NEPTUNE SPECTRAL ELEMENT GRANTS

Ed Threlfall

NEPTUNE Workshop (The Cosener's House, Abingdon)

5 September 2022

UK Atomic Energy Authority

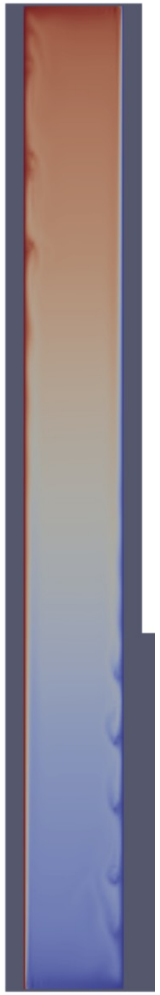
Grants

- T/NA078/20 Examining the performance of Nektar++ for fusion applications; 01/01/2021-30/06/2022
- T/AW084/21 Solving high-dimensional plasma kinetics using Nektar++; 01/09/2021-22/09/2022
- T/AW085/22 (Nektar++ for fusion applications - work is continuation of T/NA078/20); 01/09/2022-15/02/2024

All are joint KCL / Imperial College London.

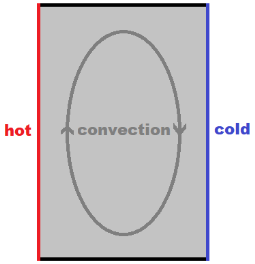
Main UKAEA personnel: Ed Threlfall (since June 2020), Owen Parry (joined early this year).

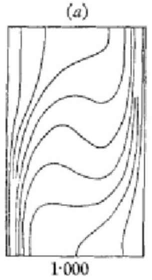
T/NA078/20 Examining the performance of Nektar++ for fusion applications

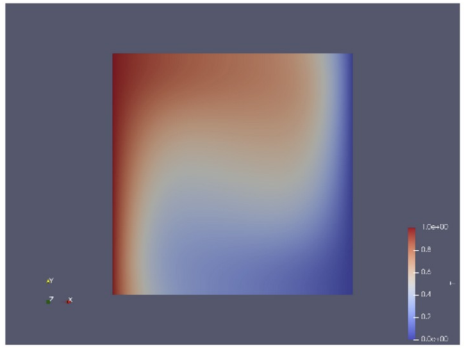


- Approach: use Nektar++ for studying problems in heat transport – slot convection problem.
- Compare outputs with results in literature.
- Learn Nektar++ / note any issues discovered / Nektar-users mail list (or DM/CC) for queries.

$$
\begin{aligned}
\frac{1}{Pr}\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) &= -\nabla p + Ra\, T\, \hat{\mathbf{y}} + \nabla^2 \mathbf{u} \\
\left(\frac{\partial T}{\partial t} + \mathbf{u}\cdot\nabla T\right) &= \nabla^2 T \\
\nabla\cdot\mathbf{u} &= 0.
\end{aligned}
$$







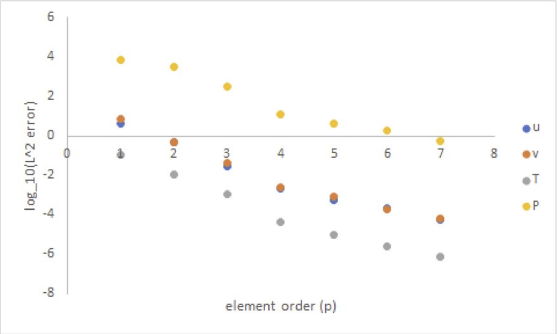
- Cf. J.W. Elder's experiments / numerics (1965).

- See UKAEA report Finite Element Models: Complementary Activities I ([Documents/CD-EXCALIBUR-FMS0051-M6.1.pdf at main · ExCALIBUR-NEPTUNE/Document (github.com)](github.com)).

