Towards scalable numerical weather and climate prediction with mixed finite element discretizations

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Università di Trieste, 7 April 2016

The GungHo team. . .

- Met Office
- U Exeter
- Imperial College London
- U Bath
- U Reading
- U Leeds
- U Manchester
- U Warwick
- Hartree Centre

Plan

Plan

- **Introduction - Atmospheric modelling**

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- Introduction - Atmospheric modelling
- Unified Model and dynamical core

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- A new dynamical core - GungHo

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- Unified Model and dynamical core
- A new dynamical core - GungHo
- Mixed finite elements - Dynamo
- Where we are and where we are headed

Atmospheric modelling

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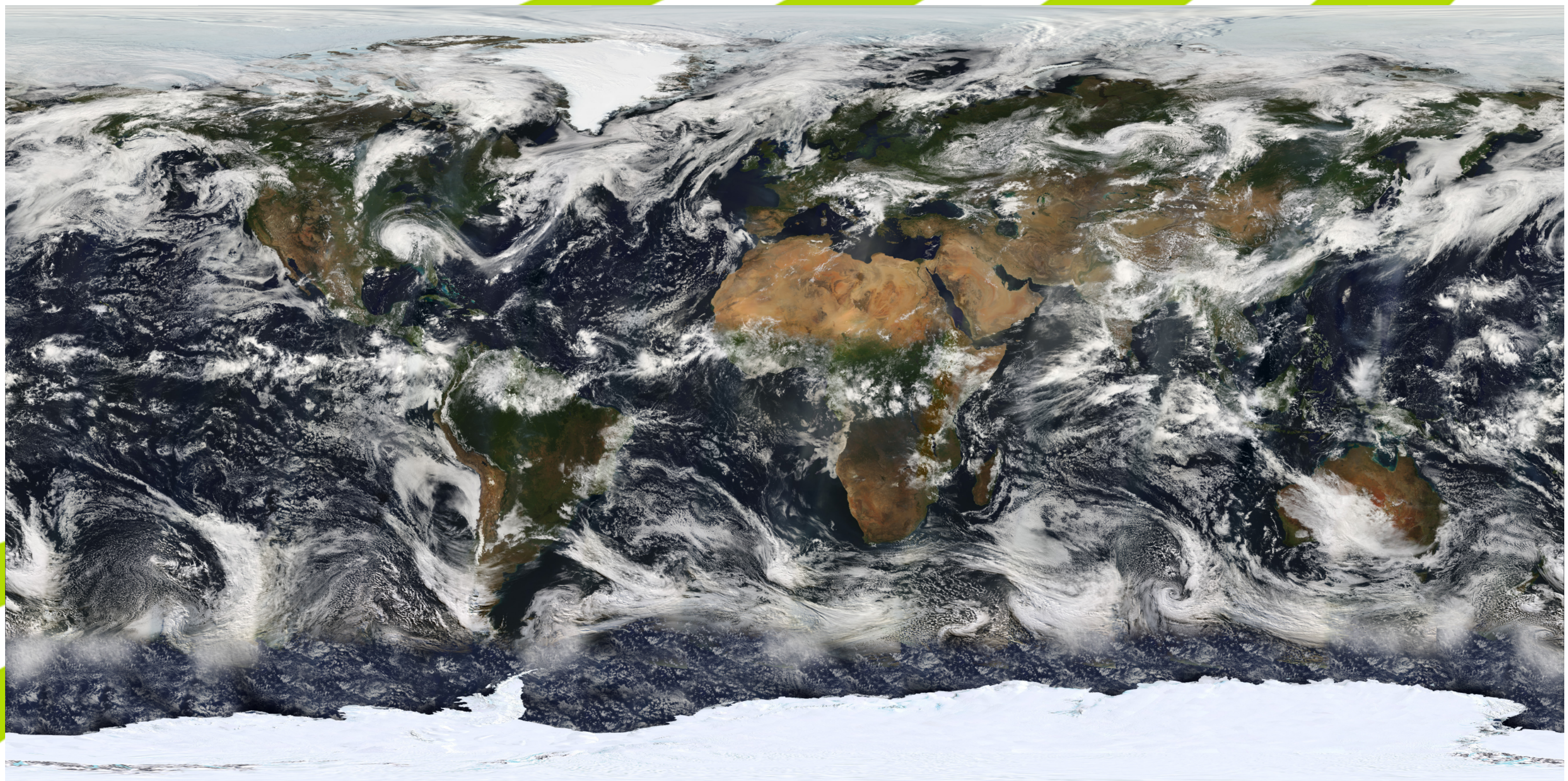
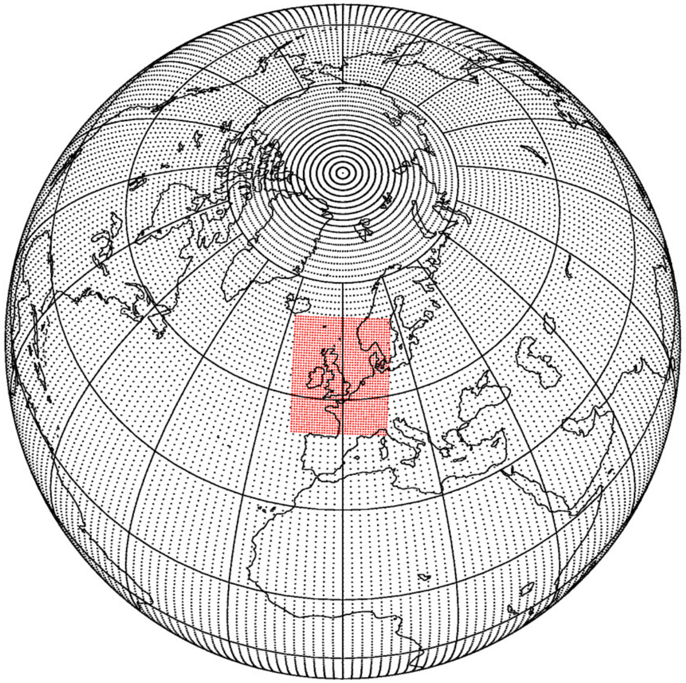


