Science and Technology Facilities Council

Application of computational methods for modelling of scientific and technological processes at STFC

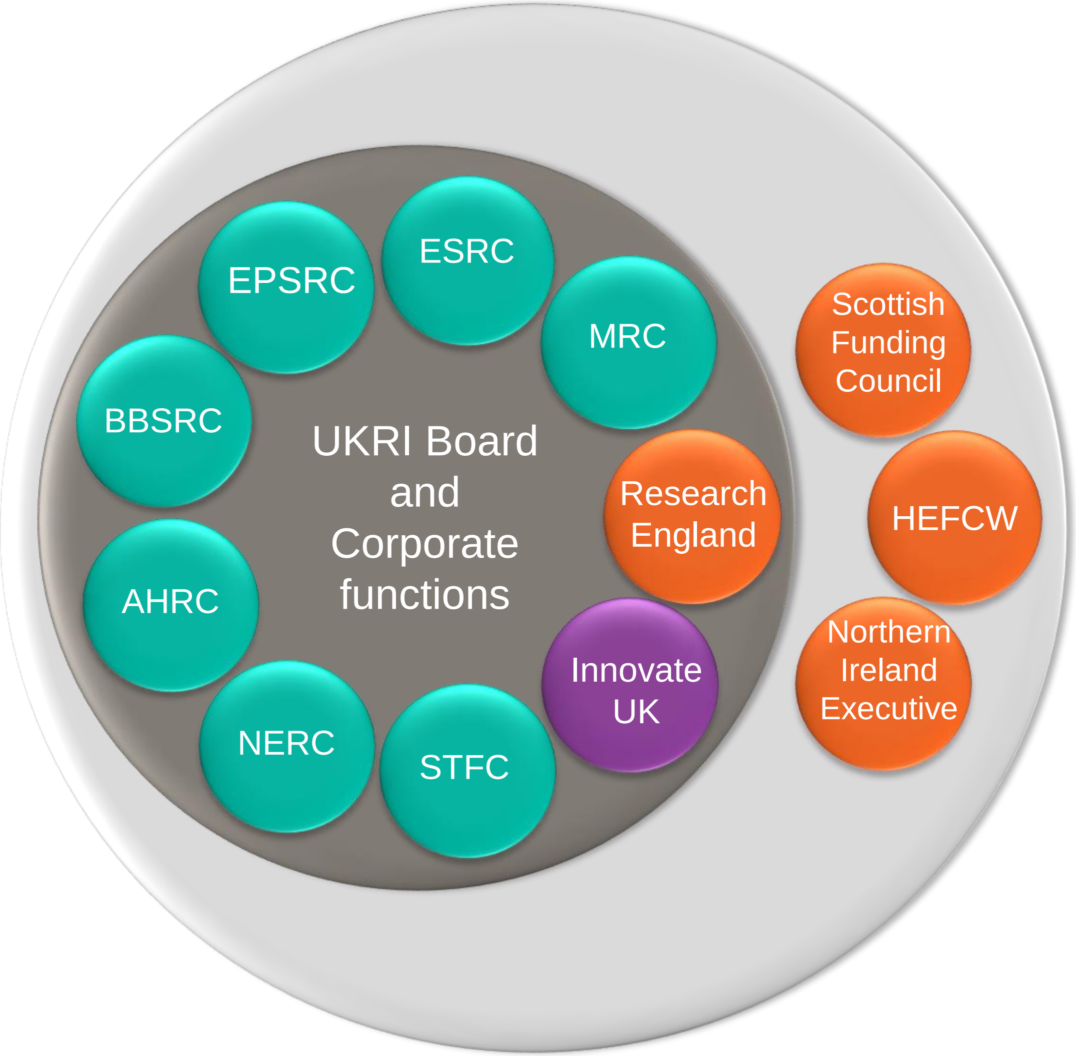
Andrew Ian Duff

Modelling in Nuclear Science and Engineering Seminar 2020
5th Nov 2020

UK Research and Innovation

From 1st April 2018 a single research and innovation funding body was formed

- Seven research councils (inc. STFC, Science and Technology Facilities Council), Research England and Innovate UK to merge into UK Research and Innovation
- Councils, Research England and Innovate UK continue in name as UKRI committees with separate budgets and delivery plans aligned to overall UK Research and Innovation strategy



Science and Technology Facilities Council

What we do

World class research, innovation and skills

- Broad range of physical, life and computational sciences
- Around 2,300 permanent scientists and engineers
- Access for 7,500 scientists to world-leading, large-scale facilities
- Science and Innovation Campuses at Daresbury and Harwell
- Globally-recognised capabilities and expertise in technology R&D
- Inspiring young people to undertake STEM

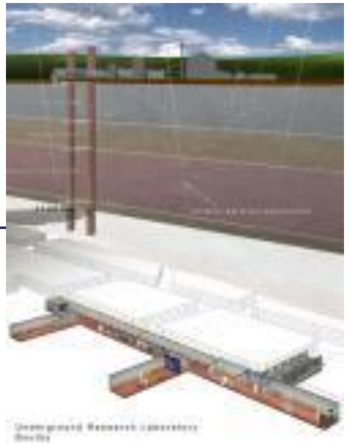
Science and Technology Facilities Council

Our UK locations

UK Astronomy Technology Centre
Edinburgh,
Scotland

Polaris House
Swindon, Wiltshire

Chilbolton Observatory
Stockbridge, Hampshire



Boulby Underground Laboratory
North Yorkshire

Daresbury Laboratory
Sci-tech Daresbury Campus,
Liverpool City Region

Rutherford Appleton Laboratory
Harwell Campus, Oxfordshire

Science and
Technology
Facilities Council

Computational Science and Engineering Division

(within the Scientific Computing Department)

What we are about

Science & engineering knowledge and skills

- Computational science & engineering research
- Training in methods and software
- Career paths for computational scientists and research software engineers

