Results and challenges with Dynamo, the Met Office's next generation dynamical core

S. Adams, M. Ashworth, T. Benacchio, R. Ford, M. Glover, M. Guidolin,
M. Hambley, M. Hobson, I. Kavcic, C.Maynard, T. Melvin, E. Mueller,
S. Mullerworth, A. Porter, S. Pring, M. Rezny, G. Riley, S. Sandbach, R. Sharp,
B. Shipway, K. Sivalingam, P. Slavin, J. Thuburn, R. Wong , N. Wood

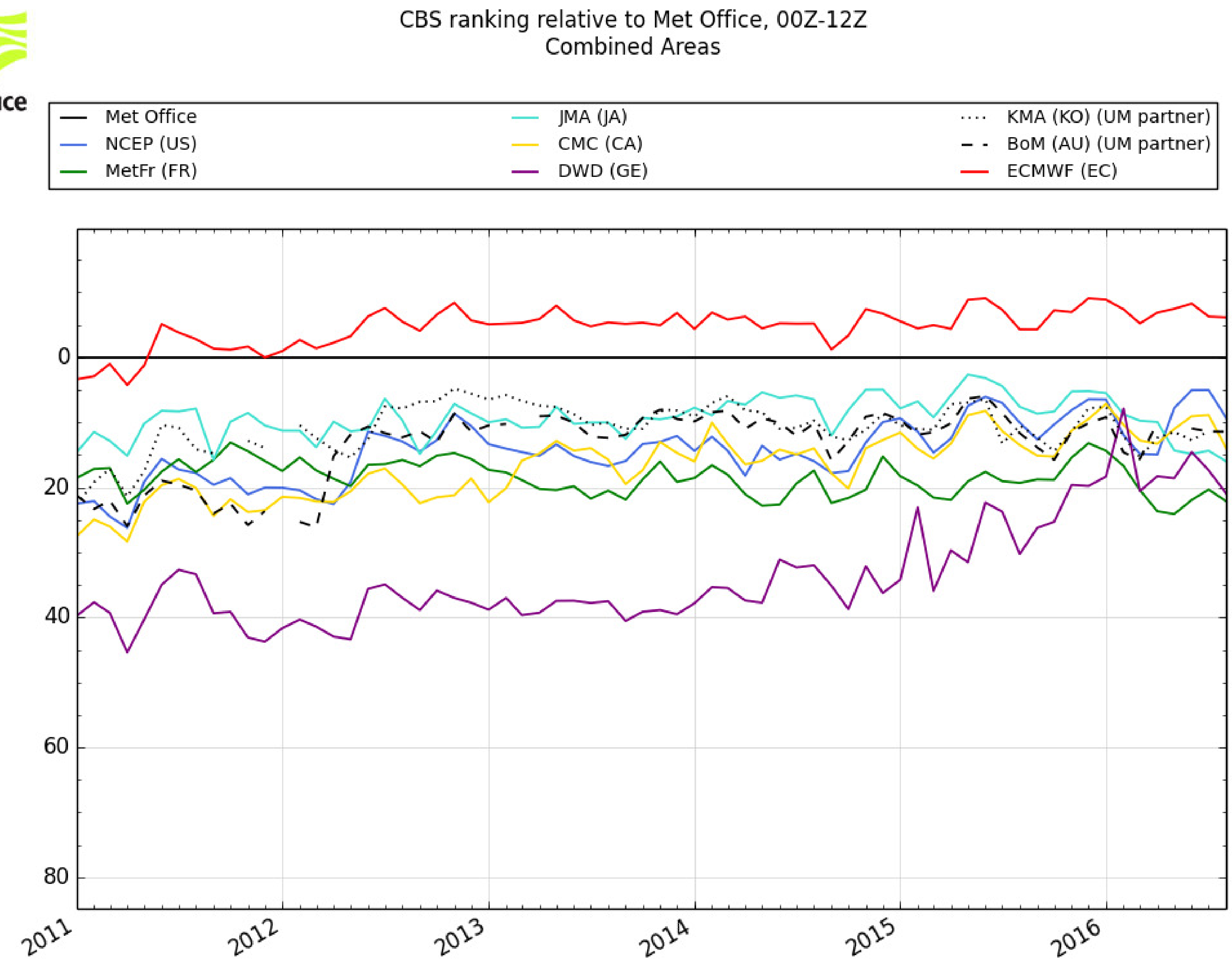
ECMWF, 3 October 2016

Plan

- ENDGame and scalability
- A new dynamical core - GungHo
- Mixed finite elements
- Results

The name of the game

Global NWP index



Met Office's Unified Model

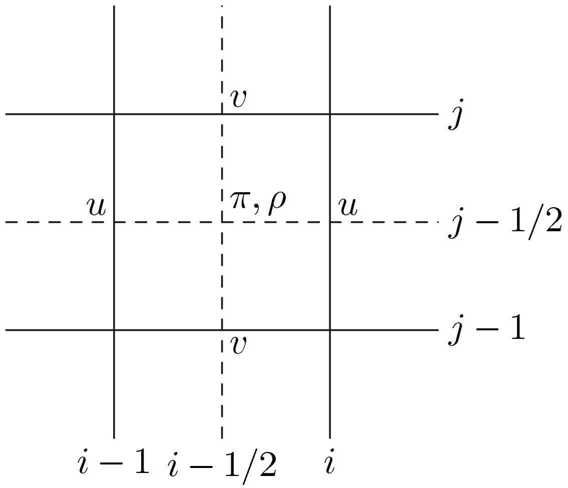
Single atmospheric model for

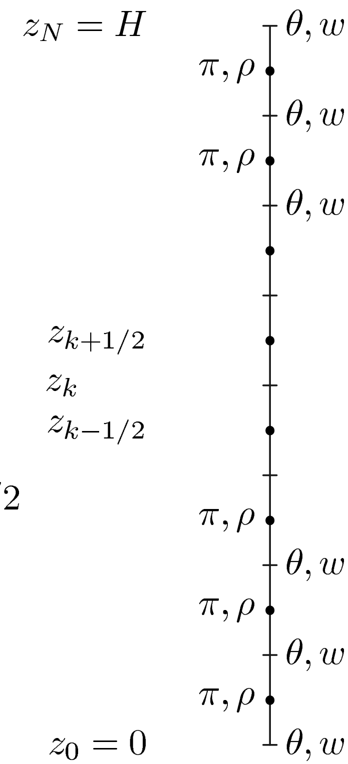
- **Global ($\Delta x \approx 17$ km) and mesoscale ($\Delta x \approx 4.4 - 1.5$ km) operational forecasts**
- **Climate predictions ($\Delta x \approx 120$ km, $T > 10$ yrs)**
- **Research mode ($\Delta x < 1$ km)**
- **26 years old**

ENDGame

Semi-implicit semi-Lagrangian **time integration, no** $\Delta t \leq \dfrac{\Delta x}{U}$

Finite differences **in space**





C-grid horizontal, Charney-Phillips vertical staggering

Wood et al. 2014, B. and Wood, 2016

Computational size

Global model at 17 km resolution

- $1536 \times 1152 \times 70 \approx 124M$ **points**
- $T = 7$ **days** 3 **hrs,** $\Delta t = 7$ **min** 30 **sec** $\Longrightarrow N_t = 1368$
- **To be completed in one hour**
- **Efficient implementation needed!**

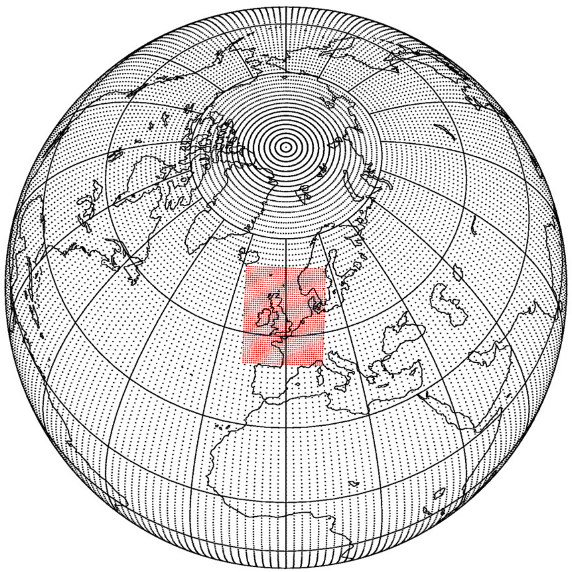
The bottleneck - Scalability

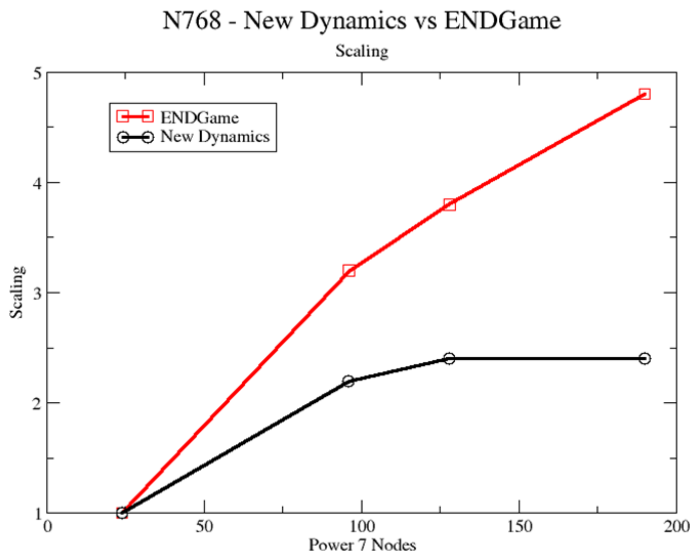
Lat-long grid:

