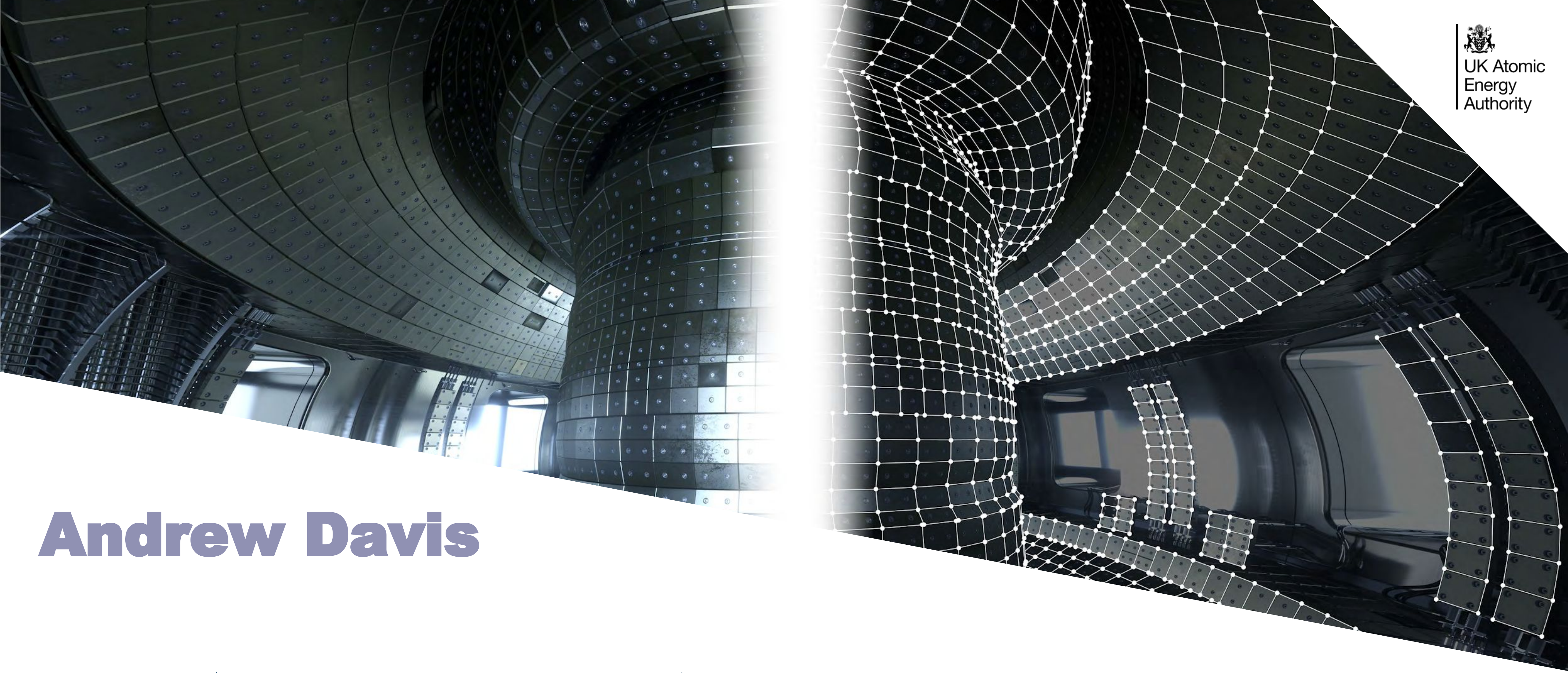
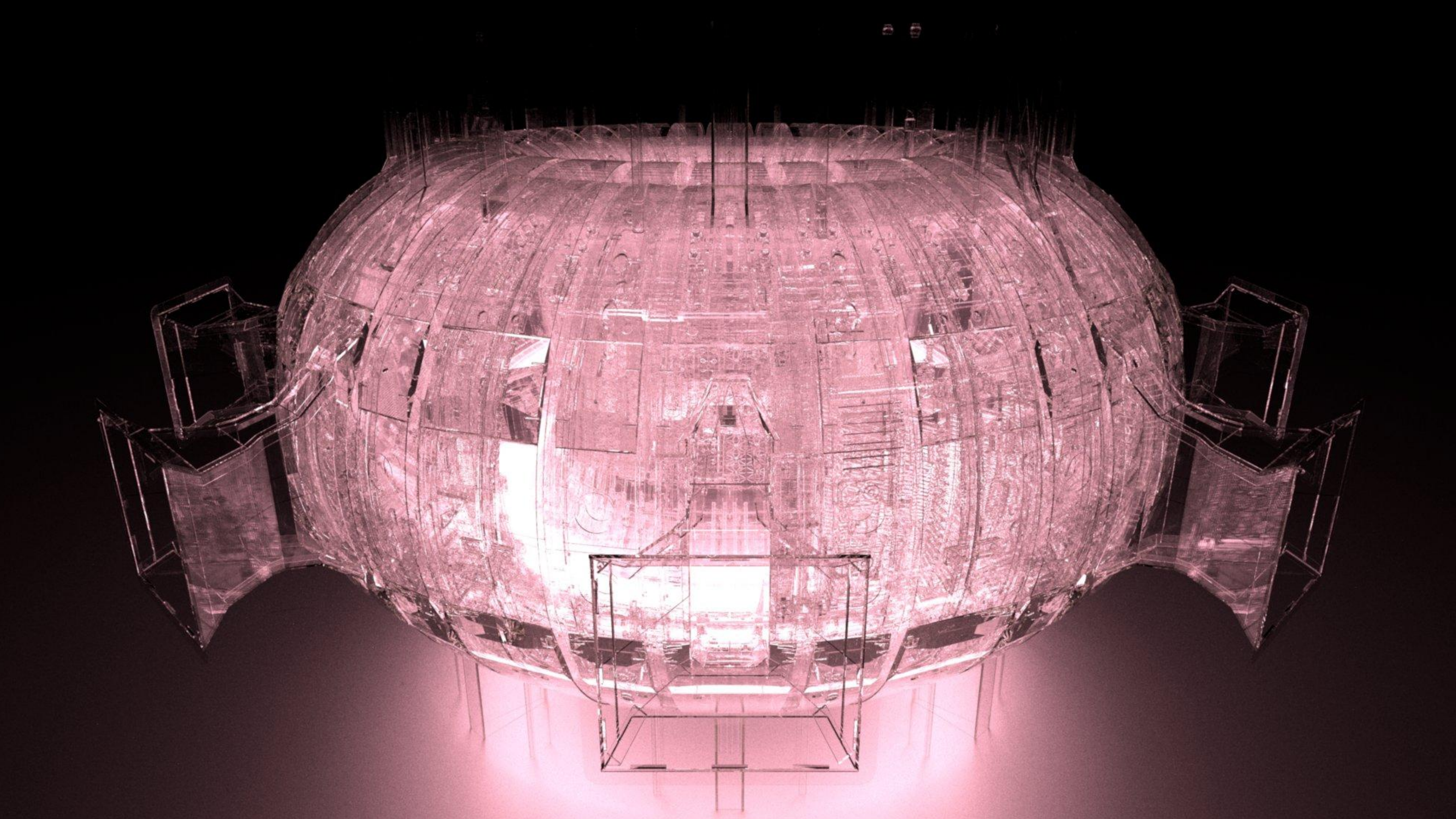


UK Atomic Energy Authority

Andrew Davis

Multiphysics at UKAEA

2020 Modelling in Nuclear Science and Engineering - 4-5th November 2020 - Bangor



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Aleks Dubas
Helen Brooks
Arun Balasubramanian
Julita Inca
Matthew Mavis

Thanks!

UKAEA History

UK Atomic Energy Authority

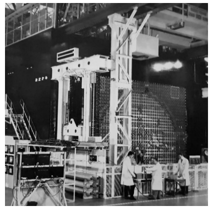
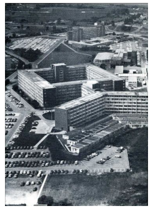
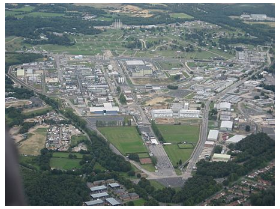
The UK Atomic Energy Authority was formed in 1954 when the British Government set up a new body to oversee the nation's nuclear research programme. The role was to provide Britain's atomic weapons deterrent and develop reactor technologies for the nuclear power stations of the future.

1954	1971	1973	1995	2004	2009
Atomic Energy Authority Act	**Atomic Energy Authority Act**	**Atomic Energy Authority (Weapons)Act**	**Atomic Energy Authority Act**	**Energy Act**	**Restructuring**
UKAEA established from AWRE & AERE Harwell	BNFL created to look after fuel, Radio Chemical Centre created for isotopes	Weapons functions transferred to AWE	Commercial parts of UKAEA privatised into AEA Technology	NDA Created legacy research sites transferred to NDA, UKAEA Ltd created	Babcock acquires RSRL and DSRL, UKAEA only doing fusion







UKAEA Since 2009

UK Atomic Energy Authority

UK Atomic Energy Authority

CCFE
CULHAM CENTRE FOR FUSION ENERGY

MATERIALS RESEARCH FACILITY

RACE

STEP

CAS

H3AT

Who are UKAEA?

UK Atomic Energy Authority

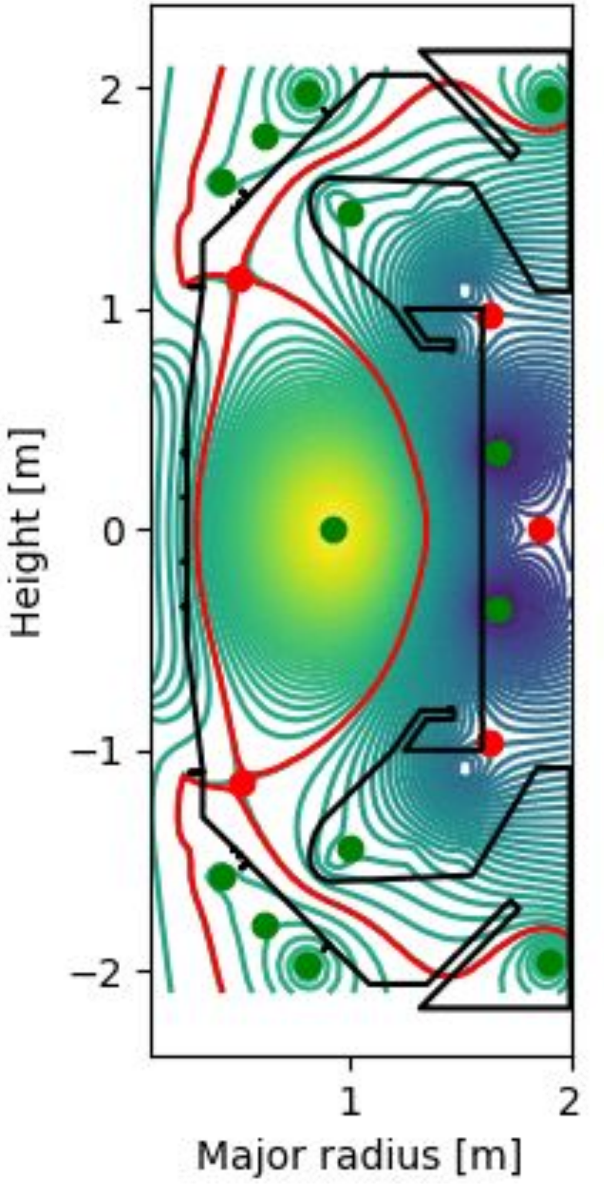
UKAEA's mission is to deliver sustainable fusion energy and maximise scientific and economic impact.

