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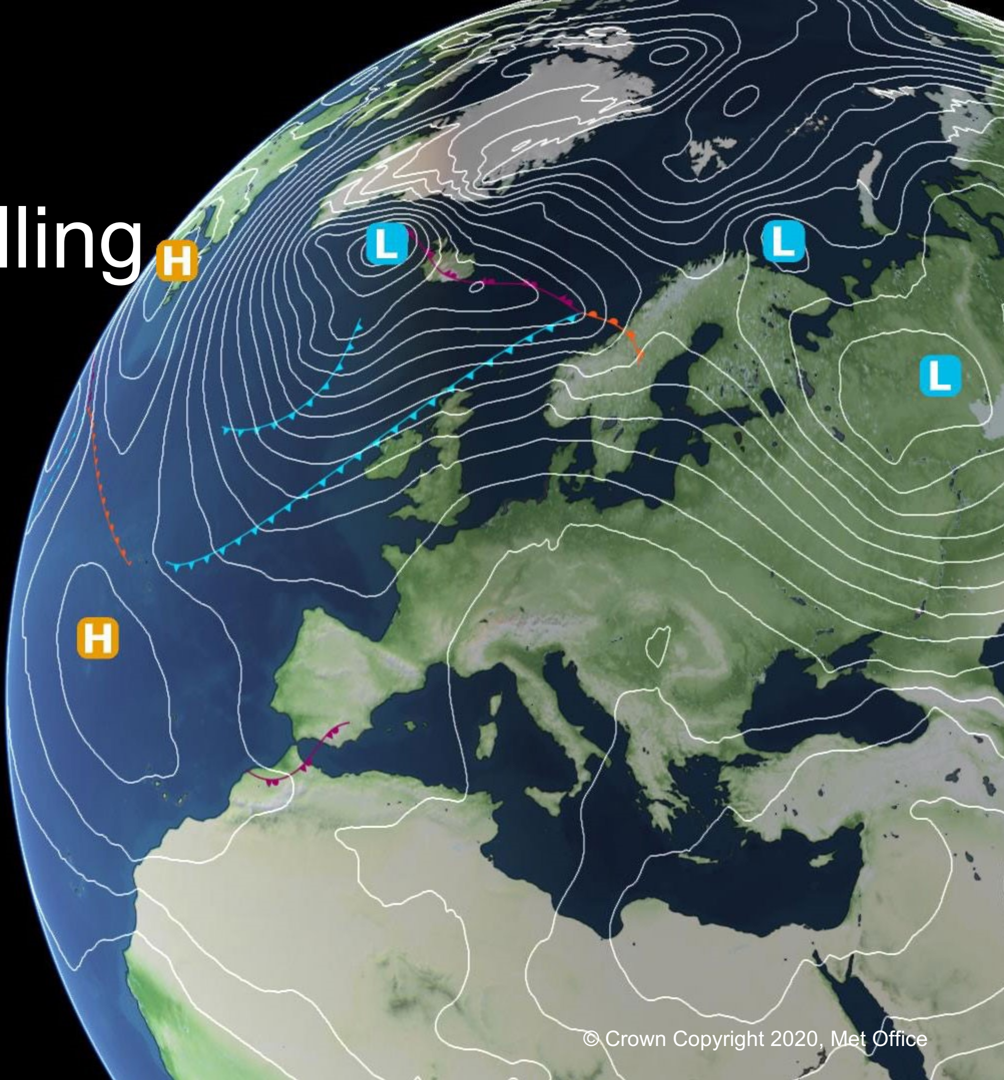
Next generation modelling with LFRic

UKCA Chemistry and Aerosol Tutorials

7 December 2022

Ben Shipway

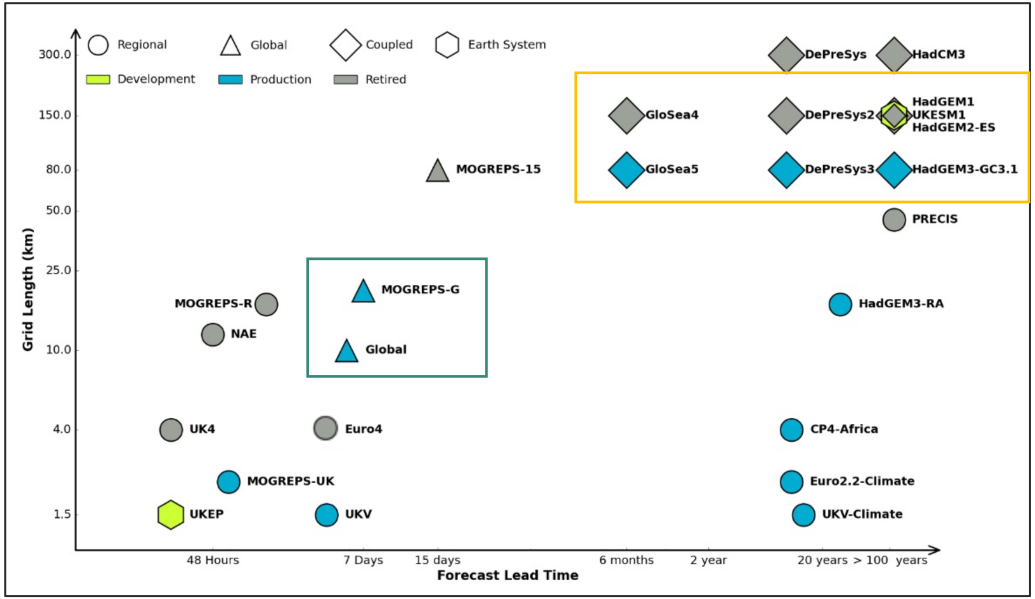


Outline

- Current Generation Modelling
  - UM atmosphere and ENDGame dynamical core
- Motivation
  - Why do we need a ‘Next Generation’
- Next Generation Modelling
  - LFRic atmosphere and GungHo dynamical core
  - Look a bit at the code
- Current status and plans
  - When with LFRic be ready?

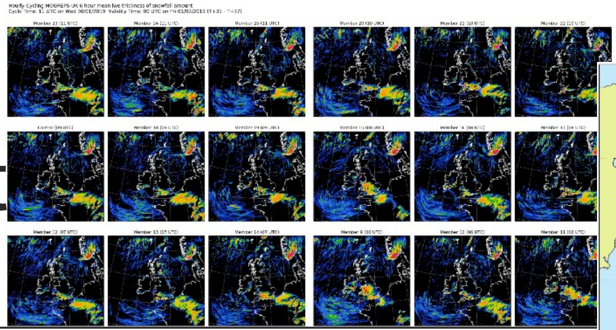
Seamless development

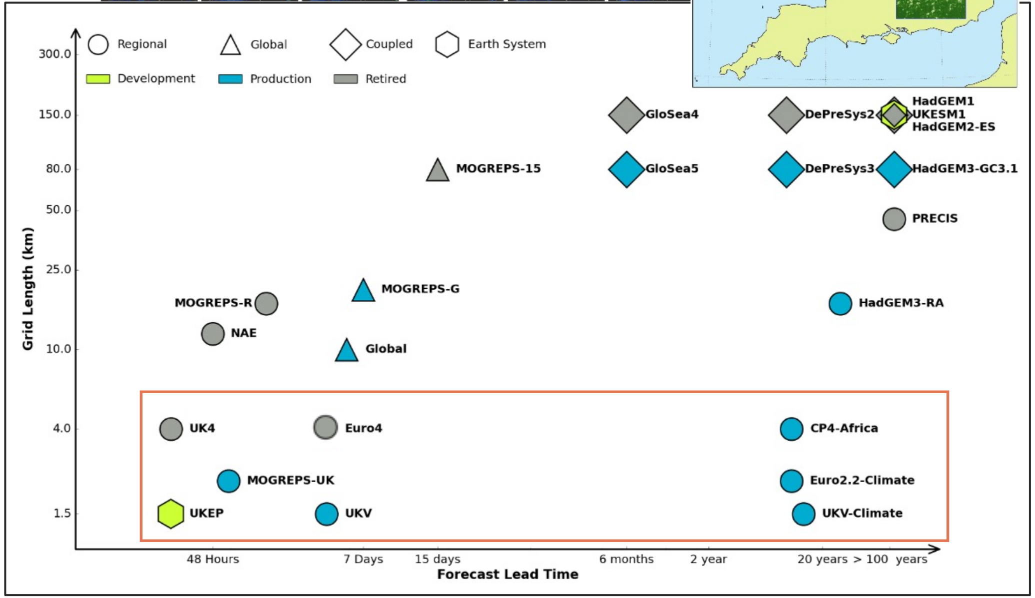
Global configurations	Horizontal resolution	Vertical levels
Deterministic NWP	0.14° x 0.09° (~10 km at mid-latitudes)	70 levels to 80 km
Ensemble NWP	0.28° x 0.18° (~20 km at mid-latitudes)	70 levels to 80 km
Seasonal/ Decadal climate	0.83° x 0.55° (~50 km at mid-latitudes)	85 levels to 85 km
Centennial/ ESM climate	1.875° x 1.25° (~140 km at mid-latitudes)	38 levels to 40 km



Seamless development

Regional configurations	Horizontal resolution	Vertical levels
UKV	1.5x1.5 km 950 x 1025 grid points	70 levels to 40 km
Ensemble	2.2x2.2 km 740 x 752 grid points	70 levels to 40 km
London Model	300mx300m 380x420	90 levels to 40 km
Relocatable LAM	various	various



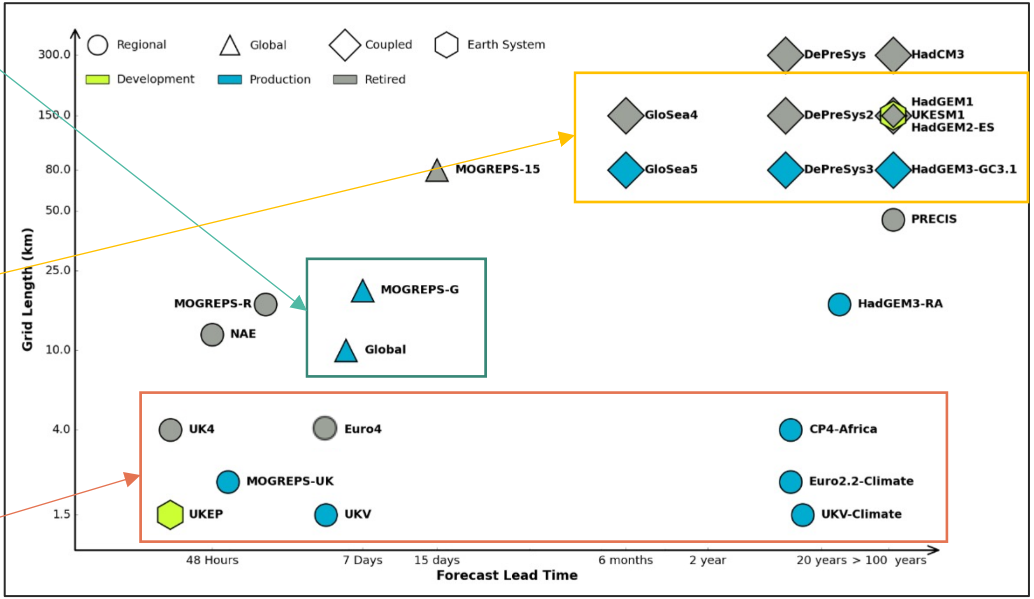


Seamless development

Global hi-resolution (NWP):
- Reaching limit of strong scaling
- Primary motivation for GungHo

