UK Atomic Energy Authority

1st Spanish Fusion HPC Workshop

Evaluating Exascale FEA Backends for Fusion Digital Twins

2020-11-27

Aleksander J. Dubas

Outline

UK Atomic Energy Authority

Motivation

Selection Criteria

Shortlist

Benchmarking Methodology

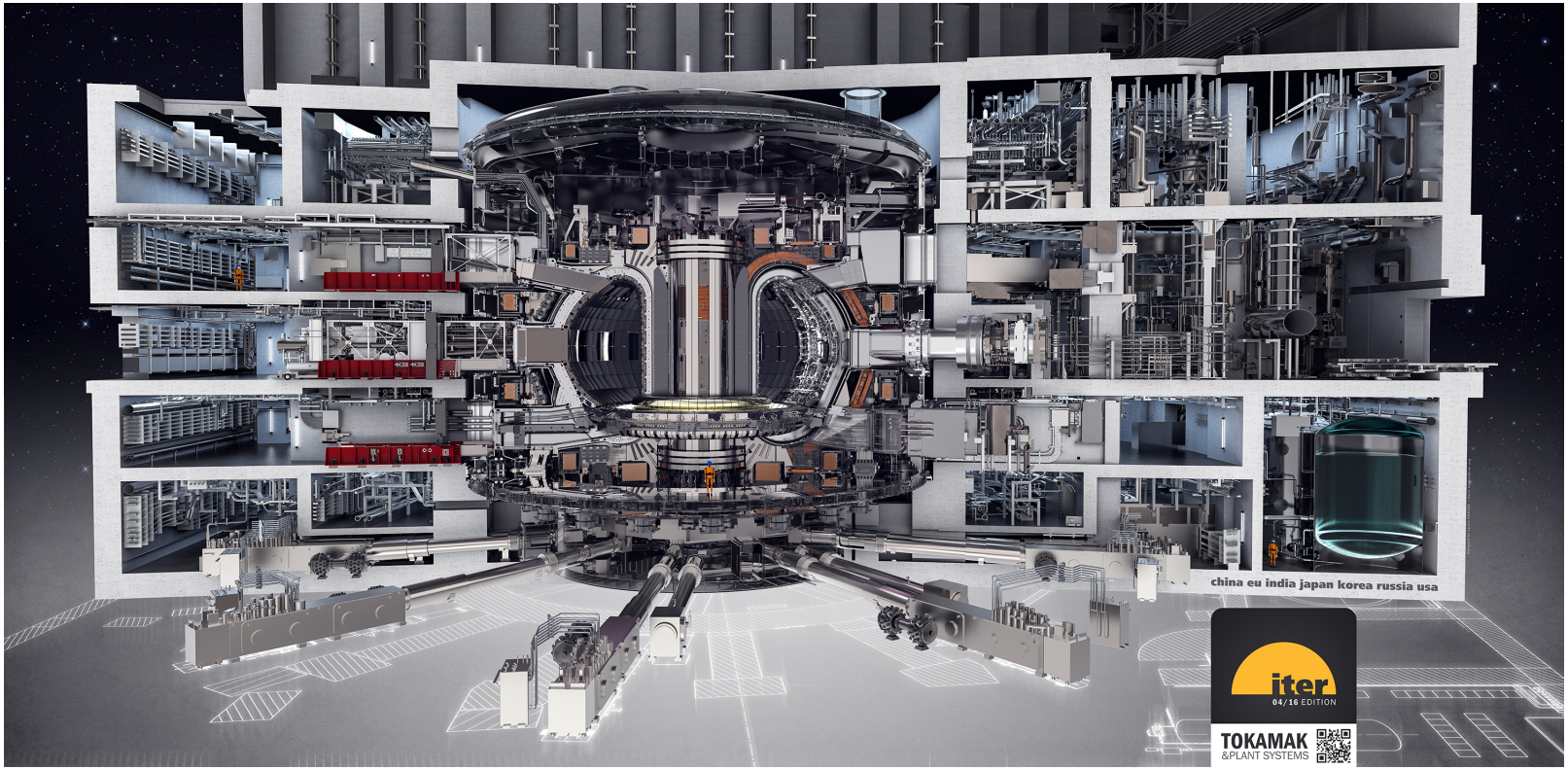
Results

Section 1

Motivation

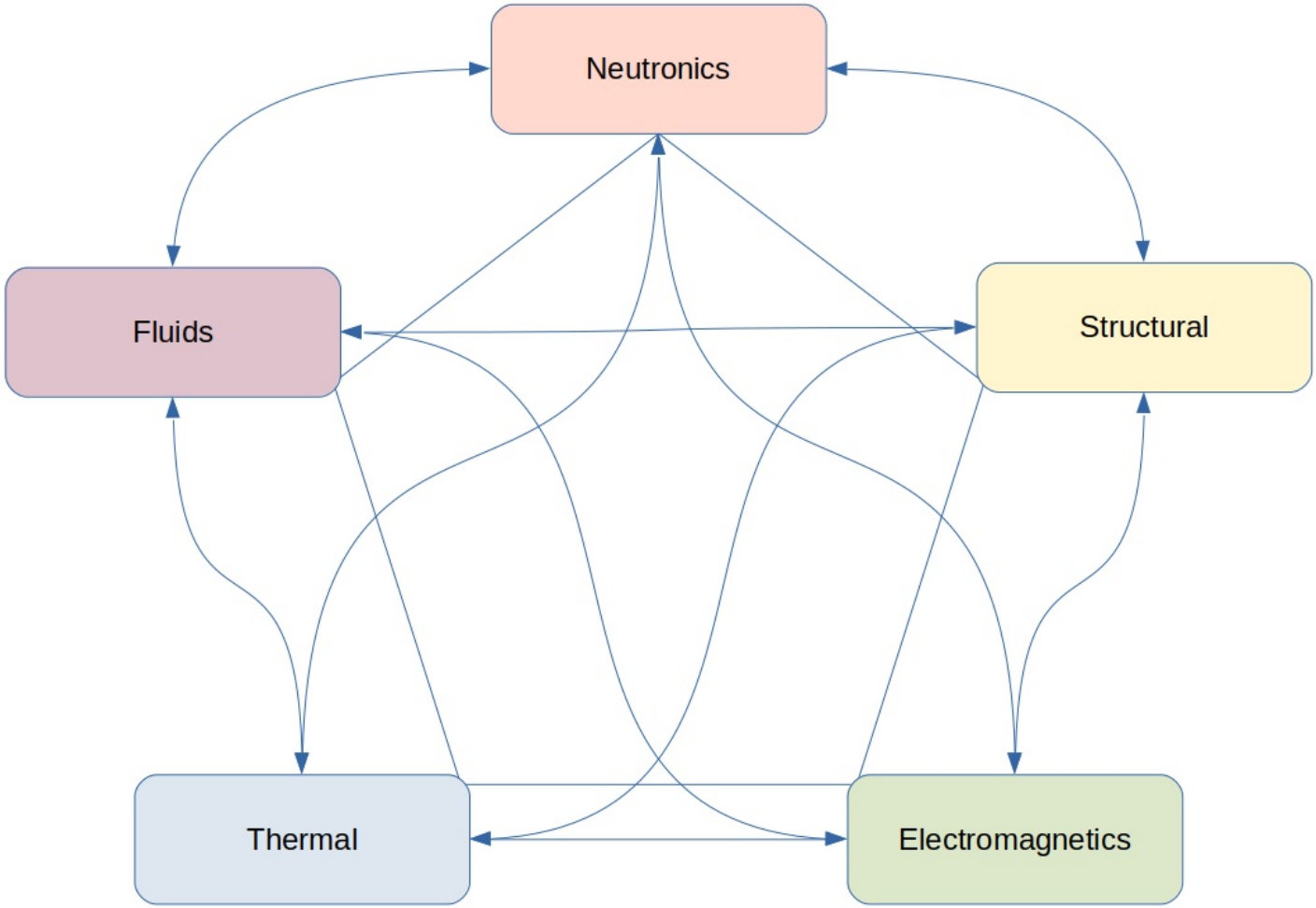
Why Digital Twin?

