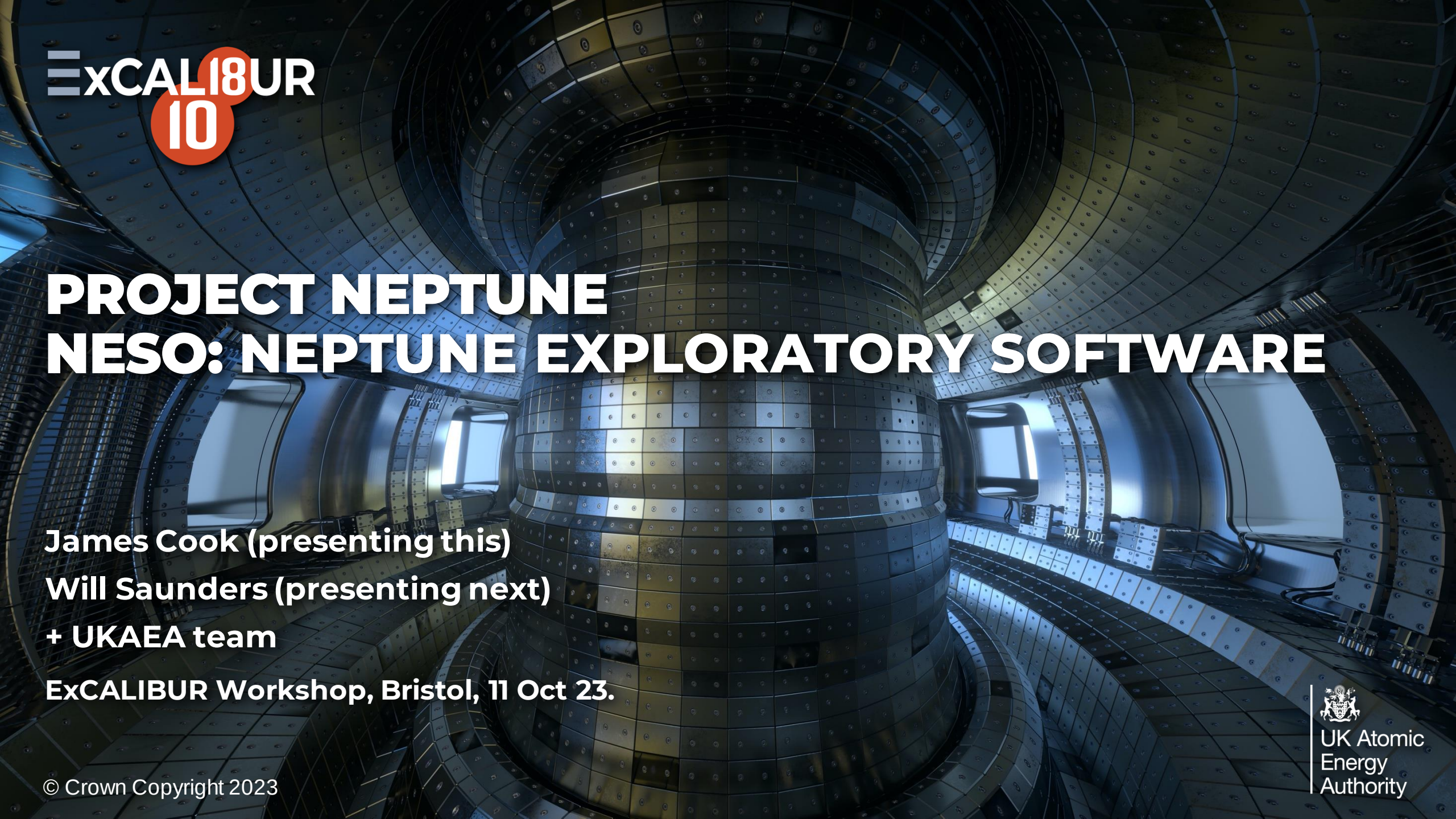


PROJECT NEPTUNE
NESO: NEPTUNE EXPLORATORY SOFTWARE

James Cook (presenting this)
Will Saunders (presenting next)
+ UKAEA team

ExCALIBUR Workshop, Bristol, 11 Oct 23.