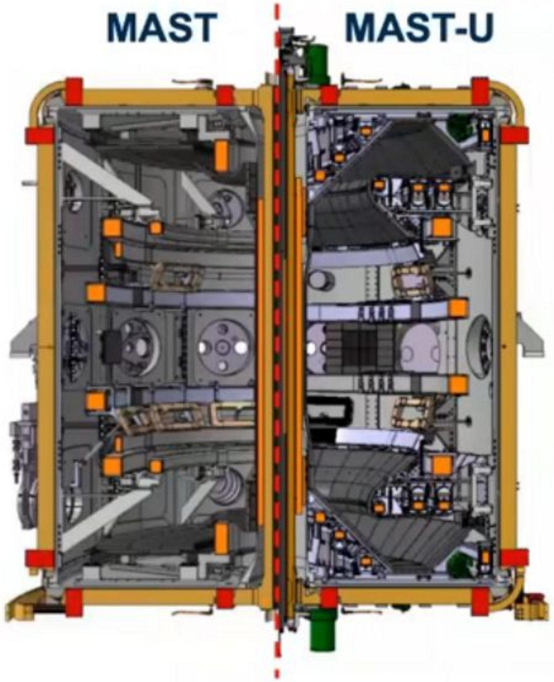
This is underpinned by four goals:

- **Goal 1** - Be a **world leader** in fusion research and development;
- **Goal 2** - Enable the delivery of **sustainable** fusion power plants;
- **Goal 3** - Drive **economic growth** and high-tech jobs in the UK; and
- **Goal 4** - Create places that **accelerate innovation** and develop skilled people for **industry to thrive**.

What is Fusion?

- Take hot gas of deuterium (D) & tritium (T), make it hot {and keep it hot} (> 150 MK) and bang -> you've done fusion…. easy right?
- Toroidal field coils (and sometimes solenoid) drive a (plasma) current that flows around the middle of the tokamak
- Plasma current self generates a poloidal field, the combination of both provide stability (relative)
- Poloidal field coils shape and control plasma





What is Fusion?

UK Atomic Energy Authority

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- Toroidal field coils (and sometimes solenoid) drive a (plasma) current that flows around the middle of the tokamak
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- Poloidal field coils shape and control plasma

Map of a Tokamak

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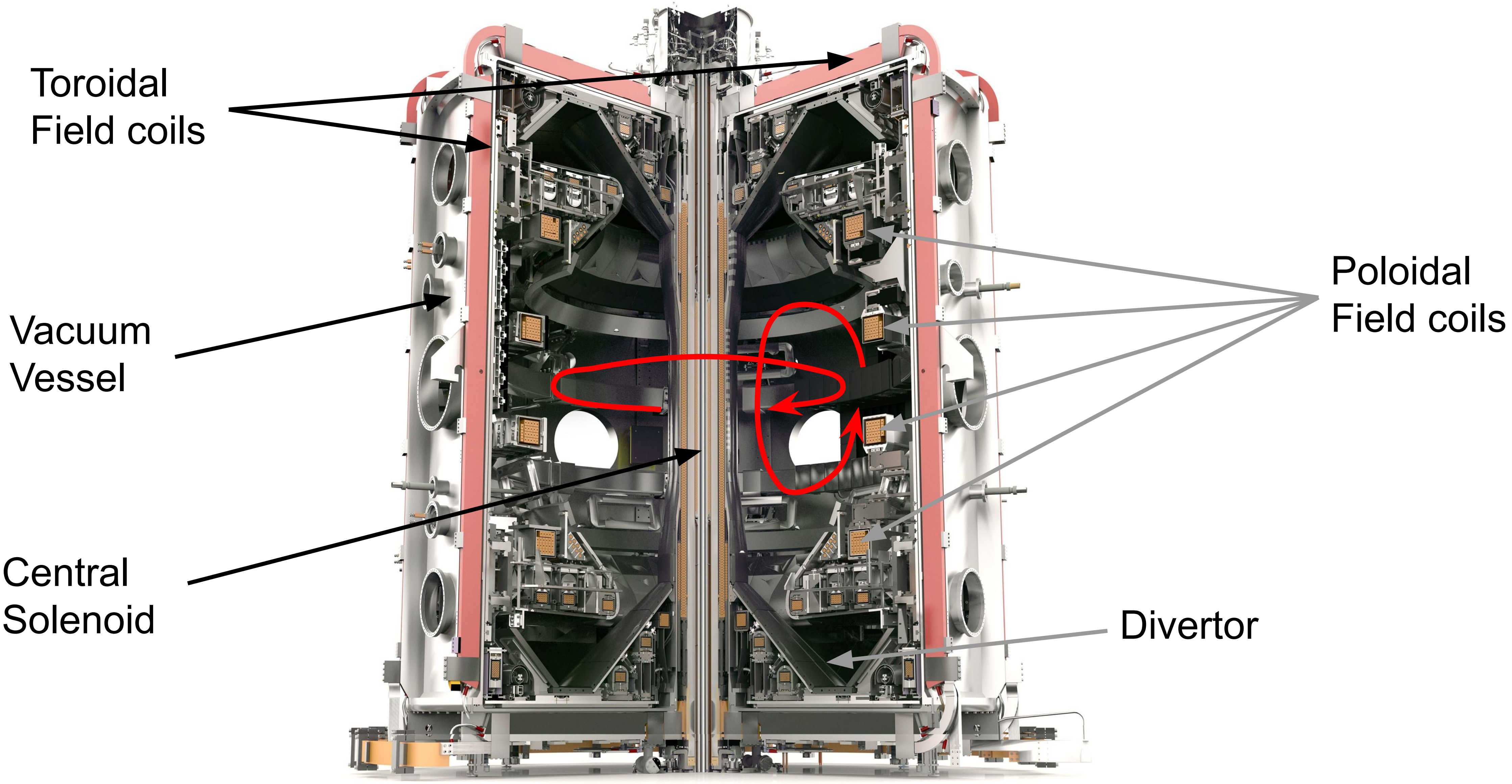

Power flow in a reactor is …..

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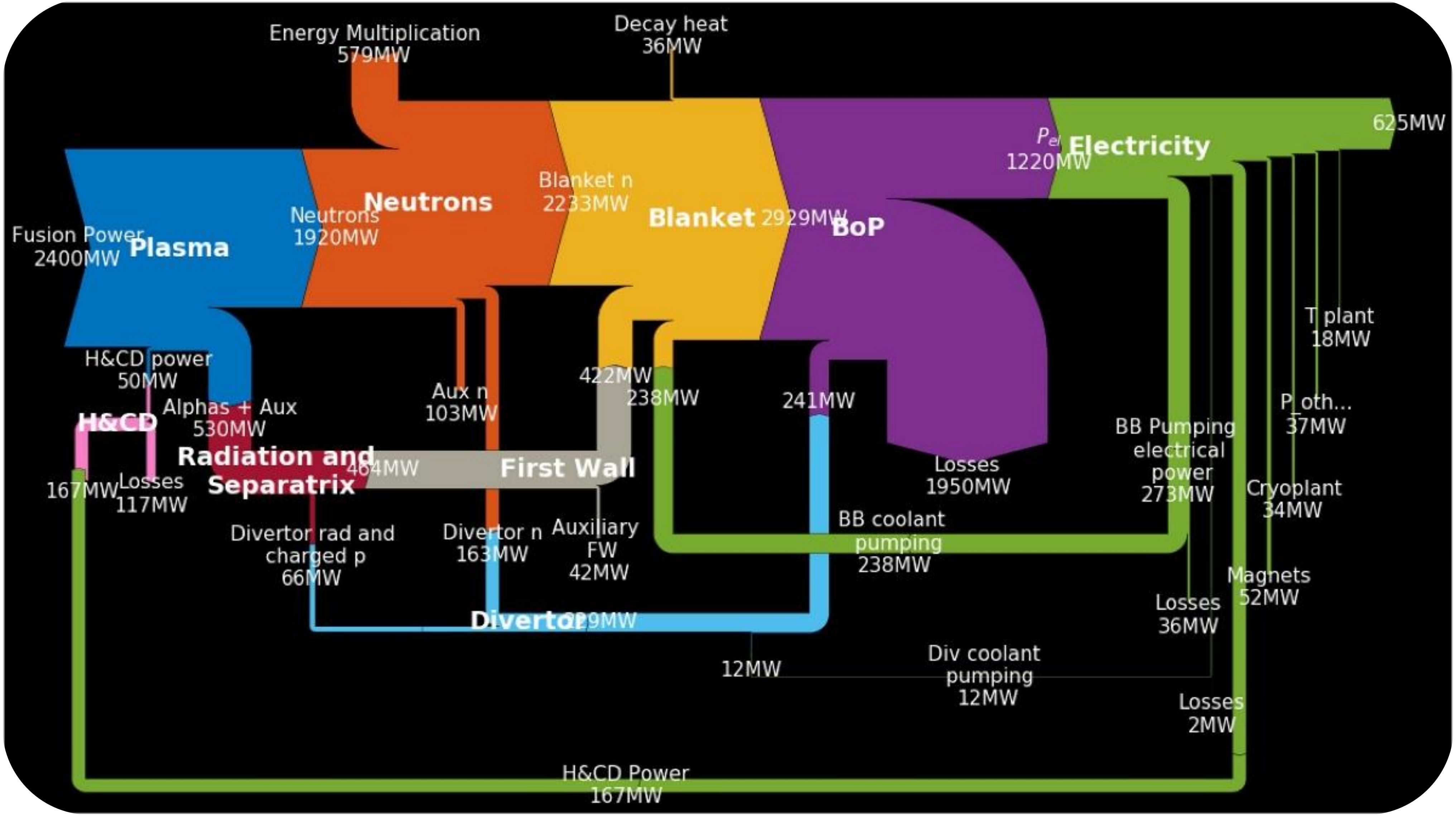
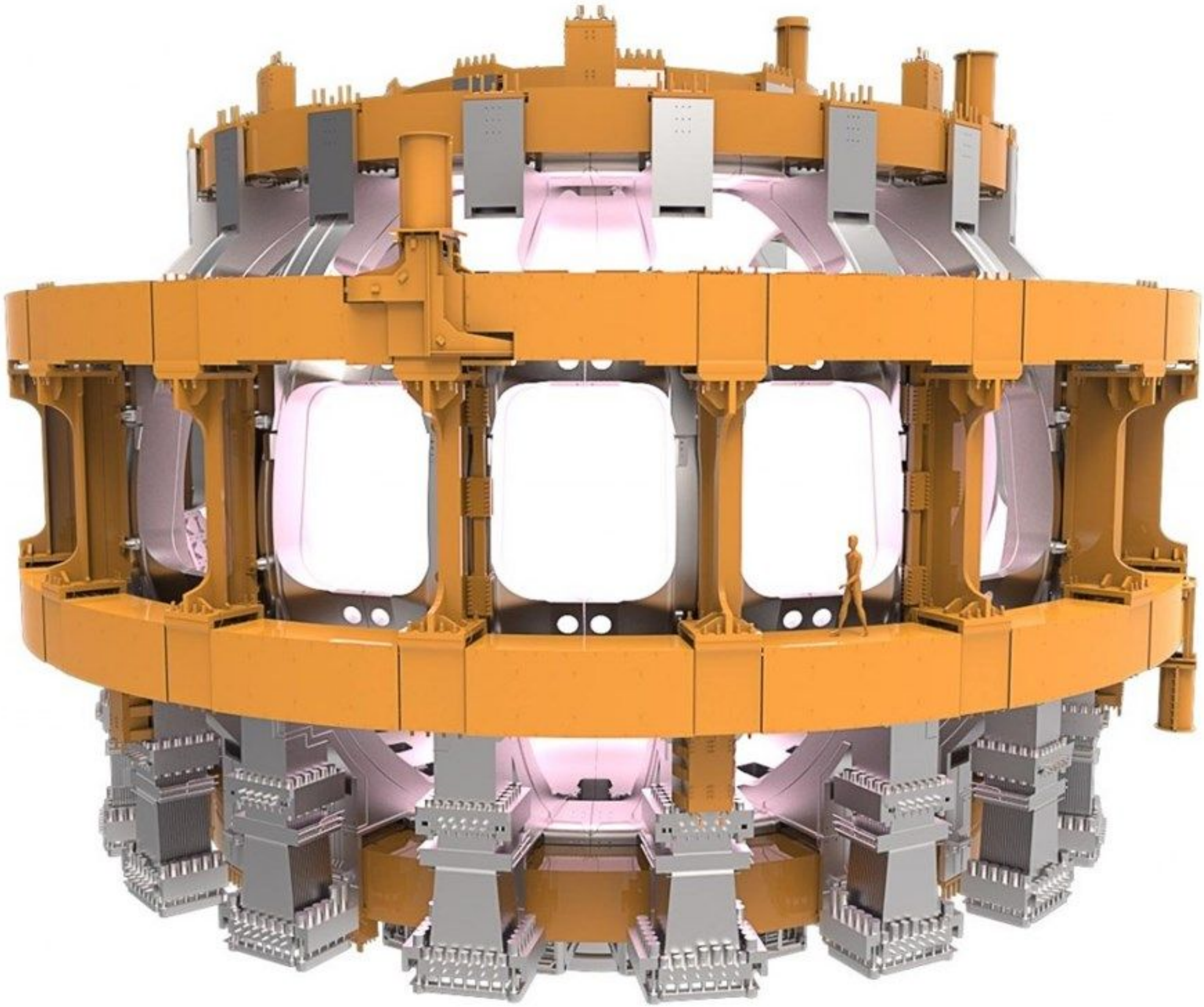


So what's the problem?