UK Atomic Energy Authority



Complex Multiphysics

UK Atomic Energy Authority



Two Approaches

UK Atomic Energy Authority

Single tightly coupled simulation

- One single program
- Solve a large linear system for all the physics involved
- Ensures capture of strongly coupled physical phenomena
- Solution may be numerically stiff

Many loosely coupled simulations

- Use best in class for each domain
- Couple together with a third party library and iterate
- Temporal accuracy may suffer
- Easy to decouple irrelevant physics

Section 2

Selection Criteria

1 - Parallel First

UK Atomic Energy Authority

Exascale simulation

Designed as a parallel code from the outset

Optimised for HPC environment

2 - Permissively Licensed

UK Atomic Energy Authority

Any location, including w/o internet

Any number of processes

Extension and modification permitted

Open source?

3 - Portable

UK Atomic Energy Authority

What does the exascale look like?

Vectorised? Mixed-mode? GPU?

4 - Extensible

UK Atomic Energy Authority

Open to external contribution

Good software engineering practices

5 - Supported

UK Atomic Energy Authority

User community - forums, mailing lists, IRC, workshops and tutorials

Documentation - for both users and developers

Compiled Language?

UK Atomic Energy Authority

Interpreted languages incur an overhead

Example: FEniCS vs. DOLFIN

At scale, overheads add up

Stable API, Actively Developed

UK Atomic Energy Authority

A reliable library must have a stable API, thus not in ’alpha’ or ’beta’ development

To be actively supported, it must be actively developed

Section 3

Shortlist

Initial Survey and Elimination

UK Atomic Energy Authority

Initial survey found 35 potential candidates

Eliminated those the were:

- not parallel first or HPC oriented,
- in early development,
- poorly supported,
- inextensible or
- abandoned.

Benchmarking Shortlist

UK Atomic Energy Authority

deal.ii	www.deallii.org
DUNE	www.dune-project.org
DOLFIN	fenicsproject.org
libMesh	libmesh.github.io
MFEM	mfem.org
MOOSE	mooseframework.org
Nektar++	www.nektar.info

