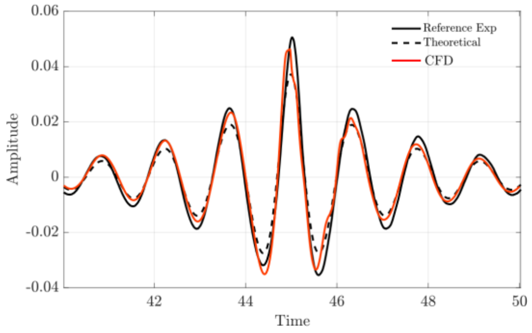
Far-field: Potential flow for fluid dynamics and aerodynamics

Flexible tethering

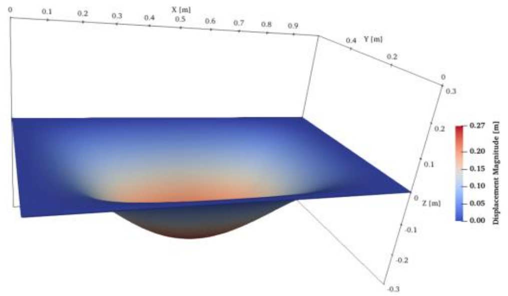
Multi-physics nature of floating offshore wind turbine



Schematic of test case



Wave generation in fluid domain



Membrane deformation in structure domain

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Group 3

X. Gu, C. Moulinec, G. Cartland-Glover,
W. Wang, B. Liu, C. Tsinginos, S. Rolfo

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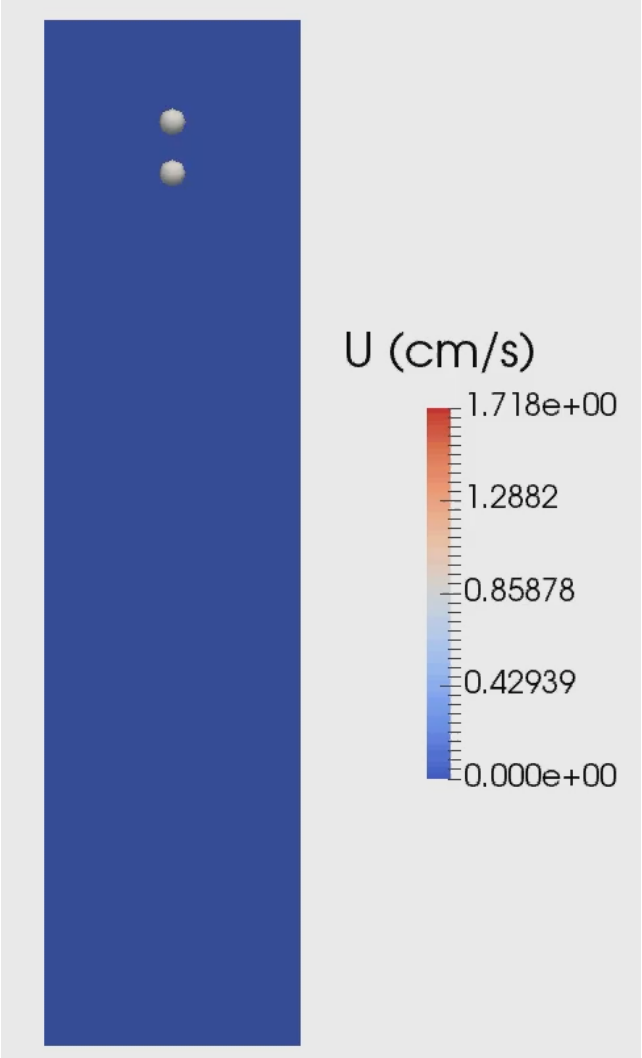
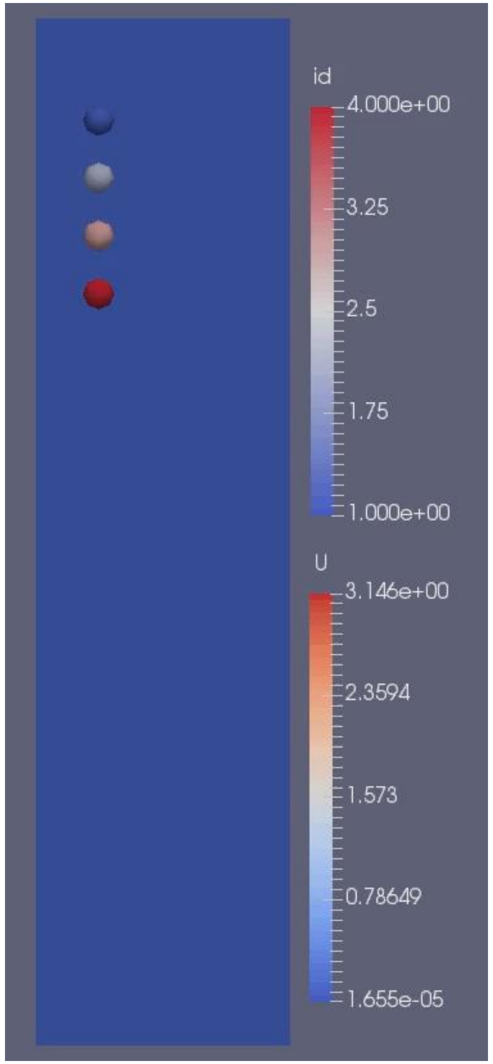
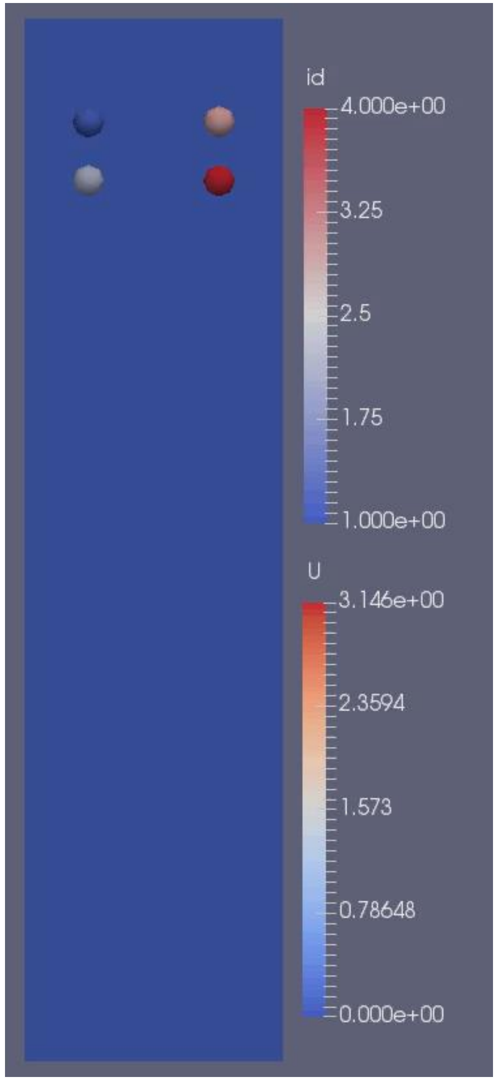
Direct Modelling Fluid Particle Systems

