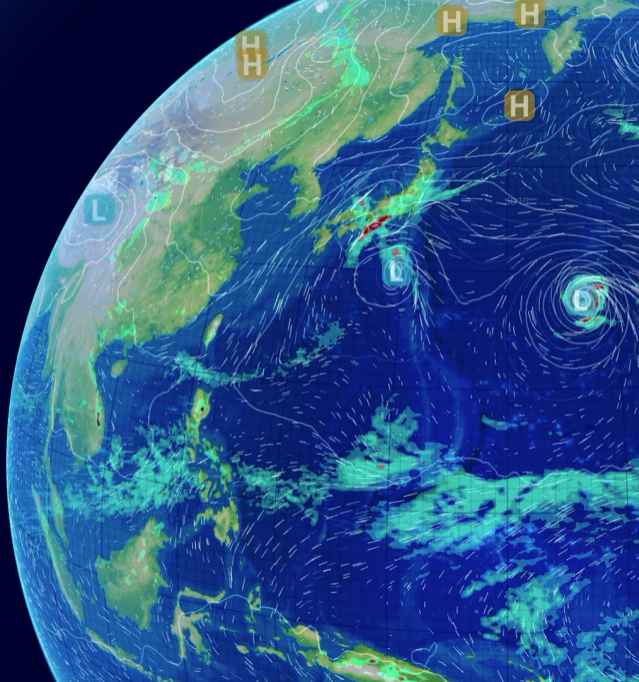


# Implementation of Lateral Boundary Conditions in the Met Office Dynamical Core, GungHo

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Dynamics Research

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# Contents

- 1 Introduction to next-generation atmospheric modelling
- 2 Adding lateral boundary conditions to the linear gravity wave system
- 3 Application to the full Gungho/LFRic model
- 4 Results and Conclusions

## Weather and climate forecasting with the Unified Model (UM)

The Unified Model (UM) is a numerical model of the atmosphere, used for both weather and climate applications.

- Compressible, non-hydrostatic
- Semi-Lagrangian advection
- Semi-implicit timestepping
- Orthogonal lat-lon grid
- Charney-Phillips Vertical staggering
- C-grid horizontal staggering



## The Exascale computing challenge



Over the next decade, supercomputers are expected to reach Exascale:  $10^{18}$  calculations per second.

- Radical changes in their design
- More parallel processing
- A new approach is required

## Next generation model development

Aim: Maintain the benefits of the current weather and climate forecast model (the Unified Model, UM) whilst improving the scalability and flexibility.

- GungHo: A new dynamical core
- LFRic: A new infrastructure



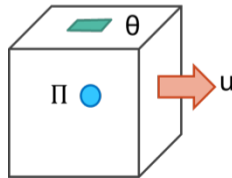
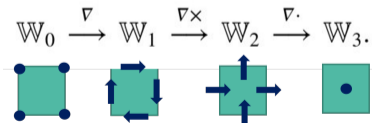
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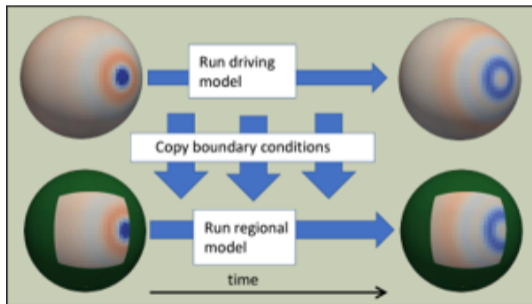
# Mixed Finite Element Discretization, with Finite Volume Advection

- Finite elements can be used with a non-orthogonal, unstructured mesh.
- The finite element function spaces are related by the de Rham complex.
- This gives an equivalence to the staggering in the UM.
- The momentum,  $u$ , is placed in  $\mathbb{W}_2$  - which is then easily linked to finite volume advection.



## Limited area models (LAMs)

- Run the weather and climate model over a small region - rather than the whole globe.
- This allows us to run at much higher resolution.
- Lateral boundary conditions (LBCs) are required.
- Nest the LAM in a (global) driving model.



