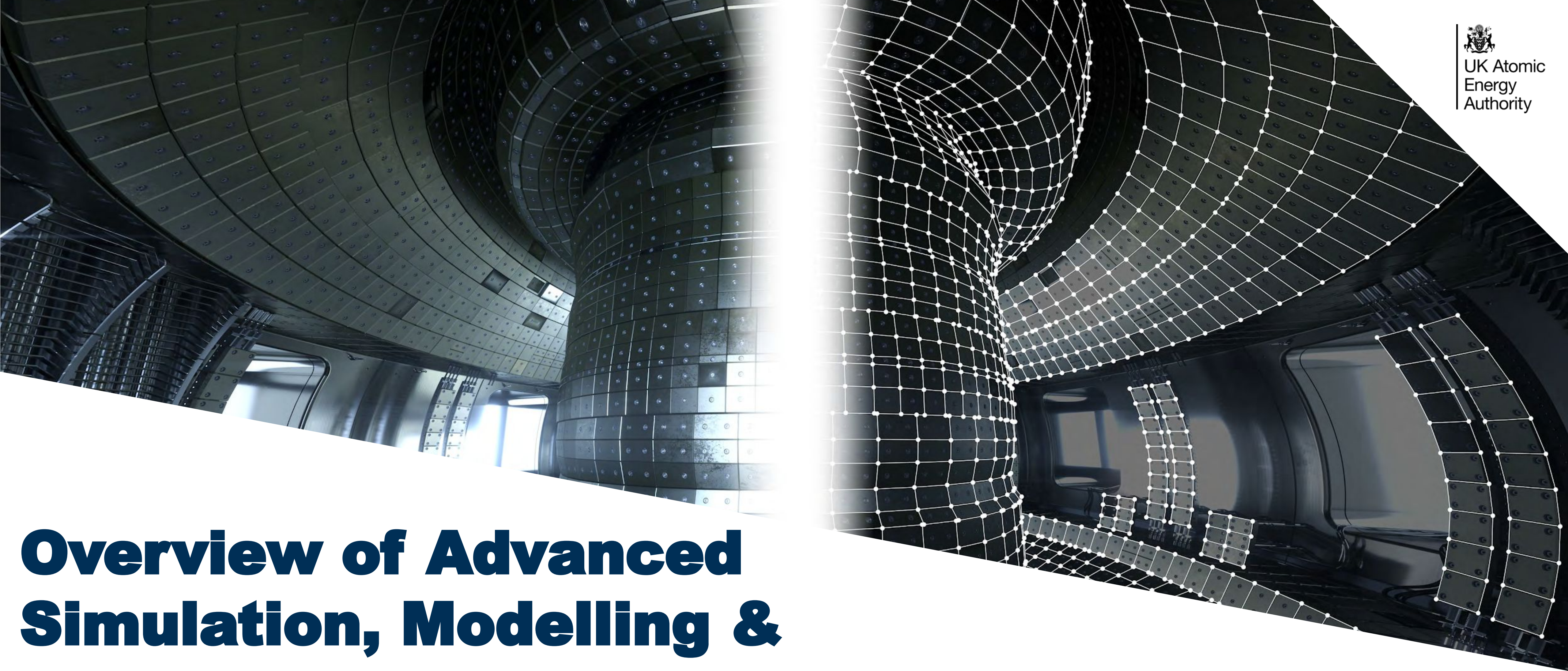

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Overview of Advanced Simulation, Modelling & Digital Twins in the UK

Prof. Andrew Davis, Head of Advanced Engineering Simulation, UKAEA

Eurofusion ETASC Meeting - November 11th 2024

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The following slides represents the work of several individuals, teams, groups and divisions, Computing, Integrated Engineering, Fusion Technology, Tokamak Science, ….

UK Funding Landscape (Computing)

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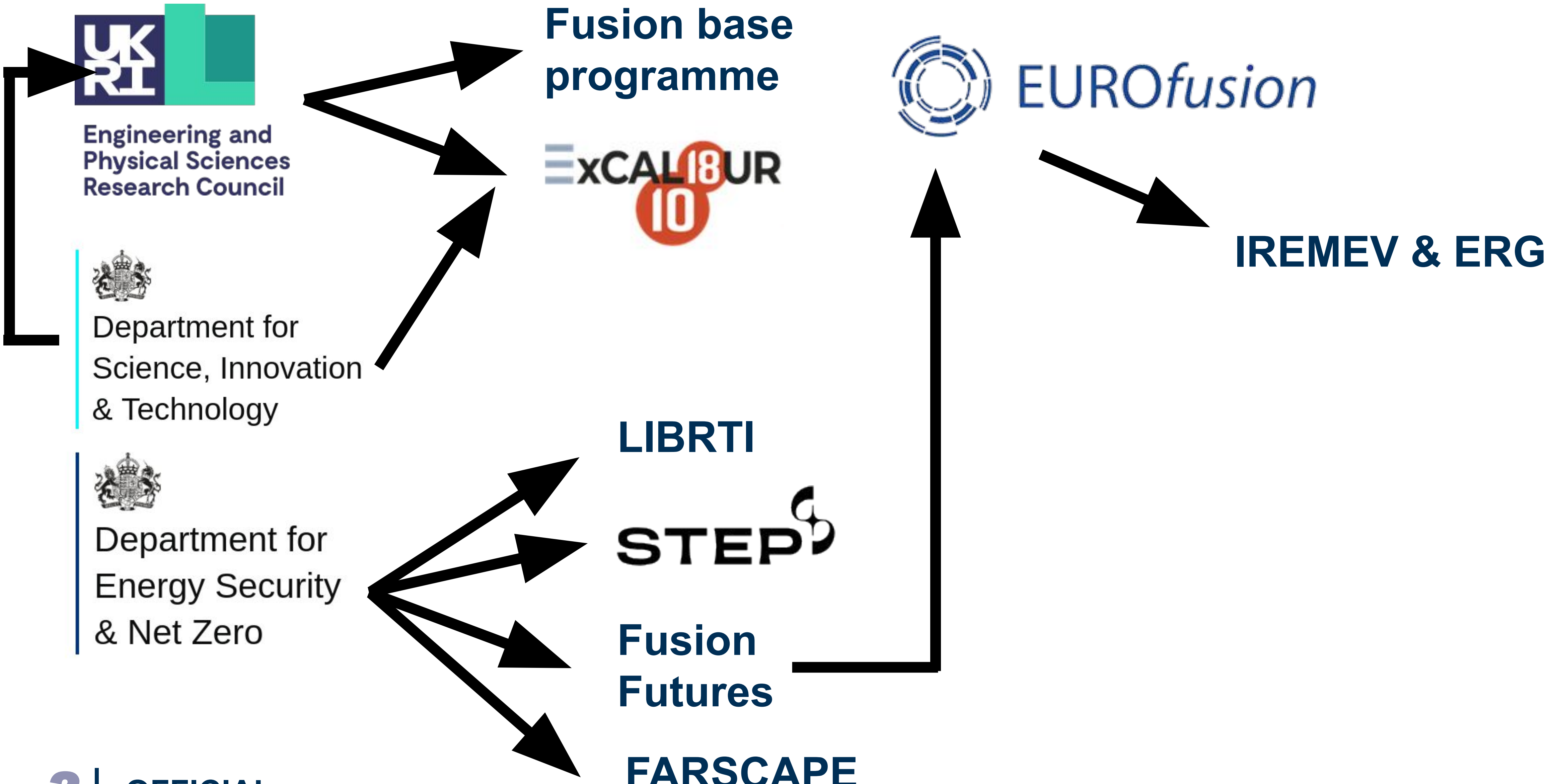

UK HPC Landscape

UK Atomic Energy Authority

Isambard-3

Archer 2

#EuroHPC Joint Undertaking

The European High Performance Computing Joint Undertaking (EuroHPC JU) will pool European resources to develop top-of-the range exascale supercomputers for processing big data, based on competitive European technology.

Member countries are Austria, Belgium, Bulgaria, Croatia, Cyprus, Czechia, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Iceland, Ireland, Israel, Italy, Latvia, Lithuania, Luxembourg, Malta, Montenegro, Netherlands, North Macedonia, Norway, Poland, Portugal, Romania, Serbia, Slovakia, Slovenia, Spain, Sweden, Türkiye and United Kingdom.

EuroHPC Joint Undertaking

All models are wrong, some are useful…

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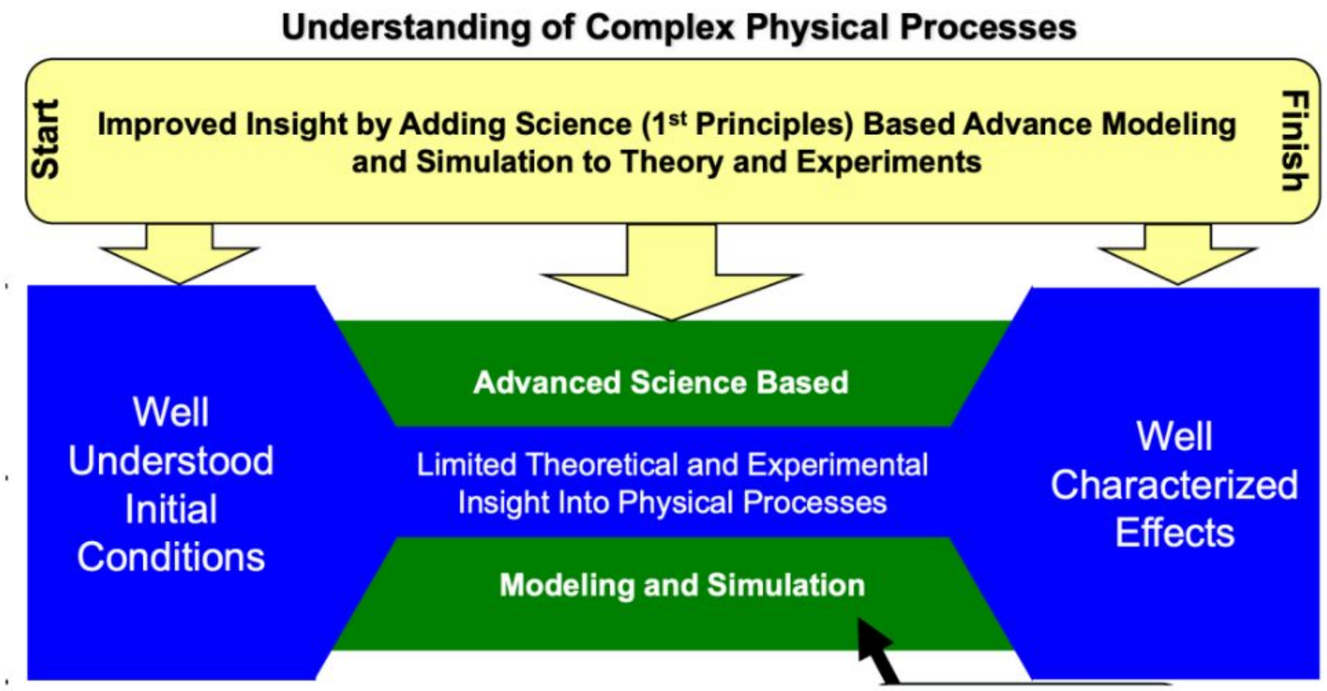
- Multiphysics modeling and simulations (M&S) enable insights into nuclear systems in ways not possible with traditional approaches alone

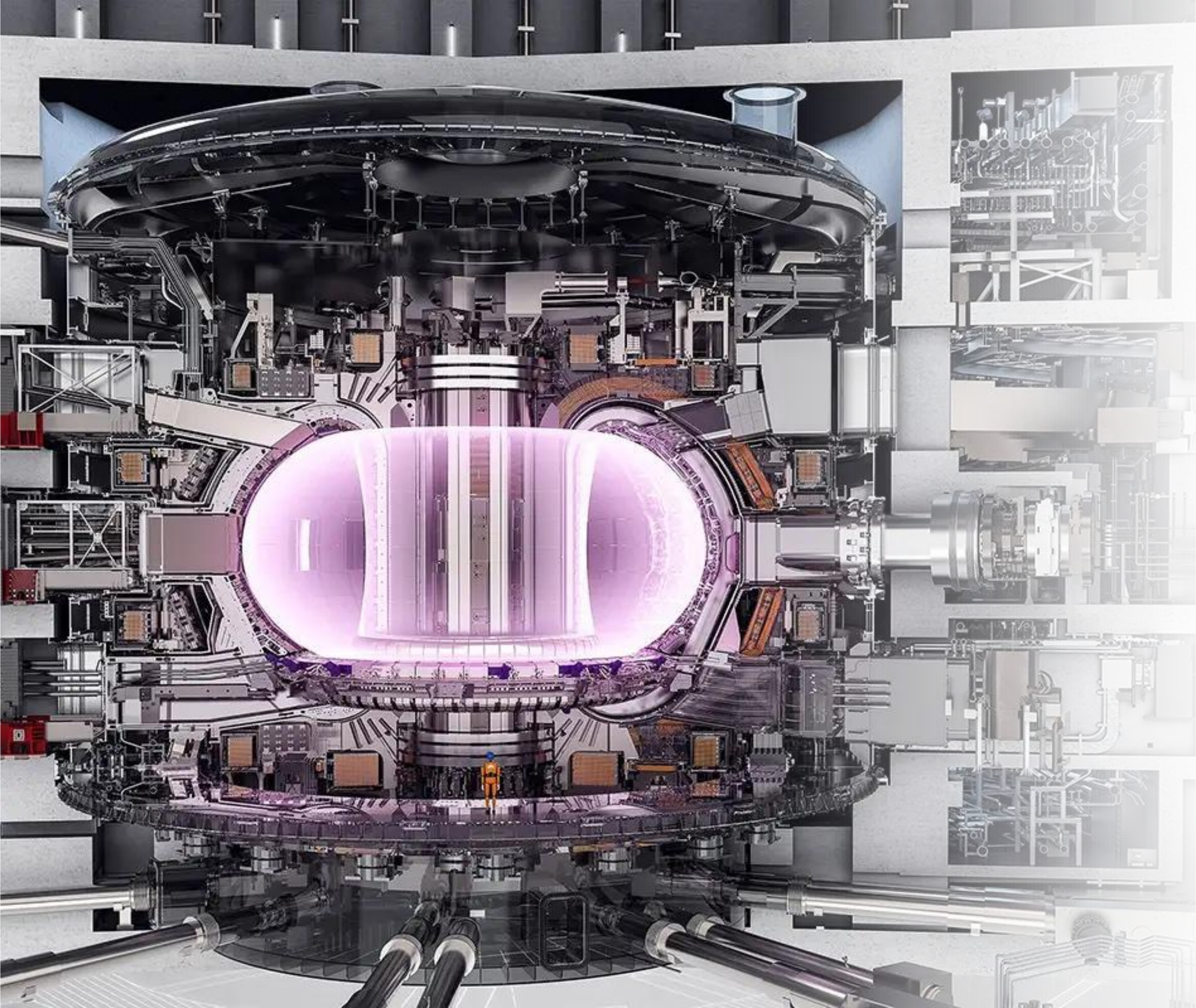
From: Lazelere 2010 DOE-NE



"All Models are wrong, but models that know when they're wrong are useful" - Lakshmiarayanan et al 2021

Validation and quantification of uncertainties is preferred to replace traditional conservative analysis for safety assessment and licensing
(Reitsma et al. 2017; IAEA Program on Uncertainty Analysis)

- Advanced science (Physics) based M&S can augment understanding when there is limited theoretical and experimental insights
- However, M&S can be uncertain needs to include VVUQ - our models need ot be probabilistic (Bayesian)



Simulation:

Everything, everywhere, all at once…

- **Radiation**
- **Electromagnetism**
- **Structural forces and Gravity**
- **Heat transport** (conductivity, thermal hydraulics)
- **Chemical transport** (Diffusion, radio-nuclide transport through fluids)
- **Temporal coupling –** transmutation, radiation induced embrittlement, fatigue, tribology/wear

What is a Digital Twin?

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I might throughout this talk drop the phrase “digital twin” - by which we mean the Grieves and Vickers definition of a digital twin (https://doi.org/10.1007/978-3-319-38756-7_4)

“It is based on the idea that a digital informational construct about a physical system could be created as an entity on its own. This digital information would be a “twin” of the **information** that was **embedded within the physical system itself** and be **linked with that physical system** through the **entire lifecycle** of the system.”