UK Atomic Energy Authority

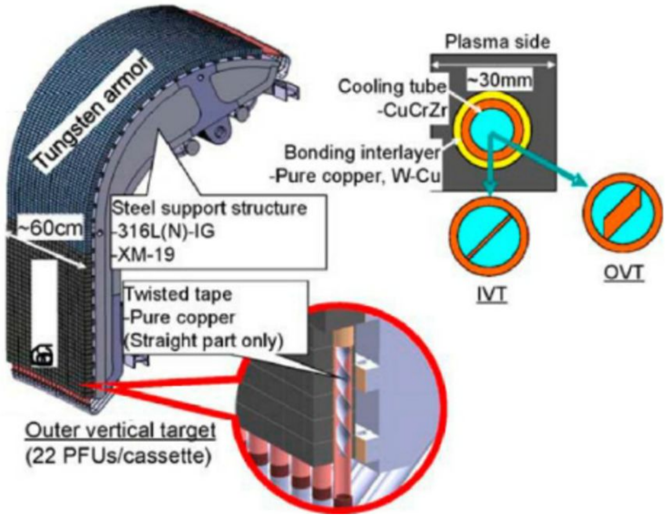
- Lots of forces
  - Magnets push the plasma, plasma push back
    - coil currents upwards of 70 MA
    - Forces upwards of 0.5 GN
    - Cross talk between coils
- High temperature gradients
  - PFC temperature can be upwards of 4000K
  - SC coils 4-40 K
  - Thermal expansion drives stress/strain
- Rapid heat transients in very cold things

  Non-Fourier hyperbolic heat model



So what's the problem?

- Flowing fluids
  - Mostly high pressure water/steam
  - CO_2, He, H, etc
  - Sometimes liquid metal + magnetic field ➡️ MHD
- Turbulence
  - We have fairly large fluid volumes that split and branch multiple times with fairly high Re numbers
- FSI in divertor & blankets
  - e.g. swirl vanes in divertor cooling channels



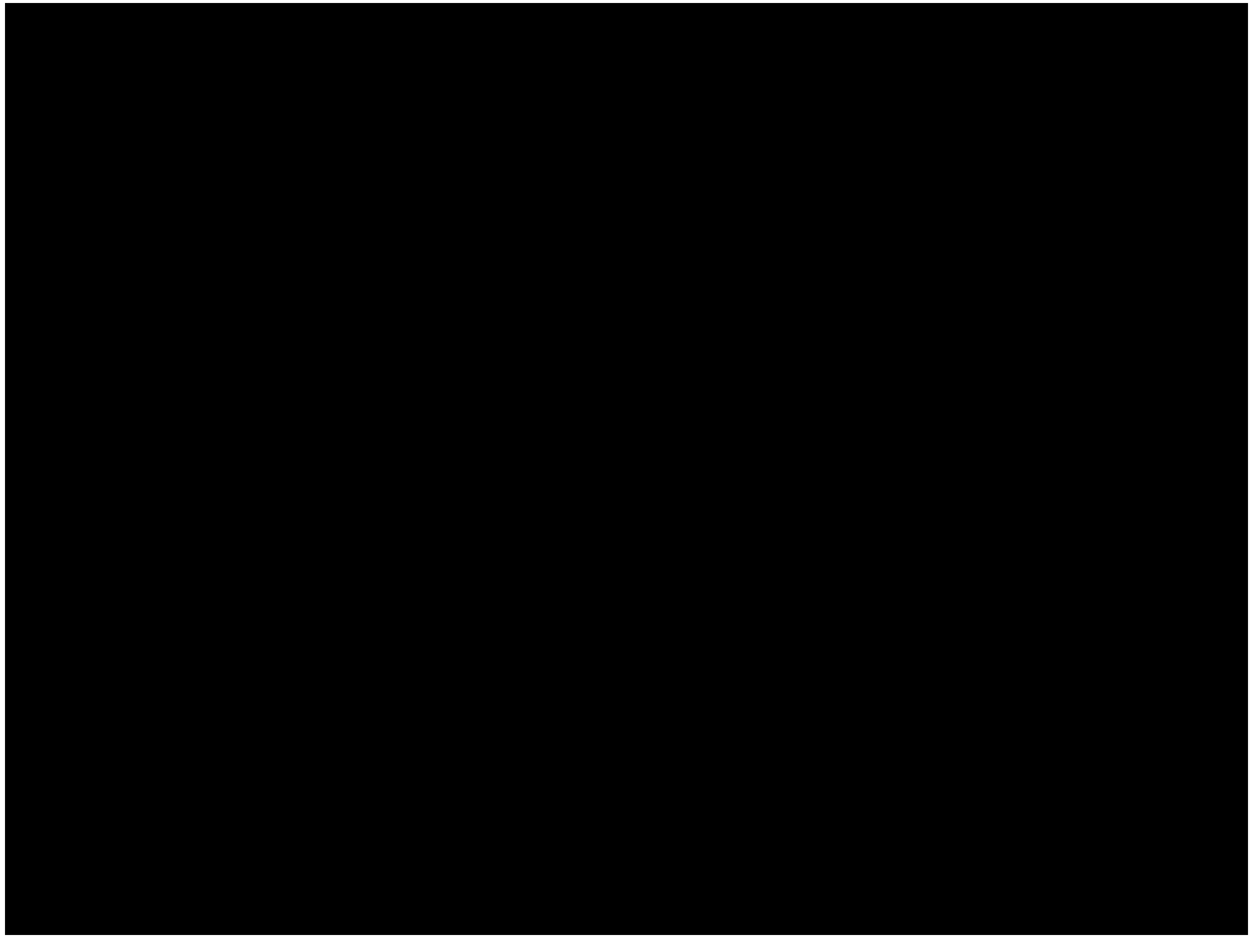
So what's the problem?

UK Atomic Energy Authority

- Plasma emits heat in the form of charged particles & radiation (neutrons, x-rays and gamma rays)
  - Can be distributed over a larger area
  - Or can be concentrated - a la divertor ➡️ 5-20 MW m^{-2}
  - Can be concentrated even further under off-normal scenarios e.g. runaway electrons
- Radiation loads
  - Plasma releases 80% of the fusion energy as neutrons
    - radiation damage drives another source of stress/load
    - nuclear heating drives another
    - further nuclear reactions increase energy deposition by 50%
  - Don't forget hot stuff radiating heat to colder stuff!
    - Complex transfer of IR from surfaces

So what's the problem?

- Vacuum ➡️ around 100x more dense than lunar atmosphere - 1×10^{-11} bar
- Tritium permeation
  - tritium diffuses through materials easily, driven by temperature gradients, material properties (adsorption rates) - really tied to the microstructure
  - tritium prediction is critical ➡️ tritium is our fuel - accurate predictions are critical
- In solid, regular diffusion applies, at escape boundary - monte carlo approach



So what’s the problem?

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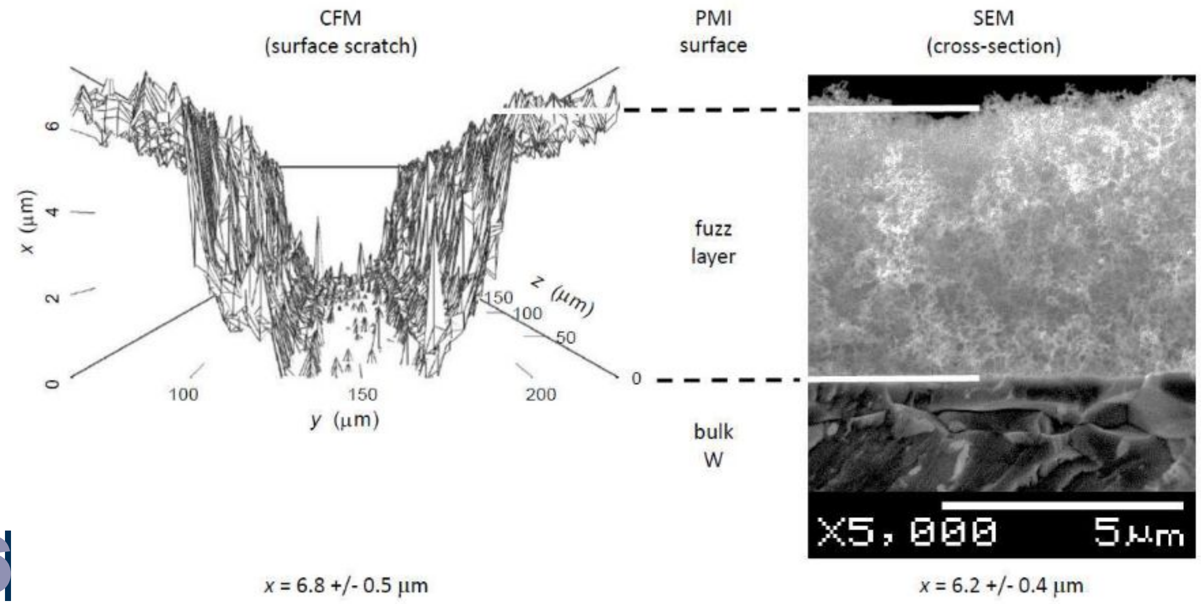
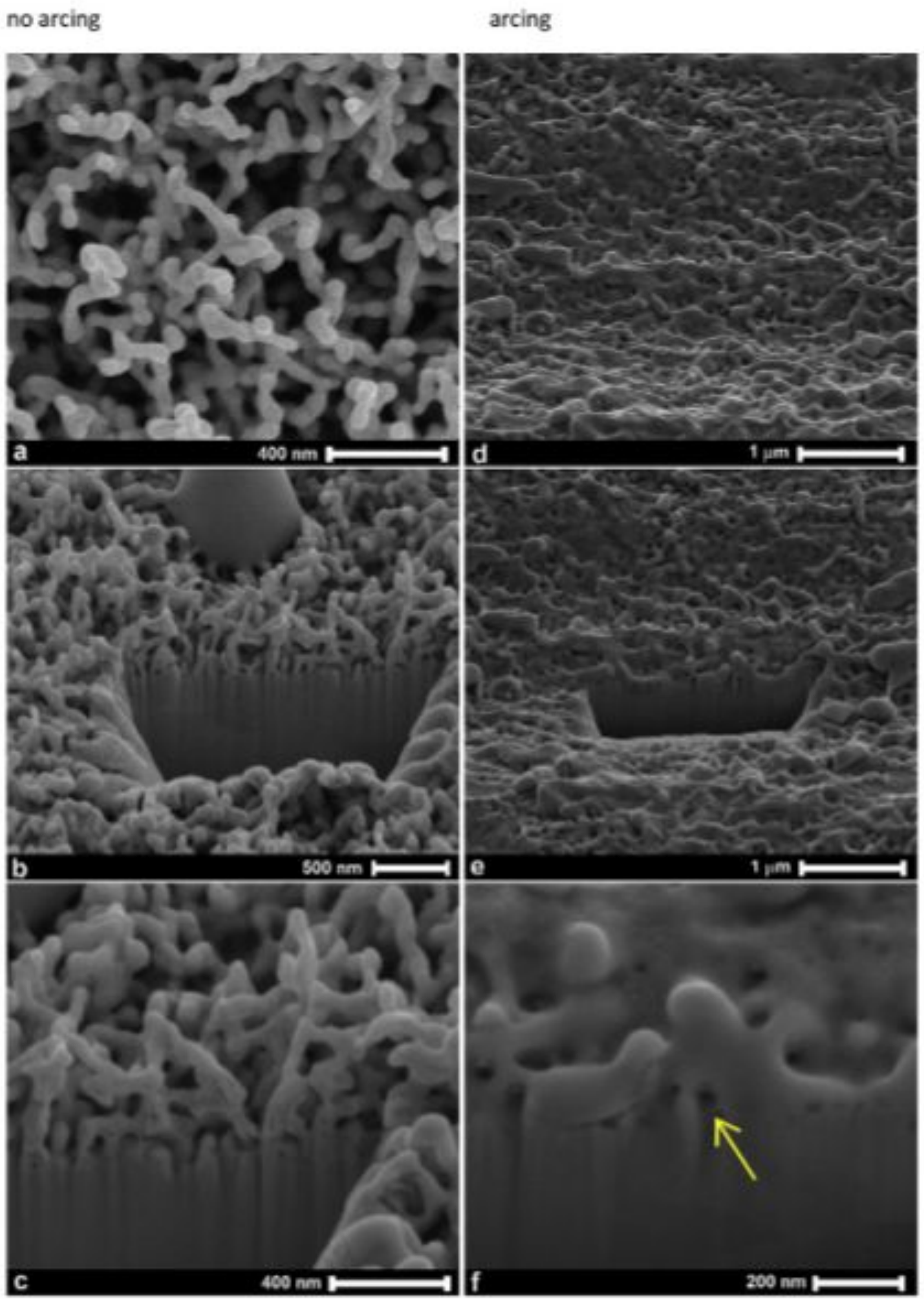
- Erosion
  - plasma heat (particles) leads to localised melting, field redeposits melt pool material over the first wall
- Divertor constantly exposed to ion flux, leads to tungsten fuzz (if divertor PFC is tungsten)





http://dx.doi.org/10.1016/j.jnucmat.2017.05.032

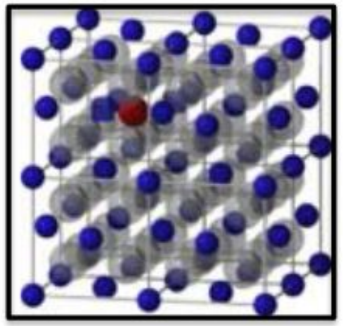
So what's the problem?