- Coupled LBM (Fluid) + DEM (particles)
- Applications:
  - Fluidised beds
  - Powders
  - Saturated soil mechanics
- Work is ongoing for direct modelling based on a multi-phase approach

Coupled LBM-DEM simulations using the partially saturated method: Theoretical and computational aspects
C Tsinginos, J Meng, XJ Gu, DR Emerson
Powder Technology, **405**, 117556, 2022





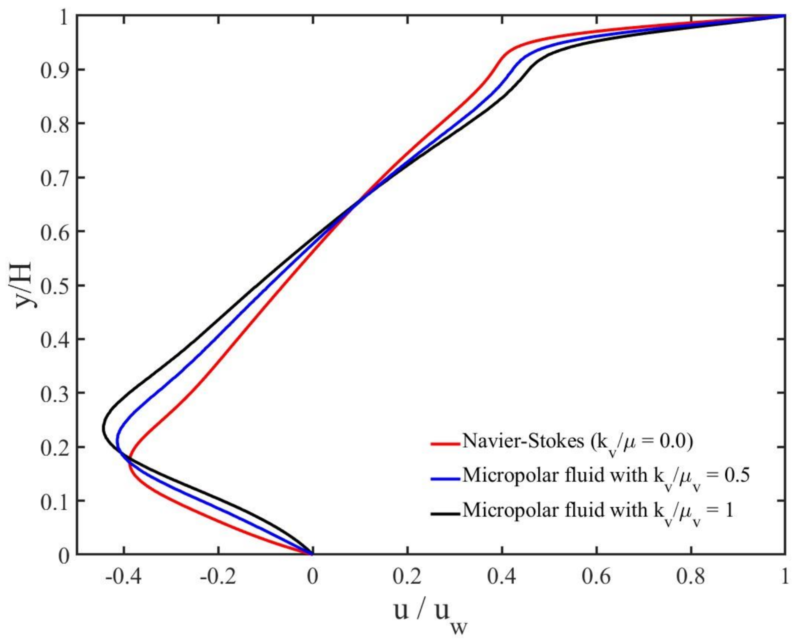


A multiscale continuum framework for fluids with microstructure

Higher-grade theories in a nutshell

Classical cont. **Micropolar cont.**

- Additional degrees of freedom and shape effects (material points)
- Additional transport equations
- Coupled equations
- Asymmetry of stress tensor
- Time & length scales involved



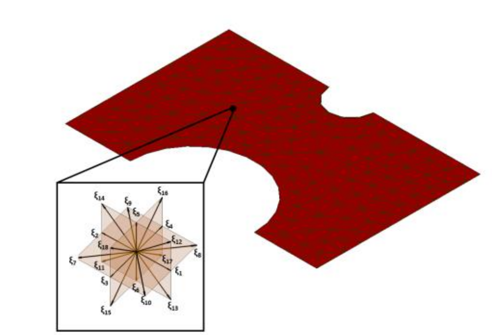
What can we do with such theories?

- Large-scale modeling of materials of complex molecules
- Coarse-grain modelling at the continuum level.
- Multiscale modelling of materials with complex structure due to consistency of micro/macro degrees of freedom

Current developments: Finite volume solver of micropolar fluids

- Compressible and incompressible solvers with the PISO approach
- Free surfaces modelled with the volume of fluid method
- Non-homogeneous viscosities

Implementation of the Discrete Unified Gas Kinetic Scheme (DUGKS)



What is DUGKS ?
Numerical method for solving **Boltzmann-like** equations introduced for multiscale modelling of fluids

Treatment of mol. vel. space: (like LBM) ⟹ N Boltzmann type equations
Treatment of physical space: Finite volume with an LBM treatment of the convection term

Timestep independency of mean free path ➡ **Inherent multiscale capabilities**

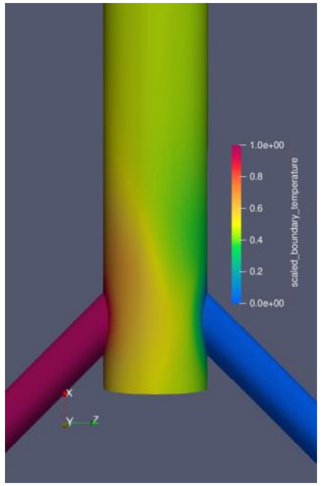
CS_DUGKS: Implementation of DUGKS into Code_Saturne

- Implicit and semi-implicit finite volume solvers
- Three different collision operator models (BGK, Shakov and ellipsoidal model)
- Three different quadratures for the discretization of the molecular velocity space
- Potential application in continuum-rarefied flow
- Potential application for neutronics => nuclear application including target stations