- Must predict future state
- Must allow emergent behaviour
- Inherently multiscale (atoms to macroscale)
- Digital twin can exist before the physical system
- Must connectivity of sensor data

Grieves test of **virtuality** (Sensory, Performance, Reflectivity) **(akin to Turing test)**

Towards a full plant Digital Twin

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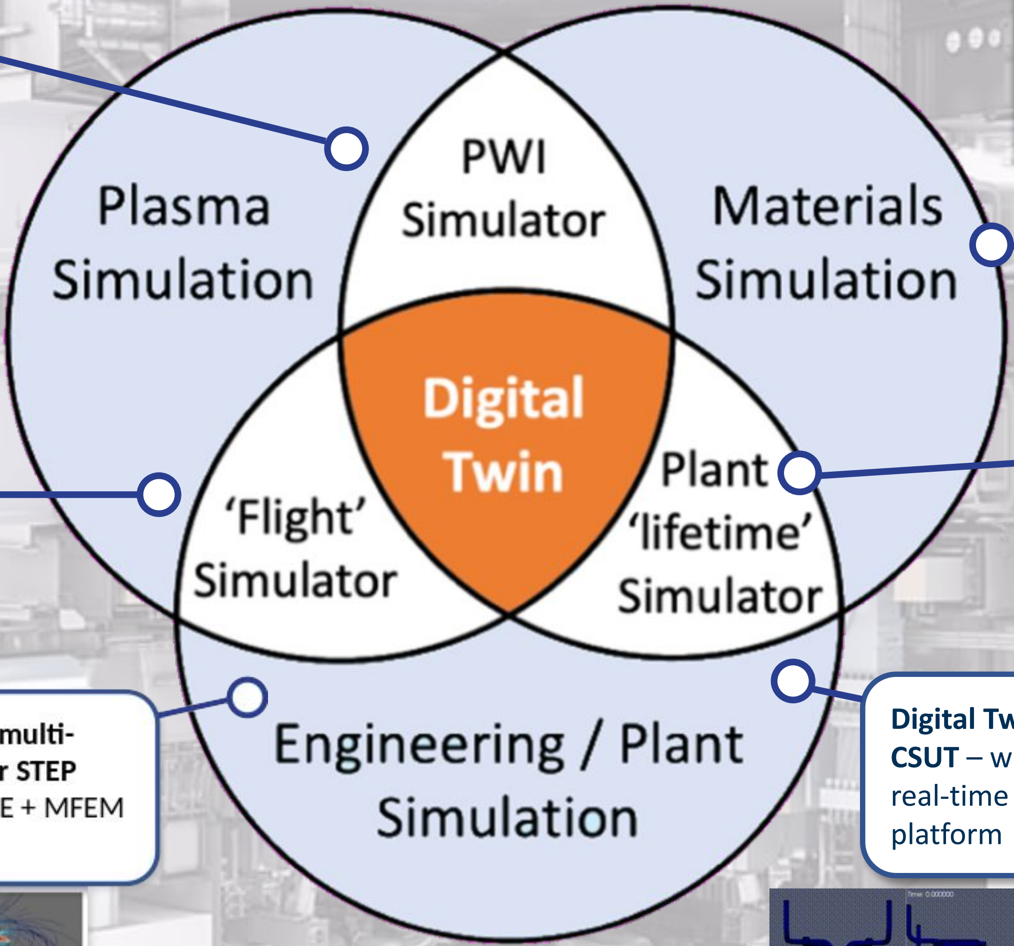
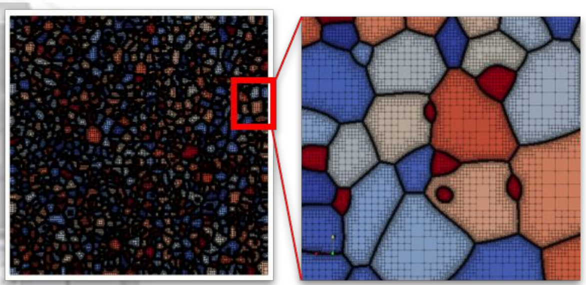
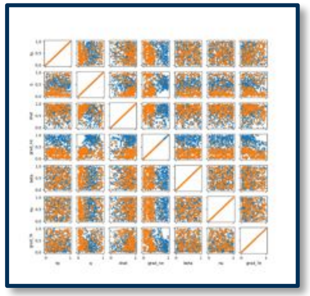
Building **exascale targeted, performance portable plasma simulation** capability



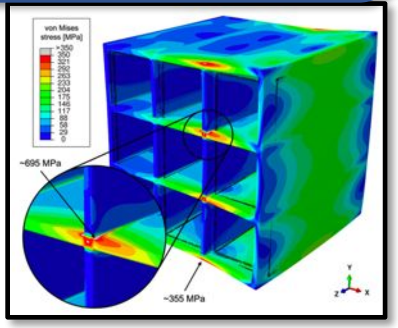


Coupling Multiscale materials modelling materials modelling necessarily has many scales to it

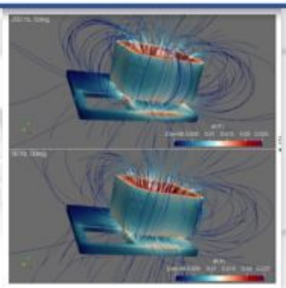
Gaussian Processes, Active Learning etc. to construct **Gyrokinetic emulators**



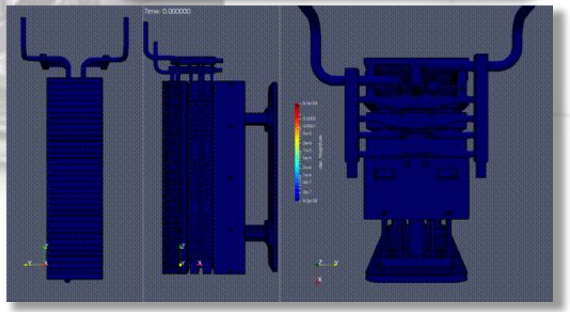
Coupling neutronics to FE (Crystal Plasticity Finite Elements) to optimise stress-strain across load assembly



Building a scalable multi-physics platform for STEP (based upon MOOSE + MFEM from LLNL)



Digital Twin of CHIMERA CSUT – within a factor 10 of real-time using MOOSE platform



Akers et al, ISC23

Advanced Computing

NEutrals and Plasma TUrbulence Numerics for Exascale

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Edge plasma physics – two major areas for NEPTUNE:

- Plasma turbulence (**fluid**);
- Neutral species (**particles**).

Main goal: **open-source** & **scalable** edge plasma code.

- Main phase ran 2019-2024.
- 2/3 of work defrayed to externals.

Edge plasma physics is complex, hence proxyapps approach.

Grantee	subject
University of Exeter	surrogates
King's College London	finite elements
Imperial College	finite elements
University of Oxford (Maths)	PDE theory
University of Oxford (Physics)	theory
STFC	numerical analysis
University College London	UQ, surrogates
University of Warwick	Particle methods
University of York (Computer Science)	hardware and software support
University of York (Physics)	plasma physics

NEPTUNE Proxy Apps

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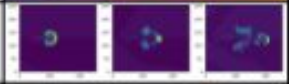
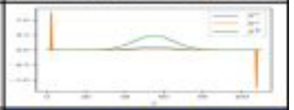
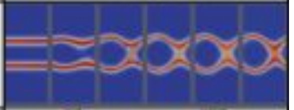
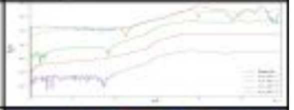
Proxyapp	Framework	Language	Comments	Sample output
nektar-driftwave	*Nektar++*	C++	2D plasma turbulence	
nektar-diffusion	*Nektar++*	C++	strongly anisotropic diffusion	
vertical natural convection in spectral / hp, 2D and 3D	*Nektar++*	C++	heat transport by fluid	
2D plasma fluid equations in spectral / hp	*Nektar++*	C++	*Hermes-3* equation system	
1D fluid solver with UQ and realistic boundary conditions	*Nektar++*	C++	1D model of scrape-off layer	
Vlasov-Poisson kinetic solver in spectral / hp	*Nektar++*	C++	Uses finite elements to do kinetic theory	
moment-kinetics	new code (Univ. Oxford)	Julia	moment-kinetic gyro-averaged code	
minepoch	*EPOCH* (Univ. Warwick)	Fortran	used for testing particle implementations	
electrostatic PIC proxyapp	NESO / NESO-Particles	C++ / SYCL	UKAEA code	
2D3V coupled fluids-neutral particles proxyapp	NESO / NESO-Particles	C++ / SYCL	UKAEA code	

NEPTUNE Software

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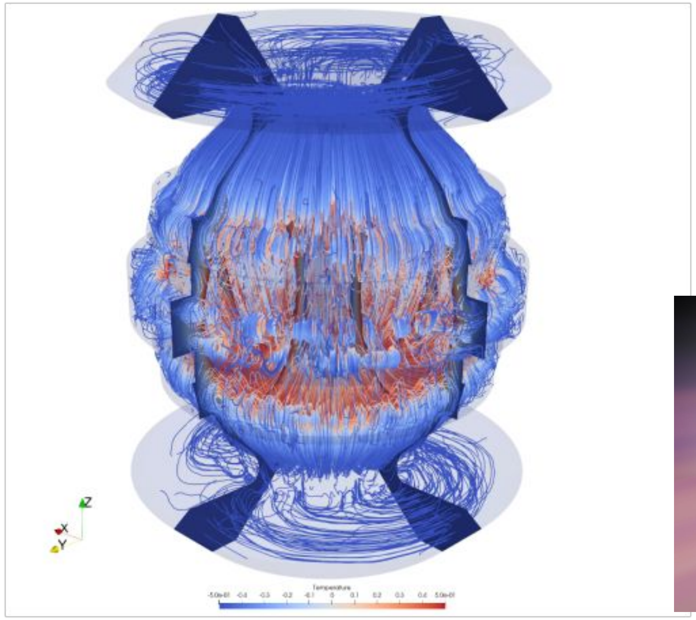
NESO Public
C++ · ☆ 4 · MIT · 3 forks · 49 (2 issues need help) · 13 · Updated 4 days ago

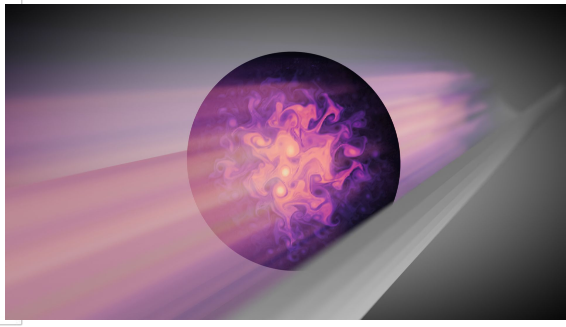
NESO-Particles Public
C++ · ☆ 2 · MIT · 1 fork · 6 · 4 · Updated 4 days ago

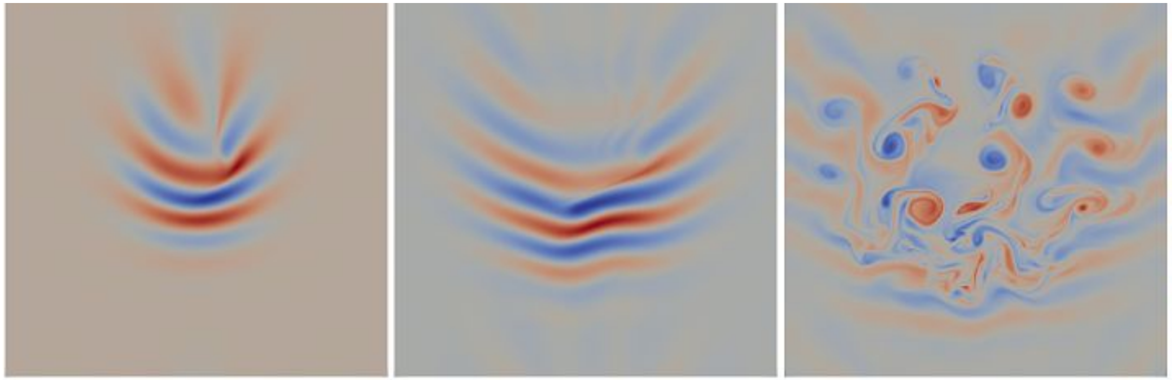
NESO-fame Public
Field Aligned Mesh Extrusion
Python · ☆ 1 · GPL-3.0 · 0 forks · 2 · 0 · Updated 2 weeks ago

NESO-Spack Public
Spack repository for installing NESO components and dependencies.
Python · ☆ 2 · 1 fork · 2 · 1 · Updated last month

NESO-UQ Public
Python · ☆ 0 · MIT · 0 forks · 1 · 0 · Updated on May 26, 2023







- NESO - NEPTUNE Exploratory Software - core NEPTUNE software.
- Nektar++ is used as finite-element method library.
- NESO-Particles library for kinetic theory
- NESO-fame: meshing magnetic flux surfaces; NESO-UQ uses SEAVEA.

https://github.com/ExCALIBUR-NEPTUNE

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FARSCAPE

In its final year, FARSCAPE includes

- Over 100 members
- 7 UK institutions (private & public)
  - Hartree Centre (STFC)
  - STFC – SCD – SciML
  - digiLab ltd
  - UK Universities (Oxford, Manchester, Bristol, York)
- Held/supported several training events
- Projects with several UKAEA Divisions

(Plasma, FTF, IED, MAST-U)

https://github.com/farscape-project/

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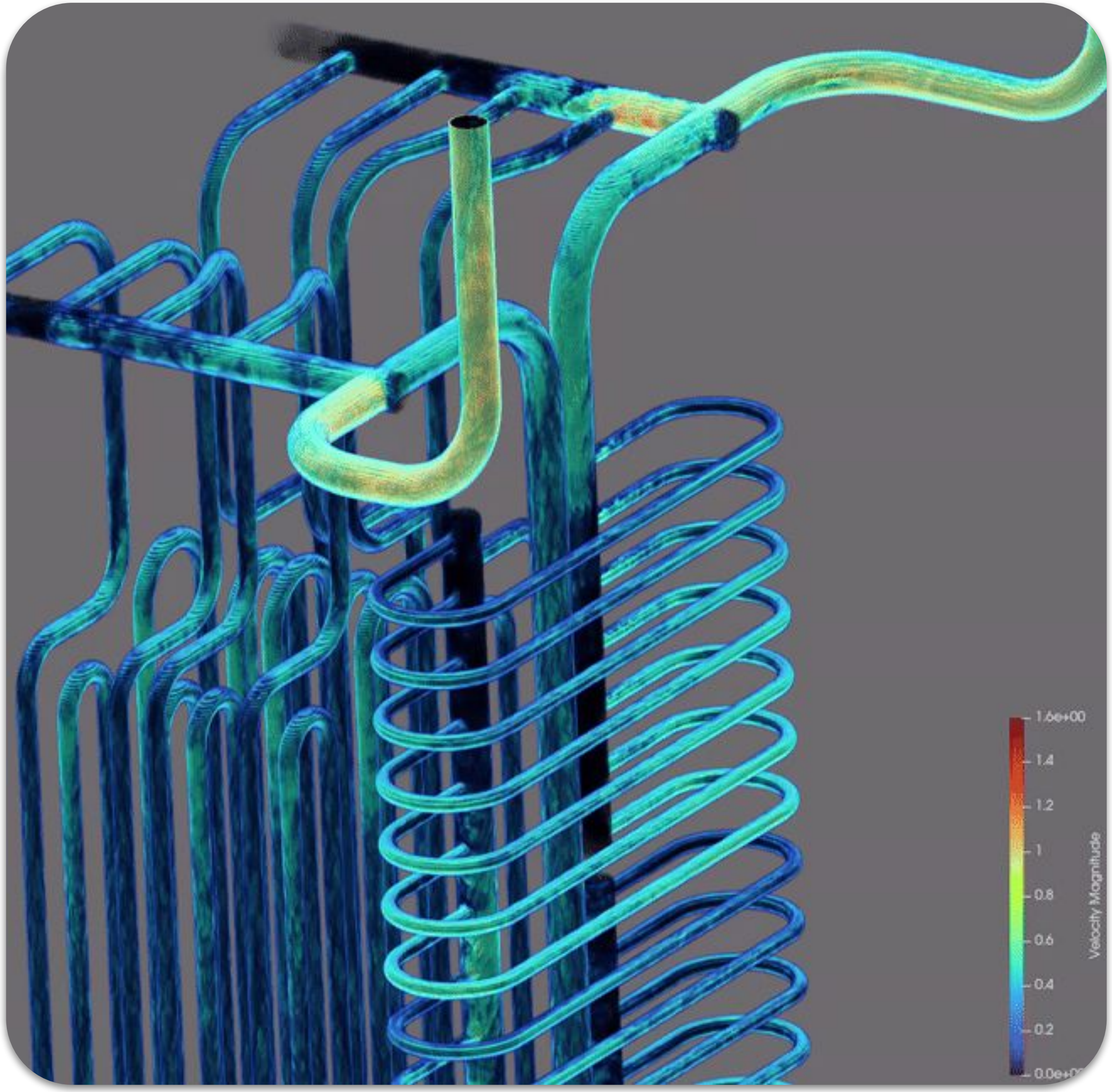
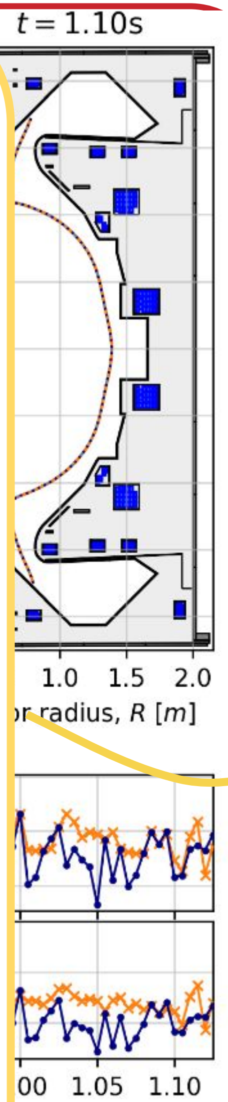
NekRS simulations of CHIMERA coolant network; 35k GPUs of Frontier used to solve the largest DNS (LES) conjugate heat transfer ever attempted. Data used to test turbulence models e.g. k-e

0.2 second per timestep





https://arxiv.org/pdf/2409.19119

odels

ainst

true coil voltages

AMRpx (AMReX)

ML surrogate models for core turbulence

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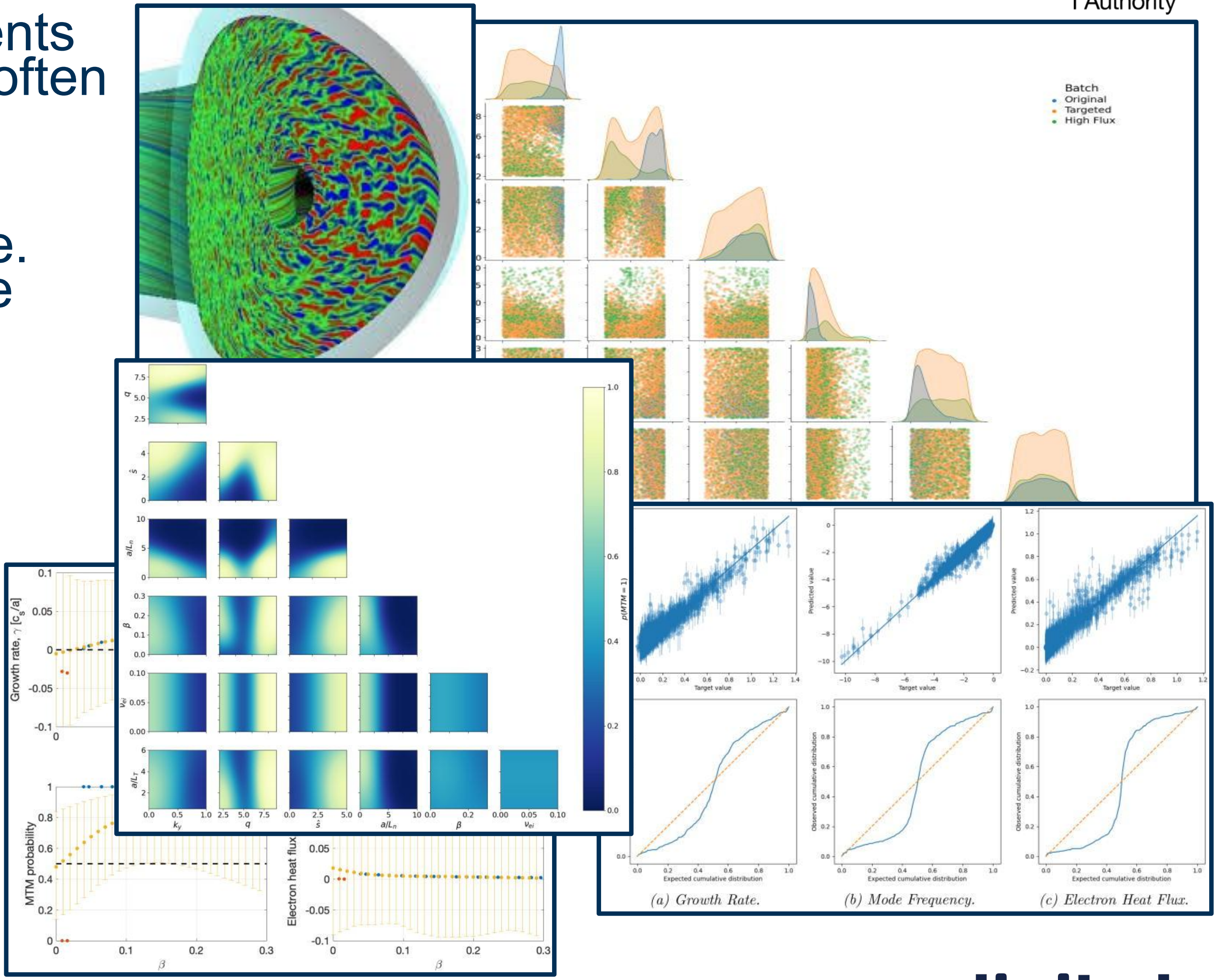
One of the most expensive components in integrated modelling workflows is often the **transport model**

Transport is dominated by turbulence. Simulations of plasma turbulence are very computationally expensive.