Global low-resolution (climate/ESM):
- Dynamical core a smaller proportion of overall cost
- Greater cost from chemistry and diagnostics
- Motivates equations that are accurate on long timescales (e.g., conservation, no systematic bias)

Regional hi-resolution (NWP):
- Spatial domain scales well
- Motivates non-hydrostatic equation set



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Constraints for GungHo design

Algorithmic drivers

- Minimize total number of (expensive) operations required to get to solution. E.g.,
  - # of timesteps
  - # of iterations
  - # of stages
  - # of substeps
- Flexible design to mitigate against ‘dead ends’
- Flexible design for different science configurations

Computational drivers

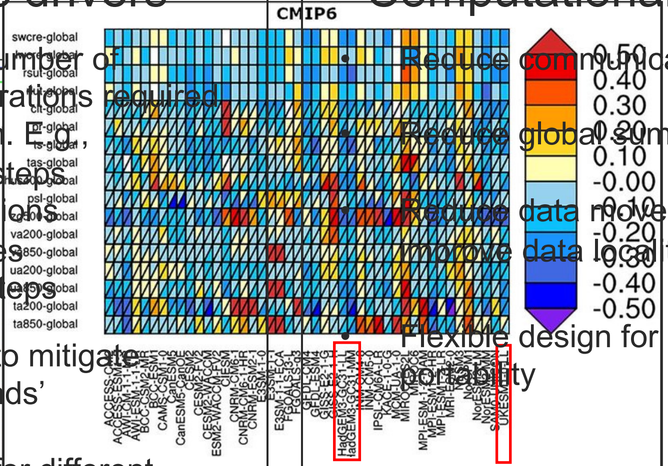
- Reduce communication
- Reduce global sums
- Reduce data movement and improve data locality
- Flexible design for performance portability

Science drivers

- Retain characteristics of ENDGame numerics:
  - Accurate representation of physical equations
  - Accurate dispersion
  - No computational modes (grid staggering)
  - Semi-implicit timestep (physics coupling)
  - Retain physical parametrizations
- Additionally want to improve inherent conservation properties

We have good NWP skill

Climate skill



Bock et al. 2020

Current generation modelling

Unified Model and ENDGame dynamical core

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Governing Equations

Momentum Equation

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} + 2\boldsymbol{\Omega}\times\boldsymbol{u} + \nabla\Phi + \frac{c_p\theta}{1+\Sigma m_x}\nabla\Pi = \boldsymbol{S}_{\boldsymbol{u}}$$

Thermodynamic Equation

$$\frac{\partial \theta}{\partial t} + \boldsymbol{u}\cdot\nabla\theta = S_\theta$$

Continuity Equation

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\boldsymbol{u}) = 0$$

Moisture Transport Equation

$$\frac{\partial m_x\rho}{\partial t} + \nabla\cdot(m_x\rho\boldsymbol{u}) = S_x$$

Equation of State

$$\Pi^{\frac{1-\kappa}{\kappa}} + \frac{R}{p_0}\rho\theta = 0$$

Moisture

Wave motion

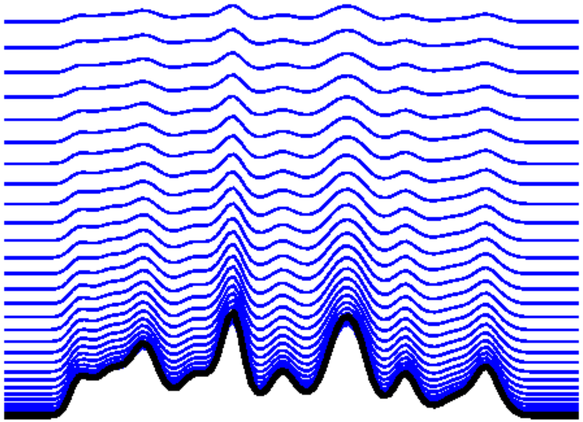
Transport terms

Subgrid forcings

Structure of the Grid

Horizontal: latitude-longitude

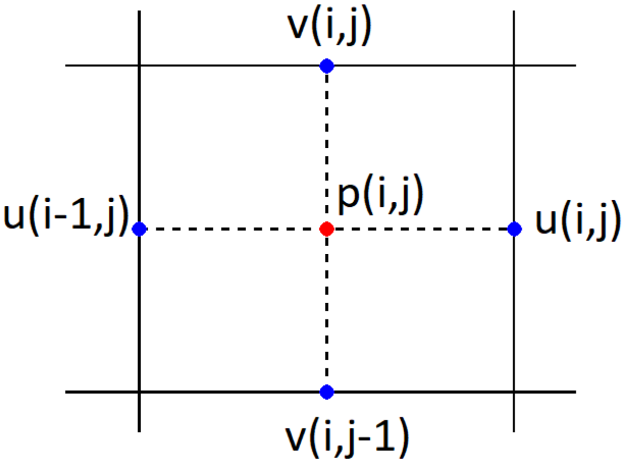
Vertical: terrain following



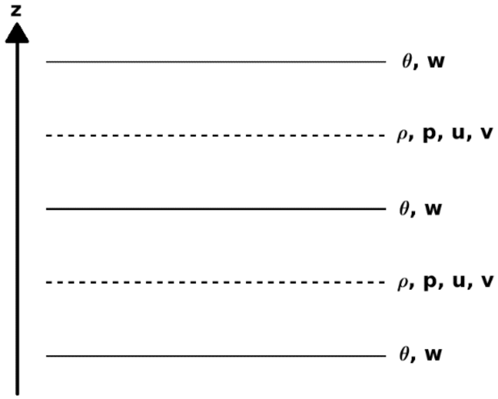
Spatial Discretisation: Staggered Finite Differences

Approximate spatial derivatives by finite differences: $$\frac{\partial X}{\partial z} \rightarrow \frac{X\left(t, z + {}^{\Delta z}/_{2}\right) - X\left(t, z - {}^{\Delta z}/_{2}\right)}{\Delta z}$$

Horizontal:
C-grid



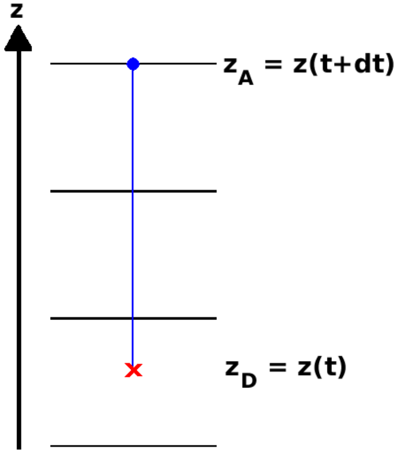
Vertical:
Charney-Phillips grid



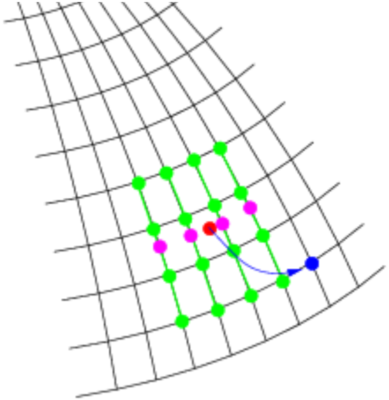
Transport: Semi-Lagrangian

Finite difference along a fluid parcel trajectory:

$$\frac{DX}{Dt} \rightarrow \frac{X\left(t+\Delta t, z(t+\Delta t)\right) - X\left(t, z(t)\right)}{\Delta t}$$



Interpolate *X* at time *t* to the departure point



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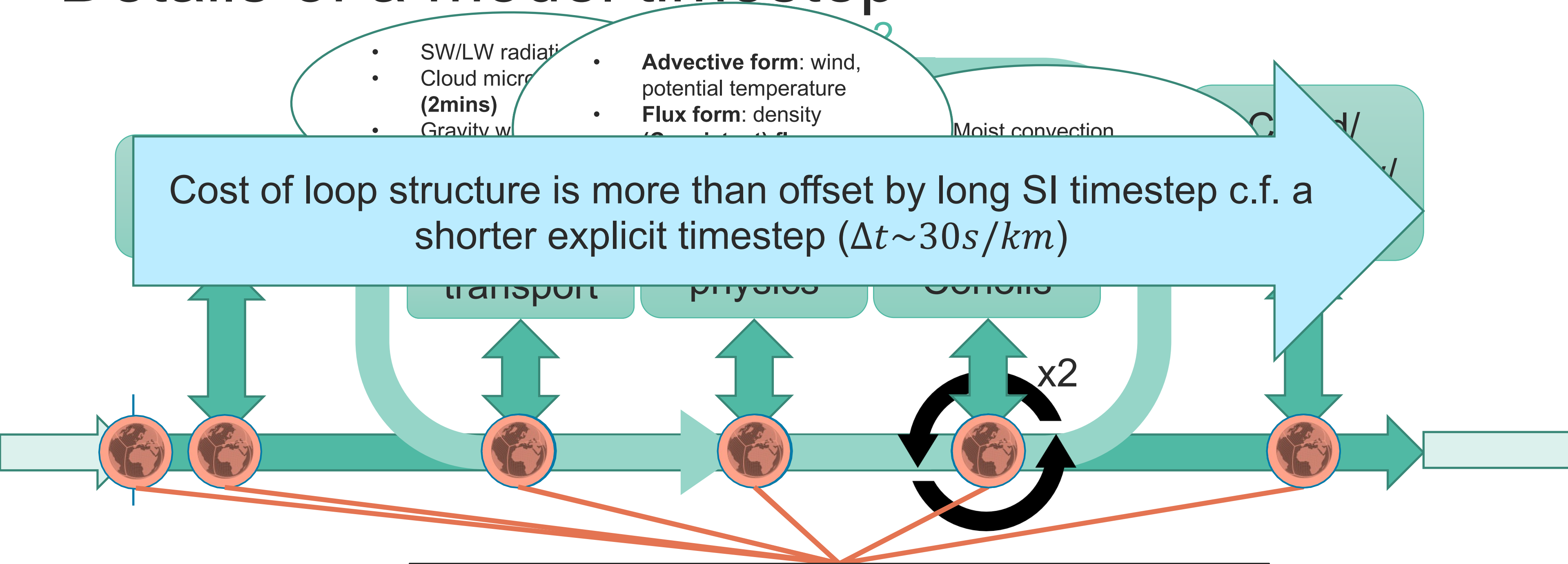
Semi-implicit timestep

