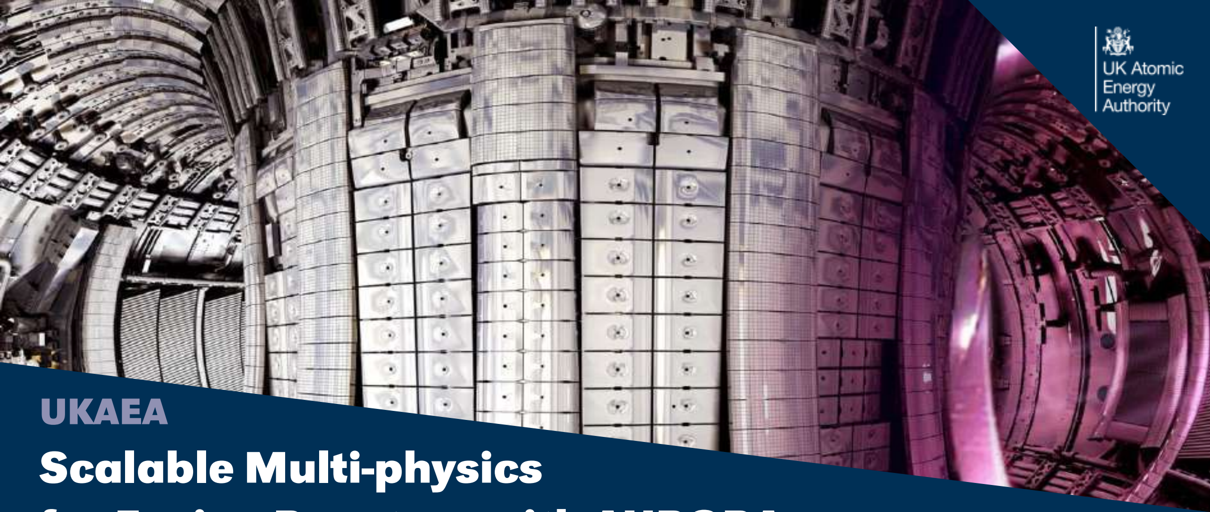

UKAEA

Scalable Multi-physics for Fusion Reactors with AURORA

2nd Fusion HPC Workshop

02/12/2021

Helen Brooks (speaker), Andrew Davis

Overview

UK Atomic
Energy
Authority

1. Introduction
2. A New Tool for Multi-physics: AURORA
3. Illustrative Results
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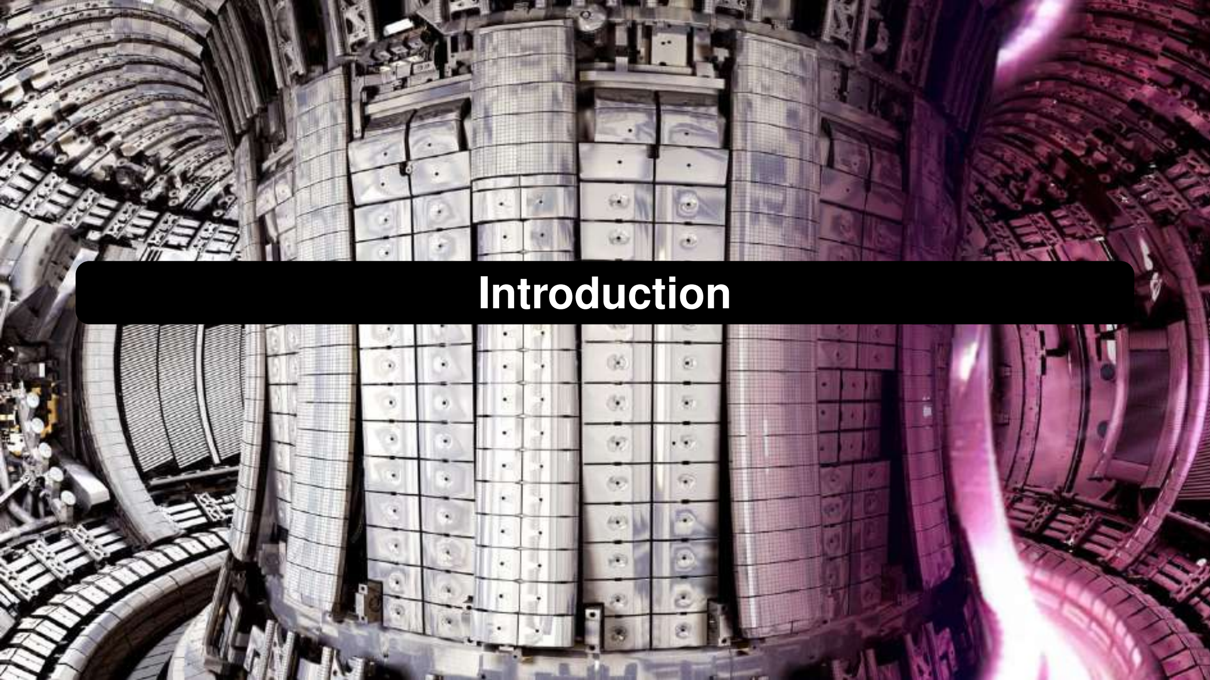
Introduction



