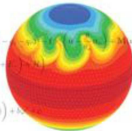


A finite-volume module for the IFS

Christian Kühnlein, Piotr Smolarkiewicz, Sylvie Malardel

$$\begin{aligned}
 \frac{\partial Q_p}{\partial t} + \nabla \cdot (\mathbf{v}Q_p) &= 0 \\
 \frac{\partial Q_m}{\partial t} + \nabla \cdot (\mathbf{v}Q_m) &= Q_p \left(-\mathbf{H}_p \cdot \mathbf{G} \nabla \mathbf{v}' - \frac{\mathbf{H}_p}{R_p} (\mathbf{v}' + \mathbf{R}_p \mathbf{v}_c') - \frac{1}{R_p} \mathbf{v}' \cdot \nabla \mathbf{H}_p + \mathbf{H}_p (\mathbf{u} + \mathbf{D}) \right) \\
 \frac{\partial Q_p'}{\partial t} + \nabla \cdot (\mathbf{v}Q_p') &= Q_p \left(-\mathbf{G}^T \mathbf{u} \cdot \nabla \mathbf{H}_p - \frac{\mathbf{H}_p}{r_p^2} \left(\frac{\Delta \mathbf{H}_p}{\Delta t} + \mathbf{v}' \cdot \nabla \mathbf{H}_p \right) \right) \\
 \frac{\partial Q_{m0}}{\partial t} + \nabla \cdot (\mathbf{v}Q_{m0}) &= Q_p R^{2m} \\
 \frac{\partial Q_p'}{\partial t} + \nabla \cdot (\mathbf{v}Q_p') &= Q_p \sum_{s=1}^S \left(\frac{\partial}{\partial t} \nabla \cdot \zeta(\psi - \mathbf{G}^T \mathbf{C} \nabla \psi') \right) + \mathbf{v}' \cdot \nabla \zeta(\psi - \mathbf{G}^T \mathbf{C} \nabla \psi')
 \end{aligned}$$

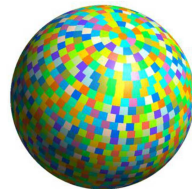


Smolarkiewicz P. K., Deconinck W., Hamrud M., Kühnlein C., Mozdzyński G., Szmelter J., Wedi, N. P.: A finite-volume module for simulating global all-scale atmospheric flows. *J. Comput. Phys.*, 2016



Current operational configuration of the Integrated Forecasting System (IFS):

- hydrostatic primitive equations (nonhydrostatic option available; see Benard et al. 2014)
- hybrid $\eta - p$ vertical coordinate (Simmons and Burridge, 1982)
- spherical harmonics discretisation in horizontal (Wedi et al., 2013)
- finite-element discretisation in vertical (Untch and Hortal, 2004)
- semi-implicit semi-Lagrangian (SISL) integration scheme (Temperton et al. 2001, Diamantakis 2014)
- cubic-octahedral (" T_{co} ") grid (Wedi, 2014, Malardel et al. 2016, Smolarkiewicz et al. 2016)
- HRES: $T_{co}1279$ (O1280) with $\Delta_h \sim 9$ km and 137 vertical levels
- ENS (1+50 perturbed members): $T_{co}639$ (O640) with $\Delta_h \sim 16$ km and 91 vertical levels

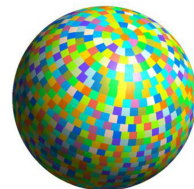


*IFS parallel decomposition
with 1600 MPI tasks*

- in the near future, spectral approach (as in IFS) is assumed to remain highly competitive in terms of time-to-solution
- however, uncertainties concerning scalability/efficiency of spectral discretisation with respect to future HPC architectures

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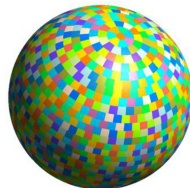
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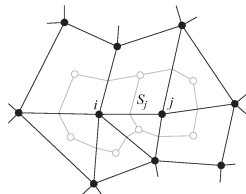
European Research Council
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⇒ PantaRhei project at ECMWF: prepare the mathematical-numerical technology for future cloud-resolving earth-system

Supplement IFS with a finite-volume module (FVM) that introduces:

- finite-volume (→ compact stencil, conservative)
- all-scale compressible Euler equations
- flexible meshes
- steep orography capability