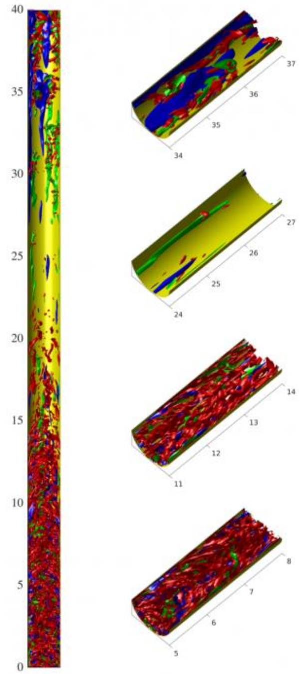
Working with UK research communities

Working with UK research communities to provide numerical methods to address challenges in low carbon/net zero economy

- CCP-Turbulence-UKTC: Porting to modern HPC architectures (CPUs+GPUs) CFD codes to address challenges related to net-zero (such as Wind-Farm development) using different paradigms
- CCP-NTH (Nuclear Thermal Hydraulics): The aim is to support a community to develop and maintain computational methods and software packages for nuclear thermal hydraulics. CCP-NTH aspires to achieve community building with networking and code development with long-term maintenance.
  - CHAPSim
  - Code_Saturne



Thermal field in Y junction with liquid metal (*Code_Saturne*)



Turbulent streaks and vortical structures in an upward heated flow of supercritical carbon dioxide (with the Boussinesq approximation applied, Re=5234).

Jundi He, Wei Wang et al
Study of fluid-to-fluid scaling for upward pipe flows of supercritical fluids using direct numerical simulation, International Journal of Heat and Mass Transfer, Volume 189, 2022

Numerical simulation of thermal mixing of liquid sodium in a Y-junction
W Wang, C Moulinec, S He, J Uribe, DR Emerson
Nuclear Engineering and Design, **417**, 112853, 2024

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SubChCFD

What is SubChCFD?

- SubChCFD is a coarse-grid approach for thermal hydraulics. It combines the traditional subchannel codes and CFD, offering CFD-like 3-D predictions ensuring consistency of the results with empirical correlations.

Key concepts

- Solving the 3-D CFD on a very coarse mesh
- Employing engineering subchannel correlations as replacement of wall functions for closure modelling
- Using simple turbulence model for turbulence mixing

Dual-mesh approach

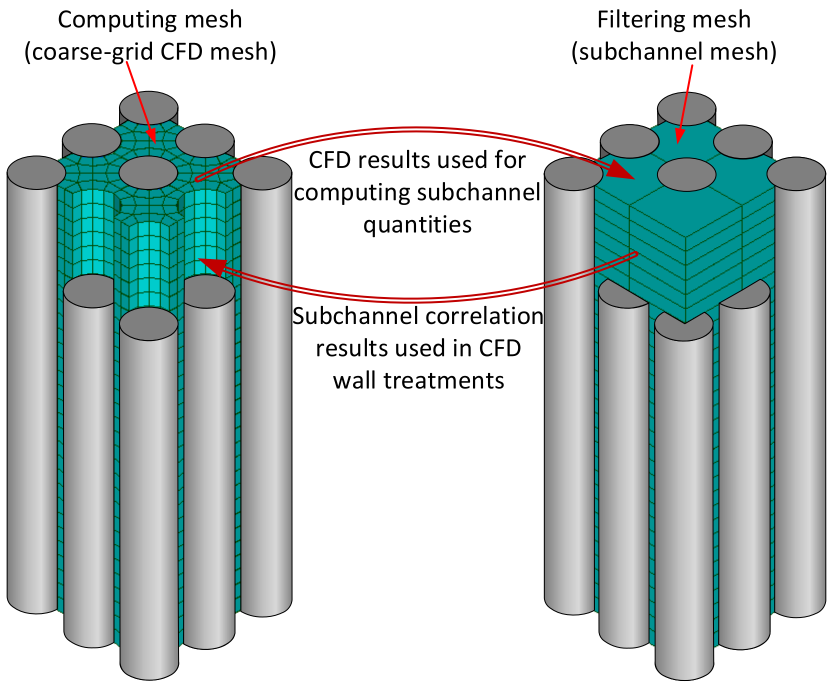
- A coarse-grid computing mesh, to perform CFD simulations
- A subchannel filtering mesh, to average the CFD result for a pseudo subchannel solution
- A data exchange carried out between the two meshes at each iteration/time step

Multi-scale capability

- Coupling with resolved CFD
- Coupling with porous media approaches

Applicability to ALC

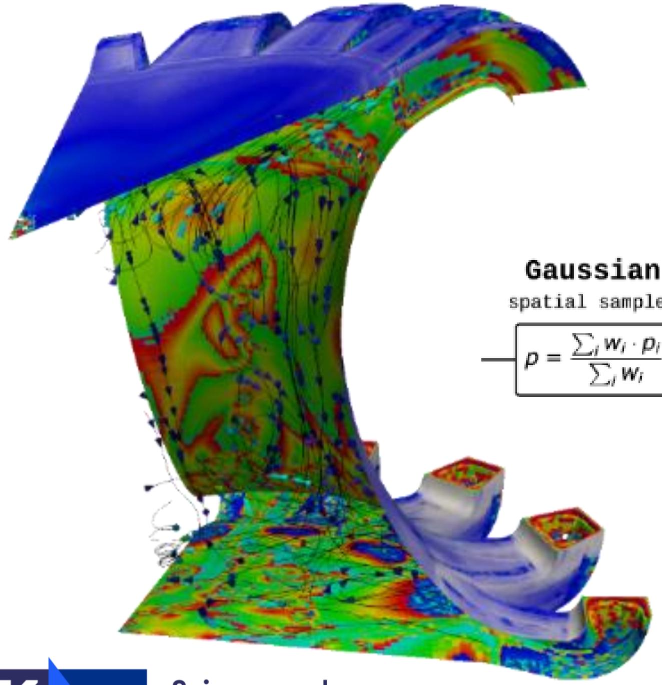
- Development of engineering digital twin for the current and next generation facilities

