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Scalable Tightly-Coupled Multi-physics for Fusion Reactors with AURORA

IAEA Technical Meeting on the Development and Application of Open-Source Modelling and Simulation Tools for Nuclear Reactors

Helen Brooks (speaker), Andrew Davis

UKAEA

22/06/2022

Overview

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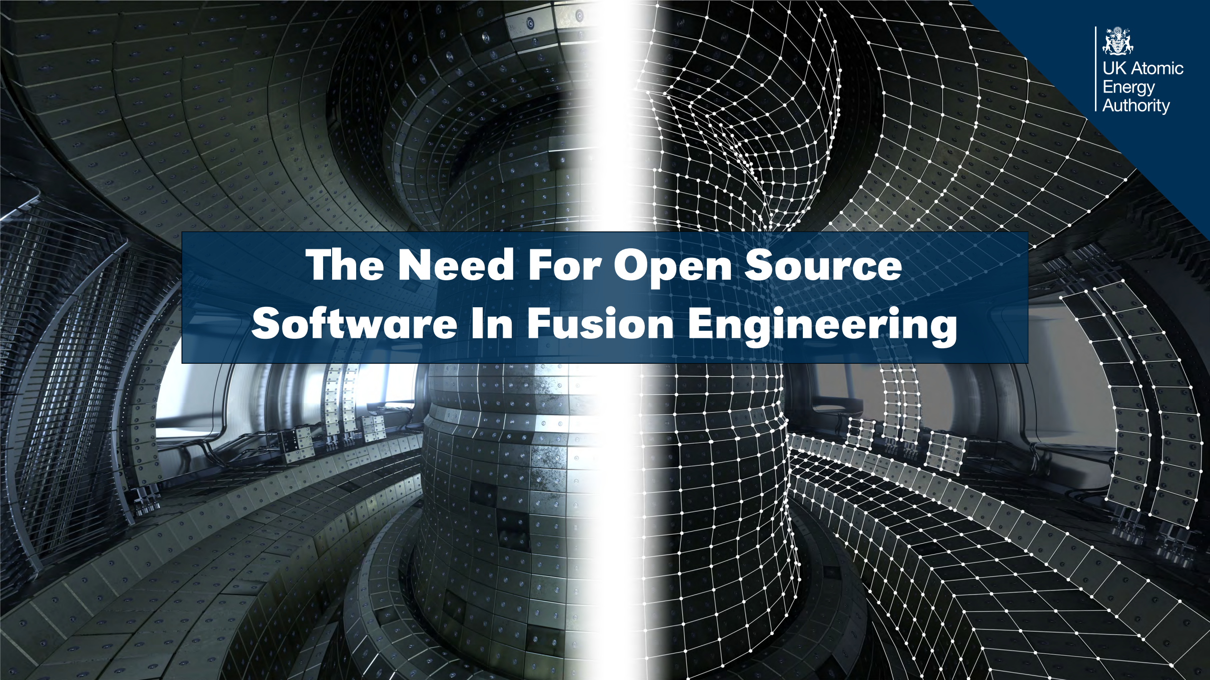
1. The Need For Open Source Software In Fusion Engineering
2. Open Source Dependencies
3. AURORA and The Pantheon for Fusion Multi-physics
4. Outlook and Summmary

The Need For Open Source Software In Fusion Engineering



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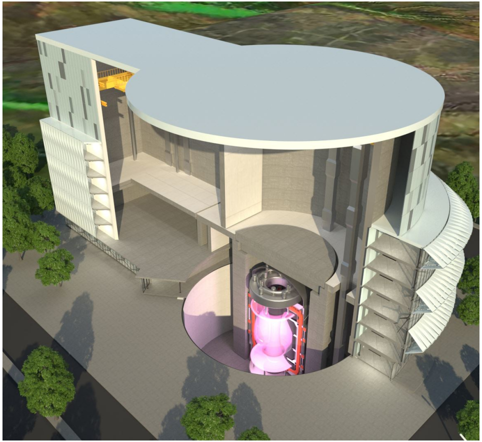
Context: Fusion for Energy Production



Artist's impression of STEP (Image credit: UKAEA)

The STEP (Spherical Tokamak for Energy Production) project has the mission:

" to deliver a prototype fusion energy plant, targeting 2040, and a pathway to viable commercial fusion."

There is an urgent need for high-fidelity engineering software tools to facilitate the design of future fusion reactors.