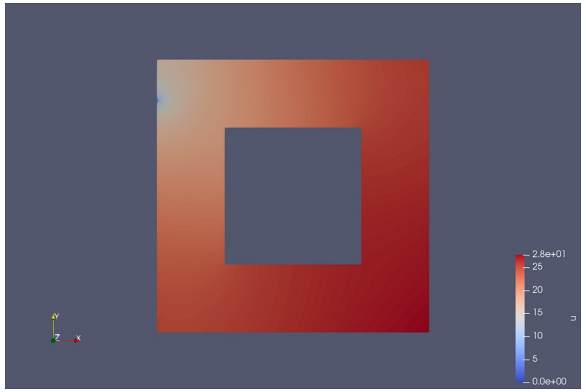
- MIT numerical benchmark very similar … [MIT Benchmark - Featflow (tu-dortmund.de)](tu-dortmund.de)

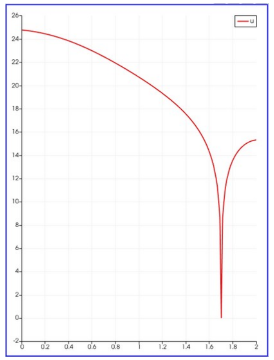
T/NA078/20 Examining the performance of Nektar++ for fusion applications

- Spectral convergence verified for a laminar convective flow (evaluate error vs. converged solution).



- Uncovered issue with VelocityCorrectionScheme algorithm (is in pressure Poisson solve – also emerges generally in Helmholtz solver algorithm). Solution is to use alternate VCSWeakPressure algorithm.





T/NA078/20 Examining the performance of Nektar++ for fusion applications

- Added new "filters" to Nektar++ to obtain heat flux (Nusselt number) and to study properties of hot spot on cavity wall where heat transfer is maximal, all as time series.

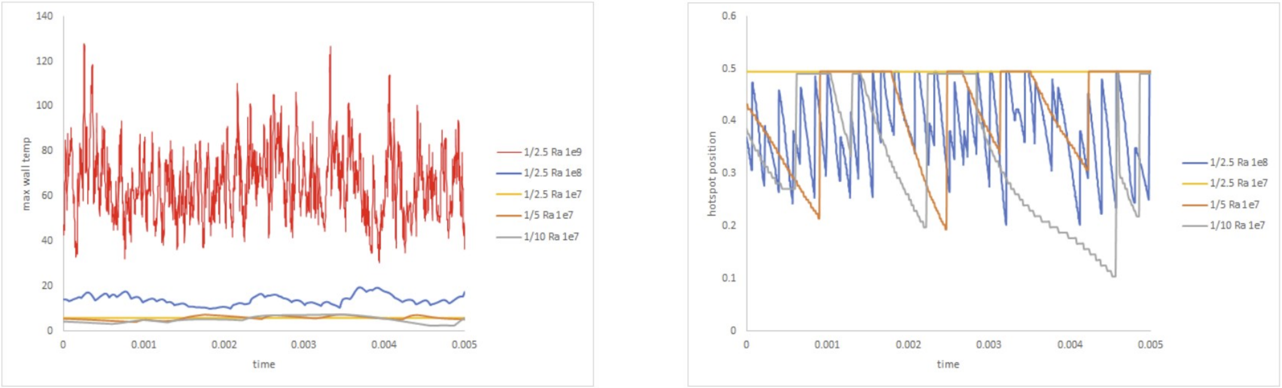


Figure 7: Transient behaviour associated to boundary-layer waves. The left-hand-side plot shows the maximum temperature at a small displacement from the cold-side wall and the right-hand-side one shows the vertical position of the hottest point near the cold wall, both as time series.

- Also constructed a GP fit to time series … used VECMA toolkit to drive Nektar++ UQ campaign (in hackathons organized by UCL).

T/NA078/20 Examining the performance of Nektar++ for fusion applications

- Further comparison with literature / exploration of Nektar++ capabilities …

- MIT benchmark convection problem; Nu = 4.57946. (See MIT Benchmark - Featflow (tu-dortmund.de))

- Same problem; time-dependent component of field near turbulent transition.

Element order p	time-av. Nusselt number Nu	Execution time / s (16 logical cores)
1	3.66566	38
2	4.95898	97
3	4.62167	171
4	4.54045	336
5	4.56850	601
6	4.57956	799
7	4.57977	1047
8	4.57943	1627
9	4.57936	1903
10	4.57935	2466
11	4.57935	3029

Table 1: Table of time-averaged Nusselt number values for $Ra = 3.4 \times 10^5$ obtained from *Nektar++*.