nasa.gov

Numerical Weather Prediction

Numerical Weather Prediction



ATMOSPHERIC DATA

$\Downarrow$

NUMERICAL MODEL

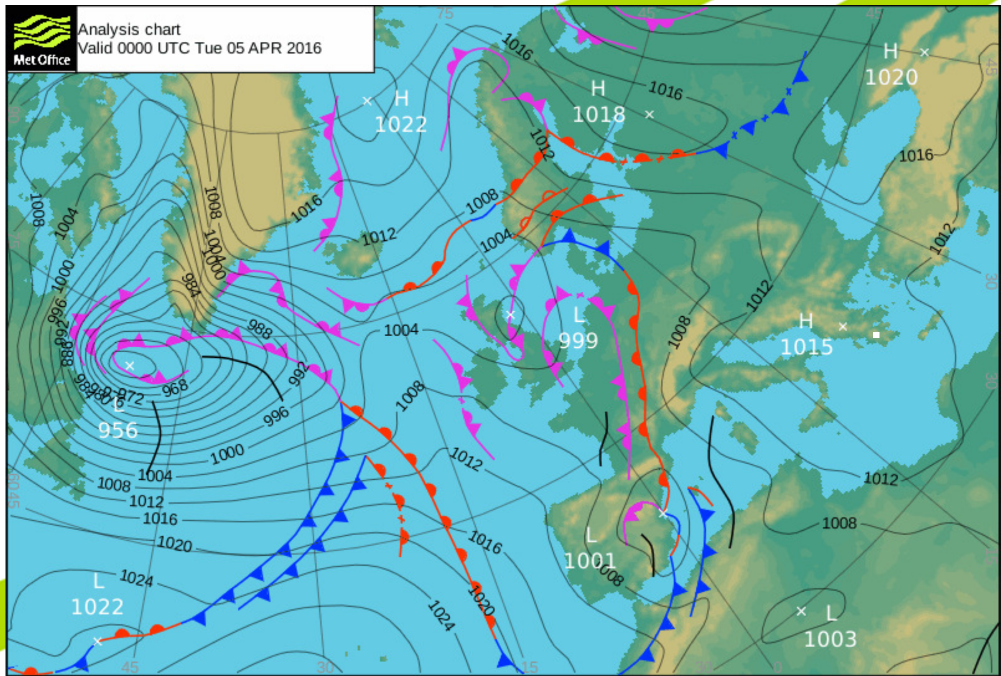
Δt, Δx

$\Downarrow \quad \int_0^T dt$

FORECAST AT TIME T

Numerical Weather Prediction

Numerical Weather Prediction



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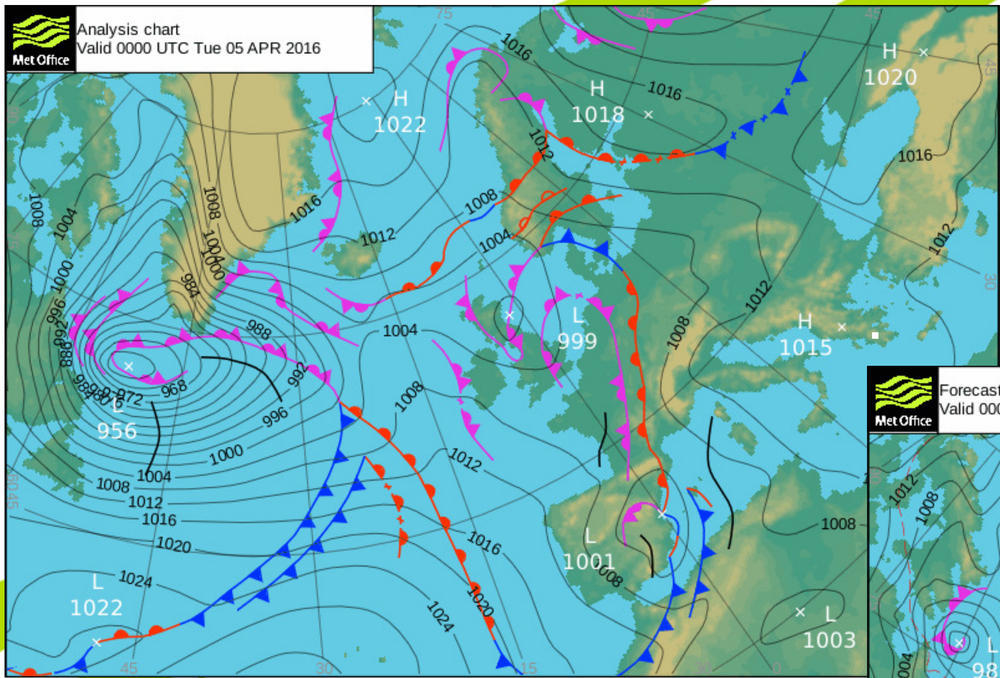

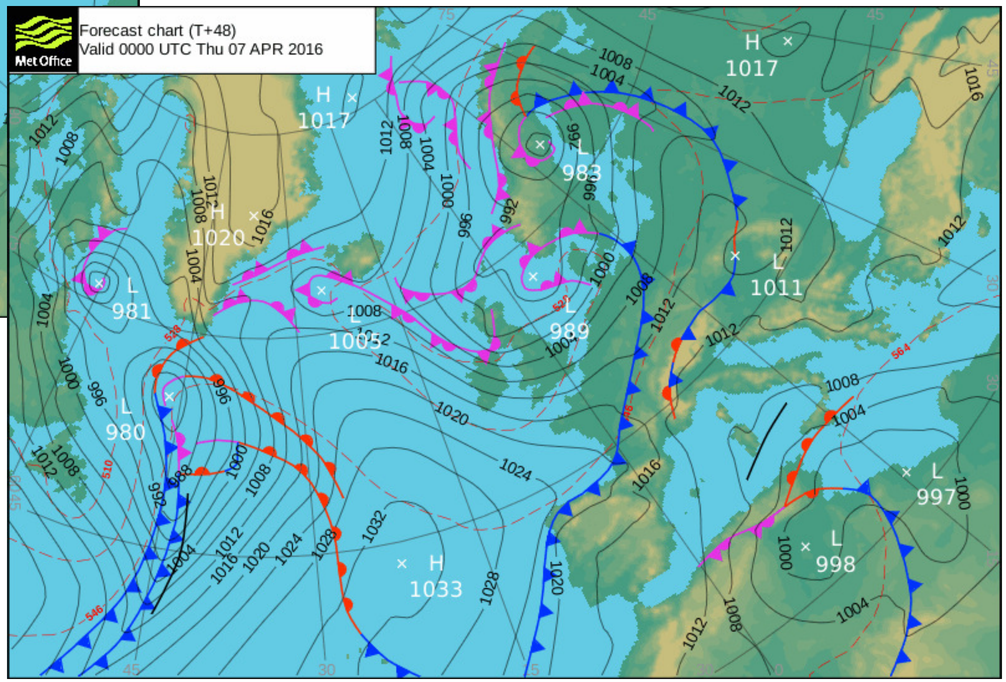

Unified Model

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Single atmospheric model for

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- **Global ($\Delta x \approx 17$ km) and mesoscale ($\Delta x \approx 4.4 - 1.5$ km) operational forecasts**

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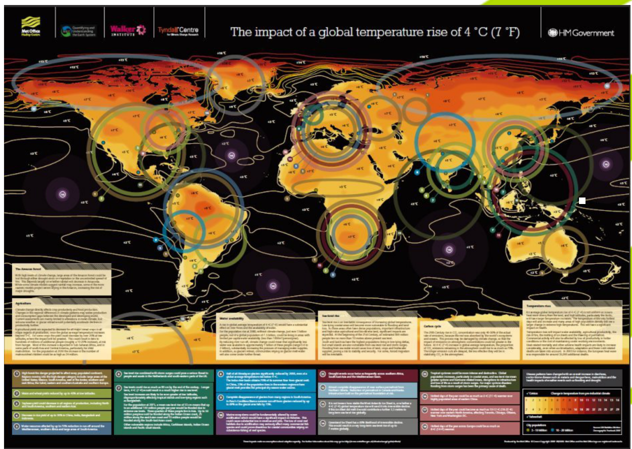
- 26 years old

Unified Model

Unified Model

$\Delta x = 300$ km



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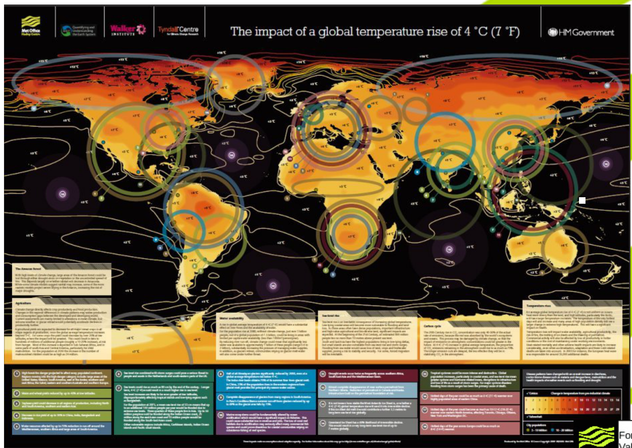

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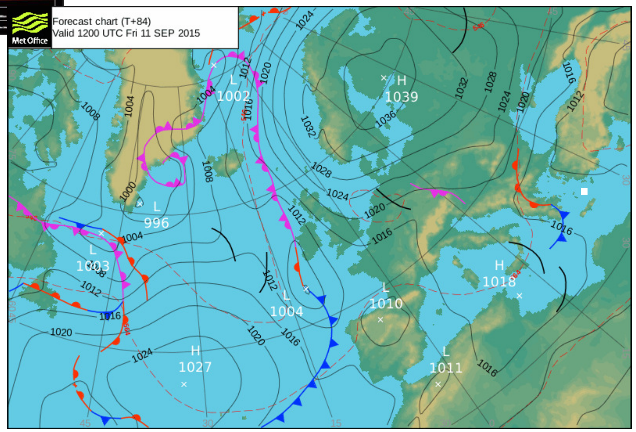

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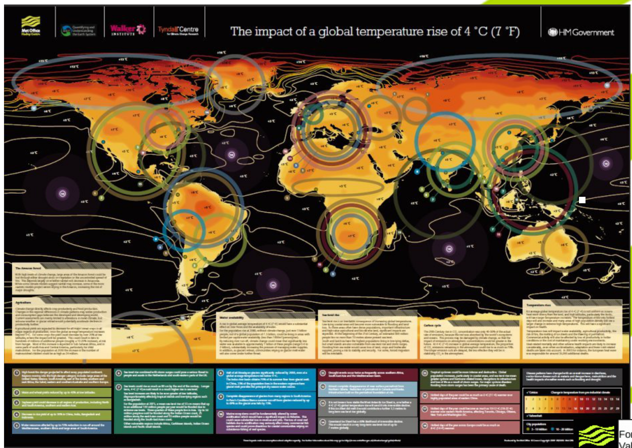

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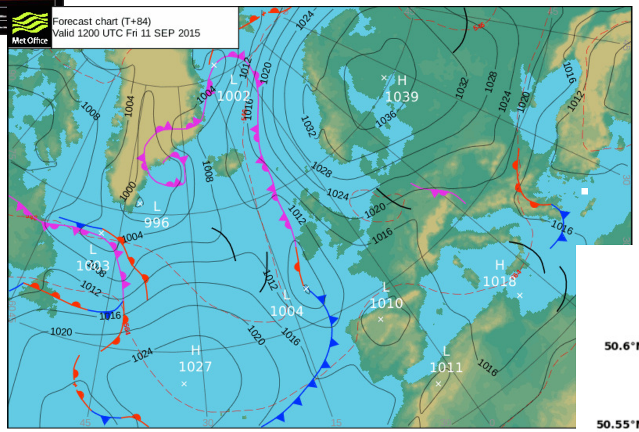
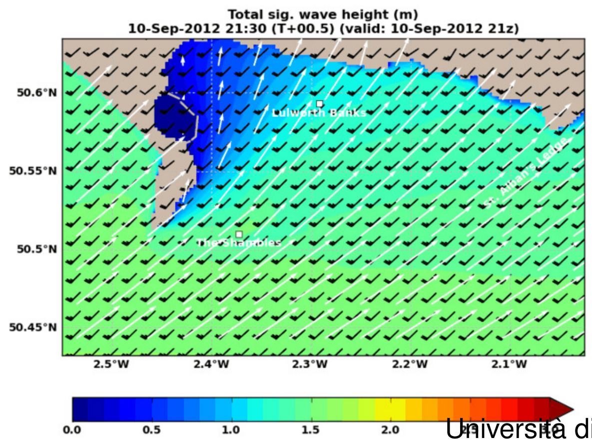