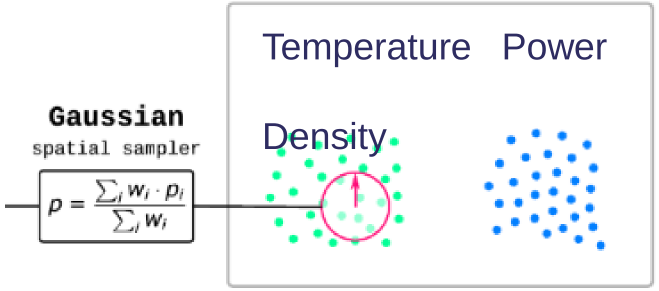


Dual-mesh system for a PWR rod bundle

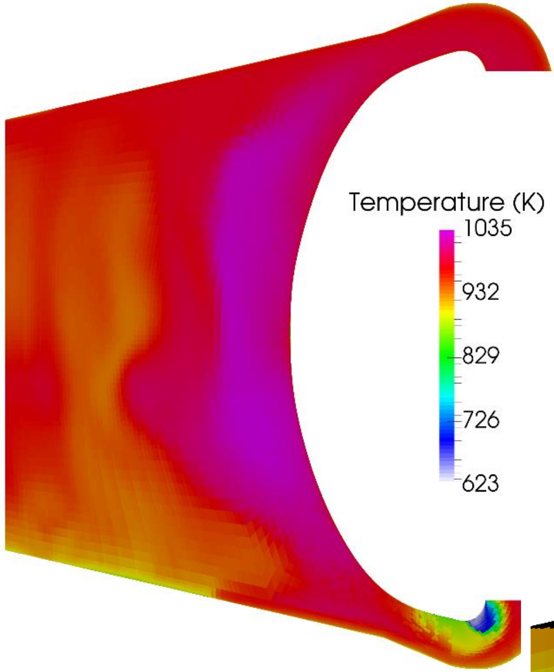
Designing the next GenIV reactors: MSFR

Coupled Neutronics-CFD simulations of the EVOL design of a Molten Salt Fast Nuclear Reactor (MSFR). Main objective was to investigate the possibility of using frozen wall technology to protect the core vessel from corrosion

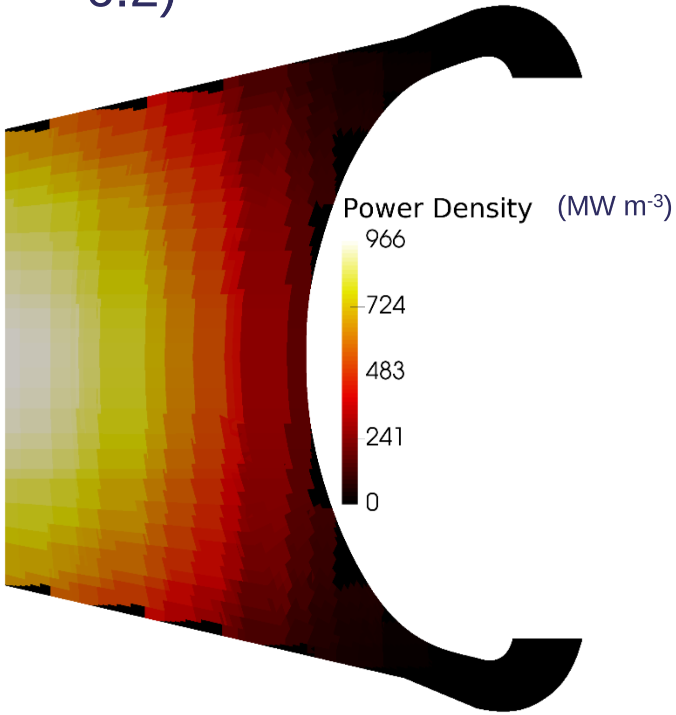




MUI code coupling https://github.com/MxUI



Neutronics and depletion simulations have also been done to study the long-term evolution of salt content with operation time (Polaris 2D from Scale 6.2)



Coupled simulations are between *Code_Saturne* for the CFD and DYN3D-MG for the **Neutronics**. Coupling has been implemented using the MUI library

