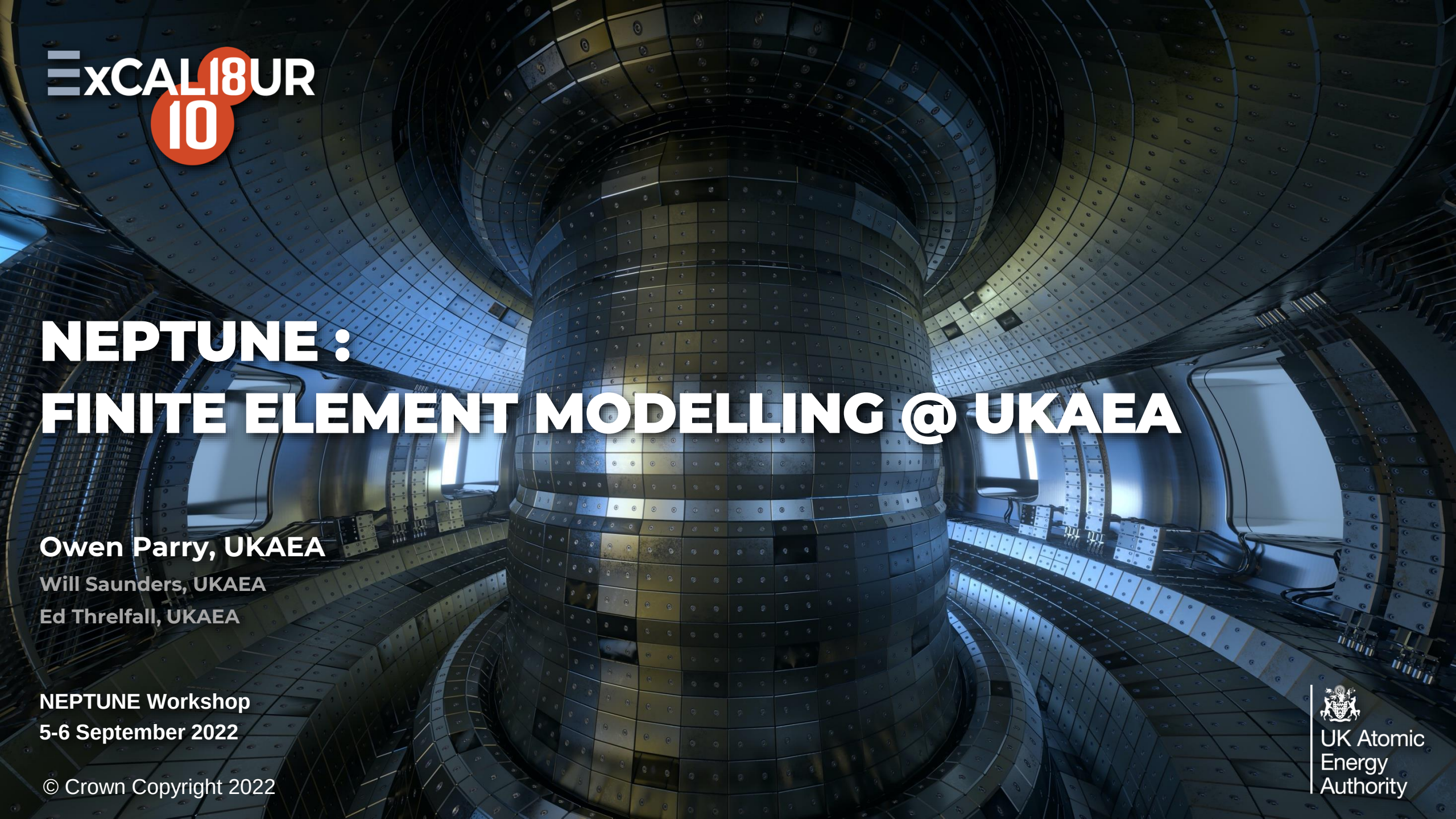


NEPTUNE : FINITE ELEMENT MODELLING @ UKAEA

Owen Parry, UKAEA
Will Saunders, UKAEA
Ed Threlfall, UKAEA

NEPTUNE Workshop
5-6 September 2022

UK Atomic Energy Authority

FEM in NEPTUNE

Summary of UKAEA activities

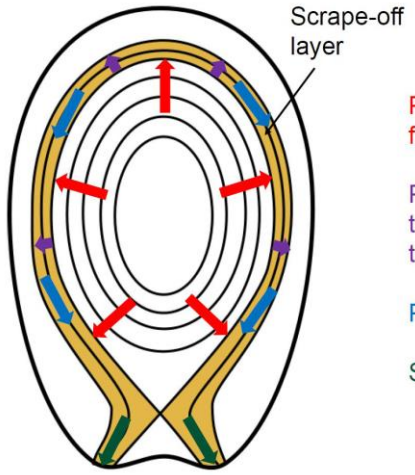
1. 1D scrape-off layer modelling with finite elements
   (Will Saunders, Owen Parry)