Context: Fusion for Energy Production

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

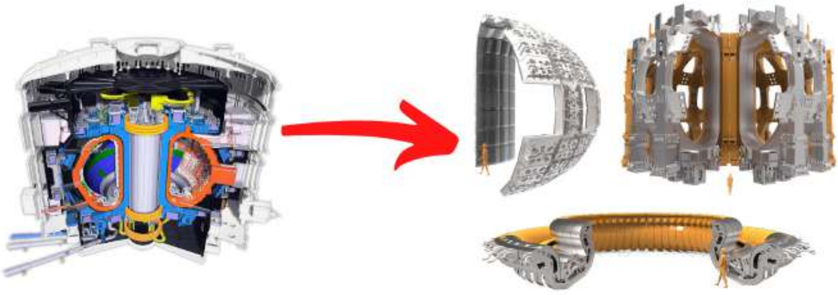
The STEP (Spherical Tokamak for Energy Production) project has the mission:

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

There is an urgent need for accessible and user-friendly engineering software tools to facilitate the design of future fusion reactors.

Vision: Digital Twins for Tokamaks

Digital twinning of tokamaks is widely acknowledged to be an exascale problem.



ITER systems (Image credit: iter.org)

- To start, focus on critical components: blanket, magnets, and divertor.
- Requires all key physics areas: neutronics, thermodynamics, mechanics and contact, electromagnetism, fluid dynamics, damage, and tritium production.

