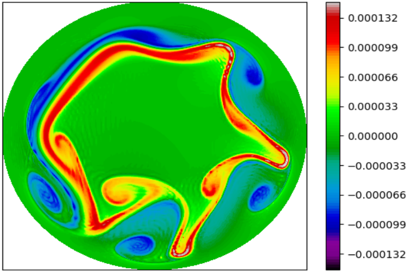
Structure preserving methods in non-hydrostatic atmospheric modeling using mixed finite elements

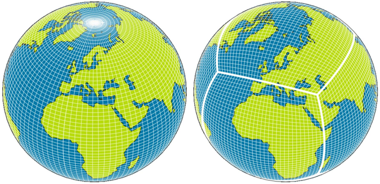
Dave Lee (Model Systems; Bureau of Meteorology)

June 7, 2021



Context

- In 2026 the UM will be deprecated by the UKMO, and replaced by a new code: LFRic
- LFRic will be based on a mixed finite element discretisation on a cubed sphere



- This talk will focus on ways to exploit the properties of finite elements to improve the representation of dynamics within atmospheric models

Why use mixed finite elements for atmospheric modelling?

- Geometric flexibility (ie: cubed sphere)
- Parallel efficiency (smaller data transfers)
- Exact preservation of balance relations:
  - Geostrophic balance (horizontal)
  - Hydrostatic balance (vertical)
- Exact preservation of conservation laws:
  - mass
  - energy
  - vorticity and potential enstrophy (shallow water)

The preservation of these properties can help to mitigate against biases in the internal representation of dynamical processes

These properties are satisfied due to the *compatible* mappings between finite element spaces via the differential operators (∇,$\nabla\times$,$\nabla\cdot$):

$$\mathbb{R} \longrightarrow \mathbb{V}_0 \xrightarrow{\nabla} \mathbb{V}_1 \xrightarrow{\nabla\times} \mathbb{V}_2 \xrightarrow{\nabla\cdot} \mathbb{V}_3 \longrightarrow 0$$

$$0 \longleftarrow \mathbb{V}_0 \xleftarrow{\tilde{\nabla}\cdot} \mathbb{V}_1 \xleftarrow{\tilde{\nabla}\times} \mathbb{V}_2 \xleftarrow{\tilde{\nabla}} \mathbb{V}_3 \longleftarrow \mathbb{R}$$

for $\mathbb{V}_0 \subset H_1(\Omega)$, $\mathbb{V}_1 \subset H(\text{curl}, \Omega)$, $\mathbb{V}_2 \subset H(\text{div}, \Omega)$, $\mathbb{V}_3 \subset L^2(\Omega)$.

What do we mean by *structure* for atmospheric models?

The 3D compressible Euler equations can be cast in *Hamiltonian* form:

$$\frac{\partial \boldsymbol{a}}{\partial t} = -\mathbf{S}(\boldsymbol{a})\frac{\delta \mathcal{H}}{\delta \boldsymbol{a}}$$

where $\mathbf{S}(\boldsymbol{a})$ is a skew-symmetric matrix; $\mathbf{S}(\boldsymbol{a}) = -\mathbf{S}(\boldsymbol{a})^\top$. Energy is conserved as

$$\frac{\partial \mathcal{H}}{\partial t} = \frac{\delta \mathcal{H}}{\delta \boldsymbol{a}} \cdot \frac{\partial \boldsymbol{a}}{\partial t} = -\frac{\delta \mathcal{H}}{\delta \boldsymbol{a}} \cdot \mathbf{S}(\boldsymbol{a})\frac{\delta \mathcal{H}}{\delta \boldsymbol{a}} = 0$$