- Continuous: $\frac{\partial x}{\partial t} = f\left(x(t)\right)$
- Explicit: $\frac{x^{n+1} - x^n}{\Delta t} = f(x^n)$
- Implicit: $\frac{x^{n+1} - x^n}{\Delta t} = f(x^{n+1})$
- Semi-implicit: $\frac{x^{n+1} - x^n}{\Delta t} = \alpha f(x^{n+1}) + (1-\alpha) f(x^n)$
- Picard iteration: $x^{k+1} = x^n + \Delta t(\alpha f\left(x^k\right) + (1-\alpha) f(x^n))$, take $x^{n+1} = x^{k+1}$after k iterations

Details of a model timestep



Slow physics = 1 call
Core transport = 2 calls
Tracer transport = 1 call

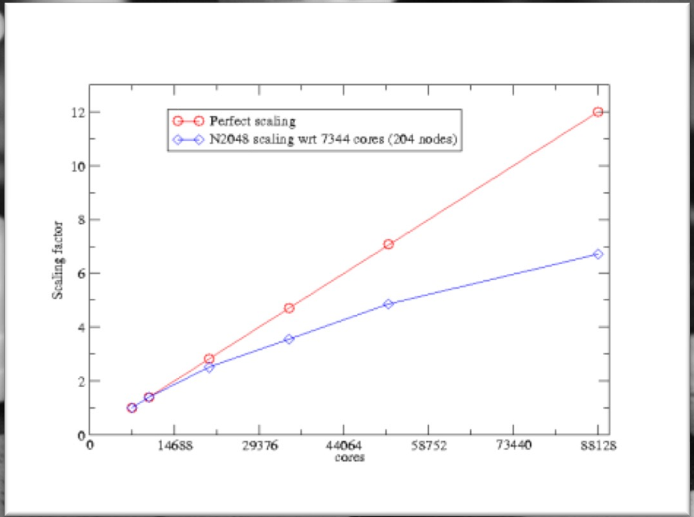
Fast physics = 2 calls
Linear solver = 4 calls
Chem/aerosol = 1 call

Why the next generation?

LFRic and GungHo dynamical core

Story begins at the ENDGame

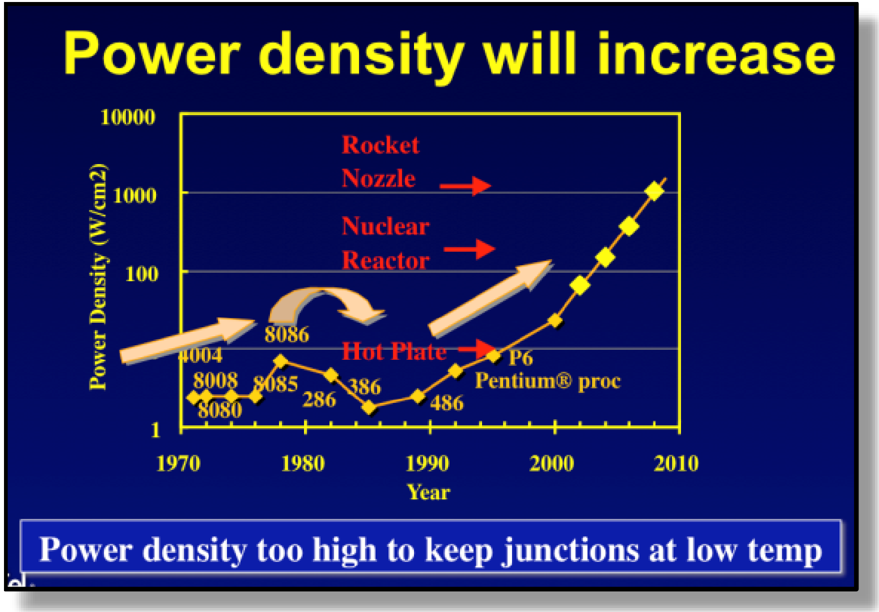
- ENDGame operational 2014
- Greatly improved scalability…
- …but not enough for Exascale



Andy Malcolm, Paul Selwood

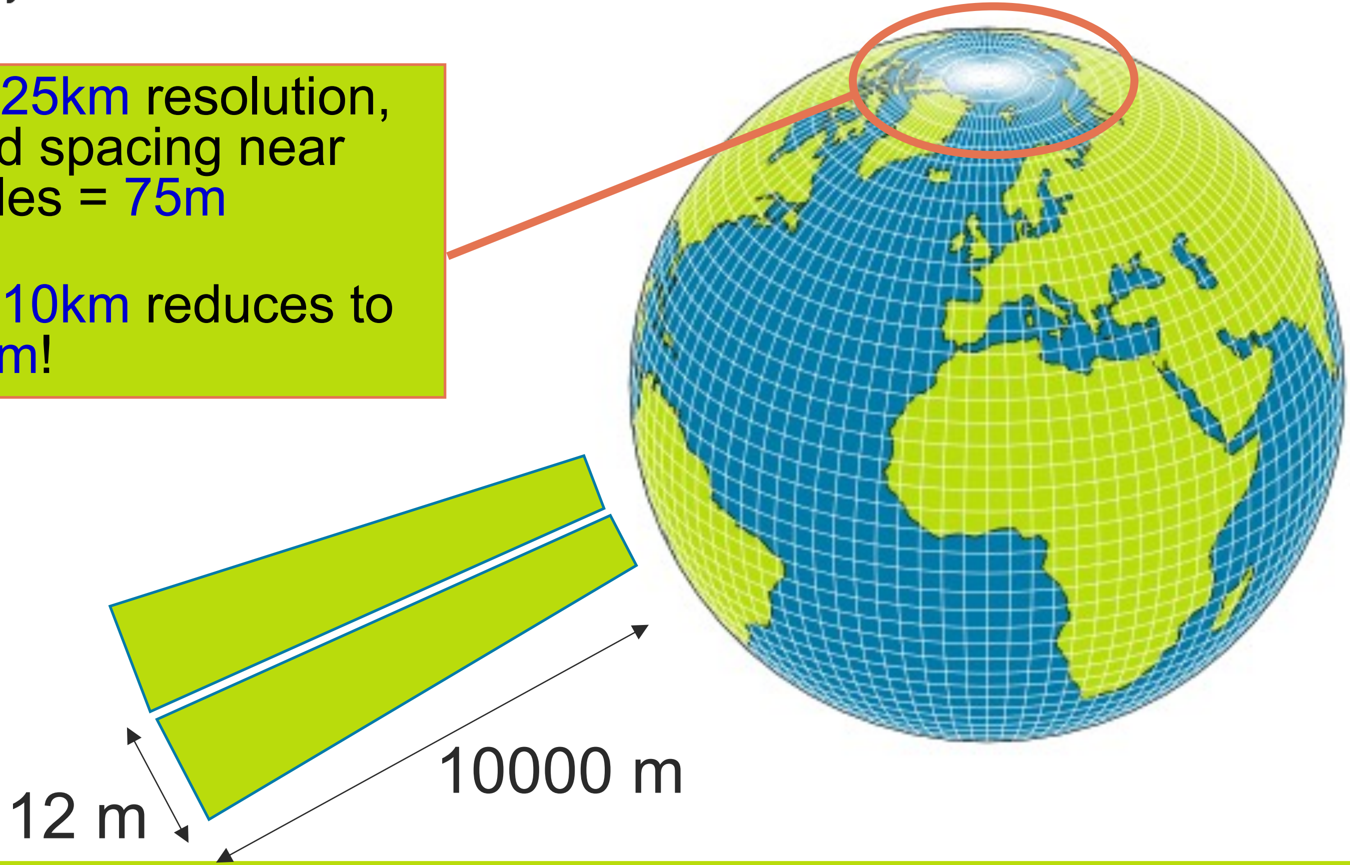
Met Office Hadley Centre

The problem is hardware

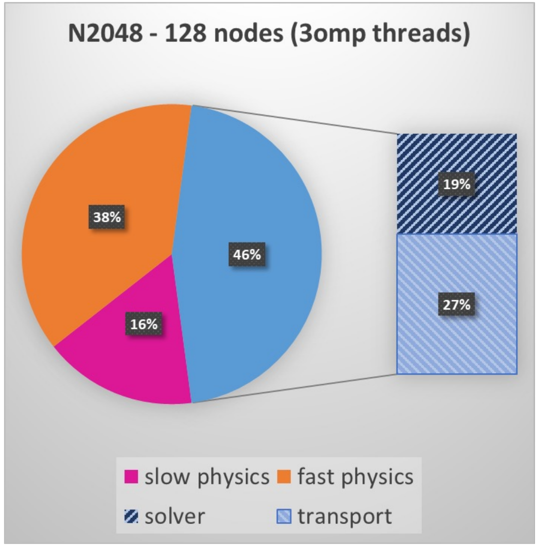


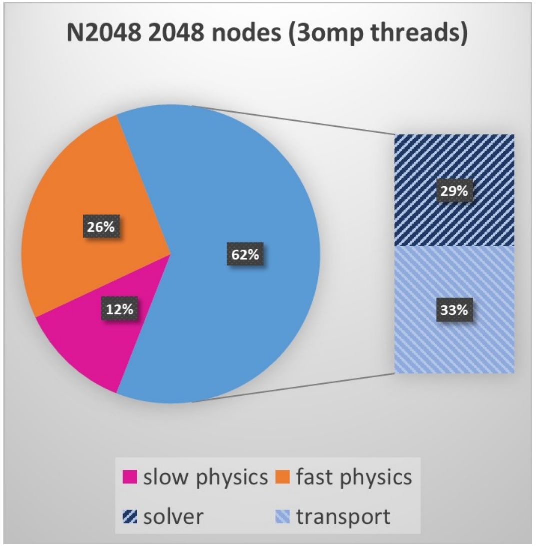
Intel, 2000

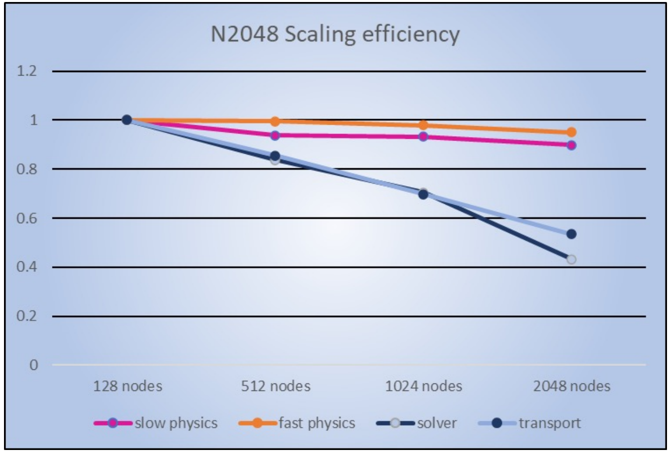
- At 25km resolution, grid spacing near poles = 75m
- At 10km reduces to 12m!