Section 4

Benchmarking Methodology

Test Problem

UK Atomic Energy Authority

Steady State: Poisson Equation

$$-\nabla^2 u = f$$

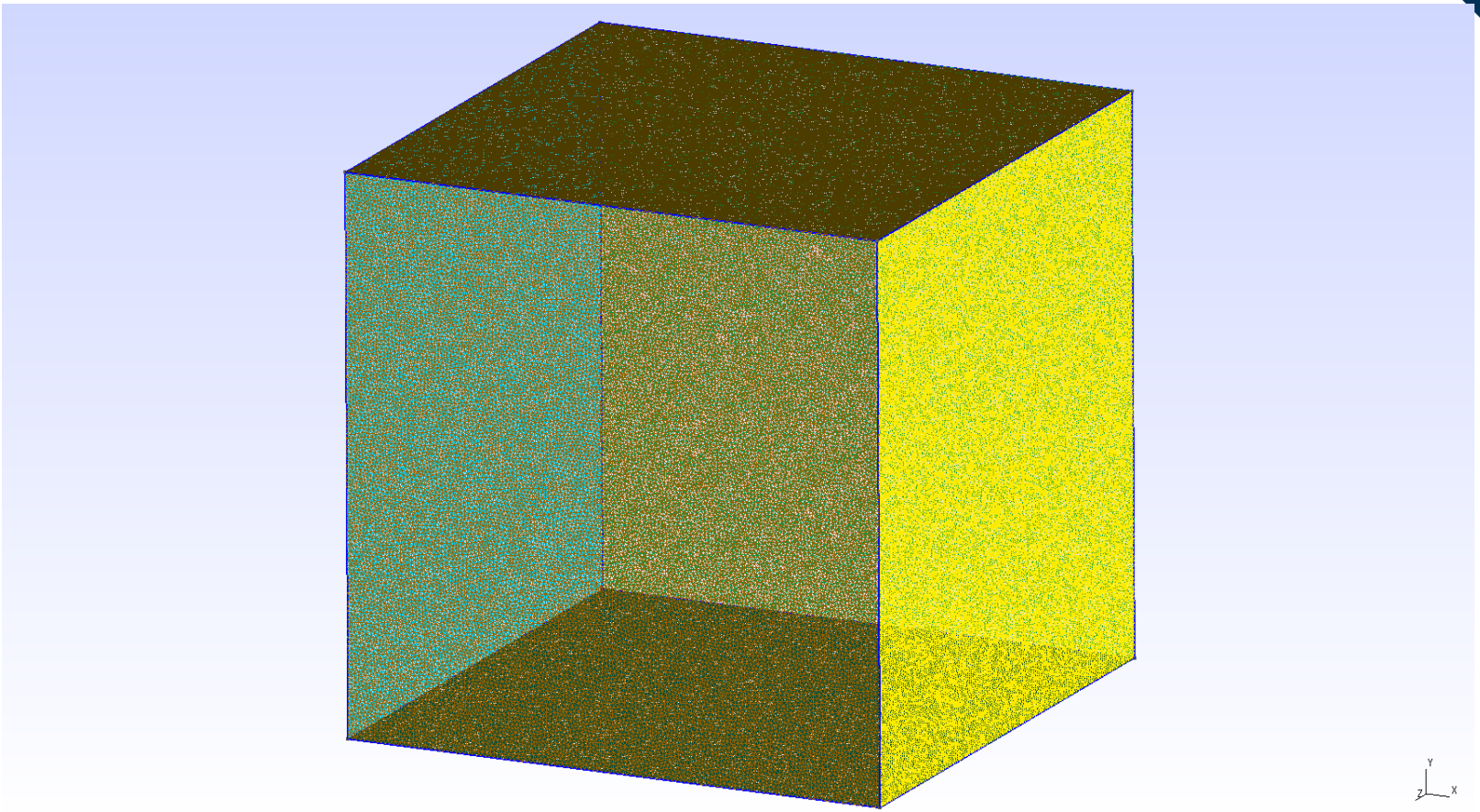
Time Dependent: Heat Equation

$$\frac{\partial u}{\partial t} - \nabla^2 u = f$$

using Method of Manufactured Solutions (MMS) to verify correctness

Geometry and Mesh

UK Atomic Energy Authority



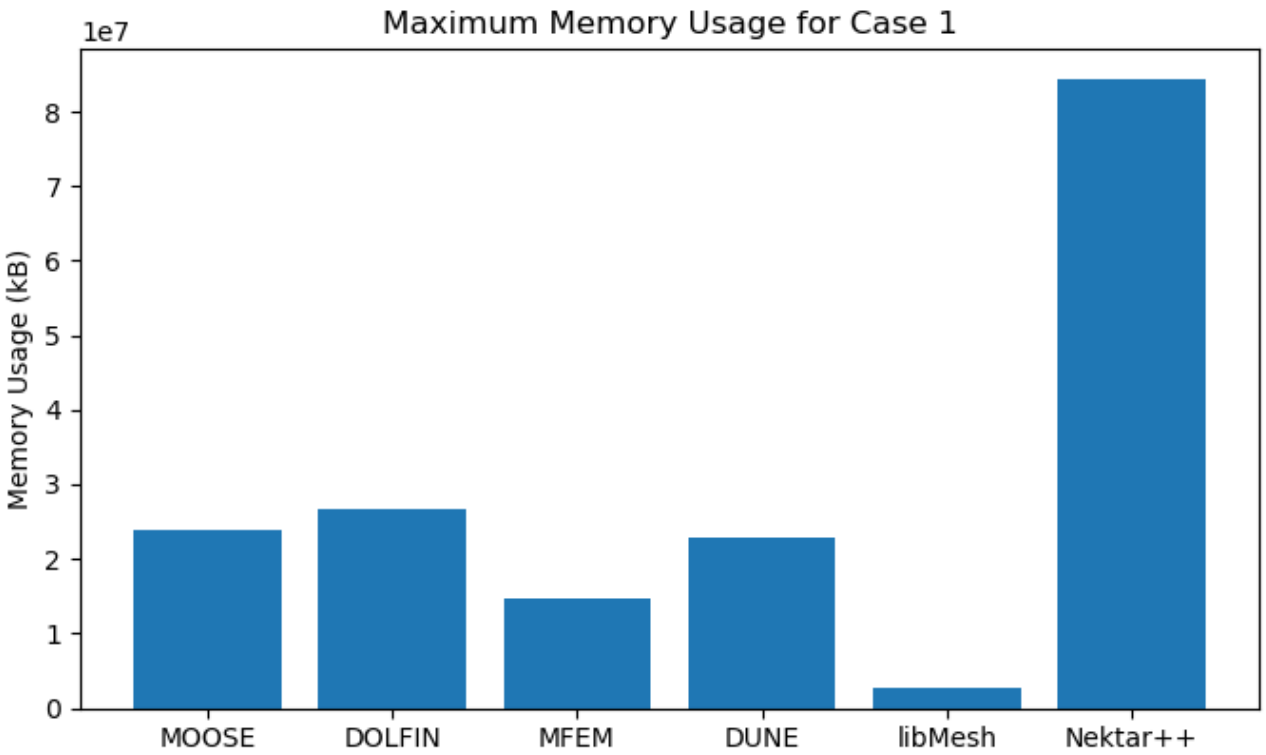
deal.ii ruled out (designed for quad/hex meshes)