2. Nektar++ changes for NEPTUNE integration
   (Owen Parry)

3. Finite element exterior calculus
   (Ed Threlfall)

1D SOL Proxyapp

Model description



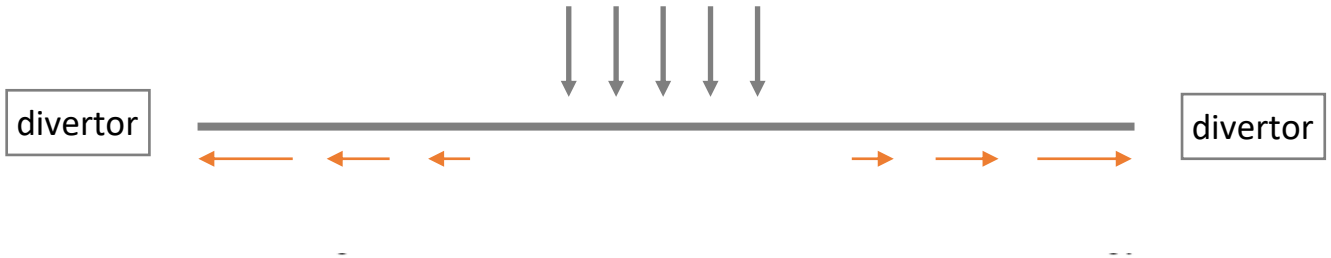
Plasma outflowing from the core

Perpendicular transport driven by turbulence

Parallel flows

Sheath losses

Image from Riva, 2019



$$U_r \frac{\partial n}{\partial t} = -\frac{\partial}{\partial s}(nu) + S^n,$$

$$U_r \frac{\partial}{\partial t}(nu) = -\frac{\partial}{\partial s}(nu^2) - \frac{\partial}{\partial s}(nT) + S^u,$$

$$U_r \frac{\partial}{\partial t}\left((g-2)nT + nu^2\right) = -\frac{\partial}{\partial s}(gnuT + nu^3) + \kappa_d \frac{\partial^2 T}{\partial s^2} + S^E,$$

g: Specific heat capacity

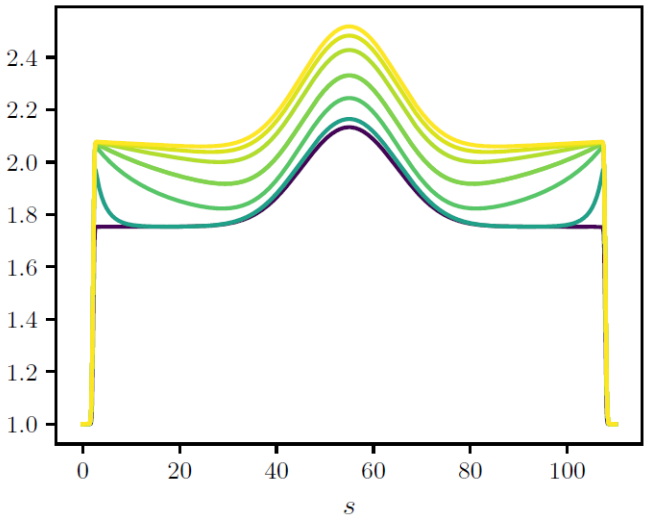
κ_d: Conduction coefficient

- Simple, 1D model of the tokamak scrape-off layer
- Flux tube aligned with a magnetic field line
- Mass deposited into the domain by perpendicular transport
- Single fluid of electrons and ions
- Sonic outflow at either end to approximate sheath BCs
- No neutrals

