Firedrake

Multigrid for numerical weather prediction

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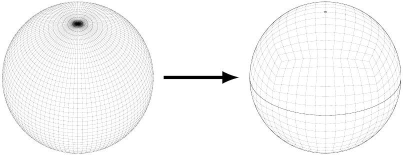
Introduction

Weather forecasting centres moving from orthogonal lat-lon to non-orthogonal meshes (e.g. cubed sphere, or icosahedral sphere).



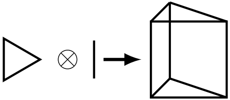
Can no longer use traditional staggered finite differences.

Compatible finite elements (FEEC) a plausible solution (Cotter and Shipton 2012).

Choose discrete spaces that match the properties of the continuous equations.

$$
\begin{array}{ccccccc}
H^1 & & H(\mathrm{curl}) & & H(\mathrm{div}) & & L^2 \\
\cup & & \cup & & \cup & & \cup \\
\mathbb{W}_0 & \xrightarrow{\mathrm{grad}} & \mathbb{W}_1 & \xrightarrow{\mathrm{curl}} & \mathbb{W}_2 & \xrightarrow{\mathrm{div}} & \mathbb{W}_3
\end{array}
$$

Tensor product spaces on wedges



Dynamical core needs to handle fast acoustic waves implicitly.

Need a solver that is *scalable* and *fast*.

5km horizontal, 100 vertical layers, around $2 \cdot 10^9$ dofs.

Large aspect ratio of the domain is challenging for black box solvers.

Formulation

Linear system for velocity $\boldsymbol{v}$, pressure p, and buoyancy b.

$$\frac{\partial \mathbf{v}}{\partial t} = \nabla p + b\hat{\mathbf{z}},$$
$$\frac{\partial p}{\partial t} = -c^2 \nabla \cdot \mathbf{v},$$
$$\frac{\partial b}{\partial t} = -N^2 \mathbf{v} \cdot \hat{\mathbf{z}}.$$

Enforce $\boldsymbol{v} \cdot \hat{\boldsymbol{n}} = 0$ at top and bottom.

$R \approx 6000\text{km}$, $H \approx 80\text{km}$.

After discretising in space and time we obtain a linear operator for $\boldsymbol{v} \in H(\mathrm{div})$, $p \in L^2$, b scalar, collocated with vertical part of $\boldsymbol{v}$ space.

$$\begin{pmatrix} M_v & -\frac{\Delta t}{2} D^T & -\frac{\Delta t}{2} Q \\ \frac{\Delta t}{2} c^2 D & M_p & 0 \\ \frac{\Delta t}{2} N^2 Q^T & 0 & M_b \end{pmatrix}$$

Eliminate buoyancy pointwise in preconditioner. Exact for spherical earth, approximate when mountainous.

Obtain a velocity-pressure system

$$\begin{pmatrix} M_v & -\frac{\Delta t}{2} D^T \\ \frac{\Delta t}{2} c^2 D & M_p \end{pmatrix}$$

Block diagonal

Using the appropriate function space inner products (Mardal and Winther 2011; Kirby 2010)

$$\begin{pmatrix} (I - \operatorname{grad}\operatorname{div})^{-1} & 0 \\ 0 & I \end{pmatrix}$$

- All operators sparse
- $H(\mathrm{div})$ multigrid (Arnold, Falk, and Winther 2000) is challenging

Schur complement

Block elimination and back substitution

$$\begin{pmatrix} M_v^{-1} & 0 \\ 0 & (M_p + \omega_c^2 D M_v^{-1} D^T)^{-1} \end{pmatrix}$$

- $S = M_p + \omega_c^2 D M_v^{-1} D^T$ is *dense*, but elliptic
- Can use similar methods as a *distributive* smoother.

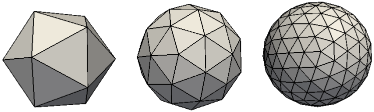
- Strong coupling in vertical direction, need to treat this exactly.
- Use a multigrid cycle with horizontal coarsening and vertical line relaxation.
- Exploit tensor-product structure to split horizontal and vertical components.