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

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

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





HPC

nextplatform.com

New supercomputer

- **Cray XC40**, complete in Q1/2017
- **≈ 500K cores**, 16 PFlops, 1.2 EB storage

A new dynamical core - GungHo

GungHo

Globally

Uniform

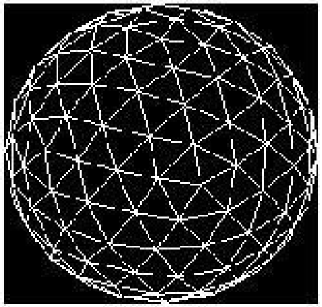
Next

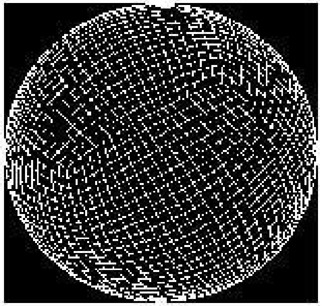
Generation

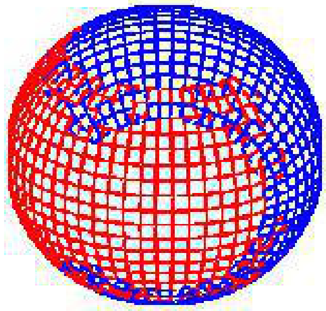
Highly

Optimized

工合







GungHo institutions

Met Office

U Exeter

Imperial College London

U Bath

U Reading

U Leeds

U Manchester

U Warwick

Hartree Centre

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

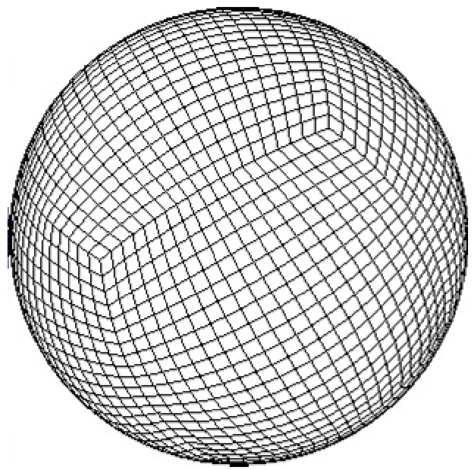
Staniforth-Thuburn 2012

GungHo - aims

- Achieve sustainable scalability

- Keep the good properties and maintain the same accuracy ($\approx$ 2nd order) of the current dynamical core

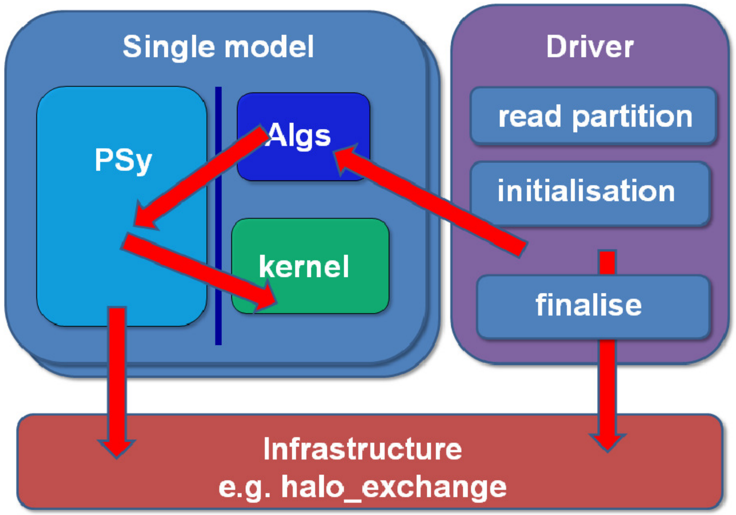
- More homogeneous grid: cubed sphere

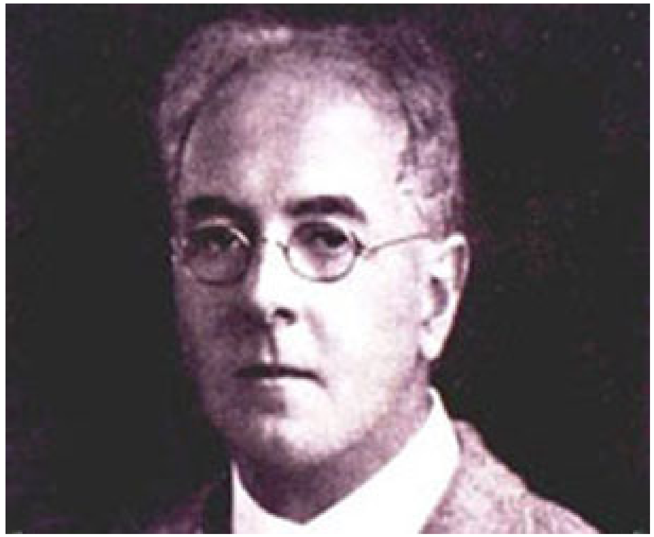


Step change, UM $\rightarrow$ LFRic

LFRic

- **Joint scientific - software engineering work**
- **Separation of concerns**





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

Mixed finite elements

Compatibility

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

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

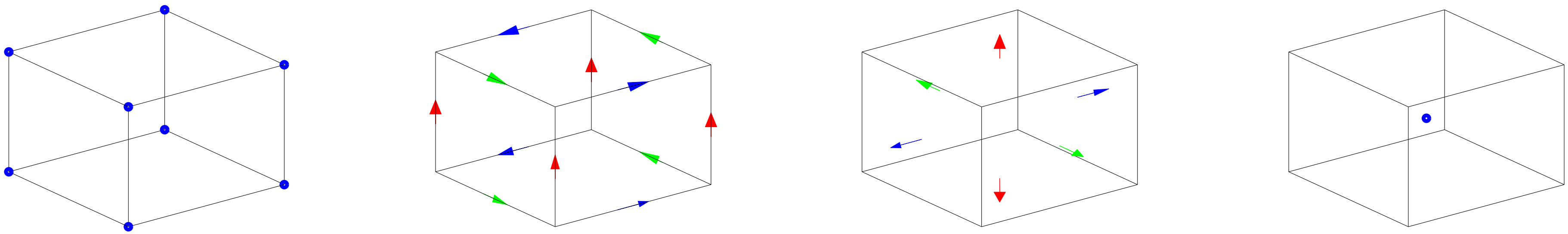
$$\nabla \times \nabla g = 0$$

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

Mixed finite elements

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

At lowest order:



Equivalent to C-grid, Charney-Phillips staggered grid

Cotter and Shipton, 2012

Vector-invariant form

On a domain Ω, solve:

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

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

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

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

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

Weak formulation

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

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

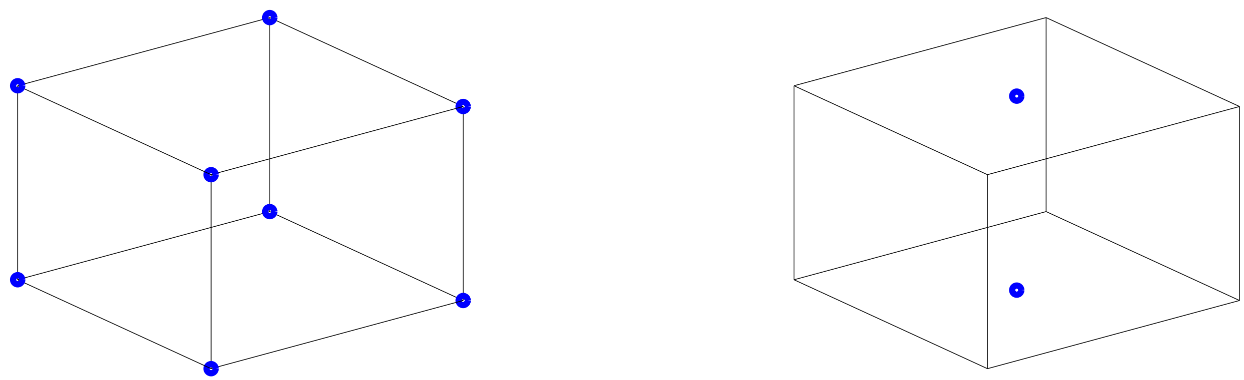
$$\left\langle \sigma, \frac{\partial \rho}{\partial t} \right\rangle = -\langle \sigma, \nabla.\mathbf{F} \rangle ,$$