We aim to replace these with ML surrogate models where appropriate reduced models don't exist.

Gaussian process regression and classification used in active learning pipeline to efficiently create training databases.

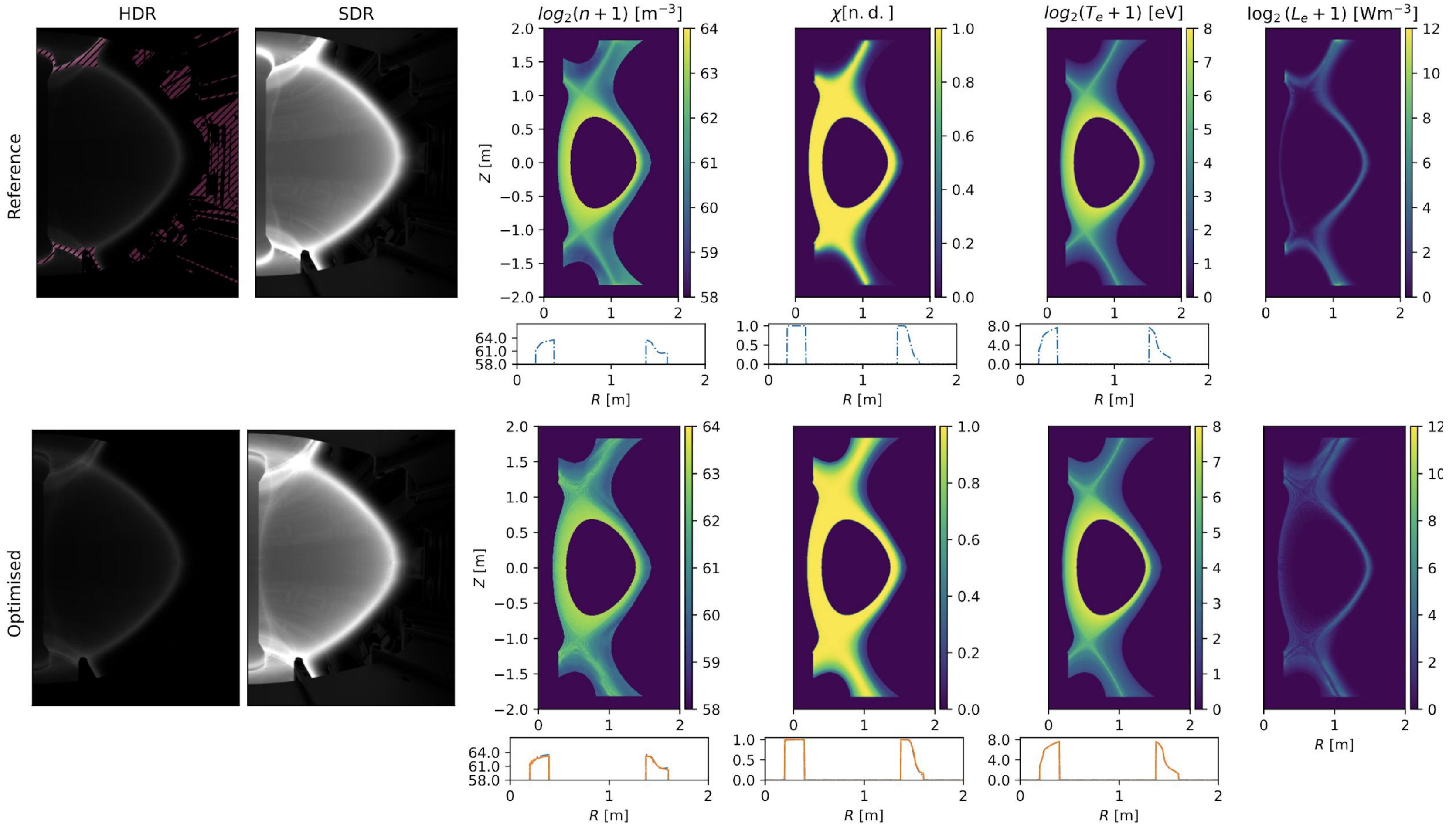


W Hornsby

digiLab

Using AI to create new Diagnostics

- Use synthetic data and synthetic rendering
- Train NN to infer plasma shape and 2D plasma composition
- Given camera image => 2D neutrals distribution (cannot be measured otherwise)



Ekin Ozturk

https://arxiv.org/pdf/2408.07555

(submitted to Nuc.Fus.)

FAIRMAST: a FAIR database of MAST for AI

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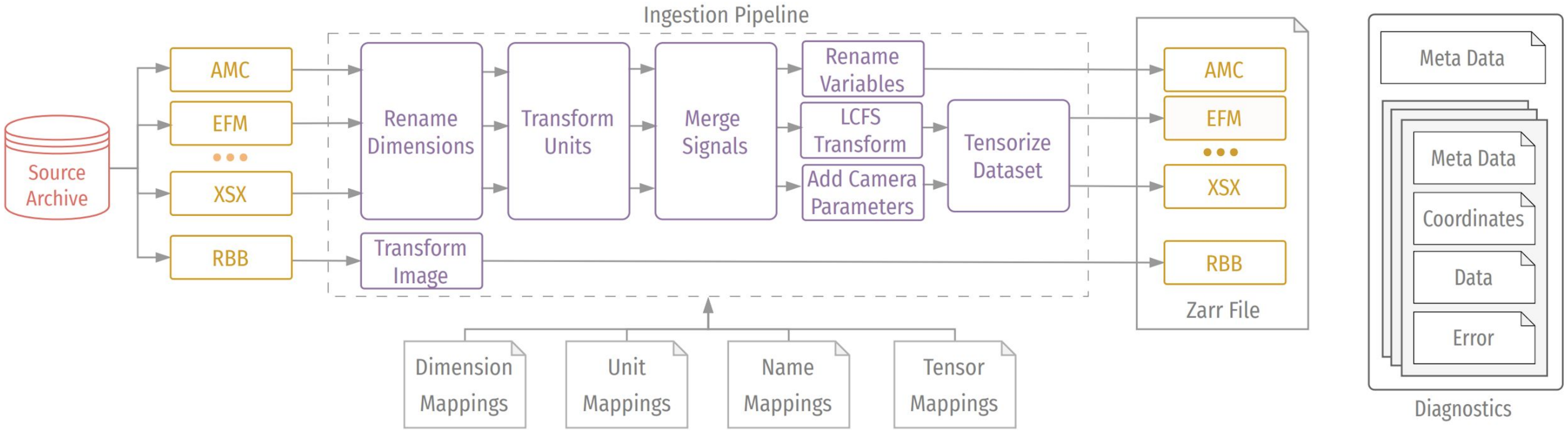
- Designed a modern database for MAST experimental data
- => Follow FAIR Principles
- => Efficient for AI applications
- => Easily mapped to other standards (eg. IMAS)

Sam Jackson et al., SoftwareX 27 (2024) 101869

https://doi.org/10.1016/j.softx.2024.101869

Extension submitted to IEEE



Accelerating MHD simulations

- Neural-Parareal: Combine Parallel-in-Time method with Neural Operators
- As more simulations are being run, new data makes Neural Operator more accurate
- => Time-parallelisation becomes more efficient
- => Simulations become faster

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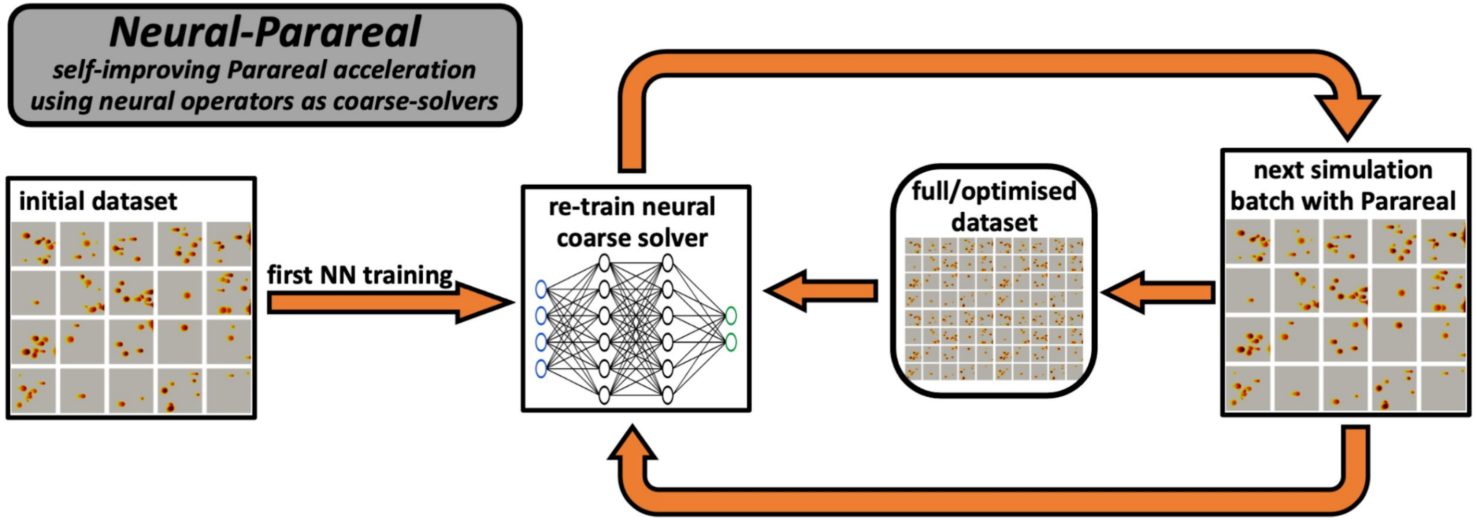
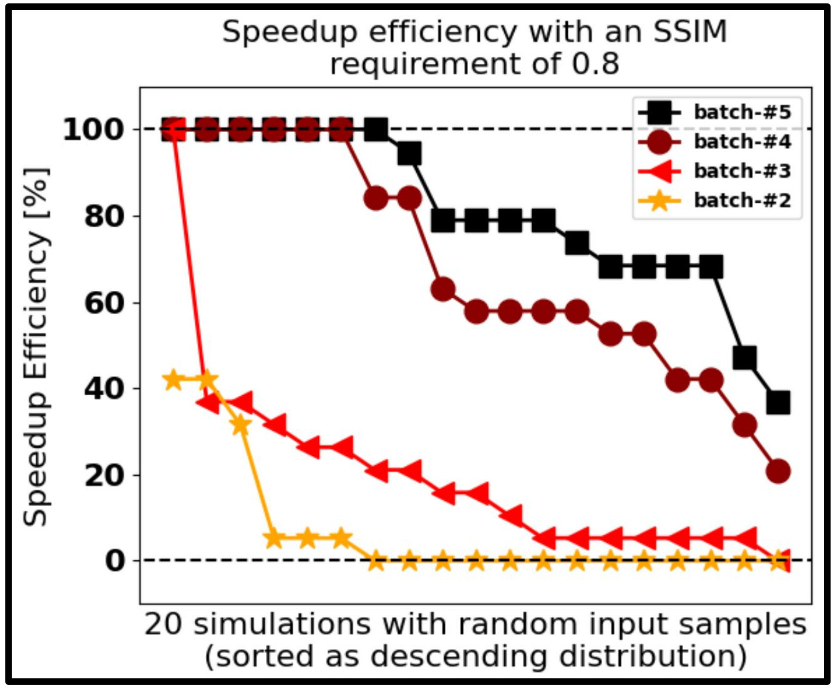
Stan Pamela, CPC 307 (2025) 109391

https://doi.org/10.1016/j.cpc.2024.109391





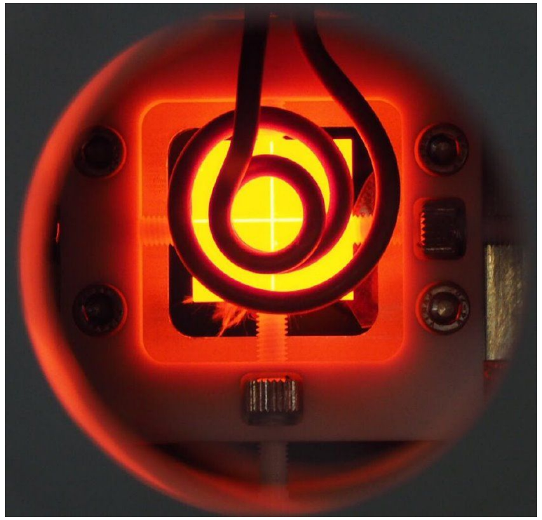
FARSCAPE

Stakeholders are our experimental facilities

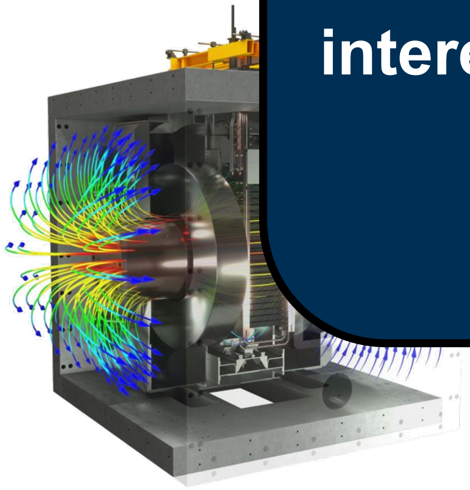
- trying to find and fill the gaps and connect **Digital Engineering** to **Exascale & AI**
    - https://www.youtube.com/wa
    - https://www.youtube.com/w
    - https://ccfe.ukaea.uk/case-s

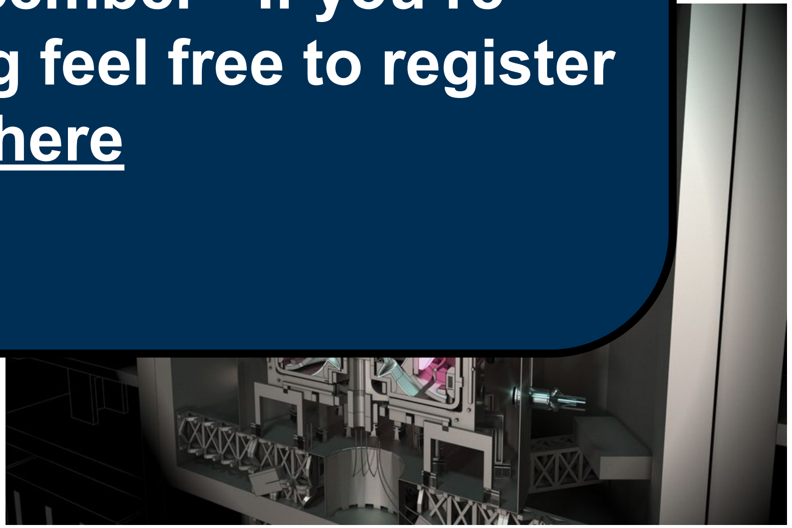
Fusion Computing Lab (nee FARCAPE) will have a yearly showcase held at Culham, on the 2nd and 3rd of December - If you're interested in coming along feel free to register to attend here