The Need For In-Silico Design

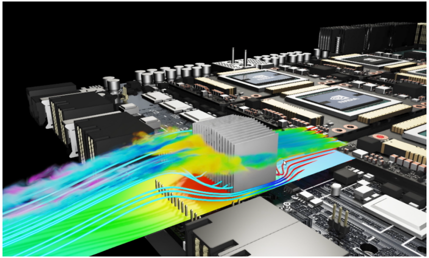
Don't have time to:

- wait for other fusion plants to come online.
- prototype everything.

But, if we combine

- Parametrisable CAD
- High-fidelity engineering simulation
- Verification and validation
- Uncertainty quantification
- Intelligent optimisation algorithms

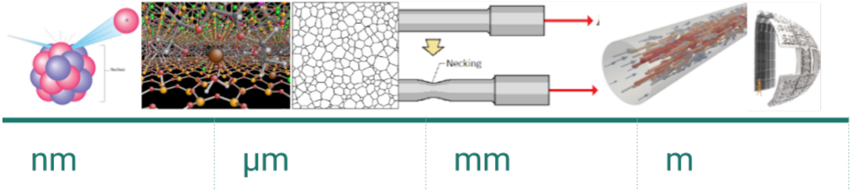
we could explore the design landscape **in-silico**.



AI-driven design is not a novel concept: for example, here NVidia Modulus utilises AI to design a heat sink for a computer chip. [Image credit: developer.nvidia.com]

The Need for Multiphysics Modelling

Modelling the fusion environment requires many domains of physics spanning multiple lengthscales.



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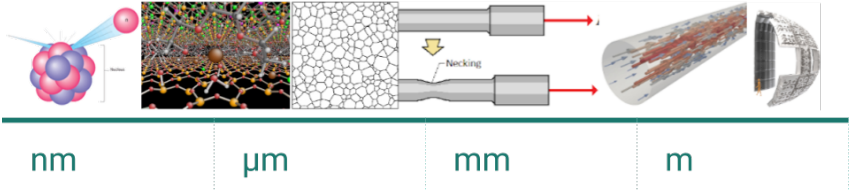

Validation of all physics is **critical** if our simulations are to be trustworthy.

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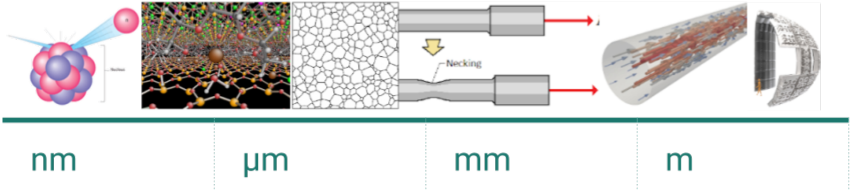

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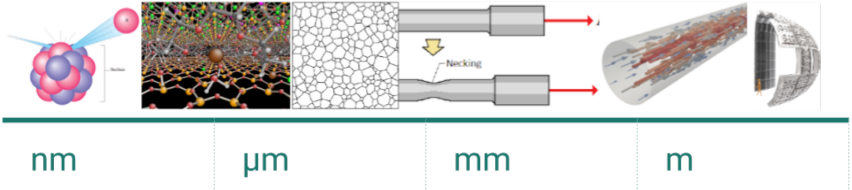

Validation of all physics is **critical** if our simulations are to be trustworthy.

But, validation takes **time**.

Use of pre-validated physics packages can **accelerate development**.

The Need for Performance

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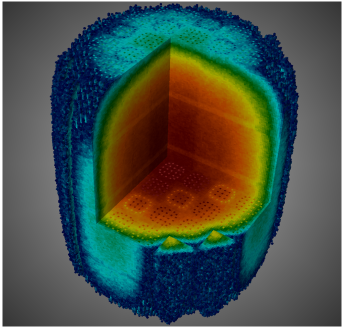
Modelling of a fusion reactor is arguably **more complex** than a small modular reactor (SMR).

- Similarities with fission modelling:
  neutronics, heating, thermal expansion, fluids
- Additionally need to model:
  tritium transport, electromagnetism, MHD ...
- Extreme conditions:
  e.g. in ITER: neutron heat loads $\sim 0.5MWm^{-2}$,
  magnetic fields $\sim 12T$ toroidal tension $\sim 100MN$
- More intricate geometries (e.g. ports): will require **billions** of elements



Modelling an SMR is already acknowledged to be an exascale challenge. [Image credit: exascaleproject.org]

Modelling of entire devices for fusion is an **exascale** endeavour!

Open Source Fusion Simulation

The need for rapid development necessitates adoption of dependencies.
But, typical commercial tools do not scale well beyond the desktop:
Need new tools!

