From symbolic mathematics to fast solvers for finite element problems

Lawrence Mitchell[1,*]

C.J. Cotter, P.E. Farrell, T.H. Gibson, D.A. Ham, P.H.J. Kelly, R.C. Kirby, M.G. Knepley, E.H. Müller, F. Wechsung, ...

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Outline

- Overview
  - Automated finite elements
  - Multigrid preconditioning for numerical weather prediction
- In depth
  - Parameter-robust preconditioning for the Navier–Stokes equations
- Future directions

Automated finite elements

Code that captures mathematical structure

Find $(u, p, T) \in V \times W \times Q$ s.t.

$$\int \nabla u \cdot \nabla v + (u \cdot \nabla u) \cdot v$$

$$-p\nabla \cdot v + \frac{\mathrm{Ra}}{\mathrm{Pr}} T g\hat{z} \cdot v \,\mathrm{d}x = 0$$

$$\int \nabla \cdot u q \,\mathrm{d}x = 0$$

$$\int (u \cdot \nabla T) S + \mathrm{Pr}^{-1} \nabla T \cdot \nabla S \,\mathrm{d}x = 0$$

$$\forall\, (v, q, T) \in V \times W \times Q$$

```
from firedrake import *
mesh = Mesh(...)
V = VectorFunctionSpace(mesh, "CG", 2)
W = FunctionSpace(mesh, "CG", 1)
Q = FunctionSpace(mesh, "CG", 1)
Z = V * W * Q
Ra = Constant(...)
Pr = Constant(...)
upT = Function(Z)
u, p, T = split(upT)
v, q, S = TestFunctions(Z)
bcs = [...]

F = (inner(grad(u), grad(v))
     + inner(dot(grad(u), u), v)
     - inner(p, div(v))
     + (Ra/Pr)*inner(T*g, v)
     + inner(div(u), q)
     + inner(dot(grad(T), u), S)
     + (1/Pr)*inner(grad(T), grad(S)))*dx

solve(F == 0, upT, bcs=bcs)
```

The computer should work for *you*

- Mathematics just says “here is the integral to compute on each element, do that everywhere”
- Code specifies an *implementation*

Assertion(s)

Having chosen a discretisation, writing the element integral is “mechanical”.

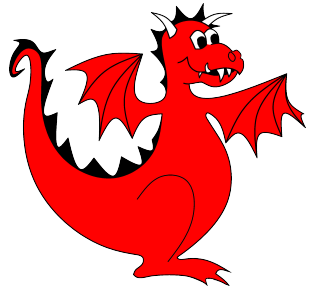
With an element integral in hand, integrating over a mesh is “mechanical”.

Corollary

Computers are good at mechanical things, why don’t we get the computer to write them for us?

Firedrake `www.firedrakeproject.org`

[...] *an automated system for the solution of partial differential equations using the finite element method.*



- Written in Python.
- Finite element problems specified with *embedded* domain specific language, UFL (Alnæs, Logg, Ølgaard, Rognes, and Wells 2014) from the FEniCS project.
- Domain-specifc optimising compiler.
- *Runtime* compilation to optimised, low-level (C) code.