Section 5

Results

Memory Usage

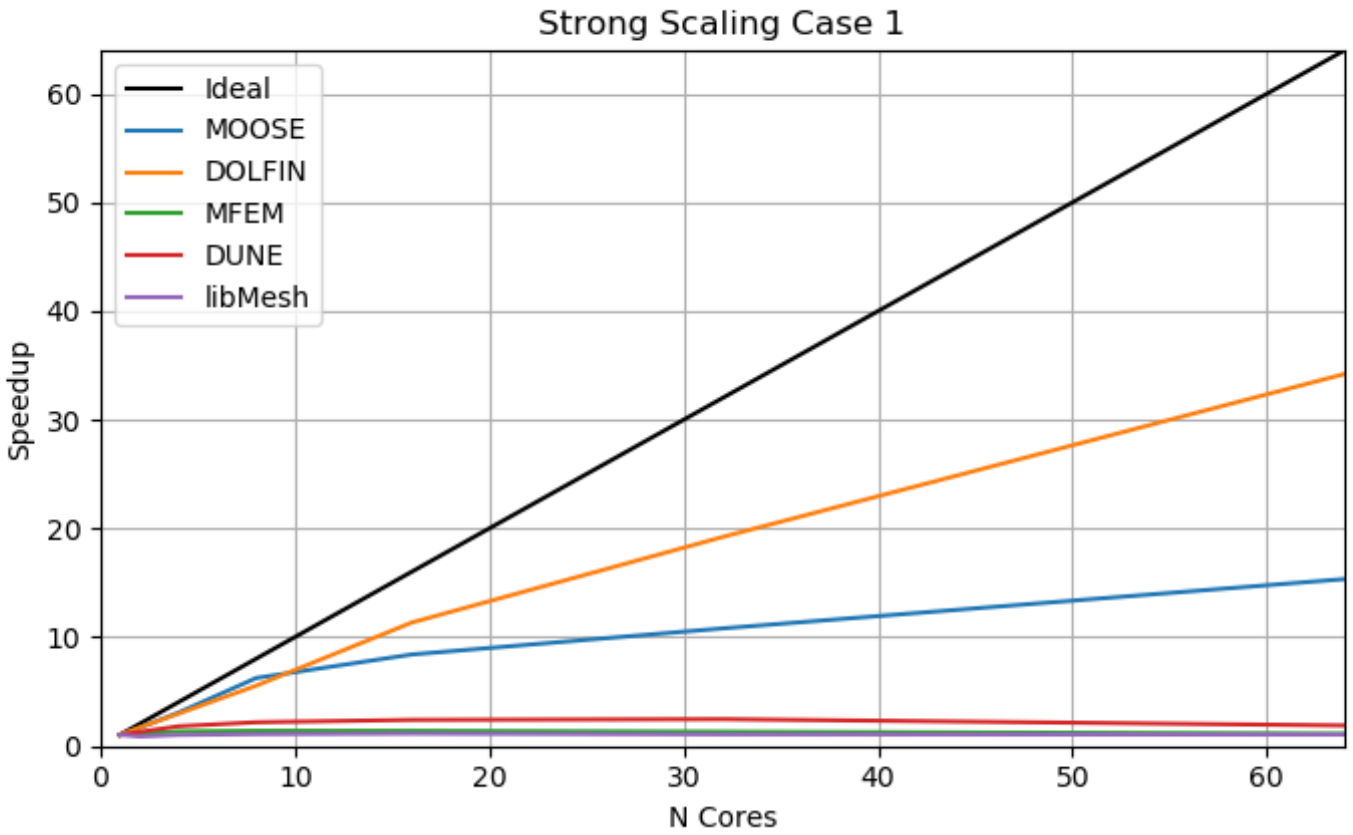
UK Atomic Energy Authority



Nektar++ ruled out (memory usage)