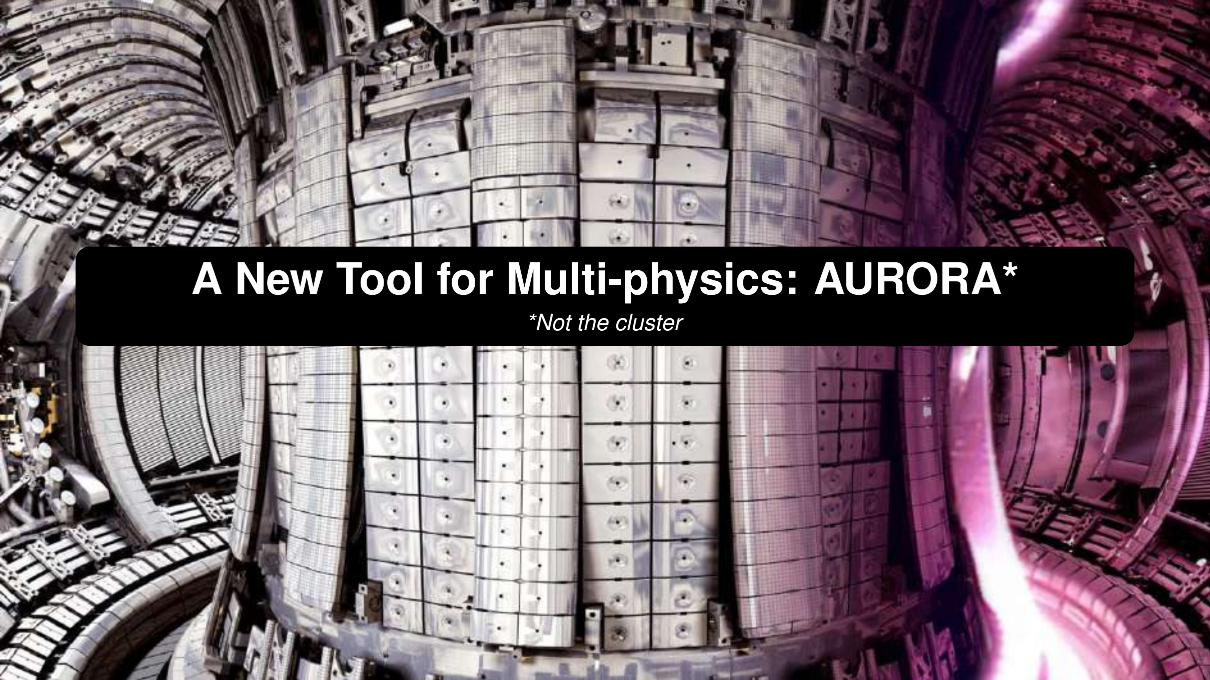
Goal: Open Fusion Engineering Software

Typical engineering analysis workflows use commercial tools which do not scale well beyond the desktop: need to develop a suite of HPC engineering analysis tools.

Key requirements:

- Adoptable: must be **easy-to-use**.
- Portable: must be **architechture-independent**.
- Reliable: must adhere to **regulatory standards**.
- Future-proof: must be **maintainable and extensible**.

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



A New Tool for Multi-physics: AURORA*

**Not the cluster*

A New Tool for Multi-physics: AURORA

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

AURORA is a tool created with the MOOSE framework, designed to tightly couple Monte Carlo neutron transport with thermomechanics through finite element analysis.

- AURORA is fully open-source, licensed under LGPLv2, and available at `https://github.com/aurora-multiphysics/aurora`.
- Idea is to feed back the impact of temperature and density changes that result from neutron heating back into the neutronics calculation.

Roman goddess of the dawn, Aurora, depicted in ceiling fresco by Guido Reni (1614).

AURORA Dependencies

We leverage a host of proven, scalable, open-source, community-driven, user-focused libraries.

MOOSE

libMesh

PETSc

OpenMC

DAGMC

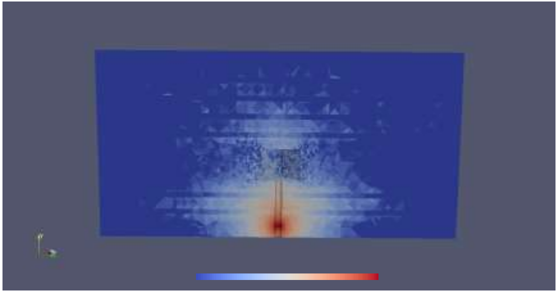
MOAB

- **MOOSE** is a finite element framework built upon **libMesh** for meshing and **PETSc** for linear algebra / preconditioning. It is modular, extensible, hierarchical, performant (scales to 32000 cores), and adheres to software quality standards.
- **OpenMC**: modern, scalable Monte Carlo neutronics code.
- **DAGMC**: library to enable performant particle transport on CAD geometries.
- **MOAB**: meshing library utilised by DAGMC.

The Algorithm

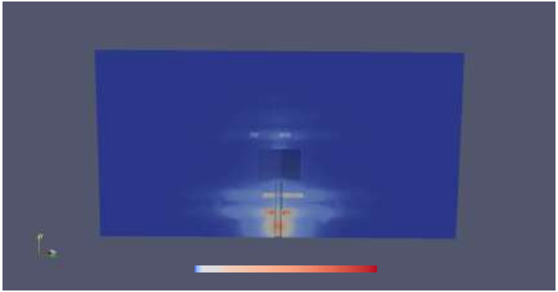
1. OpenMC performs transport of neutrons upon a geometry with DAGMC surfaces.

Tallies such as flux and heat are scored upon an unstructured volume mesh that is initialised by MOOSE and passed to OpenMC in memory.



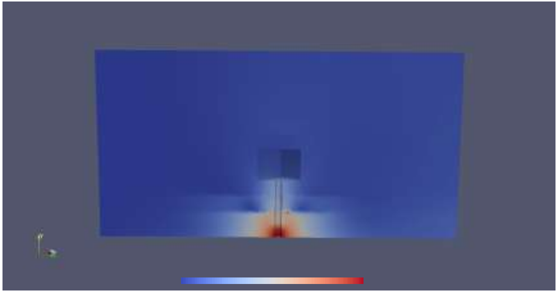
The Algorithm

2. The tallied heat is returned to MOOSE and stored as a variable where it provides a source term for transient heat conduction.