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

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

Potential temperature space

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



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

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

$$\langle \mathbf{u}\cdot\nabla\theta, \gamma\rangle = \langle\!\langle\theta, \gamma\mathbf{u}\cdot\mathbf{n}\rangle\!\rangle - \langle\nabla\cdot(\gamma\mathbf{u}), \theta\rangle$$

Equations on reference domain

Pulling back the equations through the Piola transform

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

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

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

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

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

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

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

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 $\mathrm{R}\left(\mathbf{x}^n\right)$

Do $o = 1, n\_outer$

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

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

Do $i = 1, n\_inner$

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

Solve for increment $\mathbf{x}'$

End inner loop

End outer loop

End timestep loop

In progress - density advection

Conservative, flux-form

- Mass flux in $\mathbb{W}_2$ space, density in $\mathbb{W}_3$ space
- Piecewise parabolic method, flux = Δt-accumulated mass

Dimensionally split scheme for flux calculation

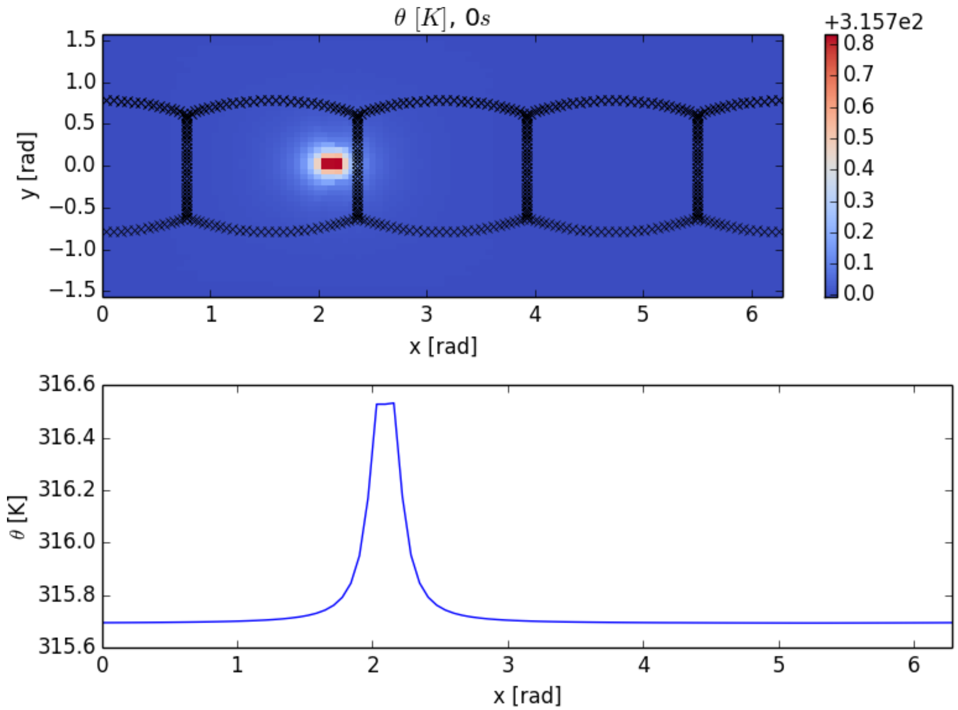
- 1D swept area approach
- No 2d calculations on complicated geometry
- PPM $\Longrightarrow$ use of $CFL > 1$

- Other options in code base: Method of Lines, FE advection.

Putnam and Lin, 2007

Results

Results - 3D Gravity Wave with rotation



Thermal perturbation over a stably stratified, 10-km deep atmosphere on reduced planet

Serial runs with auto-generated code, lowest-order elements

Ullrich et al. 2012

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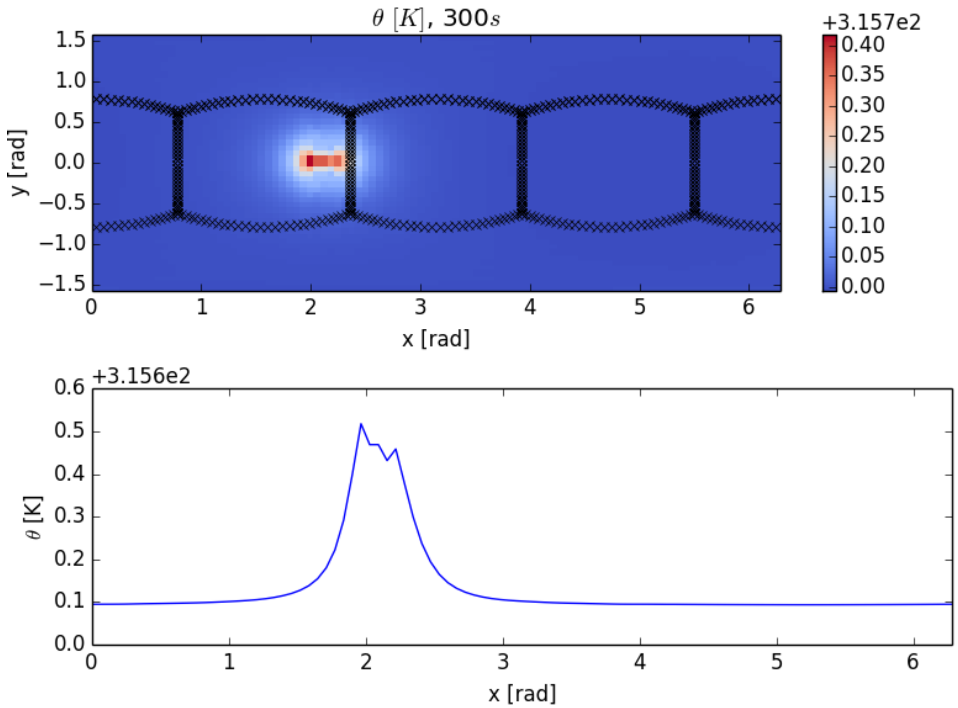

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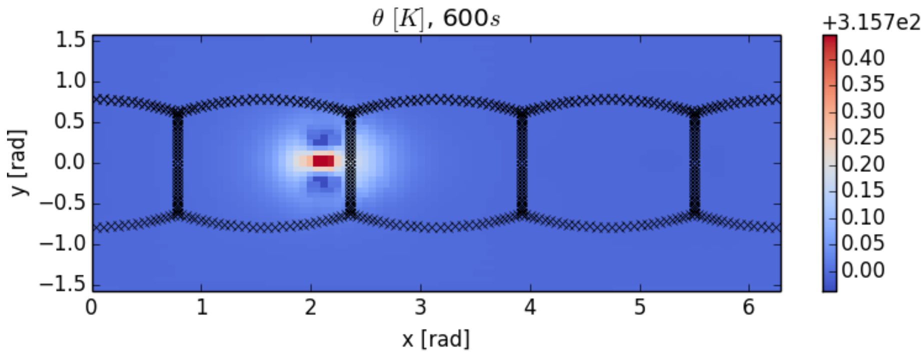