HIVE

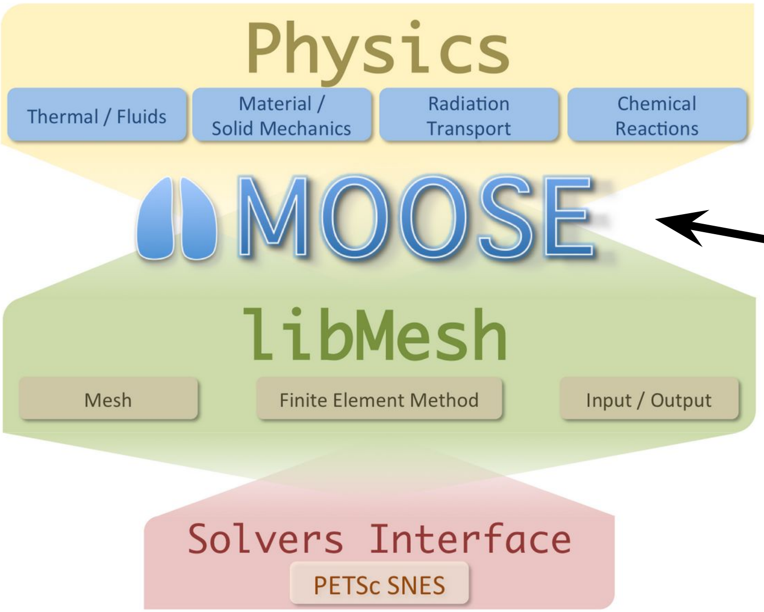


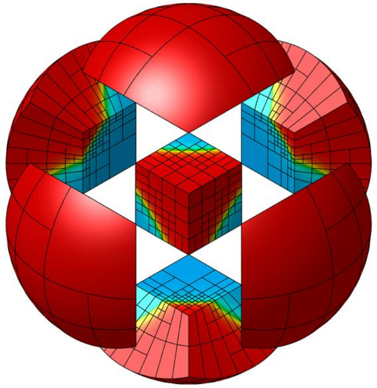
CHIM



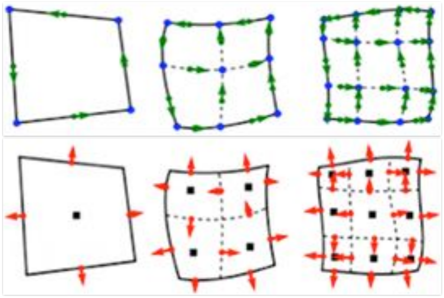


Fusion Futures (INL)

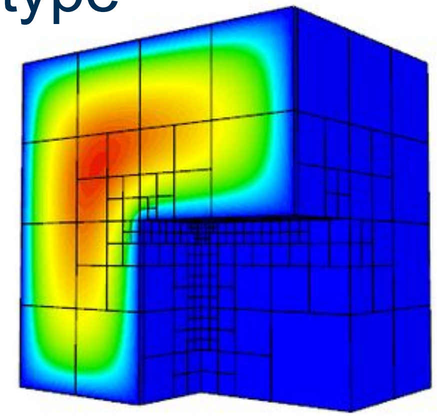




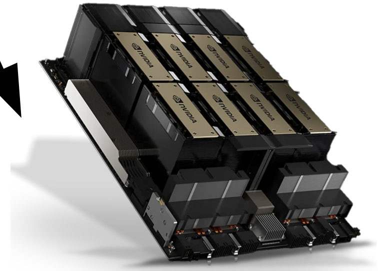
MFEM (LLNL)



Wide range of FE type



Arbitrary H & P order



Excellent GPU support

- Collaboration with INL & LLNL to replace the FE backend of MOOSE (libMesh) with an alternate MFEM (from CEED [ECP])
- Will provide scalable GPU solving to wide range of problems, e.g. structural, thermal, neutronic, fluids, MHD

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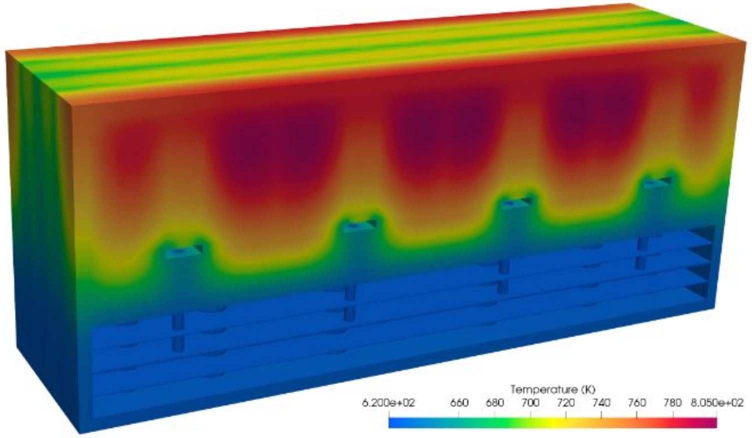
Fusion Futures (ANL)

OpenMC

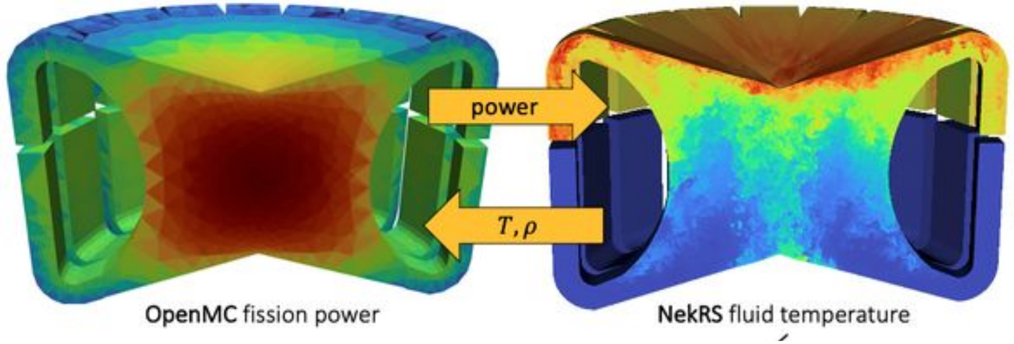
NekRS

Cardinal



- Collaboration with ANL (UW-Madison, UUIC) around OpenMC (neutron transport), NekRS (Spectral fluids solver) and Cardinal (MOOSE application that links OpenMC & NekRS).
    - GPU acceleration of OpenMC
    - GPU acceleration of DAGMC

https://shorturl.at/mrCTJ



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Modelling

bluemira

See TSVV-14 poster on Tue afternoon

Karlsruher Institut für Technologie

UK Atomic Energy Authority

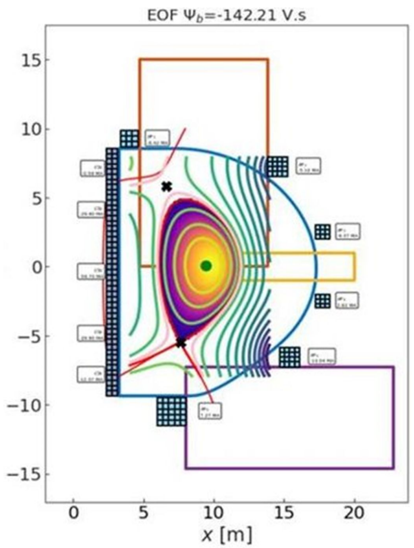
Aim is to create an open-source reactor concept tool capable of integrated modelling at multiple levels of fidelity (0-D □ 3-D). For rapid exploration of design space and an extension of low fidelity systems codes.

It isn't a digital twin, pulse design tool or "tokamak simulator". It is a whole plant concept tool (primarily workstation, i.e. not distributed).

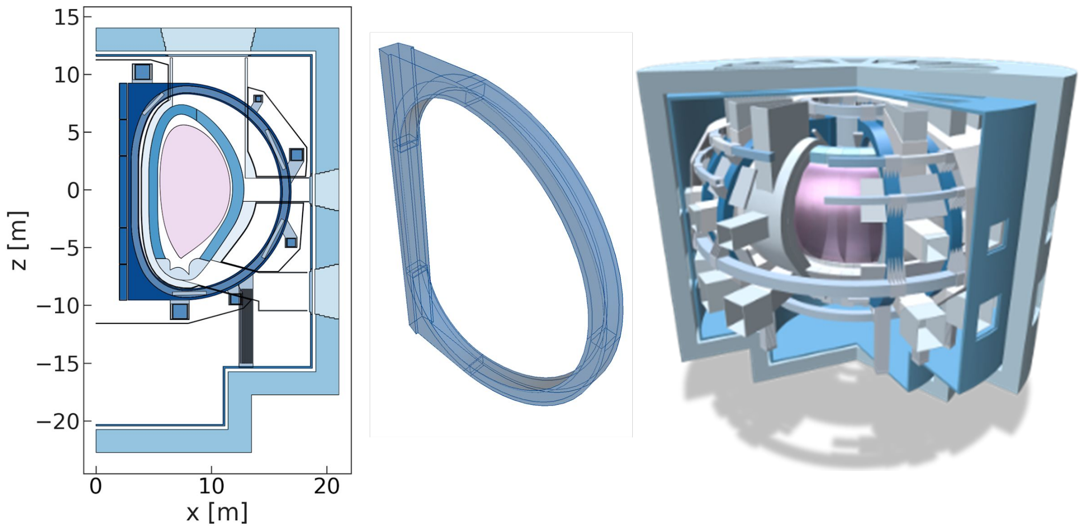
WPRM

Specification of constraints on remote maintenance. Space availability and with optimisation constraints, manipulator constraints (eg. mass).

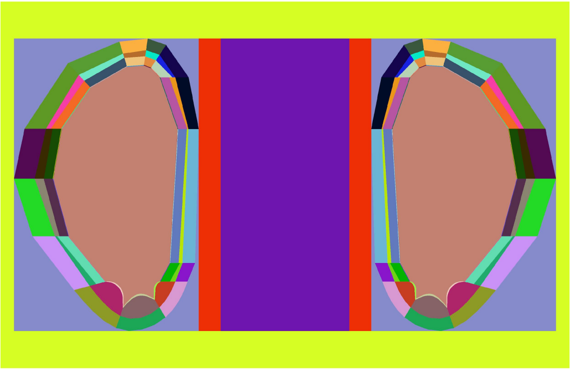
Early concept stage integration of RM considerations □ Integrated with all other systems, 2-D Keep out zones for ports part of automated PF coil positioning and blanket segmentation, access restrictions respected, immediate generation of space claim CAD expedites further analysis.



EU-DEMO Workflow



Neutronics



Created axisymmetric OpenMC (CSG) models from the bluemira wires, to calculate neutronics quantities such as the TBR and heat loads on various components.

What is the High Fidelity Plasma Simulator?

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- The HFPS is a set IMAS actors used together in a python workflow
- HFPS is a coupling *framework* (aka "JINTRAC IMAS driver") in **python**
  - Data exchange using **IDS**
  - New components interfaced as **plug-ins**
  - Communication using **MUSCLE3** (Persistent Actor Framework)

External models ideally meet a minimum set of requirements to be incorporated in HFPS workflow:

1. They must be launchable as stand-alone processes
2. They must use IMAS IDS data structures for input and output
3. They must communicate IDS inputs and outputs via the MUSCLE3 framework
4. A plug-in must be provided which describes the model's usage and interface

Currently supported actors / components

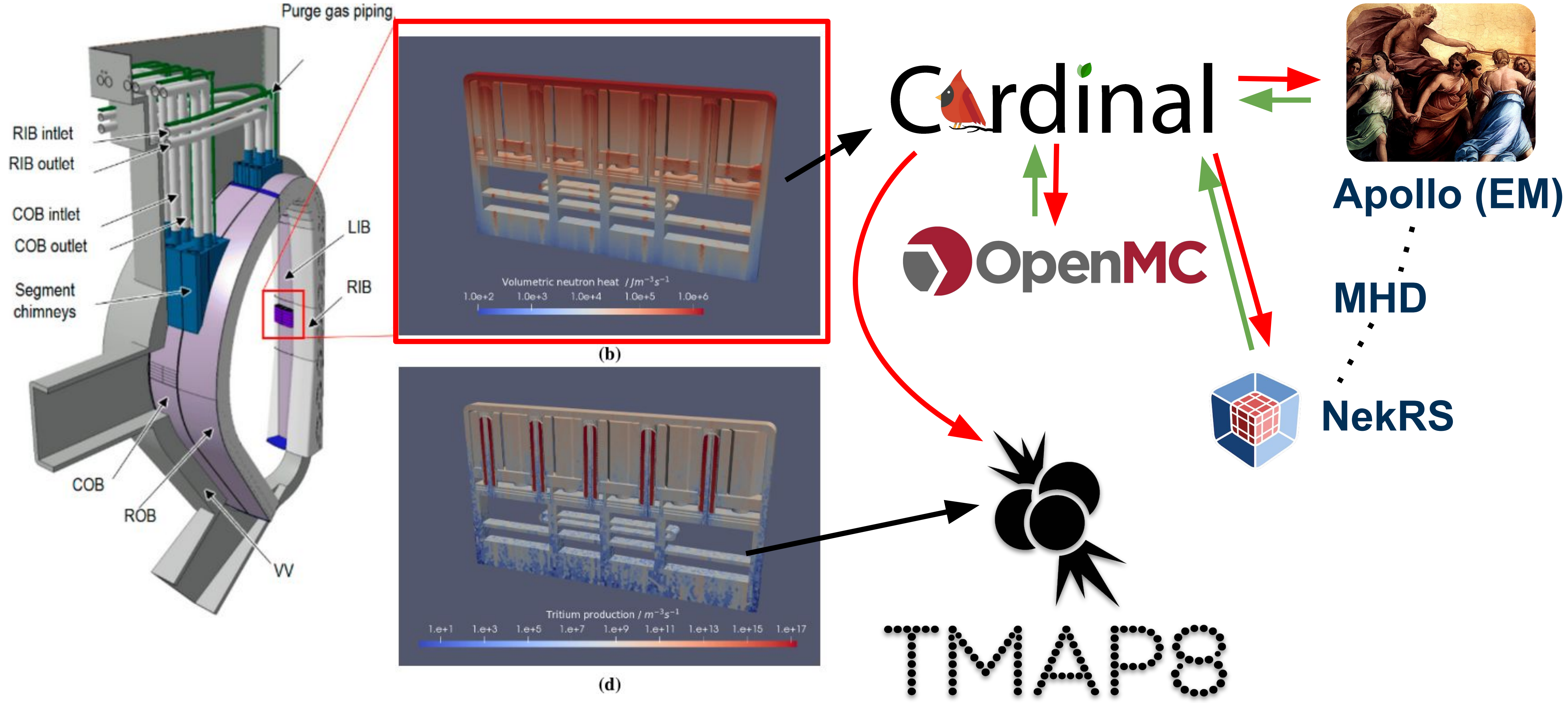
- JETTO - for 1D core transport
- EDGE2D-EIRENE – for 2D SOL / nuetrals
- COCONUT – coupled core / SOL
- HCD python – (from ETS / ITER)
- MHD python – (from ITM)
- DINA – for FBE with mag. control.
- Grid2D – for updating SOL grid
- KinMPC – for density control (from DIFFER)
- Controllers – in matlab / python

https://muscle3.readthedocs.io/

https://jintrac-mirror.pages.eufus.psnc.pl/docs/wiki/JINTRAC_IMAS_External_Models.html

See Francis Casson's slides Thursday 1330 (parallel session 2)

MOOSE Ecosystem - Blanket Example



Water water everywhere....

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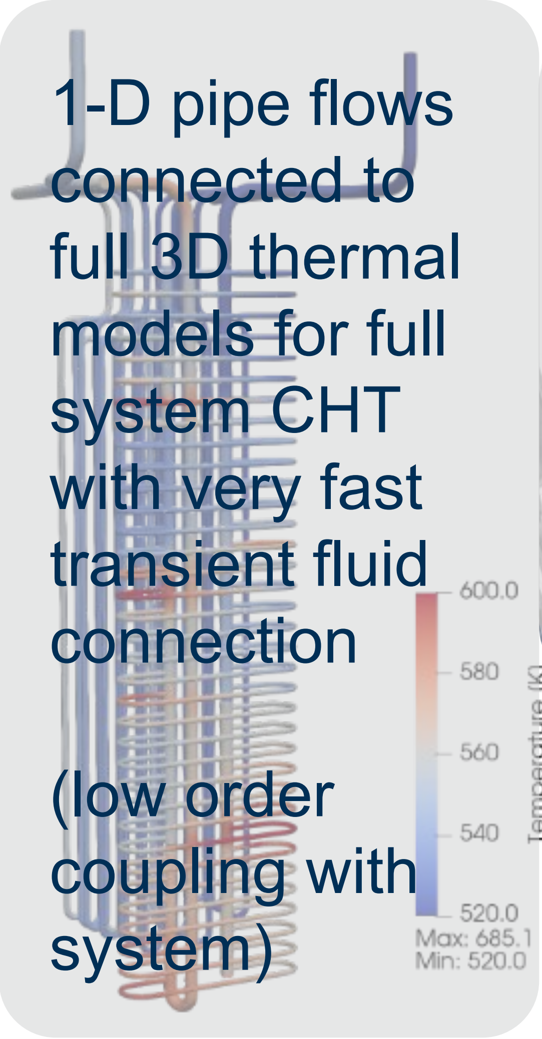
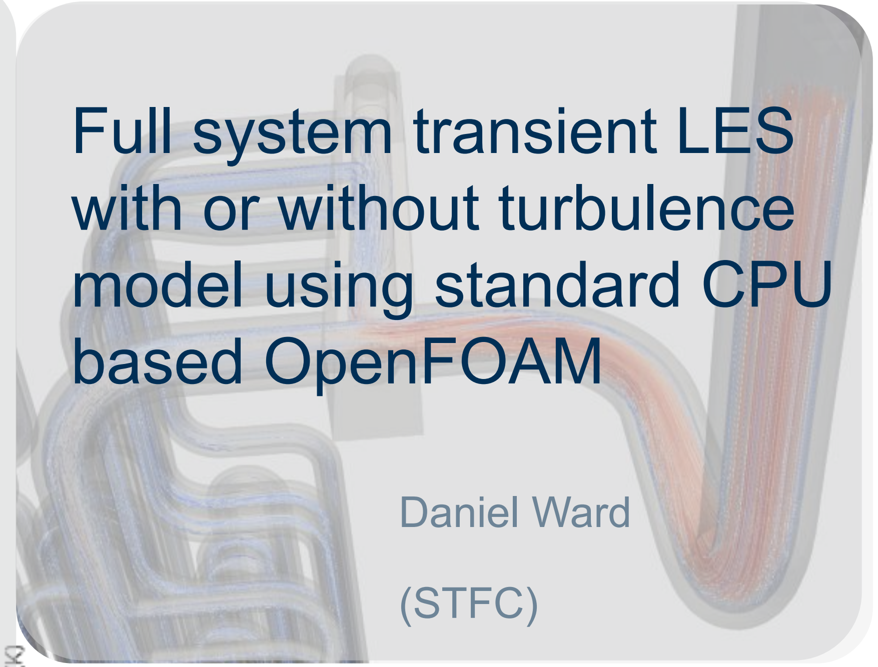