Specifically for the 3D compressible Euler equations

$$\mathcal{H} = \int \frac{1}{2}\rho|\boldsymbol{u}|^2 + \rho g z + \frac{c_v}{c_p}\Theta\Pi \mathrm{d}\Omega$$

$$\frac{\delta \mathcal{H}}{\delta \boldsymbol{u}} = \rho\boldsymbol{u} = \boldsymbol{U}, \qquad \frac{\delta \mathcal{H}}{\delta \rho} = \frac{1}{2}|\boldsymbol{u}|^2 + gz = \Phi, \qquad \frac{\delta \mathcal{H}}{\delta \Theta} = \Pi$$

$$\frac{\partial}{\partial t}\begin{bmatrix} \boldsymbol{u} \\ \rho \\ \Theta \end{bmatrix} = -\begin{bmatrix} \boldsymbol{q}\times & \nabla & \theta\nabla \\ \nabla\cdot & \mathbf{0} & \mathbf{0} \\ \nabla\cdot(\theta\cdot) & \mathbf{0} & \mathbf{0} \end{bmatrix}\begin{bmatrix} \boldsymbol{U} \\ \Phi \\ \Pi \end{bmatrix} \qquad \boldsymbol{q} = \frac{\nabla\times\boldsymbol{u} + f}{\rho} \qquad \theta = \frac{\Theta}{\rho}$$

If our code preserves this structure, then we conserve energy and balance energy exchanges

So how do we do this in numerical models?

Recalling the Hamiltonian form of the equations:

$$\frac{\partial \boldsymbol{a}}{\partial t} = -\mathbf{S}(\boldsymbol{a})\frac{\delta \mathcal{H}}{\delta \boldsymbol{a}}$$

We need a numerical method that:

- Exactly preserves the skew-symmetry of

  $$\mathbf{S}(\boldsymbol{a}) = -\mathbf{S}(\boldsymbol{a})^{\top}$$

  (compatible finite elements; mimetic finite volumes)
- Exactly integrates the variational derives in time

  $$\int_t^{t+\Delta t} \frac{\delta \mathcal{H}}{\delta \boldsymbol{a}} \mathrm{d}\tau$$

- A good preconditioner!!!

Exact (2nd order) temporal integration of the variational derivatives as [Bauer and Cotter JCP, 18; Eldred et. al. JCP, 18]

$$\left\langle \boldsymbol{\beta}_h, \frac{\delta\mathcal{H}_h}{\delta\boldsymbol{u}_h}\right\rangle = \langle\boldsymbol{\beta}_h, \overline{U}_h\rangle = \frac{1}{3}\langle\boldsymbol{\beta}_h, \rho_h^n\boldsymbol{u}_h^n\rangle + \frac{1}{6}\langle\boldsymbol{\beta}_h, \rho_h^n\boldsymbol{u}_h^{n+1}\rangle + \frac{1}{6}\langle\boldsymbol{\beta}_h, \rho_h^{n+1}\boldsymbol{u}_h^n\rangle + \frac{1}{3}\langle\boldsymbol{\beta}_h, \rho_h^{n+1}\boldsymbol{u}_h^{n+1}\rangle$$

$$\left\langle \gamma_h, \frac{\delta\mathcal{H}_h}{\delta\rho_h}\right\rangle = \langle\gamma_h, \overline{\Phi}_h\rangle = \frac{1}{6}\langle\gamma_h, \boldsymbol{u}_h^n\cdot\boldsymbol{u}_h^n\rangle + \frac{1}{6}\langle\gamma_h, \boldsymbol{u}_h^n\cdot\boldsymbol{u}_h^{n+1}\rangle + \frac{1}{6}\langle\gamma_h, \boldsymbol{u}_h^{n+1}\cdot\boldsymbol{u}_h^{n+1}\rangle + \langle\gamma_h, gz_h\rangle$$

$$\left\langle \gamma_h, \frac{\delta\mathcal{H}_h}{\delta\Theta_h}\right\rangle = \langle\gamma_h, \overline{\Pi}_h\rangle = \frac{1}{2}\langle\gamma_h, \Pi^n\rangle + \frac{1}{2}\langle\gamma_h, \Pi^{n+1}\rangle$$

such that [Lee and Palha JCP, 20]