The Algorithm

3. MOOSE solves for coupled temperature and displacement arising from thermal expansion for a user-defined time step.

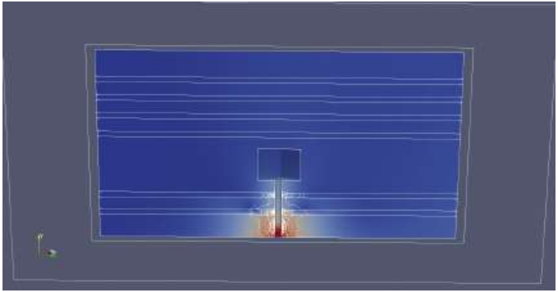


The Algorithm

4. Elements are sorted into local temperature and density regions that are defined through binning.

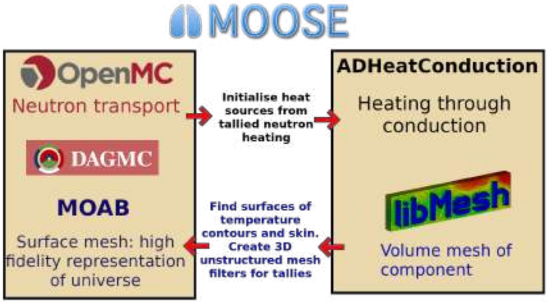
The surfaces of these regions are found using MOAB’s in-built skinning operation.

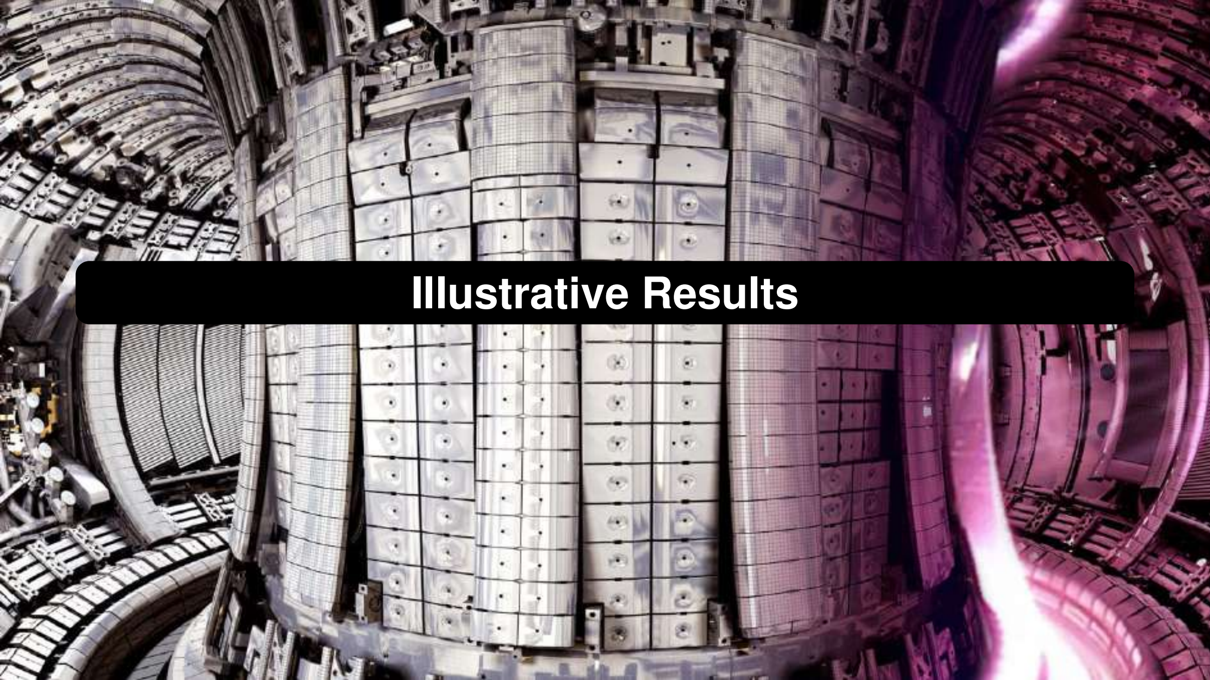
These regions define new OpenMC materials having updated DAGMC surfaces and nuclear cross sections.