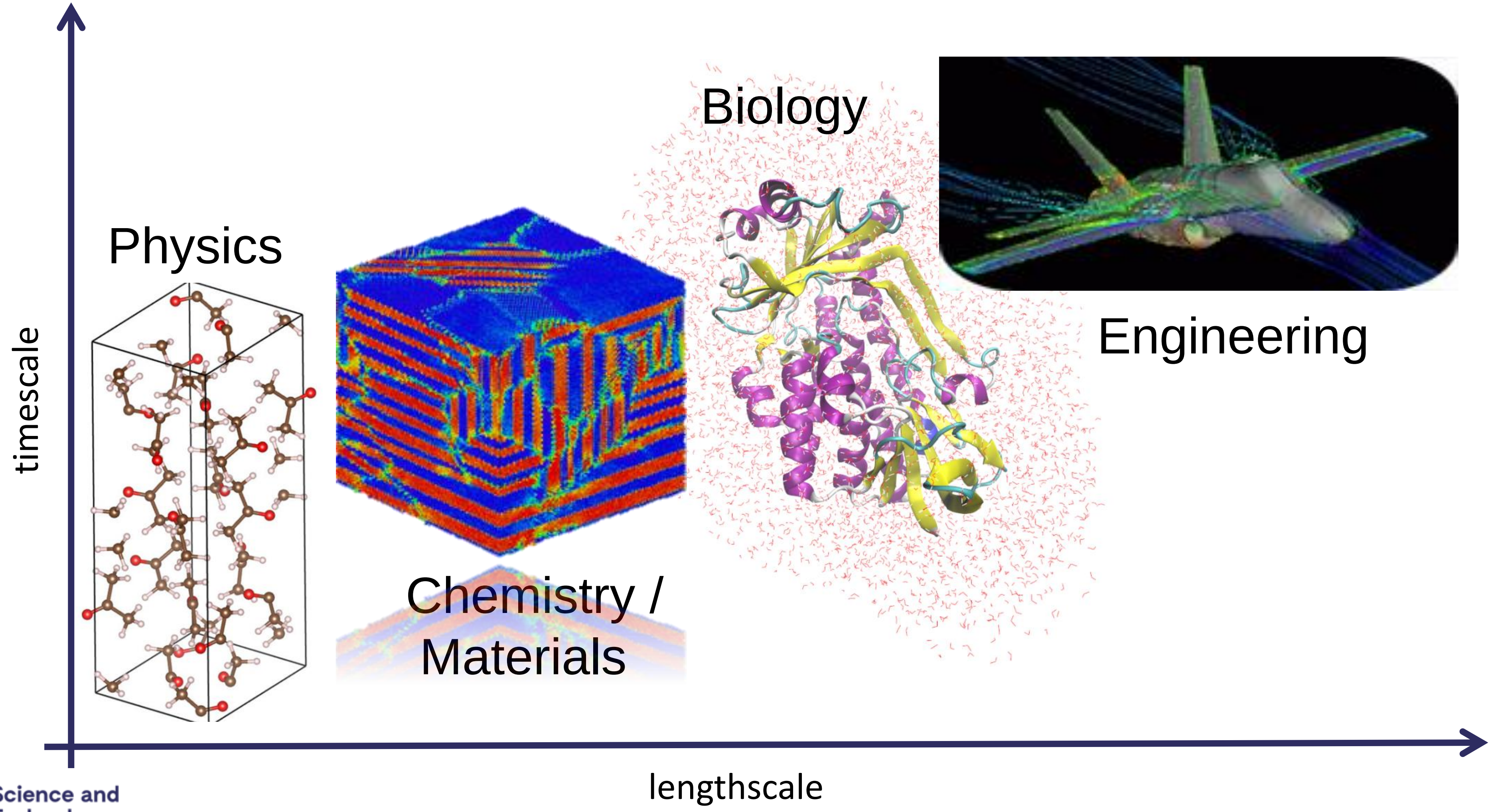
Research methods and software

- Theory and method development and validation
- Software distribution, licensing and support
- Research software engineering (incl HPC)

Collaborations and partnerships

- Collaboration with researchers in Academia, and industry
- Coordination of collaborative research communities (CCPs, HECs)
- Partnership with experimental Facilities and Research Councils

Science & engineering knowledge and skills



Who We Are

There are about 70 of us, organised in four groups:

- Computational **Biology** (led by Martyn Winn)
  including structural biology, molecular simulation and bioinformatics
- Computational **Physics** (led by Gilberto Teobaldi)
  electronic structure of the solid state and surfaces, atomic and molecular physics
- Computational **Engineering** (led by David Emerson)
  HPC solutions in fluid flow modelling, with particular strength in turbulence and microfluidics
- Computational **Chemistry** (led by Ilian Todorov)
  molecular dynamics, material science, quantum chemistry and QM/MM techniques, and mesoscale methods

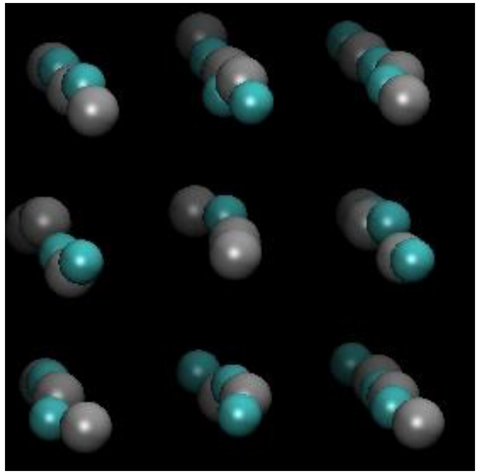
Science and Technology Facilities Council

Scientific methodologies

- I develop and apply scientific software to address challenges in nuclear, aerospace and automotive industries

TU-TILD

- Treatment of high-temperature properties is a complex and difficult challenge in material science
- TU-TILD provides fully anharmonic, *ab initio*-accurate free energies, and reliable property predictions of high-temperature melting-point materials
- Properties that can be predicted: thermal expansion; melting points; thermal conductivity; etc



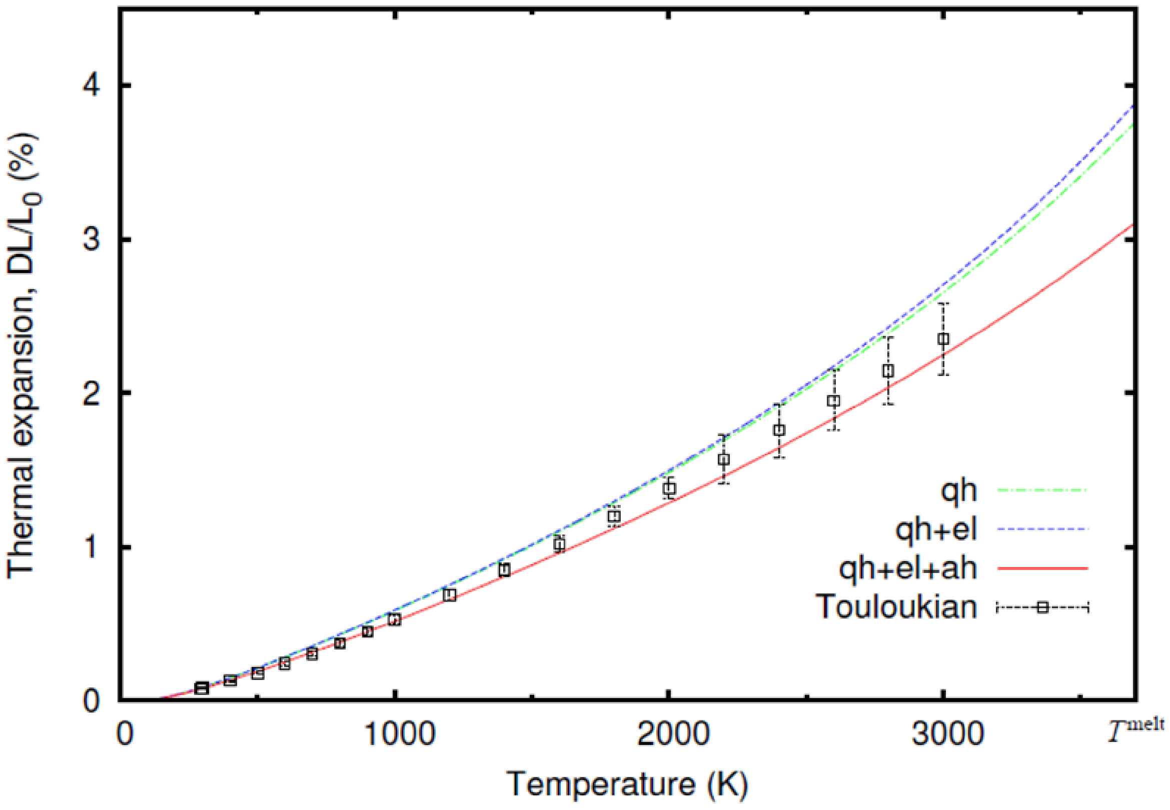
Zirconium carbide atomic vibrations at 3000 K