1-D pipe flows connected to full 3D thermal models for full system CHT with very fast transient fluid connection

(low order coupling with system)

Josh Williams (STFC)

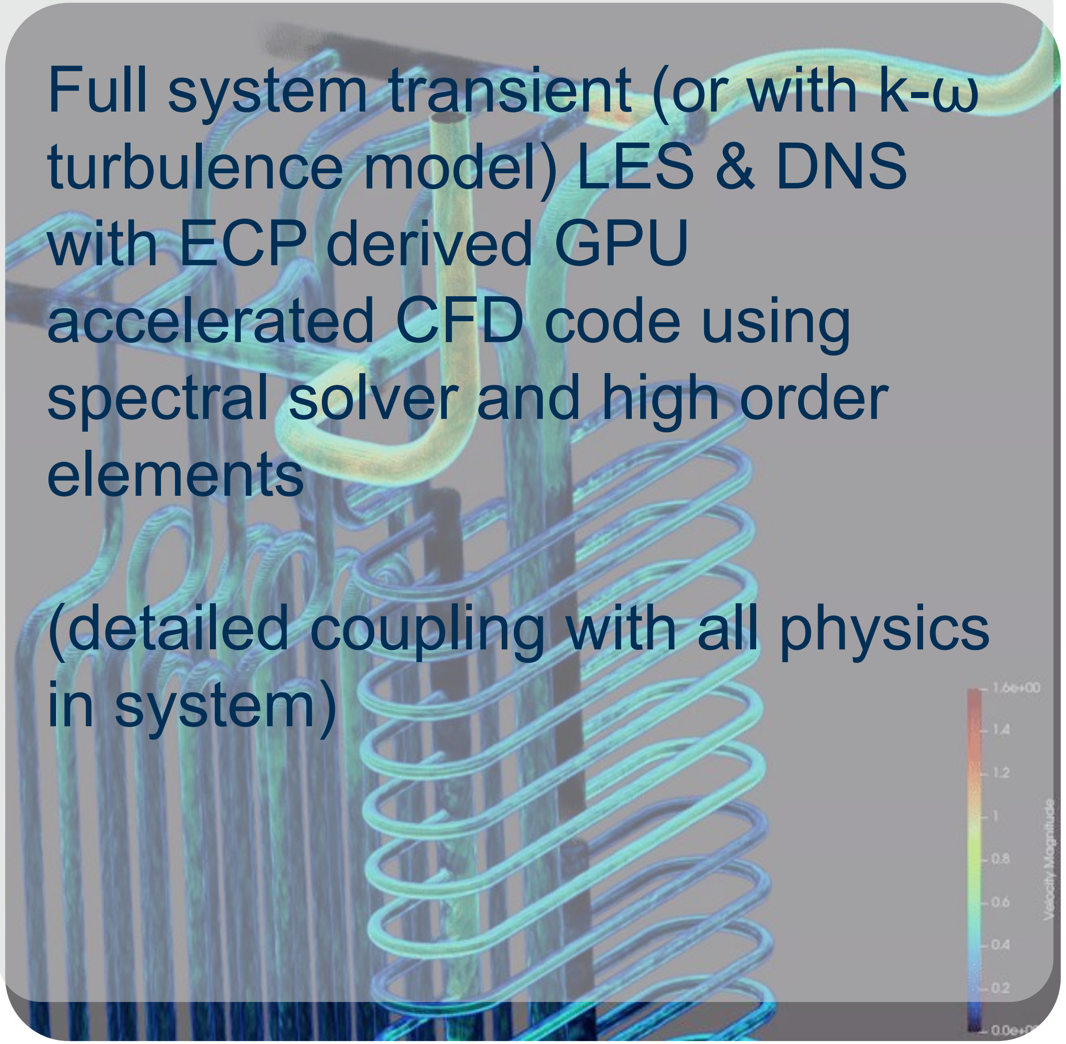


Full system transient LES with or without turbulence model using standard CPU based OpenFOAM

Daniel Ward

(STFC)

Use the high fidelity DNS to stress test turbulence models, to figure out when approximations and LO methods work - tricky with multiphase problems



Full system transient (or with k-ω turbulence model) LES & DNS with ECP derived GPU accelerated CFD code using spectral solver and high order elements

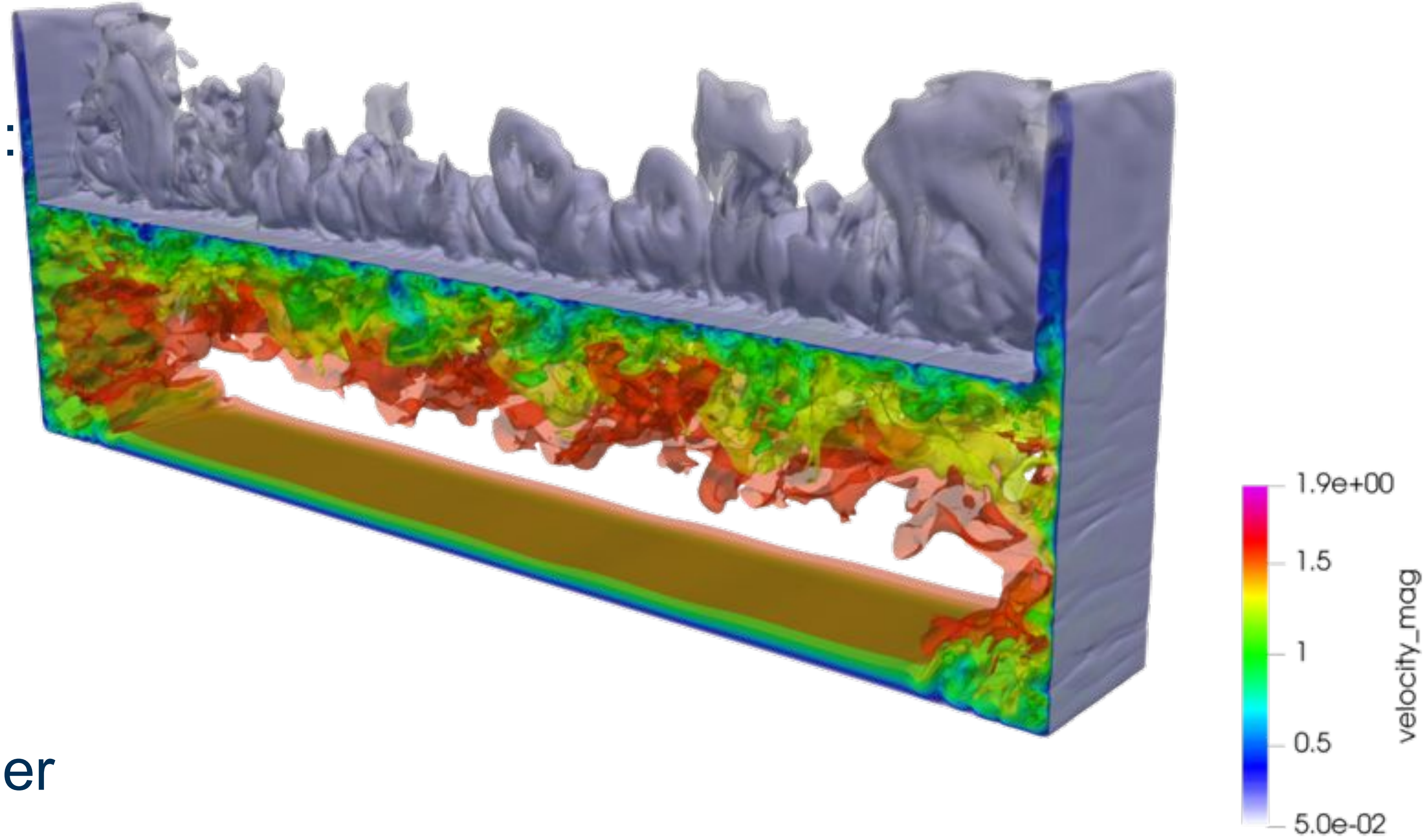
(detailed coupling with all physics in system)

Minchin Li (ANL), Paul Fischer (ANL), Elia Merzari (Penn State), Rupert Eardley-Brunt (UKAEA), Aleks Dubas (UKAEA)

Heat Transfer in Highly Turbulent Fluid Regimes

NekRS on a fusion CFD use case:
- JET Mk1 HypervapotronFluid only, isothermal
- 1 repeating unit with periodic BCs
- Re=10,000
- 43M gridpoints

Future extensions:
- >1 repeating unit.
- Higher Reynolds number, higher resolution.
- Multiphase + boiling (requires NekRS developments)

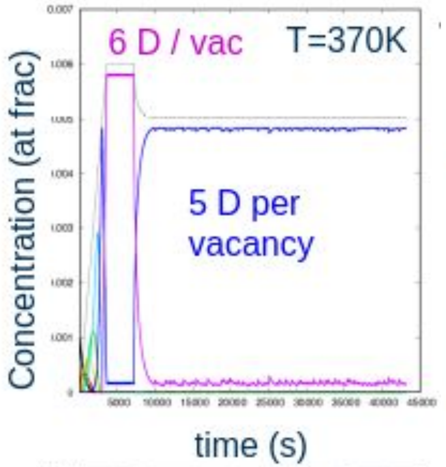


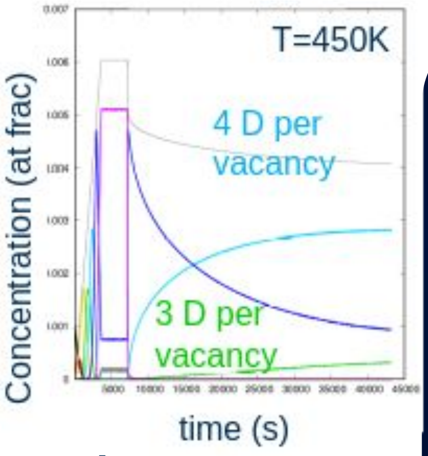
System	GPU	Nodes	Ranks per node	DOFs/rank	Time per timestep [s]
CSD3 Ampere	Nvidia A100	4	4	2.67 M	0.066
Dawn*	Intel PVC	1	8	5.37M	0.203

** Currently investigating multi-node NekRS on Dawn.*

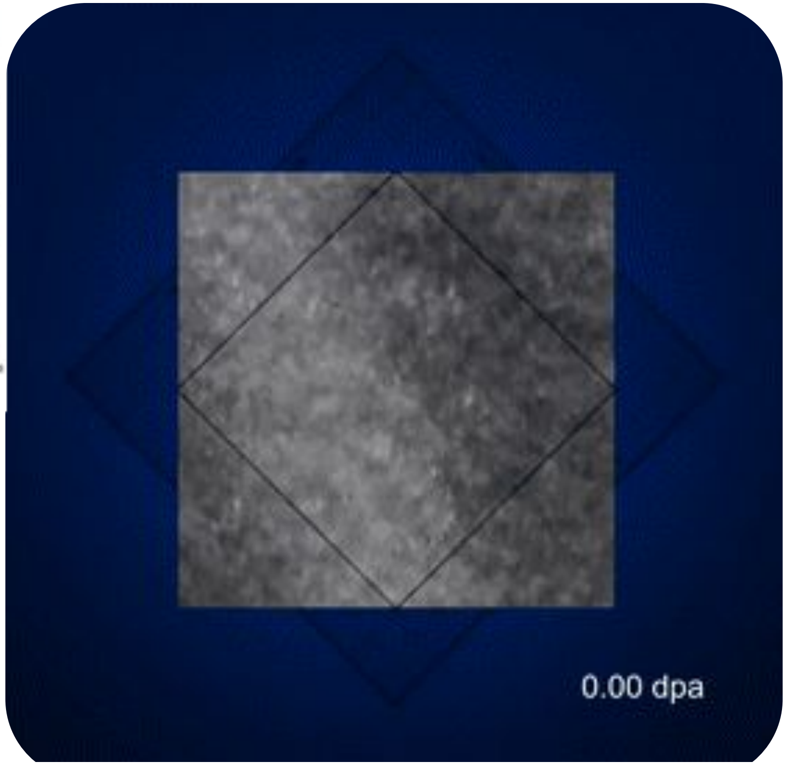
Overlapping cascade simulations

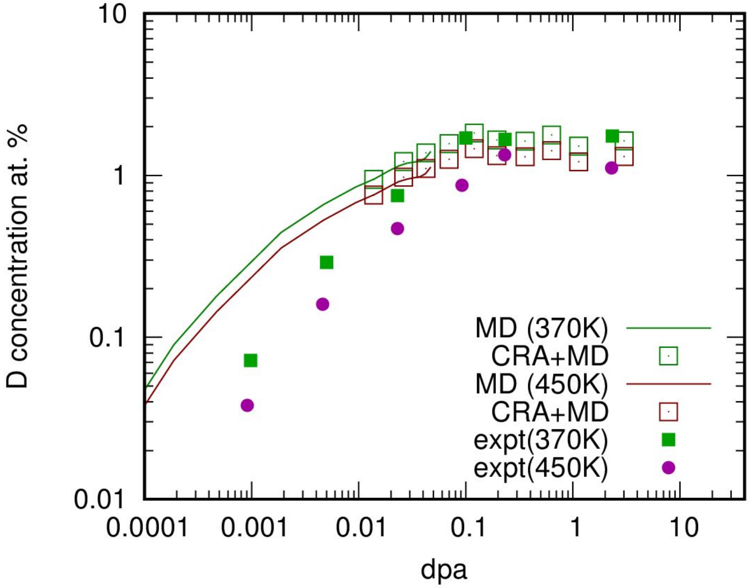
- Previously work considered massively overlapping cascade simulations
- Complex microstructure of network dislocations and monovacancies develops at 0.1 dpa
- Find the voids, and long-lived transient number of D atoms per vacancy





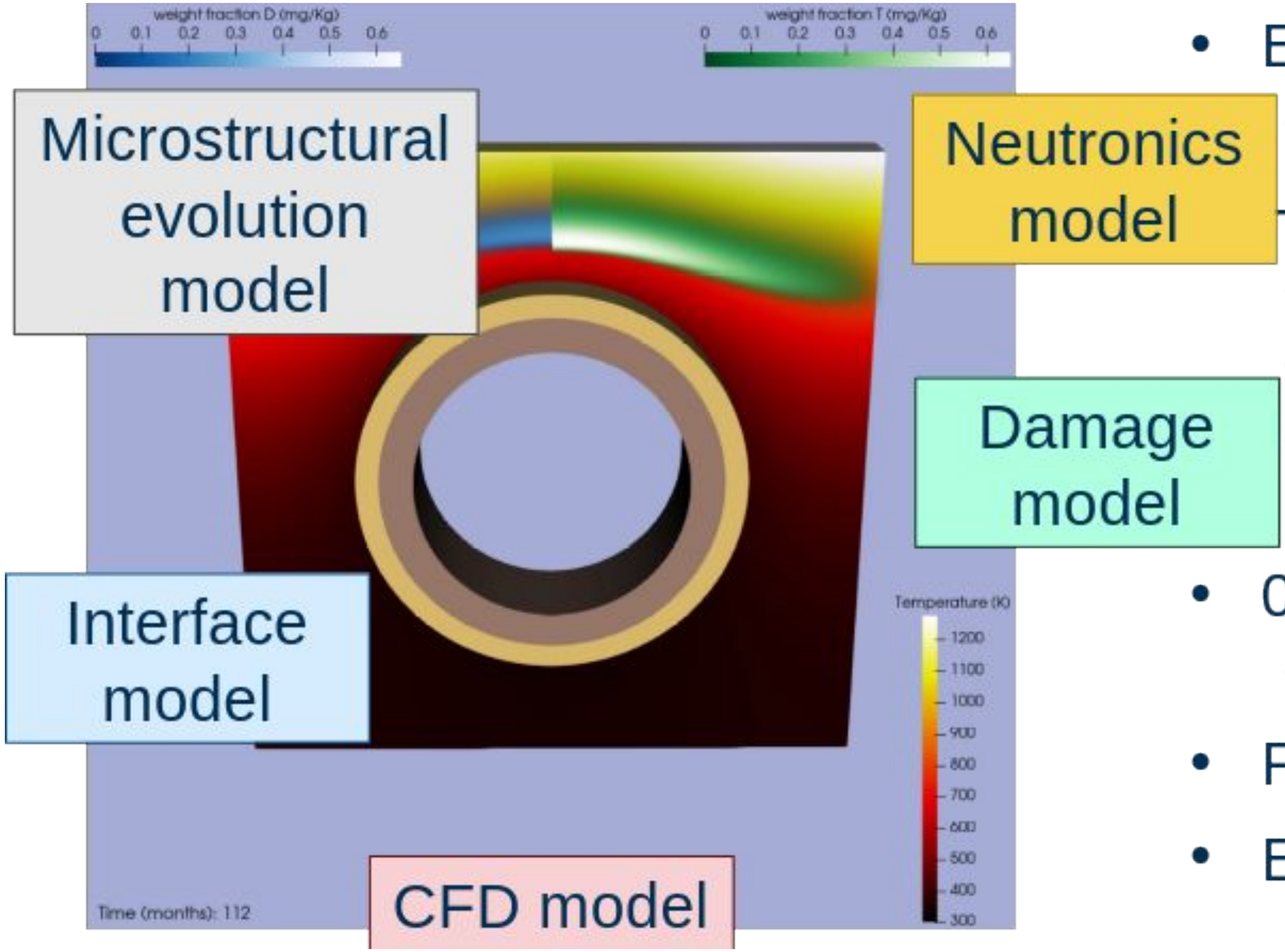
- Single crystal pure W 20 M atoms
- 6×10^5 10 keV cascades
- Low temperature
- Simulated TEM g=[200],ng=4
- + von Mises stress





- Predict D retention in the microstructure
- Experimental D retention results from Thomas Schwarz-Selinger

3d Monoblock multi-isotope multi occupancy test calculation



- Equal plasma flux of D, T at surface
  - 10^{19} ions/m^2/s
- Heat load
  - top surface 8 MW/m^2
  - W, Cu-Cr-Zr, Cu layers
  - Inside pipe convective cooling bc 10^5 W/m^2/K to water at 320K.
- 0.1 at % Heinola monovacancies
  - static & homogeneous (ie unrealistic)
- Final frame 10 years exposure
- End point < 1 gas atom per vacancy

D.R. Mason, S. Dixon, D. Nguyen-Manh et al.

