A primal-dual mixed finite element method for accurate and efficient atmospheric modelling on massively parallel computers

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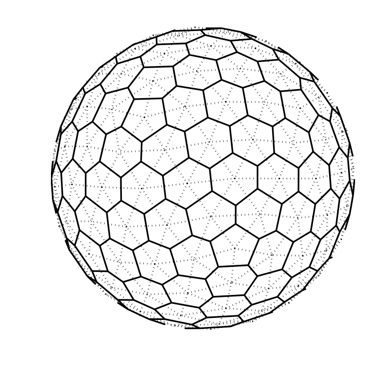
Outline

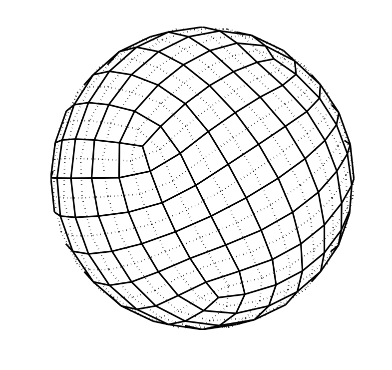
- Context and motivation
- Mixed finite elements
- Primal and dual grids and function spaces
- Challenges for massively parallel computing
- Preliminary shallow water results

Context and motivation

GungHo project: 5 year collaboration (Feb 2011 - Feb 2016) between Met Office and RCUK, to develop a dynamical core suitable for operational weather prediction and climate research on massively parallel computers.

Need for quasi-uniform spherical grid.





Examine candidate grids and schemes for spherical shallow water equations.

Qualitatively important aspects of the solution

Conservation

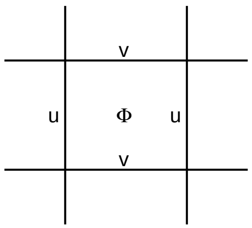
$\Phi_t + \nabla.(\mathbf{v}\Phi) = 0$

$\mathbf{v}.\nabla\Phi + \Phi\nabla.\mathbf{v} = \nabla.(\mathbf{v}\Phi)$

$\mathbf{v}.\mathbf{v}^{\perp} = 0$

Wave propagation

Suitable grid staggering; avoid or control computational modes (matching dofs)



Balance

$\mathbf{k} \cdot \nabla \times \nabla\Phi \equiv 0$;

Steady geostrophic modes for $f = \mathrm{const}$: ($\zeta_t + f\nabla.\mathbf{v} = 0$)

Accurate advection

Especially PV; conservation, boundedness, compatibility between mass and tracers, etc.

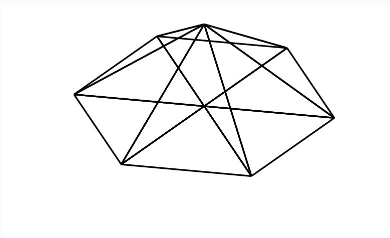
as well as stability, accuracy, and efficiency.

We have a mimetic finite-volume / finite-difference scheme that satisfies all these properties.

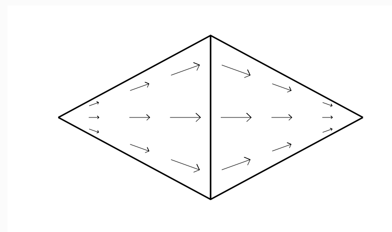
However, one part of the discretization (the construction of the Coriolis terms) is not consistent in the L_∞ norm on arbitrarily structured grids. (See INI/PDES talk 24/09/12)

Is there a better alternative?