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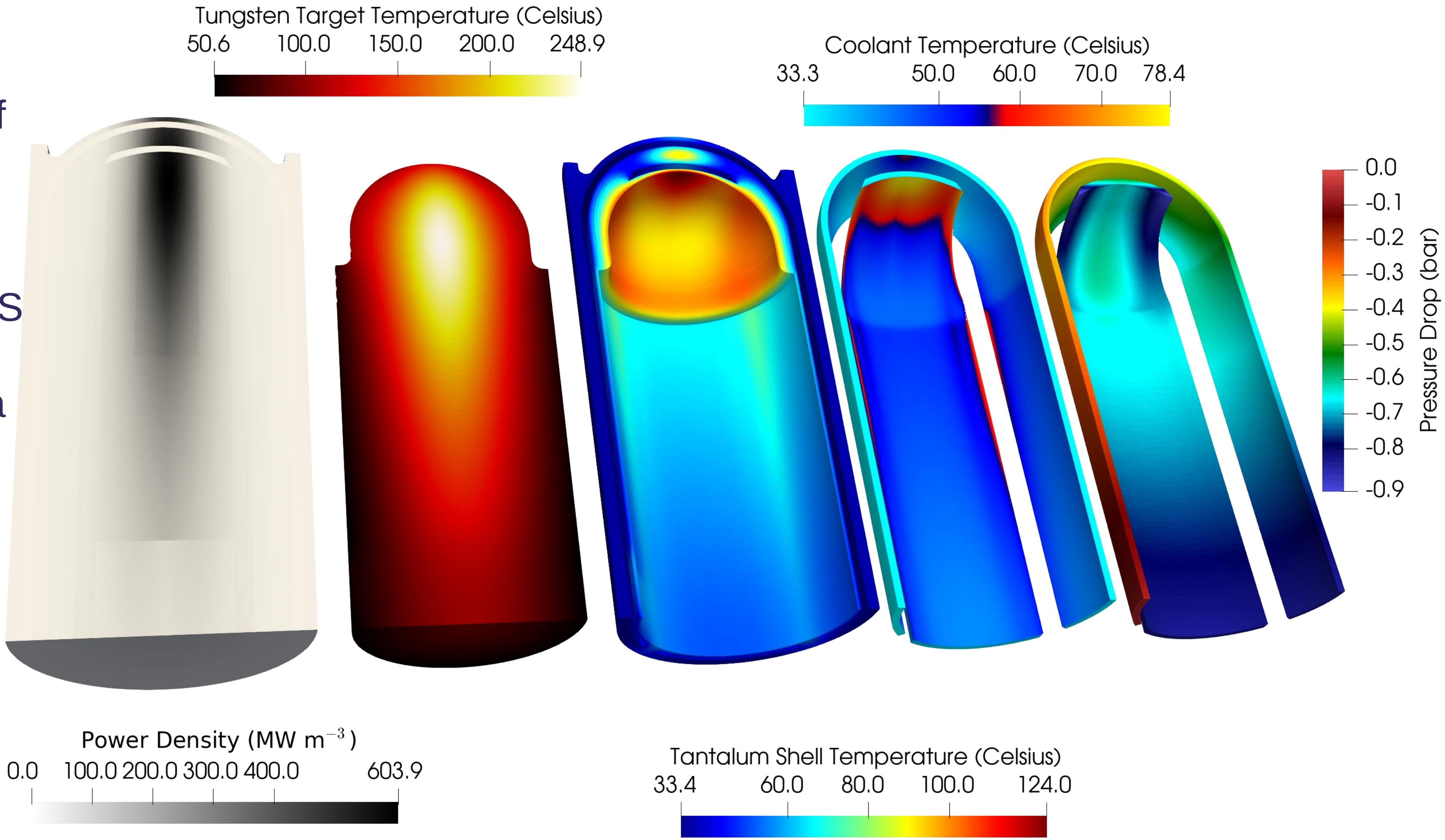
Modelling TS2

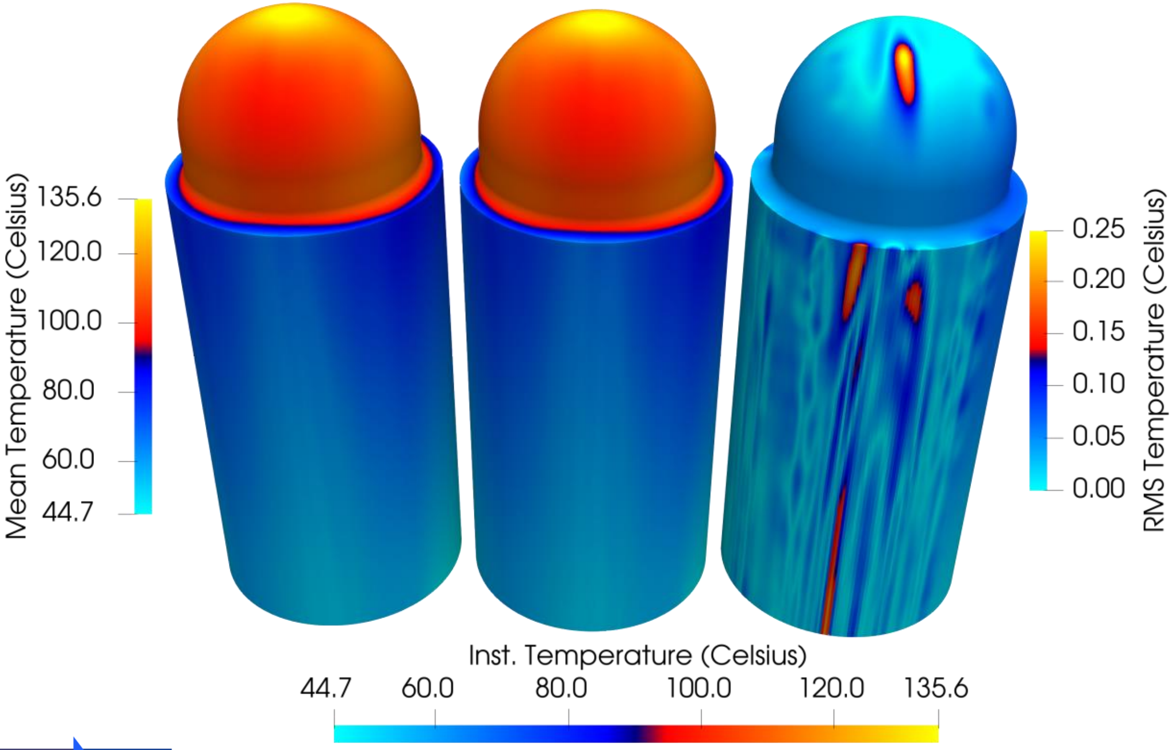
- Conjugate heat transfer simulations of Target Station 2 of the ISIS Muon & Neutron Source
- Several turbulence models including LES
- Gain insight of physical phenomena
  - Radiolysis
  - Cavitation
  - Thermal fatigue