Adding lateral boundary conditions to the linear gravity wave system



## Linear gravity wave system

Model perturbations around a basic state. This gives the acoustic wave equation, plus gravity/buoyancy in the vertical.

$$\begin{aligned}\frac{\partial \mathbf{u}}{\partial t} &= -\nabla p + bz \\ \frac{\partial p}{\partial t} &= -c^2 \nabla \cdot \mathbf{u} \\ \frac{\partial b}{\partial t} &= -N^2 \mathbf{u} \cdot \mathbf{z}\end{aligned}\tag{1}$$

where  $\mathbf{u}$ =momentum,  $p$ =pressure (normalized by the basic state density),  
 $b = -g\rho'/\rho_0$ =buoyancy,  $N$ =Brunt Vaisala frequency,  $c$ =speed of sound,  $\mathbf{z}$ =upward normal.

## Time discretization - iterated implicit method

Solve with an iterated implicit scheme:

$$\frac{\partial x}{\partial t} = F \quad (2)$$

is discretized in time as follows

$$x_{i+1}^{n+1} = x_i^n + \Delta t(F_i^{n+1} + F_i^n)/2 \quad (3)$$

where  $n$  is timelevel, and  $i$  is iteration.

## Time discretization of the system

Extending to the general system vector,

$$\mathcal{R}(\mathbf{x}_{i+1}^{n+1}) = 0 \quad (4)$$

which can be solved as

$$\begin{aligned} \mathbf{x}_{i+1}^{n+1} &= \mathbf{x}_i^{n+1} + \mathbf{x}'_i \\ \mathcal{L}(\mathbf{x}^*)\mathbf{x}'_i &= \mathcal{R}(\mathbf{x}_i^{n+1}) \end{aligned} \quad (5)$$

where  $\mathcal{L}$  is an approximation of the Jacobian of  $\mathcal{R}$ , and setting  $\mathbf{x}_{(i=0)}^{n+1} = \mathbf{x}^n$ .

## Application to the linear gravity wave system

$$\begin{aligned} \mathbf{u}' &= -\alpha (\nabla p' - b' \mathbf{z}) + \mathbf{R}_u \\ p' &= -c^2 \alpha \nabla \cdot \mathbf{u}' + R_p \\ b' &= -N^2 \alpha \mathbf{u}' \cdot \mathbf{z} + R_b \end{aligned} \tag{6}$$

where  $\alpha = \Delta t/2$ , and

$$\begin{aligned} \mathbf{R}_u &= (\mathbf{u}_i^{n+1} - \mathbf{u}^n) + \alpha \nabla (p_i^{n+1} + p^n) - \alpha (b_i^{n+1} + b^n) \mathbf{z} \\ R_p &= (p_i^{n+1} - p^n) + c^2 \alpha \nabla \cdot (\mathbf{u}_i^{n+1} + \mathbf{u}^n) \\ R_b &= (b_i^{n+1} - b^n) + N^2 \alpha (\mathbf{u}^{n+1} + \mathbf{u}^n) \cdot \mathbf{z} \end{aligned} \tag{7}$$

## Solution via the Helmholtz equation

Eliminate buoyancy,  $b'$ , to give the **Mixed system**

$$\begin{aligned} \mathbf{u}' &= -\alpha \mathbf{S} \nabla p' + \tilde{\mathbf{R}}_u \\ p' &= -c^2 \alpha \nabla \cdot \mathbf{u}' + R_p \end{aligned} \tag{8}$$

where  $\mathbf{S} = \text{diag}(1, 1, 1/(1 - N^2\alpha))$ ,  $\tilde{\mathbf{R}}_u = \mathbf{S}(R_u - \frac{\Delta t}{2} R_b \mathbf{z})$

Then eliminate momentum,  $\mathbf{u}'$ , to give the **Helmholtz equation**

$$p' - c^2 \alpha^2 \nabla \cdot \mathbf{S} \nabla p' = \tilde{R}_p \tag{9}$$

where  $\tilde{R}_p = R_p + c^2 \alpha \nabla \cdot \tilde{\mathbf{R}}_u$

## Boundary conditions for the Helmholtz equation

To solve a Helmholtz equation of the form

$$p' - \nabla \cdot \nabla p' = R \quad (10)$$

There are 2 options:

- 1 **Dirichlet** boundary conditions  
Define  $p'$  on the boundary
- 2 **Neumann** boundary conditions  
Define  $\nabla p'$  on the boundary

The time discretization has introduced an extra boundary condition.