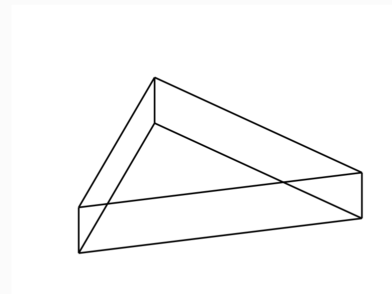
Mixed finite elements



$\nabla^\perp \longrightarrow$



$\nabla\cdot \longrightarrow$



$\mathbb{E}$ $\xi, \quad \psi$

$\mathbb{S}$ $\mathbf{u}$

$\mathbb{V}$ ϕ

DoFs placed like a C-grid

$\nabla \cdot \nabla^\perp \equiv 0$

∇ and $\mathbf{k} \cdot \nabla \times$ defined by integration by parts, then $\mathbf{k} \cdot \nabla \times \nabla \equiv 0$

Steady geostrophic modes

Linear SWEs:

$$\begin{aligned} \dot{\phi} + \phi_{ref} \nabla \cdot \mathbf{u} &= 0 \\ \dot{\mathbf{u}} + f\mathbf{u}^{\perp} + \nabla\phi &= 0 \end{aligned}$$

Any non-divergent flow $\mathbf{u} \in \mathbb{S}$ can be written $\mathbf{u} = \nabla^{\perp}\psi$ for some $\psi \in \mathbb{E}$.

Define $\phi \in \mathbb{V}$ such that $\langle \alpha, \phi \rangle = f\langle \alpha, \psi \rangle$ for any $\alpha \in \mathbb{V}$.

Then, for any $\mathbf{v} \in \mathbb{S}$,

$$\begin{aligned} f\langle \mathbf{v}, \mathbf{u}^{\perp} \rangle + \langle \mathbf{v}, \nabla\phi \rangle &= -f\langle \mathbf{v}, \nabla\psi \rangle + \langle \mathbf{v}, \nabla\phi \rangle \\ &= f\langle \nabla \cdot \mathbf{v}, \psi \rangle - \langle \nabla \cdot \mathbf{v}, \phi \rangle \\ &= 0 \end{aligned}$$

Fully discrete nonlinear governing equations

Inspiration: semi-implicit treatment of fast waves coupled with accurate advection of mass and PV

$$\phi_t + \nabla \cdot \mathbf{F} = 0, \qquad \Phi^{n+1} - \Phi^n + D_2 \widetilde{F} = 0,$$

$$\mathbf{u}_t + (f + \xi)\mathbf{u}^\perp + \nabla(\phi + k) = 0, \quad => \quad M(U^{n+1} - U^n) - M\widetilde{Q}^\perp + \overline{\overline{D}_1 L(\Phi + K)}^t = 0,$$

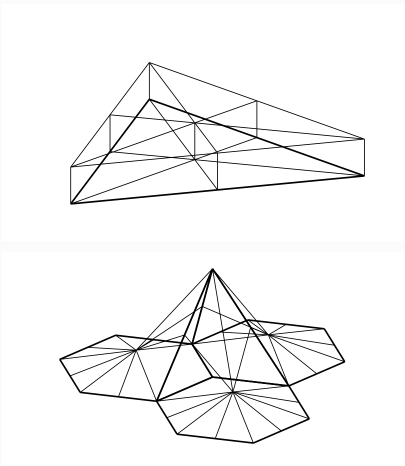
where $\overline{\psi}^t = \Delta t(\alpha \psi^{n+1} + \beta \psi^n)$.