The Algorithm

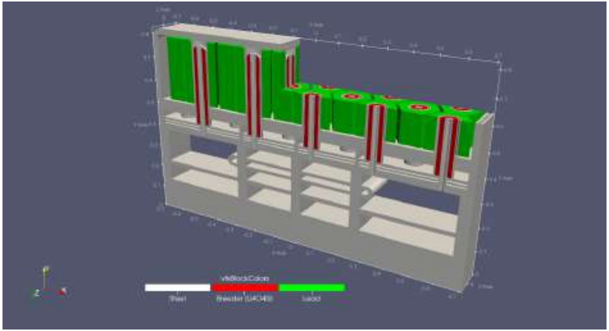
5. This procedure is repeated for the desired number of time steps or until a desirable stopping criterion is reached.





Illustrative Results

Example: Simplified Blanket Model



- Unstructured tetrahedral mesh with 1.6×10^5 DOFs
- Dimensions: $1.4 \times 0.8 \times 0.1m^3$
- Materials:
  - Steel support structures
  - Lithium orthosilicate breeder
  - Lead neutron multiplier

Analysis Set up

FEA:

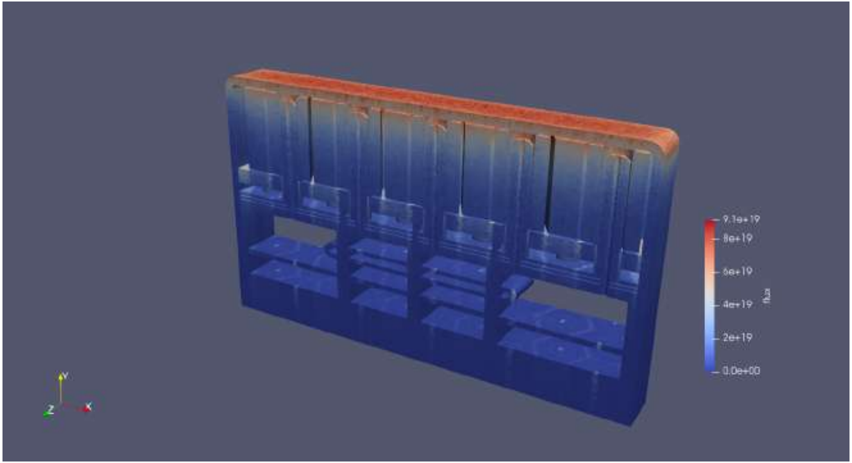
- Transient heat conduction over $1000s$.
- Initial $T_0 = 293.15$ K
- Emulate cooling from pipes with 2 heat transfer coefficient (HTC) BCs with $T_\infty = 293.15$ K :
    - Inner HTC = 309 $Wm^{-2}K^{-1}$
    - Outer HTC = 7.8 $Wm^{-2}K^{-1}$

MC:

- Monodirectional uniform neutron source in $x - z$ plane with at $y = 0.88m$ (proxy for plasma).
- Neutron source strength: $10^{17}s^{-1}$
- 10 batches of 2.5×10^5 particles.

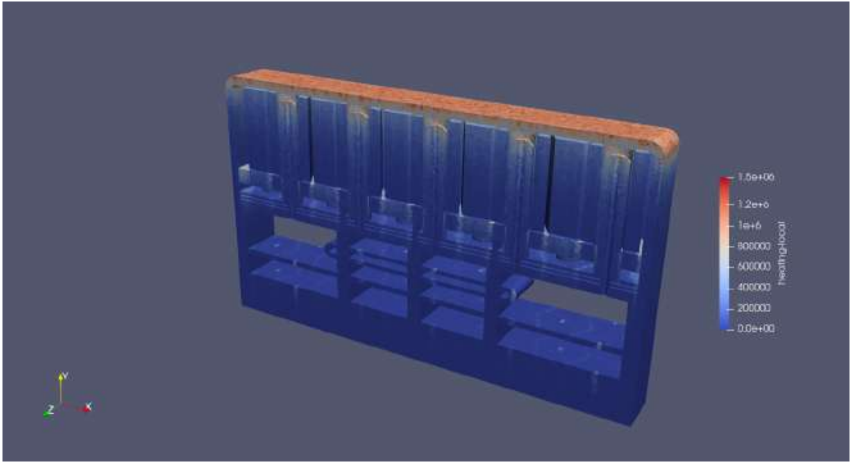
N.B.: Analysis is only demonstrative, not necessarily fully accurate.