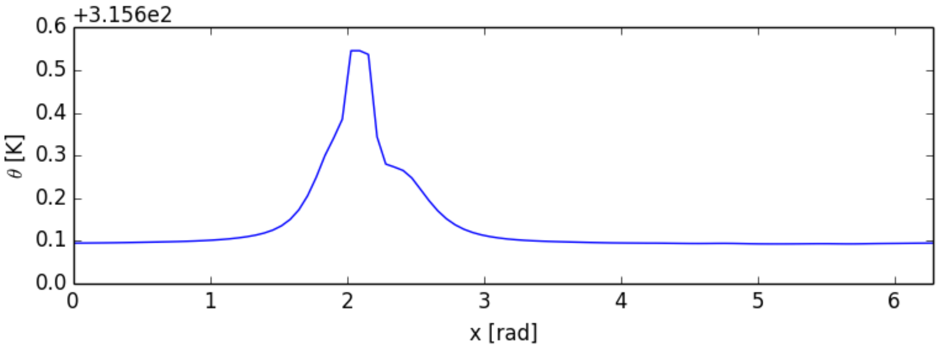

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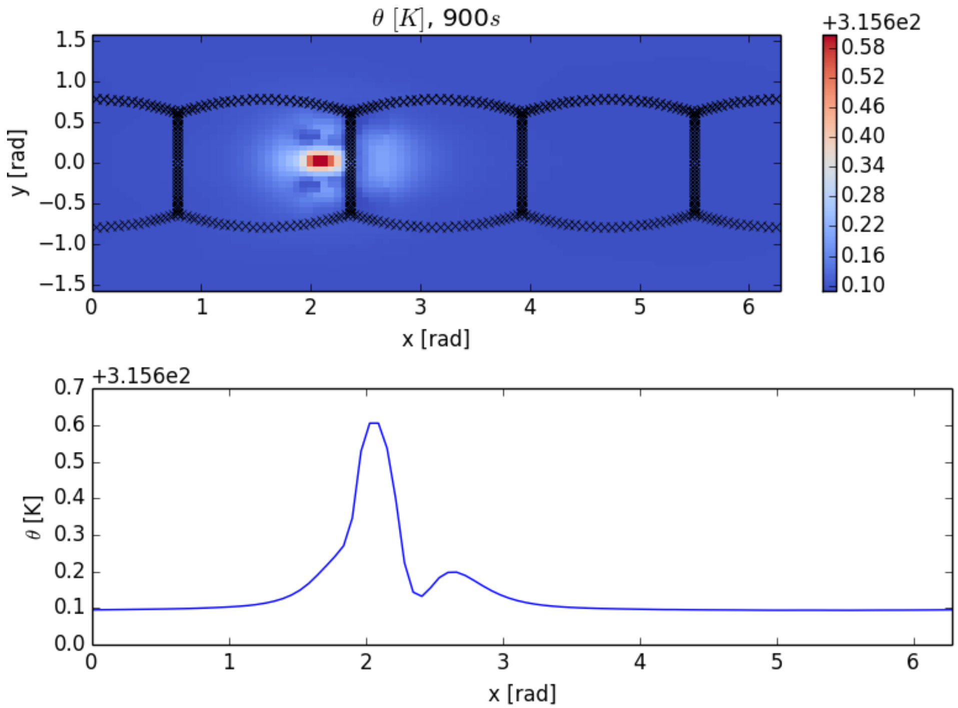

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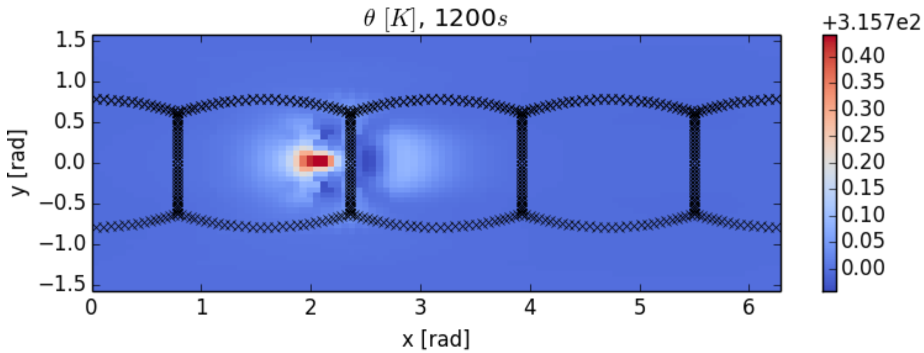

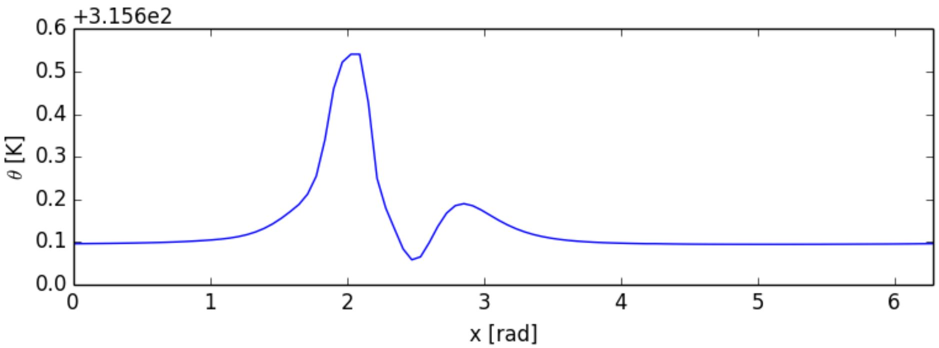

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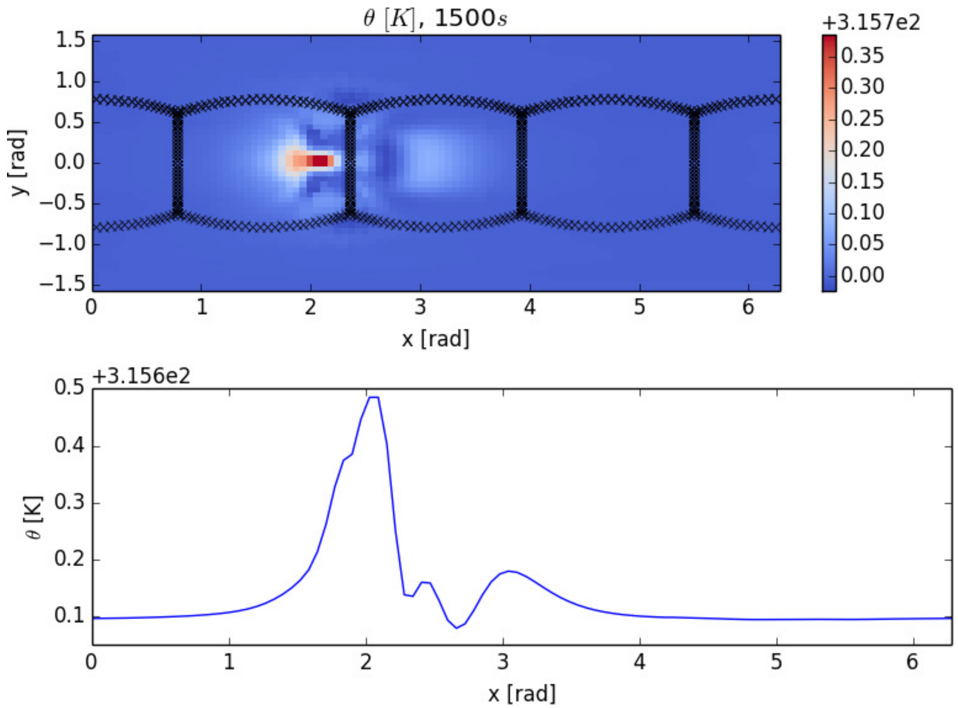

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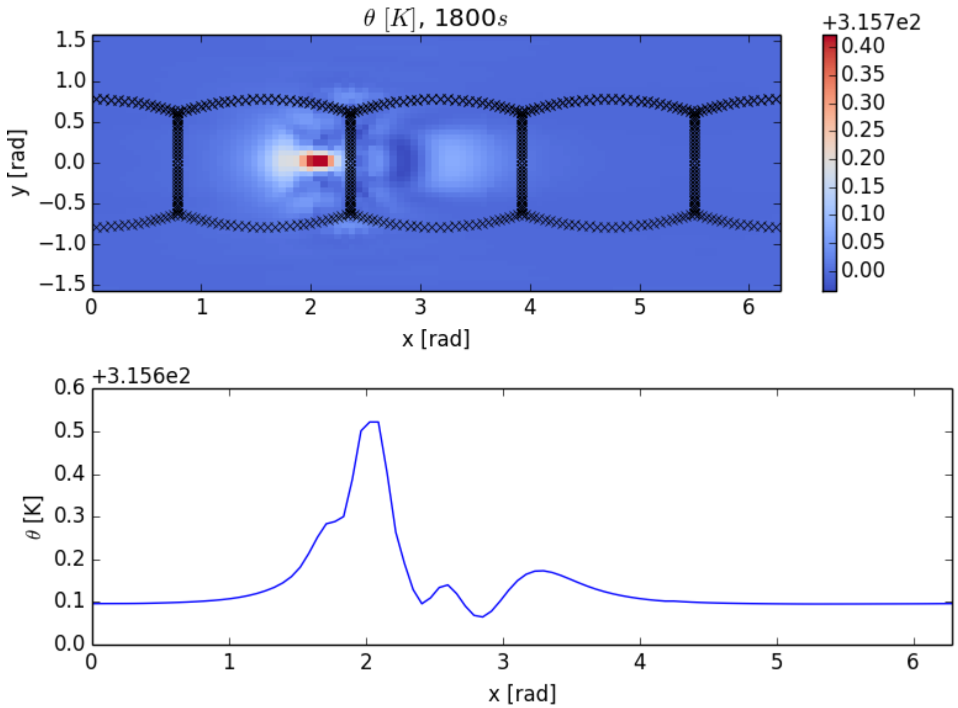