Key requirements:

- Scalable: must be **high-performance**.
- Portable: must be **architechture-independent**.
- Flexible: must be **easily extensible**.
- Adoptable: must be **easy-to-use**.
- Future-proof: must be **maintainable**.
- Reliable: must adhere to **regulatory standards**.

These requirements must underpin our implementation decisions and motivate a fully **open-source** approach.

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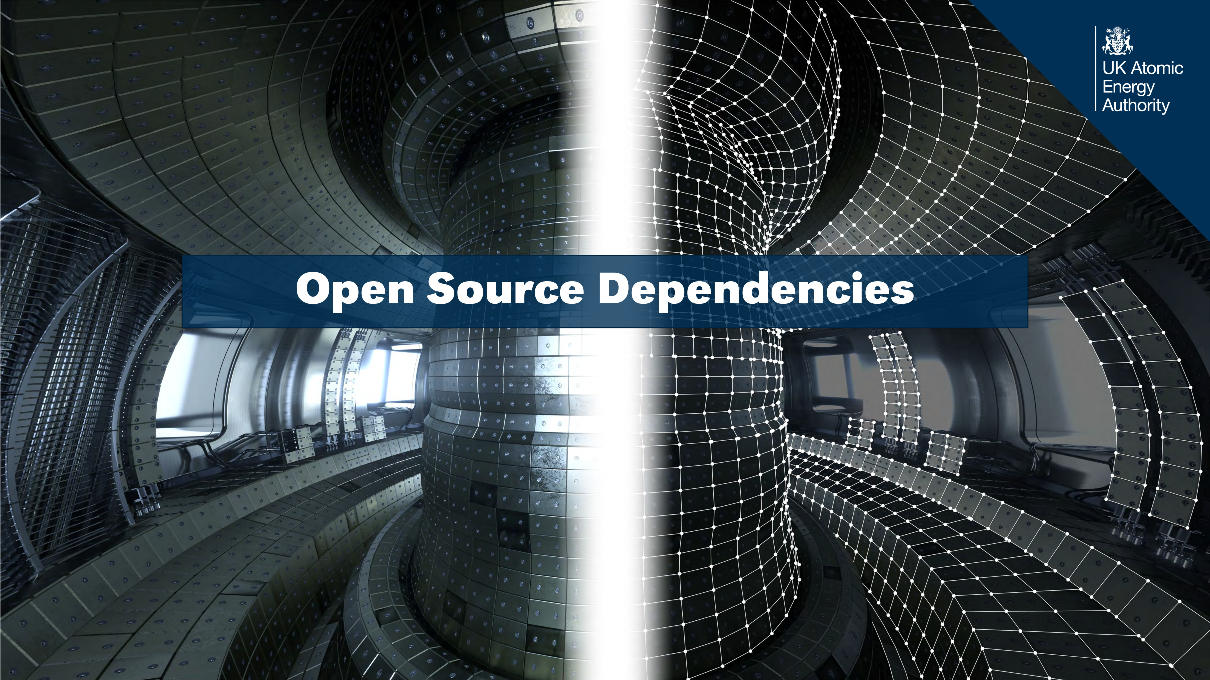
Open Source Dependencies



The MOOSE Framework for FEA

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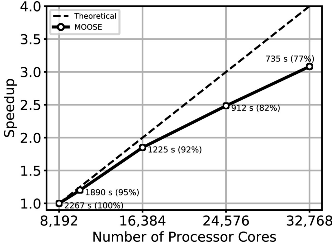
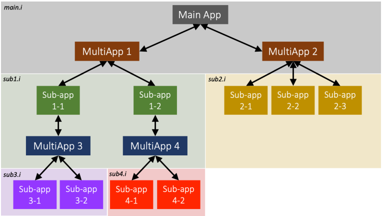
MOOSE selected for provision of finite element analysis based on the features:

- Performance
- Extensive existing physics modules
- Organising structure (e.g. MultiApps) conducive to tackling multiphysics / multiscale problems
- Open-source, easily extensible
- Support, documentation, usability
- Quality assurance





OpenMC for Neutron Transport

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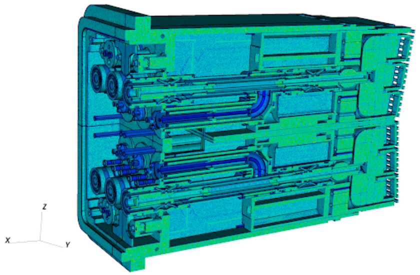
OpenMC:

- is a modern, scalable, open source Monte Carlo neutron transport code.
- performs tallying of scores on unstructured volume mesh with **MOAB**, **LibMesh**.
- natively employs constructive solid geometry (cells are enclosed by quadratic surfaces)
- employs **DAGMC** for particle tracking across arbitrary geometries.