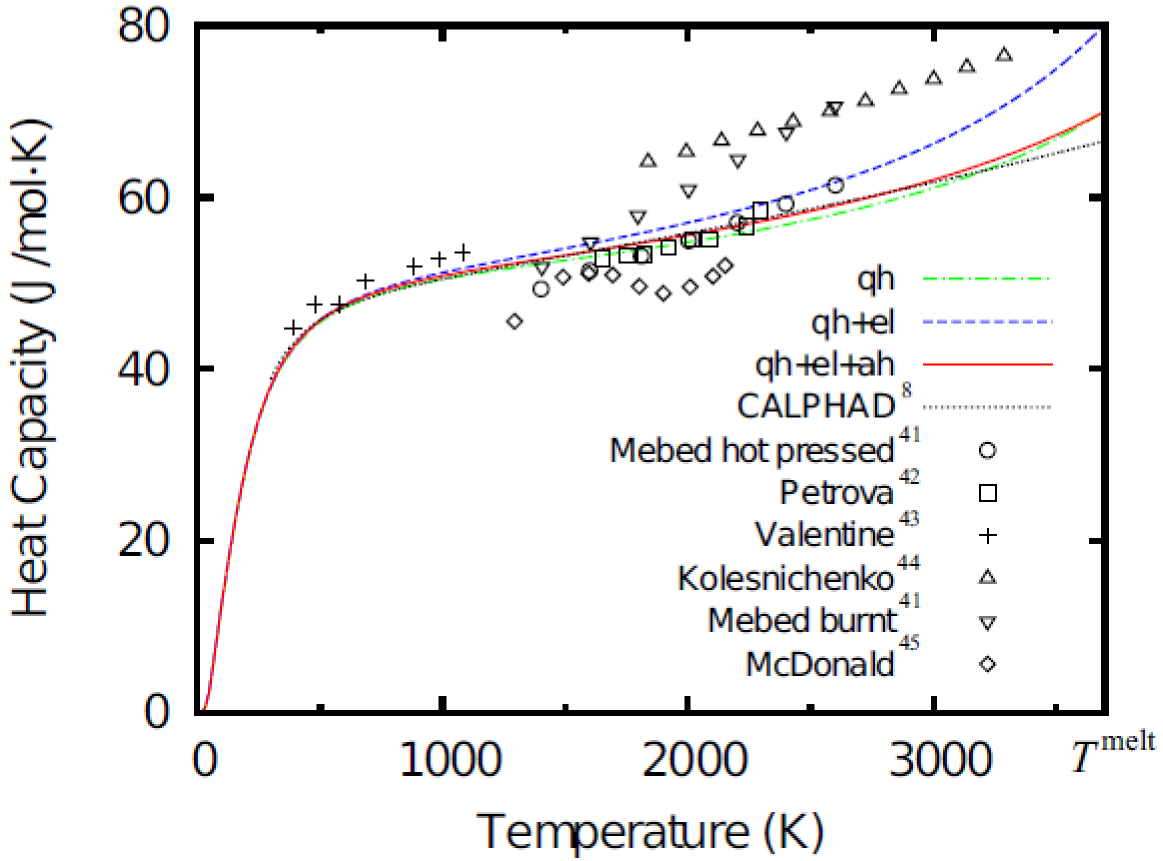
Science and Technology Facilities Council

Phys. Rev. B **91**, 214311 (2015), A. I. Duff, B. Grabowski M. Finnis et. al.

Scientific methodologies: TU-TILD

- I develop and apply scientific software to address challenges in nuclear, aerospace and automotive industries



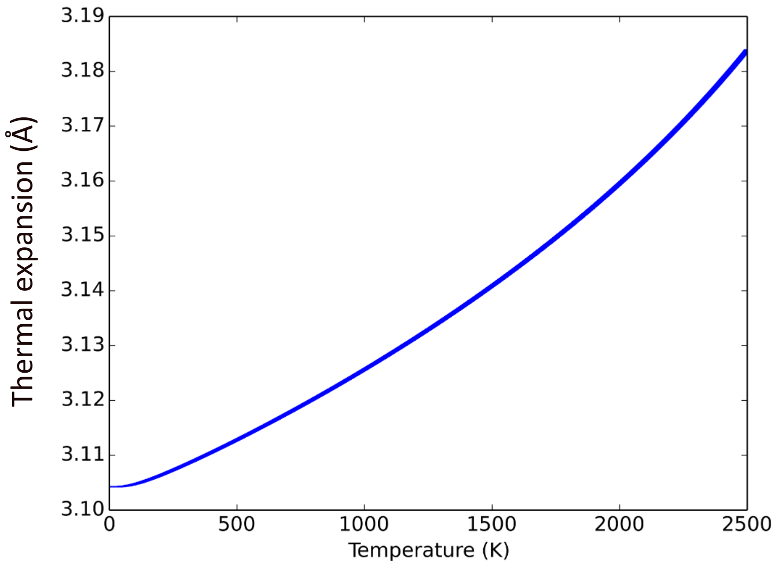


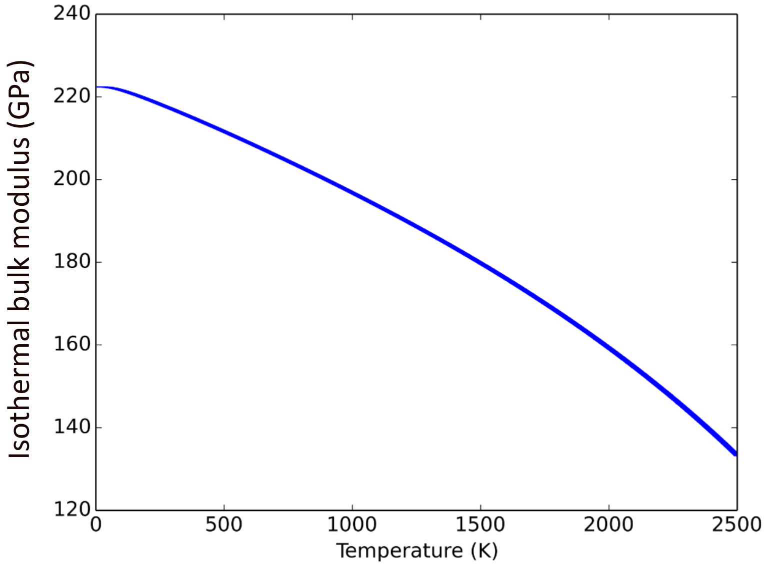
Science and Technology Facilities Council

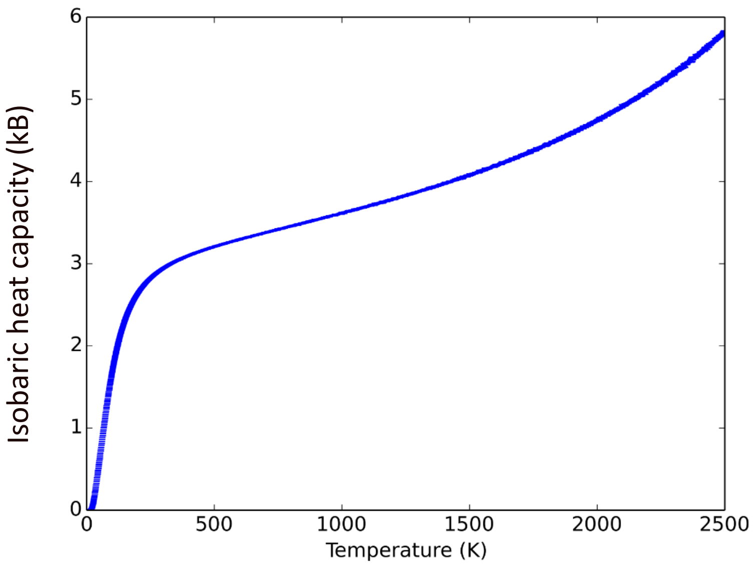
Phys. Rev. B **91**, 214311 (2015), A. I. Duff, B. Grabowski M. Finnis et. al.

TU-TILD results: TaVCrW

- Modelling radiation resistant low activation High Entropy Alloys (EP/S032835/1, EP/S032819/1), collaboration with Roger Smith (PI), Pooja Goddard, Ying Zhou at Loughborough University
- Aim to discover 'low-activation' materials for cleaner next generation nuclear reactors; and future commercial fusion reactors
- Results for TaVCrW by Ying Zhou. Now to roll out over wider composition range.