UM strong scaling at N2048 (~6km)

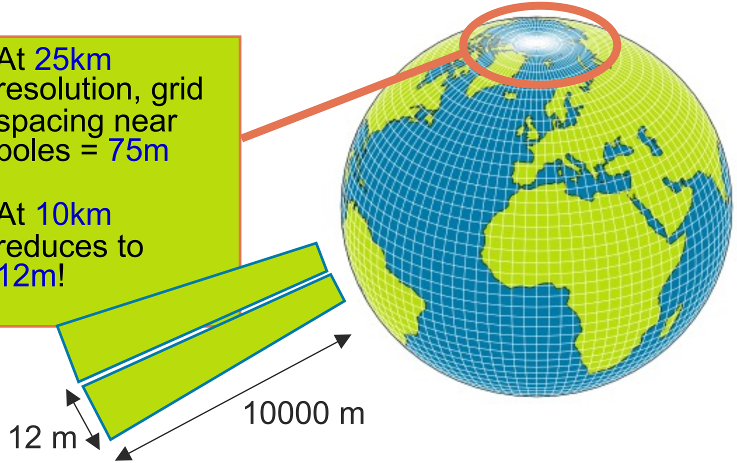






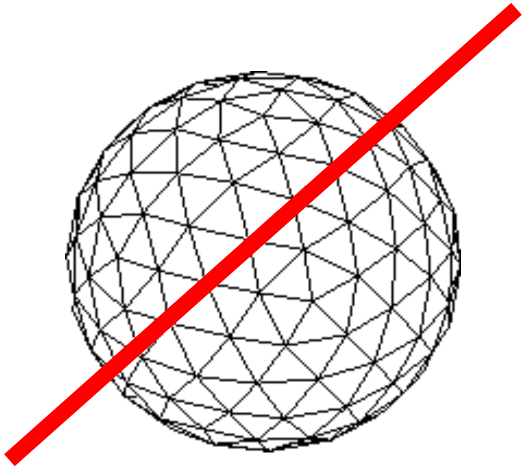
Performance Motivation

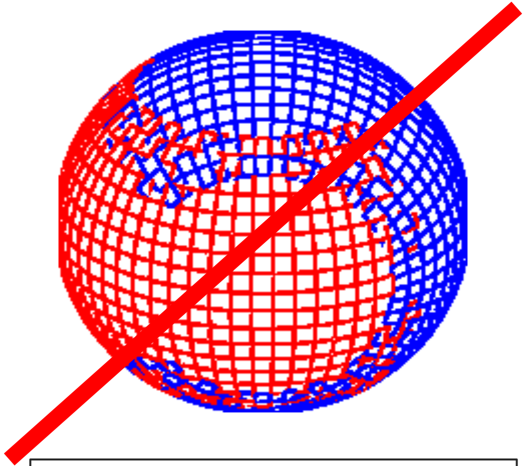
- At 25km resolution, grid spacing near poles = 75m
- At 10km reduces to 12m!



- Scalability for Lat-Lon mesh is limited by polar singularities
- Assumption of regular, orthogonal, finite difference scheme is deeply embedded in UM code
- No clear separation between computational and science code
- Choice to develop new infrastructure alongside the dynamical core

Choice of mesh (cubed-sphere)





- Triangles potentially difficult for coupling to physics and other system components.
- Not ruled out by GungHo and could be explored in future.

- Primary candidate and following assessment of scientific performance, is now becoming ‘baked into’ NGMS plans.

- Could retain ENDGame numerics.
- Not good for conservation/physics in the overlap region.

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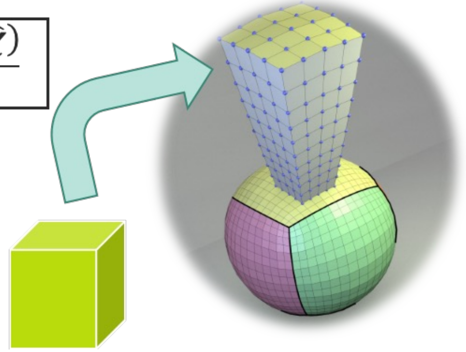
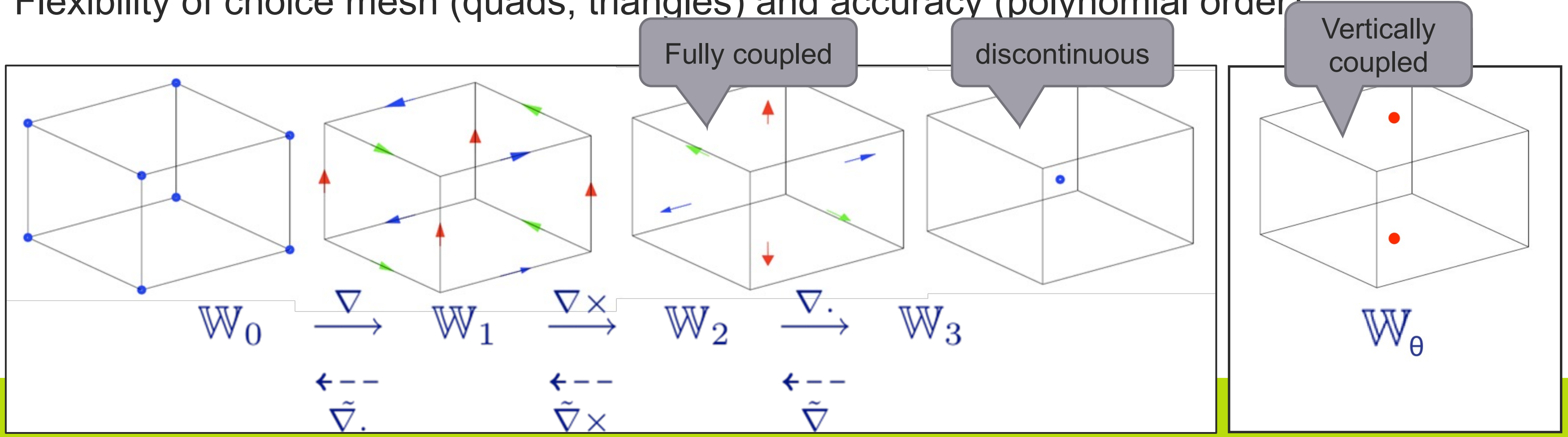
Mixed Finite Elements

$$\mathbf{J} \equiv \frac{\partial \boldsymbol{\phi}(\hat{\chi})}{\partial \hat{\chi}}$$



Mixed Finite Element method gives

- Compatibility: $\nabla\times\nabla\varphi = 0, \nabla\cdot\nabla\times\boldsymbol{v} = 0$
- Accurate balance and adjustment properties
- No orthogonality constraints on the mesh
- Flexibility of choice mesh (quads, triangles) and accuracy (polynomial order)



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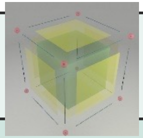
Mixed Finite Element Method

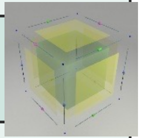
- Retains layout and properties of UM
- No requirement for orthogonality

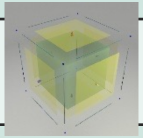
$$\mathbb{W}_0 \xrightarrow{\nabla} \mathbb{W}_1 \xrightarrow{\nabla\times} \mathbb{W}_2 \xrightarrow{\nabla\cdot} \mathbb{W}_3.$$

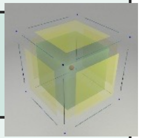
$$\mathbb{W}_\theta = \mathbf{k}\cdot\mathbb{W}_2$$

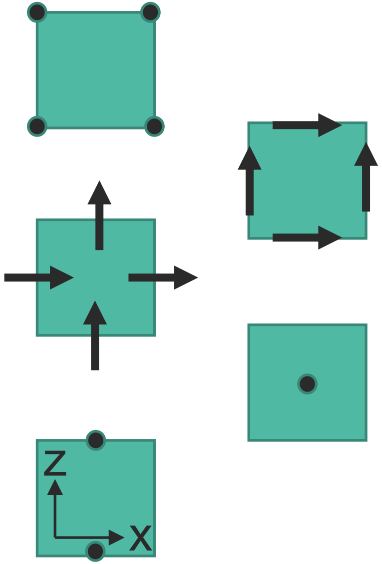
$\mathbb{W}_0$	Pointwise scalars	
$\mathbb{W}_1$	Circulation Vectors	
$\mathbb{W}_2$	Flux Vectors	Velocity
$\mathbb{W}_3$	Volume integrated Scalars	Pressure, Density
$\mathbb{W}_\theta$	Pointwise scalars	Potential Temperature, moisture











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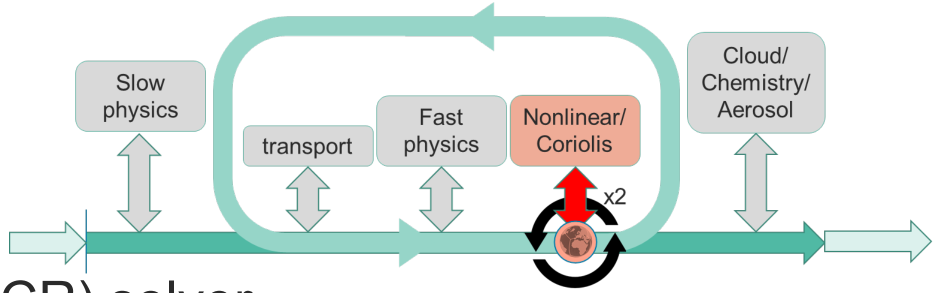


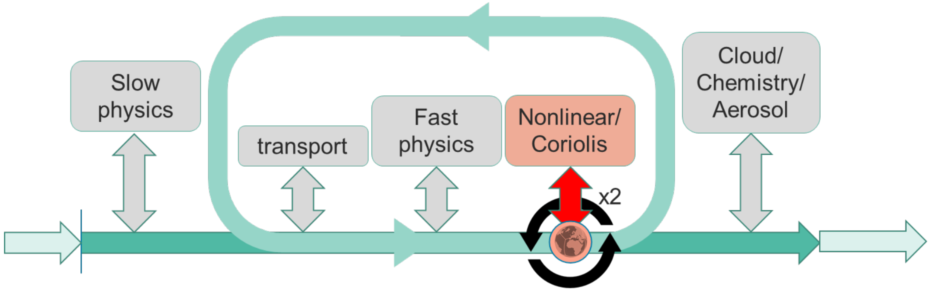
Linear Solver

- Solver Outer system with Iterative (GCR) solver

$$
\begin{pmatrix}
M_2^{\mu,C} & & -P_{2\theta}^{\Pi^*} & -G^{\theta^*} \\
D^{\rho^*} & M_3 & & \\
P_{\theta 2}^{\theta^*} & & M_\theta & \\
 & -M_3^{\rho^*} & -P_{3\theta}^{*} & M_3^{\Pi^*}
\end{pmatrix}
\begin{pmatrix}
\widetilde{u}' \\ \widetilde{\rho}' \\ \widetilde{\theta}' \\ \widetilde{\Pi}'
\end{pmatrix}
=
\begin{pmatrix}
-\mathcal{R}_u \\ -\mathcal{R}_\rho \\ -\mathcal{R}_\theta \\ -\mathcal{R}_\Pi
\end{pmatrix}
$$