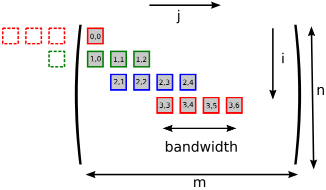
- Split horizontal and vertical $M_v^{-1} = (M_v^h)^{-1} \oplus (M_v^z)^{-1}$ (also $D = D^h \oplus D^z$)
- Diagonal approximation $M_v^{-1} \approx M_{v,\mathrm{inv}} = \delta_{ij}/(M_v)_{ii}$
- Ignore horizontal coupling, error $\mathcal{O}((\Delta z/\Delta x)^2)$

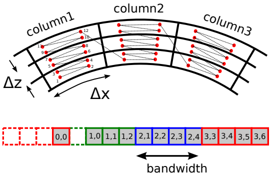
Final approximation

$$\tilde{S} = M_p + \omega_c^2 \mathrm{bdiag}\left[D^h M_{v,\mathrm{inv}}^h (D^h)^T\right] \oplus \frac{\omega_c^2}{1+\omega_N^2} D^z M_{v,\mathrm{inv}}^z (D^z)^T$$

Multigrid V-cycle using exact inverse of $\tilde{S}$ as smoother. Utilise column innermost numbering to perform fast banded matrix inverse







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Banded matrix algebra implemented as short PyOP2 kernels (Firedrake's *escape hatch*)

```
# C-kernel code for Matrix-vector product v = A.u in one vertical column
kernel_code = '''void ax(double **A, double **u, double **v) {
  for (int i = 0; i < n_row; ++i) {
    v[0][i] = 0.0;
    int j_m = (int)ceil((alpha*i - gamma_p)/beta);
    int j_p = (int)floor((alpha*i + gamma_m)/beta);
    for (int j = std::max(0, j_m); j < std::min(n_col, j_p+1); ++j)
      v[0][i] += A[0][bandwidth*i + (j - j_m)] * u[j];
  }'''
# Execute PyOP2 kernel over grid
kernel = op2.Kernel(kernel_code, 'ax', cpp=True)
op2.par_loop(kernel, hostmesh.cell_set,
             A(op2.READ, Vcell.cell_node_map()),
             u.dat(op2.READ, u.cell_node_map()),
             v.dat(op2.WRITE, u.cell_node_map()))
```

Implementation III

- Use PETSc to solve block system with fieldsplit preconditioner.
- Preconditioner for S a `PCSHELL` implementing custom multigrid.
- Allows comparison with purely algebraic approach.

Results

Compare three solvers to invert S

GMRES(30) + full schur complement factorisation tolerance 10^{-5}.

Single level

Two smoother iterations just on fine level (standard approach in Met Office Unified Model).

Custom MG

Bespoke multigrid, 5 levels. 1 smoother sweep per level. 2 smoother iterations on coarsest level.

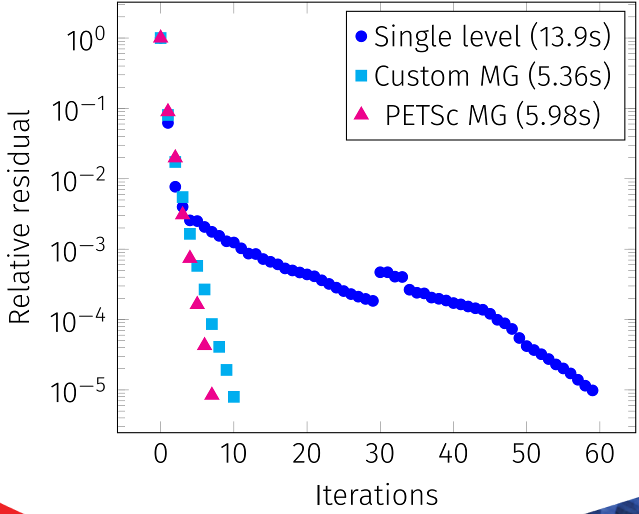
PETSc MG

BoomerAMG with ILU smoother on $\tilde{S} = M_p + \omega_c^2 D M_{v,\mathrm{inv}} D^T$

Algorithmic performance

Convergence with CFL = 8, low-order

$\boldsymbol{v} \in \mathrm{RT0}$, $p \in \mathrm{DG0}$



$18.4 \cdot 10^6$ total unknowns.

24 cores.

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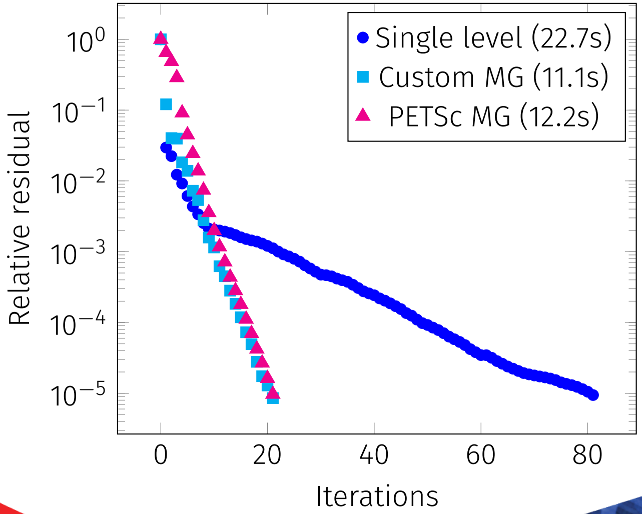
Algorithmic performance