F. Rathgeber, D.A. Ham, **L. Mitchell**, M. Lange, F. Luporini, A.T.T. McRae, G.-T. Bercea, G.R. Markall, P.H.J. Kelly.

ACM Transactions on Mathematical Software (2016). `arXiv:1501.01809[cs.MS]`

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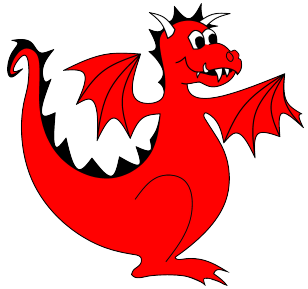
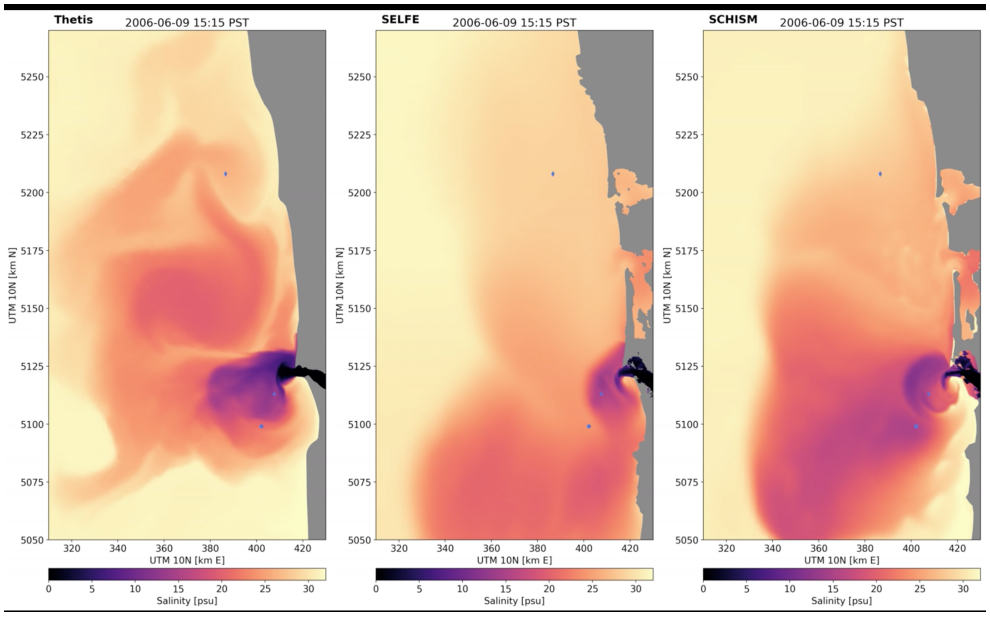


User groups at

Imperial, Oxford, Bath, Leeds, Durham, Kiel, Rice, Houston, Exeter, Buffalo, Waterloo, Washington, Baylor, Edinburgh, ...

Fourth annual (and first USA) user meeting this February (Seattle).

Application: coastal ocean modelling



Surface salinity of the Columbia river plume. Credit T. Kärnä, Finnish Meteorological Institute

- Lower numerical mixing, improved results.
- 3-8x faster than models with similar quality of results.
- Differentiable: efficient adjoint.
- Used at Finnish Met Institute; Earth Sciences at Imperial; Institute for Infrastructure and Environment (here).
- `thetisproject.org`

T. Kärnä, S.C. Kramer, **L. Mitchell**, D.A. Ham, M.D. Piggott, A.M. Baptista. Geoscientific Model Development (2018). `arXiv:1711.08552[physics.ao-ph]`

Application: numerical weather prediction

$$\begin{pmatrix} M_2 & -\frac{\Delta t}{2} D^T & -\frac{\Delta t}{2} Q \\ \frac{\Delta t}{2} c^2 D & M_3 & 0 \\ \frac{\Delta t}{2} N^2 Q^T & 0 & M_b \end{pmatrix} \begin{pmatrix} \vec{U} \\ \vec{P} \\ \vec{B} \end{pmatrix} = \begin{pmatrix} M_2 \vec{R}_u \\ M_3 \vec{R}_p \\ M_b \vec{R}_b \end{pmatrix}$$

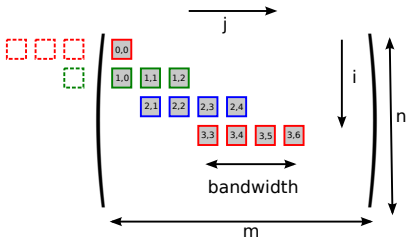
Challenge

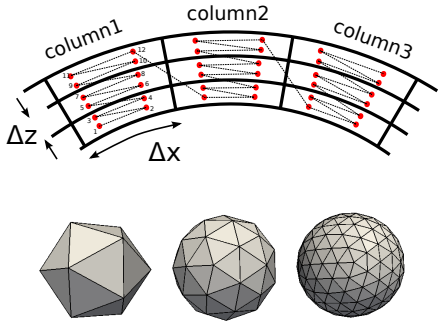
Invert elliptic operator fast enough for operational forecasting.