$\Delta x = 300$ m



Dynamical Core

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Solution of 3D rotating compressible fluid flow equations on the sphere with gravity and source terms

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Physics: motions on unresolved scales (turbulence) + clouds, radiation

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First(2002-) global, deep atmosphere non-hydrostatic model

Dynamical core

$$\frac{Du}{Dt} - \frac{uv\tan\phi}{r} - 2\Omega\sin\phi v + \frac{c_{pd}\Theta}{r\cos\phi}\frac{\partial\Pi}{\partial\lambda} = -\frac{uw}{r} + 2\Omega\cos\phi w + S^u$$

$$\frac{Dv}{Dt} - \frac{u^2\tan\phi}{r} + 2\Omega\sin\phi u + \frac{c_{pd}\Theta}{r}\frac{\partial\Pi}{\partial\phi} = -\frac{vw}{r} + S^v$$

$$\frac{Dw}{Dt} + c_{pd}\Theta\frac{\partial\Pi}{\partial r} + \frac{\partial\Phi}{\partial r} = -\frac{u^2+v^2}{r} + 2\Omega\cos\phi u + S^w$$

$$\frac{D}{Dt}(\rho r^2\cos\phi) + \rho r^2\cos\phi\left[\frac{\partial}{\partial\lambda}\left(\frac{u}{r\cos\phi}\right) + \frac{\partial}{\partial\phi}\left(\frac{v}{r}\right) + \frac{\partial w}{\partial r}\right] = 0$$

$$\frac{D\Theta}{Dt} = S^\Theta, \qquad \rho\Theta = \frac{p_{\textsf{ref}}}{R_d}\Pi^{(1-\kappa)/\kappa}, \qquad \boxed{\frac{D}{Dt} := \frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla}, \qquad \kappa = \frac{R_d}{c_{pd}}$$

Davies et al. 2005, Wood et al. 2014

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Finite differences in space

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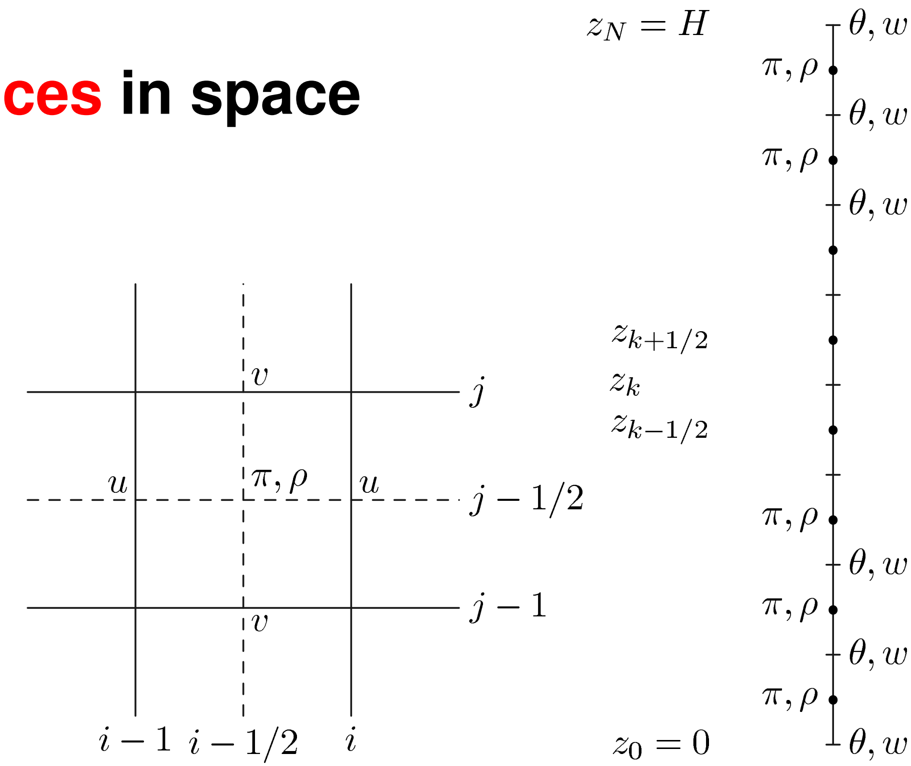

C-grid horizontal, Charney-Phillips vertical staggering

B. and Wood, 2016

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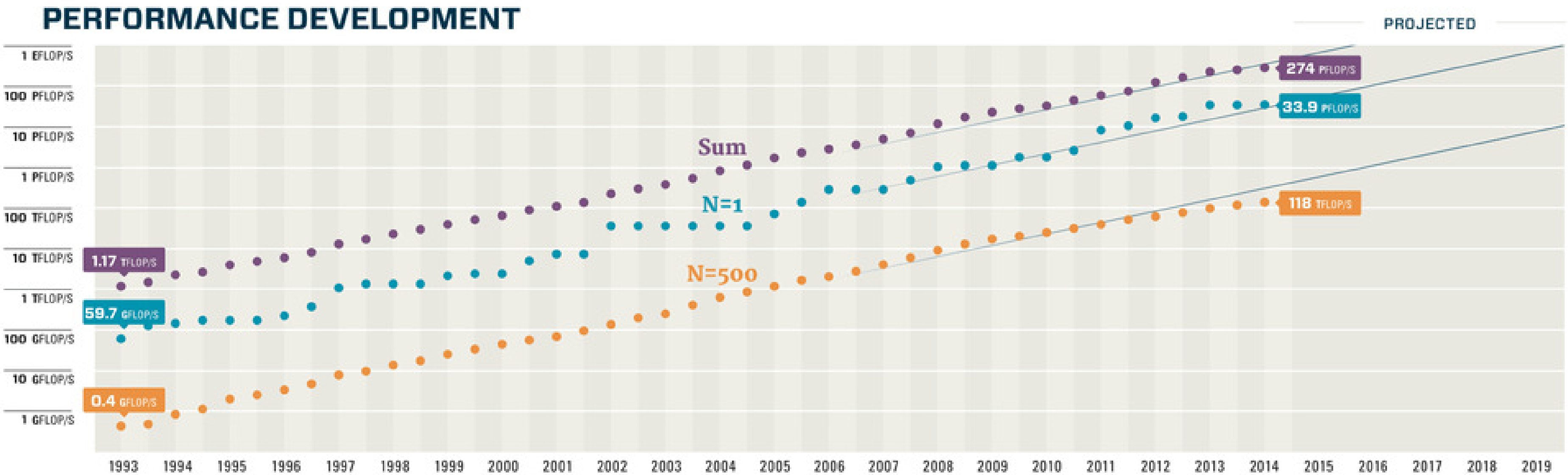
- **To be completed in one hour**
- **Efficient implementation needed!**

Dynamical core - Issues



The bottleneck - Scalability

More computing power $\Longrightarrow$ **shorter solution time**

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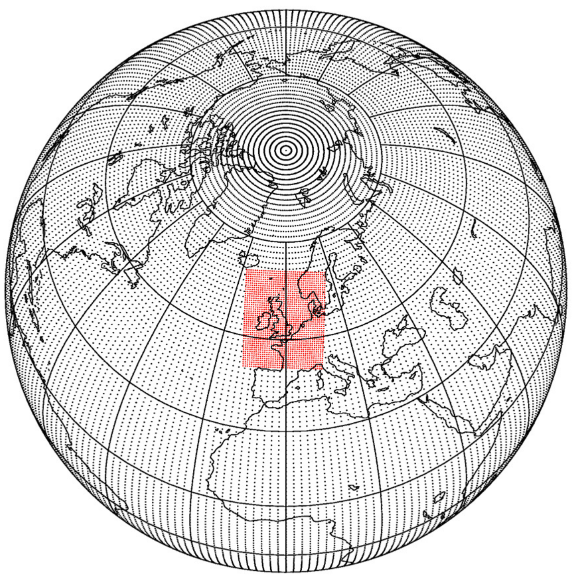
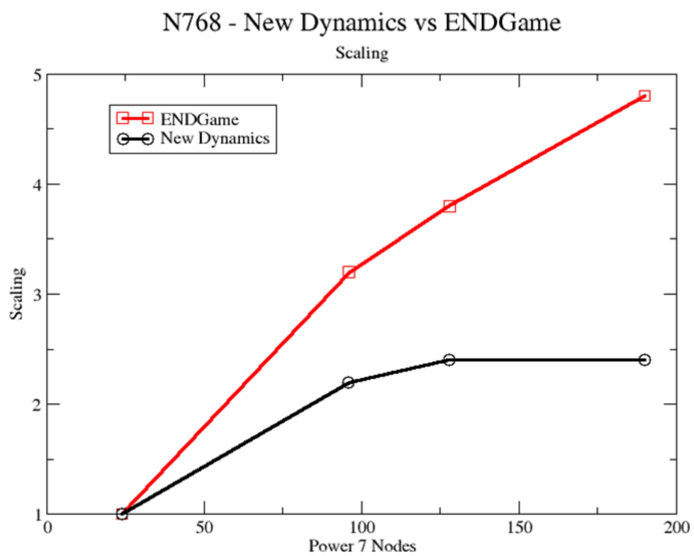
Lat-long grid:

$$\Delta x = 25 \text{ km} \Longrightarrow \Delta x_{min} = 70 \text{ m}$$

$$\Delta x = 1 \text{ km} \Longrightarrow \Delta x_{min} = 0.1 \text{ m}$$

E-W spacing vanishes at Poles $\Longrightarrow$ **grid locality lost**





A new dynamical core - GungHo

GungHo

工合

Globally

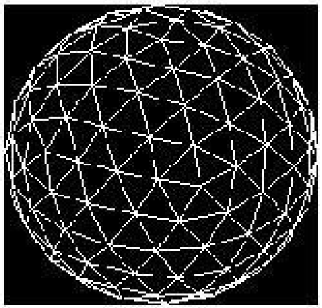
Uniform

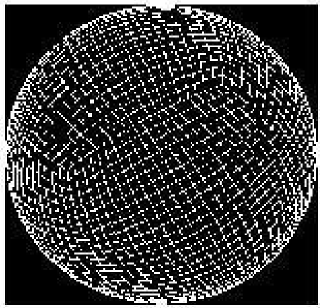
Next

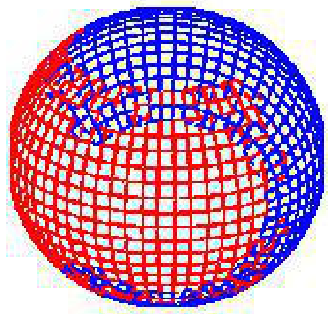
Generation

Highly

Optimized







Science & Technology Facilities Council

Parallel development at Met Office and Imperial College London

GungHo - aims

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- **Achieve sustainable scalability**

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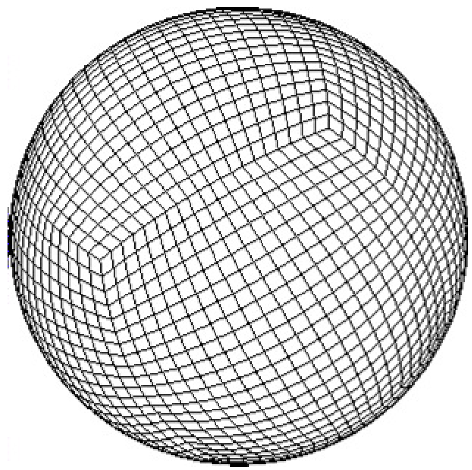
- **More homogeneous grid: cubed sphere**



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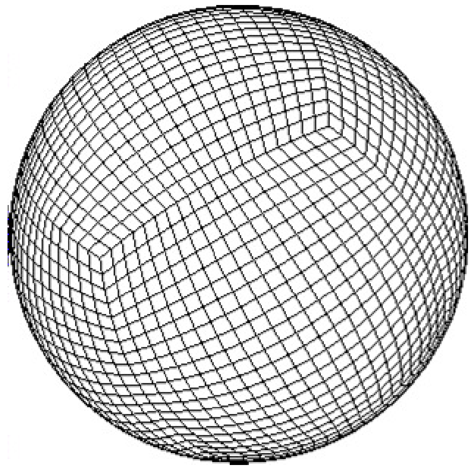

Step change → starting over

GungHo - infrastructure

- Joint scientific - software engineering work

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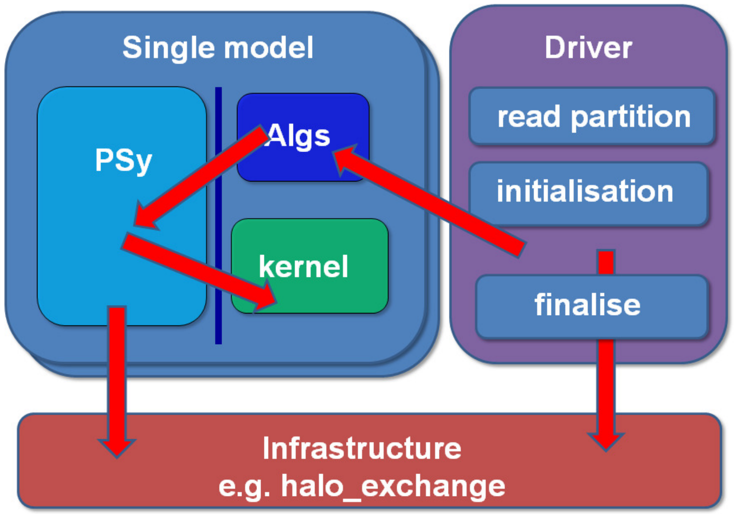
- Joint scientific - software engineering work
- Separation of concerns



- Fortran 2003 kernels + algorithm, Python parallelization engine + auto code generation

GungHo - infrastructure

- **Joint scientific - software engineering work**
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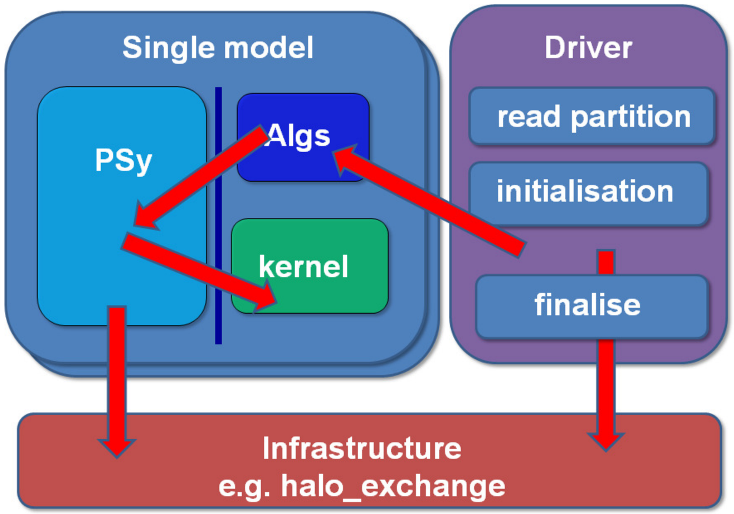

- **Fortran 2003 kernels + algorithm, Python parallelization engine + auto code generation**
- **Resilient to future technology**

GungHo - scientific requirements

- Mass conservation
- Accurate representation of balance and adjustment
- Absence of, or well controlled, computational modes
- Geopotential or pressure gradient should not produce unphysical vorticity
- Energy conserving pressure term and Coriolis term
- No spurious fast propagation of Rossby modes
- Conservation of axial angular momentum
- Accuracy at least approaching second order
- Minimal grid imprinting

Staniforth-Thuburn 2012

Mixed finite elements - Dynamo

Compatibility

Compatible numerical schemes preserve continuous properties at the discrete level, e.g.

$$\nabla \cdot (\nabla \times \mathbf{f}) = 0$$

$$\nabla \times \nabla g = 0$$

$$\nabla \cdot (\mathbf{f} g) = \mathbf{f} \cdot \nabla g + g \nabla \cdot \mathbf{f}$$

Vector-invariant form

On a domain Ω, solve:

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\boldsymbol{\xi}}{\rho} \times \mathbf{F} + 2\boldsymbol{\Omega} \times \mathbf{u} + \nabla \left(K + \Phi \right) + c_{pd}\theta \nabla \Pi = 0,$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{F} = 0,$$

$$\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta = 0,$$

$$\Pi^{\left(\frac{1-\kappa_d}{\kappa_d} \right)} = \frac{R_d}{p_0} \rho \theta$$

$$\mathbf{F} = \rho \mathbf{u}, \quad \boldsymbol{\xi} = \nabla \times \mathbf{u}, \quad K = \frac{1}{2} \mathbf{u} \cdot \mathbf{u}$$

Mixed finite elements

$$
\begin{array}{ccccccc}
\theta & & \xi & & \mathbf{u} & & \rho \\
\mathbb{W}_0 & \xrightarrow{\nabla} & \mathbb{W}_1 & \xrightarrow{\nabla\times} & \mathbb{W}_2 & \xrightarrow{\nabla .} & \mathbb{W}_3 \\
 & \underset{\tilde{\nabla} .}{\dashleftarrow} & & \underset{\tilde{\nabla}\times}{\dashleftarrow} & & \underset{\tilde{\nabla}}{\dashleftarrow} &
\end{array}
$$

Mixed finite elements

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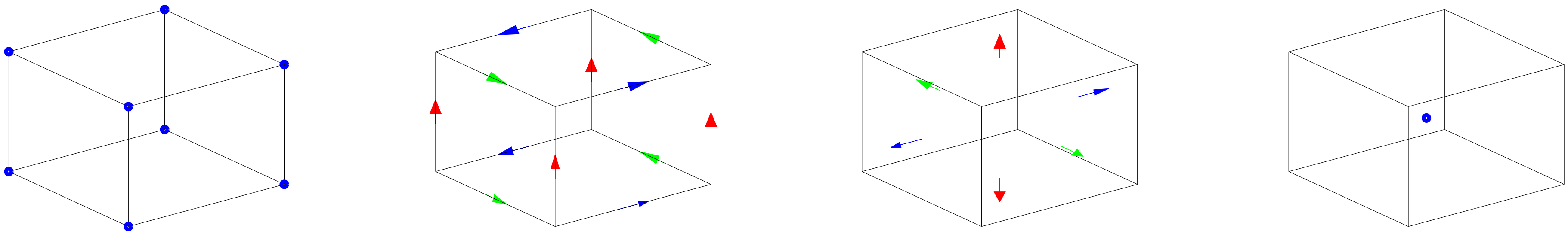
At lowest order:



Cotter and Shipton, 2012

Weak formulation

Find $(\theta,\ \mathbf{u},\ \rho) \in \mathbb{W}_0 \times \mathbb{W}_2 \times \mathbb{W}_3$ **such that**

$$\left\langle \mathbf{v}, \frac{\partial \mathbf{u}}{\partial t} \right\rangle = -\left\langle \mathbf{v}, \frac{\boldsymbol{\xi}}{\rho} \times \mathbf{F} + \nabla \Phi \right\rangle + \langle \nabla.\mathbf{v}, K \rangle + c_{pd} \langle \nabla.\left(\theta \mathbf{v}\right), \Pi \rangle - \langle \mathbf{v}, 2\boldsymbol{\Omega} \times \mathbf{u} \rangle ,$$

$$\left\langle \sigma, \frac{\partial \rho}{\partial t} \right\rangle = -\langle \sigma, \nabla.\mathbf{F} \rangle ,$$

$$\left\langle \gamma, \frac{\partial \theta}{\partial t} \right\rangle = -\langle \gamma, \mathbf{u} \cdot \nabla \theta \rangle$$

for all test functions $(\gamma,\ \mathbf{v},\ \sigma) \in \mathbb{W}_0 \times \mathbb{W}_2 \times \mathbb{W}_3$

Equations on reference domain

Equations on reference domain

Pulling back the equations through the map

$$\widehat{\Omega} \xrightarrow{\phi} \Omega$$

with Jacobian $J = d\phi$ (`div` and `curl`-conforming mapping):

$$\left\langle J\hat{\mathbf{v}}, \frac{J}{\det(J)}\frac{\partial \hat{\mathbf{u}}}{\partial t}\right\rangle = -\left\langle J\hat{\mathbf{v}}, \frac{J^{-T}\hat{\boldsymbol{\xi}}}{\hat{\rho}\det(J)} \times J\hat{\mathbf{F}}\right\rangle + \left\langle \nabla.\hat{\mathbf{v}}, \frac{1}{2}\left(\frac{J\hat{\mathbf{u}}}{\det(J)}\right).\left(\frac{J\hat{\mathbf{u}}}{\det(J)}\right)\right\rangle$$
$$- \langle \hat{\mathbf{v}}, \nabla\Phi\rangle - \left\langle \frac{J\hat{\mathbf{v}}}{\det(J)}, 2\boldsymbol{\Omega} \times (J\hat{\mathbf{u}})\right\rangle + c_{pd}\left\langle \hat{\theta}\nabla.\hat{\mathbf{v}} + \hat{\mathbf{v}}.\nabla\hat{\theta}, \Pi\right\rangle,$$
$$\left\langle \hat{\sigma}, \frac{\partial\hat{\rho}}{\partial t}\det(J)\right\rangle = -\left\langle \hat{\sigma}, \nabla.\hat{\mathbf{F}}\right\rangle,$$
$$\left\langle \hat{\gamma}, \frac{\partial\hat{\theta}}{\partial t}\det(J)\right\rangle = -\left\langle \hat{\gamma}, \hat{\mathbf{u}}.\nabla\hat{\theta}\right\rangle.$$

Discrete formulation

Expansion as a weighted sum of basis functions

$$\hat{\psi} = \sum_i \tilde{\psi}_i b_i$$

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Expansion as a weighted sum of basis functions

$$\hat{\psi} = \sum_i \tilde{\psi}_i b_i$$

$$M_2 \frac{d\tilde{u}}{dt} = RHS_u$$

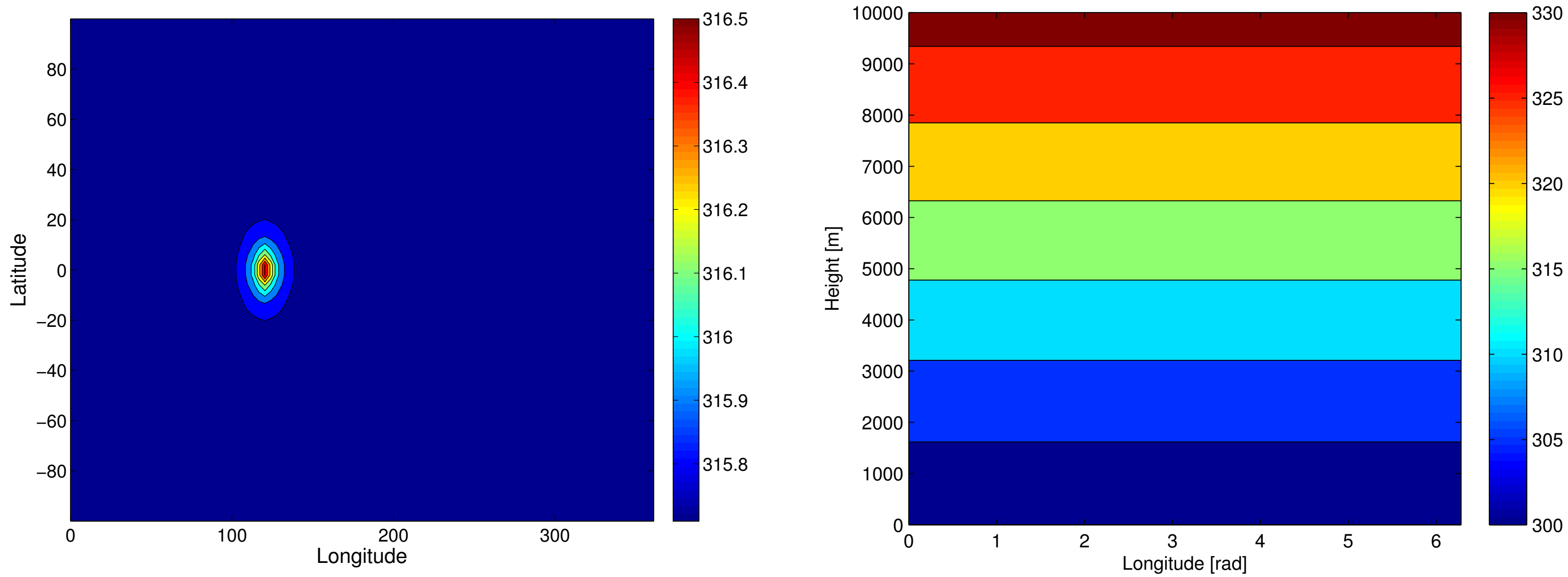
$$M_3 \frac{d\tilde{\rho}}{dt} = RHS_\rho$$

$$M_0 \frac{d\tilde{\theta}}{dt} = RHS_\theta$$

$$M_0 = \langle \hat{\gamma}, \hat{\gamma} \det(J) \rangle \,, \; M_2 = \left\langle \frac{J\hat{\mathbf{v}}}{\det(J)}, J\hat{\mathbf{v}} \right\rangle , \; M_3 = \langle \hat{\sigma}, \hat{\sigma} \det(J) \rangle$$