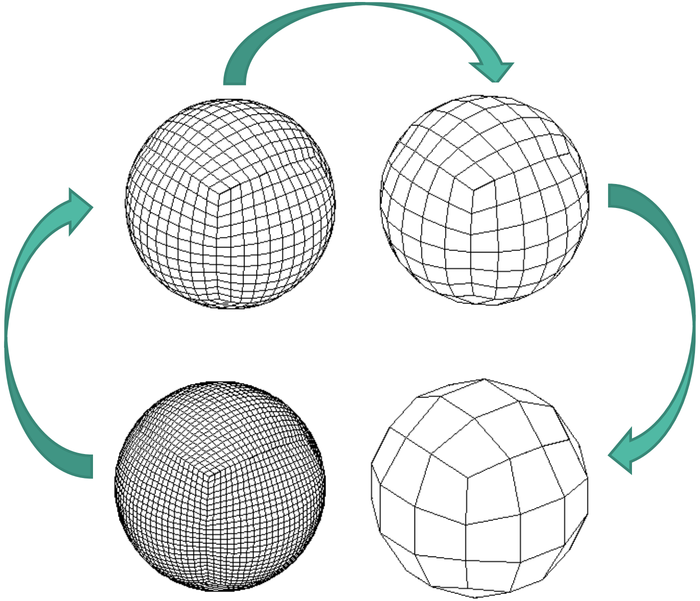
- Contains all couplings
- Velocity mass matrices couple in all directions and potential temperature mass matrices couple in the vertical
- Efficient solution requires a good preconditioner…

Multigrid preconditioner



- Helmholtz system $H\Pi' = R$ solved using a single Geometric-Multi-Grid V-cycle with block-Jacobi smoother

$$H = M_3^{\Pi^*} + \left(P_{3\theta}^{*}\mathring{M}_\theta^{-1}P_{\theta 2}^{\theta^*,z} + M_3^{\rho^*}M_3^{-1}D^{\rho^*}\right)\left(\mathring{M}_2^{\mu,C}\right)^{-1}G^{\theta^*}.$$



- Coupled mass matrices are now lumped
- Preconditioner system resembles single ENDGame solve

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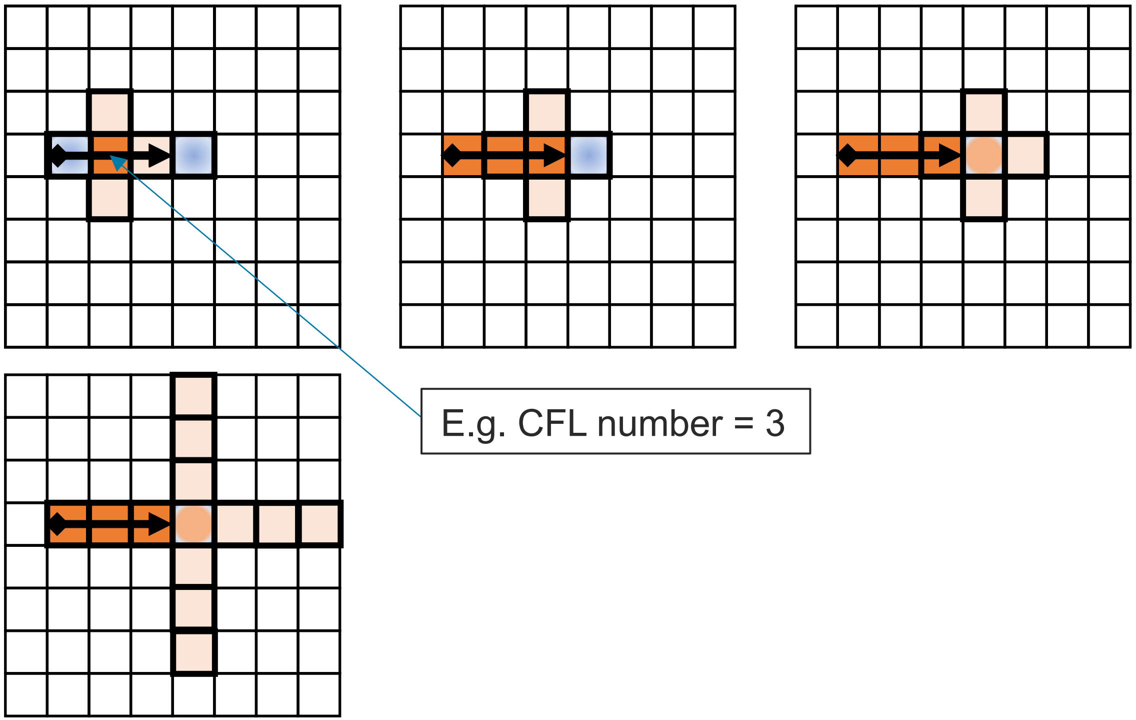
Transport – horizontal options

Stage/substep 1 Stage/substep 2 Stage/substep 3

Eulerian scheme

Flux-form Semi-Lagrangian scheme



- Small mpi halo exchange
- Multiple exchanges
- Cheap computation
- Multiple calls

- Large mpi halo exchange
- Only 1 exchanges
- More expensive computation
- Only 1 call

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UM-LFRic differences/similarities

	ENDGame/UM	GungHo/LFRic
Grid	Lat-Long	Cubed-Sphere
Equation set	Deep, non-hydrostatic	Deep, non-hydrostatic
Prognostic Variables	ρ, θ, Π, u, v, w	ρ, θ, Π, **u**
Moist Variables	**Specific humidities & mixing ratios**	**mixing ratios !**
Spatial Discretisation	**2^{nd} Order FD**	**Mixed FEM**
Temporal Discretisation	**Iterative Semi-Implicit**	**Iterative Incremental Semi-Implicit**
Advection	Semi-Lagrangian	Dimensionally split, Eulerian or FFSL
Physics parametrizations	**UM,SOCRATES,JULES**	**UM,SOCRATES,JULES**

Algorithms, kernels and Psyclone

- Algorithms work on full domain fields:

```
!!!! Compute pressure for CFL and qsat removal
call exner_wth%copy_field_properties(pressure)
inv_kappa = 1.0_r_def/kappa
call invoke(setval_X(pressure,exner_wth),         &
            inc_X_powreal_a(pressure,inv_kappa),  &
            inc_a_times_X(p_zero,pressure))
```

- No need to worry about loops, mesh structure, parallelism – this is all taken care of in the mysterious “invoke”

- Kernels work on individual grid points:

```
do k = 0, nlayers-1

  ! Pressure on layer boundaries (note, top layer is set to zero below)
  p_theta_levels(1,1,k) = real(p_zero*(exner_in_wth(map_wth(1) + k)) &
                                **(1.0_r_um/kappa), r_um)

end do   ! k
```

- Direct looping over k dimension
- Indirect looping over horizontal mesh using “map_wth”

Algorithms, kernels and Psyclone

- Psyclone is auto-generated code which sits between algorithms and kernels
- Deals with data parallelism – halo exchanges, openMP
- Does looping over horizontal mesh if required
  - Option to pass the entire horizontal domain (of MPI rank) to a kernel, to allow i-first looping if this is more performant
- Metadata is added to kernels to configure Psyclone:

```
!> Kernel metadata for Psyclone
type, public, extends(kernel_type) :: methox_kernel_type
  private
  type(arg_type) :: meta_args(3) = (/                          &
       arg_type(GH_FIELD,  GH_REAL, GH_WRITE, WTHETA), &
       arg_type(GH_FIELD,  GH_REAL, GH_READ,  WTHETA), &
       arg_type(GH_SCALAR, GH_REAL, GH_READ          )  &
       /)
  integer :: operates_on = CELL_COLUMN
contains
  procedure, nopass :: methox_code
end type methox_kernel_type
```

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Psyclone auto-generated code:

```
! Compute rhs = u + dt*grad(p)
call rhs%initialise( u%get_function_space() )
call grad%initialise( u%get_function_space() )
call invoke( setval_c(grad, 0.0_r_def),                 &
             gradient_kernel_type(grad, pressure, qr), &
             aX_plus_Y(rhs, dt, grad, u) )
```

PSy Layer

New algorithm

```
CALL rhs % initialise(u % get_function_space())
CALL grad % initialise(u % get_function_space())
CALL invoke_0(grad, pressure, rhs, dt, u, qr)
```

```
SUBROUTINE invoke_0(grad, pressure, rhs, dt, u, qr)

....

!$omp end parallel
```

MPI

```
IF (pressure_proxy%is_dirty(depth=1)) THEN
  CALL pressure_proxy%halo_exchange(depth=1)
END IF
!
```

Horizontal Looping

```
DO colour=1,ncolour
  !$omp parallel default(shared), private(cell)
  !$omp do schedule(static)
  DO cell=1,mesh%get_last_halo_cell_per_colour(colour,1)
    !
```

Kernel Call

```
    CALL gradient_code(nlayers,                                       &
                       grad_proxy%data, pressure_proxy%data,          &
                       ndf_w2, undf_w2, map_w2(:,cmap(colour, cell)), &
                       diff_basis_w2,                                 &
                       ndf_w3, undf_w3, map_w3(:,cmap(colour, cell)), &
                       basis_w3, np_xy, np_z, weights_xy, weights_z)
  END DO
  !$omp end do
  !$omp end parallel
END DO

! Set halos dirty/clean for fields modified in the above loop
CALL grad_proxy%set_dirty()
```

OpenMP

```
!$omp parallel default(shared), private(df)
!$omp do schedule(static)
```

Built-in

```
DO df=1,rhs_proxy%vspace%get_last_dof_annexed()
  rhs_proxy%data(df) = dt*grad_proxy%data(df) + u_proxy%data(df)
END DO
!$omp end do

! Set halos dirty/clean for fields modified in the above loop
```

MPI

```
!$omp master
CALL rhs_proxy%set_dirty()
!$omp end master
!
!$omp end parallel
END SUBROUTINE invoke_0
```