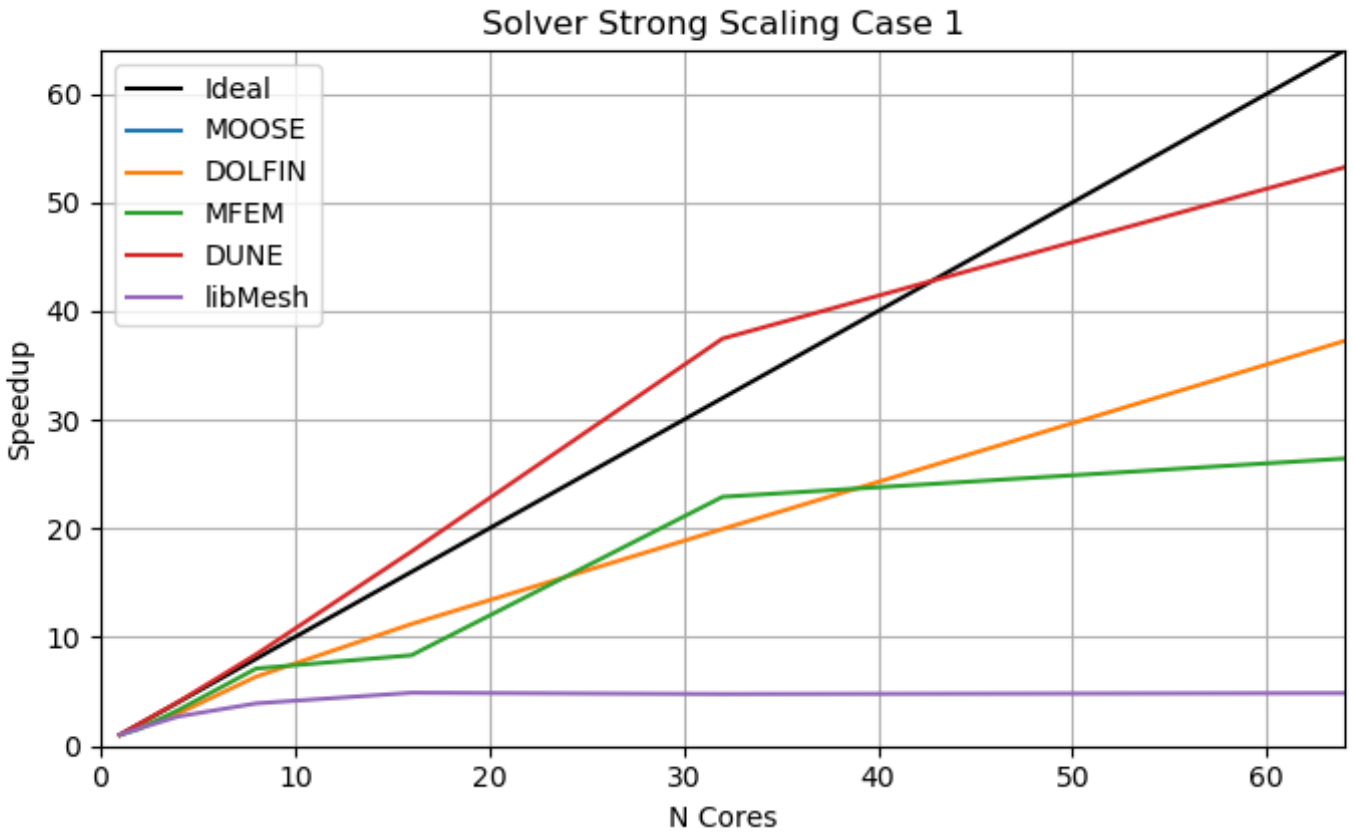
Scaling (Total Time)