UKRI Science and Technology Facilities Council

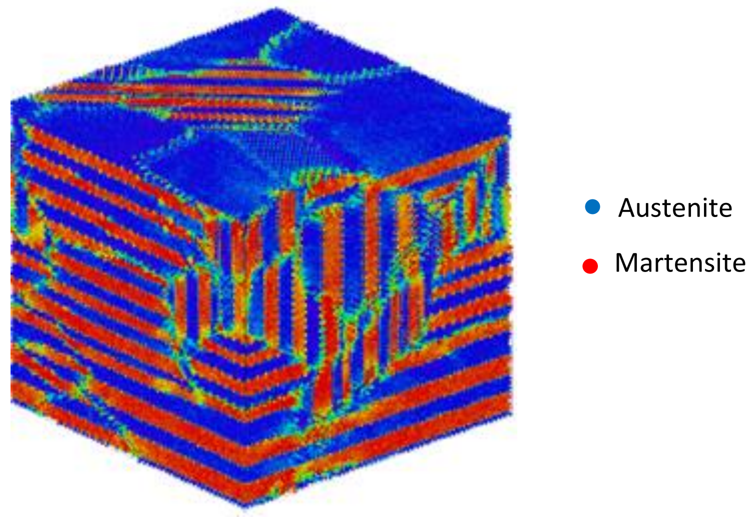
Y. Zhou, P. Srinivasan, P. Goddard, R. Smith, A. Duff

Scientific methodologies: MEAMfit

- I develop and apply scientific software to address challenges in nuclear, aerospace and automotive industries

MEAMfit

- Enables development of models ('interatomic potentials') to simulate millions of atoms, to capture realistic microstructures and processes within materials
- Versatile, able to treat a wide variety of materials
- USP: treatment of 'high entropy materials', being developed for extreme environment applications

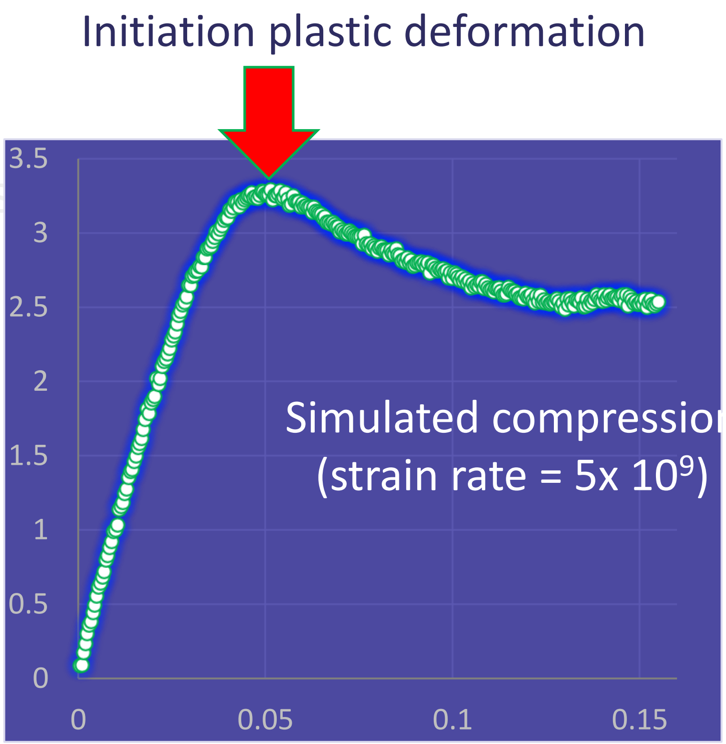


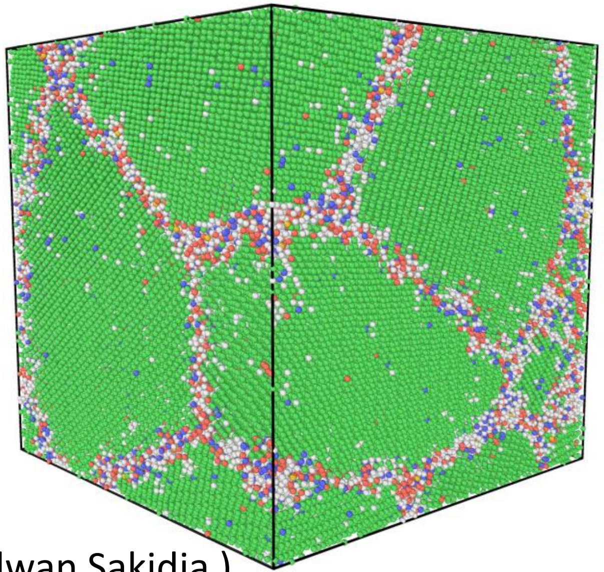
Scientific methodologies

- I develop and apply scientific software to address challenges automotive industries

MEAMfit

- Enables development of models ('interatomic potentials') to simulate millions of atoms, to capture realistic microstructures and processes within materials
- Versatile, able to treat a wide variety of materials
- USP: treatment of 'high entropy materials', being developed for extreme environment applications
- E.g. simulation of compression of polycrystalline Al-Co-Cu-Fe-Ni-Cr high entropy alloy