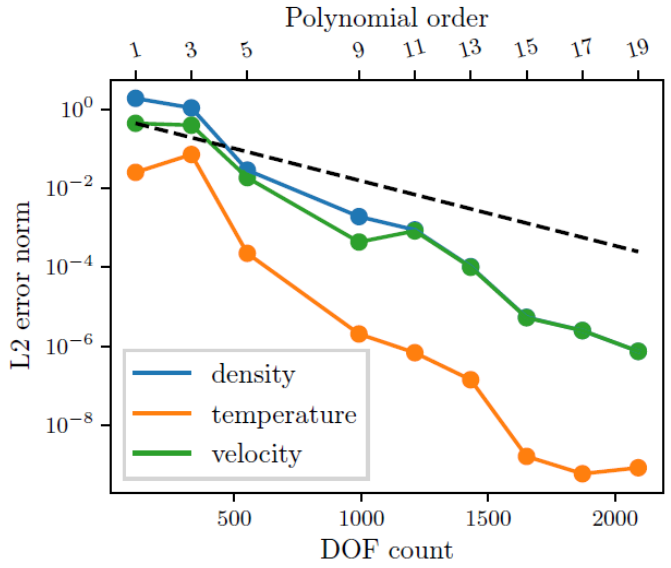
1D SOL Proxyapp

Soldrake (Will Saunders)

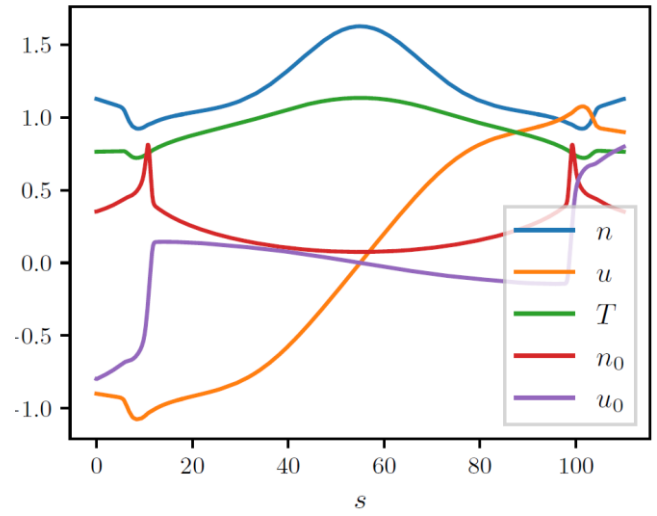
- *Firedrake* used to implement equations in weak form with Unified Form Language (UFL)
- Continuous Lagrange basis functions
- *Irksome* used for (Runge-Kutta) time integration
- Evolve to near equilibrium from ICs, add small amount of diffusion to stabilise.
- Use result as initial guess for steady state solve to speed things up



Varying conduction



Error as a function of N_{DOFs}



Including neutrals

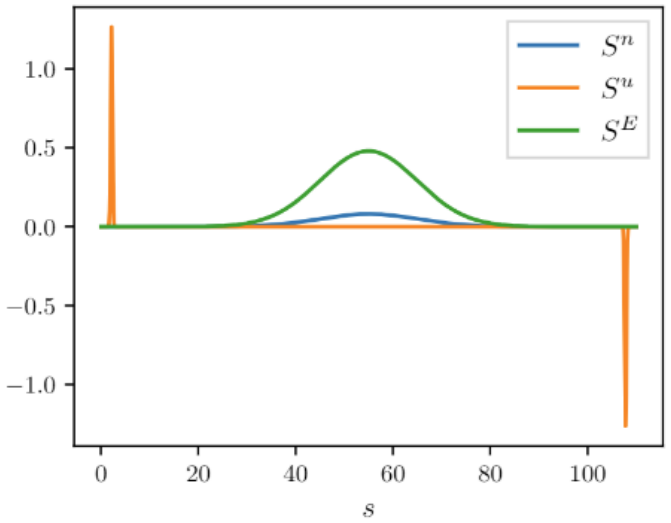
[75] W. Saunders and E. Threlfall. *Finite Element Models: Performance*. Tech. rep. CD/EXCALIBUR-FMS/0047-M2.2.2. https://github.com/ExCALIBUR-NEPTUNE/Documents/blob/main/reports/ukaea_reports/CD-EXCALIBUR-FMS0047-M2.2.2.pdf. UKAEA, 2021.