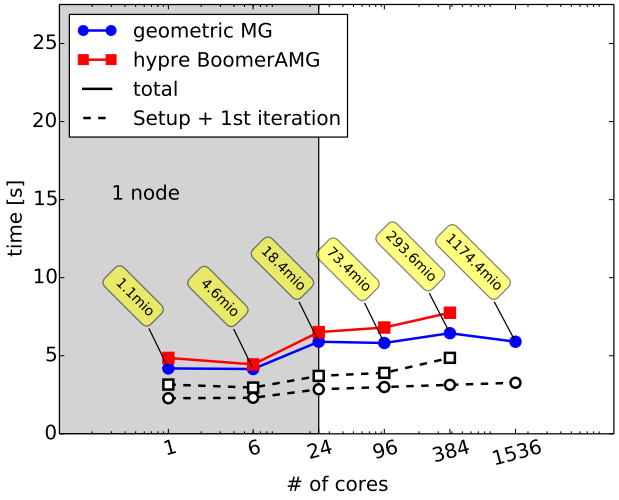
High aspect ratio: black-box numerical solvers struggle.

Need scalable, custom multigrid solver.

Multigrid approach







Developed custom tensor-product multigrid scheme, showed robustness and scalability.

L. Mitchell, E.H. Müller. JCP (2016). `arXiv:1605.00492[cs.MS]`

Future directions

Multilevel solvers for hybridised discretisations.

Approach is being explored by UK Met Office in their next generation dynamical core.

Preconditioning Navier–Stokes

Application challenge

Stationary incompressible Navier–Stokes

For $\nu \in \mathbb{R}_+$, find $(u, p) \in H^1(\Omega; \mathbb{R}^d) \times L^2(\Omega)$ such that

$$
\begin{aligned}
-\operatorname{div}(2\nu\varepsilon(u)) + (u \cdot \nabla)u + \nabla p &= f && \text{in } \Omega, \\
\operatorname{div} u &= 0 && \text{in } \Omega, \\
u &= g && \text{on } \Gamma_D, \\
2\nu\varepsilon(u) \cdot n &= pn && \text{on } \Gamma_N,
\end{aligned}
$$

Why?

Fully implicit discretisations of transient problem; bifurcation analysis of steady state.

Challenges for solvers

Desired properties

- Growth in time to solution is (at worst) $\mathcal{O}(n \log n)$ in number of degrees of freedom (resolution).
- Convergence does not degrade with $\nu \to 0$.

Direct methods

✓ Convergence independent of ν

✗ Time to solution $\mathcal{O}(n^2)$ (3D).

Krylov methods

✓ Time to solution $\mathcal{O}(n \log n)$ (with multilevel preconditioner)

✗ Convergence independent of ν challenging

Block preconditioning

Newton linearisation

$$P := \begin{pmatrix} A & B^T \\ B & 0 \end{pmatrix} \begin{pmatrix} \delta u \\ \delta p \end{pmatrix} = \begin{pmatrix} b \\ 0 \end{pmatrix}.$$

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$$P := \begin{pmatrix} A & B^T \\ B & 0 \end{pmatrix} \begin{pmatrix} \delta u \\ \delta p \end{pmatrix} = \begin{pmatrix} b \\ 0 \end{pmatrix}.$$

Block factorisations

$$P^{-1} = \begin{pmatrix} I & -A^{-1}B^T \\ 0 & I \end{pmatrix} \begin{pmatrix} A^{-1} & 0 \\ 0 & S^{-1} \end{pmatrix} \begin{pmatrix} I & 0 \\ -BA^{-1} & I \end{pmatrix}$$

PDE-specific challenge

Find good approximations $\tilde{A}^{-1}$ for A^{-1} and $\tilde{S}^{-1}$ for S^{-1}.

Choosing $\tilde{A}^{-1}$ and $\tilde{S}^{-1}$

Stokes (no advection) Silvester and A. J. Wathen (1994)

Multigrid for $\tilde{A}^{-1}$, $\tilde{S}^{-1} = -\nu M_p^{-1}$

- ✓ h-independent
- ✗ Only effective up to $\mathsf{Re} \sim 10$ for Navier–Stokes.

