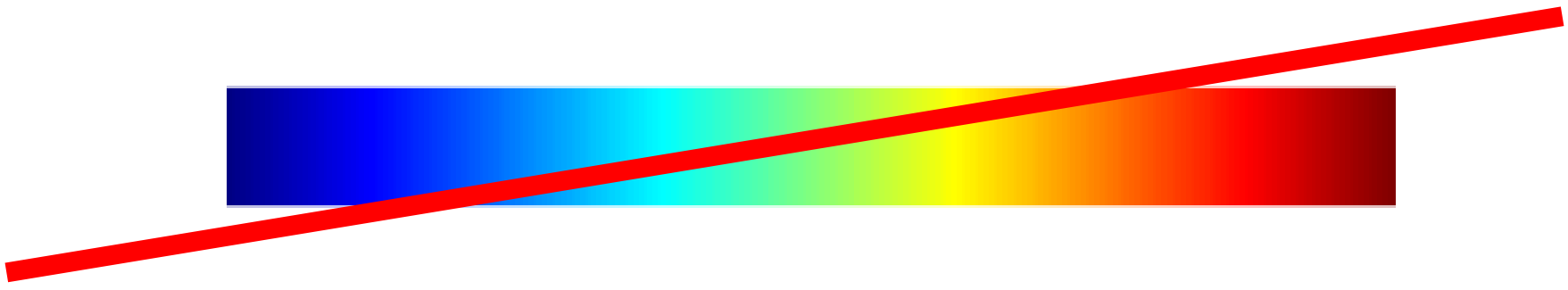
http://www.climate-lab-book.ac.uk/2014/end-of-the-rainbow/



Firedrake

Programming your (implicit) solver

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Imperial College London

Software libraries simplify writing models

Stationary Rayleigh-Bénard convection

$$-\Delta u + u \cdot \nabla u + \nabla p + \frac{\mathrm{Ra}}{\mathrm{Pr}} \hat{g} T = 0$$

$$\nabla \cdot u = 0$$

$$-\frac{1}{\mathrm{Pr}} \Delta T + u \cdot \nabla T = 0$$

```
from firedrake import *
mesh = Mesh(...)
V = VectorFunctionSpace(mesh, "CG", 2)
W = FunctionSpace(mesh, "CG", 1)
Q = FunctionSpace(mesh, "CG", 1)
Z = V * W * Q
upT = Function(Z)
u, p, T = split(upT)
v, q, S = TestFunctions(Z)
bcs = [...] # no-flow + temp gradient
nullspace = MixedVectorSpaceBasis(
   Z, [Z.sub(0), VectorSpaceBasis(constant=True),

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, nullspace=nullspace)
```

What about the solver?

- Such coupled problems are (typically) not amenable to black box solution methods.
- Direct factorisations reasonable for small problems.
- Large problems needs scalable solution, typically block factorisations.
- Gives many knobs to tweak, may require problem-specific auxiliary operators.
- How do we capture the abstraction such that automated model manipulation is still possible? (e.g. automated adjoints).

Block preconditioning

Most state of the art preconditioning for multi-variable problems is based on block LU factorisations.

$$T = \begin{bmatrix} A & 0 \\ 0 & CA^{-1}B^T \end{bmatrix}^{-1} \begin{bmatrix} A & B^T \\ C & D = 0 \end{bmatrix}$$

has minimal polynomial $T(T-I)(T^2-T-I) = 0$ (Murphy, Golub, and A. J. Wathen 2000).

See Ipsen (2001) for the case $D \neq 0$.

What does this mean

- Only need inverses of diagonal blocks (and [dense] Schur complements).
- Only need the *action* of off-diagonal blocks.
- The most efficient (time to solution) strategy is problem and parameter dependent:
  - Do I invert the blocks well or not?
  - How many couping terms should I drop?
- Need to be able to *configure* the solver without changing the code (e.g. eliminating first row or second?)
- Need to treat nested problems.

Back to Rayleigh-Bénard

Newton needs a linearisation:

$$J = \begin{bmatrix} F & B^T & M_1 \\ C & 0 & 0 \\ M_2 & 0 & K \end{bmatrix}.$$

- Navier-Stokes (top left)
- Convection-diffusion for temperature (bottom right)
- Coupling in M_1 and M_2 (non-symmetric).

Preconditioning

Write

$$N = \begin{bmatrix} F & B^T \\ C & 0 \end{bmatrix} \quad \tilde{M}_1 = \begin{bmatrix} M_1 \\ 0 \end{bmatrix} \quad \tilde{M}_2 = \begin{bmatrix} M_2 & 0 \end{bmatrix}$$

and eliminate the Navier-Stokes block, giving system for temperature:

$$S_T = K - \tilde{M}_2 N^{-1} \tilde{M}_1.$$

Howle and Kirby (2012) show that K^{-1} is a good preconditioner for S_T.