1D SOL Proxyapp

Nektar++ solver

- Nektar++ version of the same solver, implemented by Dave Moxey with support from OP
- Choose constants such that the problem reduces to solving incompressible Euler equations
- Discretisation: Discontinuous Galerkin
- Time evolution: 4th order Runge-Kutta
- Source terms, BCs chosen to match Soldrake implementation

Source terms



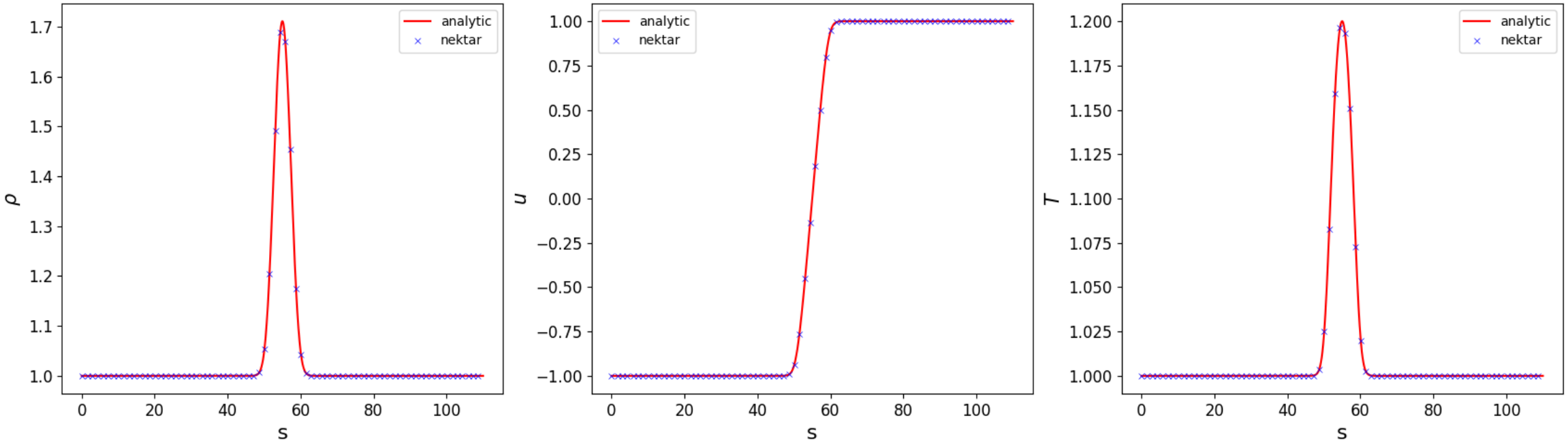
New Nektar++ solver

- Define equation system, based on existing advection solver
- Specify desired source terms via Forcing function framework
- Configure and run solver on simple 1D domain

Code at https://github.com/ExCALIBUR-NEPTUNE/nektar-1d-sol

1D SOL Proxyapp

Nektar++ results



- Good agreement with analytical solution presented by Arter (and with Soldrake)

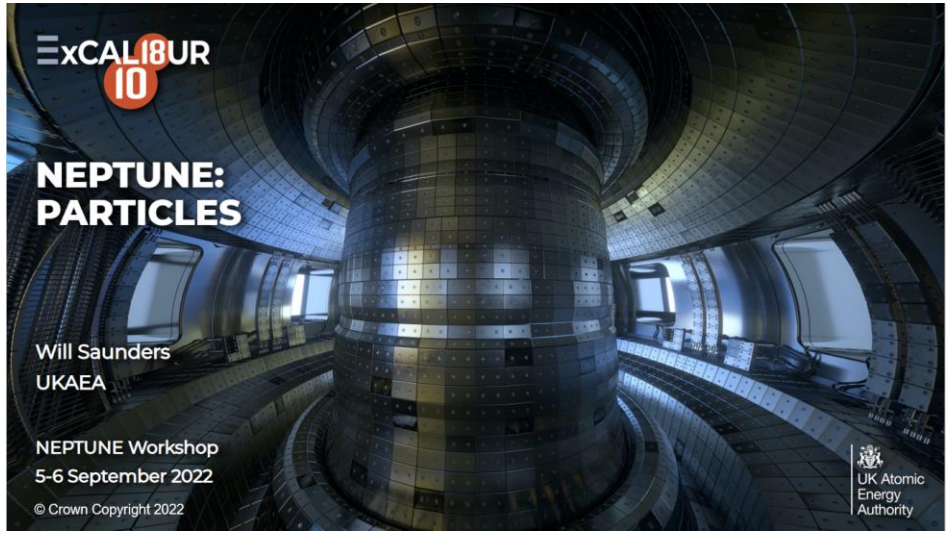
Wayne Arter. Study of source terms in the SOLF1D edge code. Technical report, Eurofusion/CCFE, 2015. CCFE-DETACHMENT-RP2-Draft.