UK Atomic Energy Authority

NESO: High level goals

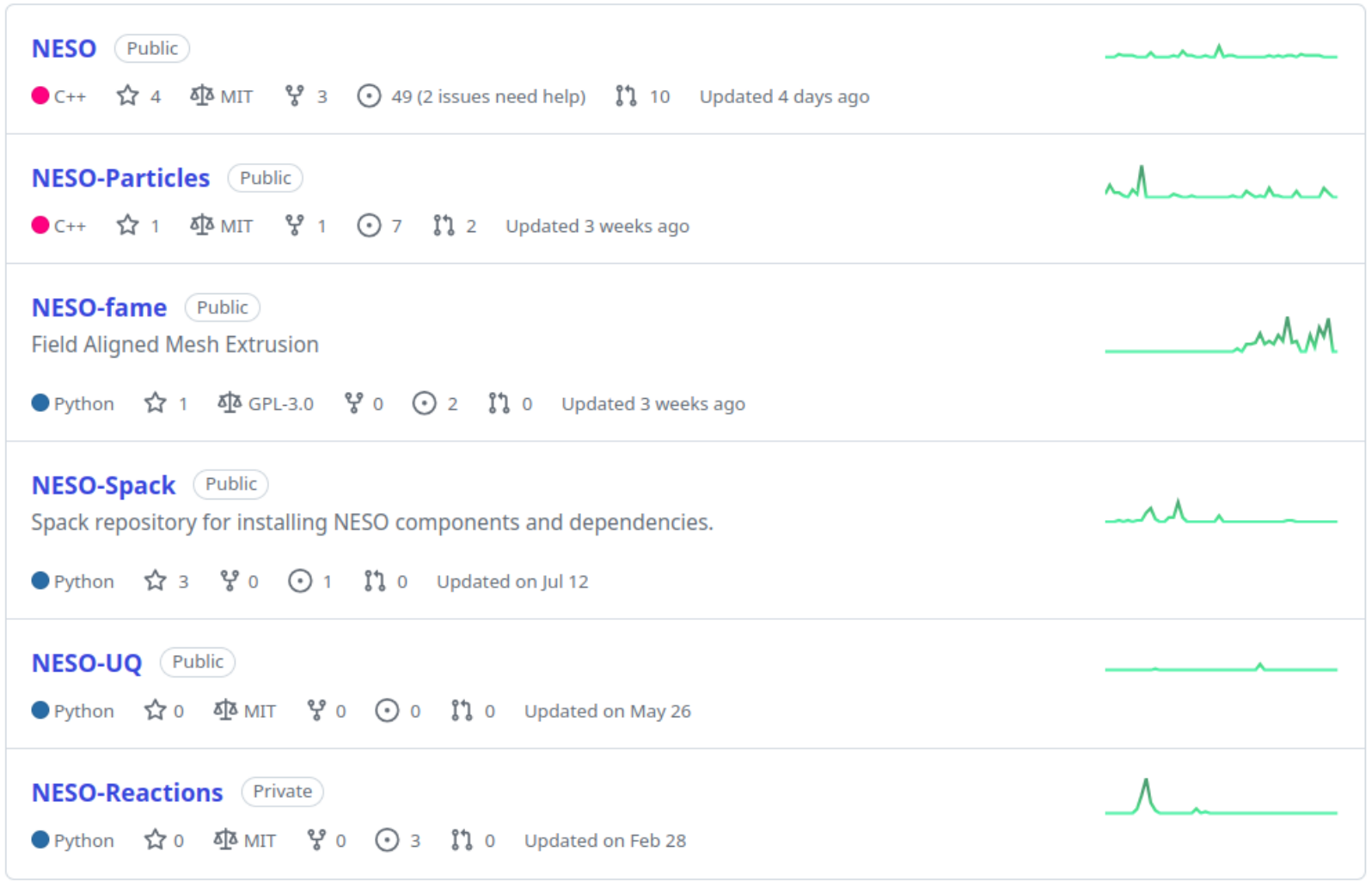
Neptune Exploratory SOftware

Bring together key technologies as foundational building blocks

- Nektar++ for its high-p DG/CG capabilities to solve generic PDEs
- NESO-Particles for SYCL-enabled charged and neutral particles
- NESO brings together Nektar++ and NESO-Particles to build mini-apps
  - An electrostatic PIC code
  - A mean field exhaust relevant system of equations
  - The turbulent reduced MHD Hasegawa-Wakatani equations
  - Capability in 2D and 3D!