Results



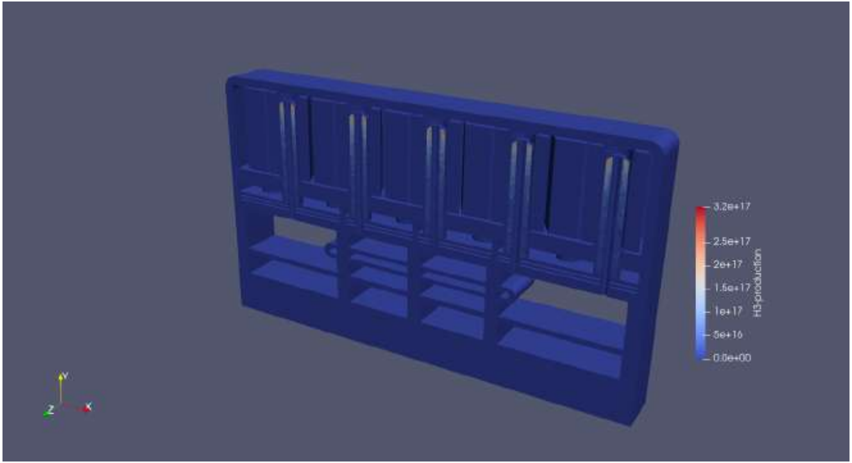
Neutron Flux [m^{-3}].