Making Best Use of our facilities

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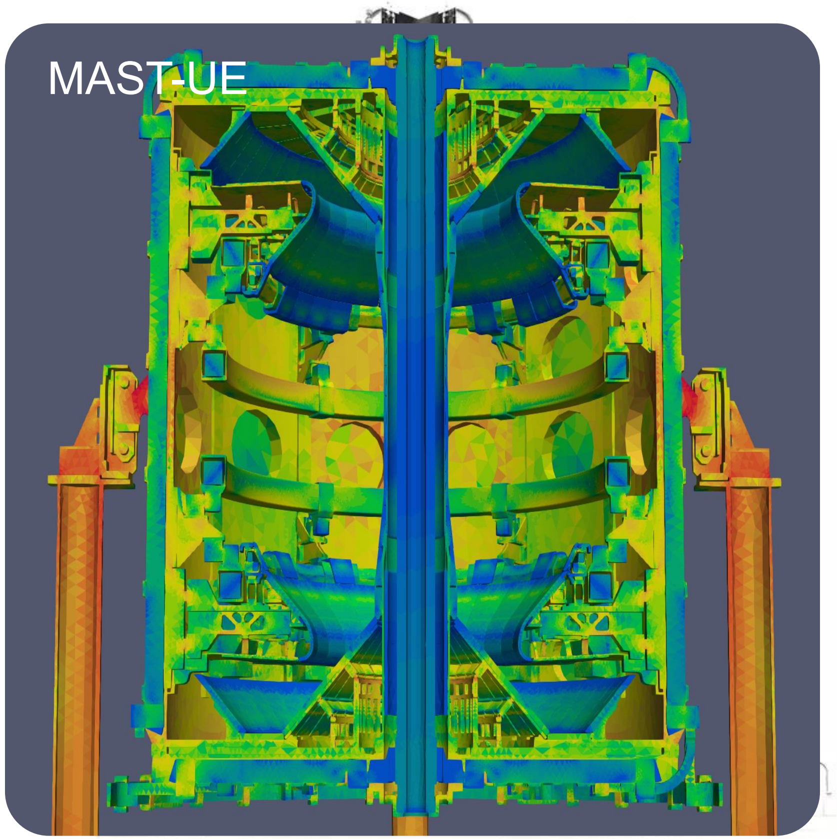
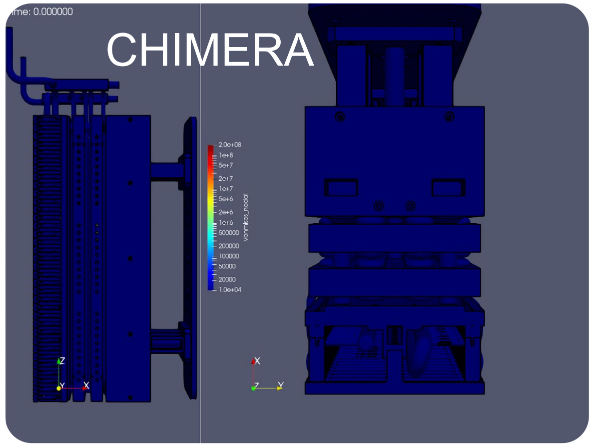
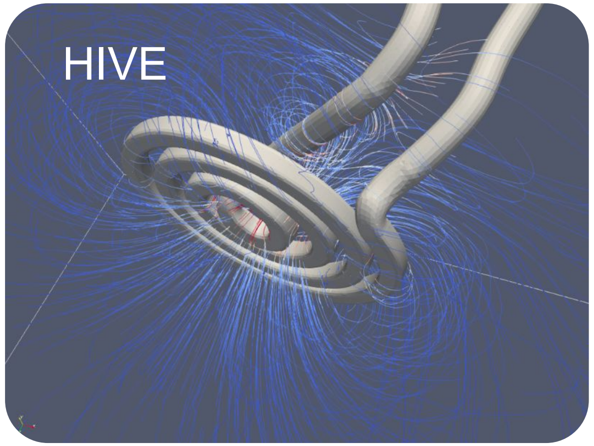
- Given the paucity of experiments that can validate fusion simulation, we must look to other domains and apply **similitude**
- Change in mindset - how can experient validate simulation?
- Need to consider doublet (or triplet) effect facilities
  - Thermal Hydraulics
  - Magnetic Test Facilities
- Need to look at actively cooled nuclear driven combined effect facilities;
  - Advanced Nuclear
  - Spallation Neutron Sources
  - Fission reactors

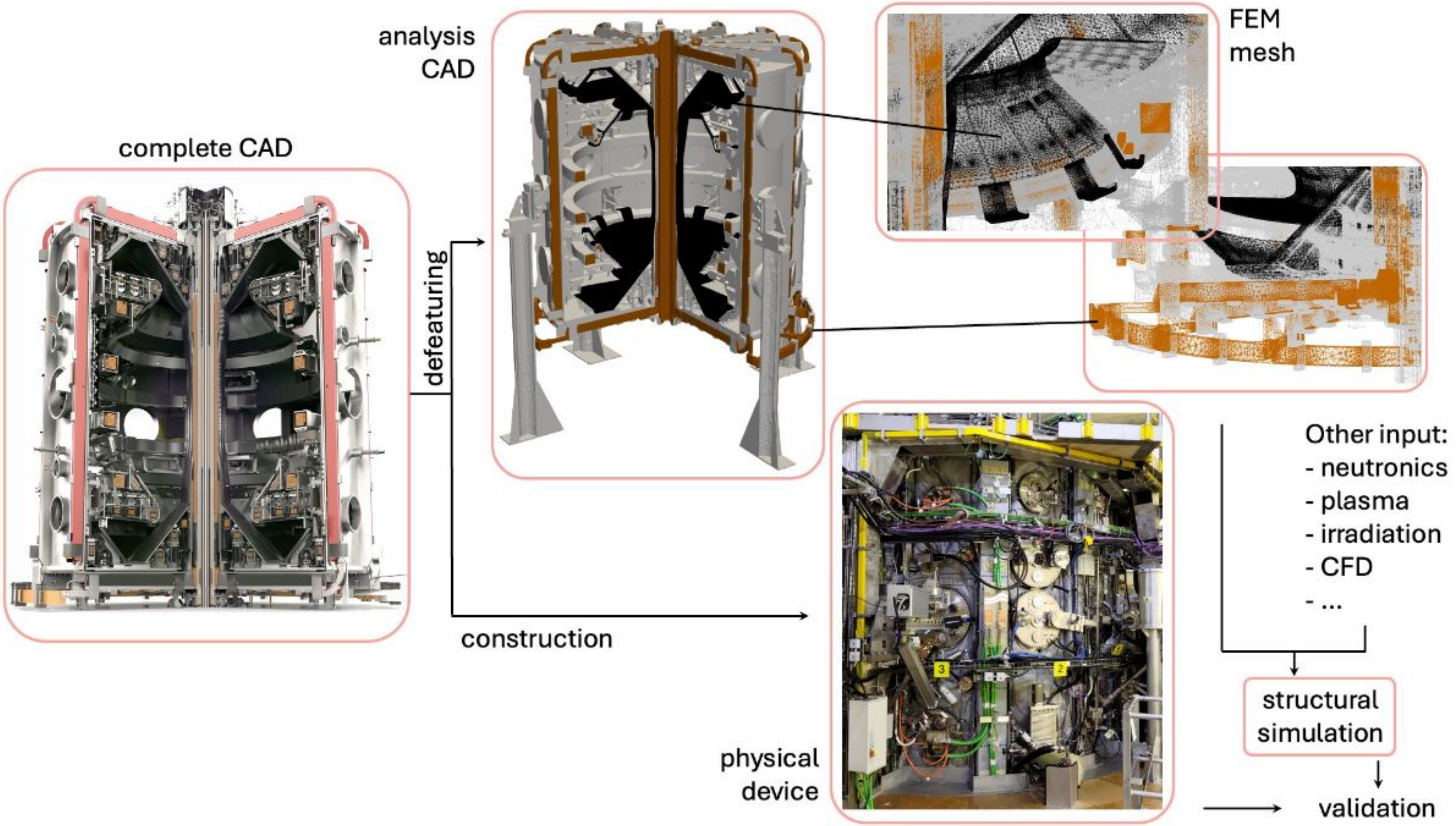






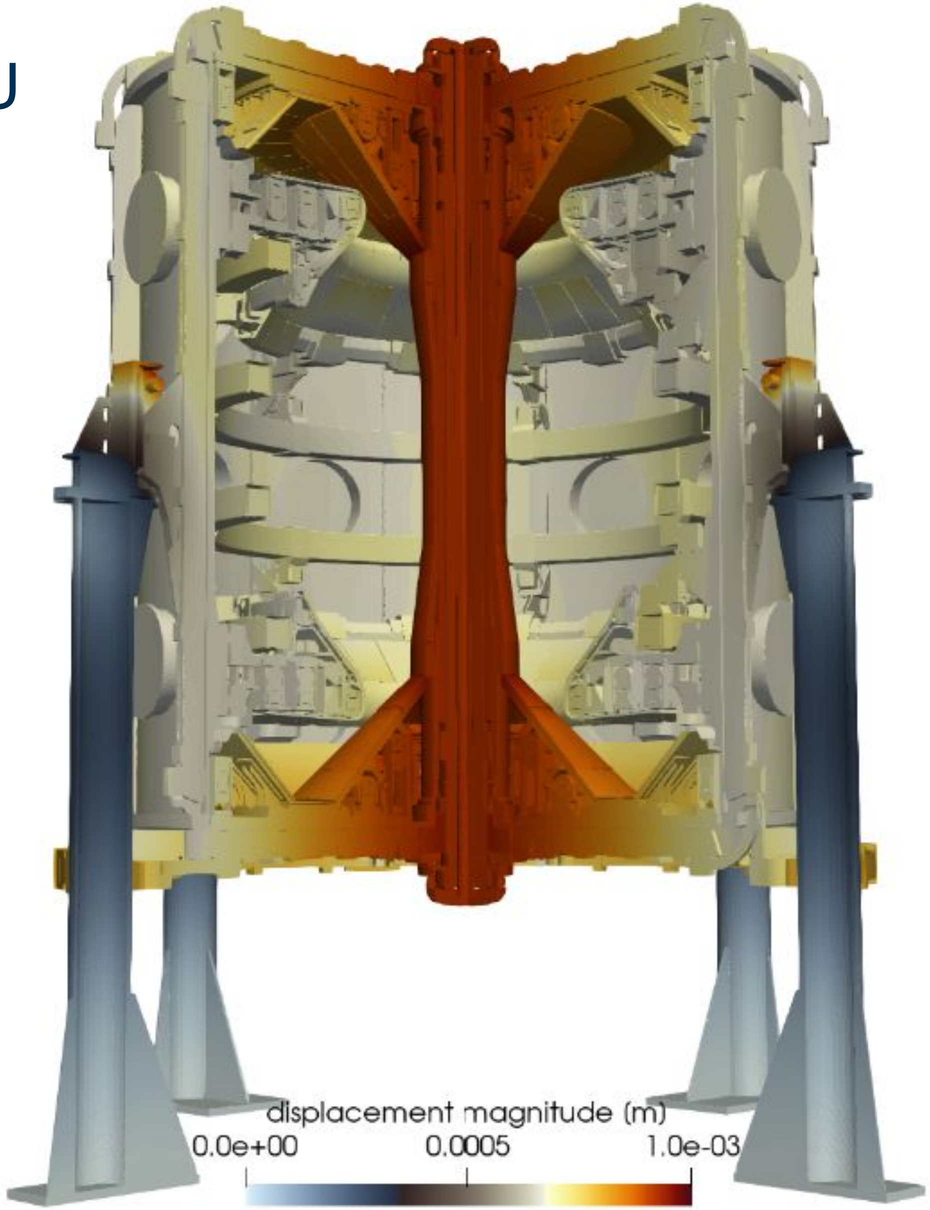
Extensive use of physically holistic digital twins to investigate emergent properties and behaviours of multiphysics systems

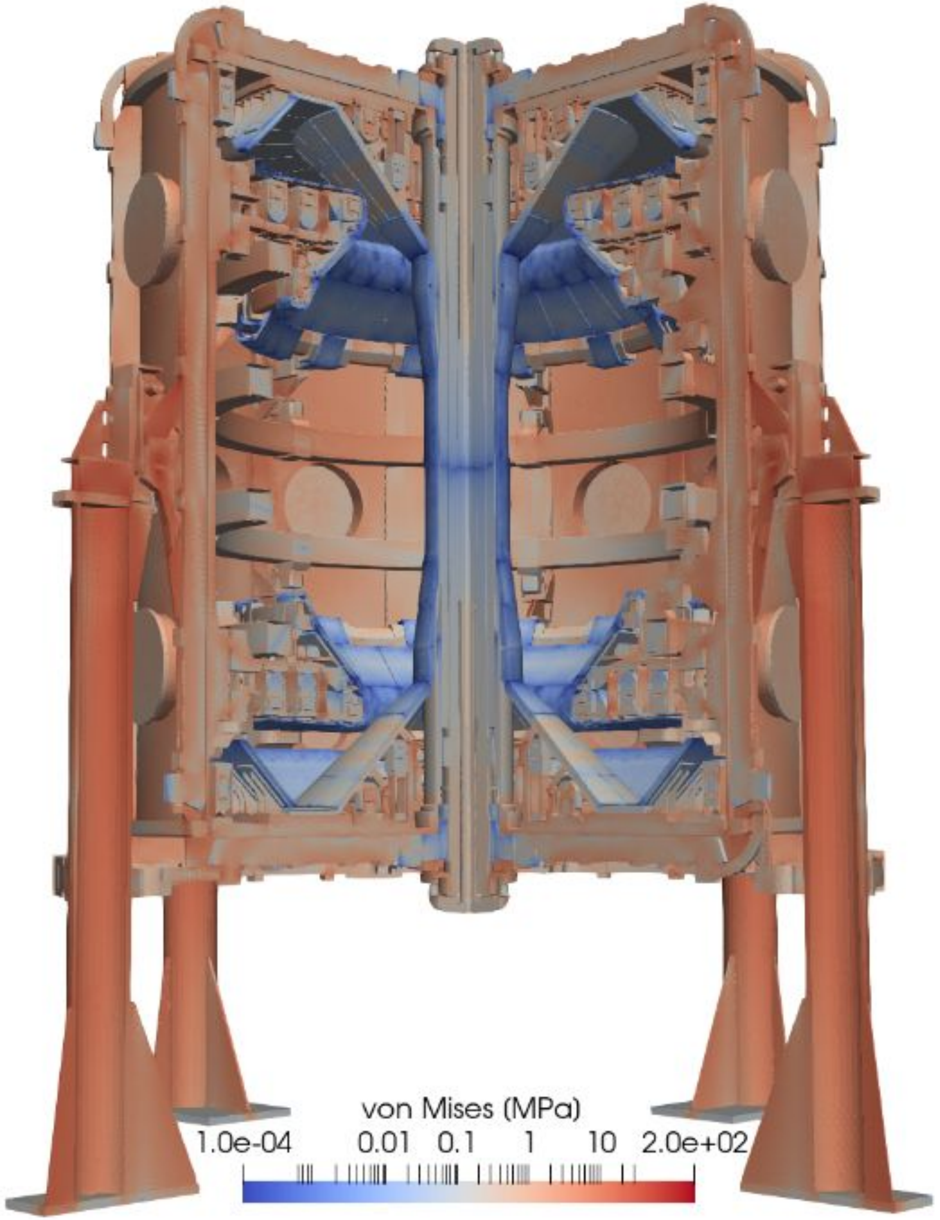
MAST-U Virtual Tokamak



MAST-U Virtual Tokamak

- Full resolution model of MAST-U
- 160M 1st order element tetrahedral mesh
- On 336 cores took 58 minutes (not optimised)
- Can be used to determine the gravitational loading and displacements
- Agrees well with reality