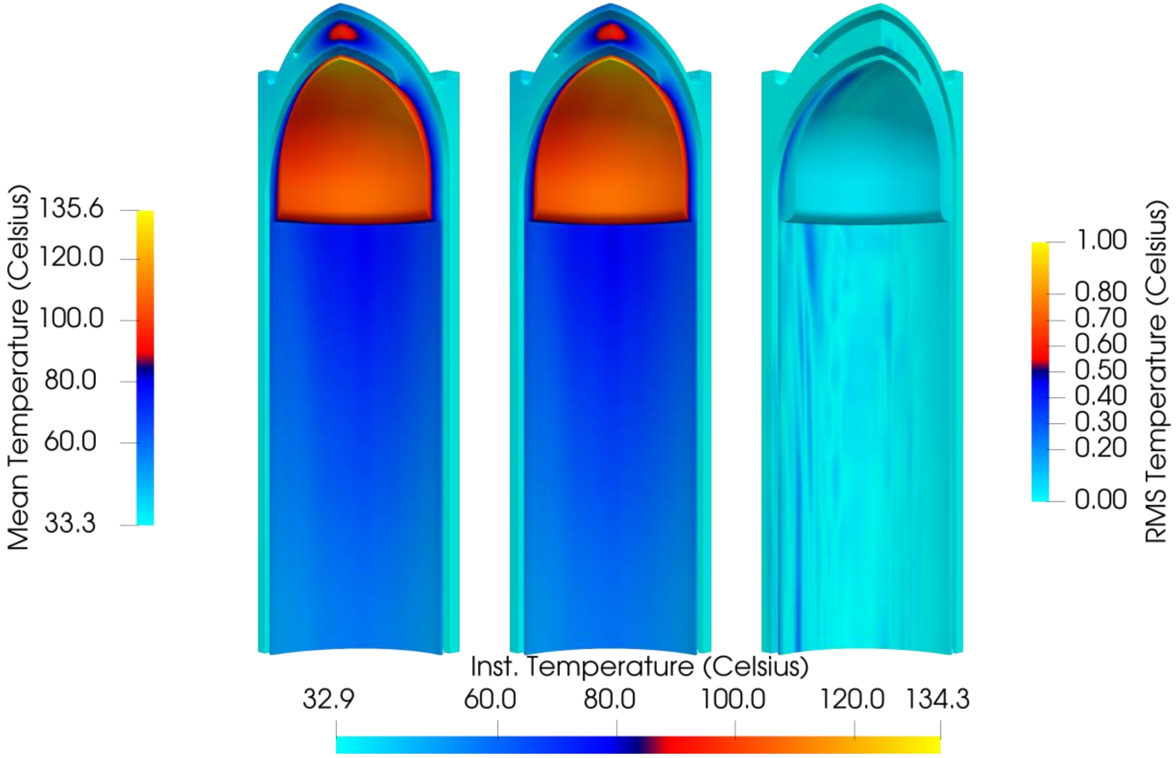
CHT with LES and steady heat source

Temperature fields

Target



Cladding



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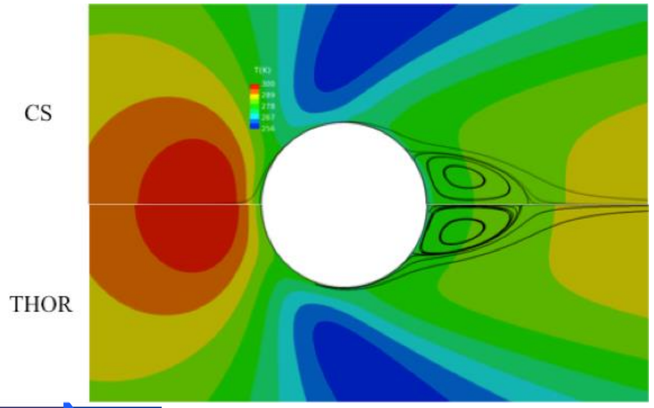
Method of Moments

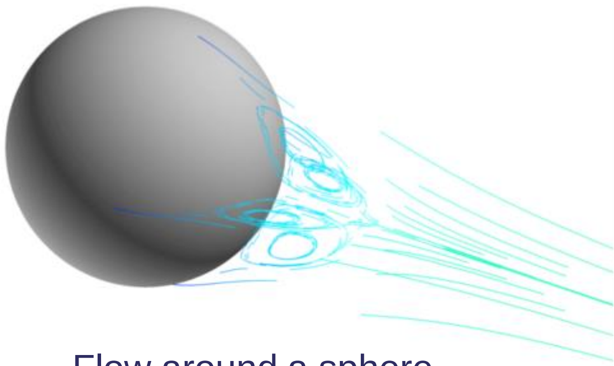
- Non-equilibrium state measured by the Knudsen number (Kn) for a rarefied gas
  - Kn<0.001 Continuum flow
  - 0.001<Kn<0.1 Slip flow
  - 0.1<Kn<10 Transitional flow
  - Kn>10 Free-molecular flow

- 3 methods are implemented, R13, R20 and R26, with velocity-slip/temp-jump boundary conditions
- Method developed with the Navier Stokes solver of Code_Saturne to handle complex geometries

Flow around a cylinder

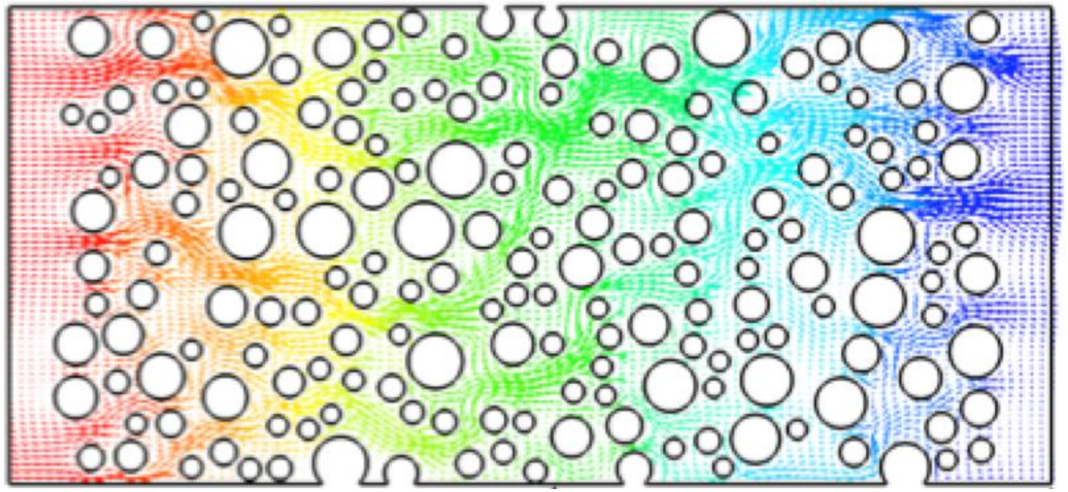
Kn = 0.02, Re=20





Flow around a sphere

Kn = 0.01, Re=50



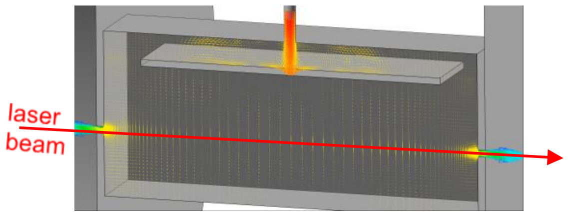
Flow past a cluster of randomly distributed cylinders (permeability of porous media)