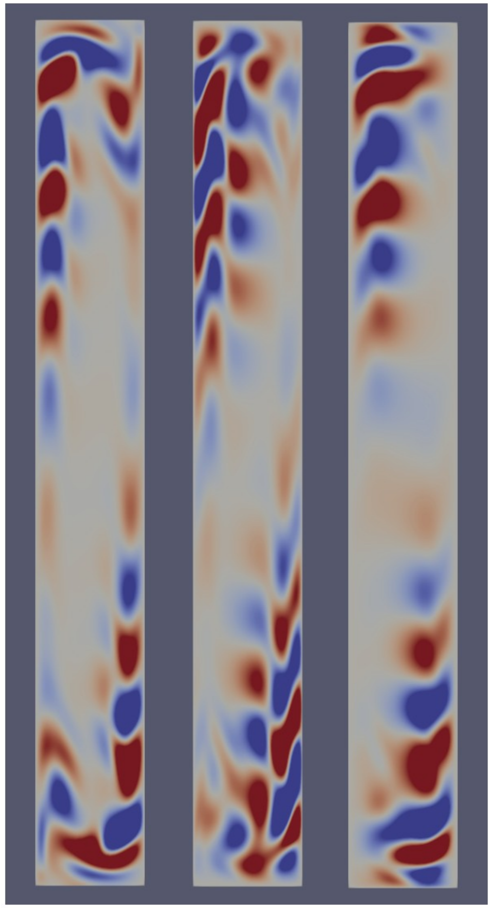


Figure 3: Nektar++ fluctuation fields for T, v, u (respectively temperature, vertical velocity, horizontal velocity), corresponding to Figs.5-7 of [8], computed by subtracting fields averaged over one period of $Ra = 3.4 \times 10^5$ case. Scales are excluded as phase does not correspond to that used in figures from the reference.

- See report Finite Element Models: Complementary Activities 2 (Documents/CD-EXCALIBUR-FMS0064-M6.2.pdf at main · ExCALIBUR-NEPTUNE/Documents (github.com))

ExCALIBUR

T/NA078/20 Examining the performance of Nektar++ for fusion applications

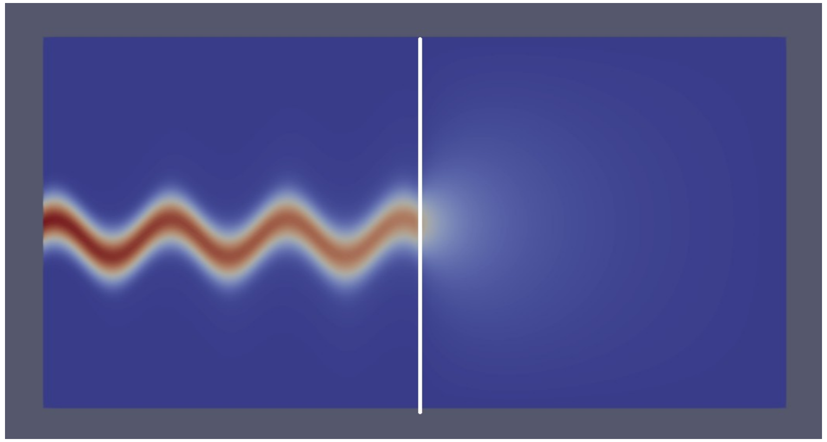
- Initial study of Nektar++-based proxyapps:
- Compared Nektar-Diffusion outputs with analytic solutions.
- Experimented with same problem in Firedrake inc. mock-up of coupled problem … ongoing. See GitHub https://github.com/ethrelfall/Heat-transport.
- Compared output of Nektar-Driftwave Hasegawa-Wakatani solver with published results.
- See report Finite Element Models: Performance (Documents/CD-EXCALIBUR-FMS0047-M2.2.2.pdf at main · ExCALIBUR-NEPTUNE/Documents (github.com)).

i) A semi-infinite domain maintained at a unit temperature at $x = 0$ at all times, for which the solution is

$$T(x;t) = 1 - \mathrm{erf}\left(\frac{x}{\sqrt{4Dt}}\right). \tag{1}$$

ii) A finite domain e.g. $x \in [0,1]$ with unit temperature at $x = 0$ and zero temperature at $x = 1$ for all times, with solution (expressible also in closed form as the integral of the Jacobi theta function of imaginary argument $\theta(x; it)$)

$$T(x;t) = 1 - x - \sum_{n=1}^{\infty} \frac{2}{\pi n}\, e^{-n^2\pi^2 Dt} \sin n\pi x. \tag{2}$$