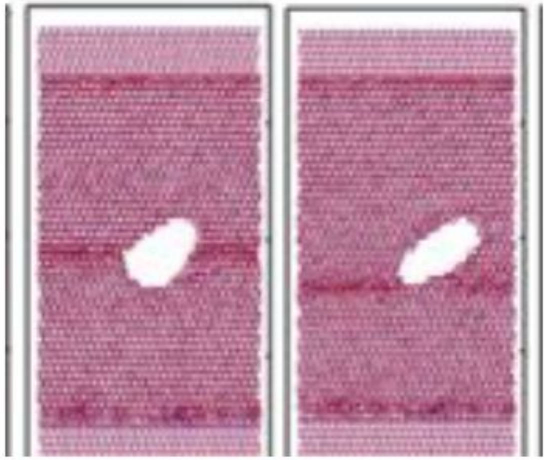
- In terms of whole device simulation we firmly have a multiscale problem

[https://icmed.engin.umich.edu/wp-content/uploads/sites/176/2016/06/Summer-School-MOOSE-talk-2016-small.pdf]

Atomic scale bulk DFT + MD

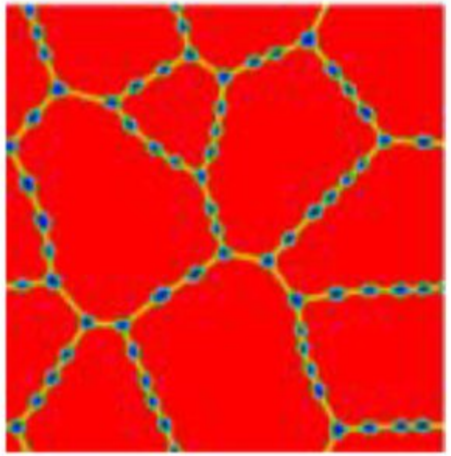
- Identify important bulk mechanisms
- Determine bulk material parameters





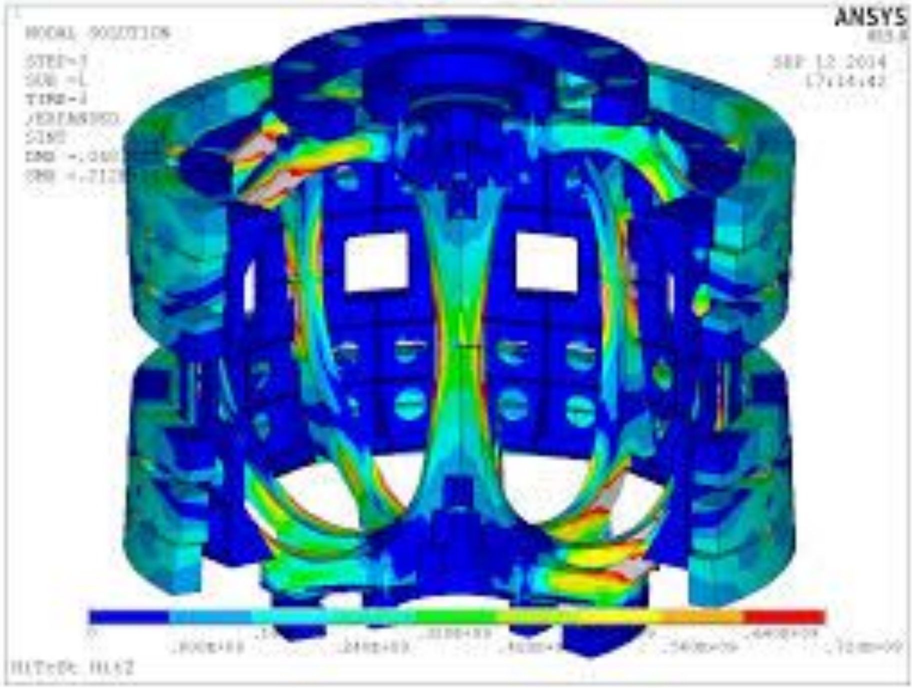
Atomic scale microstructure MD

- Investigate role of idealized interfaces
- Determine interfacial properties



Mesoscale models

- Predict and define microstructure evolution
- Determine effect of evolution on material properties



nm → µm → m

So what's the problem?

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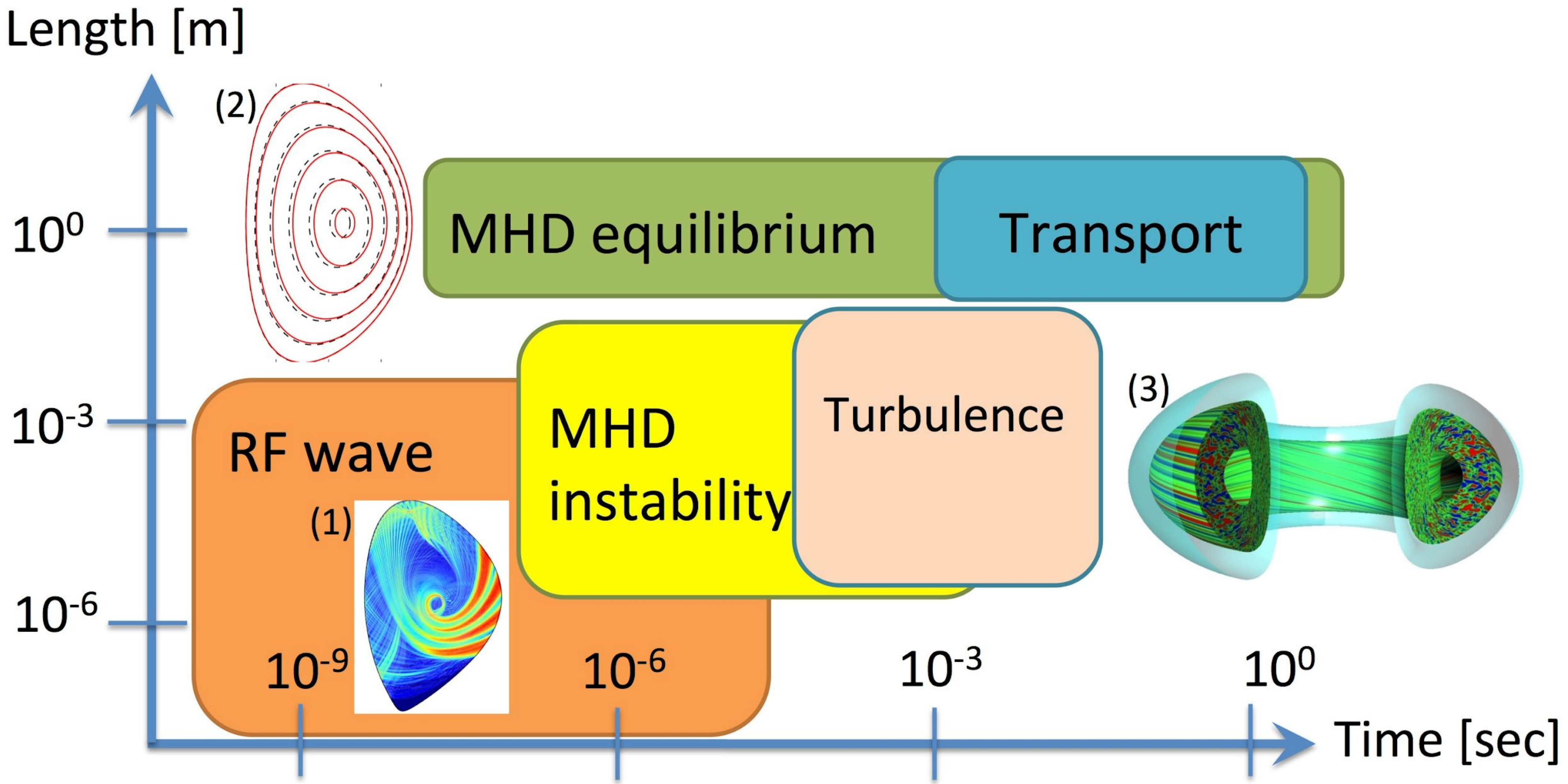
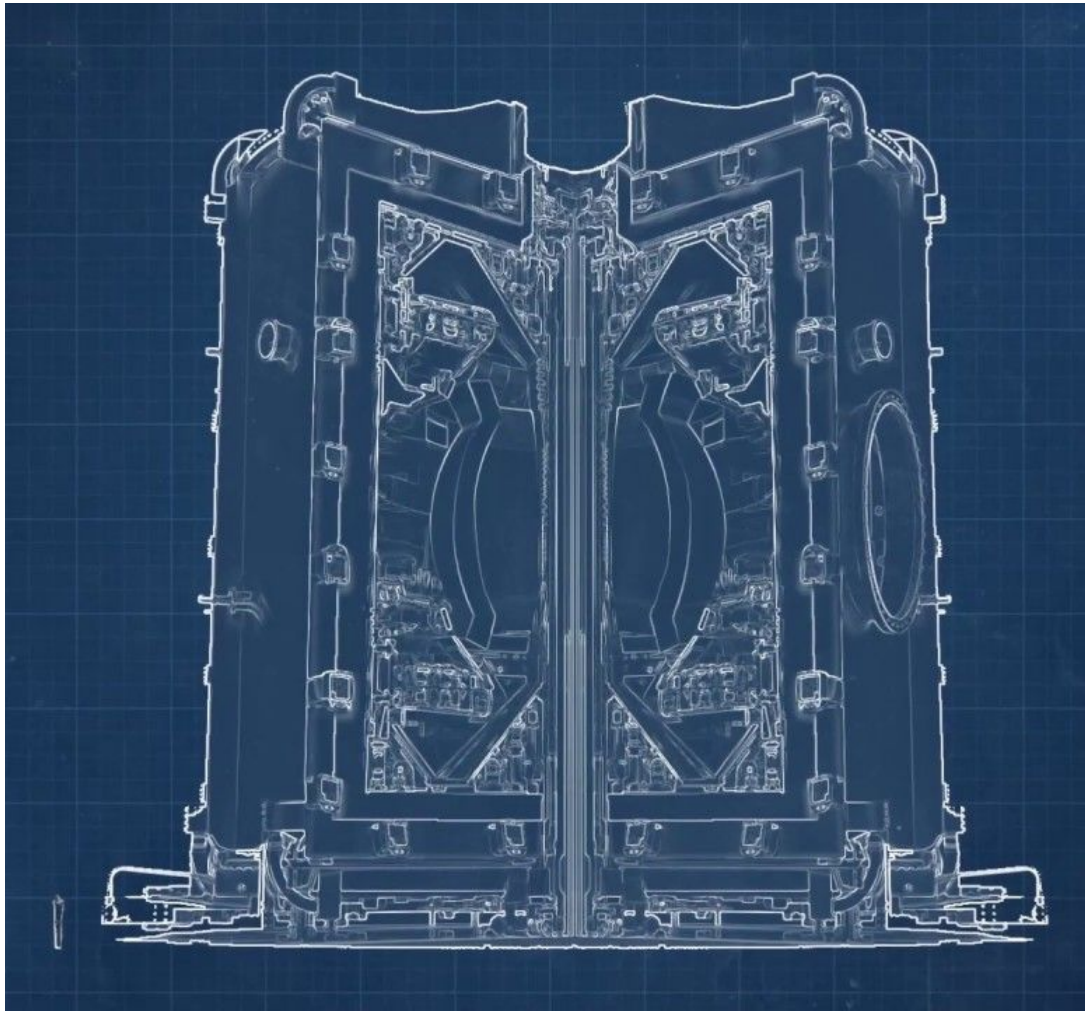


https://stuff.mit.edu/people/jungpyo/projects.html

STEP

- The Spherical Tokamak for Energy Production (STEP) is an ambitious programme to accelerate the delivery of sustainable fusion energy.
- STEP is a staged programme to design and build the world’s first compact fusion reactor, based on the spherical tokamak, by 2040.