## Weak form

Given the strong form,  $\mathbf{u} = -\nabla p + \mathbf{R}$ ,

Write in weak form, and then integrate by parts

$$\begin{aligned}\int_{\Omega} \mathbf{u} \cdot \mathbf{w} dV &= - \int_{\Omega} \nabla p \cdot \mathbf{w} dV + \int_{\Omega} \mathbf{R} \cdot \mathbf{w} dV \\ &= \int_{\Omega} p \nabla \cdot \mathbf{w} dV - \oint_{\partial\Omega} (p\mathbf{w}) \cdot \mathbf{n} s + \int_{\Omega} \mathbf{R} \cdot \mathbf{w} dV \\ &= \int_{\Omega} p \nabla \cdot \mathbf{w} dV + \int_{\Omega} \mathbf{R} \cdot \mathbf{w} dV\end{aligned}\tag{11}$$

where we have assumed periodic boundary conditions.

## Finite element spatial discretization

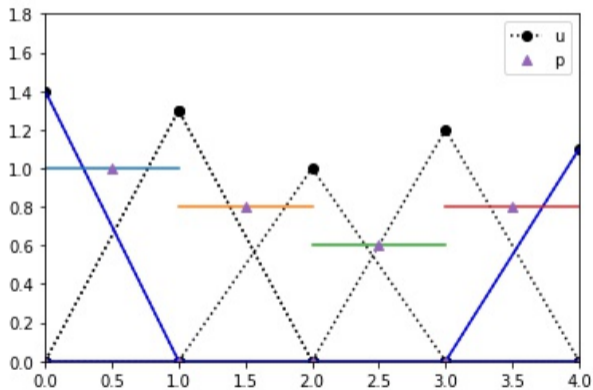
$$\begin{aligned} \mathbf{u}(x) &= \sum_i \xi_u^i \boldsymbol{\omega}_i(x) \\ p(x) &= \sum_i \xi_p^i \phi_i(x) \\ b(x) &= \sum_i \xi_b^i \theta_i(x) \end{aligned} \tag{12}$$

Choose

- $\boldsymbol{\omega}_i \in \mathbb{W}_2$  - the Raviart-Thomas space of vector functions (fluxes), continuous in both the horizontal and vertical
- $p_i \in \mathbb{W}_3$  - the discontinuous-Galerkin space of scalar functions (volumes)
- $\theta_i \in \mathbb{W}_\theta$  - discontinuous in the horizontal, and continuous in the vertical



## Compatible basis functions



- Momentum basis functions are continuous
- Pressure basis functions are discontinuous

## Discretized weak form

Given the weak form,

$$\int_{\Omega} \mathbf{u} \cdot \mathbf{w} dV - \int_{\Omega} p \nabla \cdot \mathbf{w} dV = \int_{\Omega} \mathbf{R} \cdot \mathbf{w} dV \quad (13)$$

$$\sum_i \int_{\Omega} \xi_i^u \omega_i \cdot \omega_j dV - \sum_i \int_{\Omega} \xi_i^p \phi_i \nabla \cdot \omega_j dV = \sum_i r_i^u \quad \forall j \quad (14)$$

$$\mathbf{M}_u \xi^u - \mathbf{D} \xi^p = \mathbf{r}^u \quad (15)$$

where the mass matrix  $\mathbf{M}_u$  has entries  $M_u^{ii} = \int \omega_i \cdot \omega_i dV$  and  $M_u^{ij} = \int \omega_i \cdot \omega_j dV$ .

## Comparison of Spatial Discretizations

### UM - ENDGame

- Finite difference
- Orthogonal, lat-lon grid
- Resulting mixed system of form

$$\begin{bmatrix} I & \alpha \mathbf{G} \\ \alpha c^2 \mathbf{D} & I \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{p} \end{bmatrix} = \begin{bmatrix} \mathbf{R}_u \\ \mathbf{R}_p \end{bmatrix}$$

### LFRic

- Finite element
- Unstructured, cubed-sphere mesh
- Resulting mixed system of form

$$\begin{bmatrix} \mathbf{M}_u & -\alpha \mathbf{D}^T \\ \alpha c^2 \mathbf{D} & \mathbf{M}_p \end{bmatrix} \begin{bmatrix} \boldsymbol{\xi}_u \\ \boldsymbol{\xi}_p \end{bmatrix} = \begin{bmatrix} \mathbf{r}_u \\ \mathbf{r}_p \end{bmatrix}$$

