ExCALIBUR 10

PROJECT NEPTUNE

SUSTAINABLE SOFTWARE FOR SUSTAINABLE FUSION ENERGY

Ed Threlfall, UKAEA (on behalf of the NEPTUNE team)

CIUK 2022, Manchester, 1st December 2022

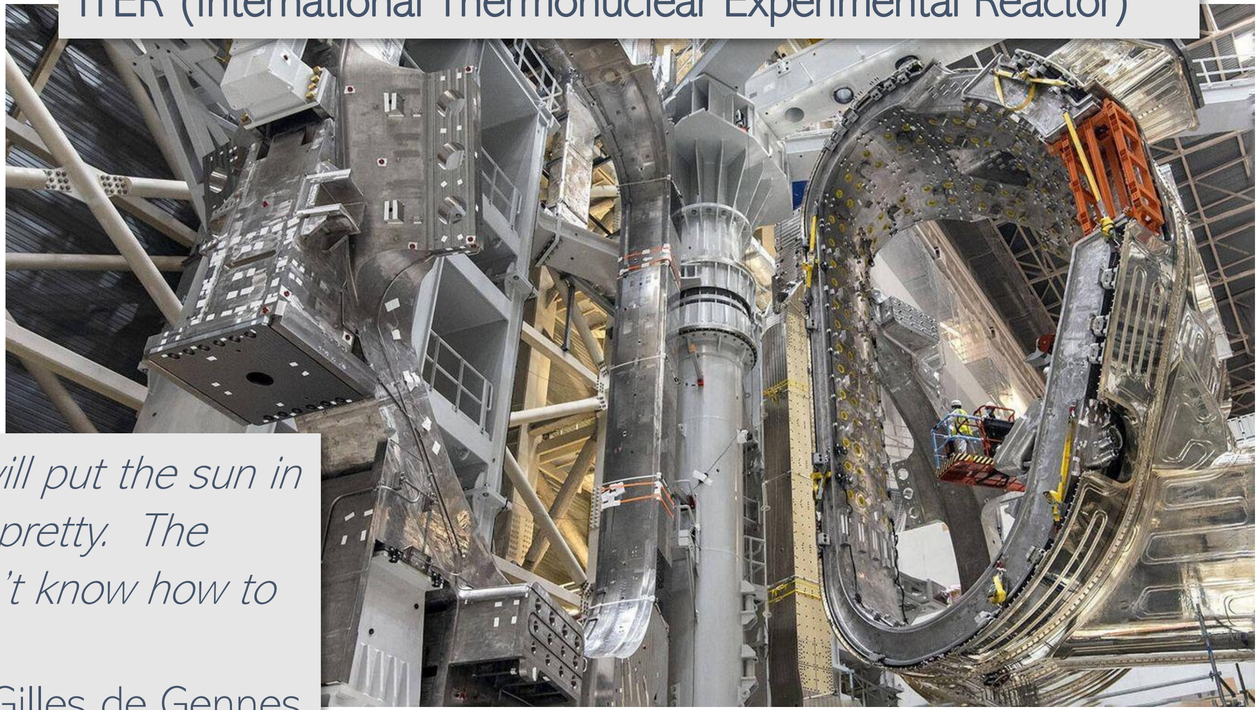
Met Office

UK Research and Innovation

UK Atomic Energy Authority

NEPTUNE – why? (1)

ITER (International Thermonuclear Experimental Reactor)



""We say that we will put the sun in a box. The idea is pretty. The problem is, we don't know how to make the box."