PCD for Navier–Stokes Kay, Loghin, and A. Wathen (2002)

Multigrid for $\tilde{A}^{-1}$, approximate $\tilde{S}^{-1}$ with convection-diffusion solves on pressure space.

- ✓ h-independent
- ✗ Only effective up to $\mathsf{Re} \sim$ 100-1000

Performance of pressure convection-diffusion (PCD)

$1/h$	# degrees of freedom	Reynolds number		
		10	100	1000
2^4	8.34×10^2	22.0	40.4	103.3
2^5	3.20×10^3	23.0	41.3	137.7
2^6	1.25×10^4	24.5	42.0	157.0
2^7	4.97×10^4	25.5	42.7	149.0
2^8	1.98×10^5	26.0	44.0	137.0

Table 1: Average number of outer Krylov iterations per Newton step for the 2D regularized lid-driven cavity problem with PCD preconditioner. Obtained with IFISS v3.5, $Q_1 - P_0$ element pair.

Augmented Lagrangian approach

SIAM J. SCI. COMPUT.
Vol. 28, No. 6, pp. 2095–2113

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MICHELE BENZI† AND MAXIM A. OLSHANSKII‡

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Observation

✓ Viscosity-robust preconditioning

✗ Only 2D, no further implementation until 2018

Objectives

- First general implementation of the method. ✓
- Extend the solver and discretisation to three dimensions. ✓
- Extend approach to *divergence-free* discretisations. ✓

Three ideas

1. Control Schur complement with an augmented Lagrangian term
2. Kernel-capturing multigrid relaxation
3. Robust multigrid prolongation

P.E. Farrell, **L. Mitchell**, F. Wechsung. SIAM SISC (2019). `arXiv:1810.03315[math.NA]`

Controlling the Schur complement

Continuous augmentation

Add γ **grad div** u term to the momentum equation.

Doesn't change solution since **div** $u = 0$

Theorem (Hestenes, Fortin, Glowinski, Olshanksii, ...)

As $\gamma \to \infty$, the Schur complement is well approximated by $\tilde{S}^{-1} = -(\nu + \gamma) M_p^{-1}$.

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Discrete augmentation

$$\begin{pmatrix} A + \gamma B^T M_p^{-1} B & B^T \\ B & 0 \end{pmatrix} \begin{pmatrix} u \\ p \end{pmatrix} = \begin{pmatrix} b \\ 0 \end{pmatrix}$$

Doesn't change solution since $Bu = 0$.

Again, as $\gamma \to \infty$, S^{-1} is well approximated by $\tilde{S}^{-1} = -(\nu + \gamma)M_p^{-1}$.

Conservation of misery

Good news

The Schur complement becomes easy to approximate as $\gamma \to \infty$

Bad news

Normal multigrid approaches for $\tilde{A}^{-1}$ don't work for $A_\gamma := A + \gamma B^T M_p^{-1} B$, and get *worse* as $\gamma \to \infty$.

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	LU for $\tilde{A}_\gamma^{-1}$	AMG for $\tilde{A}_\gamma^{-1}$
$\gamma = 10^{-1}$	15	18
$\gamma = 1$	6	40
$\gamma = 10^{1}$	3	107

Outer Krylov iterations for different choices of $\tilde{A}_\gamma^{-1}$.

Point smoother is not sufficient

- Ignorning advection, then the top-left block corresponds to discretisation of

$$a_\gamma(u, v) = \underbrace{\int_\Omega 2\nu\varepsilon(u) : \varepsilon(v)\, \mathrm{d}x}_{\text{sym. pos. def.}} + \underbrace{\int_\Omega \gamma\, \mathrm{div}\, u\, \mathrm{div}\, v\, \mathrm{d}x}_{\text{sym. pos. semi-def.}}$$

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- The semi-definite term is singular on all solenoidal fields $\Rightarrow$ the system becomes *nearly singular* as $\gamma \to \infty$

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- The semi-definite term is singular on all solenoidal fields $\Rightarrow$ the system becomes *nearly singular* as $\gamma \to \infty$
- To build a γ-robust scheme we need (Schöberl 1999)
  - a γ-robust smoother;
  - a prolongation operator with γ-independent continuity constant;

  $\Rightarrow$ overlapping Schwarz smoother with decomposition that decomposes the kernel. “The right blocks for block Jacobi”.