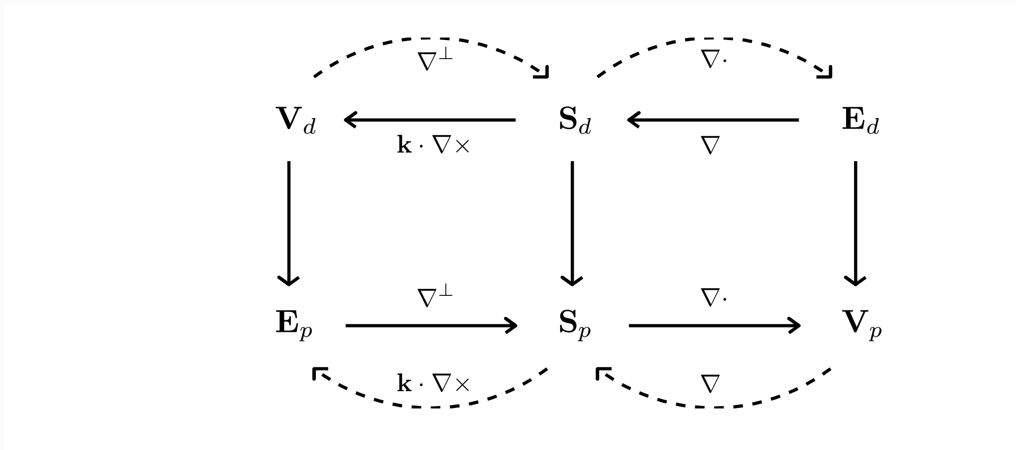
Mass flux $\widetilde{F}$ given by primal grid forward-in-time FV advection scheme.

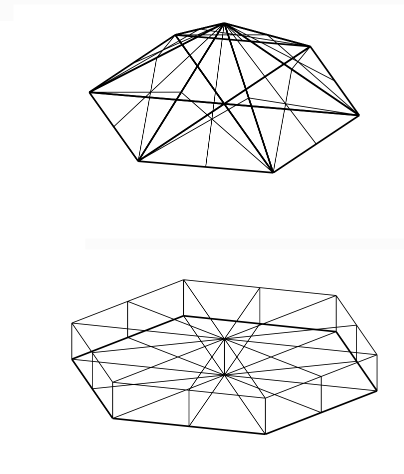
How do we construct the PV flux $\widetilde{Q}$?

(Found to be stable for $c_{adv} < 1$ with only a tiny off-centring.)

Dual grid and function spaces







Dual and primal representations of any field have matching degrees of freedom.

In $\mathbb{S}_p$ and $\mathbb{V}_p$, mass advection can be handled by a finite volume scheme.

In $\mathbb{S}_d$ and $\mathbb{V}_d$, PV advection can be handled by a finite volume scheme.

Iterative solver

Time scheme gives a coupled nonlinear problem. Solve by iterative scheme similar to ENDGame incremental formulation.

At each iteration we solve a Helmholtz problem for Φ'. Solve using one sweep of a full multigrid method.

Use 4 iterations of the incremental solver.

Challenges for massively parallel: (1) Indirect addressing

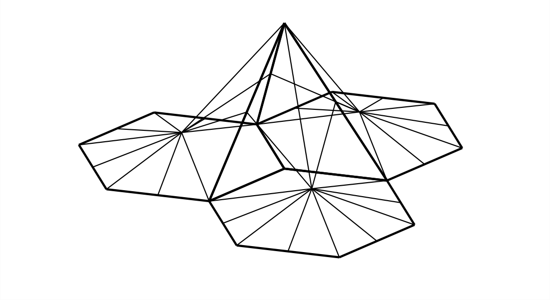
Unstructured grid algorithm $\Rightarrow$ indirect addressing.

There is growing evidence that decomposing the domain only in the horizontal and keeping the loop over levels innermost is effective.

e.g. McDonald et al. 2011, Int. J. HPC Apps.

There is work to do on the optimal domain decomposition and element numbering for different grids.

Challenges for massively parallel: (2) Complexity of quadrature



In fact it is possible to precompute the six sparse matrix operators that are needed:

$$M_{e\,e'} = \langle \mathbf{v}_e, \mathbf{v}_{e'} \rangle; \qquad H_{e\,e'} = \langle \mathbf{v}_e, \mathbf{w}_{e'} \rangle;$$

etc.

Then no quadrature is needed at run time (except in the advection scheme).

Challenges for massively parallel:
(3) Need to invert the mass matrix M and also H

M and H are both well conditioned (and the condition number does not degrade with increasing resolution).

A few Jacobi iterations are sufficient to obtain the required accuracy.

DO iter = 1, 4

...

$\widehat{F^\perp} = H^{-1} W F$

...