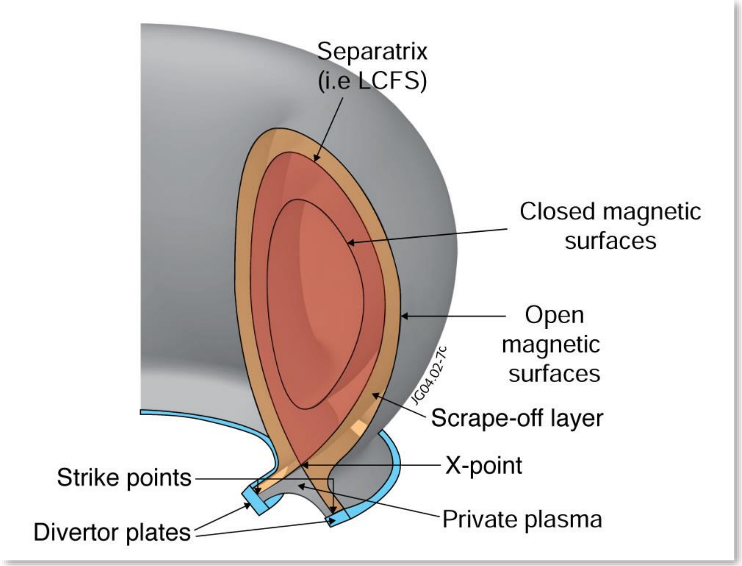
Pierre-Gilles de Gennes

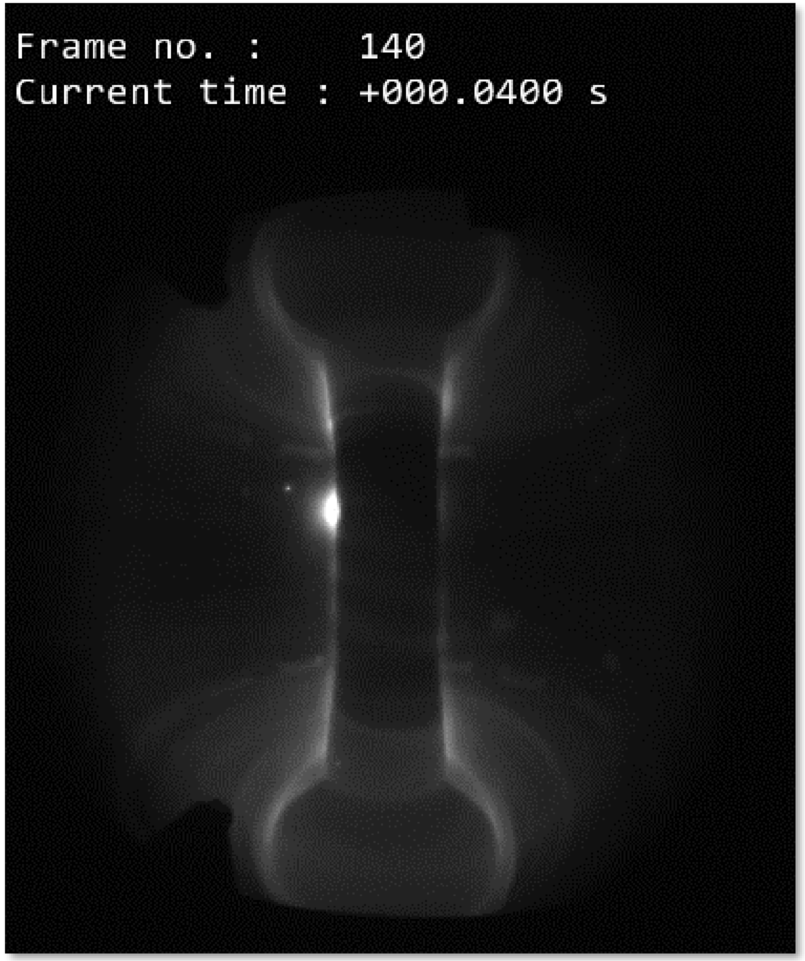
- Fusion is a potential sustainable energy solution.
- Magnetically-confined approach – 100 million degrees plasma.
- Contained in a tokamak - a toroidal `box'.
- Plasma touches side – heat loads ~ spacecraft re-entry …

NEPTUNE – why? (2)

Modelling the plasma `edge' or exhaust:

- A long-established exascale grand-challenge multi-physics, multi-scale problem.
- Complexity: turbulence (hard – outstanding Millennium Prize!), many species, atomic physics, etc.
- Kinetic effects: out-of-thermal equilibrium matter (few collisions), requires coupled fluid and particles.





~1s long H-mode MAST-U pulse

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NEPTUNE – what?

Why digital models?	Tokamaks expensive! (ITER ~€20bn, initiated 1988).
Existing software limitations	Finite-difference methods, not best suited to new HPC architectures.

NEutrals and Plasma TUrbulence Numerics for the Exascale

- *'Once-in-a-generation' opportunity for UK to improve fusion plasma physics software processes in order to develop `actionable' code i.e. code suitable for incorporation in an engineering design workflow as required for STEP.*
  (Wayne Arter, Technical Lead.)
- Interdisciplinary `rainbow' team; 60-70% of work defrayed to UKRI.
- Proxyapps development philosophy (each solves part of the problem).
- Sustainability – re-usable, reliable, efficient, scalable.

STEP (Spherical Tokamak for Energy Production) – fusion power on UK grid by 2040s.

NEPTUNE – how?

- Fluid physics module - C++ finite element library, modelling plasma turbulence.
- Particles module – C++ library for out-of-equilibrium matter.
- Uncertainty quantification for actionable code – non-intrusive.
- Sub-modules interchangeable with reduced-order models / surrogates.

Use	• Engineers, plasma physicists, software developers. • Run on anything from single laptop to exascale. • Aim for 30-year life-cycle.
Domain-specific language	DSL for user interaction - compose library components.
Languages	C++17 / SYCL 2020 for main code, Python for user DSL.

SYCL™ ExCALIBUR

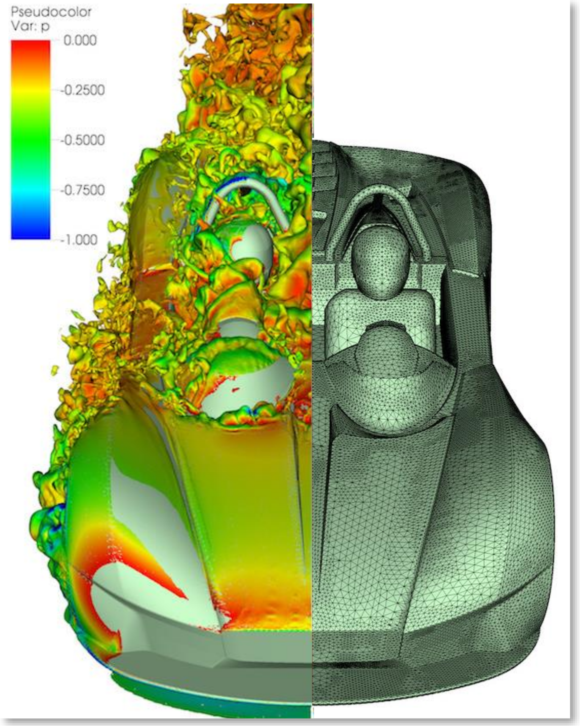
Nektar++ : spectral / hp elements

Nektar++ spectral / hp code [1] for solving plasma fluid equations.

- Arbitrary convergence order p – error $\propto h^p$ ($h \sim$ element size).
- Arithmetic intensity – increased number of operations on same data counters HPC data movement bottleneck.
- Supports complicated geometries, curved elements.

Structure	• Set of libraries. • C++ code with MPI parallelism for CPUs. • Refactoring for performance portability / GPUs / C++17.
Provenance	• Proven scaling to c.100k cores. • Well-tested code. • Established community of developers / users.
Benefit	*More rapid convergence means more energy-efficient calculations.*

NEKTAR++
SPECTRAL/HP ELEMENT FRAMEWORK



CFD simulation of Elemental RP1 track car.

