Improving algorithms within NEPTUNE for fusion energy simulations at exascale

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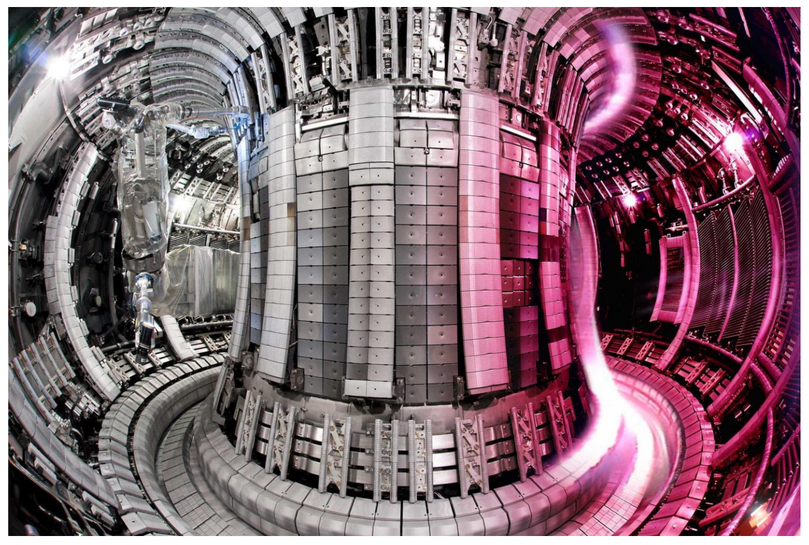
NEutrals & Plasma TUrbulence Numerics for the Exascale (NEPTUNE)

At the heart of the NEPTUNE Programme is the solution of coupled PDEs that exhibit challenging properties when trying to solve them

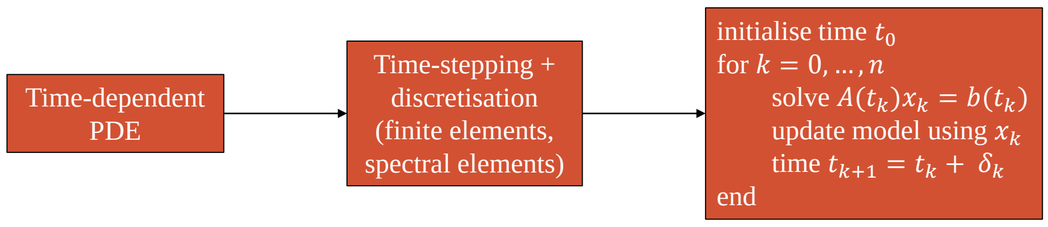
Additionally, different classes of methods may be used in different parts of the domain and these will need coupling together

Exascale performant modelling and simulation capability is needed for the ITER era

Bottlenecks that we are focusing on:
- Fluid methods/solvers
- Coupling of fluid and particle methods



Fluid methods and preconditioners



High-order finite element methods/spectral methods needed

Assembling matrix $A(t_k)$ is too expensive so use *iterative Krylov methods* which only require matrix–vector products

We require a good *preconditioner* – many approaches derived for low-order methods but struggle at high-order

Additional challenges:
- The presence of strong anisotropy (in physics and meshes)
- Effective time advance techniques for spectral elements

Prototypical 2D Poisson Example

- Continuous Galerkin with $p = 13$ on 80×80 grid
- $A \in \mathbb{R}^{n \times n}, n = 1083681, nnz = 137394401, \frac{nnz}{n} = 126$
- Firedrake with convergence threshold 10^{-7}

Preconditioner	Processors	Iterations	Time(s)
HYPRE (BoomerAMG)	256	744	18.7
Algebraic GenEO	256	23	2.1

Upcoming work to investigate:

Preconditioning
- BoomerAMG
- HPDDM (with GenEO)
- hp – multigrid
- ℓ – AIR

Time-stepping
- Crank–Nicolson
- IMEX
- ESDIRK
- Fully implicit RK

Coupling of fluid and particle models of plasma

Multiple coupling methods have been proposed.

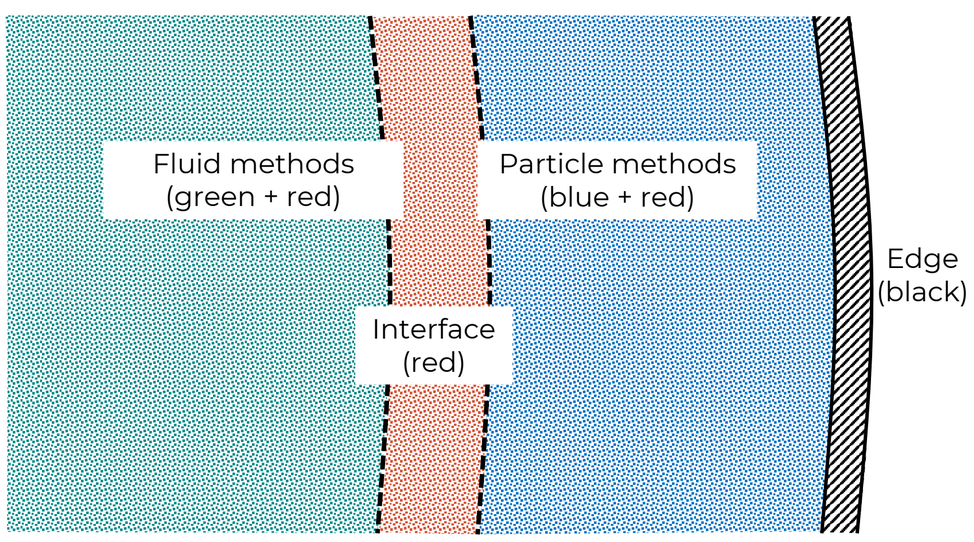
We are focussing on the *Spatial Hybridization* (SPH) method: this provides a *separation of concerns*.

The coupling of the regions at the interface is achieved by exchanging overlapping data at the interfaces. Several open-source libraries are available to manage this in an HPC environment.

Upcoming work:

Develop a *proxyapp* using CWIPI to couple fluid method (Nektar++-based) and particle method (NESO).

How do we choose interface (position and width) ?
- Maintain accuracy
- Load-balance the fluid/particle regions



Spatial Hybridization (SPH) Approach

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