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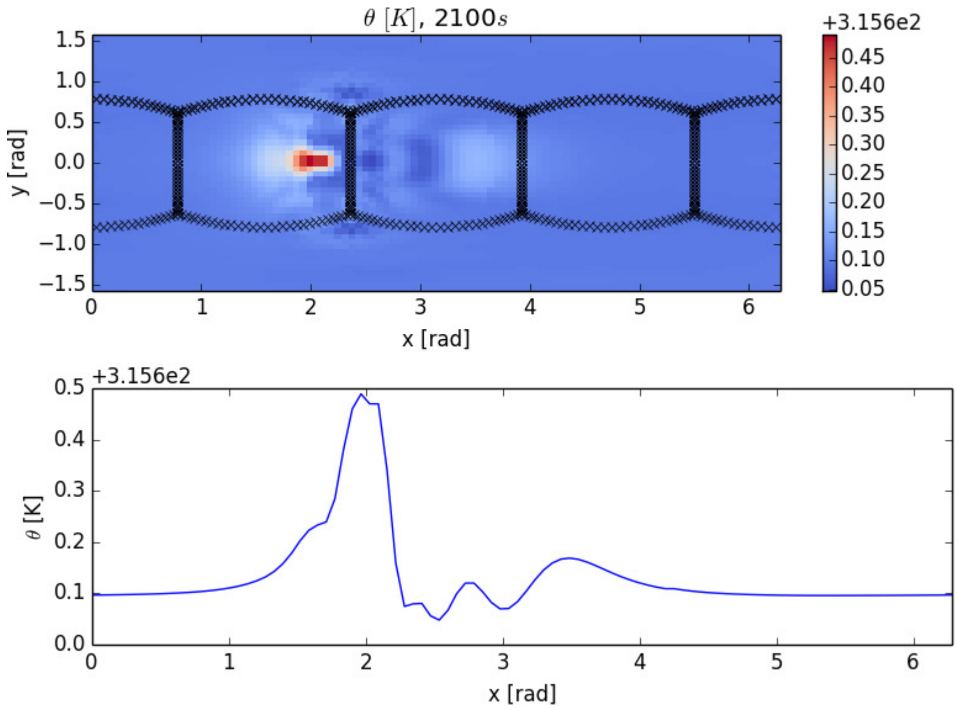

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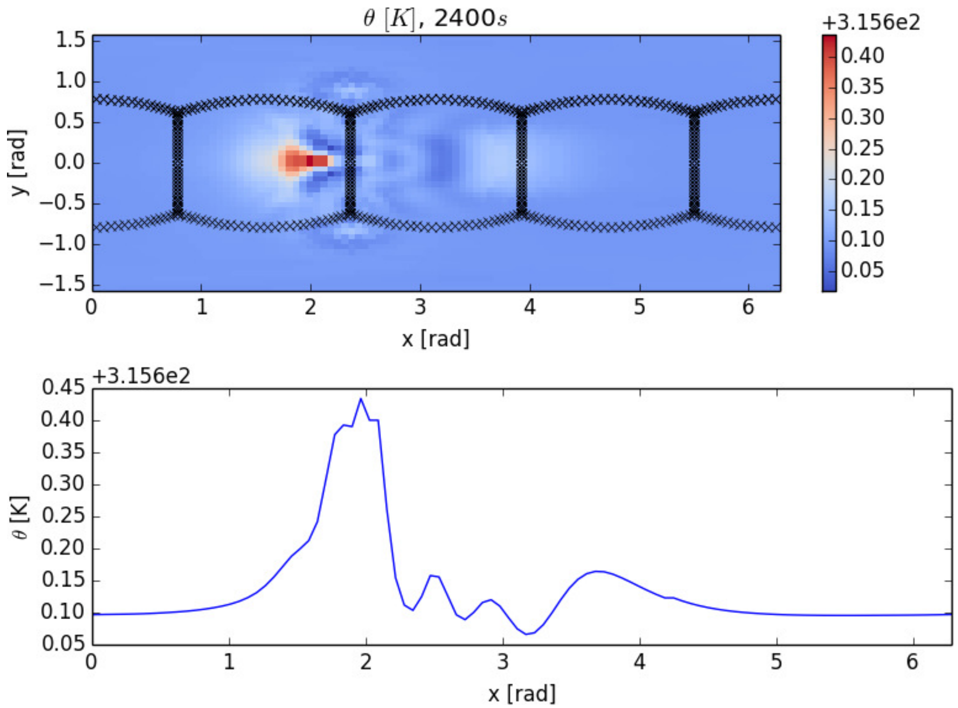

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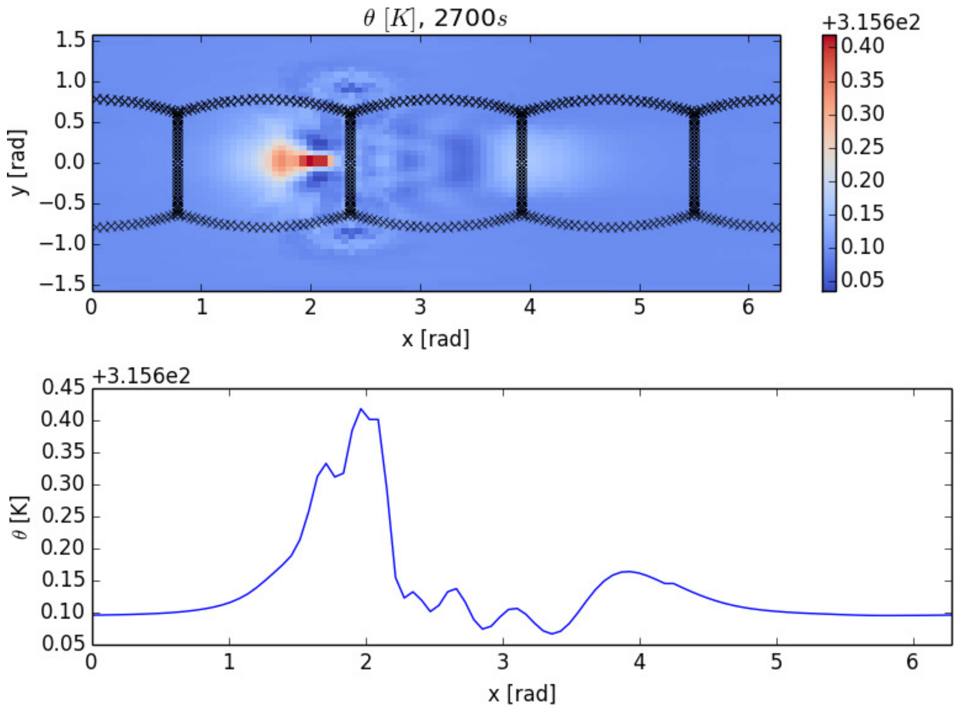

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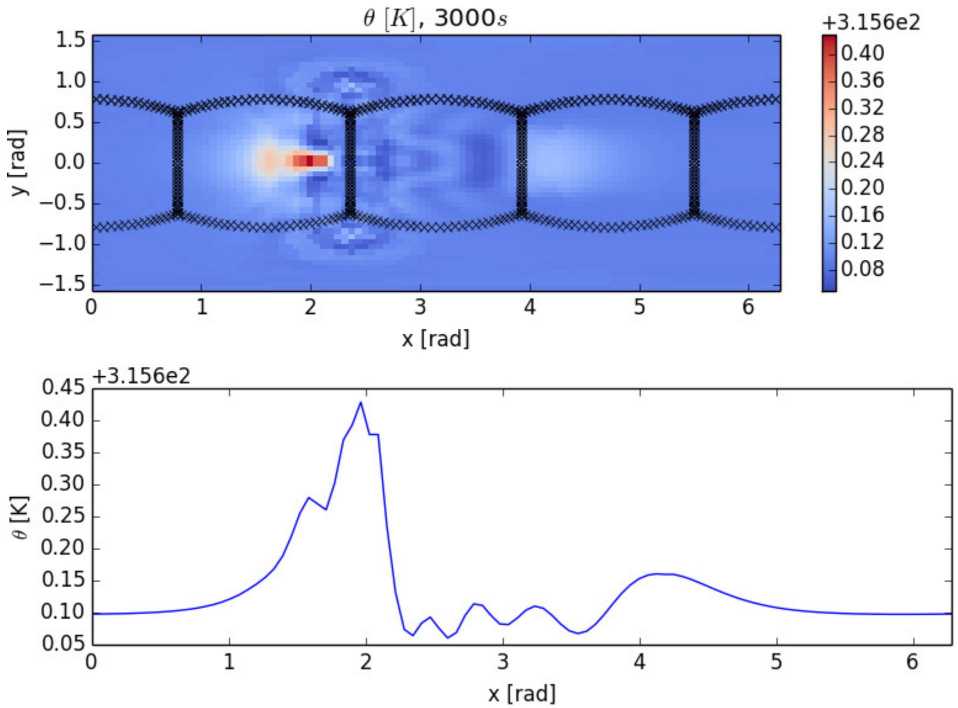