Nektar++ integration in NEPTUNE

NESO

- Nektar functionality already being used in NEPTUNE prototype code
- See *NESO* git repo at https://github.com/ExCALIBUR-NEPTUNE/NESO + Will and James' talks:

Coupling between PIC code, Nektar++ in NESO



NESO overview

Nektar++ integration in NEPTUNE

Changes to Nektar core libraries

Status quo: define session in one or more XML files

XML session file

```
<?xml version="1.0" encoding="utf-8" ?>
<NEKTAR>
    <GEOMETRY DIM="1" SPACE="1">
        <VERTEX>
        <ELEMENT>
        <COMPOSITE>
        <DOMAIN>
    </GEOMETRY>

    <EXPANSIONS>

    <FORCING>

    <CONDITIONS>
        <PARAMETERS>
        <SOLVERINFO>
        <VARIABLES>
        <BOUNDARYREGIONS>
        <BOUNDARYCONDITIONS>
        <FUNCTION NAME="InitialConditions">
        <FUNCTION NAME="ExactSolution">
    </CONDITIONS>

</NEKTAR>
```

Solver code

Session, including mesh, read here

```
SessionReaderSharedPtr session = SessionReader::CreateInstance(argc, argv);
MeshGraphSharedPtr mesh = MeshGraph::Read(session);
string driverName("Standard");
DriverSharedPtr driver = GetDriverFactory().CreateInstance(driverName, session, mesh);
driver->Execute();
session->Finalise();
```

Pass session filepath(s) to the solver at runtime:

```
my_solver.exe [path_to_session.xml]
```

Nektar++ integration in NEPTUNE

Changes to Nektar core libraries

```
<CONDITIONS>
    <PARAMETERS>
        <P> TimeStep        = 5e-4              </P>
        <P> NumSteps        = 1000000            </P>
        <P> IO_CheckSteps   = 10000              </P>
        <P> IO_InfoSteps    = 1000               </P>
        <P> Gamma           = 5.0/3.0              </P>
        <P> GasConstant     = 1.0               </P>
        <P> pInf            = 1.0               </P>
        <P> rhoInf          = 1.0               </P>
        <P> uInf            = 1.0               </P>
    </PARAMETERS>
    <SOLVERINFO>
        <I PROPERTY="EQTYPE"                VALUE="SOL"                />
        <I PROPERTY="Projection"            VALUE="DisContinuous"      />
        <I PROPERTY="AdvectionType"         VALUE="WeakDG"             />
        <I PROPERTY="TimeIntegrationMethod" VALUE="ClassicalRungeKutta4" />
        <I PROPERTY="UpwindType"            VALUE="ExactToro"          />
    </SOLVERINFO>
    <VARIABLES>
        <V ID="0"> rho </V>
        <V ID="1"> rhou </V>
        <V ID="2"> E </V>
    </VARIABLES>
```

XML session configuration

```
// Variable names
std::vector<std::string > varNames = { "rho", "rhou", "E" };

// Set params of type double
std::map<std::string, NekDouble> dblParams;
dblParams["Timestep"] = 5e-4;
dblParams["Gamma"] = 5.0/3;
dblParams["GasConstant"] = 1.0;
dblParams["pInf"] = 1.0;
dblParams["rhoInf"] = 1.0;
dblParams["uInf"] = 1.0;

// Set params of type int
std::map<std::string, int> intParams;
intParams["IO_CheckSteps"] = 10000;
intParams["IO_InfoSteps"] = 1000;
intParams["NumSteps"] = 1000000;

// Set solver properties
std::map<std::string, std::string> solverInfo;
solverInfo["EQTYPE"] = "SOL";
solverInfo["Projection"] = "DisContinuous";
solverInfo["AdvectionType"] = "WeakDG";
solverInfo["TimeIntegrationMethod"] = "ClassicalRungeKutta4";
solverInfo["UpwindType"] = "ExactToro";

// Set up session
LibUtilities::SessionConfigurableSharedPtr session;
session = LibUtilities::SessionConfigurable::CreateInstance(argc, argv,
                                                            "sol1D", varNames, dblParams, intParams, solverInfo);
```