A high-order moment approach for capturing non-equilibrium phenomena in the transition regime
X Gu and DR Emerson
Journal of Fluid Mechanics, **636**, pp. 177-216, 2009

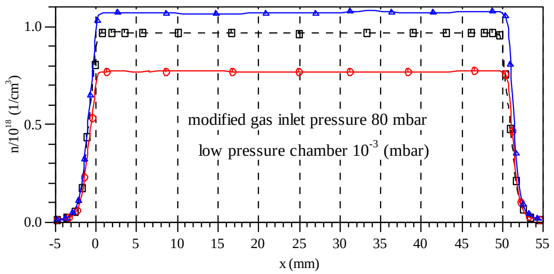
Gas Jet Design and Characterisation

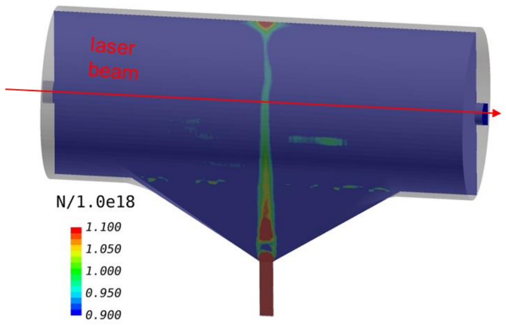
Motivation

- Thorough gas target design is crucial to operating a stable, high quality electron accelerator via LWFA.
- We will supply several different facility-maintained gas target options designed for various experimental requirements.
- The priority is a slot shaped gas nozzle.

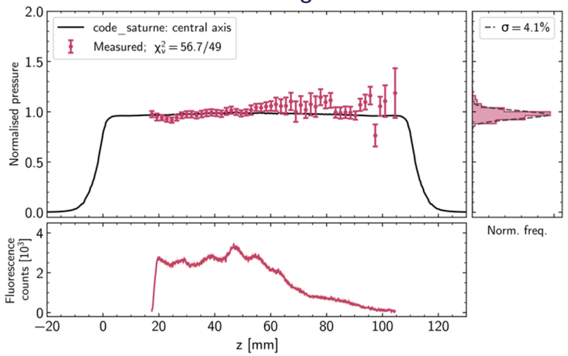


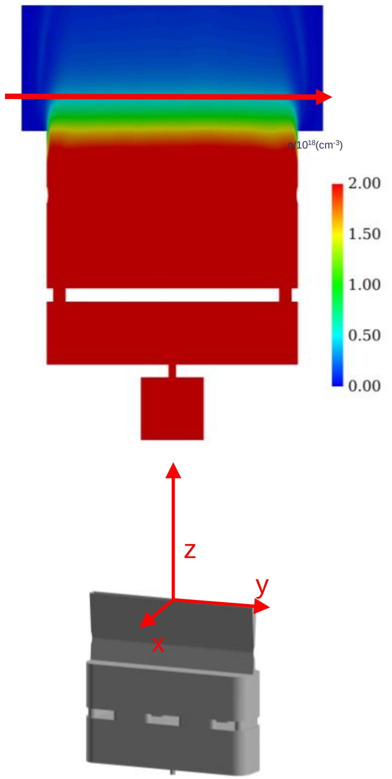
Density Profile along the Laser Beam





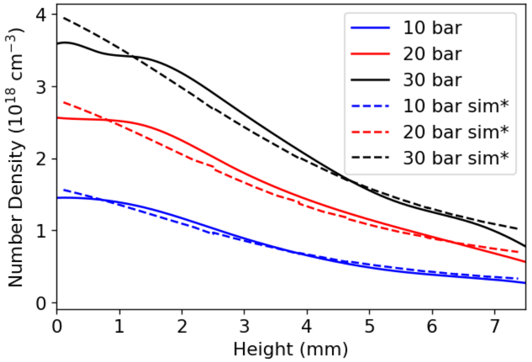
Pressure Profile along the Laser Beam





Numerical Modelling

- Simulations performed with Code_Saturne using the moment method
- Current design has a converging-diverging section to accelerate the flow, and a baffle plate above the valve inlet to homogenise the gas density in the lower region.