Modelling the ITER Ion Cyclotron Resonant Heating (ICRH) port plug: very high fidelity is needed! Image credit[Andrew Davis]

DAGMC for Particle Tracking

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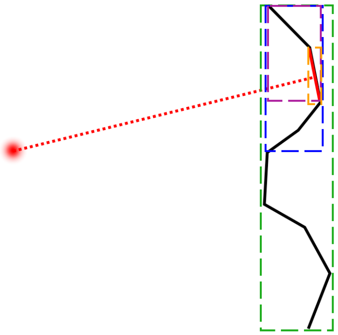
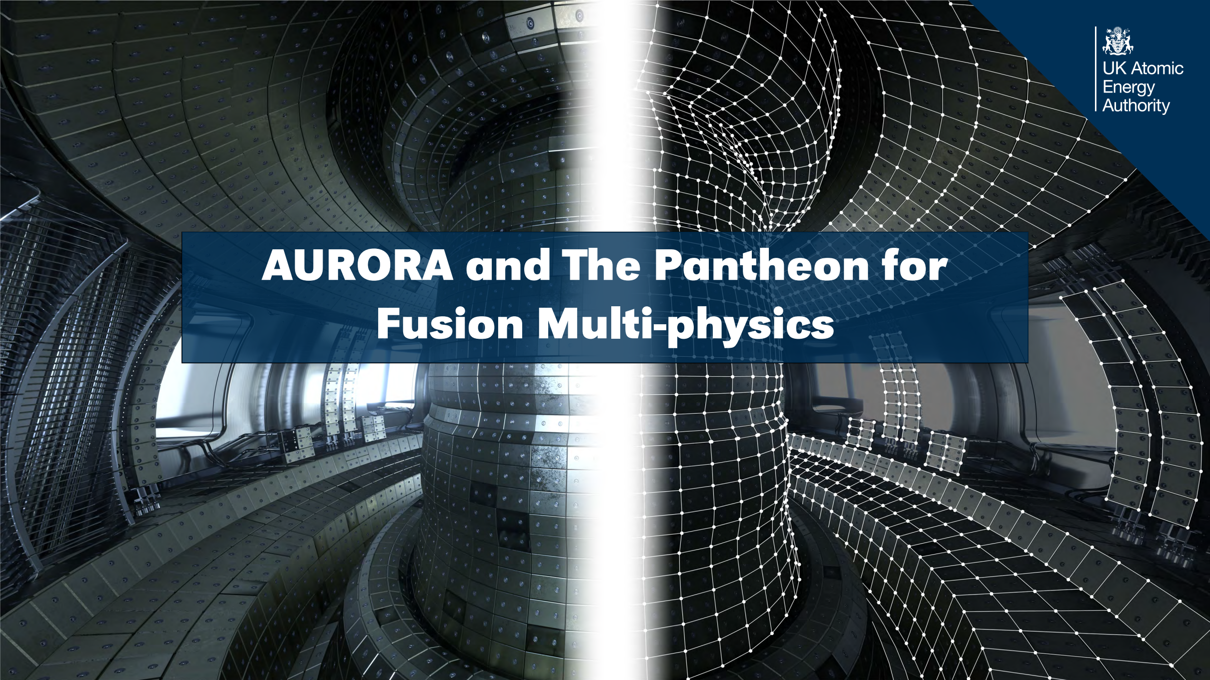
DAGMC:

- describes geometry in terms of logical volumes enclosed by faceted surfaces.
- uses **MOAB** for surface (triangle) mesh representation.
- employs ray tracing algorithms for particle tracking.
- accelerates “next surface” data queries with intelligent data structures (e.g. OBB trees).
- can optionally leverage **Intel Embree**’s ray tracing kernels via **double-down**.



Visual representation of a “next surface” query with an OBB tree.



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AURORA and The Pantheon for Fusion Multi-physics

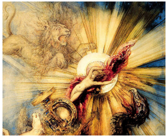
The Pantheon

A growing suite of MOOSE-based applications for fusion can be found at `https://github.com/aurora-multiphysics`.