## Using the Helmholtz as a preconditioner in LFRic

To form the Helmholtz, it requires the inverse of  $M_u$ .

$$\xi_p + \alpha^2 c^2 M_p^{-1} D M_u^{-1} D^T \xi_p = M_p^{-1} r_p - \alpha c^2 M_p^{-1} D r_u \quad (16)$$

$M_u$  is not diagonal, because the basis functions for momentum are continuous.

Instead, an approximate lumped inverse  $\mathring{M}_u^{-1}$  is used - and the Helmholtz equation is used as a preconditioner rather than as a direct solve.

This means that the boundary conditions must be added to the mixed system.

## Adding boundary conditions using splitting

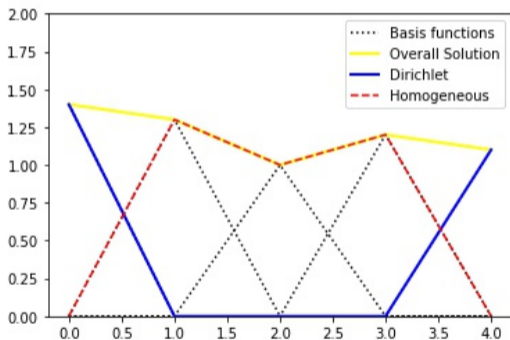
Given the mixed system  $\mathbf{Ax} = \mathbf{b}$ , split the solution into three components: homogeneous interior  $\mathbf{x}_H$ , exterior  $\mathbf{x}_E$  and boundary  $\mathbf{x}_B$ .

$$\mathbf{Ax}_H = \mathbf{b} - \mathbf{Ax}_B - \mathbf{Ax}_E \quad (17)$$

Then, apply a matrix  $\mathbf{Z}$  such that only the interior values are retained - and we choose the split such that the exterior term disappears.

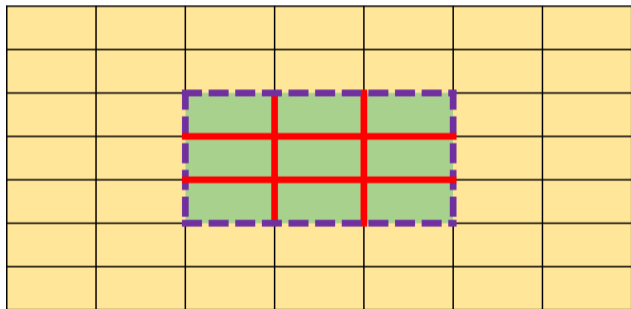
$$\begin{aligned} \mathbf{ZAx}_H &= \mathbf{Zb} - \mathbf{ZAx}_B - \mathbf{ZAx}_E \\ &= \mathbf{Zb} - \mathbf{ZAx}_B \end{aligned} \quad (18)$$

## Splitting into interior and boundary components



- Choose the interior domain such that the boundary is aligned with the cell faces/edges.
- The boundary condition is given by the momentum.
- This allows the associated divergence to be calculated, and the 'exterior term' disappears.

# Splitting



Exterior



Boundary



Interior



## Splitting in weak form

Looking back at the discretized weak form,

$$\begin{aligned}\int_{\Omega} (\mathbf{u}^H + \mathbf{u}^B + \mathbf{u}^E) \cdot \mathbf{w}_j dV &= \int_{\Omega} (p^H + p^B + p^E) \nabla \cdot \mathbf{w}_j dV + \dots \\ \int_{\Omega} (p^H + p^B + p^E) \cdot q_j dV &= - \int_{\Omega} \nabla \cdot (\mathbf{u}^H + \mathbf{u}^B + \mathbf{u}^E) q_j dV + \dots\end{aligned}\tag{19}$$

and then examining over the interior region

$$\begin{aligned}\int_{\Omega(INT)} \mathbf{u}^H \cdot \mathbf{w}_j dV + \int_{\Omega(INT)} \mathbf{u}^B \cdot \mathbf{w}_j dV &= \int_{\Omega(INT)} p^H \nabla \cdot \mathbf{w}_j dV + \dots \\ \int_{\Omega(INT)} p^H \cdot q_j dV &= - \int_{\Omega(INT)} \nabla \cdot \mathbf{u}^H q_j dV - \int_{\Omega(INT)} \nabla \cdot \mathbf{u}^B q_j dV + \dots\end{aligned}\tag{20}$$