Convergence with CFL $= 8$, high-order

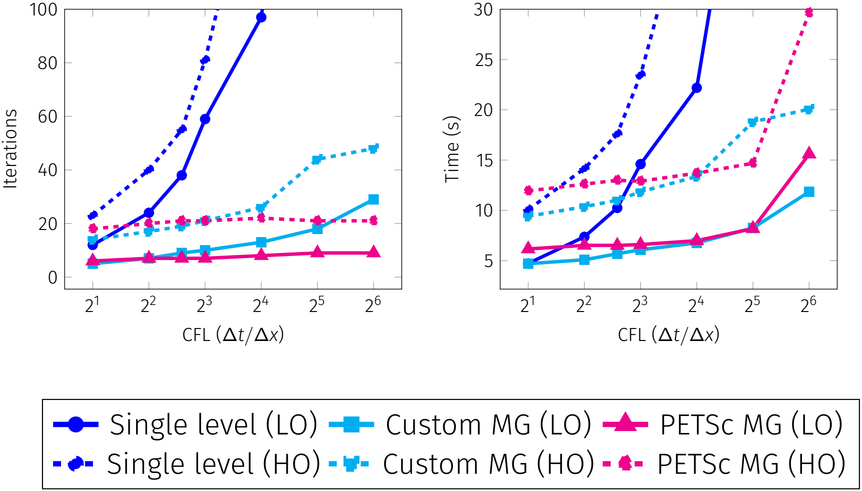
$v \in \mathtt{HDiv}(\mathrm{BDFM1} \otimes \mathrm{P2})$, $p \in \mathrm{DG1}$



$7.9 \cdot 10^{6}$ total unknowns.

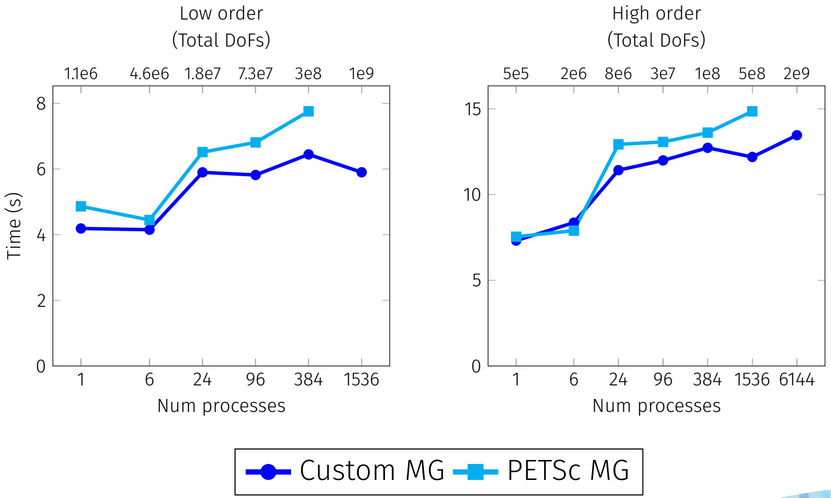
24 cores.

Varying CFL



100
80
60
40
20
0
Iterations
2^1 2^2 2^3 2^4 2^5 2^6
CFL ($\Delta t/\Delta x$)
30
25
20
15
10
5
Time (s)
2^1 2^2 2^3 2^4 2^5 2^6
CFL ($\Delta t/\Delta x$)
Single level (LO)
Custom MG (LO)
PETSc MG (LO)
Single level (HO)
Custom MG (HO)
PETSc MG (HO)

Weak scaling



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Could we go faster?

Sparse matvec is memory bandwidth limited. We count bytes moved assuming a perfect cache.

Achievable memory bandwidth for $a_i = \alpha b_i + c_i$ (STREAM triad) 74GB/s.

Measured bandwidth GB/s

	Low order		High order	
Level	$\tilde{S}$	$\tilde{S}^{-1}$	$\tilde{S}$	$\tilde{S}^{-1}$
0	2.52	1.55	0.70	0.47
1	6.65	4.50	2.30	1.60
2	14.50	4.00	7.23	5.29
3	28.09	29.29	4.69	8.99
4	39.30	40.78	45.92	12.36

Conclusions

- Scalable solver
- Performance within factor 2 of peak
  - Probably 2x available with strong scaling
  - More with judicious low-level optimisation (operational codes)
- Other approaches?
  - H(div) multigrid (Arnold, Falk, and Winther 2000)
  - Distributive smoothing (Uzawa or similar)
  - Auxiliary space (Hiptmair and Xu 2007)
- For more, see `arXiv:1605.00492 [cs.MS]`

References

Arnold, D. N., R. S. Falk, and R. Winther (2000). “Multigrid in $H(\mathrm{div})$ and $H(\mathrm{curl})$”. *Numerische Mathematik* 85. doi:10.1007/s002110000137.

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