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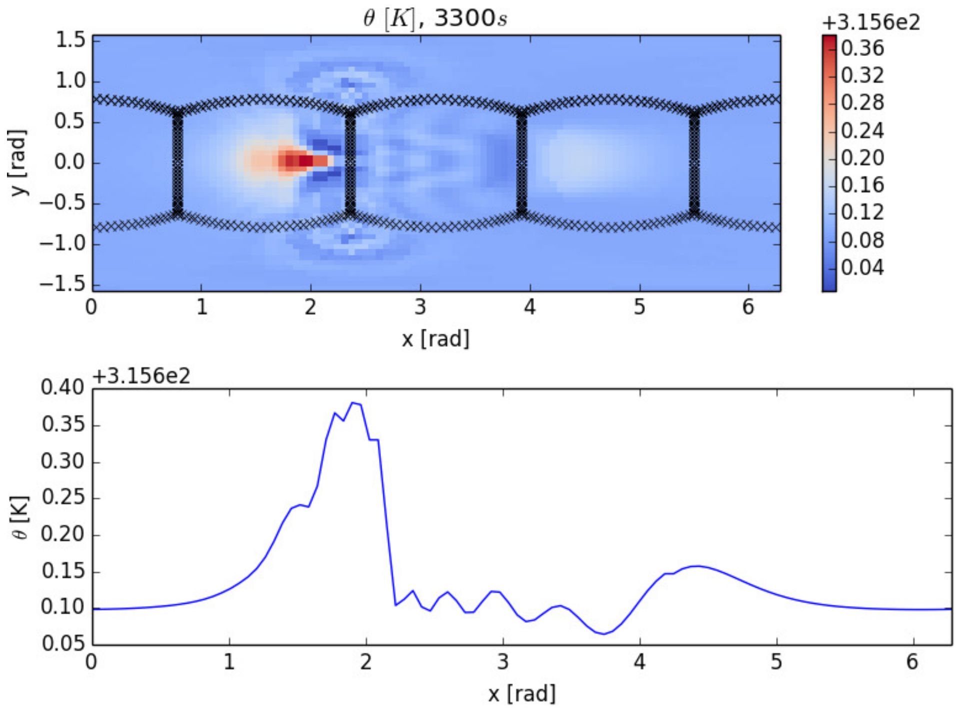

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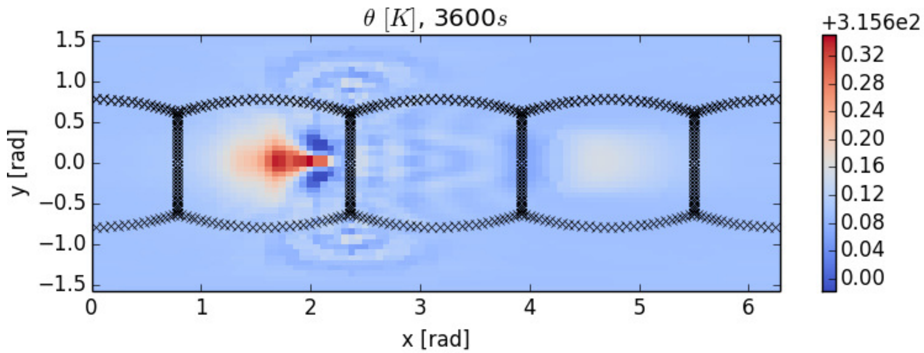

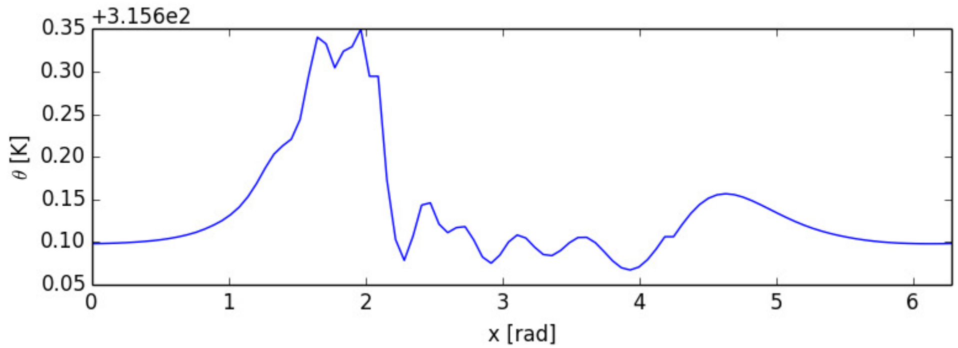

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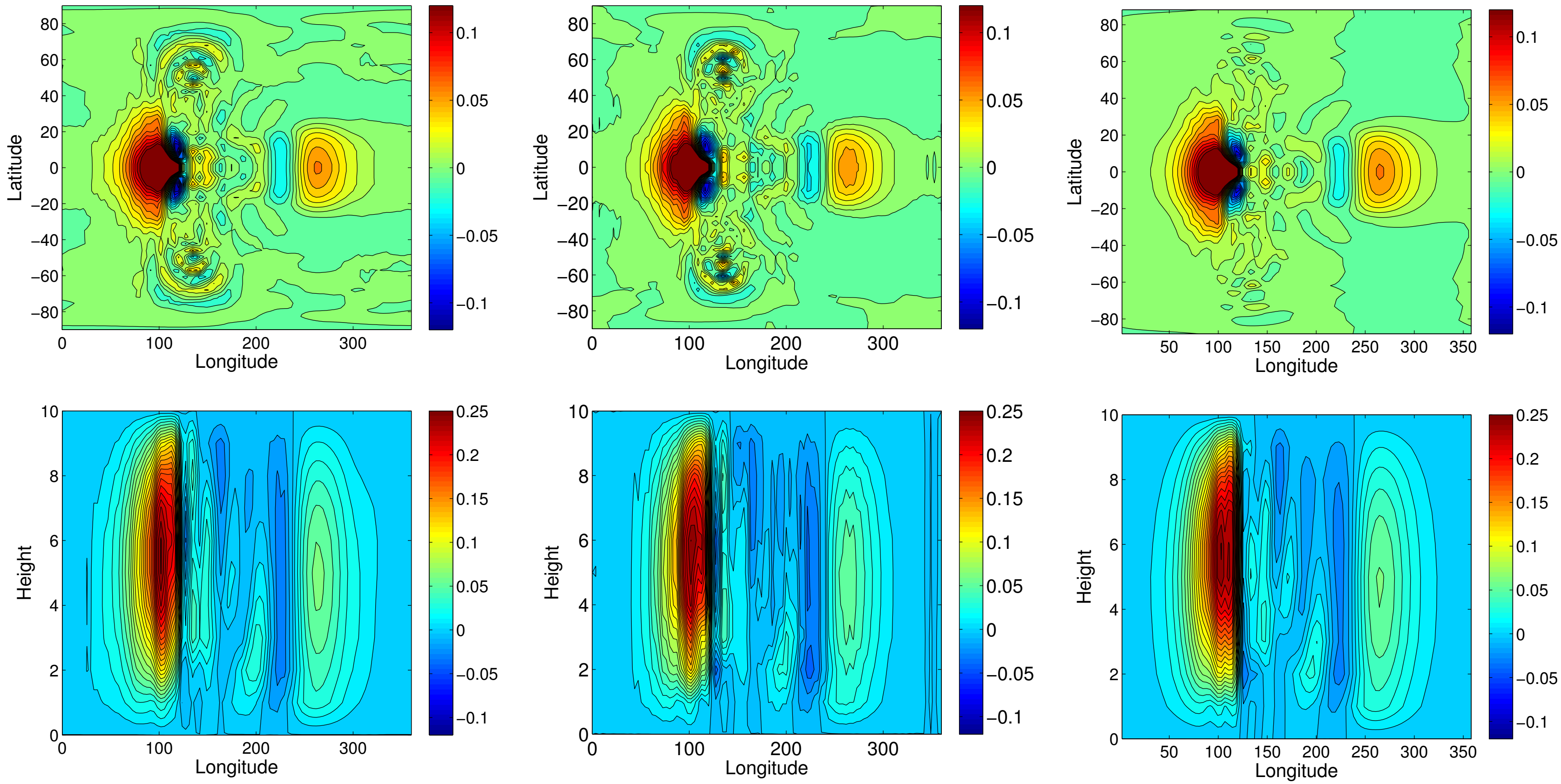