## Splitting in matrix form

The boundary conditions are added to the RHS of the mixed system, to give a new RHS

$$\begin{aligned} \begin{bmatrix} \mathbf{Z}_u \mathbf{M}_u & -\alpha \mathbf{Z}_u \mathbf{D}^T \\ \alpha c^2 \mathbf{Z}_p \mathbf{D} & \mathbf{Z}_p \mathbf{M}_p \end{bmatrix} \begin{bmatrix} \xi_u \\ \xi_p \end{bmatrix} &= \begin{bmatrix} \mathbf{Z}_u \mathbf{r}_u \\ \mathbf{Z}_p \mathbf{r}_p \end{bmatrix} - \begin{bmatrix} \mathbf{Z}_u \mathbf{M}_u & -\alpha \mathbf{Z}_u \mathbf{D}^T \\ \alpha c^2 \mathbf{Z}_p \mathbf{D} & \mathbf{Z}_p \mathbf{M}_p \end{bmatrix} \begin{bmatrix} \mathbf{b}_u \\ 0 \end{bmatrix} \\ &= \begin{bmatrix} \mathbf{Z}_u \mathbf{r}_u \\ \mathbf{Z}_p \mathbf{r}_p \end{bmatrix} - \begin{bmatrix} \mathbf{Z}_u \mathbf{M}_u \mathbf{b}_u \\ \alpha c^2 \mathbf{Z}_p \mathbf{D} \mathbf{b}_u \end{bmatrix} \\ &= \begin{bmatrix} \mathbf{r}_u^* \\ \mathbf{r}_p^* \end{bmatrix} \end{aligned} \quad (21)$$

## Boundary conditions in the Helmholtz preconditioner

Using this new RHS, a similar procedure can then be used to form the Helmholtz equation - but with the application of the  $\mathbf{Z}$  matrices.

$$\begin{aligned}\xi_p + \alpha^2 c^2 \mathbf{M}_p^{-1} \mathbf{D} \dot{\mathbf{M}}_u^{-1} \mathbf{Z}_u \mathbf{D}^T \xi_p &= \mathbf{M}_p^{-1} \mathbf{r}_p^* + \alpha c^2 \mathbf{M}_p^{-1} \mathbf{D} \dot{\mathbf{M}}_u^{-1} \mathbf{r}_u^* \\ &= \mathbf{M}_p^{-1} (\mathbf{r}_p - \alpha c^2 \mathbf{D} \dot{\mathbf{M}}_u^{-1} \mathbf{Z}_u \mathbf{r}_u) \\ &\quad - \alpha c^2 \mathbf{M}_p^{-1} \mathbf{D} (\mathbf{b}_u - \dot{\mathbf{M}}_u^{-1} \mathbf{Z}_u \mathbf{M}_u \mathbf{b}_u)\end{aligned}\tag{22}$$

The  $\mathbf{Z}$  matrices also need to be applied in the back substitution.

## Equivalence to Neumann boundary conditions

If we let  $\mathbf{M}_u = \mathbf{I}$ , then this reduces to

$$\begin{aligned} \boldsymbol{\xi}_p + \alpha^2 c^2 \mathbf{M}_p^{-1} \mathbf{D} \mathbf{Z}_u \mathbf{D}^T \boldsymbol{\xi}_p &= \mathbf{M}_p^{-1} \mathbf{r}_p^* - \alpha c^2 \mathbf{M}_p^{-1} \mathbf{D} \mathbf{r}_u^* \\ &\quad - \alpha c^2 \mathbf{M}_p^{-1} \mathbf{D} \mathbf{b}_u \end{aligned} \quad (23)$$

and, from the definition of the mixed system, the boundary momentum is related to the boundary pressure gradient as:

$$\mathbf{b}_u = \alpha \mathbf{D}^T \mathbf{b}_p \quad (24)$$

so it is similar to adding Neumann boundary conditions to the Helmholtz equation directly ... but with the addition of the momentum mass matrix.