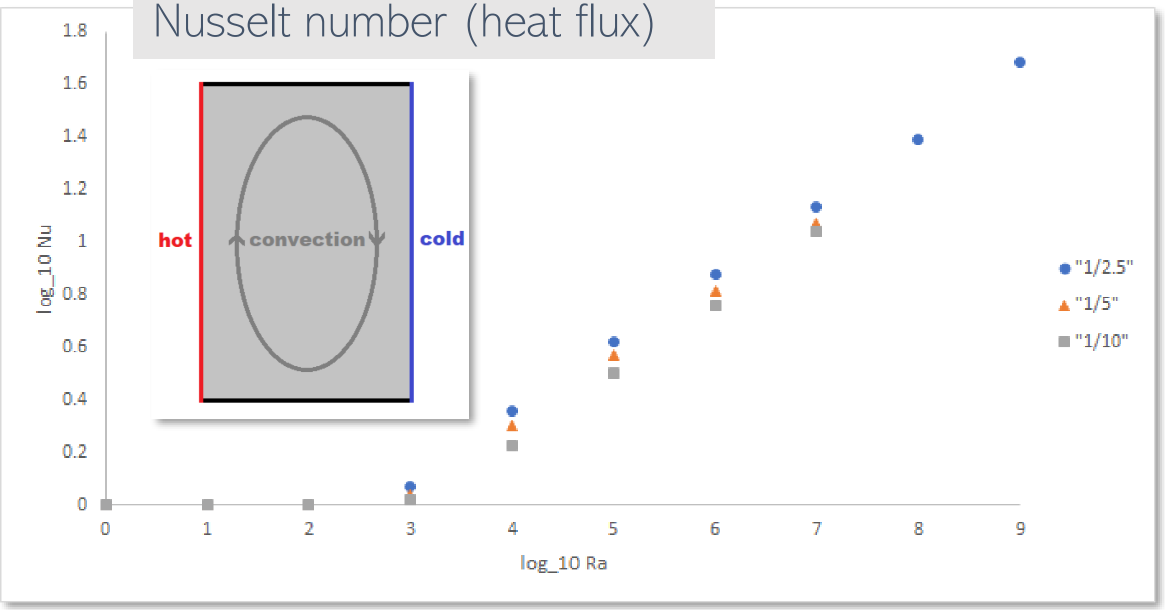
1. https://www.nektar.info

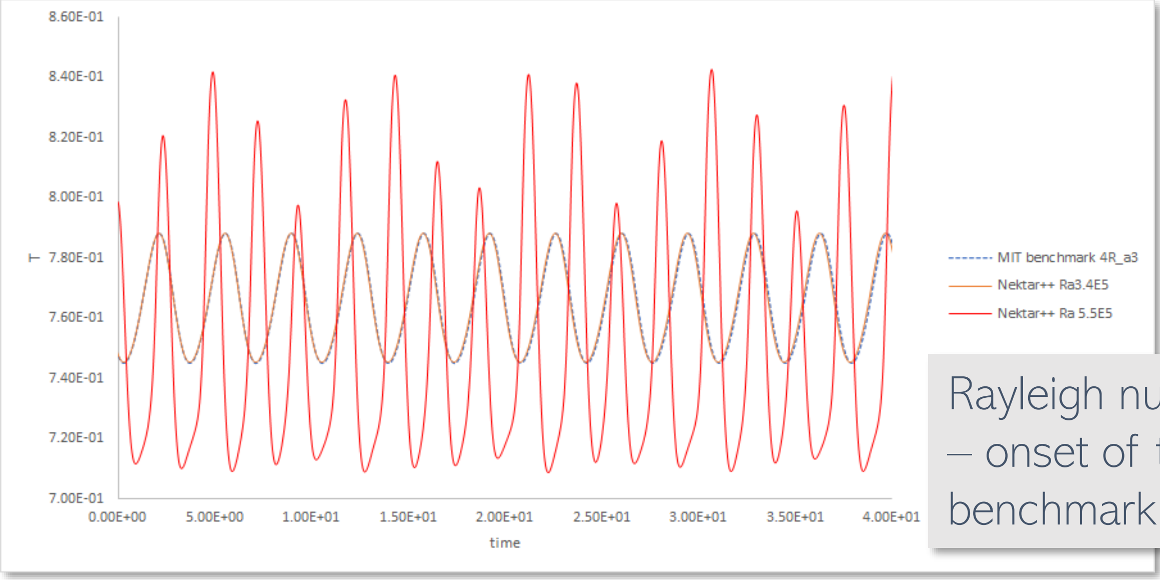
D. Moxey (King's College London); C.D. Cantwell, S.J. Sherwin (Imperial College London)

Nektar++ convection proxyapp

Temperature field - Rayleigh number (Ra) small

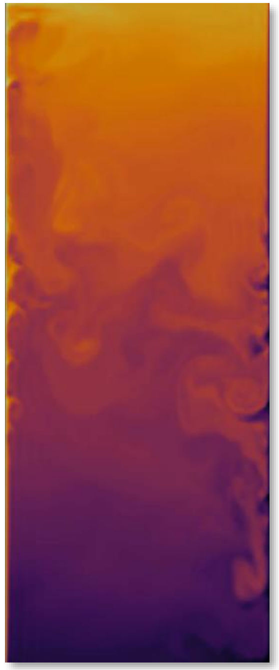
Nusselt number (heat flux)





Rayleigh number intermediate – onset of turbulence (MIT benchmark [1])

[1. https://www.mathematik.tu-dortmund.de/~featflow/en/benchmarks/cfdbenchmarking/mit_benchmark.html](https://www.mathematik.tu-dortmund.de/~featflow/en/benchmarks/cfdbenchmarking/mit_benchmark.html)