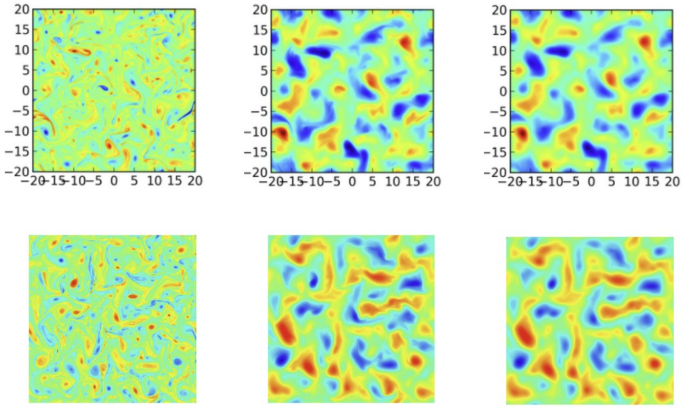
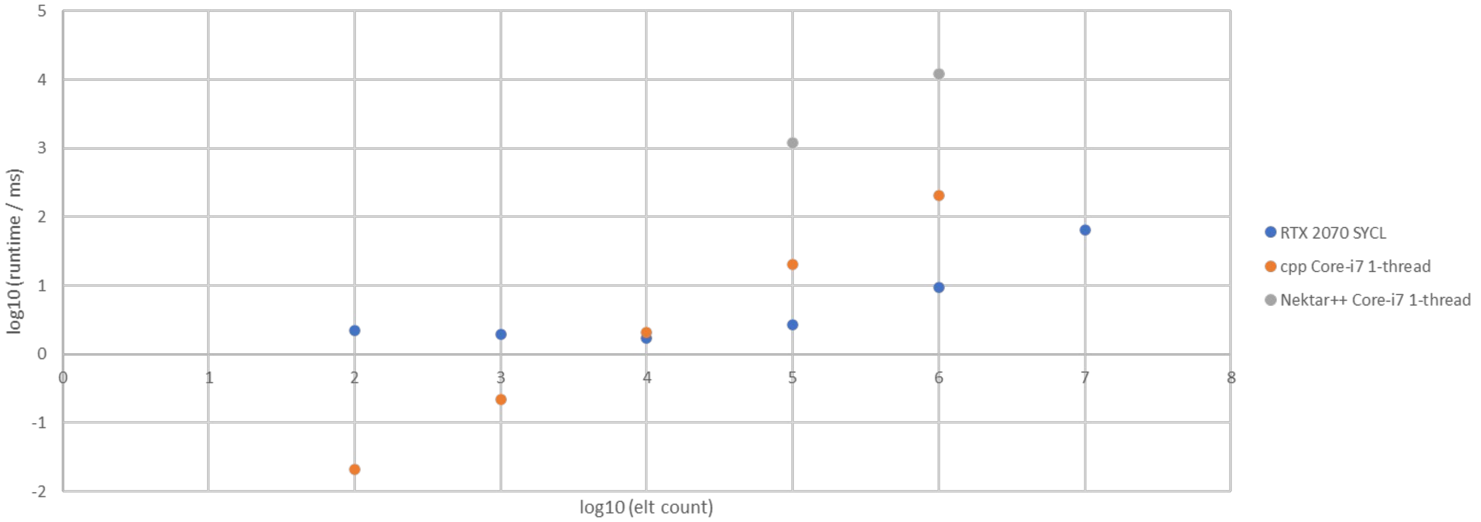


Figure 7: Example simulated vorticity, density, and electrostatic potential (left to right) from Ammar Hakim's web page (ref) (top) with corresponding proxyapp outputs (bottom), showing qualitative correspondence.

T/NA078/20 Examining the performance of Nektar++ for fusion applications

- Simple performance study in 1D plus comparison to C++ and SYCL (Nvidia GPU via Codeplay ComputeCpp) implementations of the same.



- Other performance issues … e.g. large memory use of incompressible Navier-Stokes solver – dialogue with David Moxey (established that non-essential pre-static-condensed matrix is retained).
- I have attended Nektar++ workshop events.