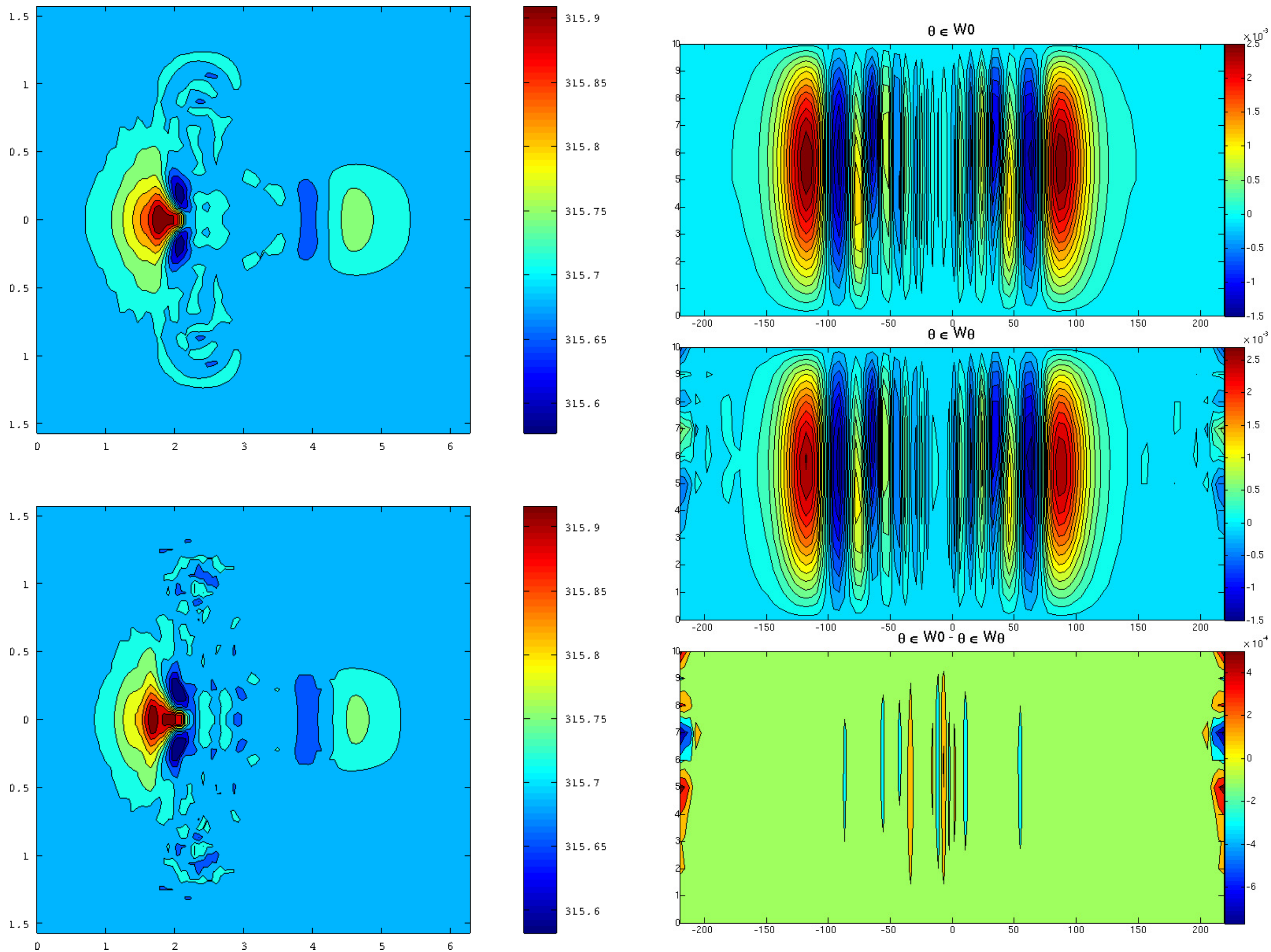
$\Delta t = 10$ **s**
RT0 (34560 ρ-dofs)

$\Delta t = 1$ **s**
RT1 (34560 ρ-dofs)