Temperature field - Rayleigh number large

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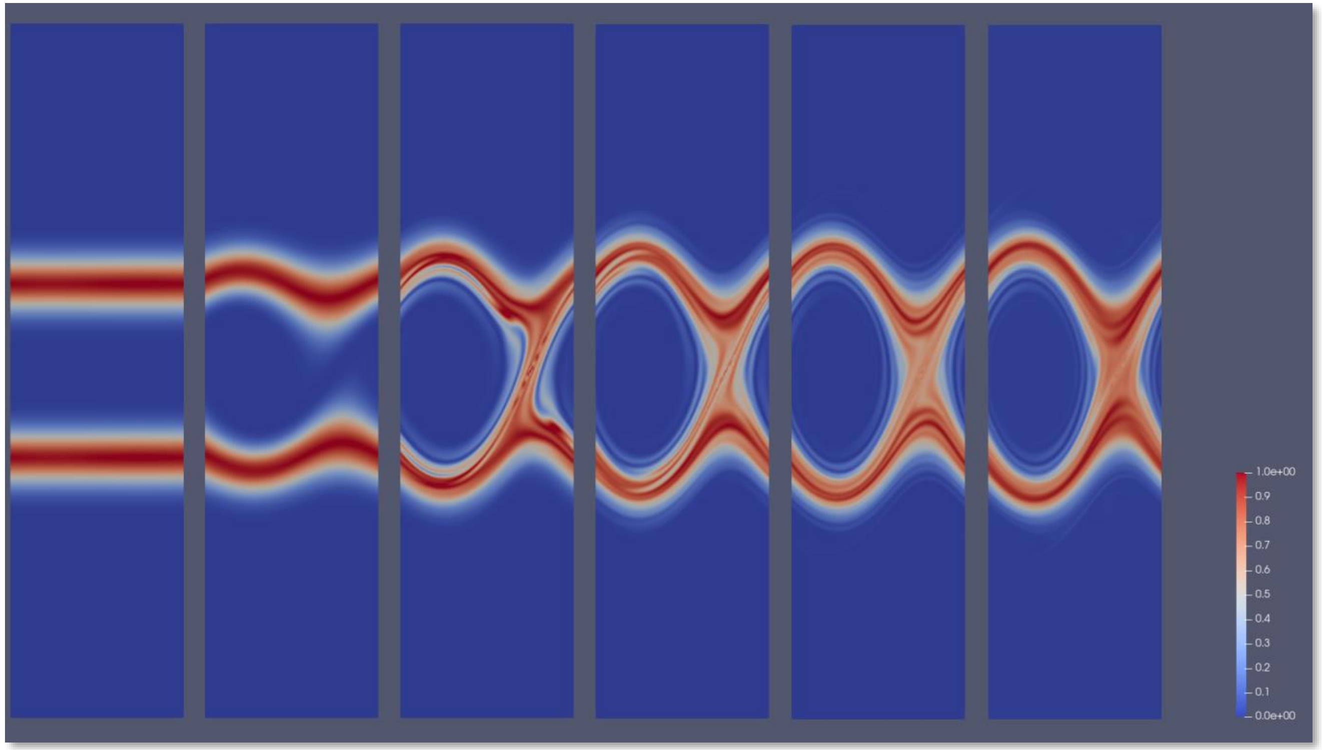
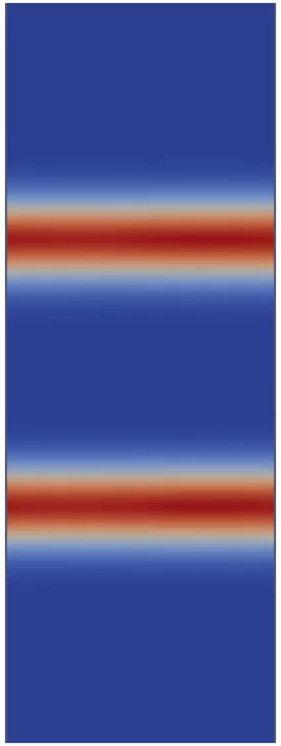
Nektar++ kinetic proxyapp

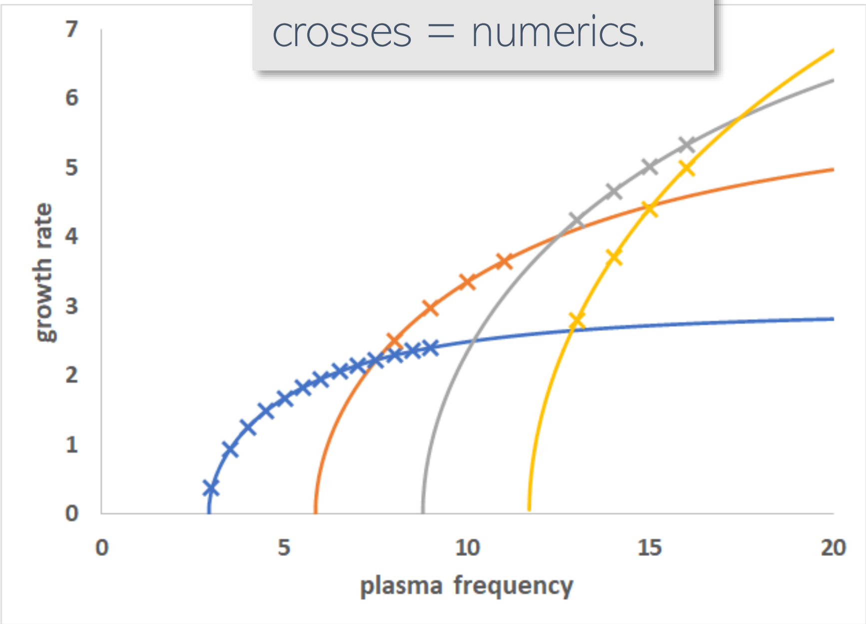
v x

Phase space!





Instability growth rates for $k_n = \frac{2\pi n}{L}$
Curves = theory, crosses = numerics.