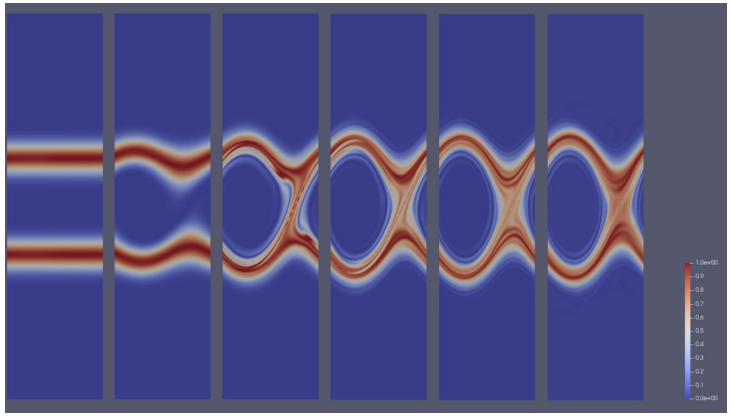
T/AW084/21 Solving high-dimensional plasma physics using Nektar++

- Grant exploring solutions of Boltzmann-type equations in phase space; allows use of two meshes (real space and velocity space).

- Wrote exploratory code solving 1+1D Vlasov-Poisson problem within Nektar++ framework (new solver; used Microsoft Visual Studio).

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} + E\frac{\partial f}{\partial v} = 0. \qquad \frac{\partial^2 \phi}{\partial x^2} = \omega_P^2 \left(\int f \frac{dv}{v_0} - 1 \right)$$

- Studied two-stream instability problem … will be useful for assessing proxyapp developed under grant to solve same problem. Internal report Support High-Dimensional Procurement ([Documents/CD-EXCALIBUR-FMS0066-M4.1.pdf at main · ExCALIBUR-NEPTUNE/Documents (github.com)](https://github.com)) provided to grantee.



T/AW084/21 Solving high-dimensional plasma physics using Nektar++

- Benchmark code against analytic solution for instability growth rate as function of plasma frequency and mode number. (Must use smooth initial data!)

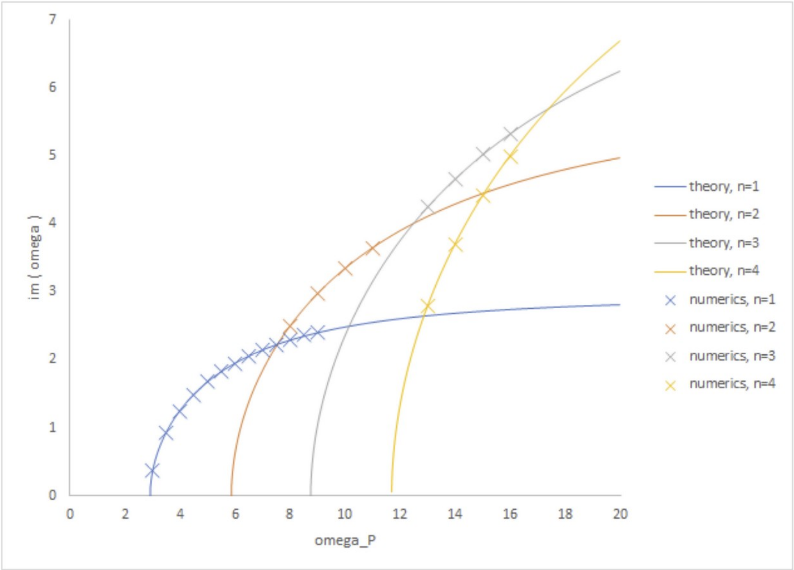


Figure 7: Theoretical predictions for the growth rates of modes $n = 1 - 4$ (spatial wavenumber $k = n\pi$) as a function of the plasma frequency ω_P. Overlain are numerical results from the *Nektar++* implementation, showing good agreement.

$$1 = -\frac{\omega_P^2}{2\sigma^2 k^2}\left(2 - \sqrt{\pi} A e^{-A^2}(\mathrm{erfi}(A) - i) - \sqrt{\pi} A' e^{-A'^2}(\mathrm{erfi}(A') - i)\right)$$

with $A \equiv \frac{\omega - k v_0}{\sqrt{2}\sigma k}$, $A' \equiv \frac{\omega + k v_0}{\sqrt{2}\sigma k}$.

- Good agreement; long-term energy conservation behaviour less nice (energy grows, even with upwinded DG).