The NESO Repositories

Software development



Top level framework

Particles with MPI & GPUs

Field Aligned Mesh Extrusion – for Gridding along magnetic field lines.

Make NESO, Nektar++, NESO-Particles easier to build with SYCL

Nascent Uncertainty Quantification repo

Placeholder for neutral particle reactions code

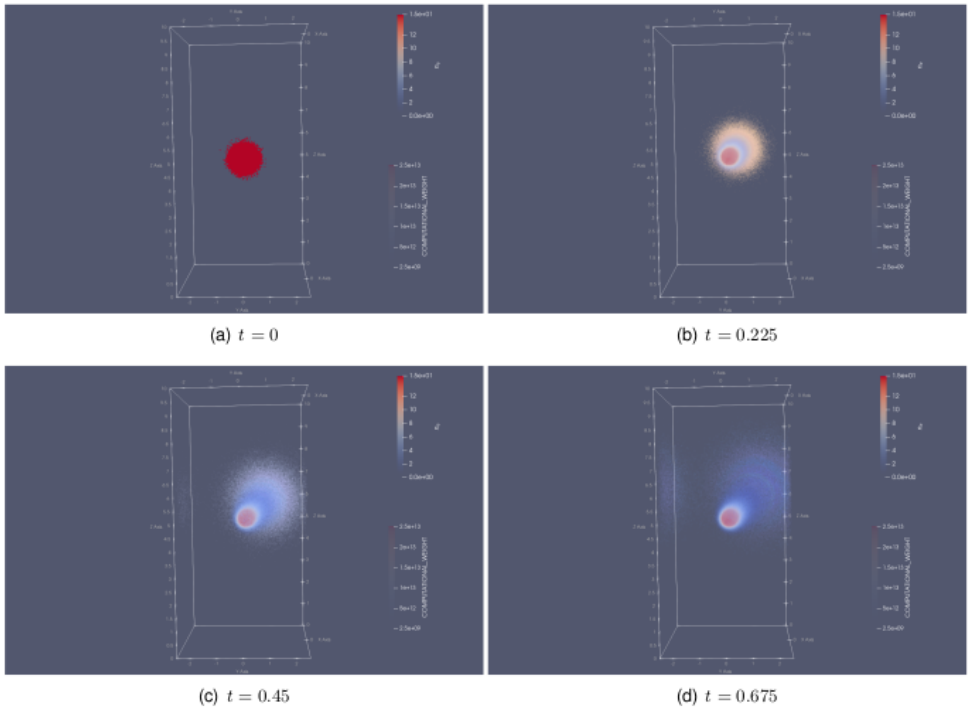
NESO: Status

Neptune Exploratory SOftware

http://en.wikipedia.org/wiki/Neso_(moon)

http://github.com/ExCALIBUR-NEPTUNE/NESO

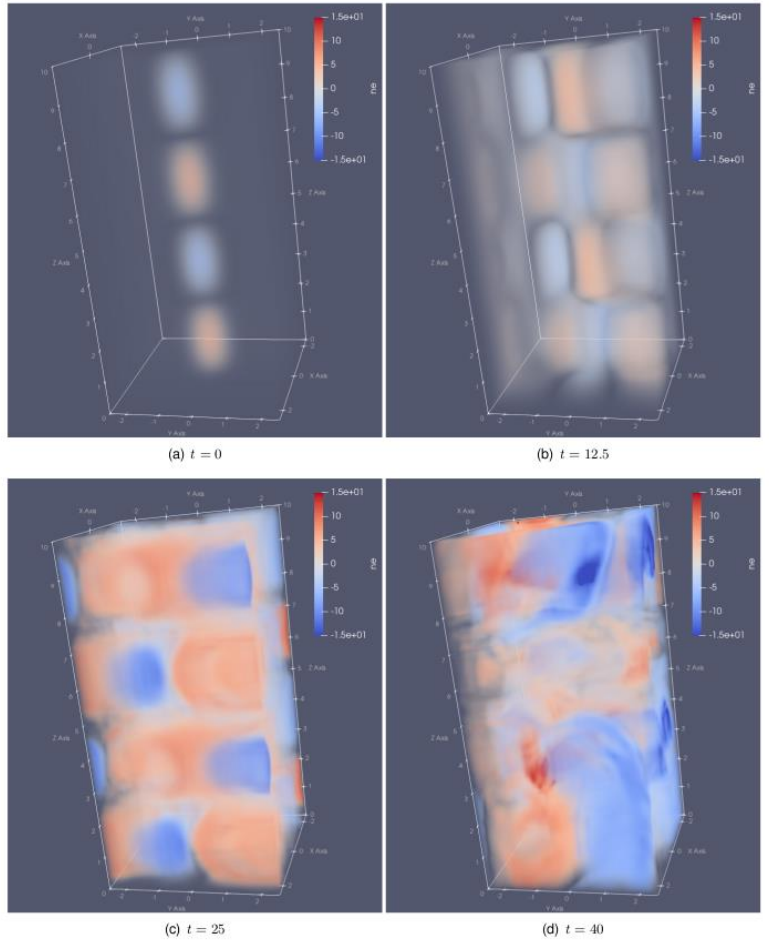
- Prototype NEPTUNE code
  - Fluid (with Nektar++) and/or particles (with NESO-Particles)
  - Implemented in SYCL (both Intel oneAPI and hipSYCL)