Results

Results - 3D Gravity Wave with rotation



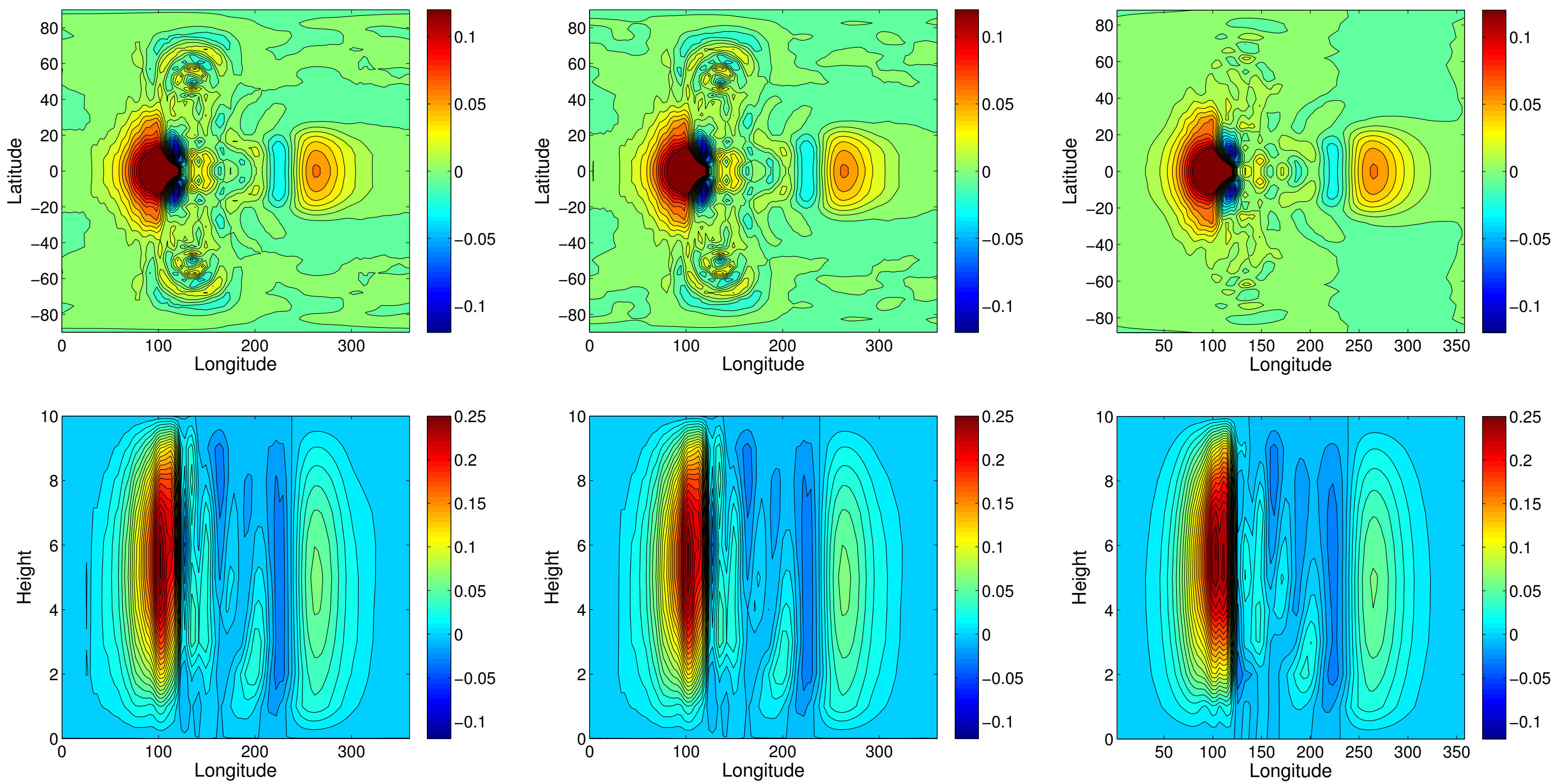
Thermal perturbation on a stably stratified, $10-$ km deep atmosphere at rest on a by $X = 125$ factor reduced planet

Serial runs with auto-generated code, $T = 3600$ s

Lowest-order elements

Ullrich et al. 2012

Results - 3D Gravity Wave with rotation



$\Delta t = 10\,$**s** $\Delta t = 1\,$**s** **REF**

T. Melvin

Results - Straka

Density current on neutrally stratified atmosphere (constant background θ).

$$T' = \begin{cases} -15\,\mathrm{K}\left[\frac{1}{2}(1+\cos(\frac{\pi}{2}r))\right] & (r \leq 1) \\ 0 & \textbf{otherwise} \end{cases}$$

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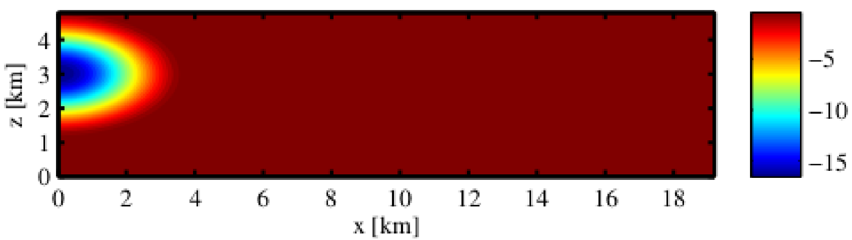

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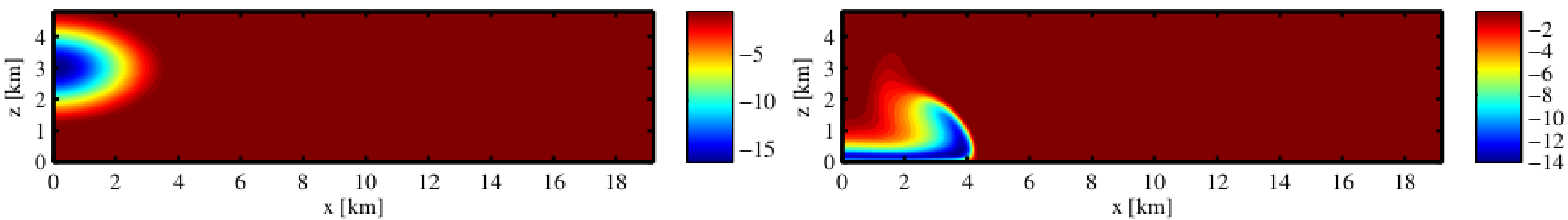

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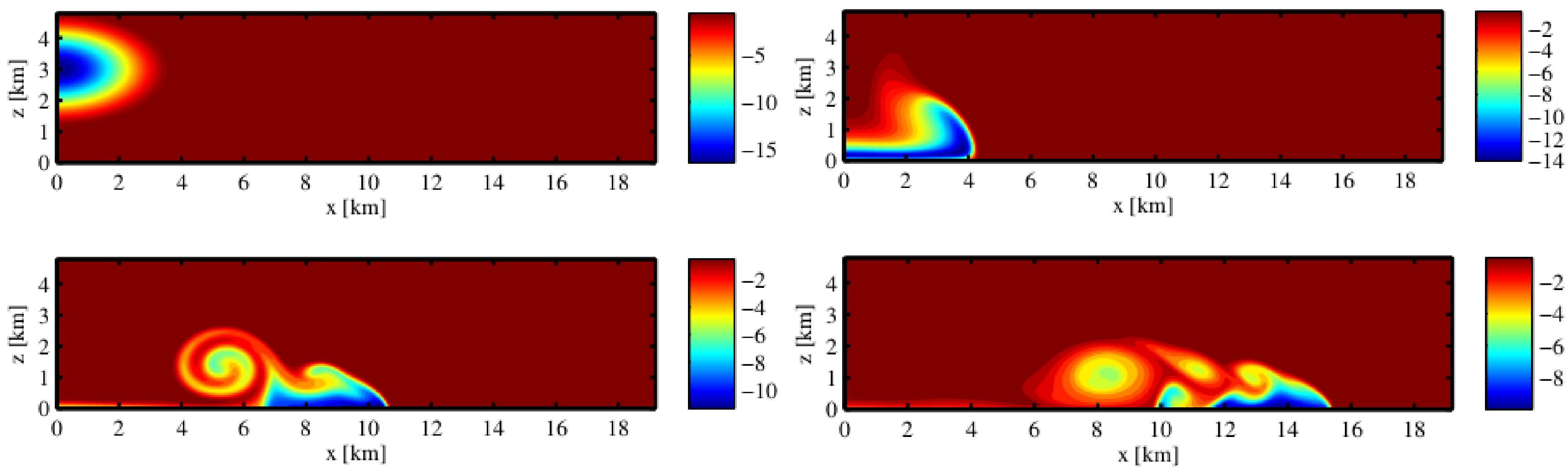

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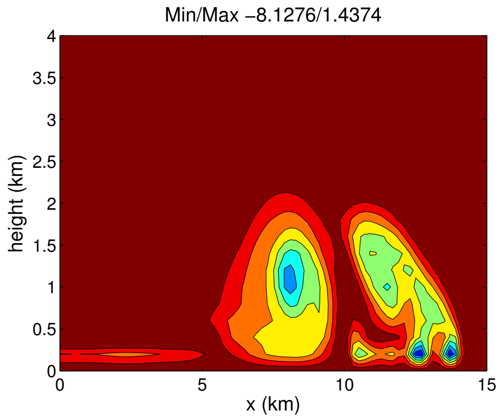

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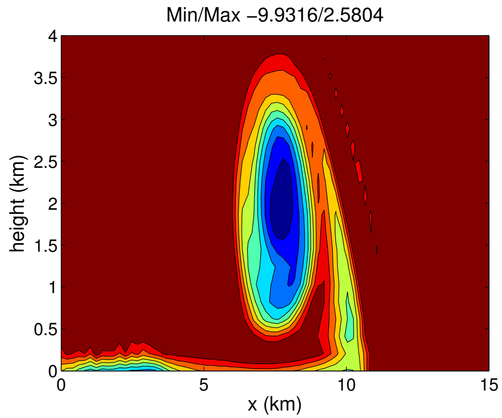
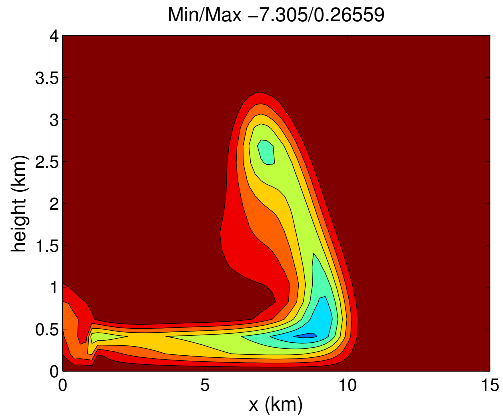