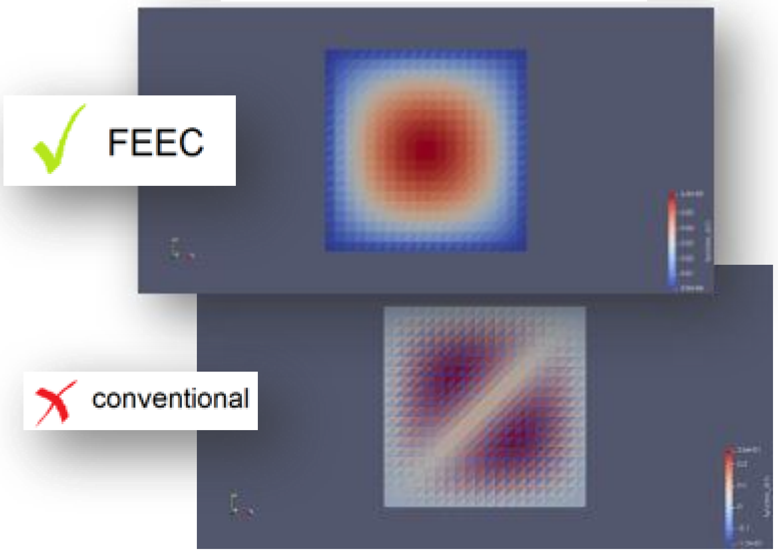


Two-stream instability – nonlinear evolution of initial Gaussian charged particle beams

Advanced techniques can guarantee numerical stability

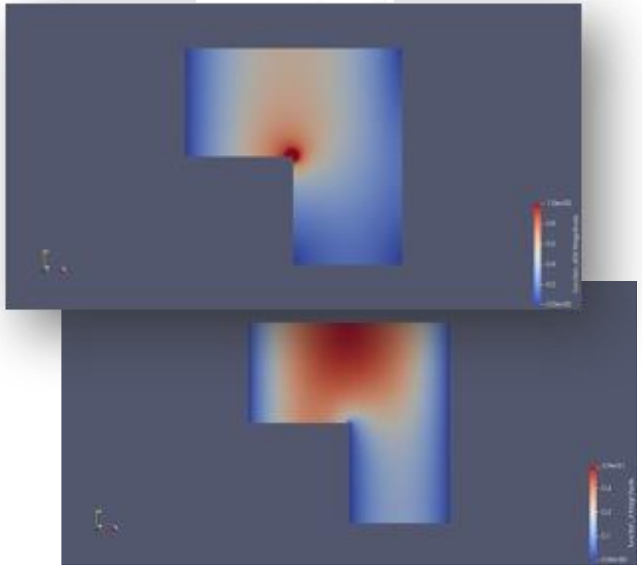
Finite element exterior calculus (FEEC)	Properties of PDE can survive discretization – conservation laws, stability, which elements to use …

$\nabla^2 u = 2y(1-y) + 2x(1-x)$



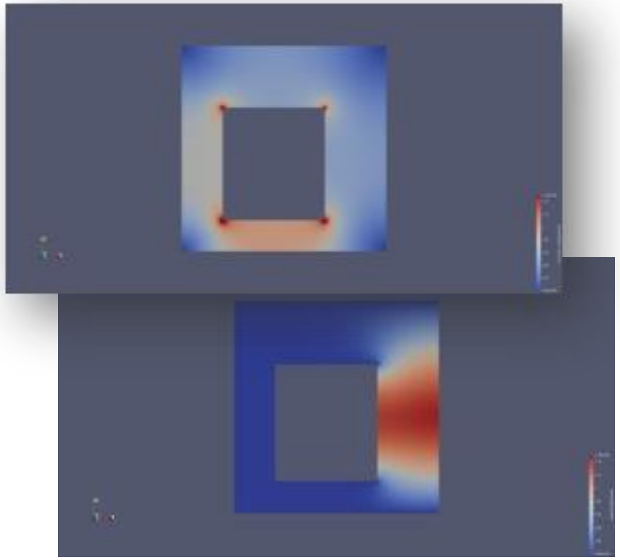
Unstable numerics

$\nabla^2 \underline{u} = (1, 0)$



Re-entrant corner field singularity

$\nabla^2 \underline{u} = \lambda \underline{u}$



Non-trivial topology

Challenge	Implement in *Nektar++* without loss in performance …
References	See textbook by D.N. Arnold [1], Firedrake ([2]) implementations of Arnold's examples [3].

1. D.N. Arnold, *Finite Element Exterior Calculus*, CBMS-NSF regional conference series in applied mathematics 93, SIAM.
2. https://www.firedrakeproject.org
3. https://github.com/ethrelfall/Finite-element-exterior-calculus

Advanced techniques can improve convergence rates

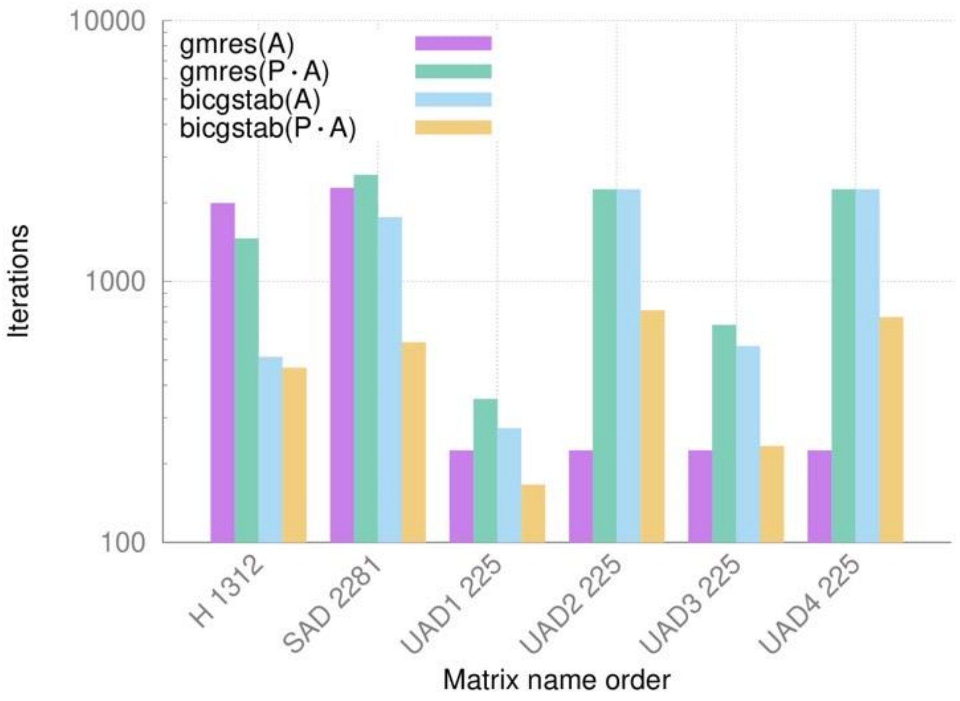
Preconditioners	Improve efficiency of $Ax = b$ matrix inversion by applying approx. solution before iterating.