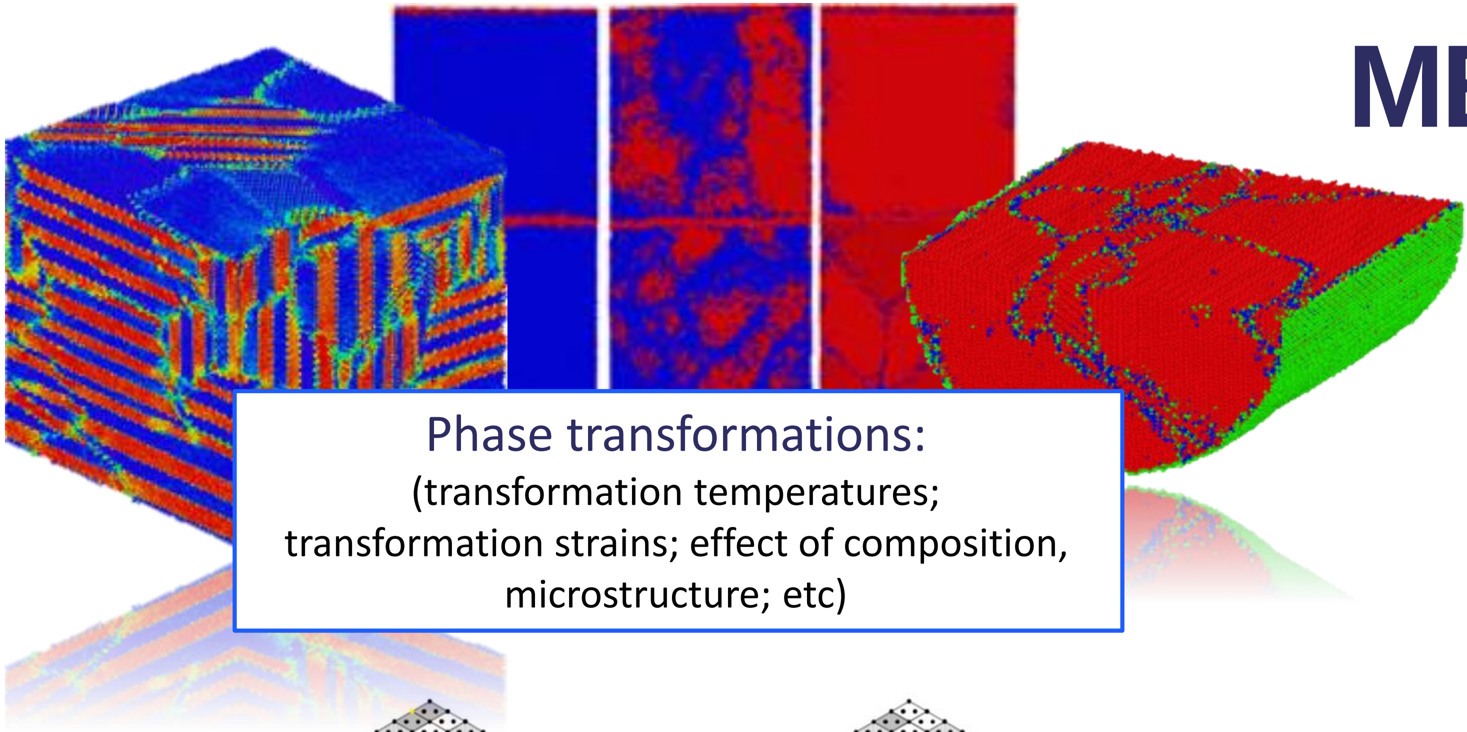




Science and Technology Facilities Council

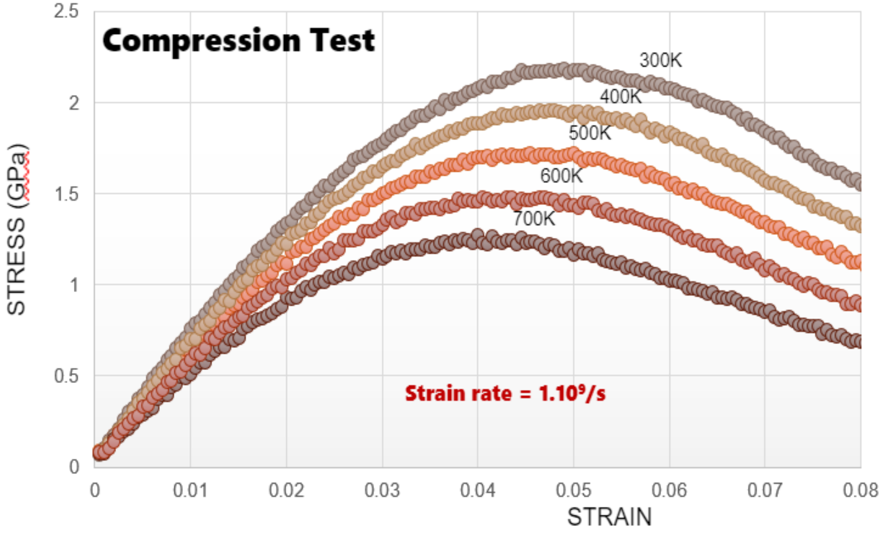
(unpublished, Tyler McGilvry-James, Andrew Duff, …, Ridwan Sakidja)

MEAMfit applications



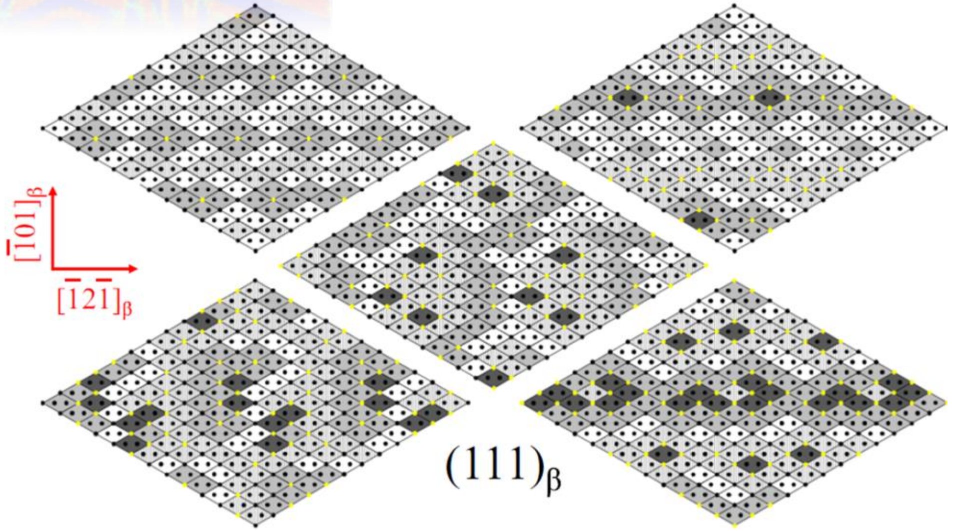
Phase transformations:

(transformation temperatures; transformation strains; effect of composition, microstructure; etc)



Mechanical properties and deformation:

(unpublished compression of AlCoCuFeNiCr polycrystal, APS March meeting 2020, Tyler, Duff, …, Ridwan Sakidja)



Prediction new phases:

(linear-chain-disorded structures in titanium)

Other applications:

Diffusion of hydrogen in Ti; Ti-H formation (Ajmalghan, Duff, Politano, International Hydrogen conference 2020)

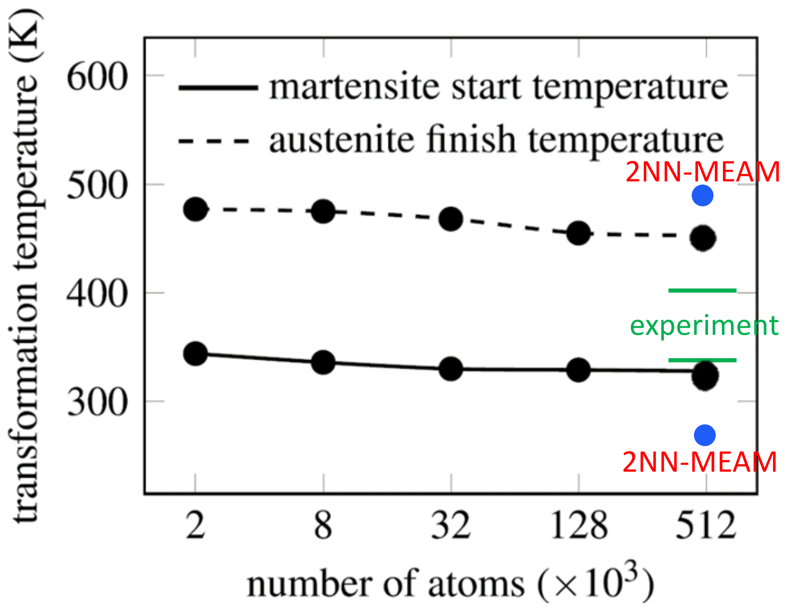
Radiation damage in UHTCs & MAX phases (In progress, Duff, et al)

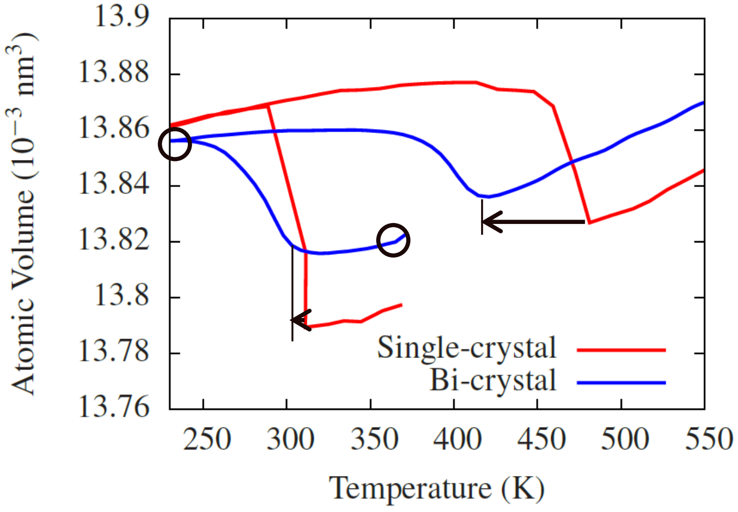
Neutron spectroscopy prediction (e.g. PRL **123** 235501 using MEAMfit)

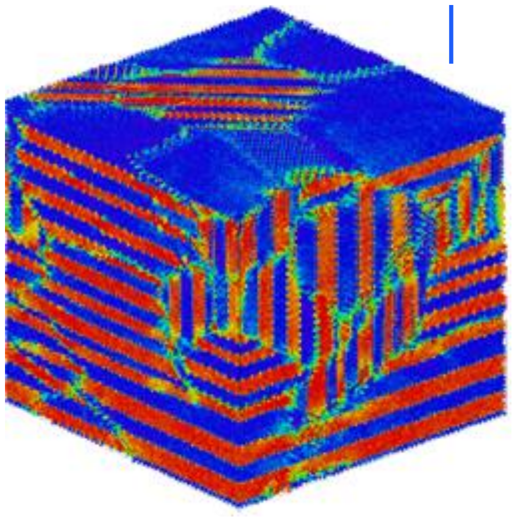
Thermal properties AlCuFe (In progess, Duff, Chtchelkatchev, et al)