(a) $t = 0$ (b) $t = 0.225$

(c) $t = 0.45$ (d) $t = 0.675$

Figure 3: Evolution of the particle distribution (points) and electron density (coloured contours) in the coupled 2D-in-3D Hasegawa Wakatani solver. Particles are coloured according to their computational weight, corresponding to the number of physical neutrals that they represent. Captions under each panel indicate the simulation time.



(a) $t = 0$ (b) $t = 12.5$

(c) $t = 25$ (d) $t = 40$

Figure 2: Evolution of the electron density in the fluid-only 2D-in-3D Hasegawa Wakatani solver.

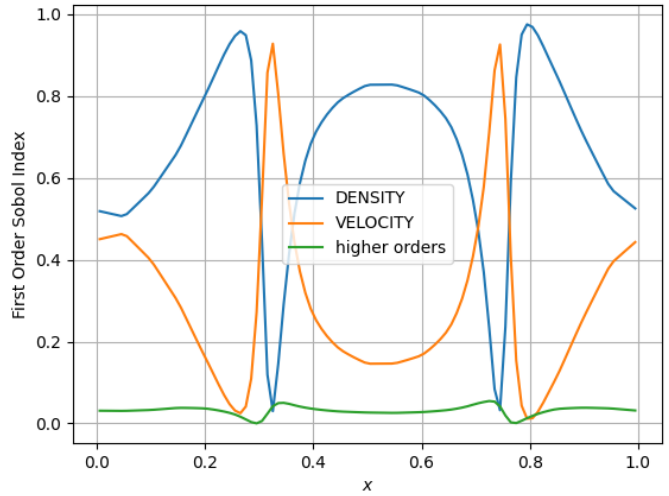
3

ExCALIBUR-NEPTUNE

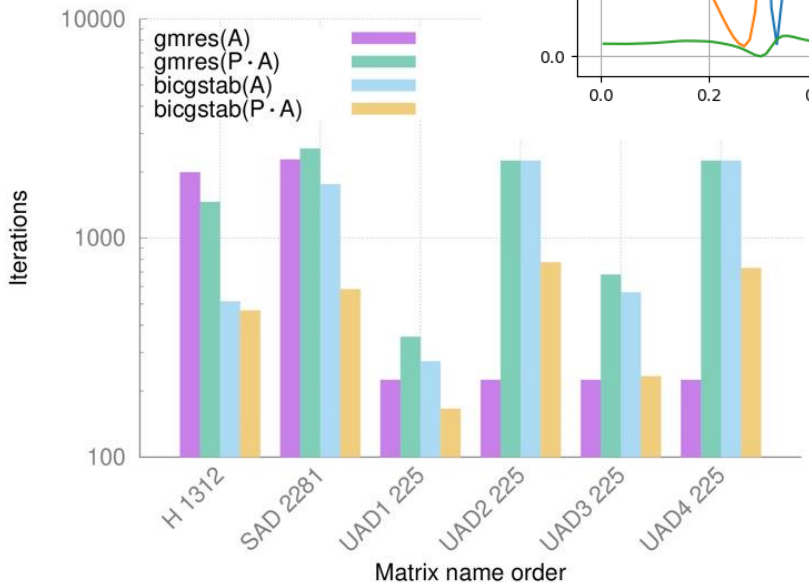
NEutrals & Plasma TUbulence Numerics for the Exascale