Operator-based preconditioner

	N_y	None	P_0	P_1
RHS Evals	200	1466071	92682	56630
Time (s)	200	1925	151	95
RHS Evals	400	-	252708	169830
Time (s)	400	-	615	413

BOUT++ / SD1D plasma-neutrals simulation: ~37% reduction in runtime over original preconditioner.

Markov-chain Monte Carlo preconditioner

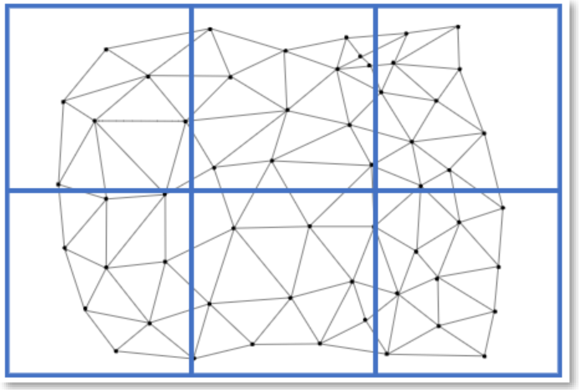


Nektar++ cases: order of magnitude speed-up.

S. Thorne, STFC Hartree Centre

DSL - enabled, performance-portable MPI particle library

NESO-PARTICLES [1] (NESO = NEPTUNE Experimental SOftware)	• UKAEA library for particle data and moving particles between MPI ranks on unstructured meshes. • Particle-mesh interface abstract - different mesh implementations possible (including *Nektar++* meshes). • Charged and neutral particles. • Header-only library.
Coupling	Initial implementations tightly-coupled to the finite element code - coupling to surrogate models anticipated.
Dependencies	• CMake • SYCL 2020 (tested with hipSYCL 0.9.2 and Intel DPCPP 2022.1.0) • MPI 3.0 (tested with MPICH 4.0 and IntelMPI 2021.6) • HDF5 (optional, if particle trajectories required)