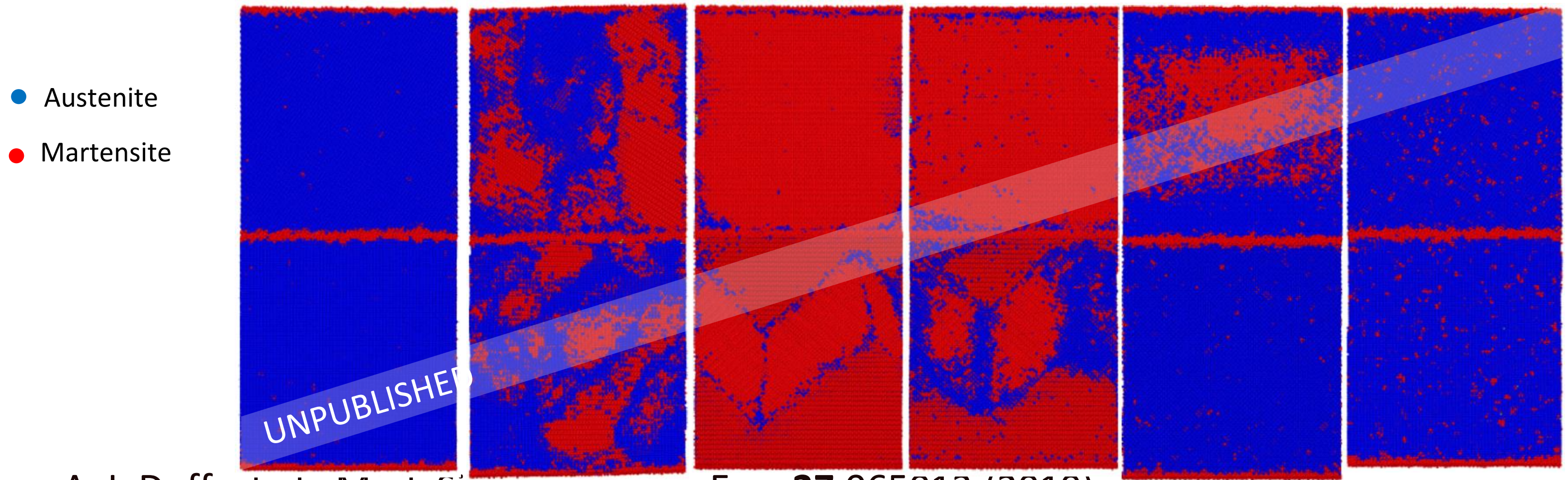
MEAMfit: Nickel-titanium phase transformation

Grain-boundary (bicrystal)





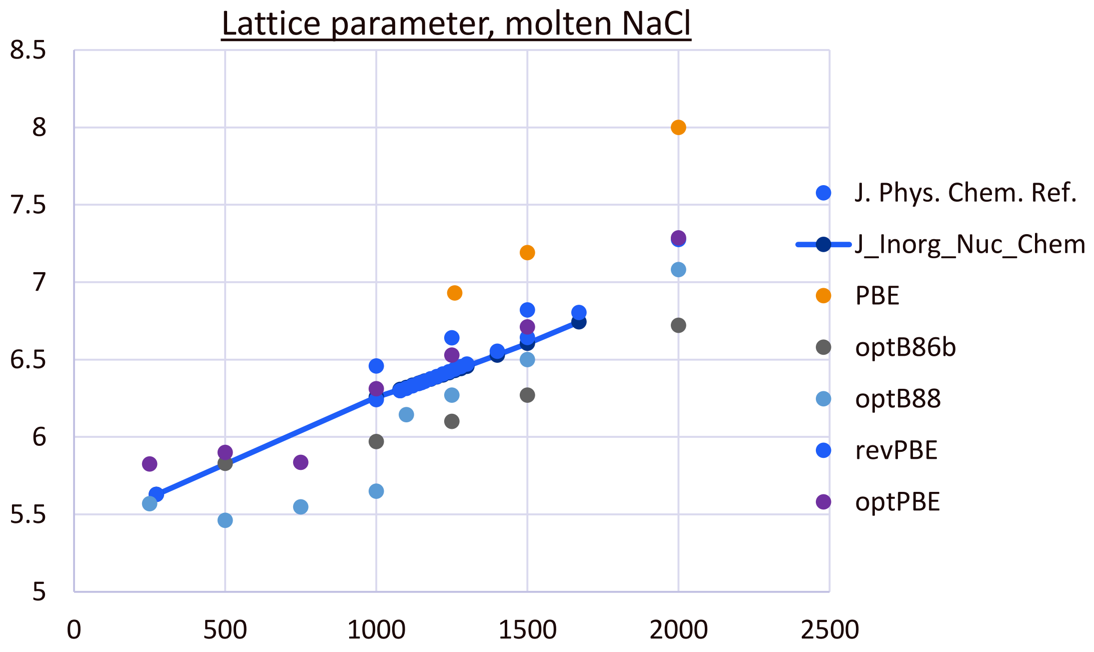


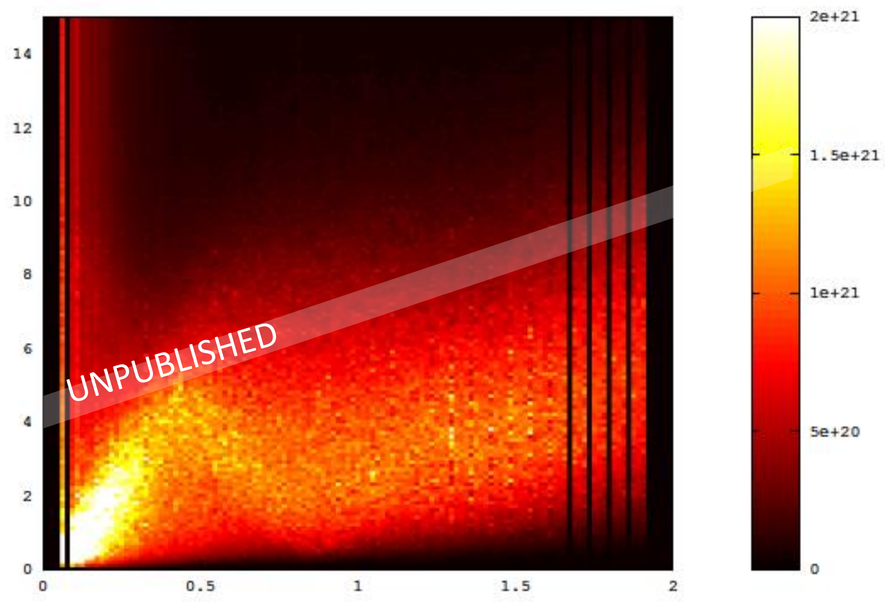


P. Srinivasan, A. I. Duff, et al., Mod. Simul. Mat. Sci. Eng. **27** 065013 (2019)

MEAMfit: Molten salts for molten salt reactors

- Aim: generate accurate high temperature data for molten-salts– highly challenging experimentally –for input into fluid dynamics simulations, in collaboration with Engineering
- Start with NaCl:
  - Develop model using *MEAMfit* to capture atomic vibrations and thermal expansion
  - Leverage model to predict neutron differential scattering cross-sections
  - Validate model against ISIS measurements (David Voneshen)
  - Apply *TU-TILD* to compute heat capacity and melting properties





Michael Leitner (FRM II)

Computational Engineering Group @ SCD

The CEG focuses on HPC to model *fluid flows*

R&D activities cover a wide range of applications, including:

- Turbulence, aero-acoustic and combustion
- Free surface and capillary flows
- Aerodynamics – high speed rarefied flow
- Environmental flow modelling
- Micro- and nano-fluidics
- Non-equilibrium fluid dynamics
- **Energy generation**
- HPC software development
- **Multi-scale and Multi-physics simulation**