AURORA
Neutronics+Thermomechanics
[Helen Brooks]

Achlys
Hydrogen ion transport
[Stephen Dixon]

Apollo
Electromagnetism
[Alexander Blair, William Ellis]



Phaeton
Fast ions with ASCOT5
[Matthew Bluteau]

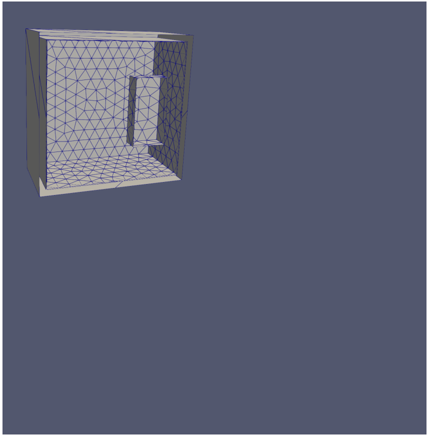
Proteus
Turbulent fluid flow
[Aleksander Dubas]

Cf. Andrew Davis' poster yesterday
"Open Source Tools in Support of Multiphysics for Fusion".

AURORA: The Algorithm

AURORA is **A** **U**nified **R**esource for **O**penMC (fusion) **R**eactor **A**pplications.

- OpenMC performs neutron transport using DAGMC to enable particle tracking across arbitrary geometries.



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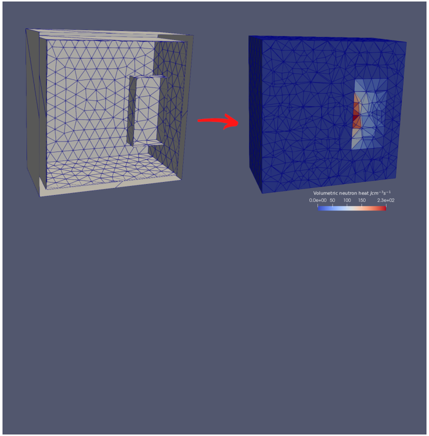

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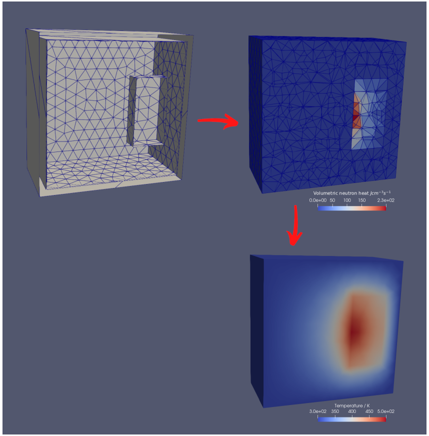

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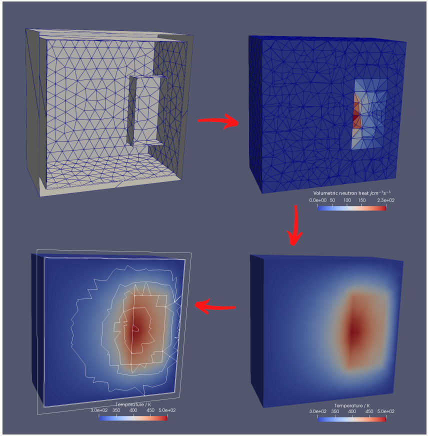
- Bin mesh elements by temperature and density to define new DAGMC surfaces and OpenMC materials.



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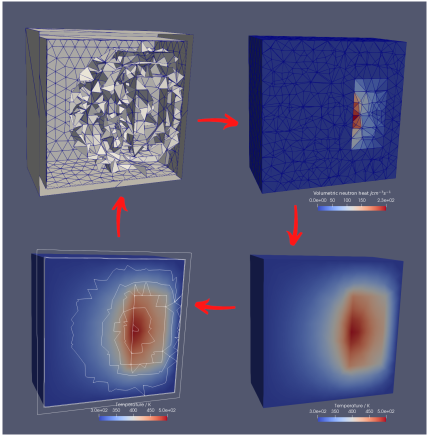
- Iterate until stopping criterion is reached.