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Coupling in the physics

- Map LFRic fields onto UM arrays
  - Example here is k-first data, but can add i-loop:

```
j = 1
do k = 1, model_levels
  do i = 1, seg_len
    ! height of levels from centre of planet
    r_rho_levels(i,j,k)    = height_w3(map_w3(1,i) + k-1) + planet_radius
```

- Call the UM scheme
  - All spatially varying information must be passed in through argument list – no use of modules

- Map UM outputs back to LFRic fields

```
!-----------------------------------------------------------------------
! For the initial implementation we pass each individual column
! of data to an array sized (1,1,k) to match the UMs (i,j,k) data
! layout.
! assuming map_wth(1) points to level 0
! and map_w3(1) points to level 1
!-----------------------------------------------------------------------
do k = 1, nlayers
  ! wet density on theta and rho levels
  rho_wet_tq(1,1,k) = wetrho_in_wth(map_wth(1) + k)
  rho_wet(1,1,k) = wetrho_in_w3(map_w3(1) + k-1)
  ! dry density on theta and rho levels
  rho_dry_theta(1,1,k) = rho_in_wth(map_wth(1) + k)
  rho_dry(1,1,k) = rho_in_w3(map_w3(1) + k-1)
```

```
call glue_conv_6a                                                          &
  ( rows*row_length, segments, n_conv_levels, bl_levels, call_number, &
   seg_num, theta_conv, q_conv, qcl_conv, qcf_conv                         &
  , qrain_conv, qgraup_conv, qcf2_conv                                     &
  , cf_liquid_conv, cf_frozen_conv, bulk_cf_conv                           &
  , p_star, land_sea_mask                                                  &
  , u_conv, v_conv, w(1,1,1)                                               &
  , tot_tracer, dthbydt, dqbydt,   dqclbydt, dqcfbydt                      &
  , dcflbydt, dcffbydt, dbcfbydt, dubydt_p, dvbydt_p                       &
```

```
if (l_mom) then
  do k = 1, n_conv_levels
    u_conv(1,1,k) = u_conv(1,1,k)    + dubydt_p(1,1,k) * timestep_conv
    v_conv(1,1,k) = v_conv(1,1,k)    + dvbydt_p(1,1,k) * timestep_conv
    ! total increments
    du_conv(map_w3(1) + k -1) = du_conv(map_w3(1) + k -1) + dubydt_p(1,1,k) * timestep_conv
    dv_conv(map_w3(1) + k -1) = dv_conv(map_w3(1) + k -1) + dvbydt_p(1,1,k) * timestep_conv
  end do
end if    !l_mom
```

Current status

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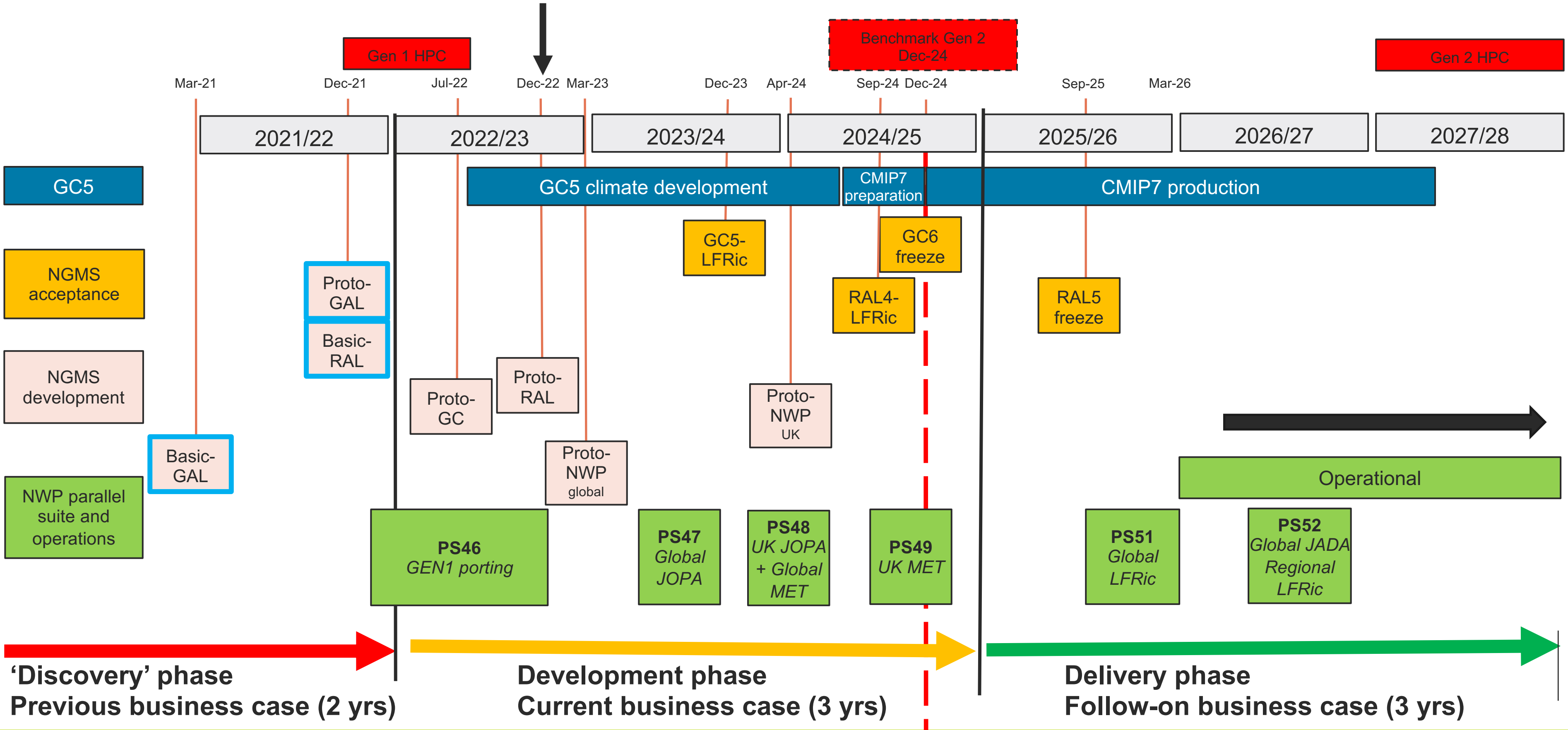
NGMS timeline



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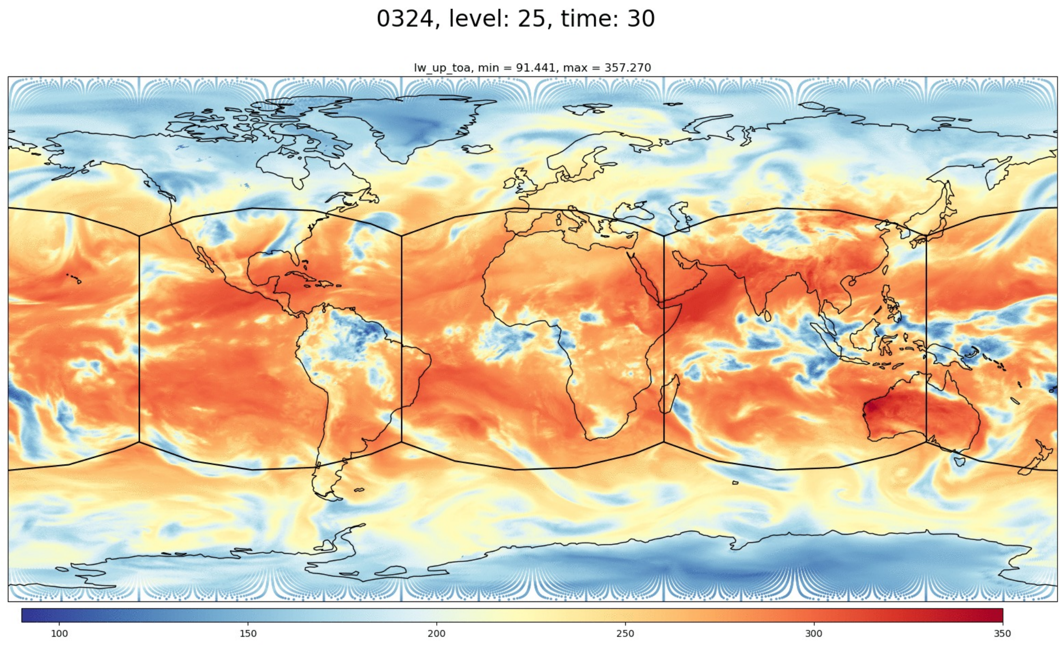
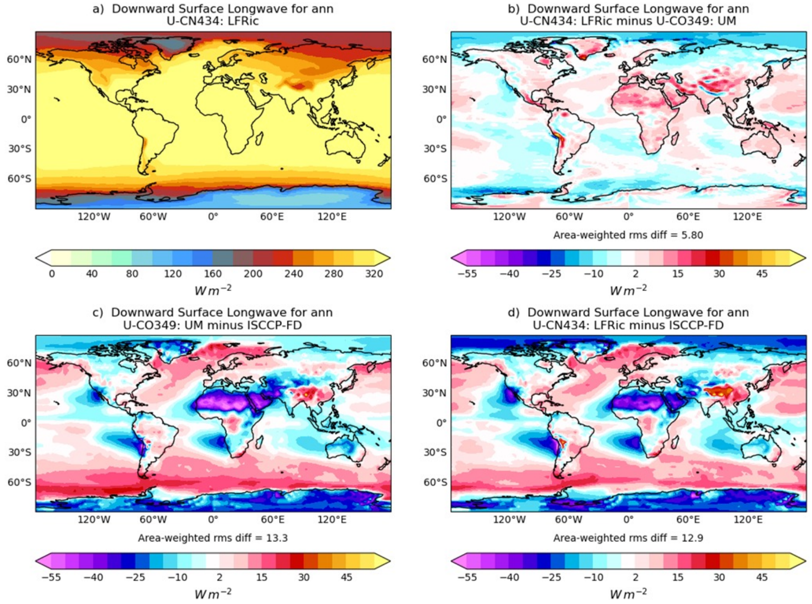
Global status