Discretisation requirements

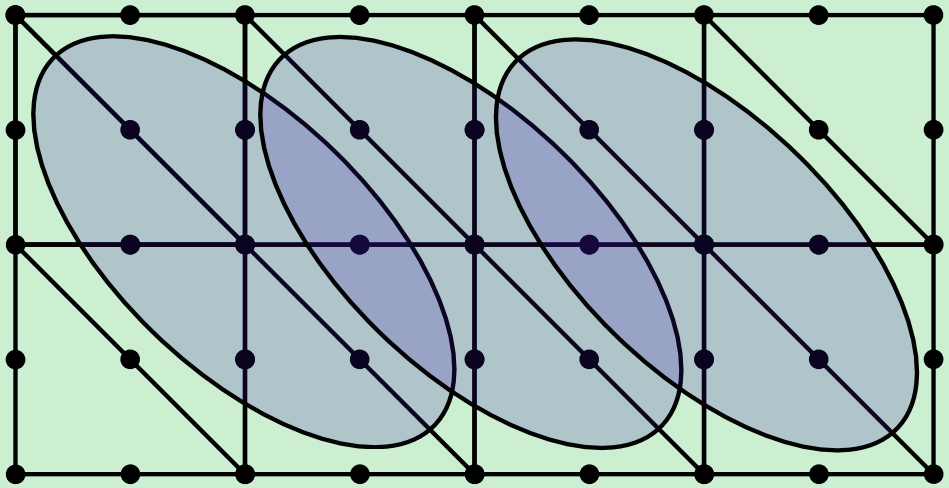
- Need inf-sup stable pair for velocity and pressure
- Need a *local basis* for the kernel of div (for efficiency).

Low-order

2D $P_2^2 - P_0$

3D $(P_1 \oplus \mathrm{FB})^3 - P_0$ (FB cubic face bubbles)

$\Rightarrow$ overlapping *star* patches



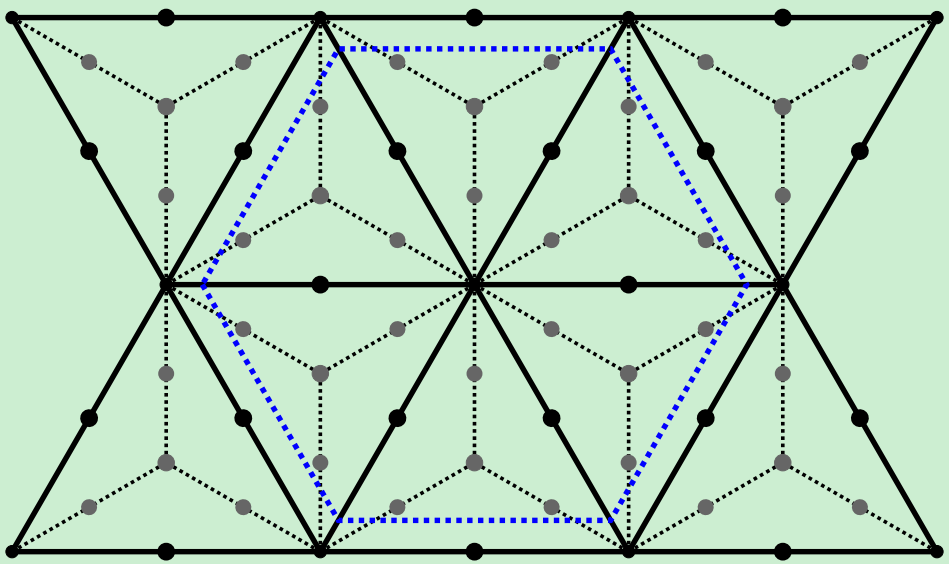
Divergence-free pair

Choose element pair from discrete subcomplex of Stokes complex

$$H^2 \xrightarrow{\mathsf{grad}} H^1(\mathsf{curl}) \xrightarrow{\mathsf{curl}} H^1 \xrightarrow{\mathsf{div}} L^2.$$

Divergence-free

- Scott–Vogelius pair: $P_k^d - P_{k-1}^{\mathrm{disc}}$ on barycentrically refined meshes ($k \geq d$).