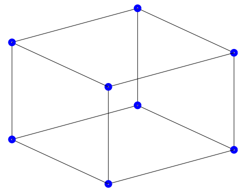
SUPG

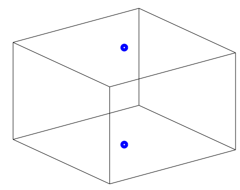


SL

In progress - $\mathbb{W}_\theta$

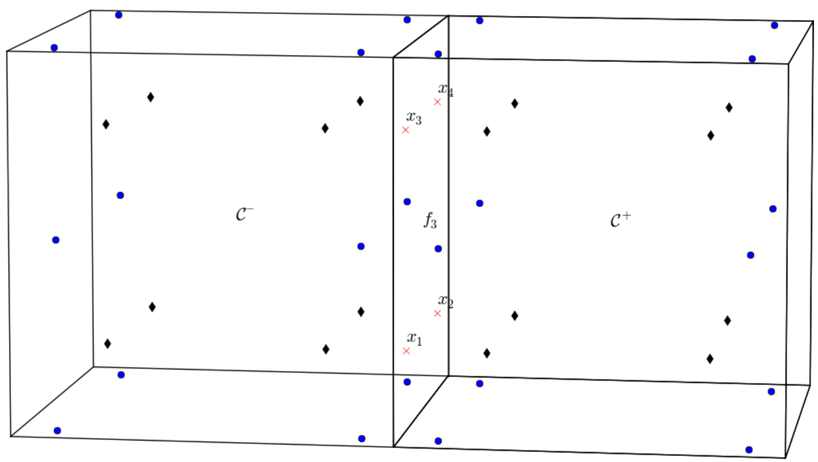
- **Moving** $\theta \in \mathbb{W}_0 \longrightarrow \mathbb{W}_\theta$





- **Quadrature formulae on faces for boundary terms:**

$$-\langle \mathbf{v},\, c_p\theta\nabla\Pi\rangle = -c_p\langle\!\langle \theta\mathbf{v}\cdot\mathbf{n},\, \Pi\rangle\!\rangle + c_p\langle\theta\Pi, \nabla\cdot\mathbf{v}\rangle + c_p\langle\Pi\mathbf{v},\, \nabla\theta\rangle$$



In progress

- **Improve semi-implicit performance**
- **Semi-Lagrangian scheme for θ advection**
- **Finite-volume like scheme for density**
- **Helmholtz problem formulation, preconditioner, multigrid solver**
- **High-order elements**

Parallel performance

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With great computing power comes great responsibility

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- **Cray XC40, complete in 2017**
- $\approx$ **500K cores, 16 PFlops, 1.2 EB (10^{18}) storage**

First runs on Cray XC40

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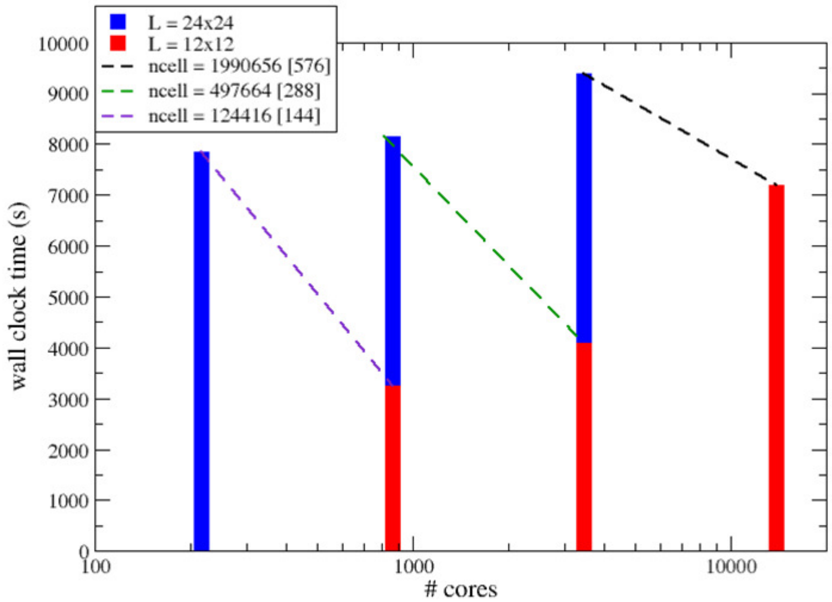
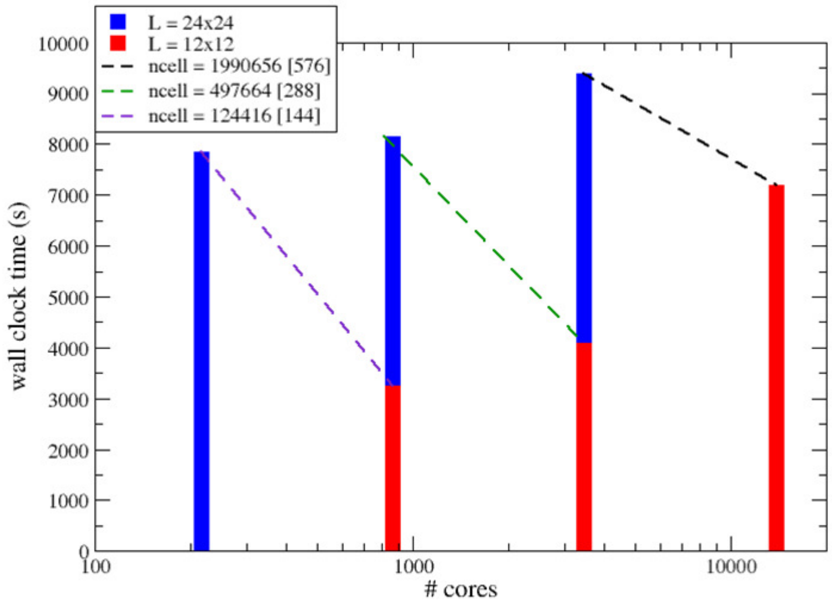
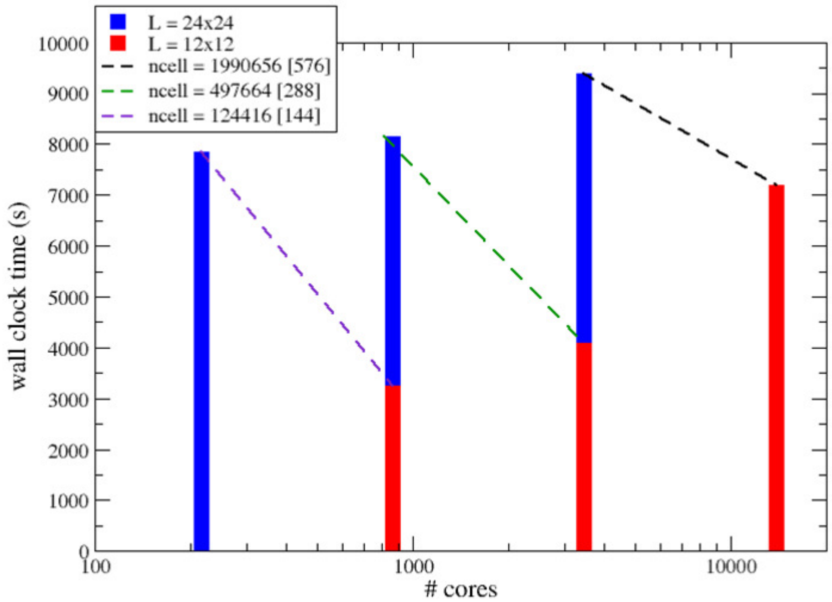


First runs on Cray XC40



- **Auto-generated parallel layer.**
- **No computational opt.**
- **Weak scaling: same amount of work per processor, perfect: straight line.**
- **Strong scaling (dashed): same global size, perfect: 4x speed-up.**

First runs on Cray XC40



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Dynamo 1.0 code release, 31.3.16

C. Maynard

Wrap-up

- Pole problem affects parallel performance of current operational dynamical core
- Mixed finite element discretization gives
  - Flexibility on order, grid
  - Mimetic properties
- Separation of concerns $\Longrightarrow$ Code adaptable to future architectures

Questions?

References

- Benacchio, T & Wood, N 2016. CAIM, in press.
- Cotter, C & Shipton, J 2012. JCP 231, 7076-7091.
- Davies T, Cullen M, Malcolm A, Mawson M, Staniforth A, White A, Wood N. 2005. QJRMS. 131, 1759–1782.
- Ullrich PA, Jablonowski C, Kent J, Lauritzen PH, Nair RD, and Taylor MA. 2012: Dynamical Core Model Intercom- parison Project (DCMIP) test case document. DCMIP Summer School, 83 pp. [Available online at http://earthsystemcog.org/ projects/dcmip-2012/.]
- Wood N, Staniforth A, White A, Allen T, Diamantakis M, Gross M, Melvin T, Smith C, Vosper S, Zerroukat M, Thuburn J. 2014. QJRMS 140, 1505–1520.