•Harness the code with a DSL for rapid physics exploration

```
ddt(rho) = -V_dot_Grad(v, rho) - rho*Div(v);
ddt(p)   = -V_dot_Grad(v, p) - g*p*Div(v);
ddt(v)   = -V_dot_Grad(v, v) + (cross(Curl(B),B) - Grad(p))/rho;
ddt(B)   = Curl(cross(v,B));
```



• Unobtrusive UQ ("error bars") and surrogates ("fits" that are quick to evaluate) will render the code base actionable for engineering design.



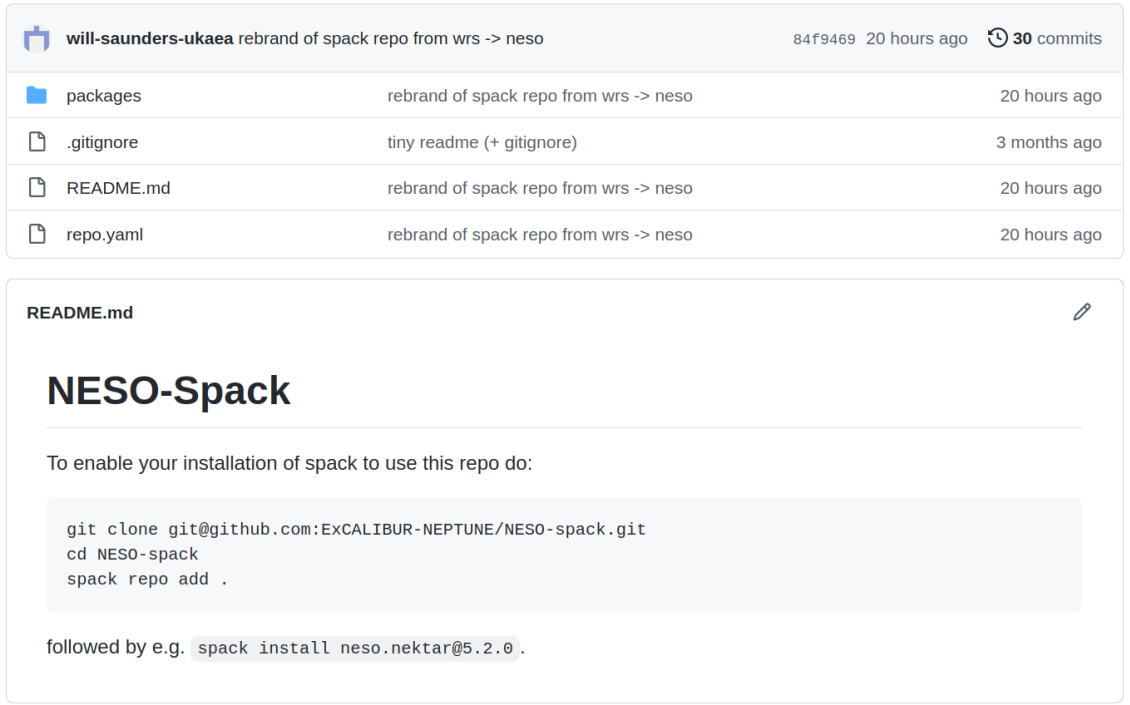
• Leverage fundamental research at the forefront of science from advanced preconditioner methods, parallel-in-time and neural methods.

NESO-Spack

Building dependencies from scratch

Users are able to build nektar++ against:

- Intel's oneapiSYCL implementation
- AMD's hipsycl SYCL implementation
- particular compilers, e.g.
- gcc@11.2.0
    - oneapi@2022.1.0 (i.e. dpcpp / icpx)
- python for NekPy
- your choice of MPI e.g. mpich



One can make a module file; `module load neso-hipsycl`

```
spack install --keep-stage -j 4 neso.nektar@5.2.0-f1598d ^python ^mpich %gcc@11.2.0
spack install --keep-stage -j 4 neso.hipsycl@0.9.2 %gcc@11.2.0
```

```
spack install --keep-stage -j 4 neso.nektar@5.2.0-f1598d +mkl %oneapi@2022.1.0 ^intel-
oneapi-mpi %oneapi@2022.1.0 ^intel-oneapi-mkl %oneapi@2022.1.0 ^python
```