Results



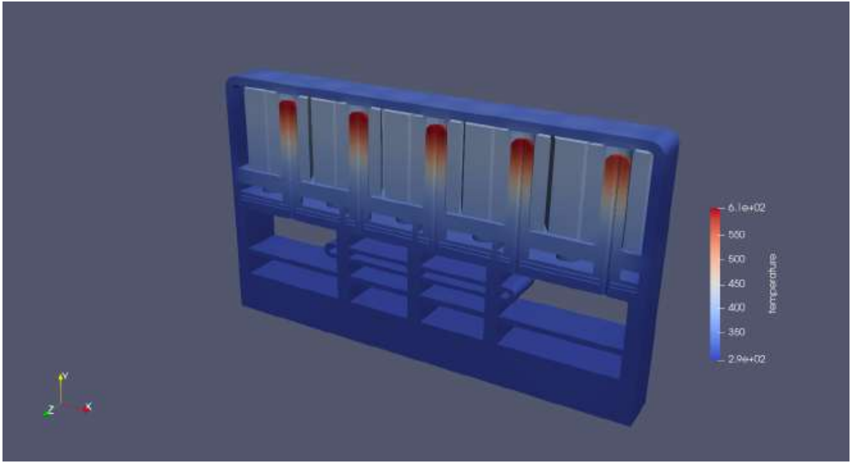
Neutron heat flux $[W m^{-3}]$

Results



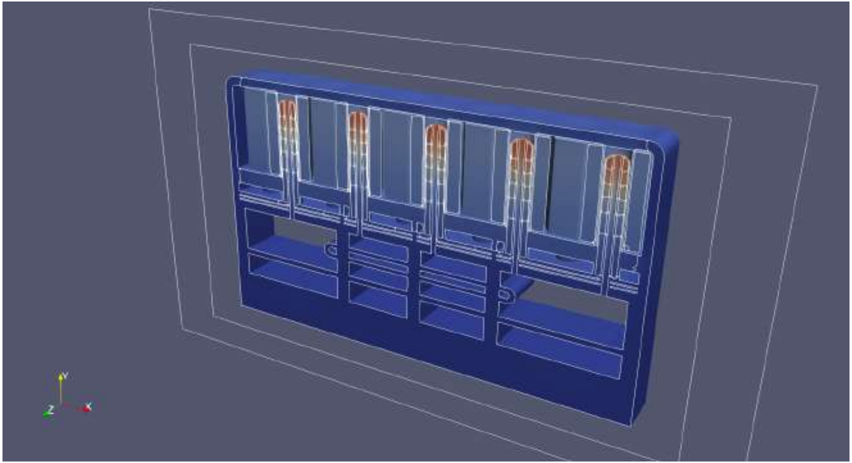
Tritium production $[m^{-3}]$

Results



Temperature $[K]$

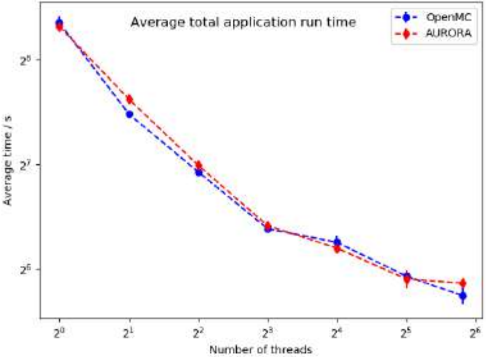
Results



Temperature $[K]$ contours

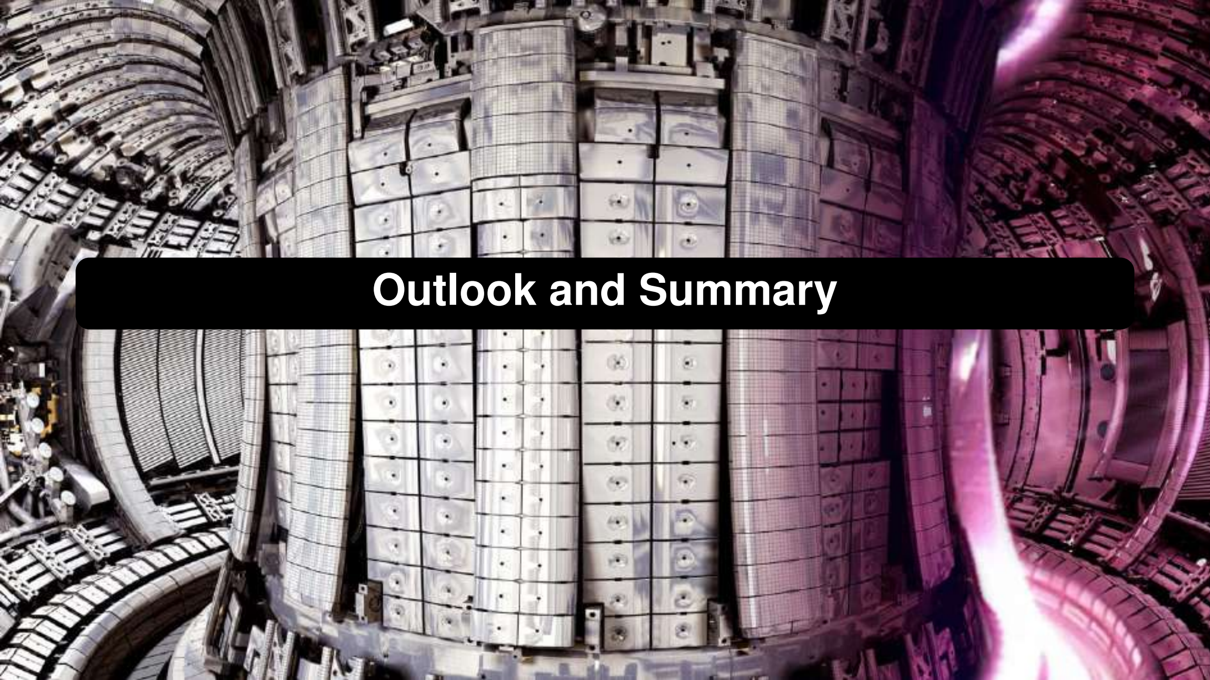
Shared-memory Parallel Scaling

Perform comparison of run times for OpenMC run directly against the MOOSE-wrapped sub-application (no FEA) used in AURORA.



- OpenMC tends to scale well with threads: so compare run-times on a single node.
- Average over 10 runs, each having 10 batches of 10^5 particles, tallying on a mesh with 1.2×10^4 elems.
- Initial results indicate that wrapping OpenMC in a MOOSE application does not introduce any significant overhead.

Outlook and Summary



Outlook: Physics Analysis

This is only the first step in our journey.

Next steps:

- Perform systematic study on impact of tightly coupling neutronics and thermomechanics.
- Couple to fluids - investigate the impact of neutronics on cooling (and vice versa).
- Couple to tritium transport - investigate impact of temperature on tritium breeding.