Find res in Φ and U eqns

Form RHS of Helmholtz $(\widetilde{M^{-1}})$

Solve Helmholtz for Φ' $(\widetilde{M^{-1}})$

Backsub for U' $(\widetilde{M^{-1}})$

Increment Φ and U

ENDDO

Challenges for massively parallel: (4) Helmholtz problem

$$\alpha^2 \, \Delta t^2 \, D_2 \, \phi^* \, \widetilde{M^{-1}} \, \bar{D}_1 \, L \, \Phi' - \Phi' = RHS$$

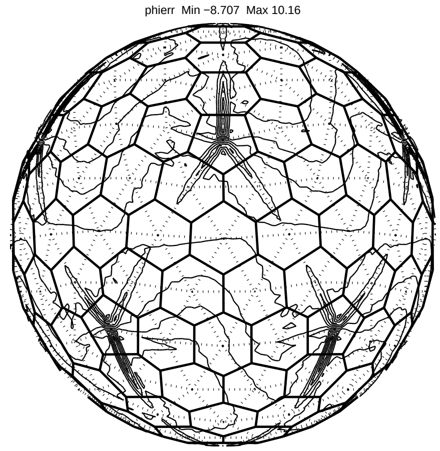
Geometric multigrid appears to scale well (see talk by Eike Müller). Only local communication at each iteration.

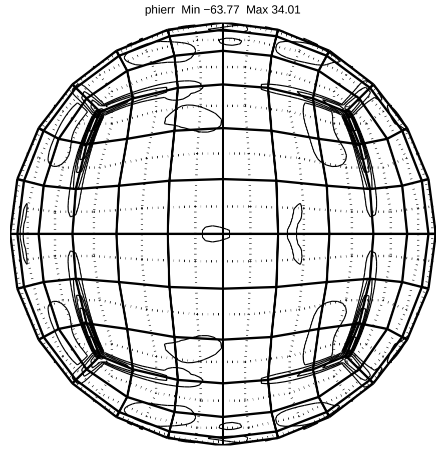
V-cycles do not need to be deep: coarsen until $\Delta x \sim (\phi^*)^{1/2} \Delta t$

Jacobi smoother is conservative and keeps open the possibility of strong bit reproducibility.

RESULTS solid body rotation (Williamson et al. 1992, J. Comput. Phys.)