FIN

UKAEA NEPTUNE:

Rob Akers
Wayne Arter
Matthew Barton
James Cook
Joseph Parker
Owen Parry
Will Saunders
Ed Threlfall

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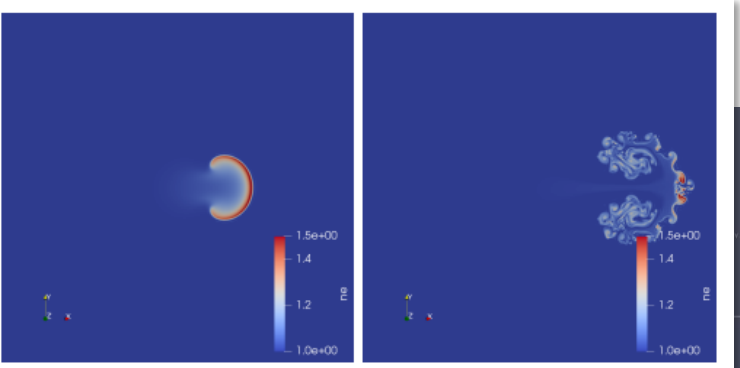
ExCALIBUR-NEPTUNE

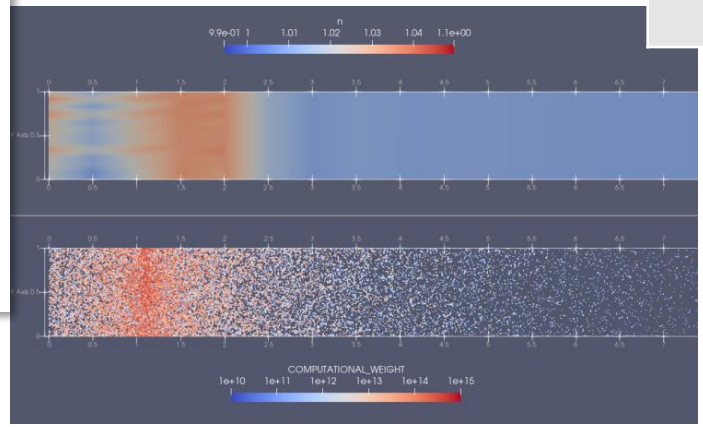
NEutrals & Plasma TUbulence Numerics for the Exascale

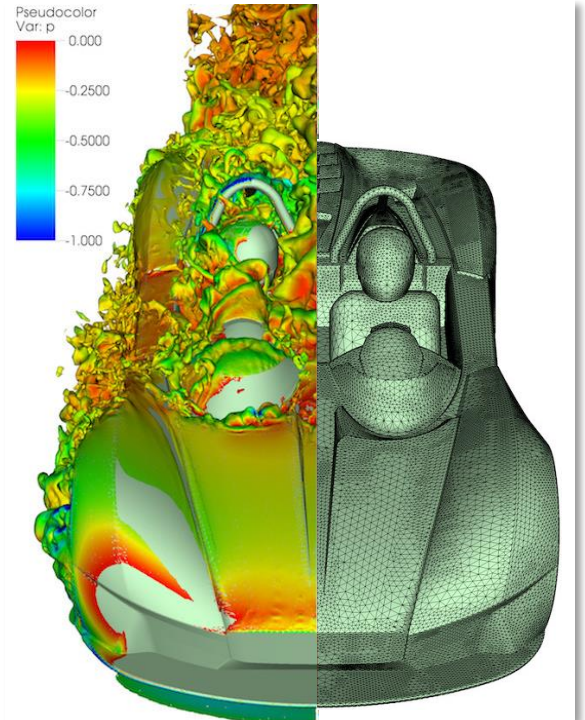
•Fusion reactors are a strongly coupled, multi-physics system of systems problem - The plasma itself requires several different models to accommodate enormous range in time- and length-scales.

NEKTAR++
SPECTRAL/HP ELEMENT FRAMEWORK

•NEPTUNE and its satellite repositories together comprise a highly scalable, arithmetically complex, performance portable next gen code, based on **Nektar++** and **SYCL**.







•One such problem is the **coupling** of plasma to the first wall, which requires **3 velocity components** of the plasma to be represented near the wall (hence > billions of particles).

SYCL™

ExCALIBUR