$$\begin{bmatrix}\langle\boldsymbol{\beta}_h, \boldsymbol{u}_h^{n+1}\rangle\\ \langle\gamma_h, \rho_h^{n+1}\rangle\\ \langle\gamma_h, \Theta_h^{n+1}\rangle\end{bmatrix} = \begin{bmatrix}\langle\boldsymbol{\beta}_h, \boldsymbol{u}_h^{n}\rangle\\ \langle\gamma_h, \rho_h^{n}\rangle\\ \langle\gamma_h, \Theta_h^{n}\rangle\end{bmatrix} +$$

$$\Delta t\begin{bmatrix} -\langle\boldsymbol{\beta}_h, \overline{q}_h\times\boldsymbol{\beta}_h\rangle & (\mathsf{E}^{3,2})^\top\langle\gamma_h,\gamma_h\rangle & \langle\boldsymbol{\beta}_h, \overline{\theta}_h\boldsymbol{\beta}_h\rangle\langle\boldsymbol{\beta}_h,\boldsymbol{\beta}_h\rangle^{-1}(\mathsf{E}^{3,2})^\top\langle\gamma_h,\gamma_h\rangle\\ -\langle\gamma_h,\gamma_h\rangle\mathsf{E}^{3,2} & \mathbf{0} & \mathbf{0}\\ -\langle\gamma_h,\gamma_h\rangle\mathsf{E}^{3,2}\langle\boldsymbol{\beta}_h,\boldsymbol{\beta}_h\rangle^{-1}\langle\boldsymbol{\beta}_h,\overline{\theta}_h\boldsymbol{\beta}_h\rangle & \mathbf{0} & \mathbf{0}\end{bmatrix}\begin{bmatrix}\hat{\overline{U}}_h\\ \hat{\overline{\Phi}}_h\\ \hat{\overline{\Pi}}_h\end{bmatrix}$$

Multiplying both sides by $[\overline{\hat{U}}_h^\top, \overline{\hat{\Phi}}_h^\top, \overline{\hat{\Pi}}_h^\top]$:

$$\left\langle \overline{U}_h, \boldsymbol{u}_h^{n+1} - \boldsymbol{u}_h^n \right\rangle + \left\langle \frac{1}{2}\overline{\boldsymbol{u}_h \cdot \boldsymbol{u}_h}, \rho_h^{n+1} - \rho_h^n \right\rangle + \left\langle gz_h, \rho_h^{n+1} - \rho_h^n \right\rangle + \left\langle \overline{\Pi}_h, \Theta_h^{n+1} - \Theta_h^n \right\rangle = 0$$

Discrete form of the continuous relation:

$$\frac{\delta K}{\delta \boldsymbol{u}} \cdot \frac{\partial \boldsymbol{u}}{\partial t} + \frac{\delta K}{\delta \rho} \cdot \frac{\partial \rho}{\partial t} + \frac{\delta P}{\delta \rho} \cdot \frac{\partial \rho}{\partial t} + \frac{\delta I}{\delta \Theta} \cdot \frac{\partial \Theta}{\partial t} = 0$$

Energetic exchanges given as

$$\begin{aligned}
\frac{\partial K_h}{\partial t} &= \overline{\hat{U}}_h^\top (\mathsf{E}^{3,2})^\top \langle \gamma_h, gz_h \rangle + \langle \overline{U}_h, \theta_h \boldsymbol{\beta}_h \rangle \langle \boldsymbol{\beta}_h, \boldsymbol{\beta}_h \rangle^{-1} (\mathsf{E}^{3,2})^\top \langle \gamma_h, \overline{\Pi}_h \rangle \\
\frac{\partial P_h}{\partial t} &= -\langle gz_h, \gamma_h \rangle \mathsf{E}^{3,2} \overline{\hat{U}}_h \\
\frac{\partial I_h}{\partial t} &= -\langle \overline{\Pi}_h, \gamma_h \rangle \mathsf{E}^{3,2} \langle \boldsymbol{\beta}_h, \boldsymbol{\beta}_h \rangle^{-1} \langle \boldsymbol{\beta}_h, \theta_h \overline{U}_h \rangle
\end{aligned}$$

Example: rotating shallow water on the cubed sphere

If we conserve energy (or just balance energy exchanges) in space + time then our code is *non-linearly stable* and can run without dissipation

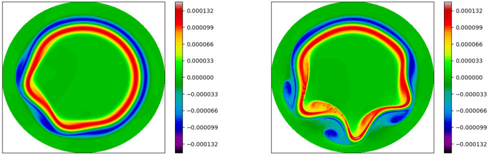


Figure: Vorticity field for the Galewsky test case, days 4 and 5.