There's still more mountain to climb.
(Image: photo of Ben Lomond, New Zealand)

Outlook: Performance

We have only scratched the surface of parallel performance so far.

Next steps:

- Perform benchmarking for models with higher fidelity: greater numbers of mesh elements and particles per batch.
- Perform benchmarking with distributed memory and hybrid parallelism.
- Attain recommendations for optimal distribution of MPI tasks and threads for fully coupled FEA+neutronics.

See also

Julia Inca Chiroque's talk *"Scalable solution of the Linear Elasticity Equations in 3D"* **today at 16.35** for a scalability benchmarking study using MOOSE for a variety different preconditioners.

Outlook: The Multiphysics Pantheon

AURORA is not intended to work alone!

A growing suite of MOOSE applications are currently under development at `https://github.com/aurora-multiphysics`:

- **Apollo** (Roman god of the sun) : a set of electromagnetism modules.
- **Phaeton** (Greek god who lost control of sun chariot) : application coupling to fast ions with ASCOT5.
- **Achlys** (Greek goddess of mist) : application modelling tritium transport.

Apollo (Guido Reni - 1614)

Phaeton (Gustave Moreau - 1878)

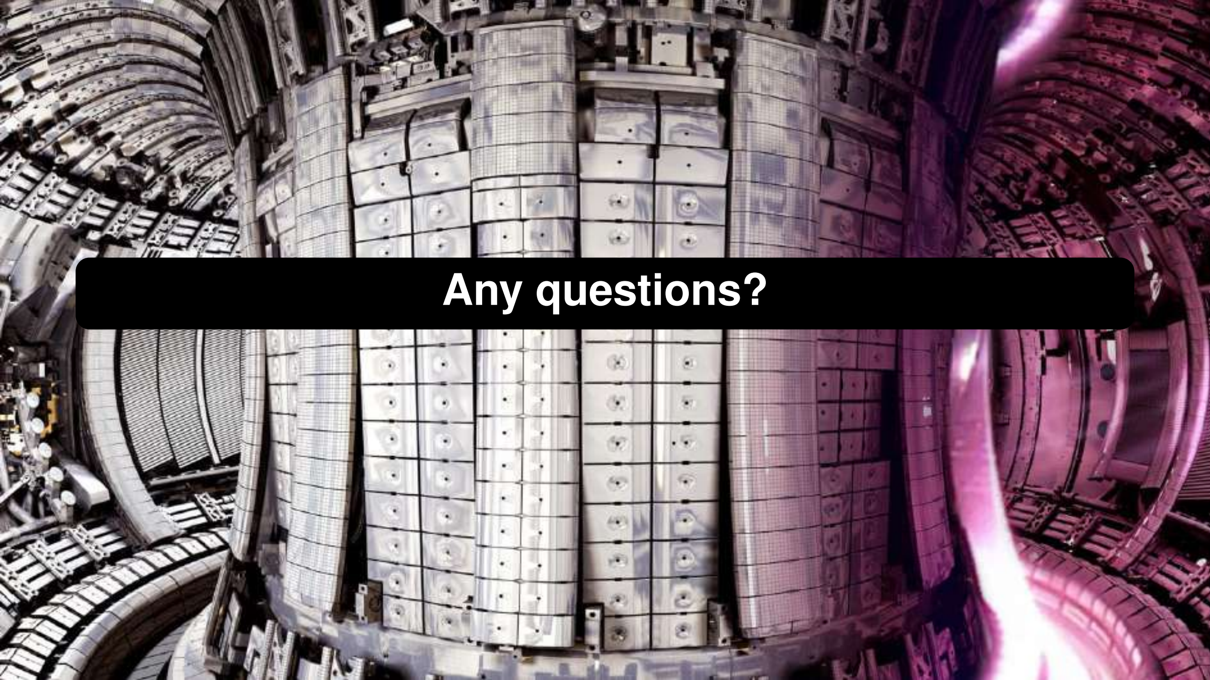
MOOSE has support for recursive multi-app structures: these can be **trivially combined**.

Conclusion

Our goal is to create user-friendly, open-source, 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 FEA and Monte Carlo transport codes (MOOSE, OpenMC, DAGMC).
3. is intended to couple with a suite of other under-development tools that focus on electromagnetism, tritium transport and fast ions.



Any questions?