T/AW085/22 Nektar++ for fusion applications

- System 2-6 plasma fluid equations supplied to grantee for Nektar++ implementation.

number density n_e, "vorticity" $(\nabla \cdot \mathbf{E}^+)$, electron energy $\mathcal{E}_e$, ion energy $\mathcal{E}_i$ and neutral number density n_n are respectively

$$\partial_t n_e + \nabla \cdot (n_e \mathbf{u}_e) = S_{n_e} - \frac{n_e}{\tau_{n_e}} \tag{94}$$

$$\begin{aligned}\partial_t \nabla \cdot \mathbf{E}^+ + \nabla \cdot (\nabla \cdot (\mathbf{u}_i \otimes \mathbf{E}^+)) = \nabla \cdot \left(n_i (\mathbf{u}_{\nabla Bi} + \mathbf{u}_{cx}) - \frac{1}{Z_i} n_e \mathbf{u}_{\nabla Be} \right) \\ + \frac{1}{Z_i} \frac{n_e}{\tau_{n_e}} - \frac{n_i}{\tau_{n_i}} + \nabla \cdot (\nu \nabla_\perp (\nabla \cdot \mathbf{E}^+))\end{aligned} \tag{95}$$

$$\partial_t \mathcal{E}_e + \nabla \cdot (\mathcal{E}_e \mathbf{u}_e + p_e \mathbf{u}_e) = S_{\mathcal{E}_e} - \frac{\mathcal{E}_e}{\tau_{Ee}} + Q_{ie} + \nabla \cdot (\chi_{\perp e} n_e \nabla_\perp T_e) \tag{96}$$

$$\partial_t \mathcal{E}_i + \nabla \cdot (\mathcal{E}_i \mathbf{u}_i + p_i \mathbf{u}_i) = S_{\mathcal{E}_i} - \frac{\mathcal{E}_i}{\tau_{Ei}} - Q_{ie} + \nabla \cdot (\chi_{\perp i} n_i \nabla_\perp T_i) \tag{97}$$

$$\partial_t n_n = S_{n_n} + \nabla \cdot (D_n \nabla_\perp p_n) \tag{98}$$

where with the usual notation for species α pressure p_α, temperature T_α, charge state Z_i, species mass m_α, electric potential Φ and magnetic field $\mathbf{B}$,

- Owen Parry embedded in Nektar++ development team at KCL.

T/AW085/22 Nektar++ for fusion applications

- Exploring use of structure-preserving methods to enforce conservation laws / provide guarantees of validity of numerical methods (e.g. immanent stability removes requirement to add numerical dissipation).

- Hasegawa-Wakatani shown earlier is candidate, but equations may need re-framing (usually presented in scalar form but need vector).

- Started with simple Discrete Exterior Calculus problems assessed using Method of Manufactured Solutions or analytic solutions.

D.S. Rufat. Spectral exterior calculus and its implementation. *PhD thesis, Caltech*, 2017.

$$\frac{\partial u}{\partial t} = \frac{\pi}{4}\frac{\partial^2 u}{\partial x^2},$$

$$u(x,t) = \theta_3(x;t) \equiv 1 + 2\sum_{n=1}^{\infty} e^{-\pi n^2 t} \cos 2nx,$$

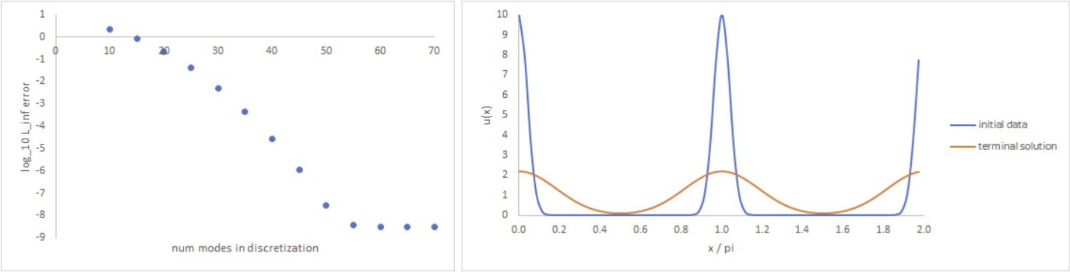
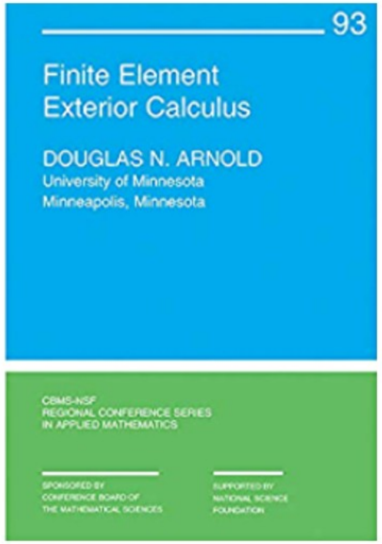


Figure 6: Convergence of the discrete exterior calculus implementation of the diffusion problem explained in the main text (left). Solution curves for $N = 70$ shown to right - the initial data corresponds to $t = 0.01$ and the terminal solution $t = 0.21$.