Newton update

Solve for the update

$$\delta x = J^{-1} r.$$

Write $\mathcal{K}(A, \mathbb{A})$ to denote approximating A^{-1} using an iteration $\mathcal{K}$ on A using $\mathbb{A}$ as a preconditioner. Then the iteration

$$\mathcal{K}\left(J, \begin{bmatrix} \mathcal{K}(N, \mathbb{N}) & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} I & -\tilde{M}_1 \\ 0 & I \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & \mathcal{K}(K, \mathbb{K}) \end{bmatrix}\right)$$

empirically converges swiftly, and requires only preconditioners $\mathbb{N}$ for Navier-Stokes and $\mathbb{K}$ for convection-diffusion.

Navier-Stokes block (Elman, Silvester, and A. Wathen 2014)

A lower Schur complement factorisation of N is a good option. Requires $\mathcal{K}(F, \mathbb{F})$ and $\mathcal{K}(S_p, \mathbb{S})$ where $S_p = -CF^{-1}B^T$.

One option is the *pressure convection-diffusion* approximation:

$$\mathbb{S} = \mathcal{K}(L_p, \mathbb{L})\, F_p \mathcal{K}(M_p, \mathbb{M}),$$

giving

$$\mathbb{N} = \begin{bmatrix} F & 0 \\ 0 & \mathcal{K}(S_p, \mathcal{K}(L_p, \mathbb{L})\ F_p\ \mathcal{K}(M_p, \mathbb{M})) \end{bmatrix} \begin{bmatrix} I & 0 \\ -C & I \end{bmatrix} \begin{bmatrix} \mathcal{K}(F, \mathbb{F}) & 0 \\ 0 & I \end{bmatrix}.$$

Things to note

- We only ever need inverses of diagonal blocks.
- Can save memory by applying operators matrix-free.
- The inverses are nested, we need ways of controlling the inner iterations.
- PCD drives an axe through the horizontal split between the PDE library and the solver library.

PCD

Needs the auxiliary discretised operator F_p and approximate inverses of the auxiliary operators L_p and M_p.

Firedrake & PETSc to the rescue

PETSc already provides a highly runtime-configurable library for *algebraically* composing solvers (Brown et al. 2012).

Firedrake makes it straightforward to build any auxiliary operators.

A new matrix type

We create a new PETSc matrix type in Firedrake that remembers the symbolic Jacobian it comes from, and implements matrix-free actions.

Firedrake-aware preconditioners

Algebraic preconditioners cannot work on shell matrices, so we create custom preconditioners that can inspect the symbolic information and do the appropriate thing.

PCD

```python
class PCDPC(PCBase):
    def initialize(self, pc):
        _, P = pc.getOperators()
        ctx = P.getContext()
        appctx = ctx.appctx
        p, q = ctx.arguments()
        M_p = assemble(p*q*dx)
        L_p = assemble(inner(grad(p), grad(q))*dx
        M_ksp = KSP().create()
        M_ksp.setOperators(M_p)
        L_ksp = KSP().create()
        L_ksp.setOperators(L_p)
        [...] # Some boilerplate elided
        u0 = split(appctx["state"])[appctx["velocity_space"]]
        F_p = assemble(inner(grad(p), grad(q))*dx + inner(u0, grad(p))*q*dx)

    def apply(self, pc, x, y):
        # y ← 𝒦(L_p, 𝕃) F_p 𝒦(M_p, 𝕄) x
        a, b = self.workspace
        self.M_ksp.solve(x, a)
        self.F_p.mult(a, b)
        self.L_ksp.solve(b, y)
```

How to configure things

PETSc provides a “programming language” for configuring objects at runtime. It has two operations

1. Value assignment
2. String concatenation

Every object has an *options prefix* which controls where in the options database it looks for configuration values.

This is verbose, but a very powerful idea. We can control the types of individual solves by ensuring that they have different prefixes.

The elided boilerplate

```
class PCDPC(PCBase):
    def initialize(self, pc):
        ...
        prefix = pc.getOptionsPrefix()
        M_ksp.setOptionsPrefix(prefix + "pcd_Mp_")
        M_ksp.setFromOptions()
        L_ksp.setOptionsPrefix(prefix + "pcd_Lp_")
        L_ksp.setFromOptions()
```

Back to the main event

We are solving

$$\mathcal{K}\left(\begin{bmatrix} F & B^T & M_1 \\ C & 0 & 0 \\ M_2 & 0 & K \end{bmatrix}, \mathbb{J}\right)$$

using

$$\mathbb{J} = \begin{bmatrix} \mathcal{K}\left(\begin{bmatrix} F & B^T \\ C & 0 \end{bmatrix}, \mathbb{N}\right) & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} I & 0 & -M_1 \\ 0 & I & 0 \\ 0 & 0 & I \end{bmatrix} \begin{bmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & \mathcal{K}(K, \mathbb{K}) \end{bmatrix}$$

with

$$\mathbb{N} = \begin{bmatrix} F & 0 \\ 0 & \mathcal{K}(S_p, \mathcal{K}(L_p, \mathbb{L})\ F_p\ \mathcal{K}(M_p, \mathbb{M})) \end{bmatrix} \begin{bmatrix} I & 0 \\ -C & I \end{bmatrix} \begin{bmatrix} \mathcal{K}(F, \mathbb{F}) & 0 \\ 0 & I \end{bmatrix}$$

and

$$S_p = -C\mathcal{K}(F, \mathbb{F})\, B^T.$$

First, the temperature solve

$$\mathcal{K}\left(J, \begin{bmatrix} \mathcal{K}\left(\begin{bmatrix} F & B^T \\ C & 0 \end{bmatrix}, \mathbb{N}\right) & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} I & 0 & -M_1 \\ 0 & I & 0 \\ 0 & 0 & I \end{bmatrix} \begin{bmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & \mathcal{K}(K, \mathbb{K}) \end{bmatrix}\right)$$