Programmatic session configuration

Finite element exterior calculus (FEEC)

(Work by Ed Threlfall)

- Framework for formulating finite element methods with useful numerical properties
- Developed by Douglas Arnold, and others, in early 2000s
- Combines ideas from homological algebra, functional analysis, exterior calculus

Can be used to ensure that a numerical method

- is naturally stable without adding artificial dissipation
- explicitly conserves certain quantities (e.g. electric charge)

Used in several major PIC codes: GEMPIC, EMPIRE

Numerous examples in the literature that illustrate FEEC utility; for instance…

Finite element exterior calculus (FEEC)

An example with Firedrake

Example from Douglas Arnold's book, run with Firedrake

D.N. Arnold, *Finite Element Exterior Calculus*, CBMS-NSF regional conference series in applied mathematics **93**, SIAM.

- "Re-entrant corner" problem:

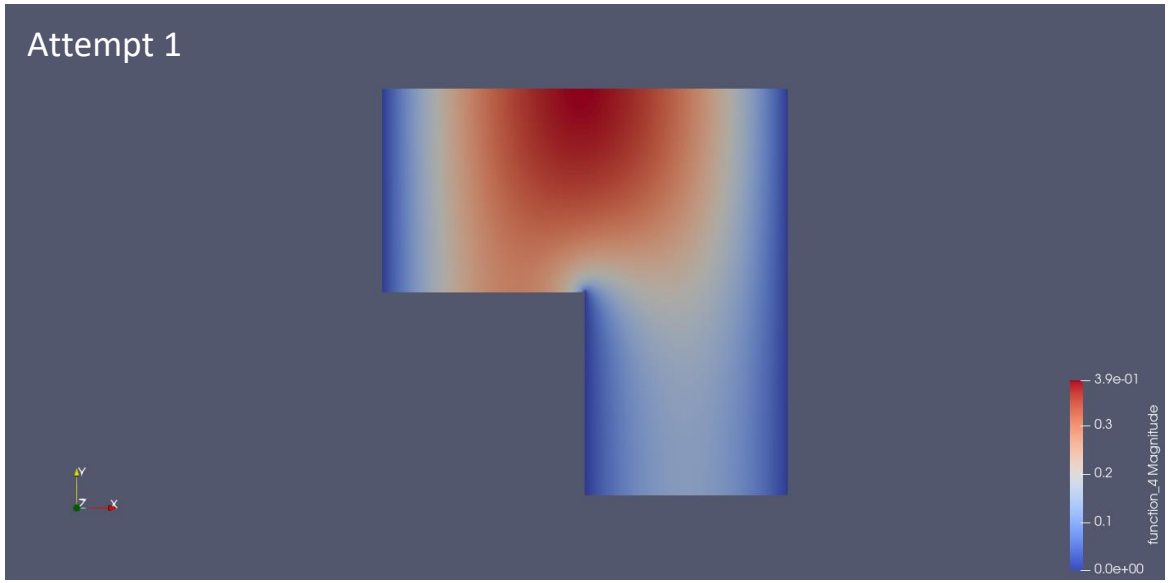
  Solve $\nabla^2 \underline{u} = \underline{f}$ on an L-shaped domain with source on interior corner

  with $\underline{f} = (1,0)$ and $\underline{u} \cdot \underline{n} = \nabla \times \underline{u} = 0$ on the boundary.

Solution: singularity of the form $r^{-\frac{1}{3}}$

(r: distance from the corner)

6th order vector Lagrange FS for $\underline{u}$



Converged, smooth… wrong! ⇒ Need *mixed* formulation

Finite element exterior calculus (FEEC)

An example with Firedrake

- "Re-entrant corner" problem:

  Solve $\nabla^2 \underline{u} = \underline{f}$ on an L-shaped domain with source on interior corner