AURORA: Quality Assurance

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- Unit and integration tests with **GTest**
- Code coverage estimates with **coveralls**
- Continuous integration with **GitHub Actions** and **docker** containers
- User documentation generated with MOOSE docs
- Developer API generated with **Doxygen**
- **GitHub Pages**
- Collaboration guidelines
- Installation instructions
- Versioning

AURORA: Scalability

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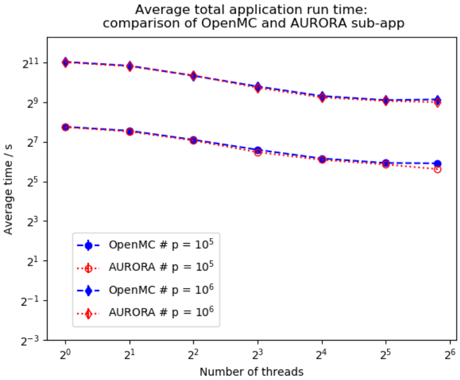

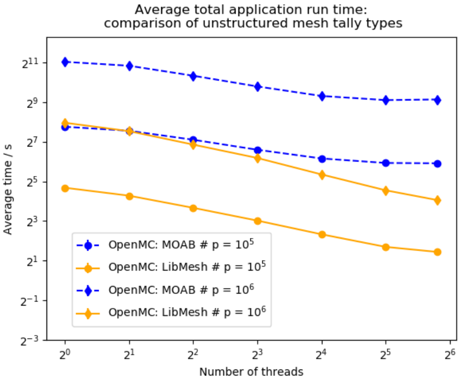

Shared memory performance: no measurable penalty in wrapping OpenMC in a MOOSE sub-app.

AURORA: Breeder Blanket Demonstration

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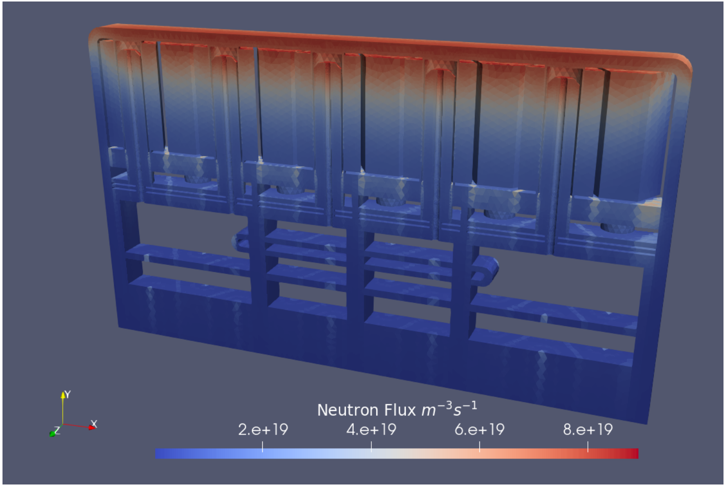

Irradiate with a monodirectional plane source of neutrons to emulate plasma. Neutrons do not propagate far into the blanket.

AURORA: Breeder Blanket Demonstration

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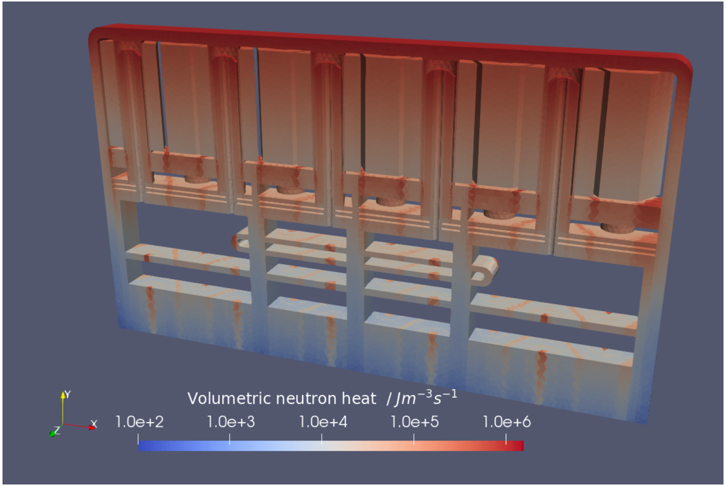
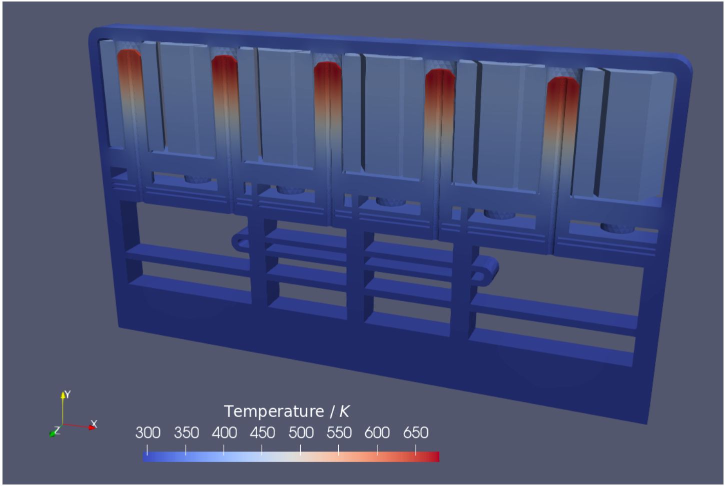


Neutrons primarily deposit heat on innermost components.