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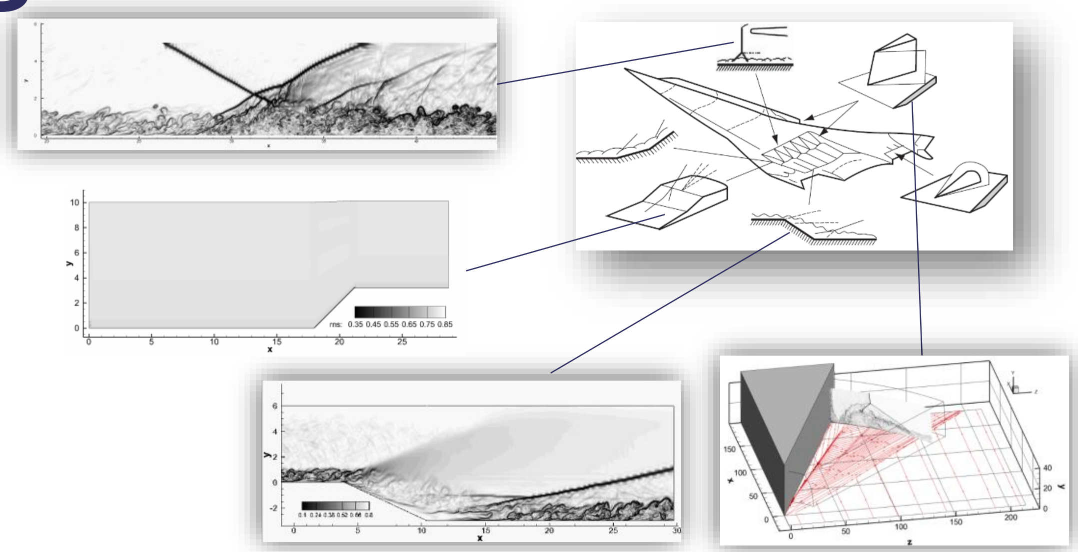
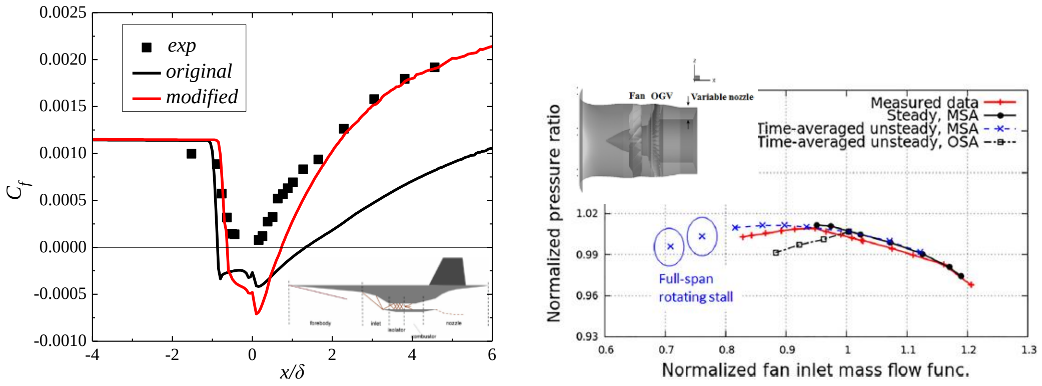
All-optical GeV electron bunch generation in a laser-plasma accelerator via truncated-channel injection
A Picksley, J Chappell, E Archer, N Bourgeois, J Cowley, DR Emerson, L Feder, XJ Gu, O Jakobsson, AJ Ross, W Wang, R Walczak, SM Hooker
Physical Review Letters, **131** (24), 245001, 2023

High-Speed Aerodynamics

- High-speed engineering flows rely on a deep understanding and accurate prediction of critical flow phenomena over **supersonic** and **hypersonic** vehicles.
- Within SCD, research related to supersonic/hypersonic engineering is being conducted in aspects of applied mathematics, high-performance computing, fundamental aerodynamics and engineering applications.
- Based on the advanced numerical tools developed in SCD, a series of key flow phenomena in hypersonic vehicle were studied, leading to discovery of new flow structures and mechanisms.
- This fundamental research has also benefitted industry. An example is the improved turbulence model based on a newly discovered mechanism that has been adopted by Rolls-Royce in aeroengine design.



Critical aerodynamic configurations over hypersonic vehicles studied in SCD



Improvement of engineering model and its application to aero-engines adopted by Rolls-Royce

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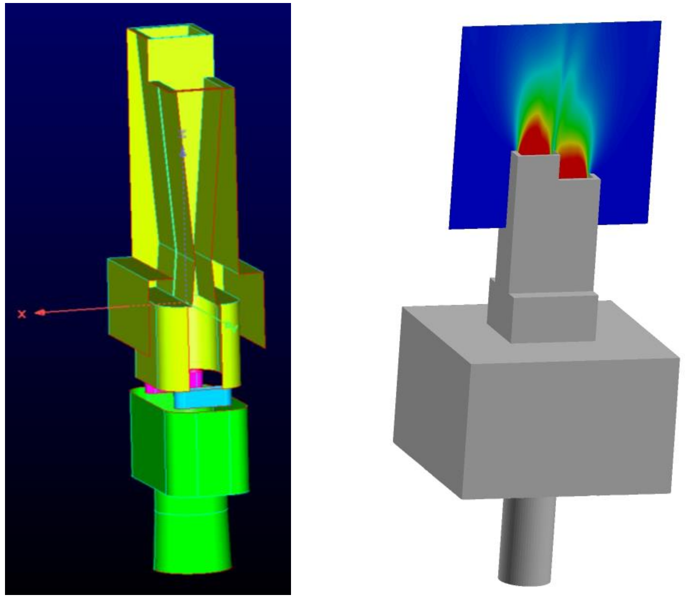
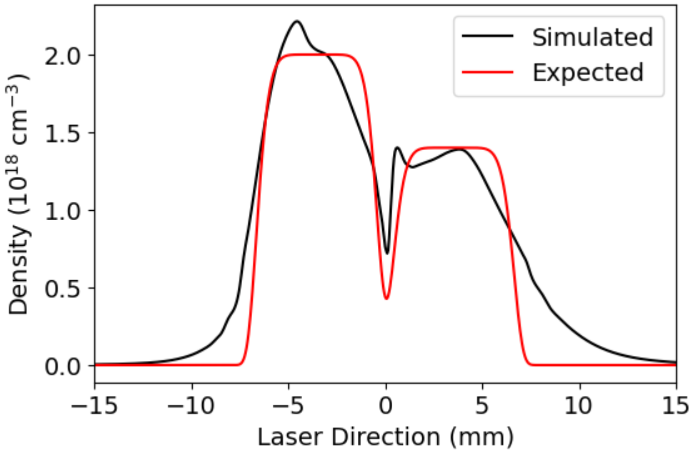
Concluding Remarks

- Slides present a whistle-stop tour of activities within the Computational Engineering Theme
- We develop our open-source software to run on a range of facilities, from laptops and PCs to small clusters (Tier 2) to national supercomputing facilities (Tier 1, ARCHER2) – with a strong focus on future exascale hardware
- If you would like to know more about any of the work presented, please get in touch

Current work in progress





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Thank you

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