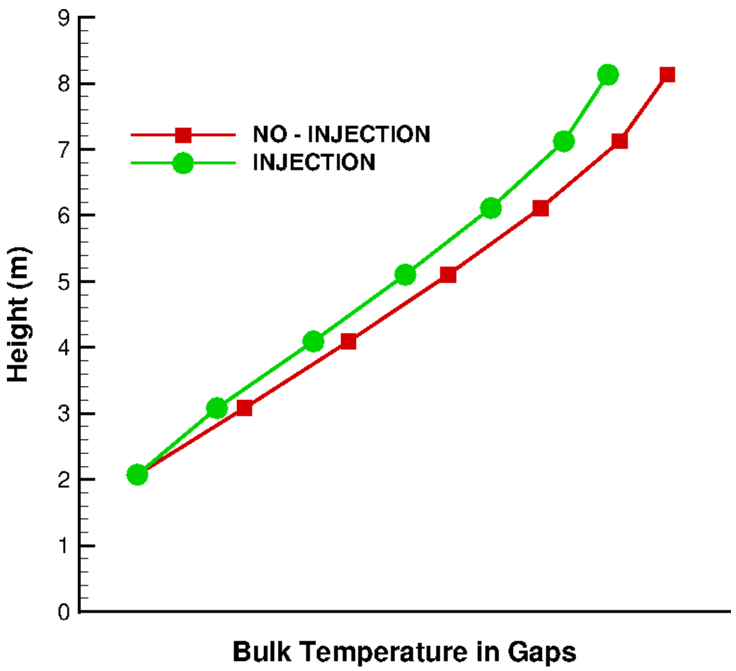
Several on-going projects related to the nuclear industry:

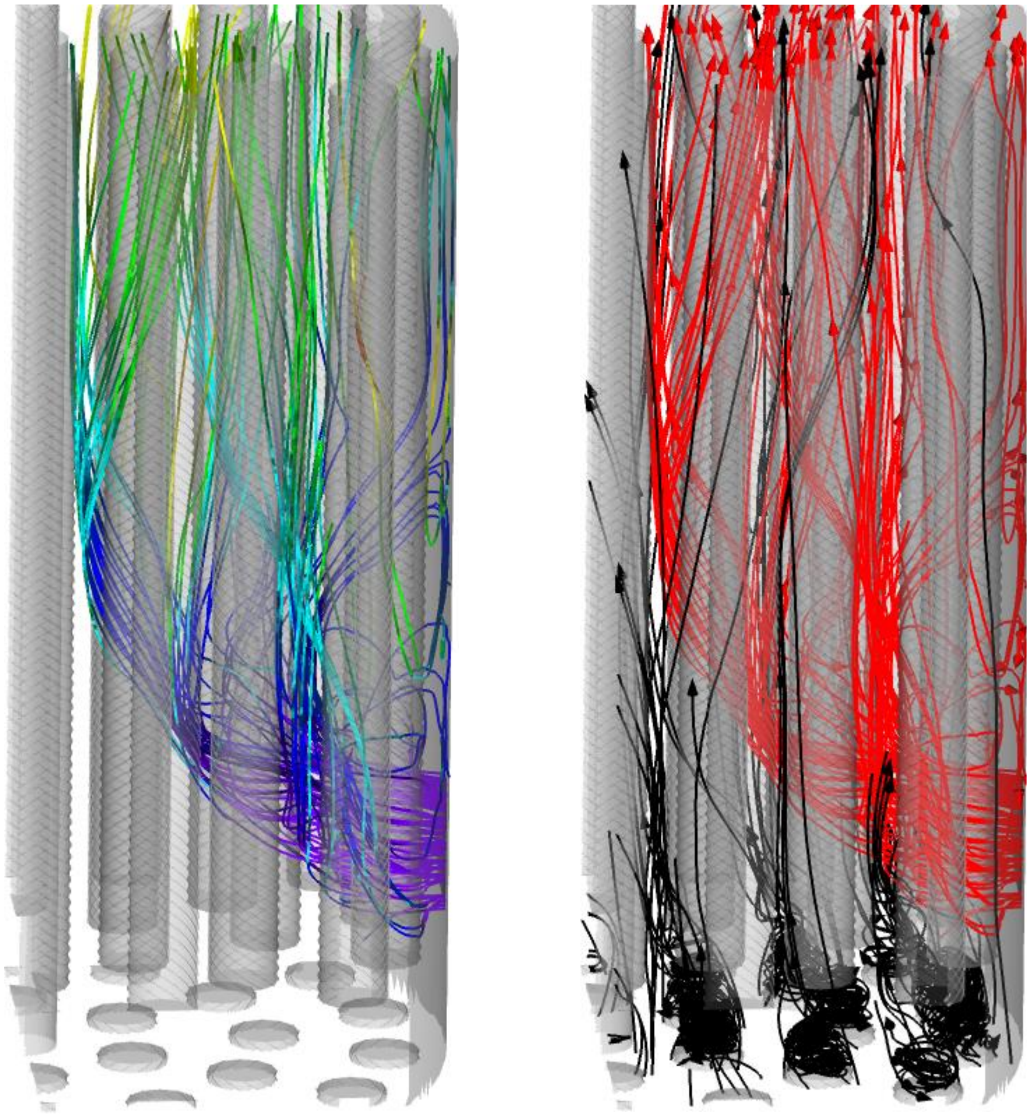
- CCP-NTH: collaborative computational project on nuclear thermal hydraulics to support the next generation of civil nuclear reactors
- High fidelity CFD for pipe break in HTGRs (EP/T002417/1)
- CFD modelling development for liquid metal fast reactors (EP/T002395/1)
- Part of the second phase of BEIS thermal Hydraulics project (led by Frazer-Nash)
- Collaborations with industrial partners such as EDF Energy R&D UK Centre, RR Nuclear, Westinghouse

Science and Technology Facilities Council

Life extension of the UK AGRs

- The Advanced Gas-cooled Reactors (AGR) in the UK make up the bulk of the fleet.
- In order to ensure safe operation, it is necessary to have a deeper understanding of the flow conditions inside the reactors.
- The designs are decades old and there is little reliable data from experiments.
- CEG has worked on a range of projects with EDF R&D UK to use HPC and CFD to extend the life of several AGR components





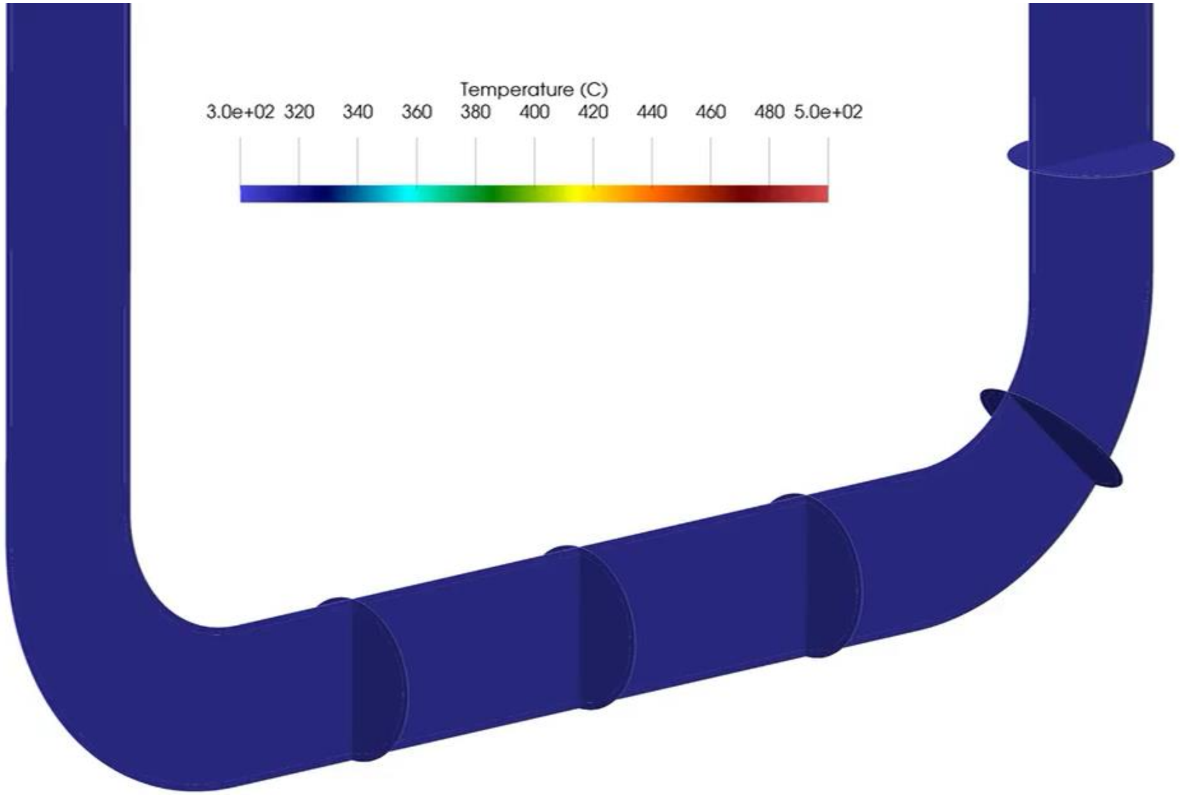
Injection of cold flow in the fuel assembly of an AGR reactor