Fusion Timelines

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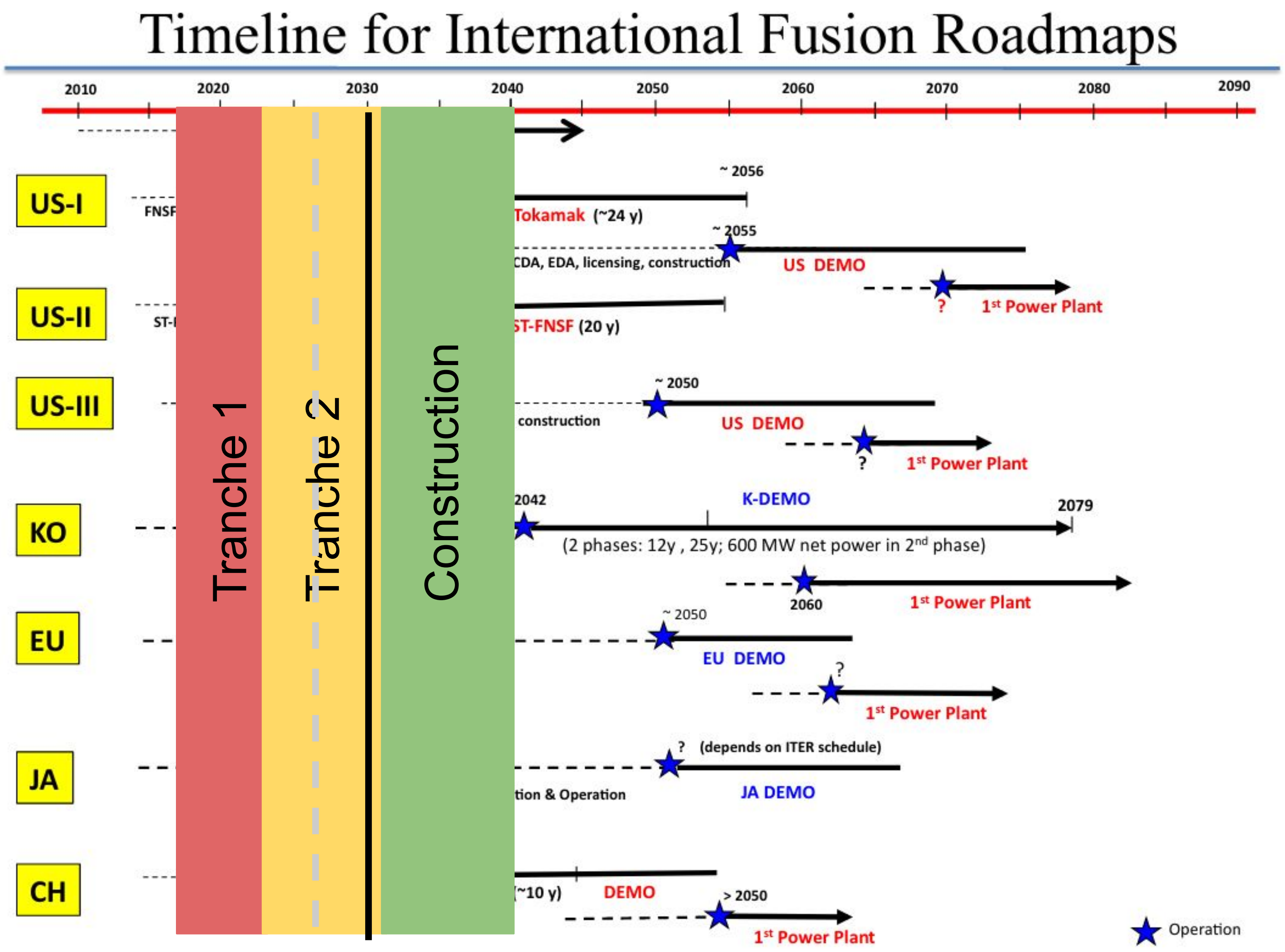
- In between now and 2040 there are a number of demonstration type plants coming online
  - ITER
  - SPARC
  - CFETR
- Nuclear Test Facilities
  - IFMIF
- Non Nuclear Test Facilities
  - CHIMERA



From L. El-Guebaly

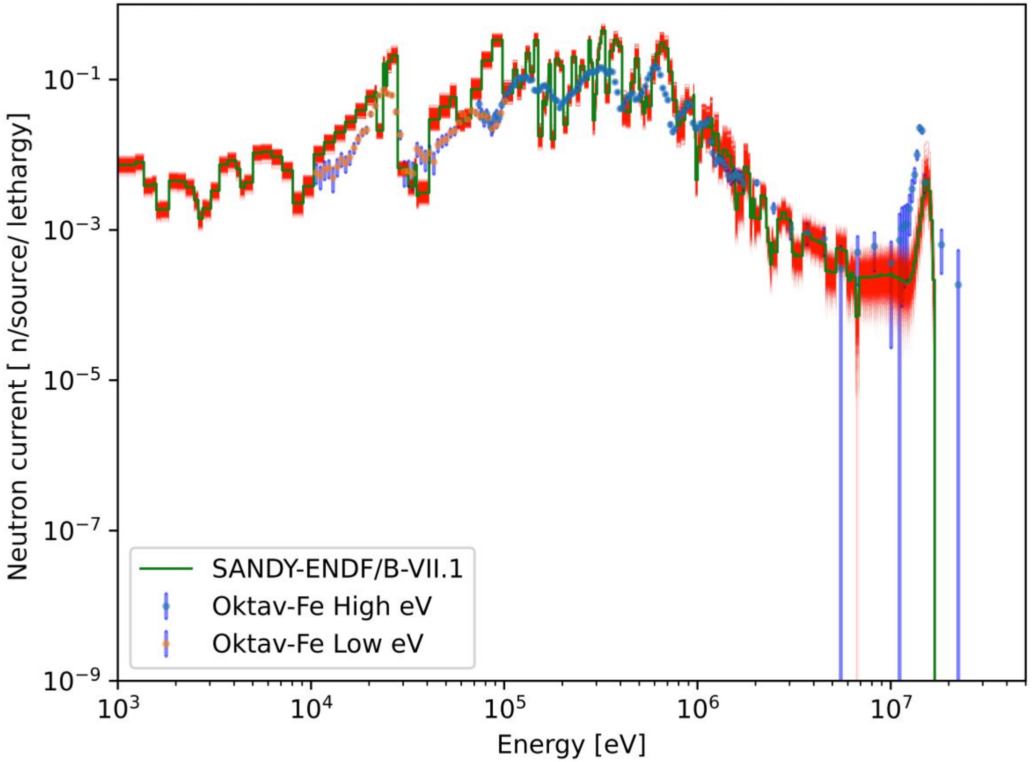
Fusion Timelines

UK Atomic Energy Authority

- In between now and 2040 there will be only 3 years, 2037 onwards of ITER experiment that will have DT neutrons and all remaining loads present
- The Commonwealth Fusion Systems SPARC device might run - will we have access to the data? 10 s pulses?
- Will need to qualify and gain regulatory compliance in absence of all the experimental evidence that may be needed
  - Cross Validation across fields & domains
  - Uncertainty Quantification & Propagation
- Small efficient directed testing will be critical

UNIVERSITY OF LIVERPOOL

Ander Grey, Andrew Davis, Eduardo Pateli



Traditional techniques lack scale

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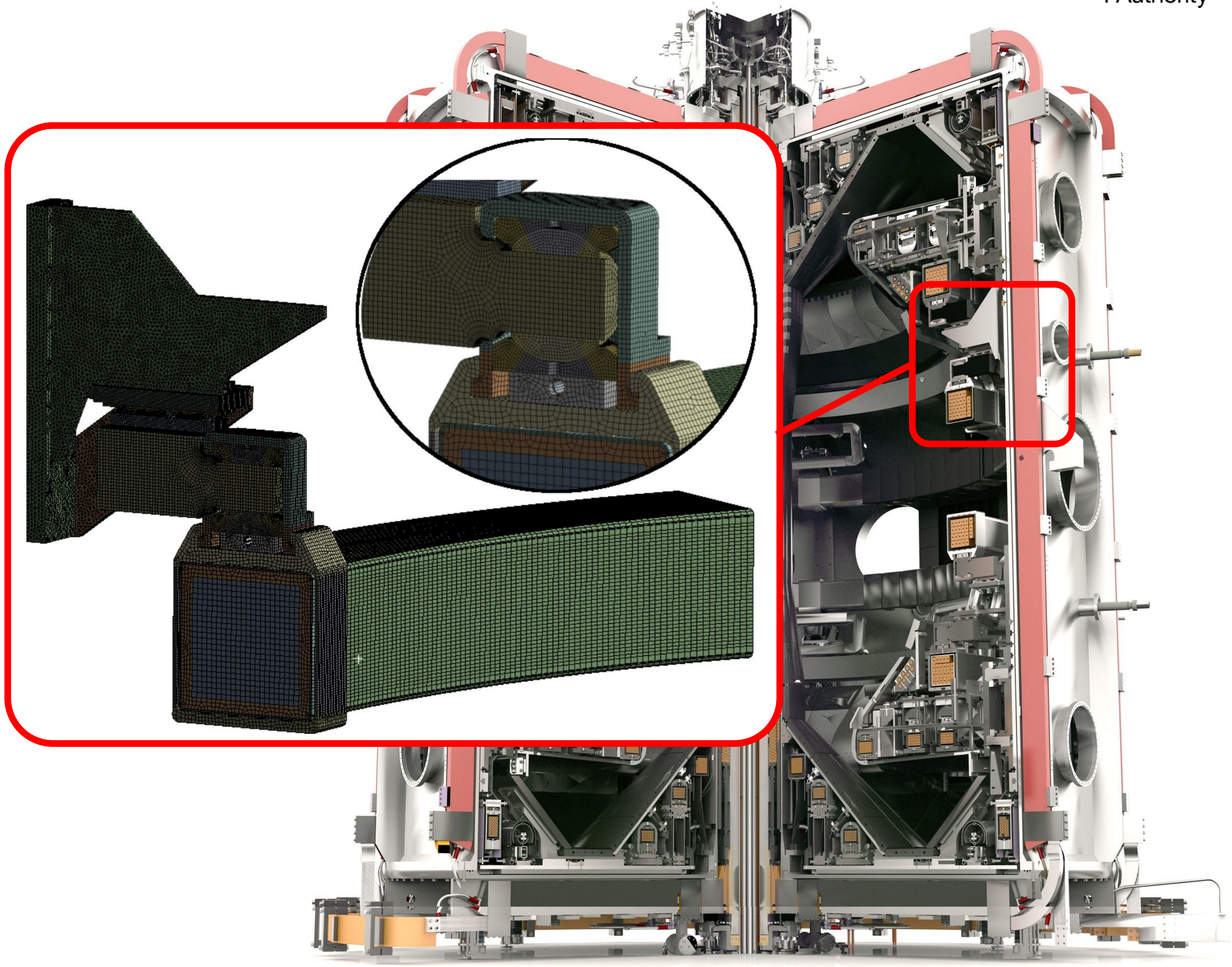
- Sub-modelling techniques limit throughput
    - Manual
    - Built on humans & approximations
- Manual mesh generation
    - Tedious
    - Slow
    - Not parallel
- Commercial solvers tend not to scale well beyond 32 cores
- Need to move the engineer off the desktop