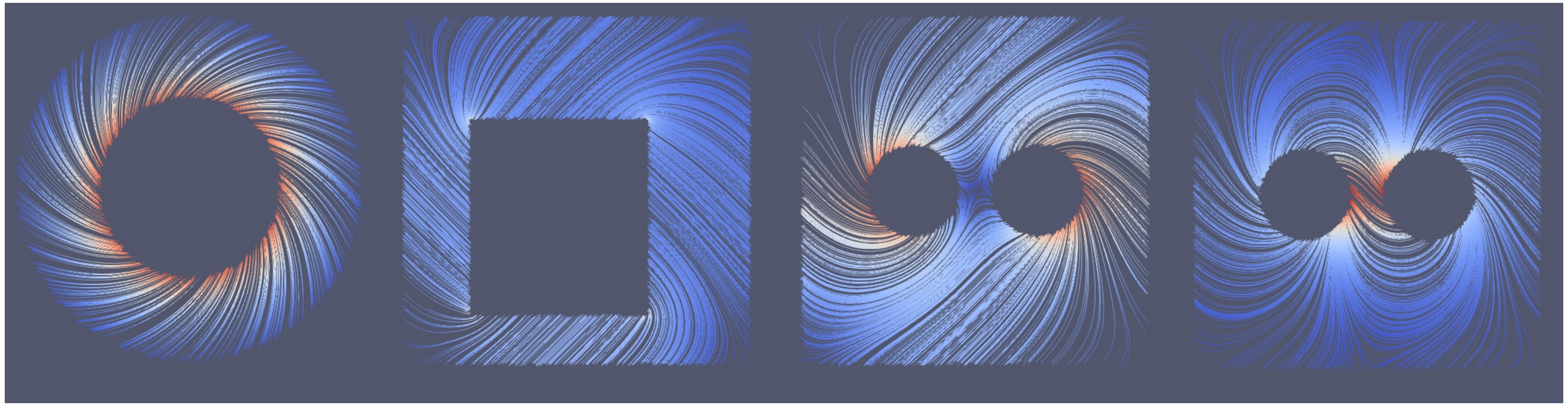
- Verified spectral convergence of toy implementations (C++ / Boost / Intel MKL).

T/AW085/22 Nektar++ for fusion applications



- Investigating Finite Element Exterior Calculus (FEEC) techniques.

- Read textbook / papers of Douglas N. Arnold.
- Implemented a number of examples in Firedrake and committed to GitHub repository; see https://github.com/ethrelfall/Finite-element-exterior-calculus.
- These are generically "challenging" for conventional FEM but work nicely if use FEEC.



$$\nabla \cdot \underline{v} = \nabla \times \underline{v} = 0; \quad \nabla^2 \underline{v} = 0; \quad \rho\, \underline{v} \cdot \nabla \underline{v} = -\nabla p$$

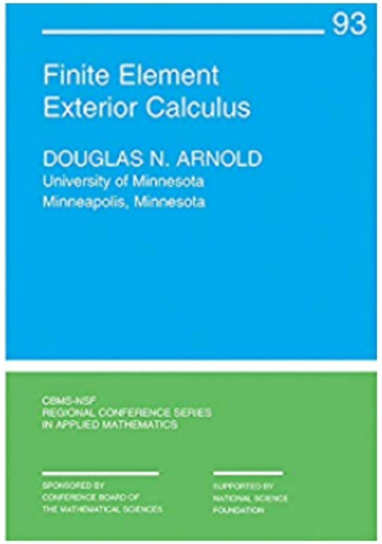
- I have canvassed opinion from members of the Firedrake community re FEEC.