ENDGame
46080 cells

T. Melvin

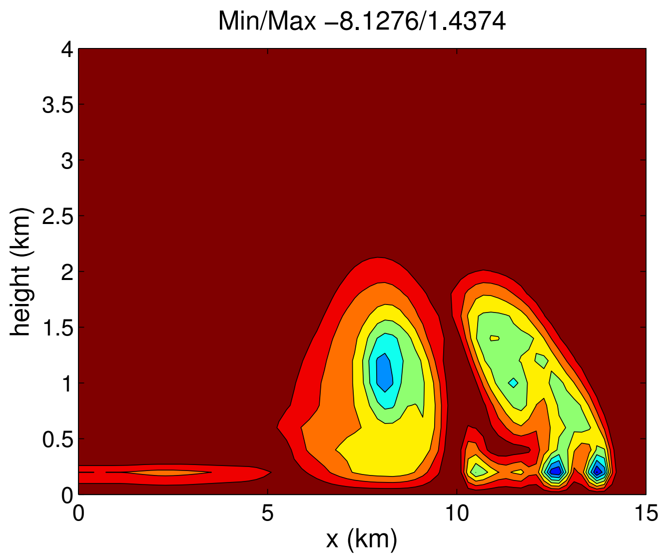
$\mathbb{W}_0$ vs. $\mathbb{W}_\theta$



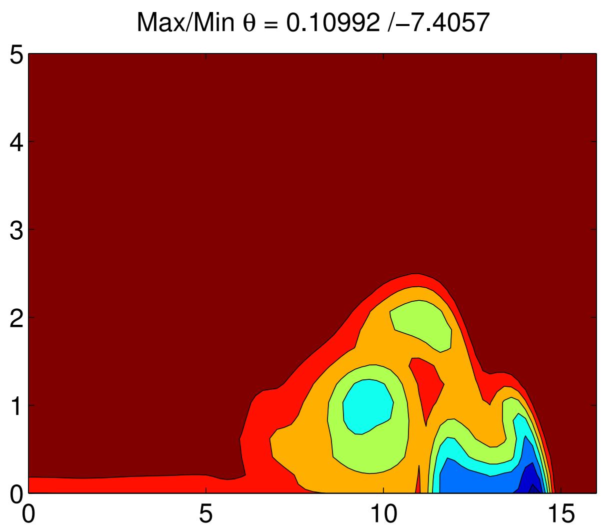
Results - Straka

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

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



ENDGame

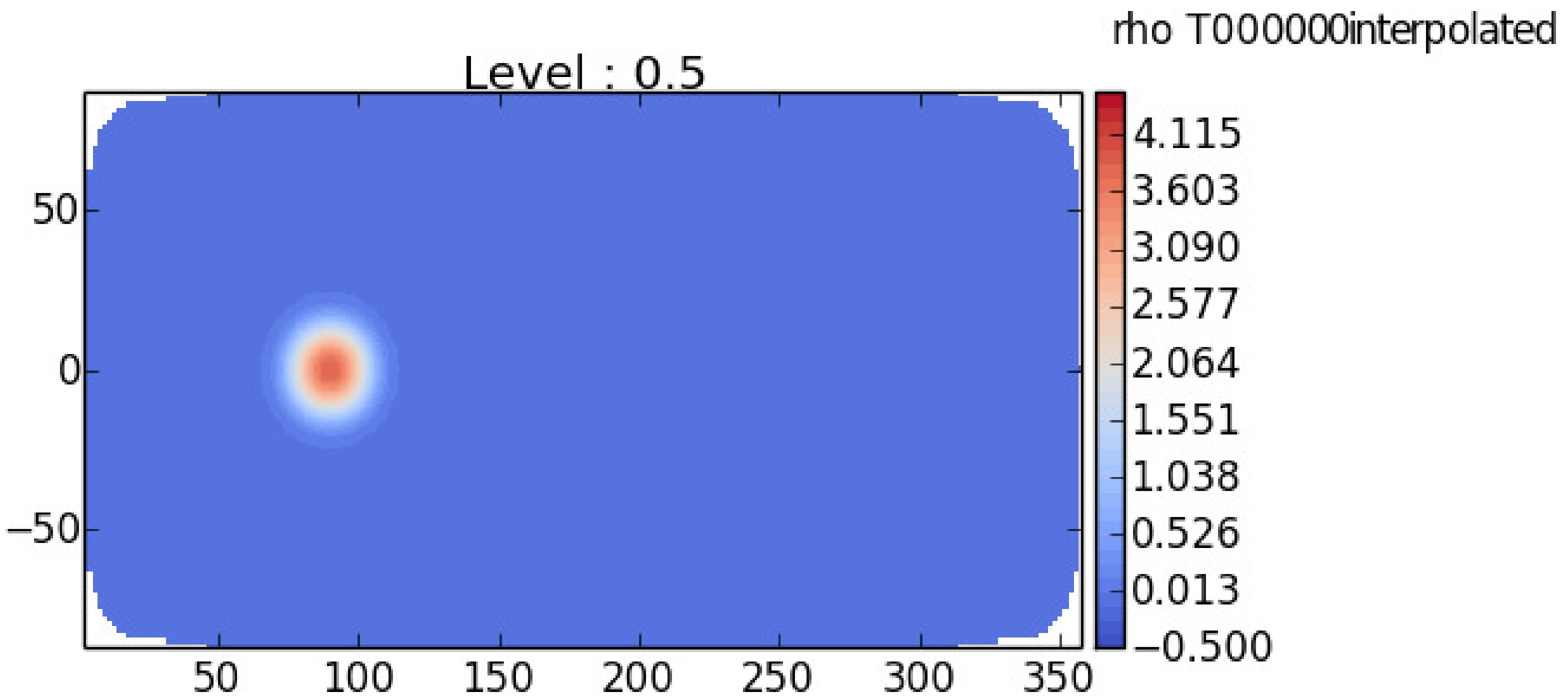


Dynamo

T. Melvin

Density advection

Solid body wind, parallel runs

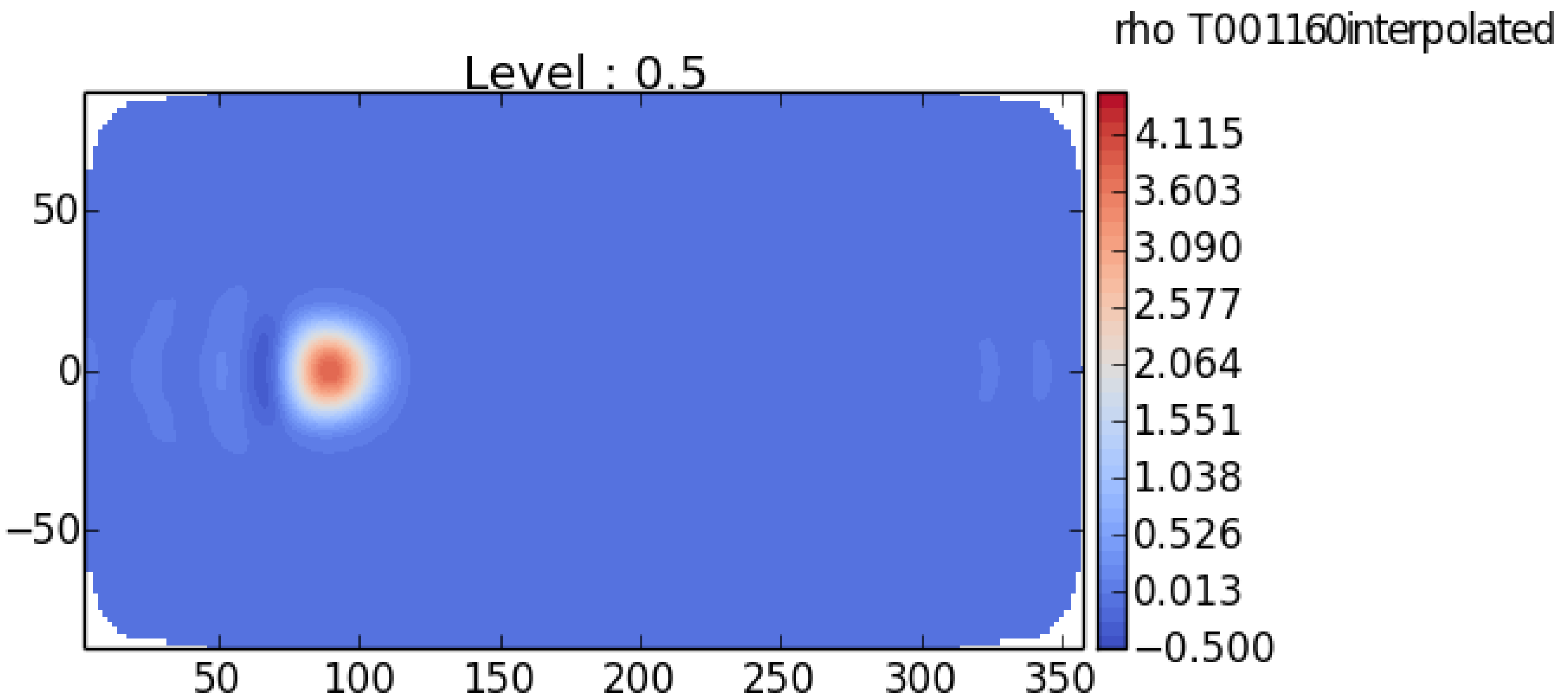


24 cells per horizontal panel, CFL≈0.1

S. Pring

Density advection

Solid body wind, parallel runs



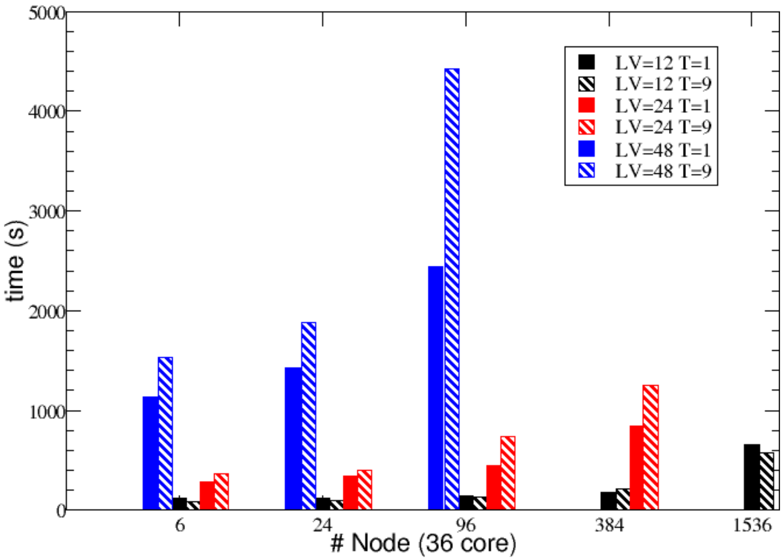
24 cells per horizontal panel, CFL$\approx$0.1

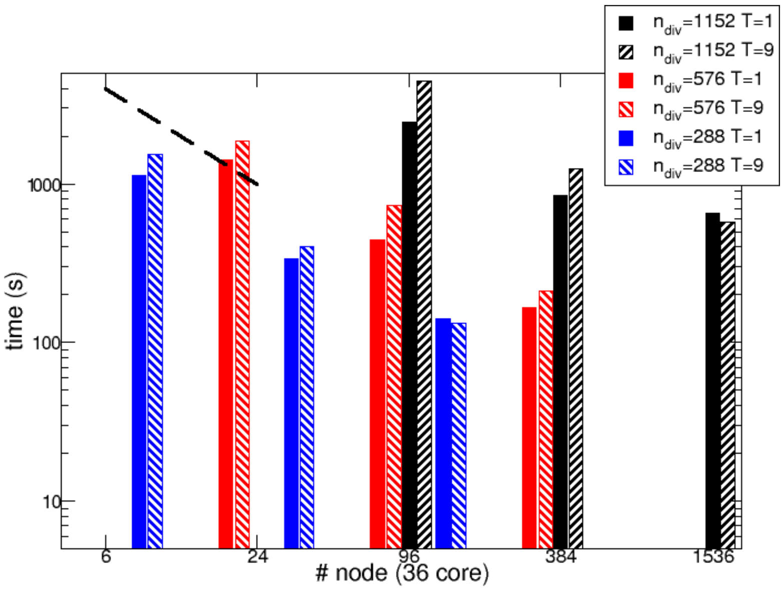
S. Pring

Outlook - To do

- Transport
- Orography
- Multigrid solver
- Physics-dynamics coupling
  - Coupling FE and FV
  - Impact of physics on dynamics

Scaling





- **Auto-generated parallel layer.**
- **Weak scaling: same amount of work per processor, perfect: horizontal line.**
- **Strong scaling (dashed): same global size, perfect: 4x speed-up.**

Dynamo 1.0 code release, 31.3.16 (now 1.1).

C. Maynard

Questions?

tommaso.benacchio@metoffice.gov.uk

References

- Cotter, C & Shipton, J 2012. JCP 231, 7076-7091.
- Putnam, WM & Lin, S-J 2007. JCP 227, 55-78.
- Staniforth, A & Thuburn, J 2012. QJRMS 138, 1-26.
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