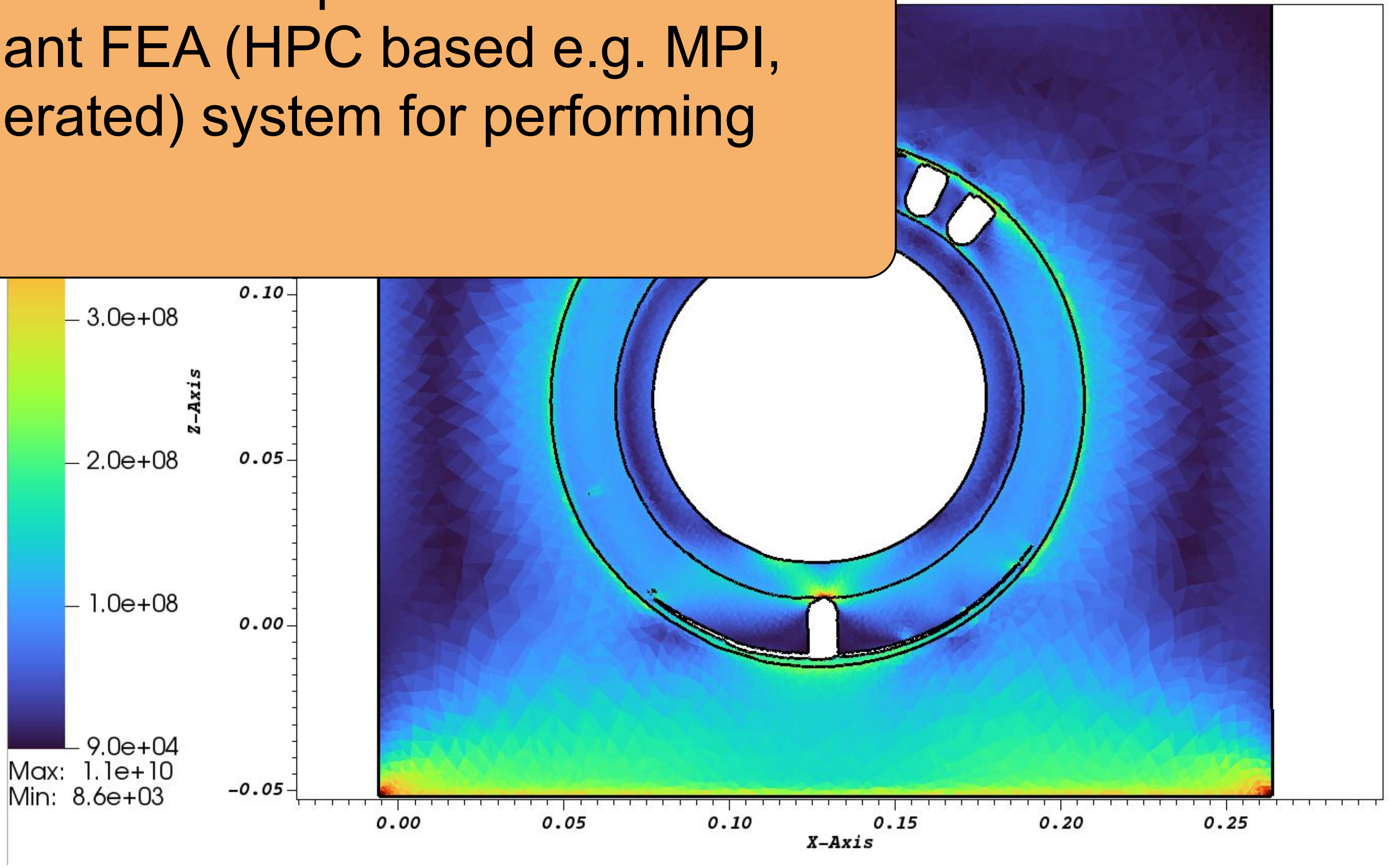


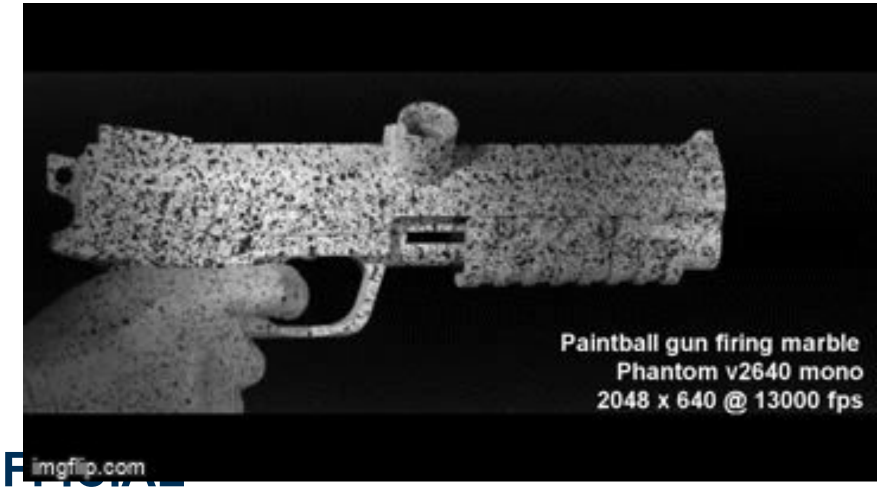
Combine as designed, with as built

UK Atomic Energy Authority

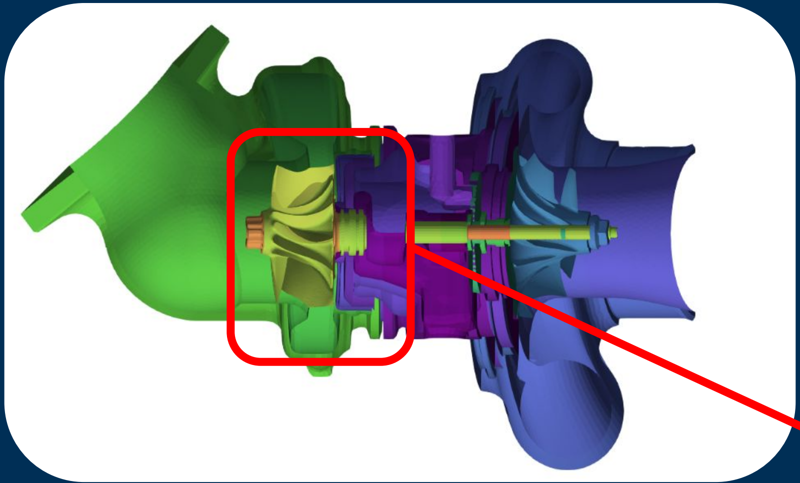
- Combine as designed FEA with Image Based Finite Element (IBFEM)
  - IBFEM allov
    built compo
  - route to con
    validation
- Combine with
  Correlation (D
  surface and depth characterisation

Modelling entire as built or IB components will necessitate a performant FEA (HPC based e.g. MPI, Threaded, GPU accelerated) system for performing calculations





Moving towards as designed FEA is ach



O(10^9) tets
2nd order mesh
25000 CPUS (25000 MPI)
Wall clock time - 400 s (!!!)
1e5 DOF per CPU

C Richardson et al - “Scalable Computation of Thermomechnical Machinery”

ITER I
simplif
PPP to
thread
eleme

Digital Twins

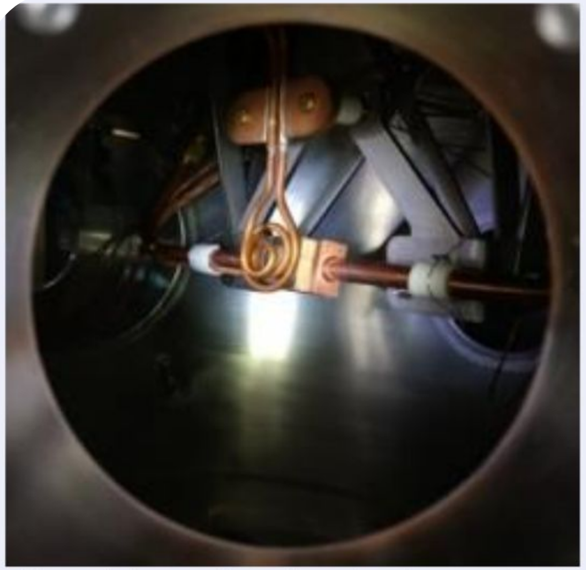


Figure 1: Image of sample undergoing experiment in HIVE [1]

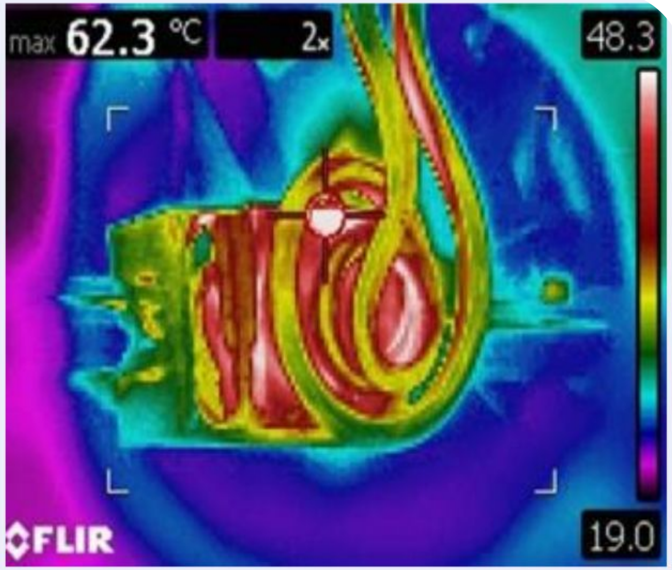
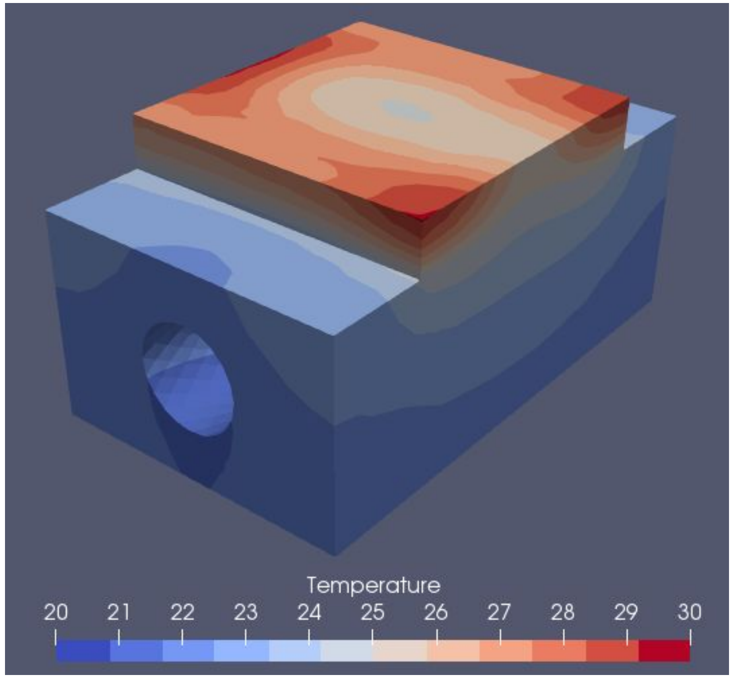
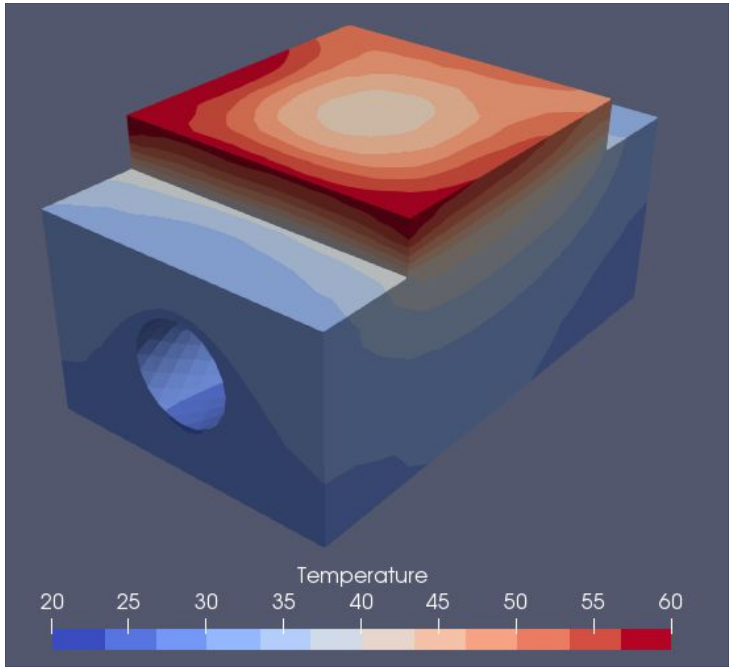