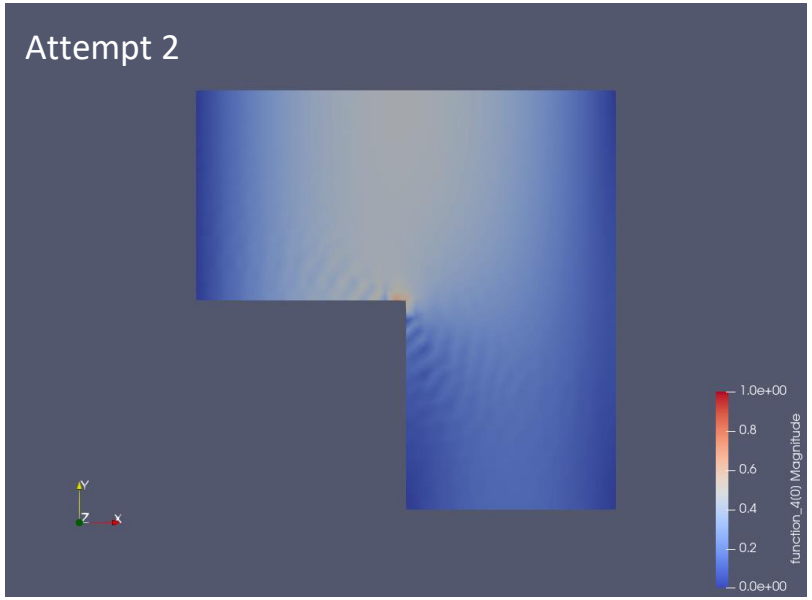
  with $\underline{f} = (1, 0)$ and $\underline{u} \cdot \underline{n} = \nabla \times \underline{u} = 0$ on the boundary.

Solution: singularity of the form $r^{-\frac{1}{3}}$

(r: distance from the corner)

6th order vector Lagrange FS for $\underline{u}$

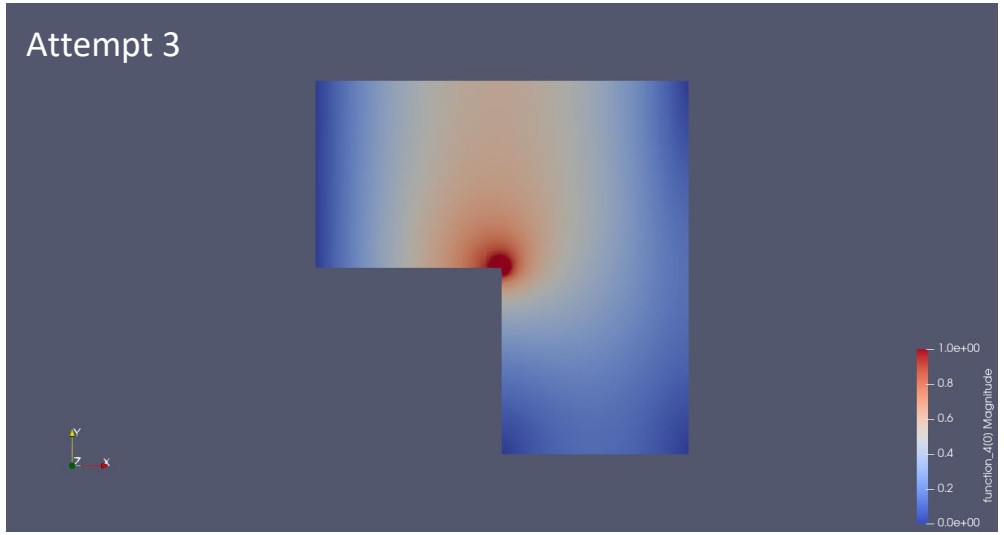
6th order scalar Lagrange FS for $\sigma \equiv \nabla . \underline{u}$



Spurious oscillations due to inconsistent choice of function spaces

6th order vector Raviart-Thomas "Edge" FS for $\underline{u}$

6th order scalar Lagrange FS for σ



Smooth, resolves singularity

Finite element exterior calculus (FEEC)

Lessons

- FEEC framework can help guarantee stability and conservation in FEM approaches
- Principles are easily demonstrated in idealised examples, but apply equally to real-world modelling
- Wide range of element types available – need to study literature to make a sensible choice
- FEEC increasingly being applied in PIC codes – may well be an essential ingredient for NEPTUNE

Conclusion

Progress towards Nektar++/NEPTUNE integration

- Nektar++ already applied to several problems relevant to edge-plasma physics
- FEEC offers a promising avenue to improve solver stability, apply conservation laws in FEM
- FEM-related NEPTUNE development:
  - PIC code / Nektar++ coupling: already started in NESO
  - Nektar++ setup without XML: almost complete
  - FEEC in Nektar++: future challenge