## Summary

### UM ENDGame

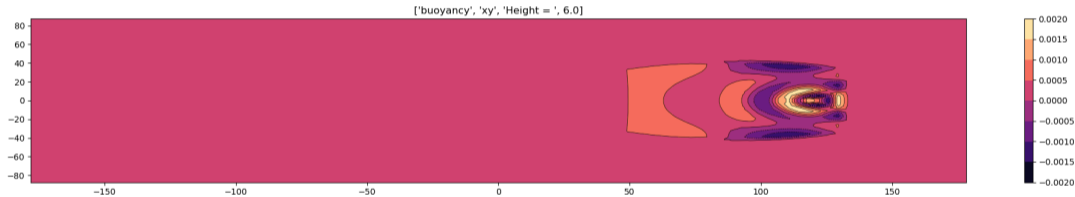
- Adds the boundary conditions directly to the Helmholtz equation
- Is free to use either Dirichlet or Neumann boundary conditions
- Chooses to use Dirichlet i.e. pressure

### LFRic

- Adds the boundary conditions to the mixed solve.
- Due to the structure of the mixed finite element basis functions, it must use momentum as the boundary condition
- These boundary conditions are indirectly used by the associated Helmholtz equation
- This is equivalent to using Neumann boundary conditions

## Gravity wave model results

Gravity waves in a box! Setting the boundary momentum to zero.

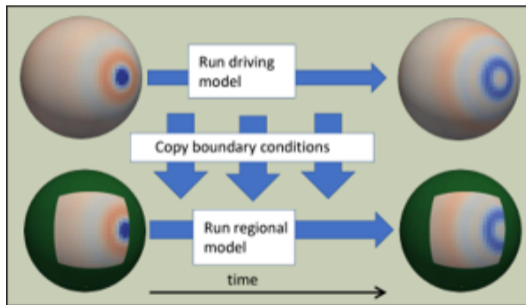


Buoyancy, C24 mesh

The solver is run over the whole mesh - but the variables are only allowed to evolve in the limited area region.

## Gravity wave model results

- Limited area model nested in a driving model
- Start with the same initial conditions
- Boundary conditions (for momentum increment,  $u'$ ) are provided by the driving model at every timestep



Application to the full Gungho/LFRic model

## Continuous Equations

The Euler equations for a perfect gas in a rotating frame, with equation of state

$$\begin{aligned}\frac{\partial \mathbf{u}}{\partial t} &= -\boldsymbol{\xi} \times \mathbf{u} - 2\boldsymbol{\Omega} \times \mathbf{u} - \nabla(K + \Phi) - c_p \theta \nabla \Pi \\ \frac{\partial \rho}{\partial t} &= -\nabla \cdot (\rho \mathbf{u}) \\ \frac{\partial \theta}{\partial t} &= \mathbf{u} \cdot \nabla \theta \\ \Pi \left( \frac{1-\kappa}{\kappa} \right) &= \frac{R}{p_0} \rho \theta\end{aligned}\tag{25}$$



## The Mixed system for the full model

Mixed-solve equations:

$$\begin{pmatrix} \mathbf{M}_2 & & -\mathbf{P}_{2\theta} & -\mathbf{G} \\ \mathbf{D} & \mathbf{M}_3 & & \\ \mathbf{P}_{\theta 2} & & \mathbf{M}_\theta & \\ & -\mathbf{M}_3^{\rho*} & -\mathbf{P}_{3\theta} & \mathbf{M}_3^{\Pi*} \end{pmatrix} \begin{pmatrix} \tilde{\mathbf{u}}' \\ \tilde{\boldsymbol{\rho}}' \\ \tilde{\boldsymbol{\theta}}' \\ \tilde{\boldsymbol{\Pi}}' \end{pmatrix} = \begin{pmatrix} -\mathbf{r}_u \\ -\mathbf{r}_\rho \\ -\mathbf{r}_\theta \\ -\mathbf{r}_\Pi \end{pmatrix} \quad (26)$$

This is associated with the Helmholtz preconditioner operator in the form

$$\mathbf{H} = \mathbf{M}_3^{\Pi*} + \left( \mathbf{P}_{3\theta} \dot{\mathbf{M}}_\theta^{-1} \mathbf{P}_{\theta 2} + \mathbf{M}_3^{\rho*} \mathbf{M}_3^{-1} \mathbf{D} \right) \dot{\mathbf{M}}_2^{-1} \mathbf{G} \quad (27)$$

where  $\dot{\mathbf{M}}_2^{-1}$  is the inverse of the diagonal mass-lumped mass matrix approximation of  $\mathbf{M}_2 + \mathbf{P}_{2\theta} \dot{\mathbf{M}}_\theta^{-1} \mathbf{P}_{\theta 2}$ .