Science and Technology Facilities Council

Reference person: C. Moulinec

Thermal Fatigue in Pipe Bends

- Thermal Fatigue is an important feature in many nuclear applications which could lead to thermal striping
- The CEG group in collaboration with the nuclear arm of Rolls Royce is looking at high fidelity coupled conjugate heat transfer calculations to simulate accurately thermal transient phenomena



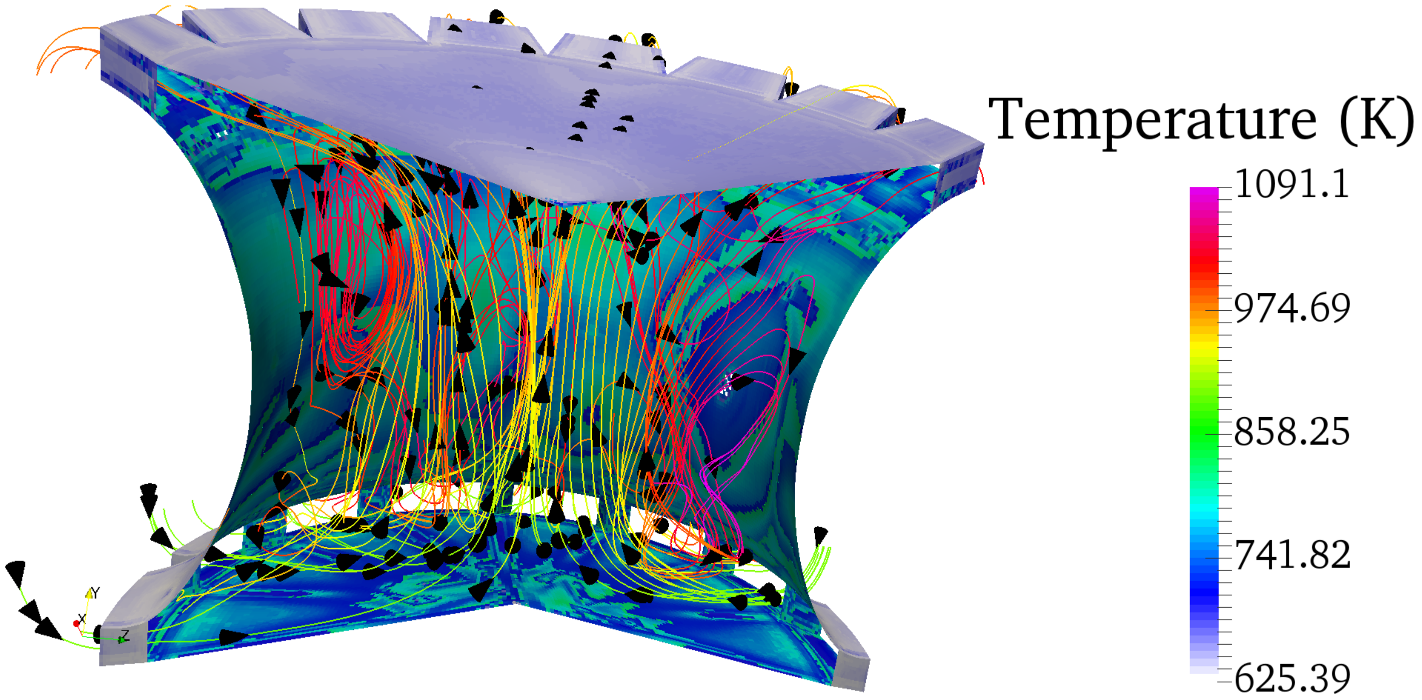
Thermal Transient in a U-bend

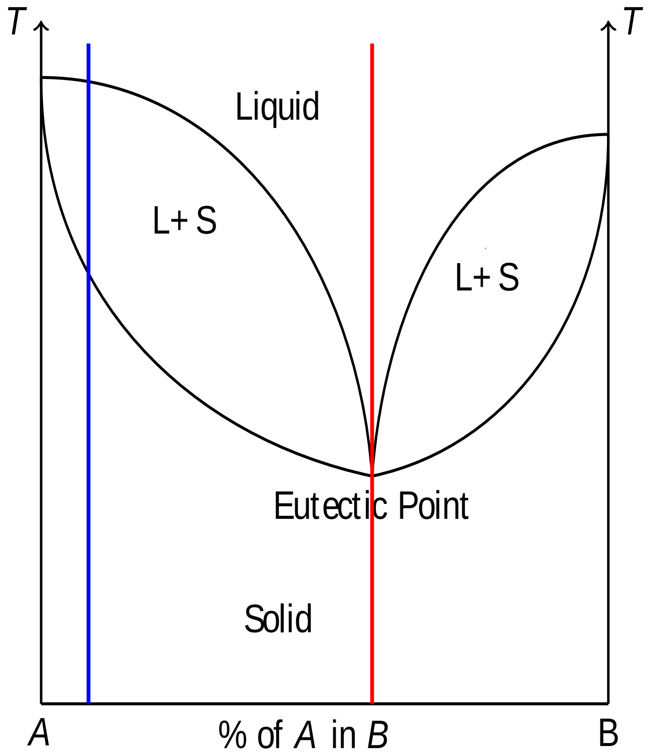
UKRI Science and Technology Facilities Council

Reference person: A. Skillen

Frozen Wall in Molten Salt Fast Reactors

- Molten Salt Fast Reactors (MSFRs) are one of the proposals for the next gen-IV reactors.
- They have the advantage of having the coolant and the fuel both mixed together as a homogeneous medium.
- One of their main disadvantages is corrosion because of the nature of the salt.
- CEG has been developing a coupled CFD-Neutronics framework for the simulation of the frozen salt dynamics on the vessel walls





Reference persons: G. Cartland-Glover and S. Rolfo

Conclusions

- STFC carries out broad range of nuclear based modelling activities

Materials modelling

- TU-TILD brings access to high temperature properties of nuclear-relevant materials for high-throughput studies, including high entropy materials
- MEAMfit enables large scale simulations of complex microstructure, e.g. to investigate mechanical properties of polycrystalline high entropy alloys
- Methodologies leveraged to investigate: low activation materials for next generation and fusion reactors; molten salts relevant to molten salt reactors; ultra high temperature ceramics

Fluid dynamics

- Involved in a range of projects and consortia, with nuclear applications to:
  - AGR lifetime extension through modelling of cold flows within fuel assemblies
  - model thermal fluctuations and turbulence within pipe-bends to reduce fatigue damage
  - investigate potential to form solid salt on the walls in connection with corrosion in MSFRs; conclusions suggesting smaller reactor designs may be necessary (Greg is in the audience!)

Science and Technology Facilities Council

Thank you for your attention!

Material science: Andrew I. Duff (andrew.duff@stfc.ac.uk)

Fluid dynamics: Stefano Rolfo (stefano.rolfo@stfc.ac.uk); Gregory Cartland Glover (greg.glover@stfc.ac.uk); A. Skillen; C. Moulinec