AURORA: Breeder Blanket Demonstration



Steel support stays cool due to thermal properties and proximity to cooling channels, while breeder pins heat up.

AURORA: Breeder Blanket Demonstration

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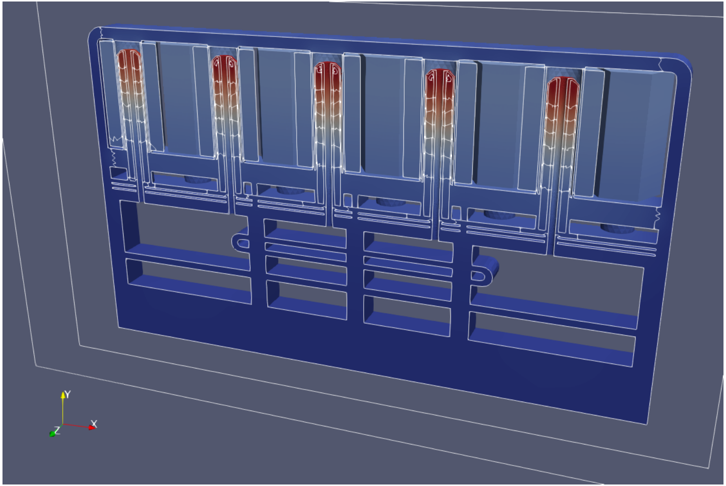
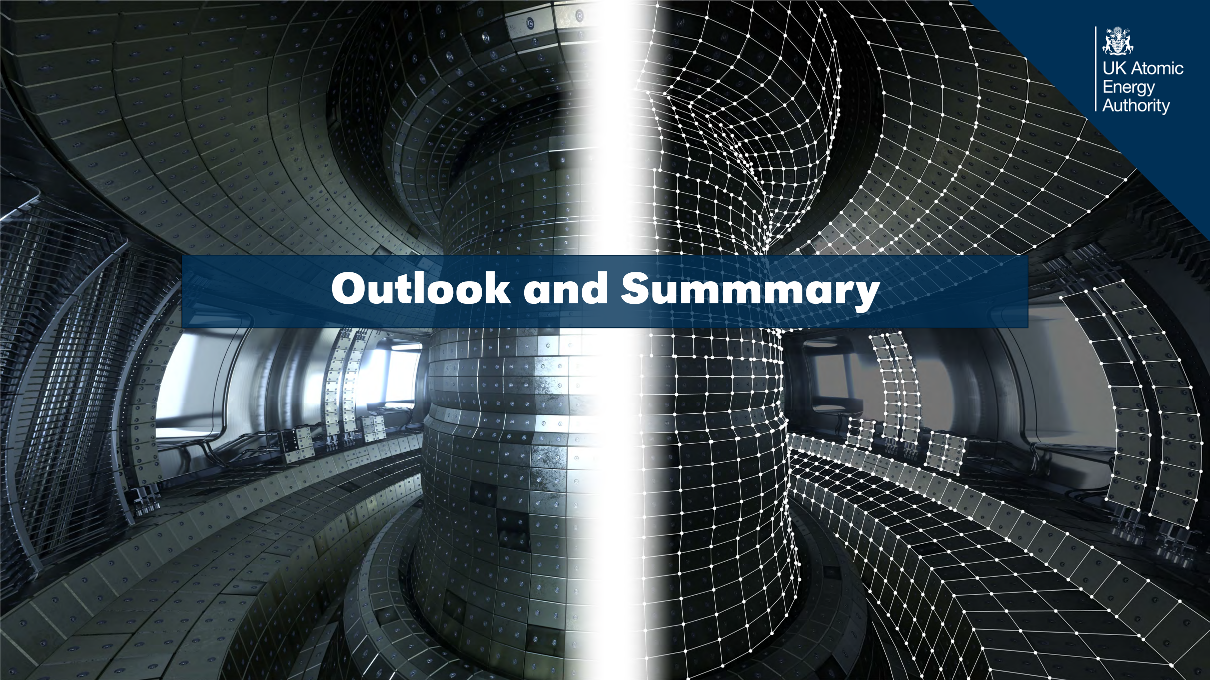


New OpenMC materials are defined in the pins.