Figure 2: Heat distribution captured in HIVE using infrared camera [1]





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The HIVE experiment mimics first wall temperatures, driven by inductive heater - digital twin & machine learning driven

Swansea University Prifysgol Abertawe

Rh. Lewis[1,2], Ll.M. Evans[1,2], A.D.L. Hancock[2], A. Davis[1,2], R. Otin[2], K. Flinders[2], J. Paterson[2], D. Stone[2], M. Dearing[2], H. Lewtas[2], P. Nithiarasu[1]

Large scale multiphysics

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- If we are to fully simulate complete systems, need scalable coupled FEA framework, it must cover:
  - Computational Solid Mechanics
    - Including dynamic contact
    - fracture mechanics
  - Computational Chemistry
    - DFT, Damage
  - Computational Electromagnetics
  - Computational Fluid Dynamics
  - Computational Radiation Transport
  - Heat Transfer
  - Microstructure (phase field, grains)
  - Diffusion (and reaction)
- Massively scalable ➡️100,000’s of CPUs
- Exascale gazing (considering support for GPU)

We are trying to build a performant multiphysics software framework

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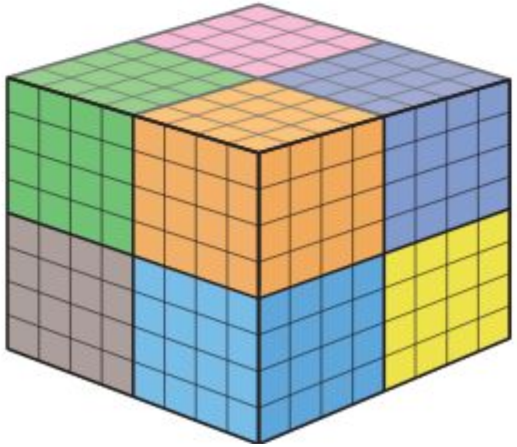
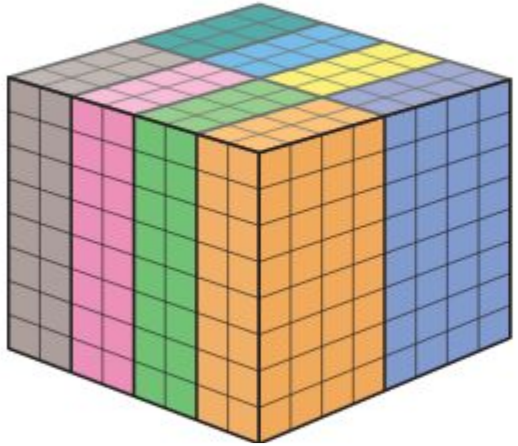
- We need to perform efficient multiphysics simulations
  - Experimenting with tightly coupled framework rather than federated model
  - This means we take a more ***holistic*** view of how we stick different codes together
  - It may be the case that taking the best/fastest physics packages and sticking them all together does not lead to the most scalable solution
    - communication of mesh or solutions could begin to dominate
    - for massively decomposed problems (where we need to be for performance)
- Still figuring out what tools, physics, scales



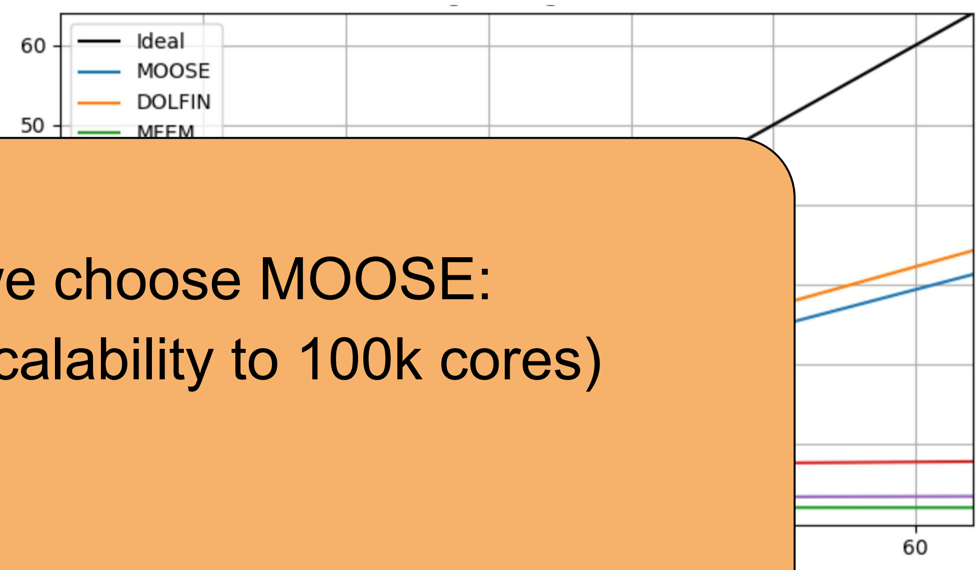
Ideal partitioning for a CFD problem

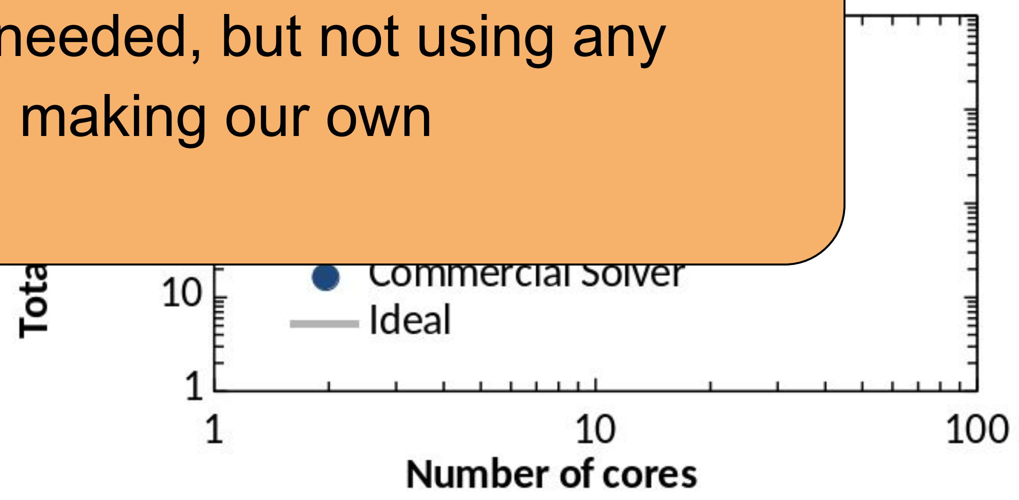


Ideal partitioning for a neutral particle problem

Initial Investigations

- Horizon scanning revealed something like 37 modern FE frameworks which we could base some tools
  - down se
  - ease of
  - software
  - scaling
  - memory
- Compariso lead to a fi
  - MFEM
  - MOOSE
  - Dolfin (Fenics/Fenics/X)





Given our limited programme duration, we choose MOOSE:

- due to its scalability (demonstrated scalability to 100k cores)
- quite wide ranging physics options
- multiscale
- ease of plugging in external physics

Make improvements to physics where needed, but not using any MOOSE Apps (Falcon, Marmot, etc) -> making our own

Initial Investigations

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- Looking at the role of turbulence in gas cooled breeding blankets
  - somewhat contrived problem, but reflective of a concept design from KIT
  - 1 MW/m^2 heat load on front surface
  - 10 MW/m^3 nuclear heat load
  - 5 ms^{-1} helium coolant (ramping flow)

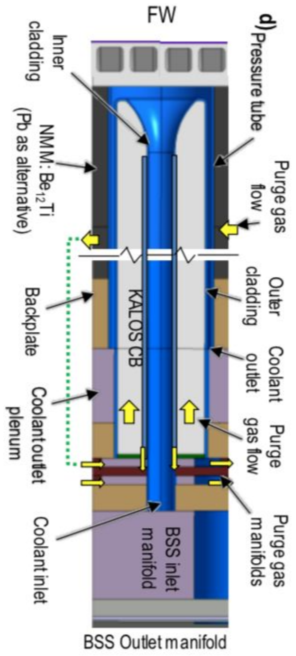
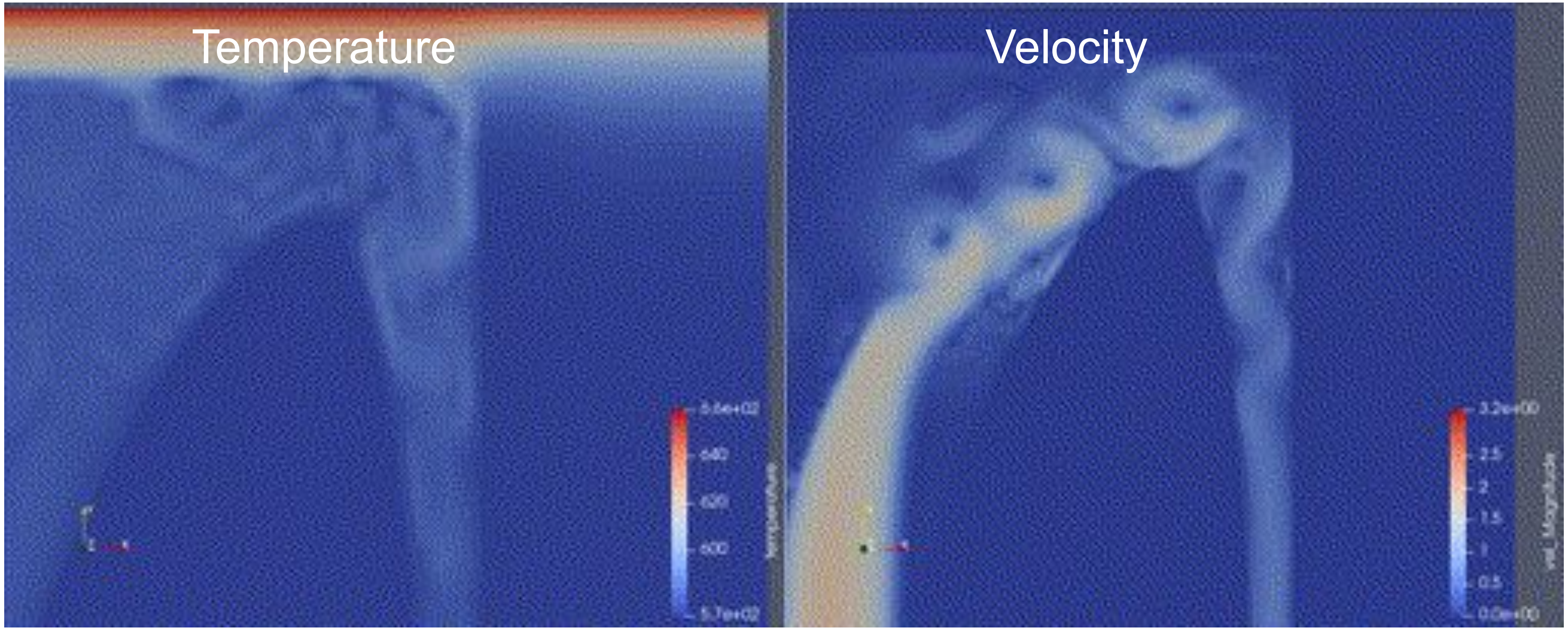
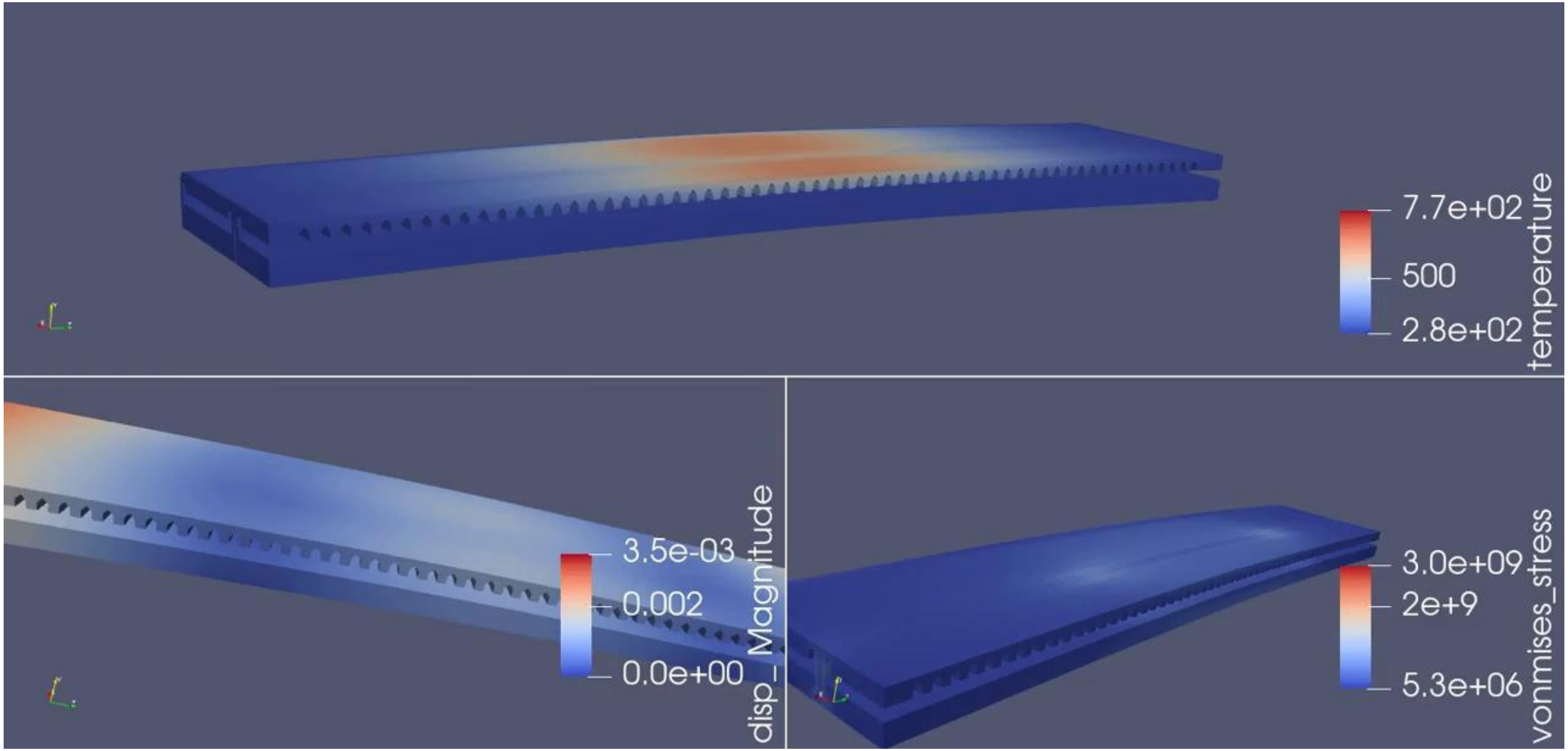