## Apply LBCs to the mixed solve

To add the LBCs, apply the same splitting method to give a new RHS

$$\begin{pmatrix} -\mathbf{Z}_u(\mathbf{r}_u + \mathbf{M}_2\mathbf{u}_B) \\ -\mathbf{Z}_\rho(\mathbf{r}_\rho + \mathbf{D}^{\rho*}\mathbf{u}_B) \\ -\mathbf{Z}_\theta(\mathbf{r}_\theta + \mathbf{P}_{\theta 2}\mathbf{u}_B) \\ -\mathbf{Z}_\Pi(\mathbf{r}_\Pi) \end{pmatrix} \quad (28)$$

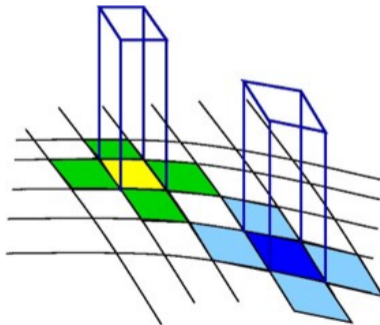
and then we can then derive the associated Helmholtz operator

$$\mathbf{H} = \mathbf{Z}_\Pi \mathbf{M}_3^{\Pi*} + \mathbf{Z}_\Pi (\mathbf{P}_{3\theta} \mathbf{M}_\theta^{-1} \mathbf{Z}_\theta \mathbf{P}_{\theta 2} + \mathbf{M}_3^{\rho*} \mathbf{M}_3^{-1} \mathbf{Z}_\rho \mathbf{D}) \mathbf{M}_2^{-1} \mathbf{Z}_u \mathbf{G} \quad (29)$$

## LFRic infrastructure

The LFRic infrastructure is designed to use unstructured meshes and uses a 'separation of concerns' approach.

- The looping over cells is separate to the science code
- Its non-trivial to identify which are the boundary cells



## LAM masks

The solution is to create masks - a field of 1s and 0s that identifies the boundary cells/nodes. The masks are equivalent to the  $Z$  matrices.

---

```
1 call invoke( X_times_Y( masked_data , data , mask ))
```

---

This allows us to easily re-use the existing operators (e.g.  $D$ ) that have been developed for the global model.

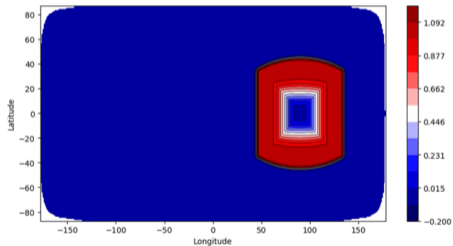
Two methods have been devised to create the masks:

- 1 Coordinate-based - query the coordinates of the node
- 2 Connectivity-based - query whether the cell is connected to other cells

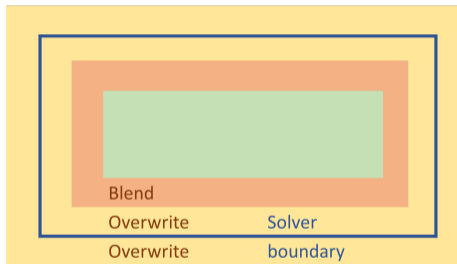
## Blending

The full model has advection, and there are differences between the driving model and the limited area model e.g. in resolution and in physics.

- Use a 'rim' of driving model LBC data, from which to calculate the advective forcings
- Add blending to prevent mismatches between the interior and the driving model.
- $x^{\text{blended}} = wx^{\text{driving}} + (1 - w)x^{\text{LAM}}$
- This is the same method as in the UM.