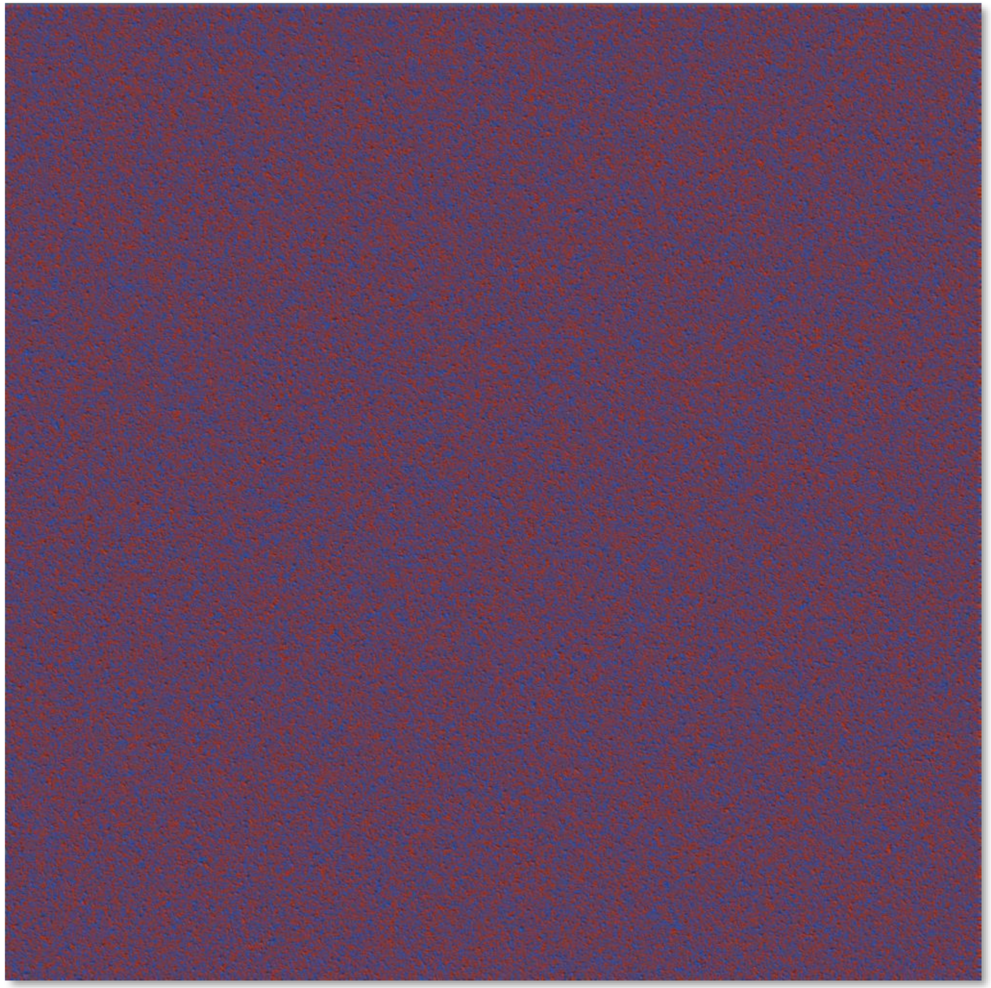


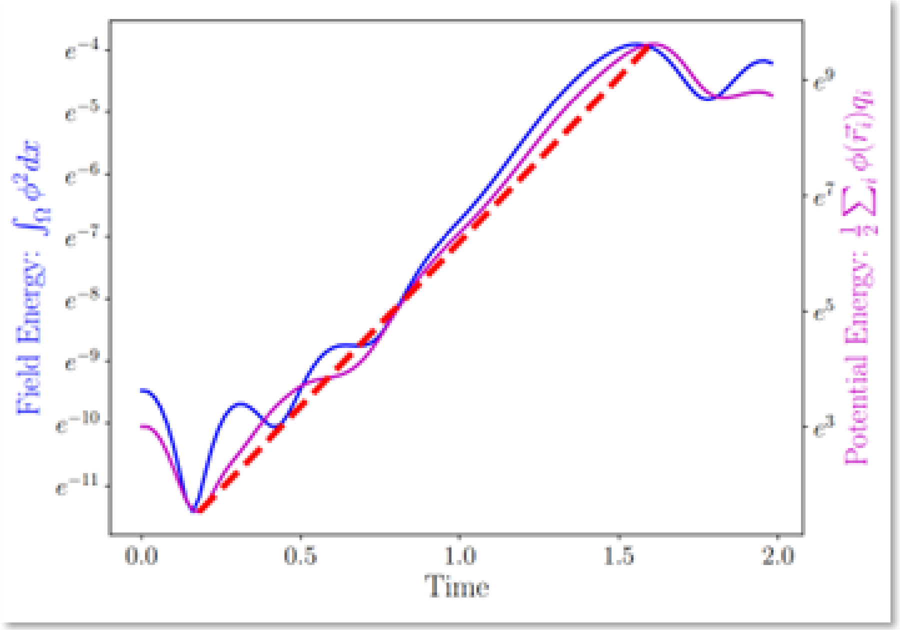
1. https://github.com/ExCALIBUR-NEPTUNE/NESO-Particles

Particles proxyapps

NESO [1]	• Test implementations integrating particle capabilities and FEM. • Can be built using Spack package manager. • 2D2V electrostatic particle-in-cell solver. • Nektar++ provides Poisson solve.
Tests	• Linear growth rates of unstable modes. • Energy conservation.

Time evolution of 512k interacting particles





Instability growth rate vs theory

1. https://github.com/ExCALIBUR-NEPTUNE/NESO

Actionable code requires Uncertainty Quantification

VVUQ	• Meaningful bounds on error in code outputs given statistical uncertainty in inputs. • Ensemble-based execution patterns. • Non-intrusive UQ – separation of concerns.
SEAVEA project synergy, SEAVEA toolkit [1]	• UQ campaigns on HPC. • Construction of surrogate models e.g. Gaussian process models, machine-learning. • Modern data science techniques e.g. data assimilation, Bayesian analysis.
FabNEPTUNE [2]	• FabSim3 plugin created specifically for NEPTUNE. • Easy execution of NEPTUNE simulations, integrated with SEAVEA toolkit. • Currently drives *Nektar++* 2D and 3D convection proxyapps - but more specific plasma applications very soon.

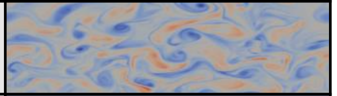
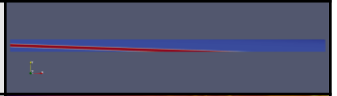
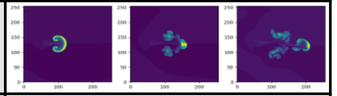
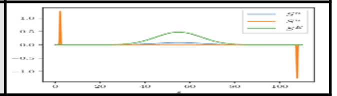
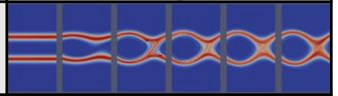
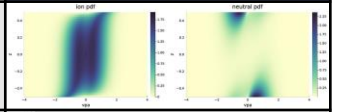
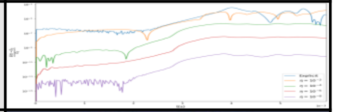
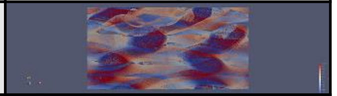
Nektar++ convection proxyapp + VVUQ to support *Smallab* experiments (Arter, Buta – Univ. Leeds)

FabNEPTUNE

1. https://www.seavea-project.org/seaveatk
2. https://github.com/UCL-CCS/FabNEPTUNE

S. Guillas, P.V. Coveney, K. Bronik (UCL)

Proxyapps inventory

Proxyapp	Framework	Language	Comments	Sample output
nektar-driftwave	*Nektar++*	C++	2D Hasegawa-Wakatani equations	
nektar-diffusion	*Nektar++*	C++	strongly anisotropic diffusion	
vertical natural convection in spectral / hp, 2D and 3D	*Nektar++*	C++	incompressible Navier-Stokes with buoyancy	
2D plasma turbulence equations in spectral / hp	*Nektar++*	C++	*Hermes-3* equation system	
1D fluid solver with UQ and realistic boundary conditions	*Nektar++*	C++	1D model of scrape-off layer	
Vlasov-Poisson kinetic solver in spectral / hp	*Nektar++*	C++	due Dec 2022	
moment-kinetics	new code (Univ. Oxford)	Julia	moment-kinetic gyro-averaged code	
minepoch	*EPOCH* (Univ. Warwick)	Fortran	used for testing particle implementations	
electrostatic PIC proxyapp	NESO-Particles	C++ / SYCL	due Dec 2022	
2D3V coupled fluids-neutral particles proxyapp	NESO-Particles	C++ / SYCL	due Mar 2023	coming soon