MAST-U Virtual Tokamak

https://arxiv.org/pdf/2409.13554

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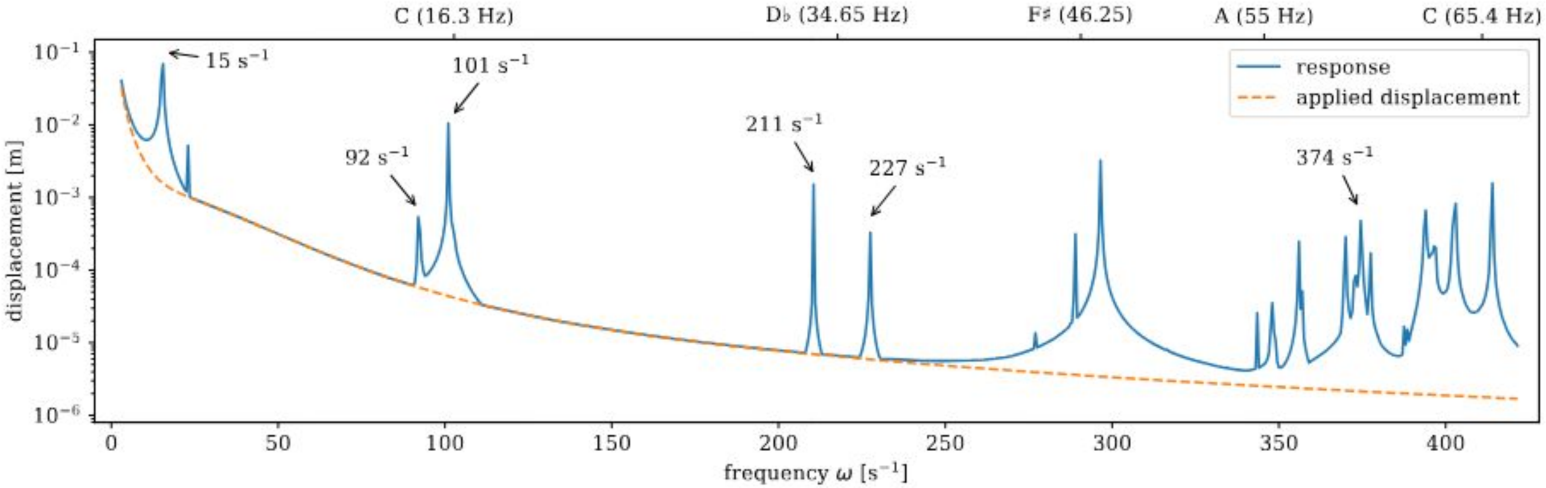
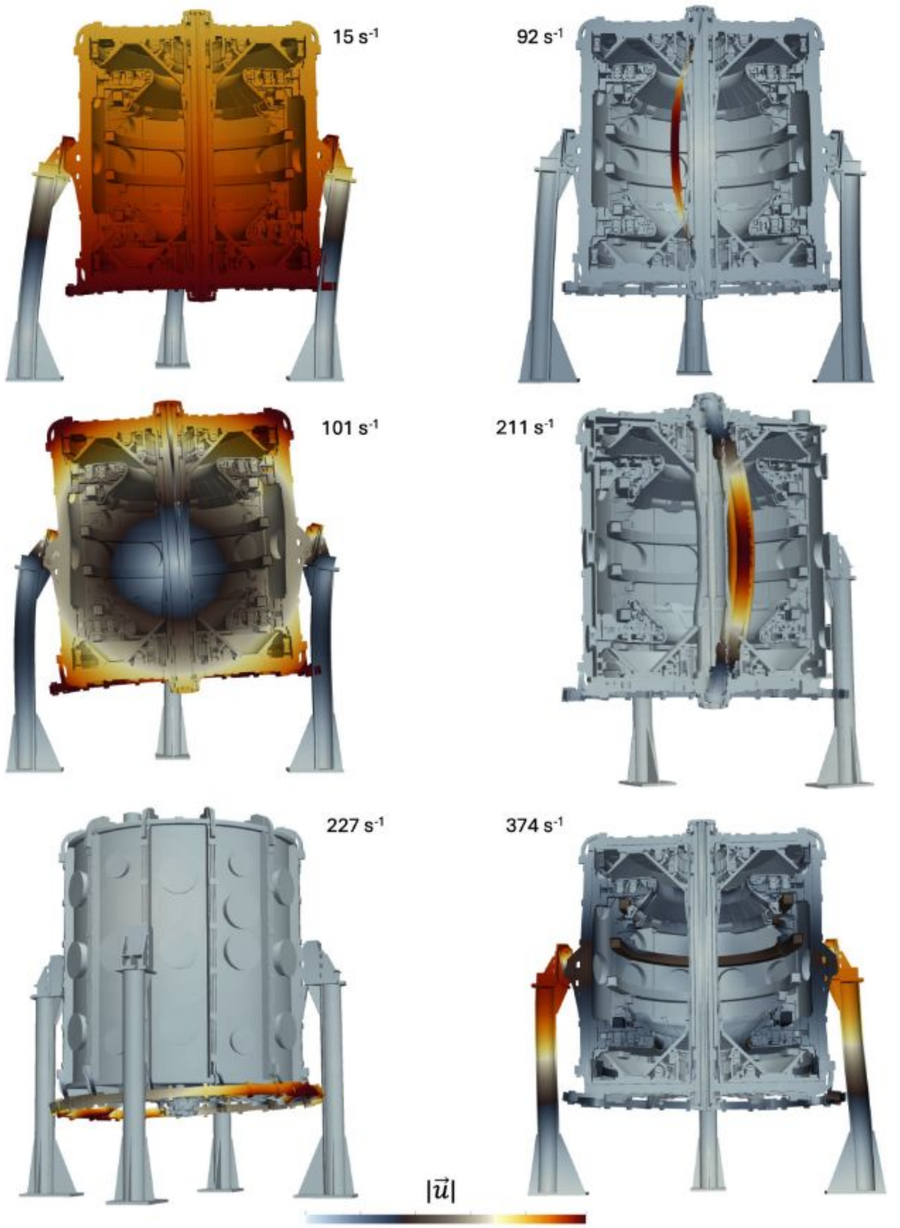
- Performing a simulation of the modes of vibration of the MAST-U load assembly
  - First time done at scale
  - First time done with the asymmetric model
- Some interesting results!

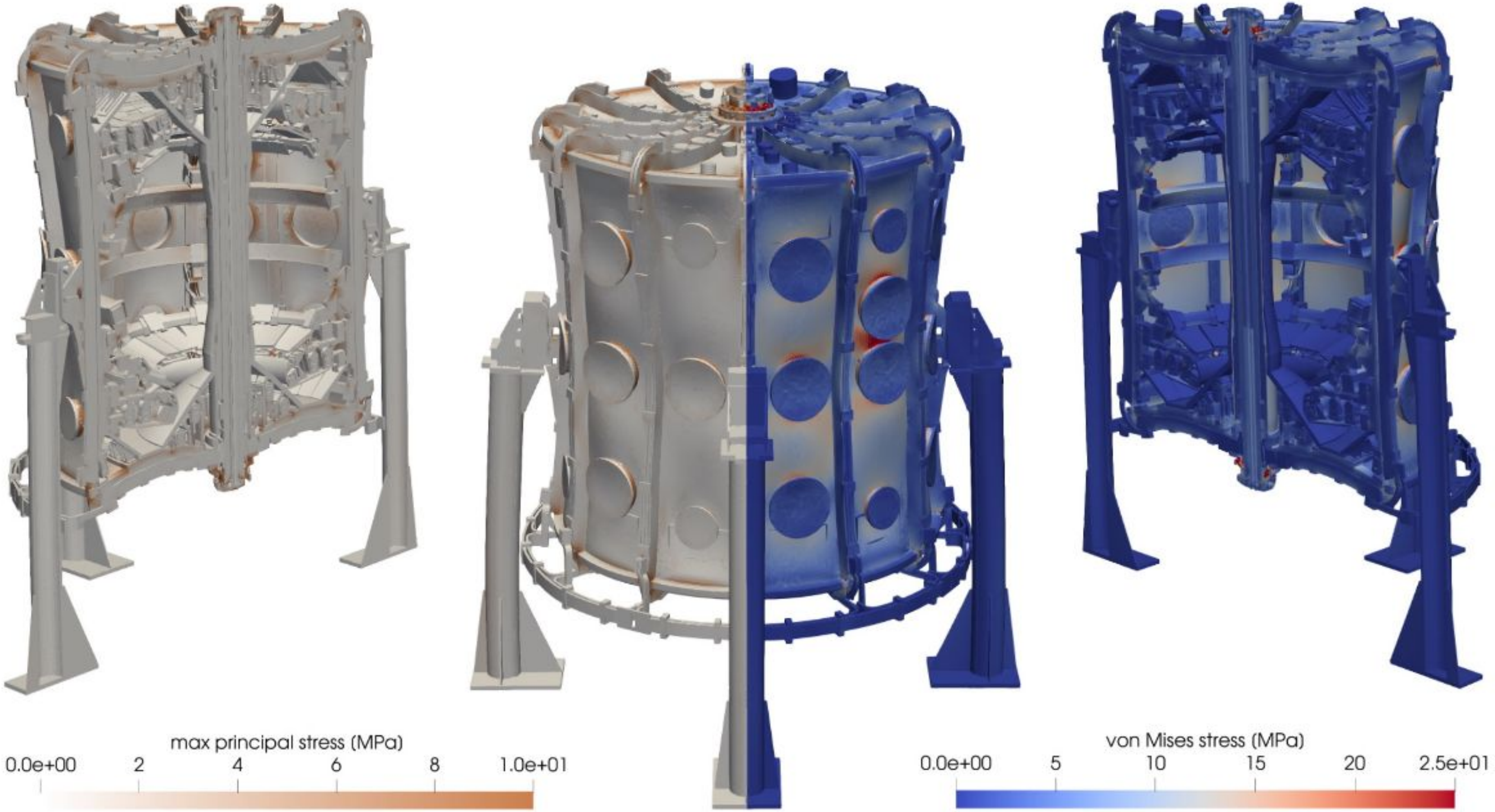
Mechanical Model for a Full Fusion Tokamak Enabled by Supercomputing

W. M. E. Ellis,* L. Reali,† A. Davis,‡ H. M. Brooks,§ I. Katramados,¶ A. J. Thornton,** R. A. Akers,†† and S. L. Dudarev‡‡
UK Atomic Energy Authority, Culham Campus, Oxfordshire OX14 3DB, UK





MAST-U Virtual Tokamak



One mesh (sort of) to rule them all

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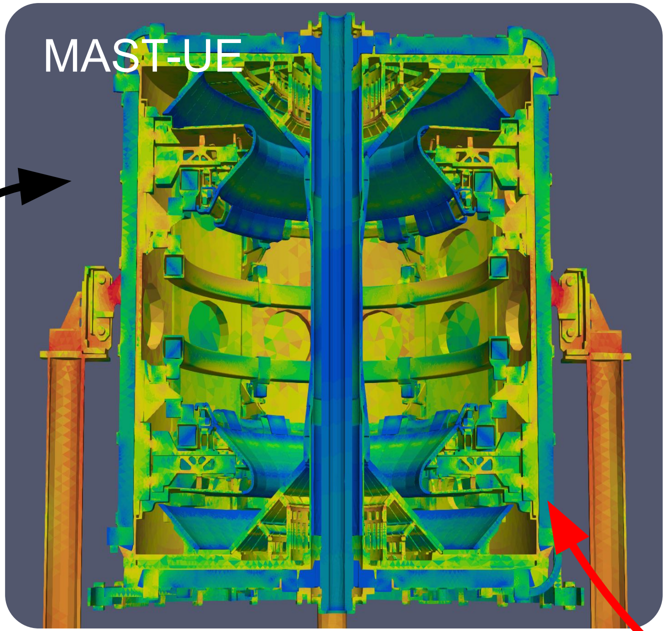
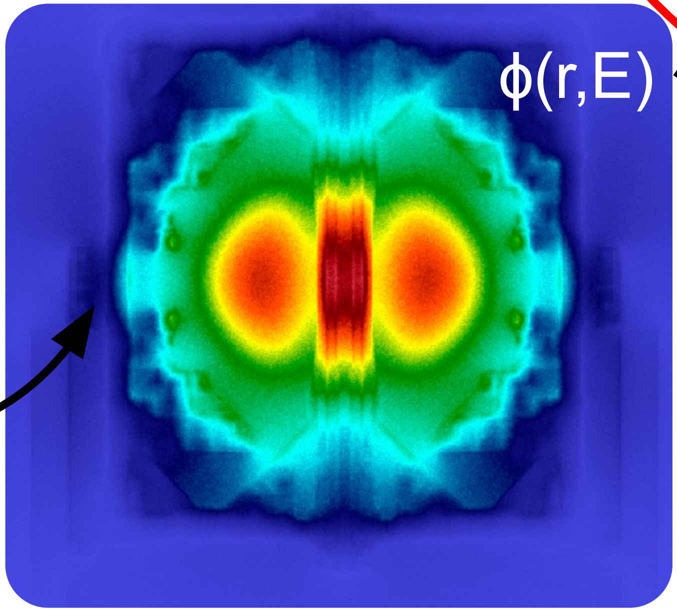
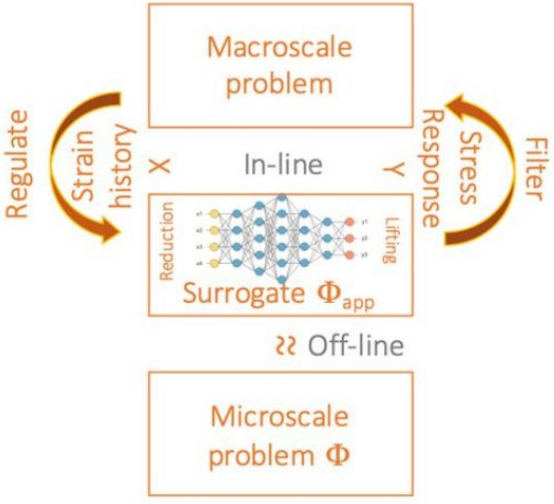
- When doing coupled analysis there are error terms related to;
  - body force terms (e.g. heat sources)
  - surface loads
- DIfficult to derive error terms when each physics analysis uses a different mesh
- With one mesh, can simulate all physics on the lowest common denominator mesh
  - Currently down to two meshes
    - ‘FE/FV’ world
    - Surface mesh world







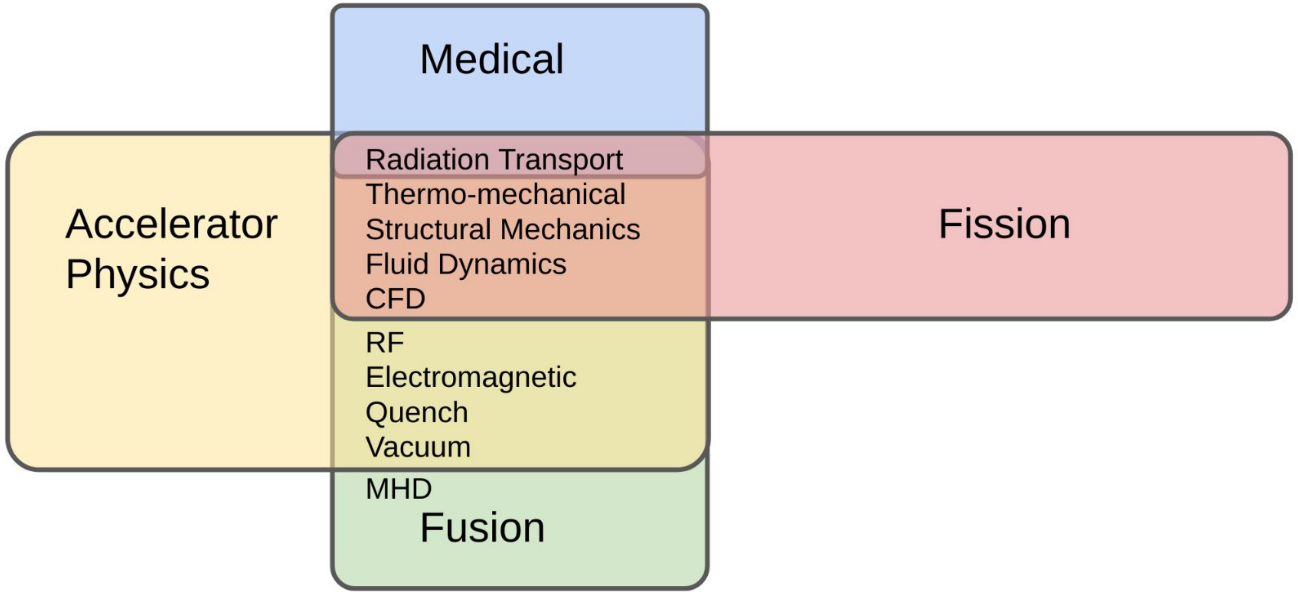
eigenstrains

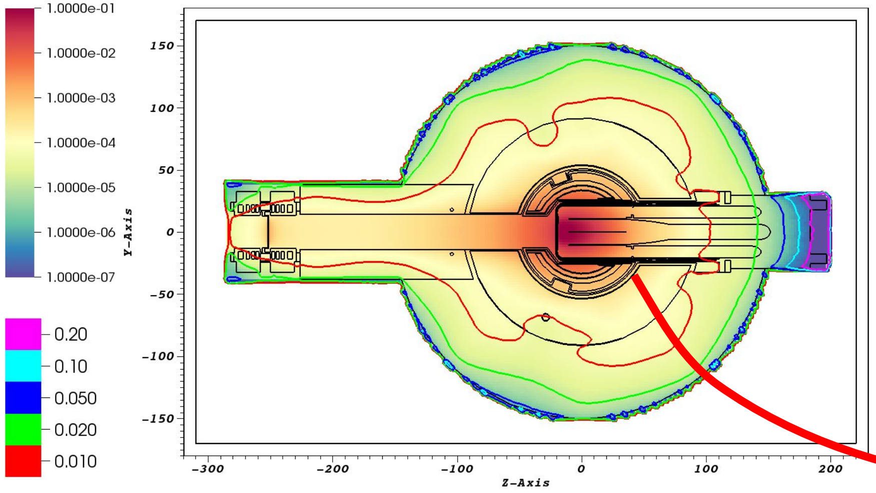
Down to two meshes, can we get it down to one? High order FE meshes could allow one mesh to rule them all

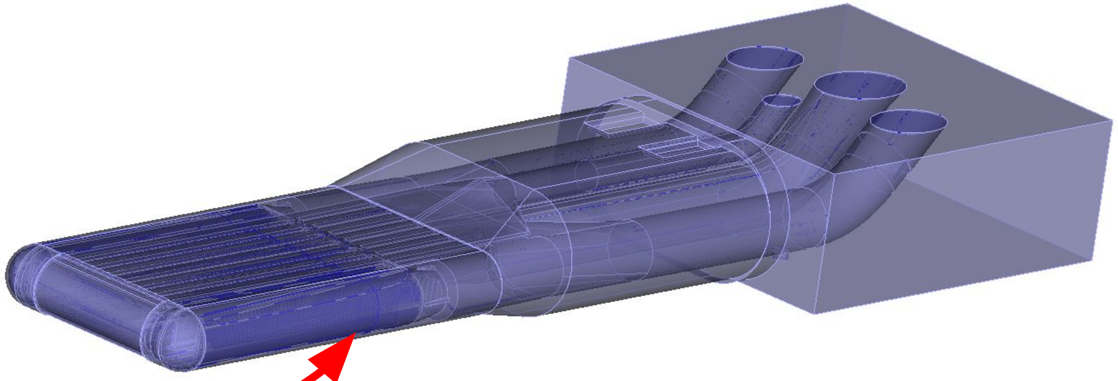
Digital Twins

Would like to deploy nuclear digital twins

- Much of the technology (computing) that we would like to deploy is also relevant beyond fusion to:
  - Small Modular Fission Reactors
  - Advanced Modular Reactors
  - Spallation Neutron Sources
  - High Energy Physics (e.g. beamstops)
- Can do a lot of parallel learning from existent nuclear systems
  - SNS
  - nTOF
-