T/AW085/22 Nektar++ for fusion applications

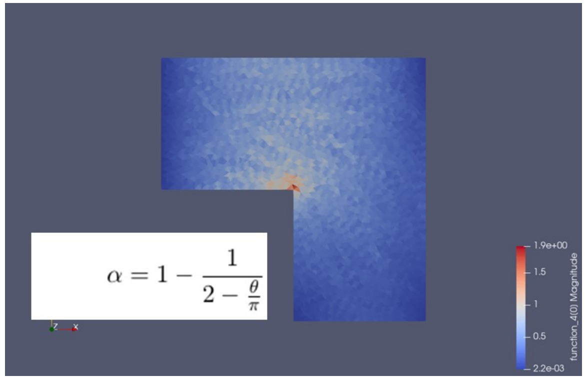
- FEEC makes sense of large "zoo" of finite-element types.

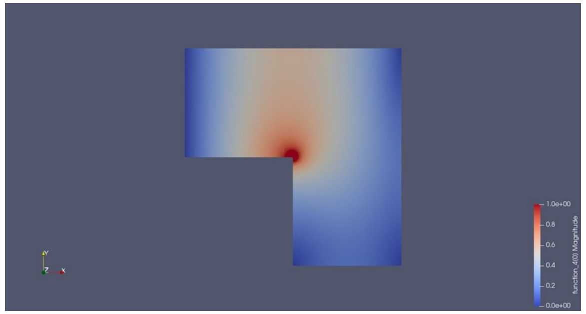
Bernstein		scalar	interval, triangle, tetrahedron
Brezzi-Douglas-Marini	BDM	vector	triangle, tetrahedron
Brezzi-Douglas-Fortin-Marini	BDFM	vector	triangle, tetrahedron
Bubble	B	scalar	interval, triangle, tetrahedron
FacetBubble	FB	scalar	interval, triangle, tetrahedron
Crouzeix-Raviart	CR	scalar	triangle, tetrahedron
Discontinuous Lagrange	DG	scalar	interval, triangle, tetrahedron, quadrilateral, hexahedron
Discontinuous Raviart-Thomas	DRT	vector	triangle, tetrahedron
Discontinuous Taylor	TDG	scalar	interval, triangle, tetrahedron
Gauss-Legendre	GL	scalar	interval
Gauss-Lobatto-Legendre	GLL	scalar	interval
HDiv Trace	HDivT	scalar	interval, triangle, tetrahedron, quadrilateral, hexahedron
Hellan-Herrmann-Johnson	HHJ	tensor	triangle
Nonconforming Arnold-Winther	AWnc	tensor	triangle, tetrahedron
Conforming Arnold-Winther	AWc	tensor	triangle, tetrahedron
Hermite	HER	scalar	interval, triangle, tetrahedron
Kong-Mulder-Veldhuizen	KMV	scalar	triangle, tetrahedron
Argyris	ARG	scalar	triangle
Mardal-Tai-Winther	MTW	vector	triangle
Morley	MOR	scalar	triangle

Bell	BELL	scalar	triangle
Lagrange	CG	scalar	interval, triangle, tetrahedron, quadrilateral, hexahedron
Nedelec 1st kind H(curl)	N1curl	vector	triangle, tetrahedron
Nedelec 2nd kind H(curl)	N2curl	vector	triangle, tetrahedron
Raviart-Thomas	RT	vector	triangle, tetrahedron
Regge		tensor	triangle, tetrahedron
DQ		scalar	interval, quadrilateral, hexahedron
Q		scalar	interval, quadrilateral, hexahedron
RTCE		vector	quadrilateral
RTCF		vector	quadrilateral
NCE		vector	hexahedron
NCF		vector	hexahedron
Real	R	scalar	interval, triangle, tetrahedron, quadrilateral, hexahedron
DPC		scalar	interval, quadrilateral, hexahedron
S		scalar	interval, quadrilateral, hexahedron
DPC L2		scalar	interval, quadrilateral, hexahedron
Discontinuous Lagrange L2	DG L2	scalar	interval, triangle, tetrahedron, quadrilateral, hexahedron
Gauss-Legendre L2	GL L2	scalar	interval
DQ L2		scalar	interval, quadrilateral, hexahedron
Direct Serendipity	Sdirect	scalar	quadrilateral



- … pick the right one!





T/AW085/22 Nektar++ for fusion applications

- FabNEPTUNE plug-in made available by UCL.
- Facilitates NEPTUNE workflows on HPC and gives integration with SEAVEAtk UQ toolkit.
- Currently set-up to run Nektar++ convection simulations in 2D and 3D (189k elements). Ongoing … 3D results have crossover with Smallab experimental program.