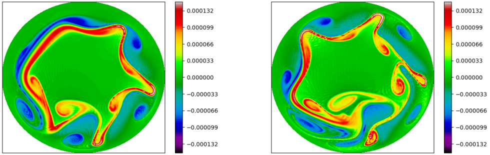
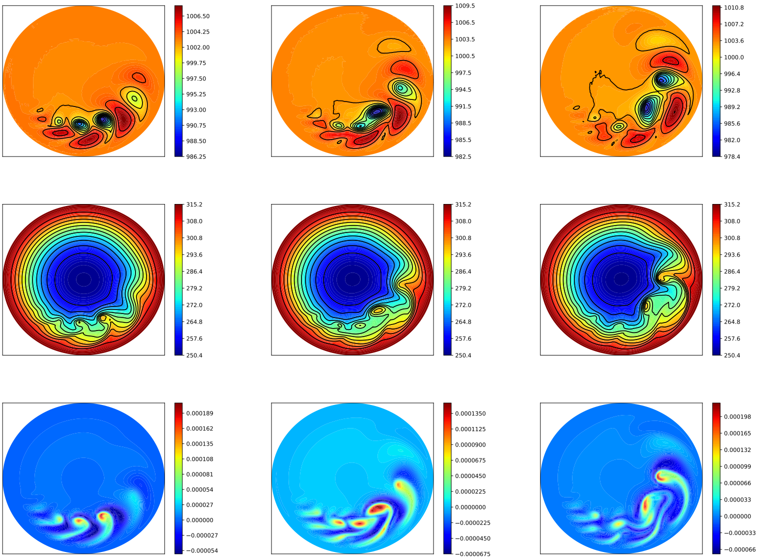


Figure: Vorticity field for the Galewsky test case, days 6 and 7.

Baroclinic instability test case (days 9–11)



Non-hydrostatic 3D warm bubble

We can systematically dissipate other moments while still conserving energy in order to suppress spurious oscillations

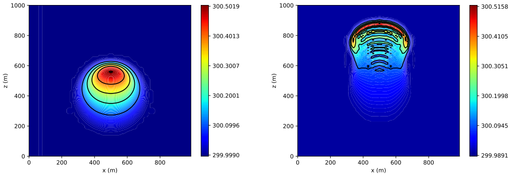


Figure: Potential temperature field at times 200s and 400s

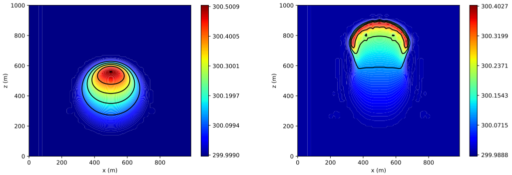


Figure: Potential temperature field at times 200s and 400s (with entropy generation)

Thanks for listening!

Code can be founds at: https://github.com/davelee2804/MiMSEM

D. Lee and A. Palha "Exact spatial and temporal balance of energy exchanges within a horizontally explicit/vertically implicit non-hydrostatic atmosphere" *J. Comp. Phys.* **440** (2021) 110432

D. Lee "An energetically balanced, quasi-Newton integrator for non-hydrostatic vertical atmospheric dynamics" *J. Comput. Phys.*, **429** (2021) 109988

D. Lee "Petrov-Galerkin flux upwinding for mixed mimetic spectral elements, and its application to geophysical flow problems" *Comput. Math. Appl.* **89** (2021) 68–77

D. Lee and A. Palha "A mixed mimetic spectral element model of the 3D compressible Euler equations on the cubed sphere" *J. Comp. Phys.* **401** (2020) 108993