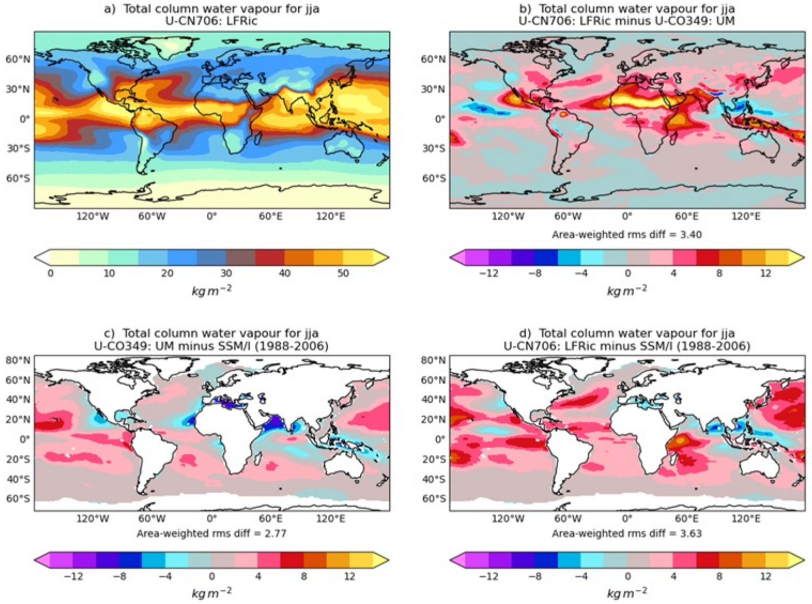


- C448 (20km) simulations running
- Currently attempting C896 (10km)…

Climate assessment

- Increased humidity over land – broadly seems like a good thing





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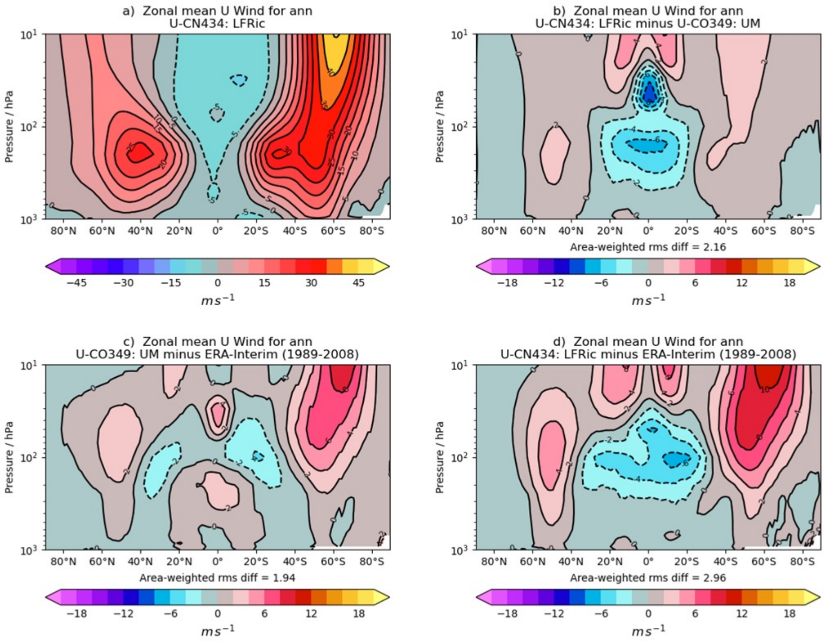
Climate assessment



- Large scale circulation is a bit different
- Jets moved polewards

- In gross terms, the mean climate looks broadly similar however

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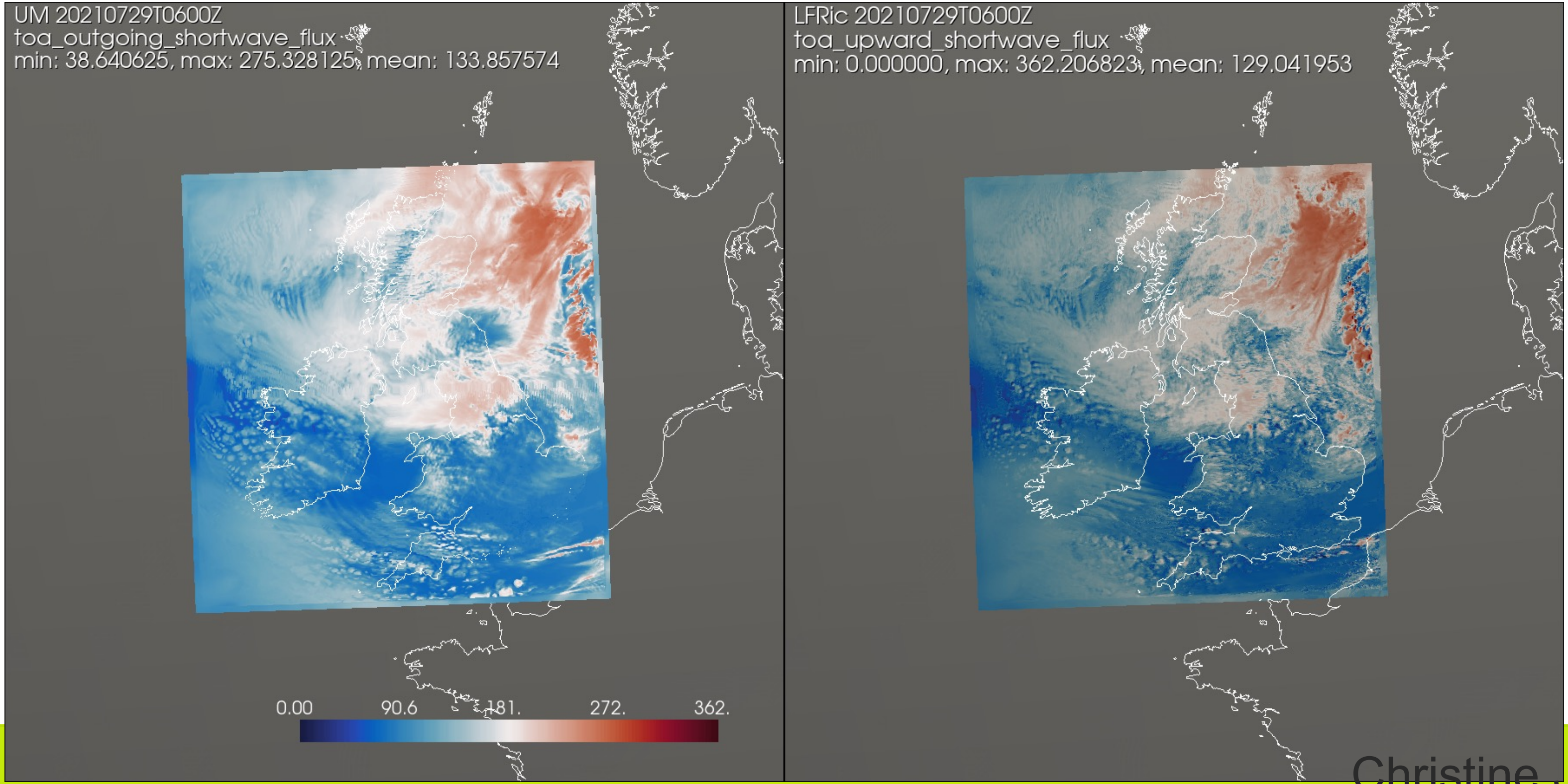
Regional status

- 1.5km UK simulations looking reasonable

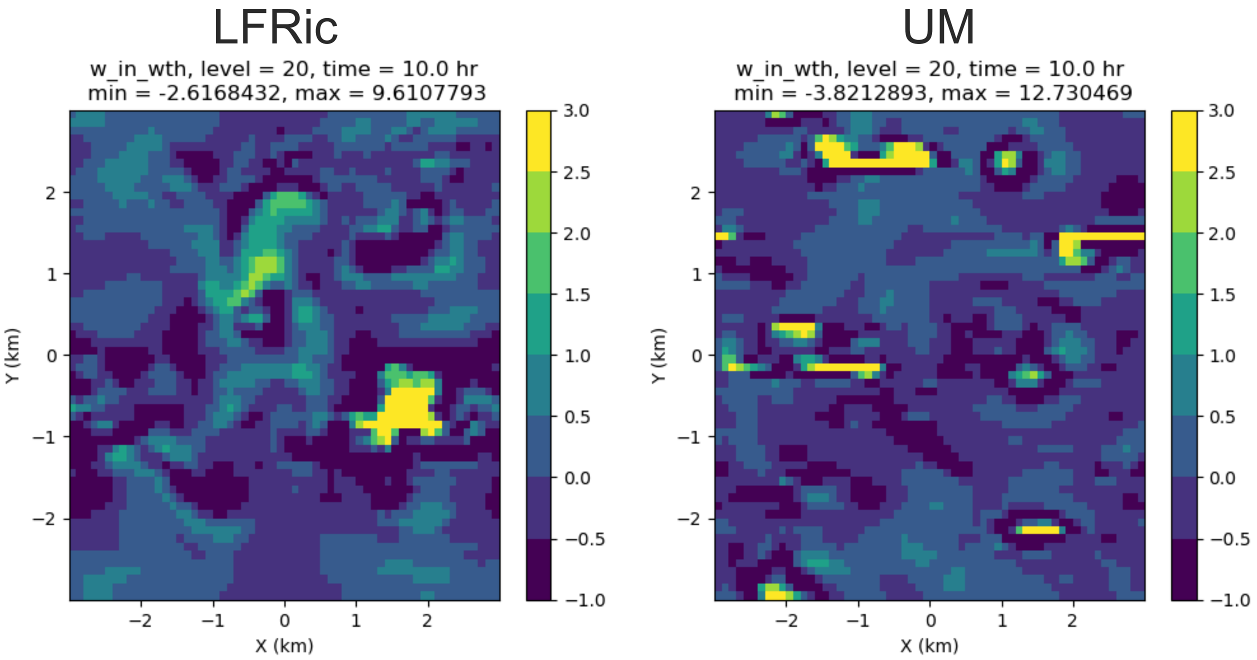


Christine Johnson

Met Office

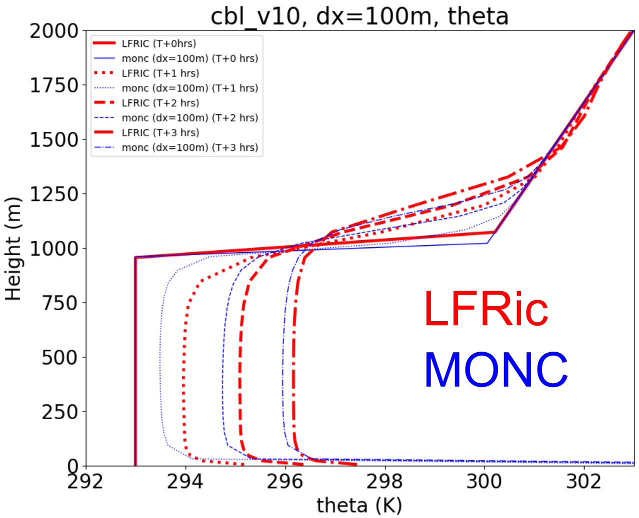
Very high resolution

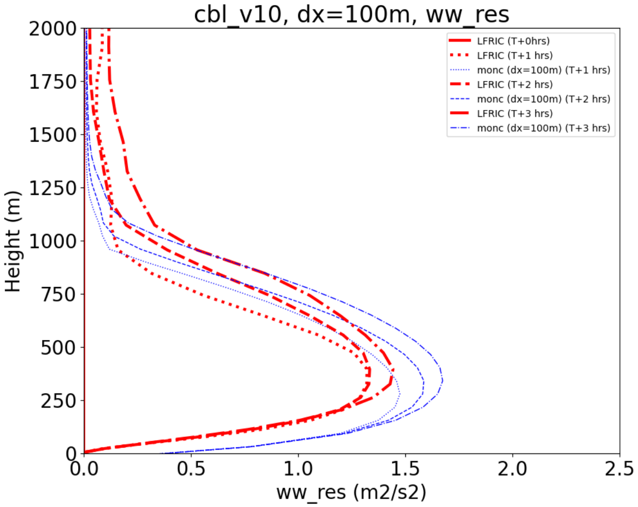
- Idealised "radiative-convective equilibrium" at 100m grid-length also shows good comparison
- Structures appear more coherent and better resolved in LFRic