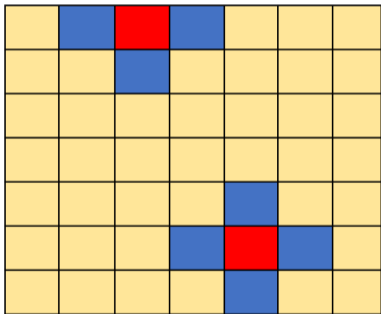


## Blending and solver boundary



- The solver boundary does not coincide with the edge of the mesh.
- There is a rim of cells around the edge of the model that are overwritten with the driving model data.
- This is the philosophy of nesting the LAM within the driving model.

## Stencils on a LAM mesh



- Stencils (indirect addressing) are used to provide information from adjacent cells.
- Stencils are modified on the boundary - so that they don't try to access non-existent cells.
- The code loops over all cells in the stencil.
- It doesn't matter what answer is provided, as the data is then overwritten in the boundary region.

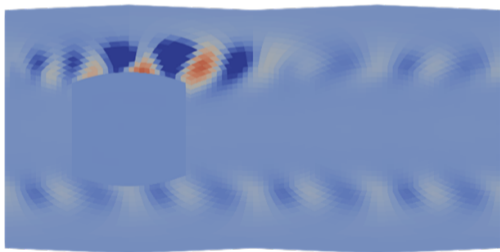
## Results and Conclusions



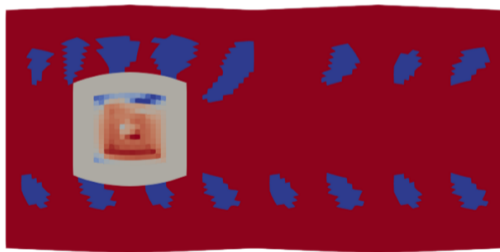
## GungHo results: Baroclinic wave

Big brother experiment - where the driving and limited area models and resolutions are identical.

Plots show differences between the driving model and LAM, for Exner pressure at the surface.

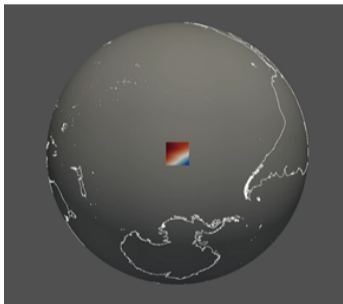


a) Contour interval  $[-0.0002, 0.006]$



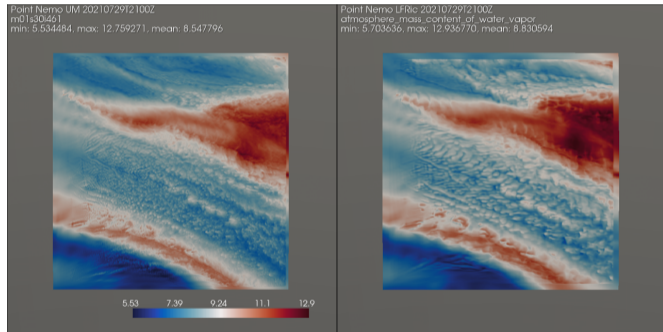
b) Contour interval  $[-5e-8, 5e-8]$

## Full Gungho/LFRic model setup



- GungHo Dynamical core + UM physics (parametrisations)
- Driving model is the UM. Data is interpolated to the limited area model mesh.
- Limited area models use a rotated-pole, lat-lon grid, with 1.5km grid length.
- 29/07/2021, with forecast run out to 144 hours.
- Domain centered on Point Nemo - a domain which is entirely located over the sea.

## Full model results: UM v LFRic



Note: These early results are only intended to demonstrate a working LFRic regional model. Work is ongoing to refine the details of the scientific configuration.

Total column water vapour from UM (left) and GungHo (right).  
Courtesy Ben Shipway and Anke Finnenkoetter.

## Conclusions

- A new formulation for the addition of lateral boundary conditions to the GungHo dynamical core.
- The design is similar to the UM, except that Neumann boundary conditions are used in the Helmholtz equation.
- Demonstrated in idealized models
- Demonstrated in the full GungHo + physics model
- Next steps are to improve the efficiency, run on domains with orography, refine the scientific configurations and complete further comparisons between the UM and LFRic.

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