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Now the Navier-Stokes block

$$\mathcal{K}\left(N, \begin{bmatrix} F & 0 \\ 0 & \mathcal{K}(S_p, \mathcal{K}(L_p, \mathbb{L})\, F_p\, \mathcal{K}(M_p, \mathbb{M})) \end{bmatrix} \begin{bmatrix} I & 0 \\ -C & I \end{bmatrix} \begin{bmatrix} \mathcal{K}(F, \mathbb{F}) & 0 \\ 0 & I \end{bmatrix}\right)$$

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$$\mathcal{K}\left(N, \begin{bmatrix} F & 0 \\ 0 & \mathcal{K}(S_p, \mathcal{K}(L_p, \mathbb{L})\ F_p\ \mathcal{K}(M_p, \mathbb{M})) \end{bmatrix} \begin{bmatrix} I & 0 \\ -C & I \end{bmatrix} \begin{bmatrix} \mathcal{K}(F, \mathbb{F}) & 0 \\ 0 & I \end{bmatrix}\right)$$

```
-fieldsplit_0_ksp_type gmres
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-fieldsplit_0_pc_fieldsplit_schur_fact_type lower
-fieldsplit_0_fieldsplit_0_ksp_type preonly
-fieldsplit_0_fieldsplit_0_pc_type python
-fieldsplit_0_fieldsplit_0_pc_python_type firedrake.AssembledPC
-fieldsplit_0_fieldsplit_0_assembled_pc_type hypre
-fieldsplit_0_fieldsplit_1_ksp_type preonly
-fieldsplit_0_fieldsplit_1_pc_type python
-fieldsplit_0_fieldsplit_1_pc_python_type firedrake.PCDPC
-fieldsplit_0_fieldsplit_1_pcd_Fp_mat_type aij
-fieldsplit_0_fieldsplit_1_pcd_Mp_ksp_type preonly
-fieldsplit_0_fieldsplit_1_pcd_Mp_pc_type ilu
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-fieldsplit_0_fieldsplit_1_pcd_Kp_pc_type hypre
```

Not shown

- Setting solver tolerances
- Configuring $\mathcal{K}(F, \mathbb{F})$ inside application of S_p (not needed because $\mathcal{K}(S_p, \mathbb{S})$ is applied `preonly`).
- More complex configurations for elliptic solves (e.g. *hp*-independent iterations using subspace corrections for high order).
- ...

Runtime composability

- Can tune implicit solve for Navier-Stokes on its own, then drop in where-ever such a block wants inverted.
- Model formulation doesn't care about variable splittings. Maybe we wanted to eliminate temperature first. Do so, without changing the code.
- Composes with nonlinear solvers that need linearisations.
- Automatically take advantage of any improvements in Firedrake (fast matrix actions, etc...)
- No need to worry about parallel!

Easy extensibility

A preconditioner for the Ohta–Kawasaki equation (Farrell and Pearson 2016)

```
class OKPC(PCBase):

    def initialize(self, pc):
        # Approximate S^{-1} ~ Ŝ^{-1} M Ŝ^{-1}
        # with Ŝ = ⟨q, w⟩ + ε√c ⟨∇q, ∇w⟩
        c = (dt * theta * eps**2)/(1 + dt * theta * sigma)
        w = TrialFunction(V)
        q = TestFunction(V)
        op = assemble(inner(w, q)*dx + sqrt(c) * inner(grad(w), grad(q))*dx)
        self.ksp = KSP().create(comm=pc.comm)
        self.ksp.setOperators(op.petscmat, op.petscmat)
        [...] # boilerplate elided
        mass = assemble(w*q*dx)
        self.mass = mass.petscmat
        work = self.mass.createVecLeft()
        self.work = (work, work.duplicate())

    def apply(self, pc, x, y):
        tmp1, tmp2 = self.work
        self.ksp.solve(x, tmp1)
        self.mass.mult(tmp1, tmp2)
        self.ksp.solve(tmp2, y)
```

Future directions

- Include ability to nest GMG solves: matrix-free multigrid.
- Take advantage of new hybridisation opportunities in Firedrake
- Extend approach to nonlinear preconditioning, DD?

All of this is available as part of the Firedrake project

`http://www.firedrakeproject.org/`

Questions?

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Elman, H., D. Silvester, and A. Wathen (2014). *Finite elements and fast iterative solvers*. Second edition. Oxford University Press.

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Murphy, M. F., G. H. Golub, and A. J. Wathen (2000). “A Note on Preconditioning for Indefinite Linear Systems”. *SIAM Journal on Scientific Computing* **21**. doi:10.1137/S1064827599355153.