Fig. 2 Enhanced HCPB for the DEMO1 baseline 2017.



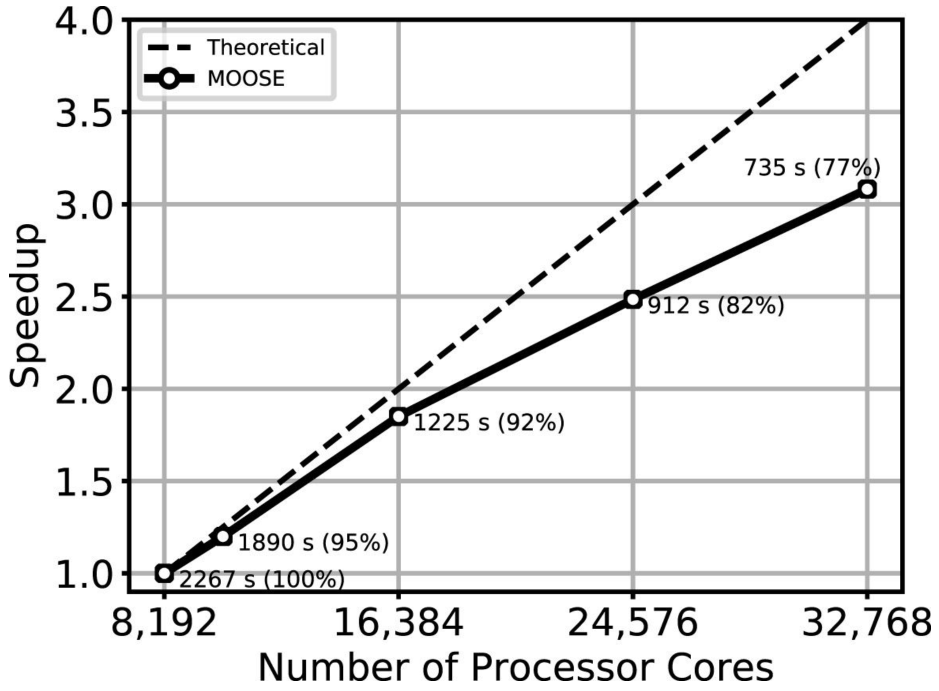
Initial Investigations

- Hypervapotron (heat exchanger) simulations

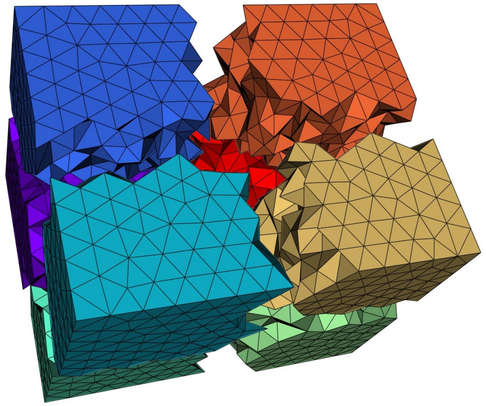


Parallel Scaling

- Some physics limits hardware scaling
  - Pre-conditioners
  - very nonlinear physics
  - temperature dependent parameters
  - long grind time
- MOOSE assembly time scales very well
- Mesh partitioning is intelligent - factors in BC's, contact
- MOOSE ➡️ libMesh ➡️ PETSc
- Allows trivial tight coupling
- MultiApp makes federation easier



Example MOOSE scaling 78M elements 713M DOF
https://doi.org/10.1016/j.softx.2020.100430



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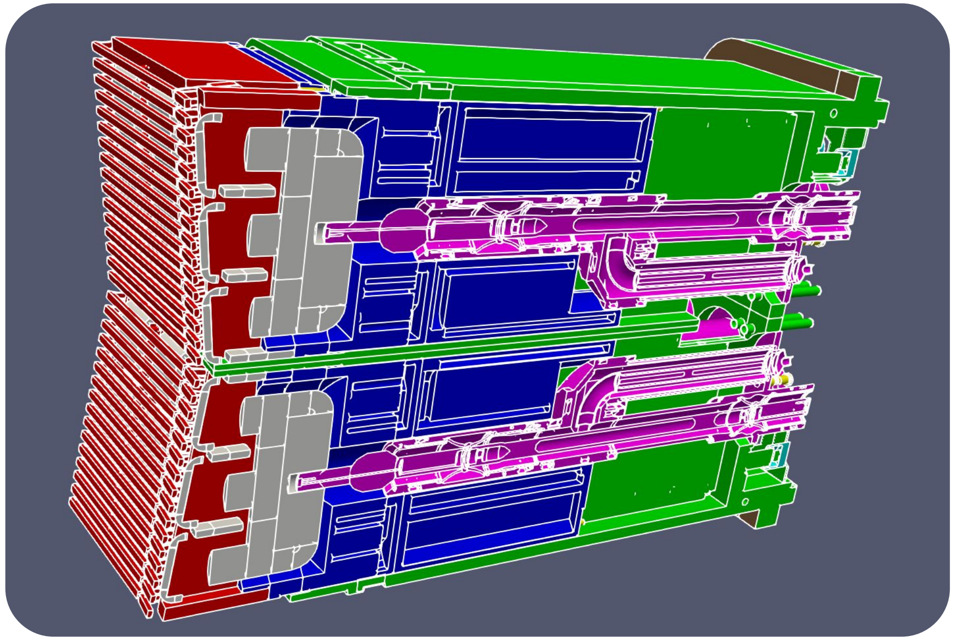
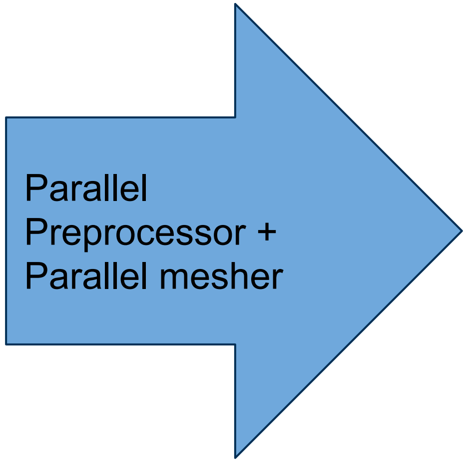
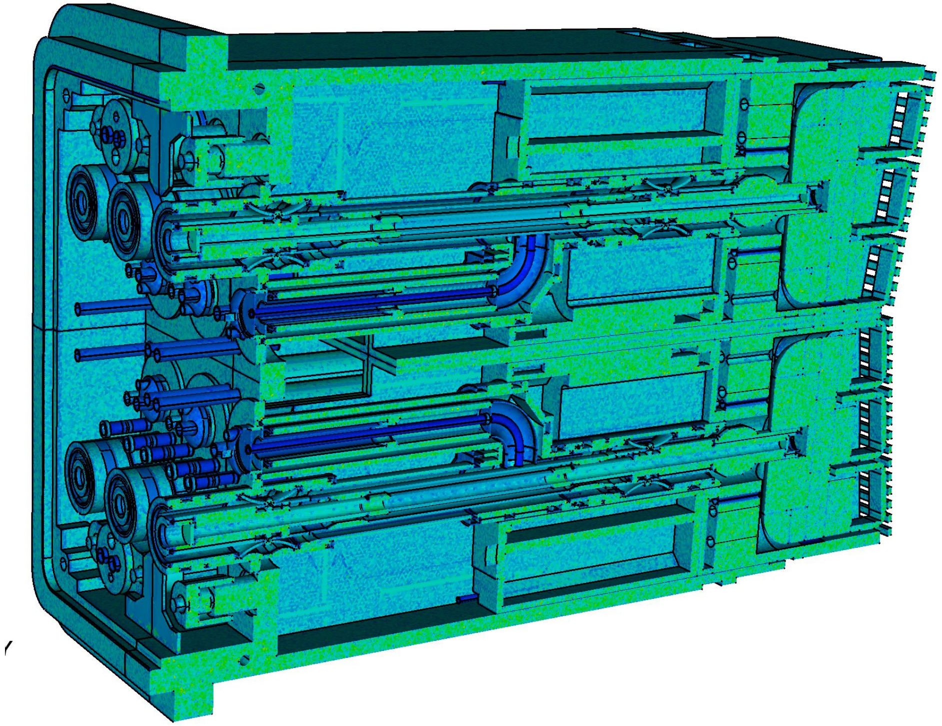
Challenges

- In-situ visualisation
  - We cannot rely on rsync/ssh/scp to transfer massive outputs for visualisation
  - Exascale problem
- Geometry preparation and meshing
  - Most (all?) parallel meshing systems do not preserve curvature - **important!**
  - All geometry preprocessing is serial with commercial tools







64 cores for 1.9 hours
78M elements

https://github.com/ukaea/parallel-processor

That being said.....

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- There are some really interesting things coming down the academic pipelines
    - Iso Geometric Analysis (IGA)
    - Spectral HP Based FE/FV
- These two combined will (1) simplify the CAE pipeline and (2) massively increase the arithmetic density (high order)
- But…..have to be pragmatic
    - we cannot wait for these tools to come on-line, we need to do things now, can phase in newer technology later

Conclusions

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- We have short timescales to deliver a working fusion reactor, in order to deliver going to need
  - Performant, scalable multiphysics
  - Uncertainty quantification to allow actionable simulation
  - Digital twins of experiments for validation
- We can’t do it alone, we can be the keepers of our domain knowledge
  - We need your help
  - We need your use cases too, every experiment is critical

Questions