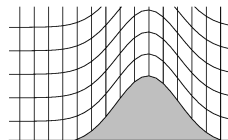
- compressible Euler equations in geospherical coordinates
- generalised curvilinear coordinates (Prusa & Smolarkiewicz JCP 2003; Wedi & Smolarkiewicz JCP 2003; Kühnlein et al. JCP 2012)
- fully unstructured edge-based finite-volume discretisation in horizontal (Szmelter & Smolarkiewicz, JCP 2010)
- structured flux-form finite-difference discretisation in vertical (Smolarkiewicz et al. JCP 2016)
- all prognostic variables are co-located
- two-time-level semi-implicit integration scheme with 3d implicit acoustic, buoyant and rotational modes (Smolarkiewicz, Kühnlein, Wedi JCP 2014)
- preconditioned generalised conjugate residual iterative solver for elliptic problems arising in semi-implicit integration schemes
- Eulerian advection with non-oscillatory forward-in-time MPDATA scheme (Smolarkiewicz and Szmelter JCP 2005; Kühnlein and Smolarkiewicz, prep. to JCP)



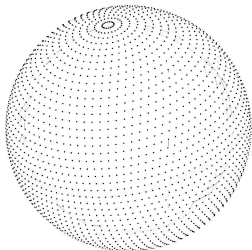
median-dual finite-volume approach

$$\int_{\Omega} \nabla \cdot \mathbf{A} = \int_{\partial\Omega} \mathbf{A} \cdot \mathbf{n} = \frac{1}{\mathcal{V}_i} \sum_{j=1}^{l(i)} A_j^{\perp} S_j$$

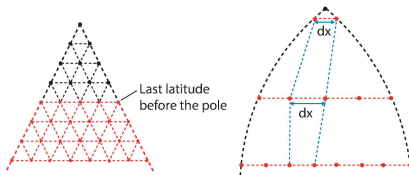
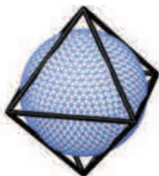
dual volume: \mathcal{V}_i , face area: S_j

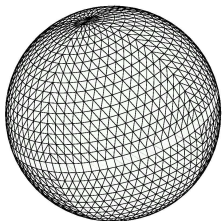


O24

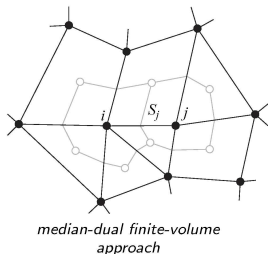
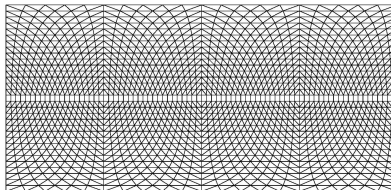


- suitable for spherical harmonics transforms applied in spectral IFS
 - Gaussian latitudes \Rightarrow Legendre transforms
 - uniform spacing of points along latitudes \Rightarrow Fourier transforms
- Notation is 'OX', for octahedral grid with X latitudes between pole and equator
- quasi-uniform resolution over the sphere
- operational at ECMWF with HRES and ENS since March 2016
- Malardel et al. ECMWF Newsletter 2016, Smolarkiewicz et al. JCP 2016





O16



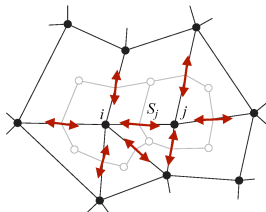
- FVM develops median-dual mesh around nodes of octahedral grid
- operational spectral IFS and FVM can operate on same horizontal grid
- FVM formulation is not restricted to this grid
- Parallel data structures and mesh generator provided by Atlas (Deconinck et al., in prep. for Comput. Phys. Commun.)

$$\begin{aligned}
 & \frac{\partial \mathcal{G} \rho}{\partial t} + \nabla \cdot (\mathbf{v} \mathcal{G} \rho) = 0 \\
 & \frac{\partial \rho \mathcal{G} \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{v} \rho \mathcal{G} \mathbf{u}) = \rho \mathcal{G} \left(-\Theta_d \tilde{\mathbf{G}} \nabla \varphi' - \frac{\mathbf{g}}{\theta_a} (\theta' + \theta_a (\varepsilon q'_v - q_c - q_p)) - \mathbf{f} \times (\mathbf{u} - \Upsilon_C \mathbf{u}_a) + \mathbf{M} \right) \\
 & \frac{\partial \rho \mathcal{G} \theta'}{\partial t} + \nabla \cdot (\mathbf{v} \rho \mathcal{G} \theta') = \rho \mathcal{G} \left(-\tilde{\mathbf{G}}^T \mathbf{u} \cdot \nabla \theta_a - \frac{L \theta}{c_p T} (C_d + E_p) + \mathcal{H} \right) \\
 & \varphi' = c_p \theta_0 \left[\left(\frac{R_d}{p_0} \rho \theta (1 + q_v / \varepsilon) \right)^{R_d / c_v} - \pi_a \right] \\
 & \frac{\partial \rho \mathcal{G} q_v}{\partial t} + \nabla \cdot (\mathbf{v} \rho \mathcal{G} q_v) = \rho \mathcal{G} (-C_d - E_p + D_{q_v}) \\
 & \frac{\partial \rho \mathcal{G} q_c}{\partial t} + \nabla \cdot (\mathbf{v} \rho \mathcal{G} q_c) = \rho \mathcal{G} (C_d - A_p - C_p + D_{q_c}) \\
 & \frac{\partial \rho \mathcal{G} q_p}{\partial t} + \nabla \cdot (\mathbf{v} \rho \mathcal{G} q_p) = \rho \mathcal{G} (A_p + C_p + E_p + D_{q_p}) - \nabla \cdot (\mathbf{v}_p \rho \mathcal{G} q_p)
 \end{aligned}$$