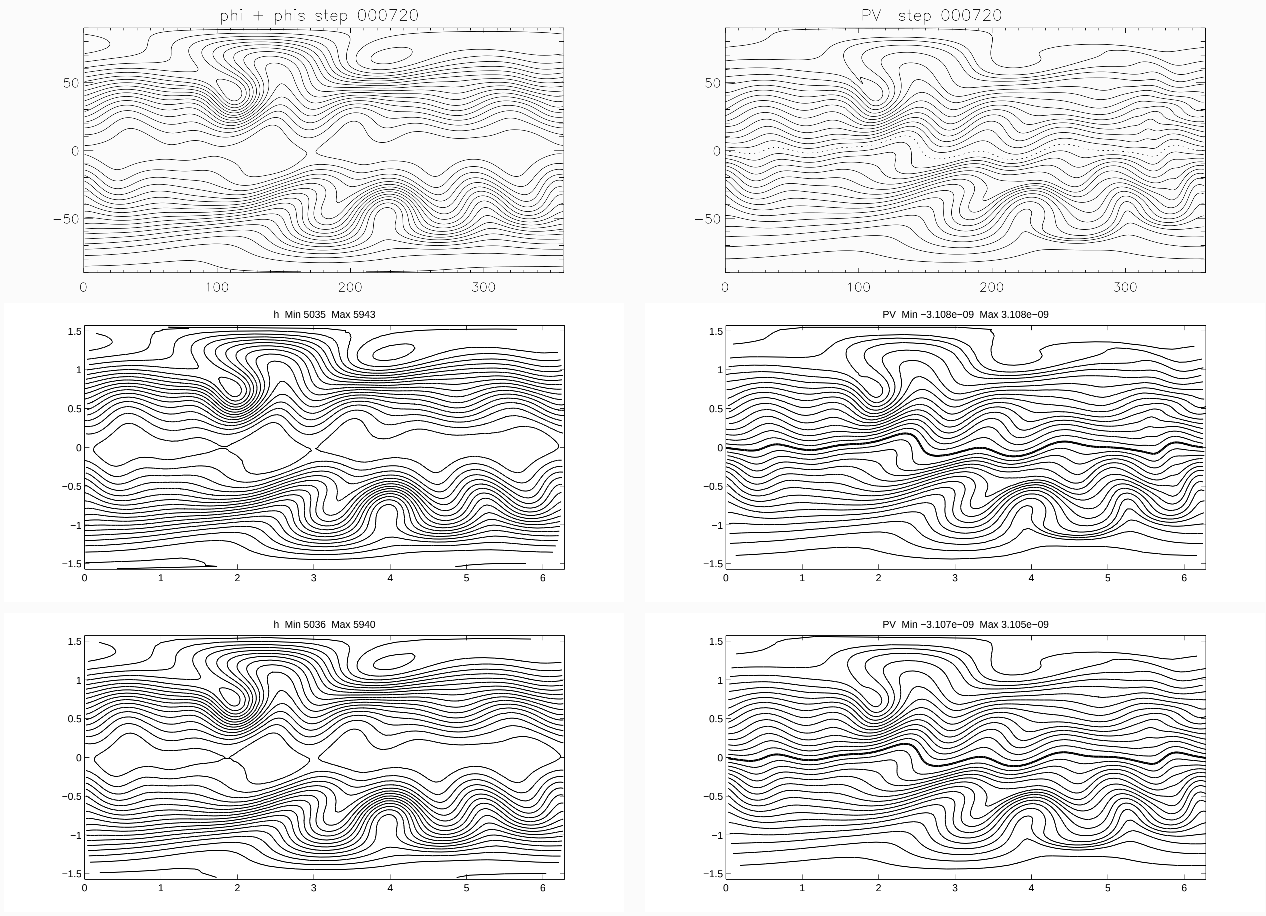
Grid	Faces	L_1	L_2	L_∞
Hex	642	39.59	49.88	133.27
FV/FD	2562	12.08	15.13	44.67
	10242	3.40	4.16	15.14
	40962	0.96	1.25	8.92
Hex	642	16.19	21.07	61.27
Dual mixed FE	2562	8.82	9.97	24.13
*	10242	2.36	2.74	10.16
	40962	0.61	0.75	4.93
Cube	864	207.75	253.65	678.15
FV/FD	3456	63.20	79.57	279.32
	13824	16.81	22.08	126.16
	55296	4.46	6.45	111.36
Cube	864	35.45	52.13	237.49
Dual mixed FE	3456	14.19	20.81	123.39
*	13824	3.89	7.07	63.77
	55296	1.13	2.54	34.31





** DO NOT overinterpret! **

RESULTS Flow over an isolated mountain



Day 15 test case 5.
Left: surface height, contour $50\,\mathrm{m}$.
Right: PV, contour $2 \times 10^{-10}\,\mathrm{m}^{-2}\mathrm{s}$.

Top: ENDGame 256x128;

middle: hex 10242 faces;

bottom; cube 13824 faces.

Summary

• We can obtain a set of desirable properties on arbitrarily structured and even non-orthogonal grids with C-grid placement of DoFs using mixed finite elements.

• We can use a finite volume scheme for advection of both mass and PV by introducing dual function spaces and suitable maps between primal and dual.

• Challenges for massively parallel computing (indirect addressing, run time quadrature, mass matrix inversion, Helmholtz solve for implicit time stepping) may not be too serious.

• Very preliminary results suggest accuracy is at least comparable to a closely related FV/FD scheme.