HIVE

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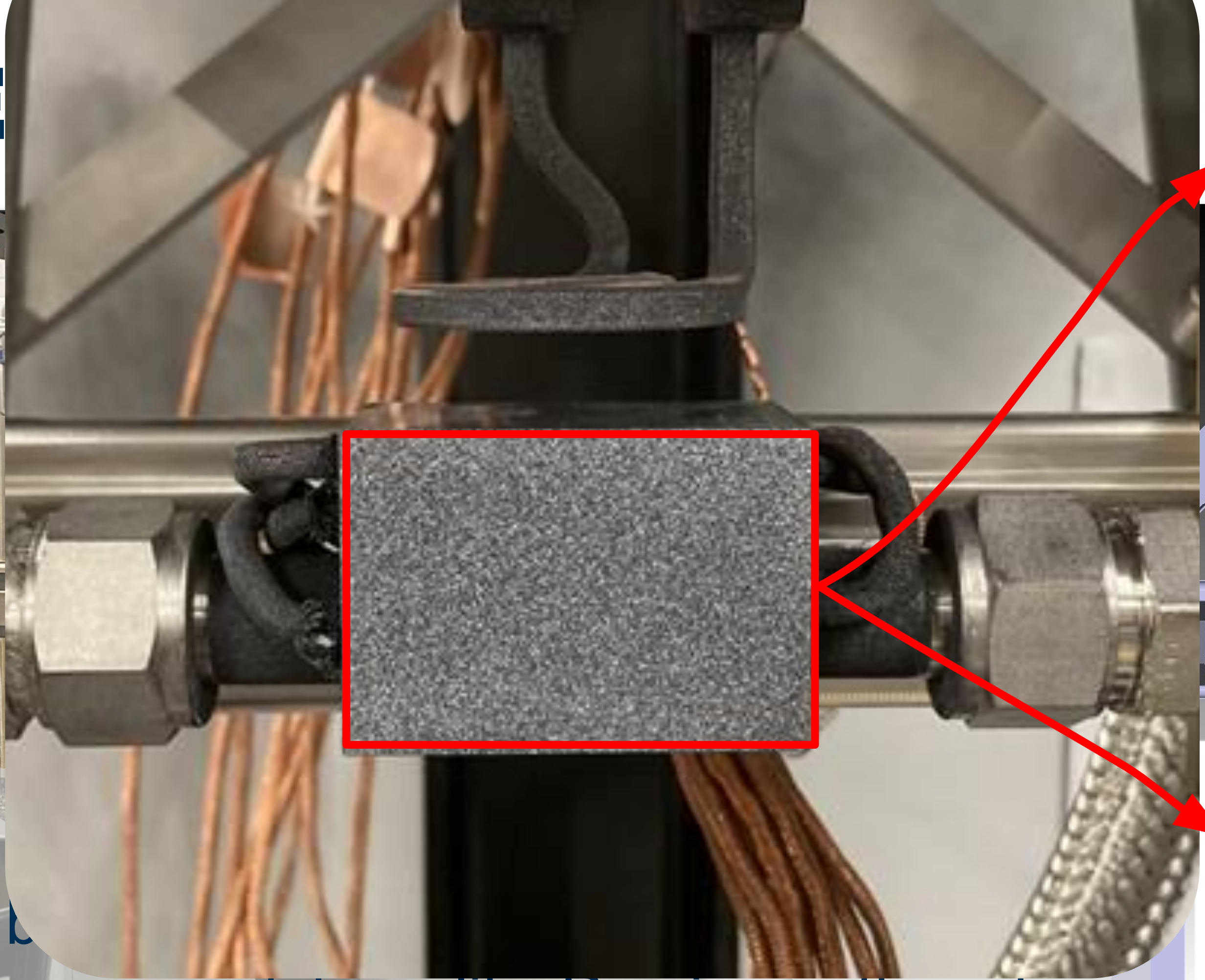

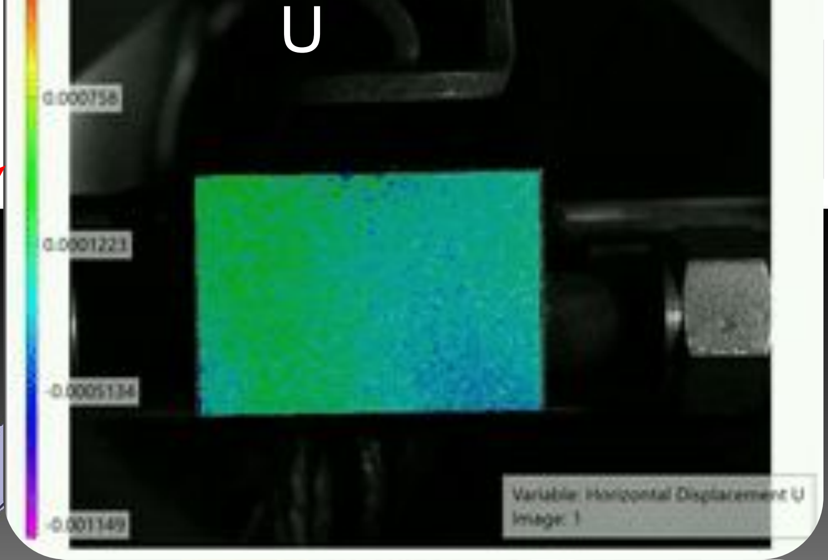

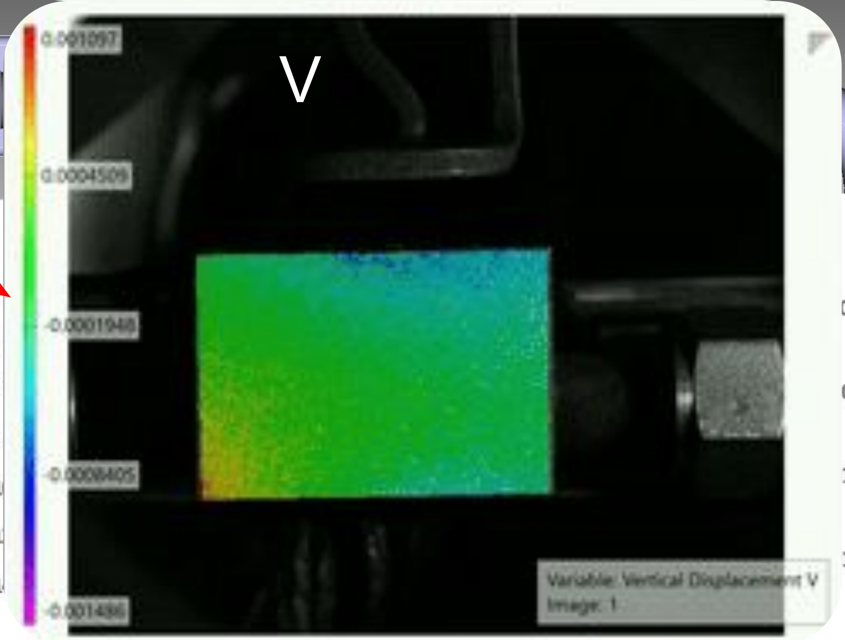

Vertical Displacement

Vertical Displacement

“Back to b
simulation can match reality. Previous attempt have encountered disagreements between simulation & measurement,

CHIMERA Digital (Instance) Shadow

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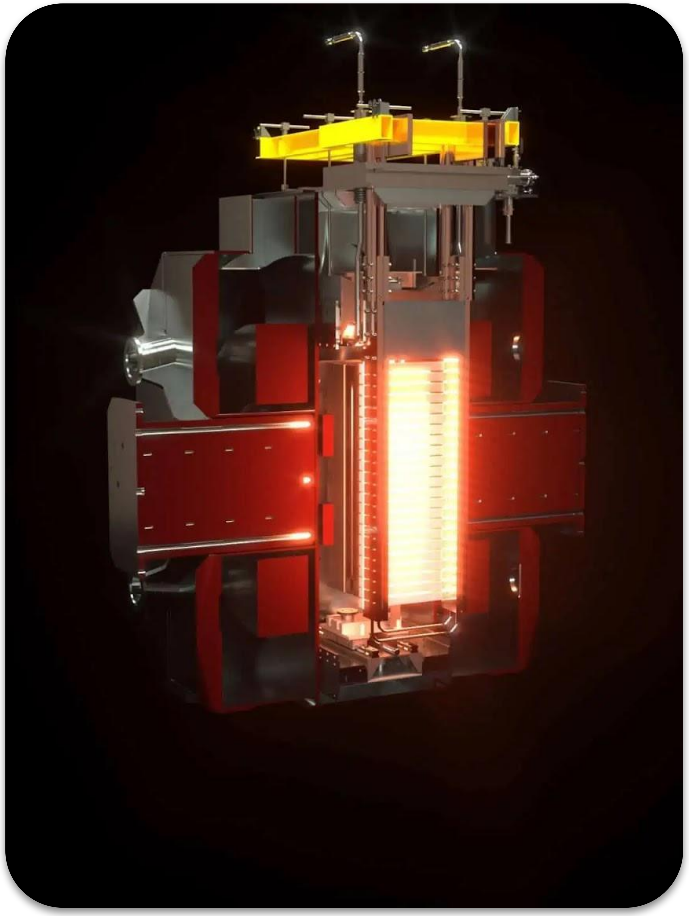
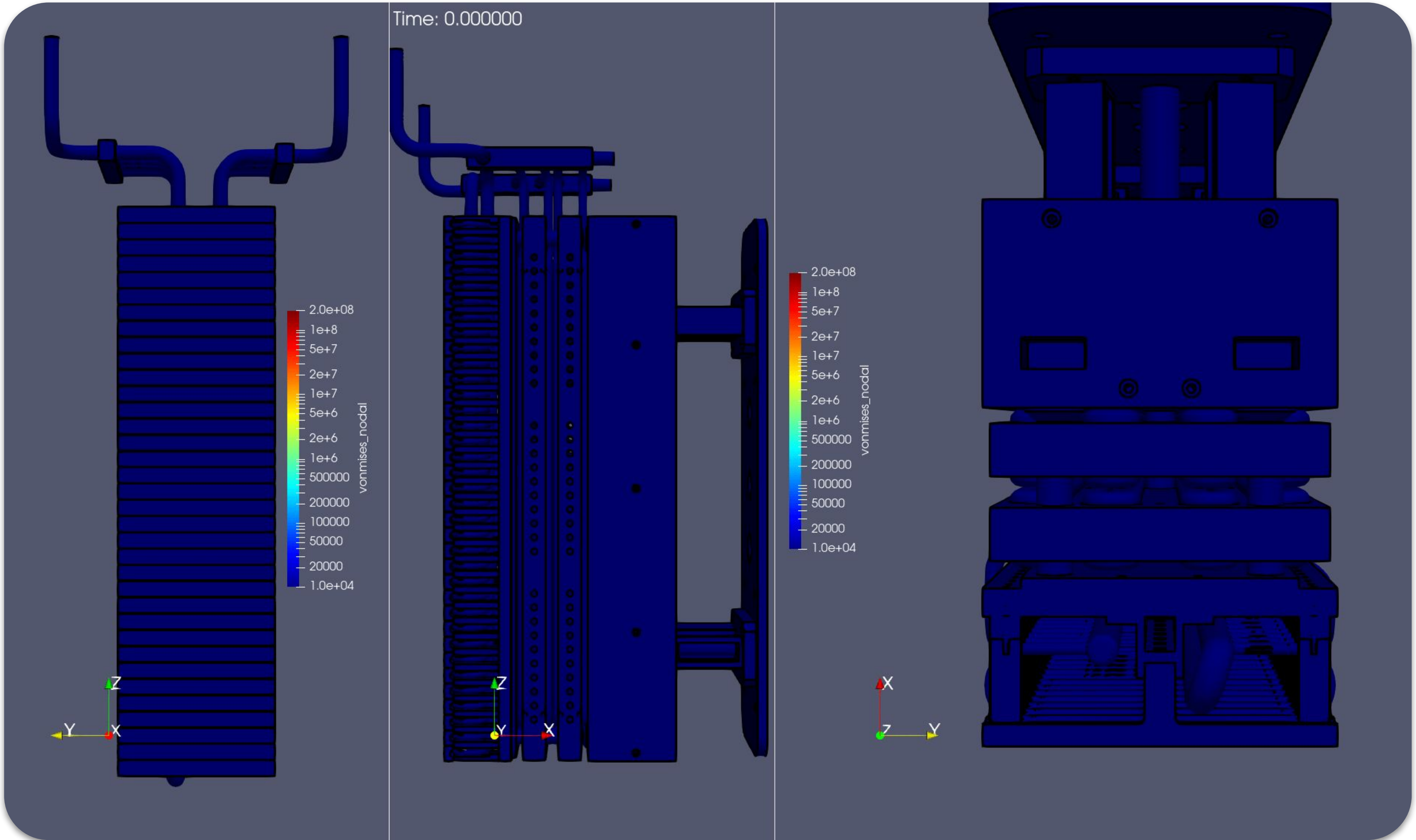
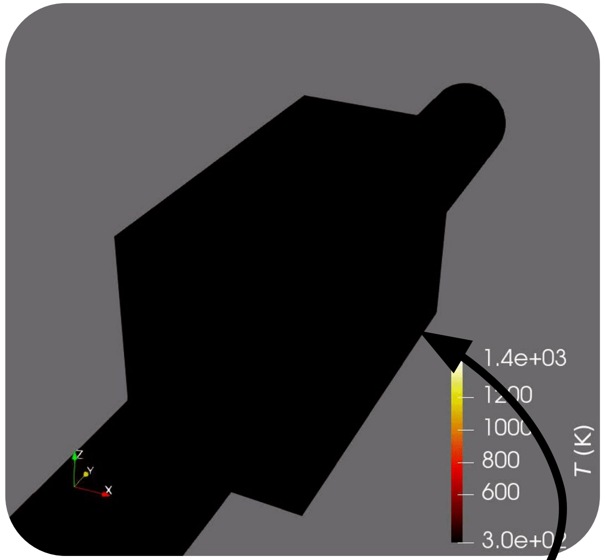
CHIMERA - high heat flux & magnetic (non nuclear) test facility, suite of diagnostics for range of measurements, example of thermal commissioning test unit



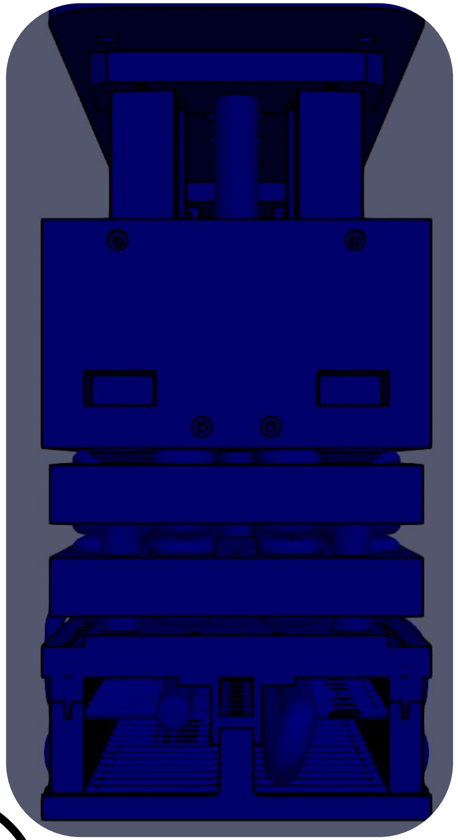


Computation will qualify fusion....

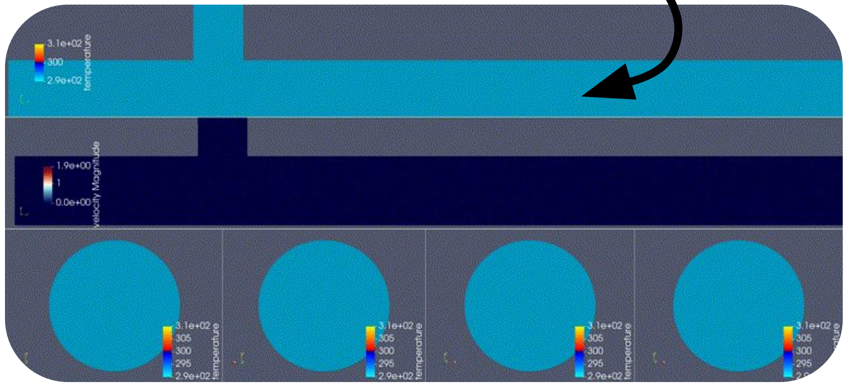
- HPC & Simulation will be a driving force in the delivery of fusion power to the grid
- More benefit can pass to industry by upskilling and uptake of HPC
  - Particularly in the engineering sector can drive unique benefits
  - Human factors dominate the uptake
- Journey is not unique to other sectors
  - advancements already being made in aerospace, advanced nuclear
  - advancements made in fusion can spill over into other domains
- Digital twins will be central to validating understanding
- We will use computation as the 3rd mode of discovery



Induction heating



Turbulent mixing



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Open Source Manifesto

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- Within the computing division we are committed to open source software
- Choose software that you can….
  - access easily access
  - inspect the workings of
  - models that you look inside of
  - can give to people
  - build upon
- Open science benefits us all we couldn't have made the progress we have in many areas with out it

open source initiative®

https://github.com/ukaea

https://github.com/aurora-multiphysics

https://github.com/openmc-dev/openmc

https://github.com/nek5000/nekrs

https://github.com/neams-th-coe/cardinal
https://github.com/idaholab/moose
https://github.com/mfem/mfem
https://github.com/Fusion-Power-Plant-Framework/bluemira

Thank you for you attention

Questions

I look forward to the rest of the meeting

andrew.davis@ukaea.uk

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COMPUTING DIVISION