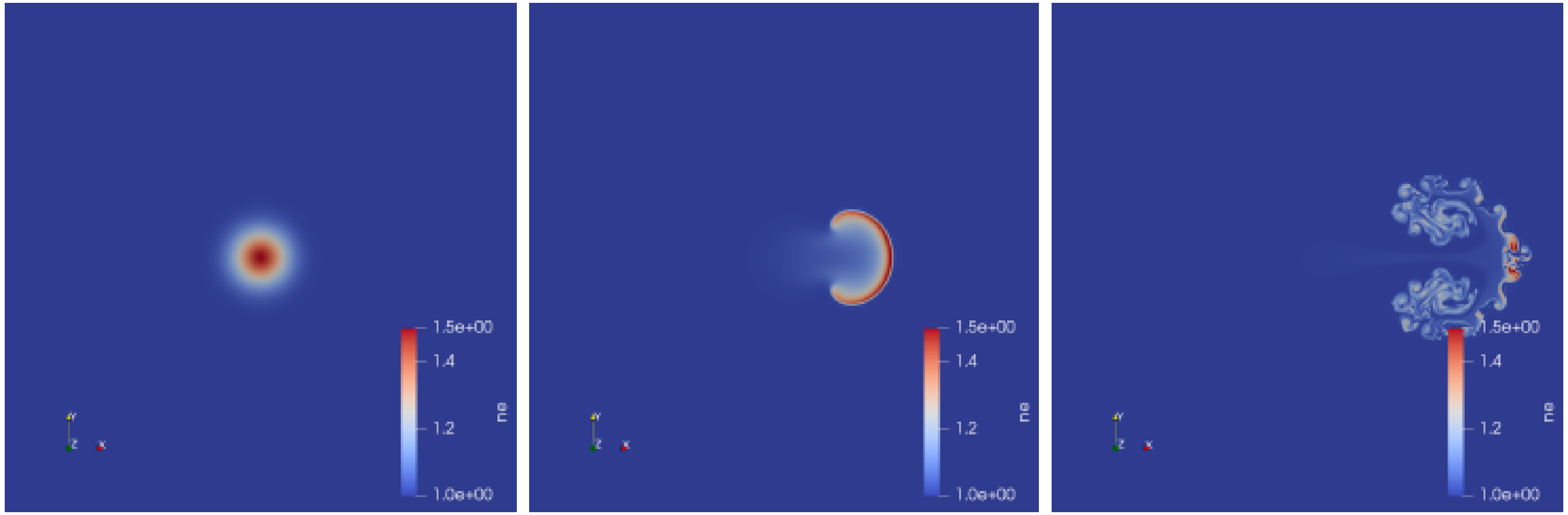
Community overview

UKAEA TEAM	Rob Akers, Wayne Arter, Matthew Barton, James Cook, John Omotani, Joseph Parker, Owen Parry, Will Saunders, Ed Threlfall.
UKRI GRANTS	• University of Exeter (VVUQ, surrogate models): Peter Challenor, Tim Dodwell, Louise Kimpton. • King's College London (Nektar++): Mashy Green, David Moxey. • Imperial College London (Nektar++): Chris Cantwell, Bin Liu, Spencer Sherwin. • University of Oxford: Michael Barnes, Patrick Farrell, Michael Hardman. • STFC Hartree Centre: Vasil Alexandrov, Hussam al-Daas, Tyrone Rees, Emre Sahin, Andrew Sunderland, Sue Thorne. • University College London (VVUQ): Kevin Bronik, Peter Coveney, Matt Graham, Serge Guillas, Tuomas Koskela, Yiming Yang. • University of Warwick (DSLs): Gihan Mudalige. • University of York (plasma physics, support & coordination, DSLs): David Dickinson, Ed Higgins, Chris Ridgers, Steven Wright.
ALUMNI	• University of Oxford: Felix Parra-Diaz. • University of Warwick (EPOCH): Ben McMillan, Tom Goffrey. • University of York: Ben Dudson.
OUTPUT (INC. CODE)	• Proxyapps code (MIT licence): see repositories on https://github.com/ExCALIBUR-NEPTUNE (some, inc. NESO and NESO-Particles, are public). • Large body of supporting documents and reports – https://github.com/ExCALIBUR-NEPTUNE/Documents (currently private). • Developer website in development.

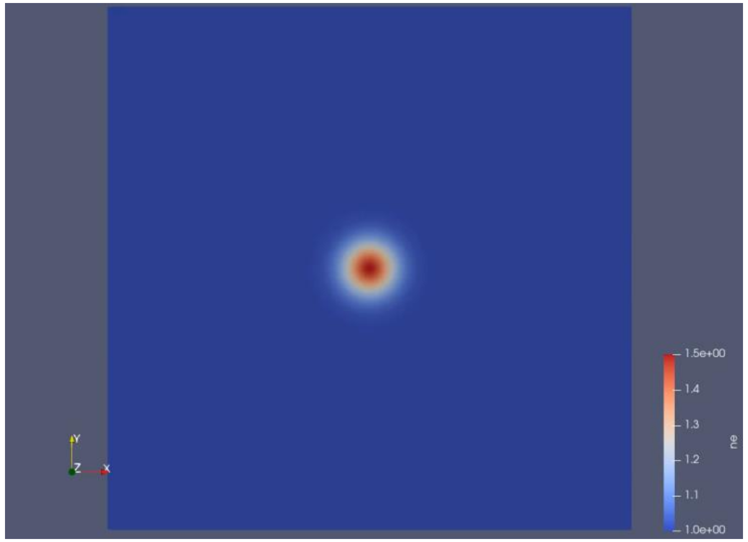
Participation welcomed!

Next steps: 2D3V plasma proxyapp

2D plasma turbulence with neutral particle source terms	• Tight-coupled integration of the spectral / hp and particles. • Kinetic neutral species in plasma background. • Due by end Mar 2023.
Plasma turbulence in *Nektar++*	*Nektar++* [1] implementation of equations from existing *Hermes-3* code (finite difference) [2].
Neutral particles	Neutral particles do not feel confining magnetic field, but ionize as they interact with plasma – source terms in fluid equations (= coupling).



(a) $t = 0$ (b) $t = 2$ (c) $t = 4$



1. https://github.com/ExCALIBUR-NEPTUNE/nektar-driftplane 2. https://github.com/bendudson/hermes-3