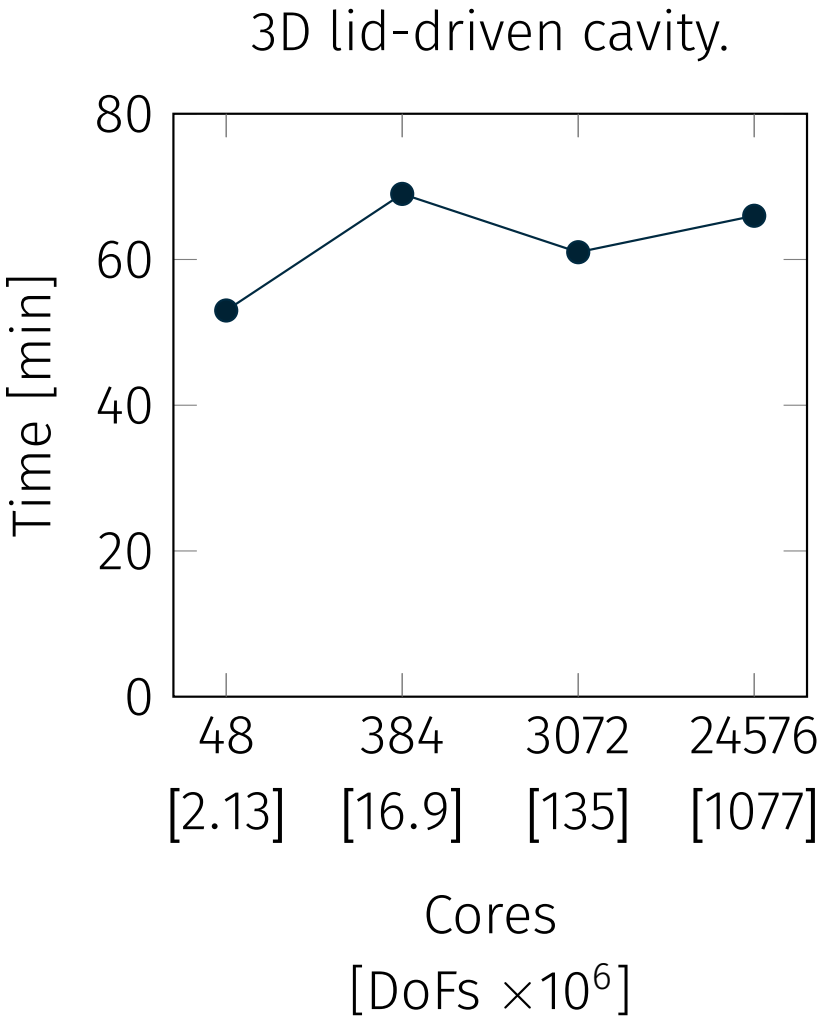


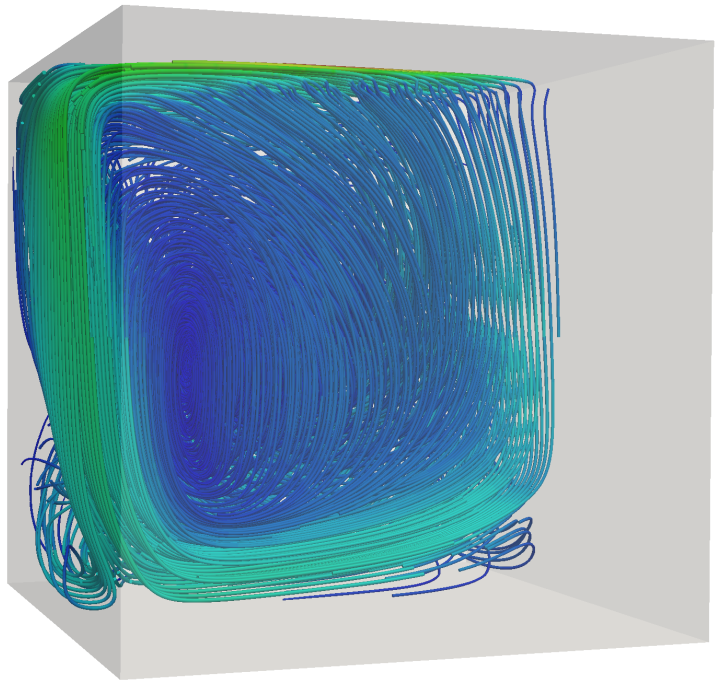
Numerical results — 3D $(P_1 \oplus \mathrm{FB})^3 - P_0$

# ref.	# dofs	Reynolds number				
		10	100	1000	2500	5000
Lid Driven Cavity						
1	2.1×10^6	4.50	4.00	5.00	4.50	4.00
2	1.7×10^7	4.50	4.33	4.50	4.00	4.00
3	1.3×10^8	4.50	4.33	4.00	3.50	7.00
4	1.1×10^9	4.50	3.66	3.00	5.00	5.00
Backwards facing step						
1	2.1×10^6	4.50	4.00	4.00	4.50	7.50
2	1.7×10^7	5.00	4.00	3.33	4.00	10.00
3	1.3×10^8	6.50	4.50	3.50	3.00	8.00
4	1.0×10^9	7.50	3.50	2.50	3.00	6.00

Table 2: Average number of outer Krylov iterations per Newton step for two 3D benchmark problems.

Computational performance — 3D





Velocity streamlines at Reynolds number 5000. Credit F. Wechsung, University of Oxford.

50 continuation steps

Numerical results — 2D $P_3^2 - P_2^{\text{disc}}$

# ref.	# dofs	Reynolds number				
		10	100	1000	5000	10000
Lid Driven Cavity						
1	9.3×10^4	2.50	2.33	2.33	5.50	8.50
2	3.7×10^5	2.00	2.00	2.00	4.00	6.00
3	1.5×10^6	2.00	1.67	1.67	2.50	3.50
4	5.9×10^6	2.00	1.67	1.50	1.50	4.00
Backwards facing step						
1	1.0×10^6	2.00	2.50	2.50	5.00	7.50
2	4.1×10^6	2.50	2.50	1.50	3.00	4.00
3	1.6×10^7	2.50	2.50	1.50	1.50	2.50

Table 3: Average number of outer Krylov iterations per Newton step for two 2D benchmark problems.

Main result

It is possible to solve the Navier–Stokes equations in a Reynolds-robust way!

Even for exactly divergence-free discretisations.

Open source implementation at `https://github.com/florianwechsung/alfi`

Enabling mathematical software

General implementation enabled by new mathematical software developments:

- Extensible block-preconditioning framework in Firedrake

  R.C. Kirby, **L. Mitchell**. SIAM SISC (2018). `arXiv:1706.01346[cs.MS]`

- New preconditioner in PETSc and Firedrake for multigrid relaxation schemes based on subspace correction methods

  P.E. Farrell, M.G. Knepley, **L. Mitchell**, F. Wechsung. `arXiv:1912.08516[cs.MS]`

Future directions

Idea

- Mathematics is the language used to derive optimal solvers.
- It *should be* the language we use to describe their implementation.

Challenges

- Is there appropriate language to describe these problems to a computer?
- Not everything is a PDE, what then?

Rewards

- Bring state-of-the-art numerical solvers to the masses.
- Enable more exploratory, and creative, mathematics.

Summary

- Broad interdisciplinary research agenda spanning:
  - finite element discretisation and implementation;
  - linear and non-linear solvers/preconditioners;
  - high-performance computing;
  - domain-specific compilers.
- Application areas:
  - coastal ocean & freshwater outflow;
  - renewable energy;
  - numerical weather prediction.

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