UK Atomic Energy Authority



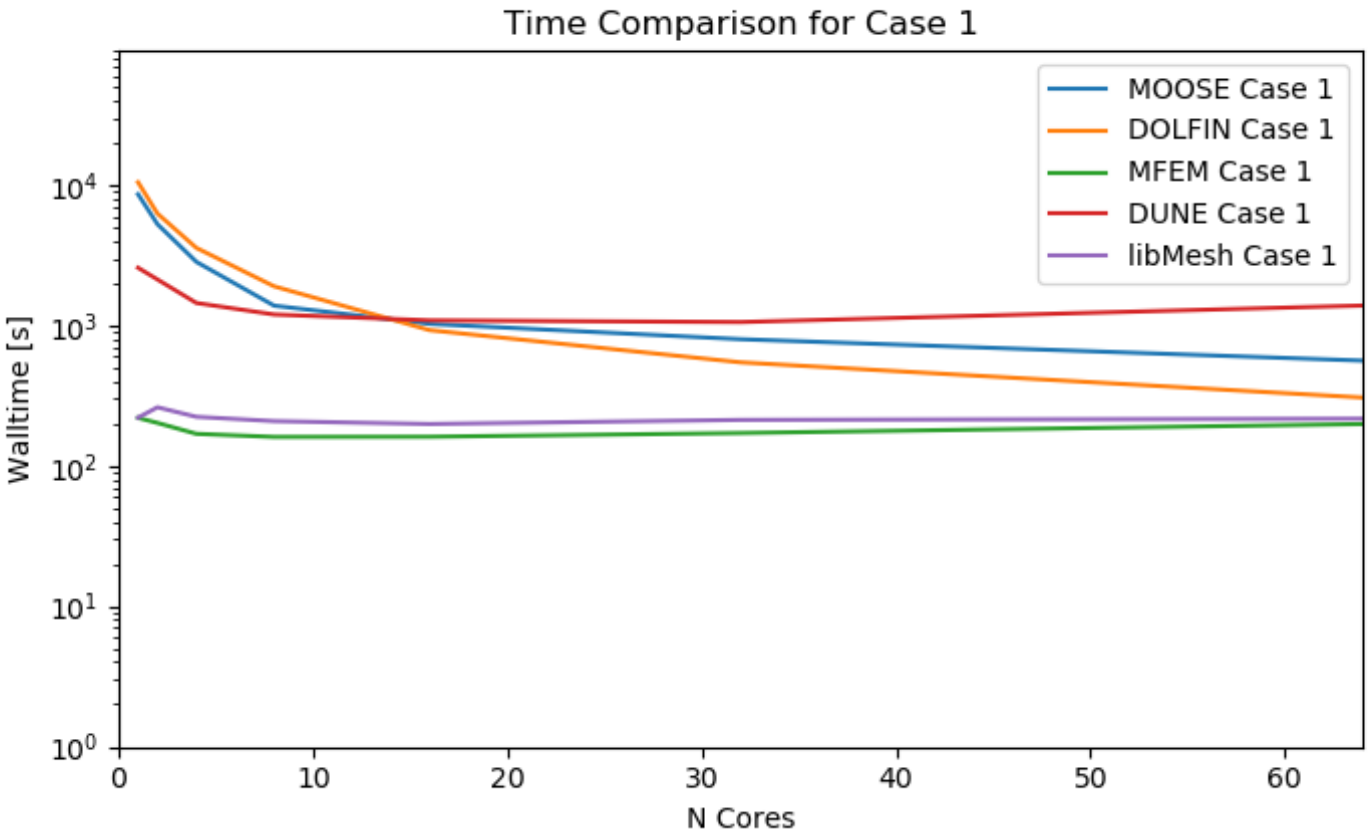
Scaling (Solver Time)

UK Atomic Energy Authority



Wall Time

UK Atomic Energy Authority



Honourable Mentions

UK Atomic Energy Authority

MFEM - Highly portable, few dependencies, clear and simple build process

MOOSE - Multiphysics coupling design, many physics domains already implemented

Thank You For Your Attention

UK Atomic Energy Authority

Any Questions?

Contact: aleksander.dubas@ukaea.uk