Outlook and Summmary

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Summary

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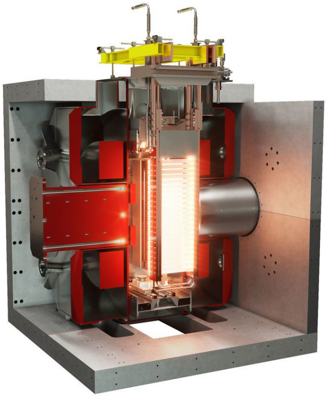
Our goal is to create open-source, performant, user-friendly, architecture-agnostic multiphysics and multiscale engineering tools for fusion reactors.

Our new code **AURORA**:

1. represents a first step towards this goal, focusing on tightly-coupled neutronics and thermomechanics.
2. leverages existing proven codes e.g. MOOSE, OpenMC, DAGMC.
3. is intended to couple with a suite of other under-development tools that focus on electromagnetism, fluids, tritium transport and fast ions.
4. would not have been possible without an open-source approach.

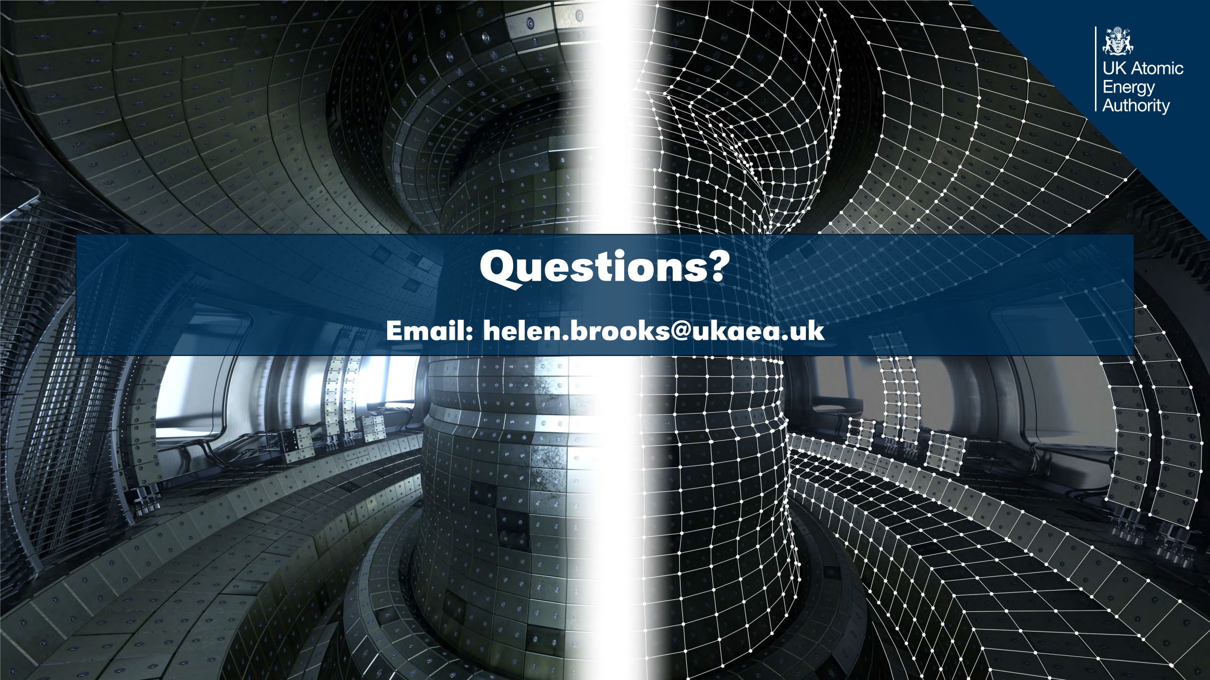
Future Work

We can only serious about fusion reactor digital twins if we can **validate** our software, not only for standalone-physics but also coupled physics scenarios.



Artist's impression of CHIMERA facility.

- Validation of neutronics using data from facilities such as n_TOF, ISIS, ESS, SNS.
- Validation of multiphysics couplings will be supported through testing facilities such as HIVE and CHIMERA.
- Digital Twinning of CHIMERA will first require couplings to other domains such as fluids and electromagnetism; inclusion of these couplings is a high priority.



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Questions?

Email: helen.brooks@ukaea.uk