Bonus slides

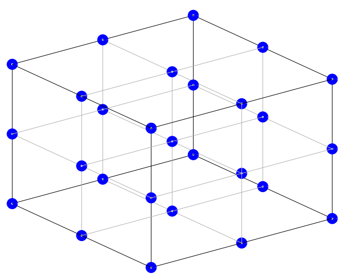
$\mathbb{W}_0$, The space of scalar functions built from the tensor product of $P^{k+1}(\chi_1)P^{k+1}(\chi_2)P^{k+1}(\chi_3)$ polynomials with full continuity;

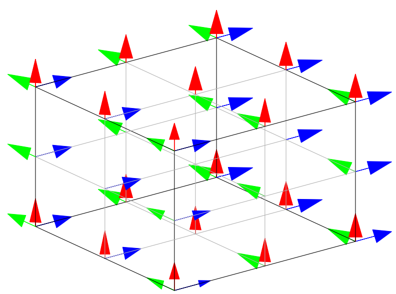
$\mathbb{W}_1$, The space of vector functions built from the tensor product of two P^{k+1} polynomials and one P^k polynomial with continuity in the tangential direction only;

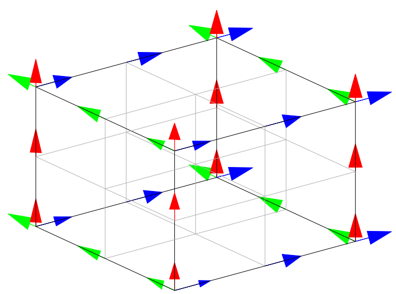
$\mathbb{W}_2$, The space of vector functions built from the tensor product of one P^{k+1} polynomial and two P^k polynomials with continuity in the normal direction only;

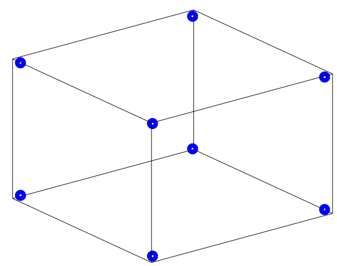
$\mathbb{W}_3$, The space of scalar functions built from the tensor product of $P^k(\chi_1)P^k(\chi_2)P^k(\chi_3)$ polynomials with no continuity.

$\mathbb{W}_\theta$, The space of scalar functions based on the vertical part of $\mathbb{W}_2$ to obtain the desired properties of a Charney-Philips grid.



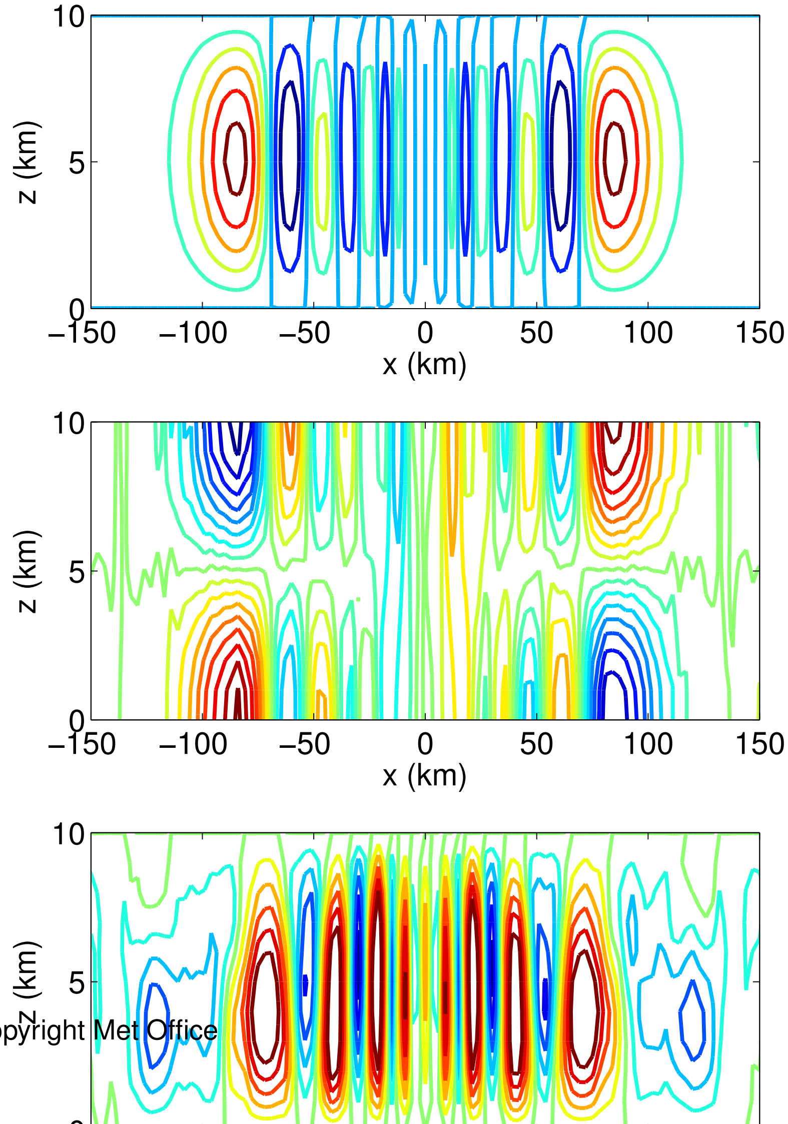






Results - 2d gravity wave

Skamarock and Klemp 1994,



Semi-implicit time discretization

$$R_{\mathbf{u}}^{n+1} + R_{\mathbf{u}}^{n} + R_{\mathbf{u}}^{adv} = 0$$

$$R_{\theta}^{n+1} + R_{\theta}^{n} + R_{\theta}^{adv} = 0$$

$$R_{\rho}^{n+1} + R_{\rho}^{n} + R_{\rho}^{adv} = 0$$

Semi-implicit time discretization

$$R_{\mathbf{u}}^{n+1} + R_{\mathbf{u}}^{n} + R_{\mathbf{u}}^{adv} = 0$$
$$R_{\theta}^{n+1} + R_{\theta}^{n} + R_{\theta}^{adv} = 0$$
$$R_{\rho}^{n+1} + R_{\rho}^{n} + R_{\rho}^{adv} = 0$$

$$R_{\mathbf{u}}^{n+1} = \left\langle \mathbf{v}, \mathbf{u}^{n+1} \right\rangle - \alpha \Delta t \left[- \left\langle \mathbf{v}, \nabla \Phi \right\rangle + \left\langle \nabla . \mathbf{v}, K^{n+1} \right\rangle + c_{pd} \left\langle \nabla . \left(\theta^{n+1} \mathbf{v} \right), \Pi^{n+1} \right\rangle - \left\langle \mathbf{v}, 2\boldsymbol{\Omega} \times \mathbf{u}^{n+1} \right\rangle \right]$$

$$R_{\mathbf{u}}^{n} = - \left\langle \mathbf{v}, \mathbf{u}^{n} \right\rangle - (1-\alpha) \Delta t \left[- \left\langle \mathbf{v}, \nabla \Phi \right\rangle + \left\langle \nabla . \mathbf{v}, K^{n} \right\rangle + c_{pd} \left\langle \nabla . \left(\theta^{n} \mathbf{v} \right), \Pi^{n} \right\rangle - \left\langle \mathbf{v}, 2\boldsymbol{\Omega} \times \mathbf{u}^{n} \right\rangle \right]$$

$$R_{\mathbf{u}}^{adv} = \Delta t \left\langle \mathbf{v}, \left(\frac{\boldsymbol{\xi}}{\rho} \right)^{n} \times \widetilde{\mathbf{F}} \right\rangle$$

Semi-implicit time discretization

Newton's method:

$$J\left(\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}\right) = -\mathbf{R}(\mathbf{x}^{(k)})$$

Semi-implicit time discretization

Newton's method:

$$J\left(\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}\right) = -\mathbf{R}(\mathbf{x}^{(k)})$$

Linearization around a reference state x^*:

$$J\left(\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}\right) \equiv J\mathbf{x}' \approx L\mathbf{x}'$$

$$L\mathbf{x}' = \begin{cases} \mathbf{u}' + \tau\Delta t c_{pd}\left(\theta^*\nabla\Pi' + \theta'\nabla\Pi^*\right) \\ \theta' + \tau\Delta t \mathbf{u}' \cdot \nabla\theta^* \\ \rho' + \tau\Delta t \nabla \cdot \left(\rho^* \mathbf{u}'\right) \end{cases}$$

Semi-implicit time discretization

Do $n = 1, n\_time$

Compute time-level n terms $\mathbf{R}\left(\mathbf{x}^n\right)$

Do $o = 1, n\_outer$

Compute advective wind $\overline{\mathbf{u}}$

Compute advective terms $\mathbf{R}^{adv}\left(\mathbf{x}^n, \overline{\mathbf{u}}\right)$

Do $i = 1, n\_inner$

Compute time-level $n+1$ **terms** $\mathbf{R}\left(\mathbf{x}^{n+1}\right)$

Solve for increment $\mathbf{x}'$

End inner loop

End outer loop

End timestep loop

Semi-implicit timestepping

- **Advective terms costly inside Newton loop, assumed fixed**
- **Recomputed in outer loop using latest $\mathbf{u}$ estimate**
- **Inside the Krylov solver the residual R is evaluated as $\mathbf{R} = \left[R_{\mathbf{u}}^{n+1},\, R_{\theta}^{*},\, R_{\rho}^{*}\right]^{T}$ where:**

$$R_{\theta}^{*} = \theta^{n+1} + \tau \Delta t \mathbf{u}^{n+1} . \nabla \theta^{n+1}$$

$$R_{\rho}^{*} = \rho^{n+1} + \tau \Delta t \nabla . \left(\rho^{n+1} \mathbf{u}^{n+1}\right)$$