Very high resolution

- Idealised dry convective boundary layer at 100m grid-length
- Comparison to large-eddy model (MONC) is pretty good
- Promising signs that LFRic could behave reasonable as a large-eddy model, and certainly be suitable for ~100m NWP





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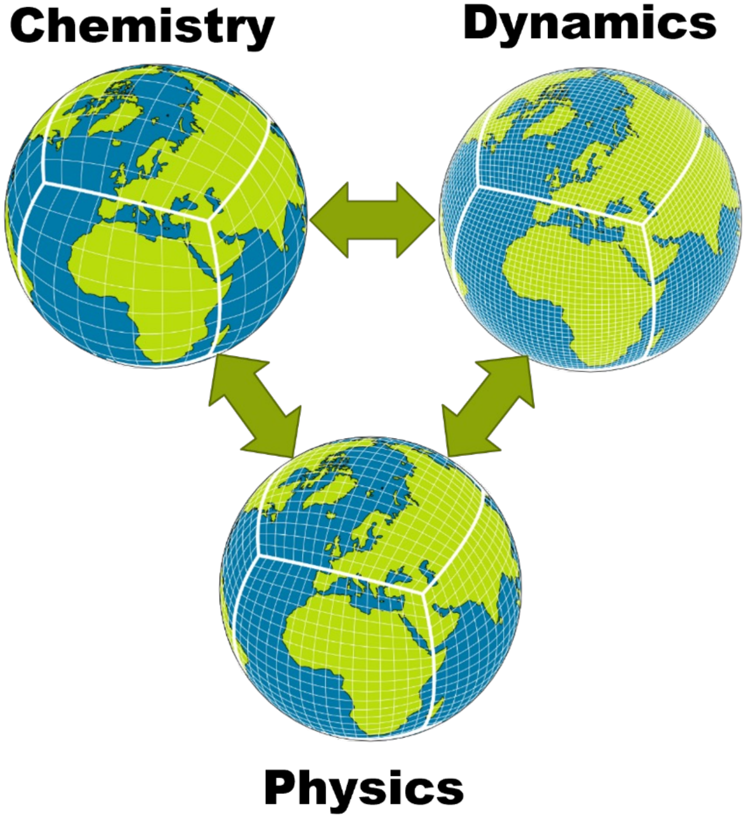
Future plans

Multi-resolution coupling

- Currently the UM runs a hybrid "junior-senior" Earth system model, coupling an N216 physical model to N96 chemistry & ES components
- Aim to design this from the bottom up with LFRic, allowing coupling between different model components (dynamics, physics, chemistry) on different meshes
- Infrastructure can be equally applicable to limited-area models



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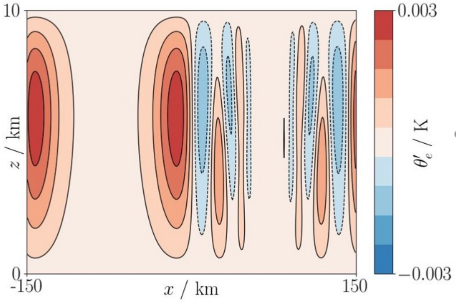
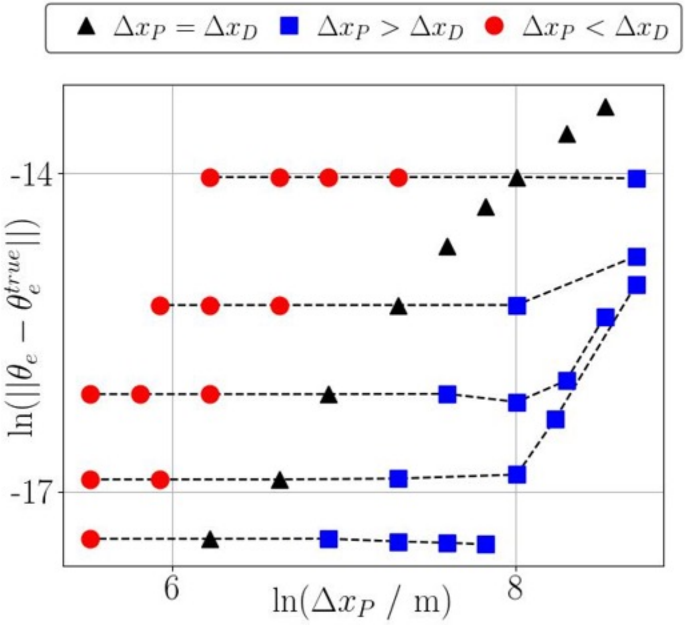
Idealised testing

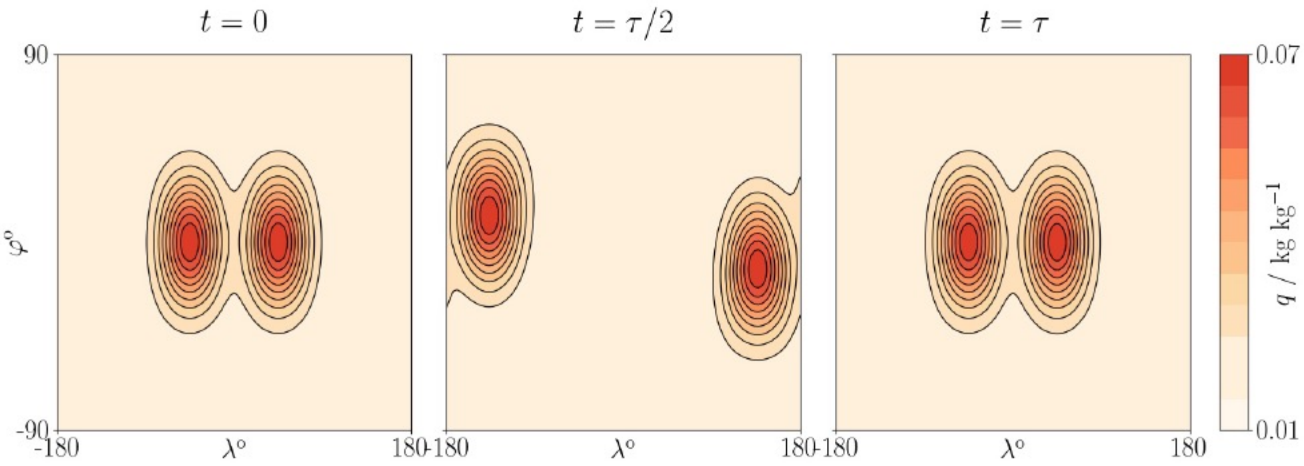


- Moist gravity wave with condensation/evaporation
- Black shows convergence of results as dynamics and physics resolution is increased
- Red shows increasing physics resolution beyond dynamics does not improve errors
- Blue shows degrading physics resolution initially has no effect, but then leads to strong degradation



Transport on a different mesh

- Tracer bubble exists at coarser resolution than model dynamics
- Dynamical winds driver tracer transport on it's native mesh
- Works, and is much cheaper than transport on dynamics mesh

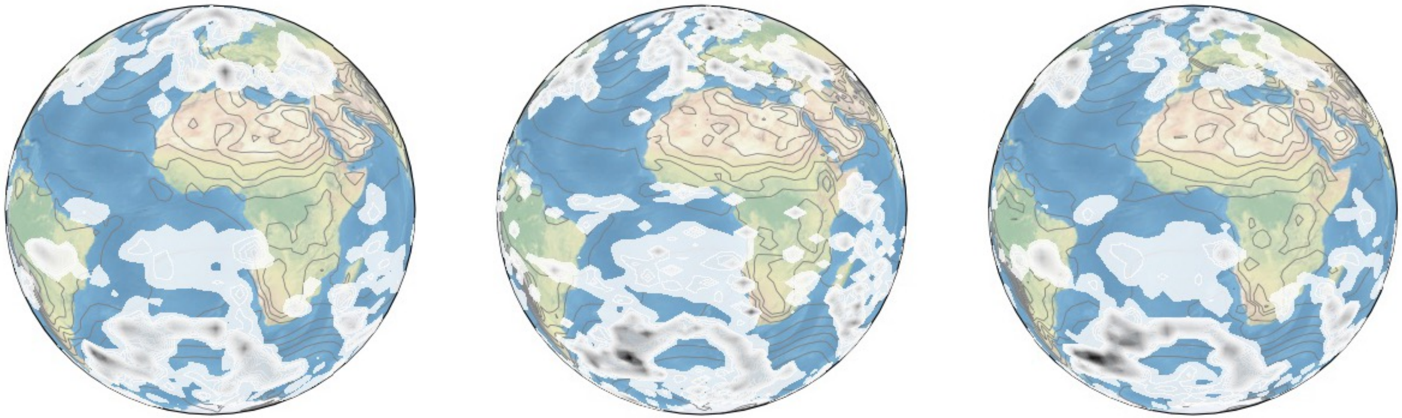


Global NWP simulations

- Initial tests demonstrate that it's possible to run full model with physics at different resolution to dynamics
- Results look plausible in all cases

t = -1.5 hr

$\Delta x_{phys} = \frac{1}{2}\Delta x_{dyn}$ $\quad$ $\Delta x_{phys} = \Delta x_{dyn}$ $\quad$ $\Delta x_{phys} = 2\Delta x_{dyn}$



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What’s changing

- Infrastructure
- Code layout (algorithms & kernels)
- Data layout (k-first ordering)
- Input/output & file format (netcdf)
- Transport (substepped method of lines or flux-form semi-lagrangian – both locally conservative)
- Solver (mixed system with multigrid preconditioner)

What’s not changing (much)

- Physical parametrizations
  - UM, Jules, Socrates, Casim, UKCA built directly from their current repositories
- Horizontal and vertical grids (C-grid horizontal, Charney-Phillips vertical)
- Timestep structure (slow/fast physics, iterative outer/inner loop dynamics)
- Use of Rose, fcm etc