with:

$$\Theta_d := \frac{\theta (1 + q_v / \varepsilon)}{\theta_0 (1 + q_t)} \equiv \frac{\theta_d}{\theta_0} \quad \Upsilon_C \equiv \frac{\theta}{\theta_a} \quad \varepsilon := \frac{R_d}{R_v} \quad \varepsilon = 1/\varepsilon - 1 \quad \mathbf{v} = \tilde{\mathbf{G}}^T \mathbf{u}$$

→ "a" subscript denotes ambient state which satisfies subset of full equations, "0" subscript refers to constant reference, all primed variables are deviations with respect to the ambient state ($\psi' = \psi - \psi_a$ $\psi = u, v, w, \theta, \dots$)



Two-time-level semi-implicit solution of compressible Euler equations (Smolarkiewicz et. al JCP 2014)

Mass continuity:

$$\rho_i^{n+1} = \mathcal{A}_i(\rho^n, (\mathbf{v}\mathcal{G})^{n+1/2}, \mathcal{G}^n, \mathcal{G}^{n+1}) \Rightarrow (v^\perp \mathcal{G}\rho)^{n+1/2}$$

Conservation laws for primitive variables Ψ ($\Psi = u, v, w, \theta', \dots$) :

$$\Psi_i^{n+1} = \mathcal{A}_i(\tilde{\Psi}^n, (v^\perp \mathcal{G}\rho)^{n+1/2}, (\mathcal{G}\rho)^n, (\mathcal{G}\rho)^{n+1}) + 0.5 \delta t R^\Psi |_i^{n+1}$$

with $\tilde{\Psi}^n \equiv \Psi^n + 0.5 \delta t R^\Psi |^n$

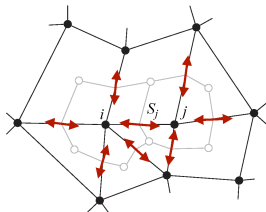
$\mathcal{A}()$ -operator is FV-MPDATA for homogeneous equation (Smolarkiewicz & Szmelter, 2005):

$$\frac{\partial \mathcal{G}\psi}{\partial t} + \nabla \cdot (\mathbf{V}\psi) = 0 \quad \rightarrow \quad \psi_i^{n+1} = \psi_i^n - \frac{\delta t}{G_i V_i} \sum_{j=1}^{l(i)} F_j^\perp(\psi_i^n, \psi_j^n, V_j^\perp) S_j$$

with normal upwind flux: $F_j^\perp(\psi_i, \psi_j, V_j^\perp) = [V_j^\perp]^+ \psi_i + [V_j^\perp]^- \psi_j$ where $V^\perp := \mathbf{V} \cdot \mathbf{n}$

- First step is classical upwind scheme with advection of ψ by physical flow \mathbf{V}
- Error-compensative step with pseudo-velocity $\tilde{V}^\perp := -\psi^{-1} \times \text{Error}(\delta r, \delta t)$ from modified equation analysis, e.g.

$$\text{Error} = -\frac{1}{2} |V_j^\perp| \left(\frac{\partial \psi}{\partial r} \right)_{s_j}^* (r_j - r_i) + \frac{1}{2} \delta t \frac{V_j^\perp}{G_j} \{ \mathbf{V} \cdot \nabla \psi \}_{s_j}^* + \frac{1}{2} \delta t \frac{V_j^\perp}{G_j} \{ \psi (\nabla \cdot \mathbf{V}) \}_{s_j}^* + \text{HOT}$$



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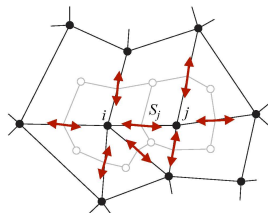
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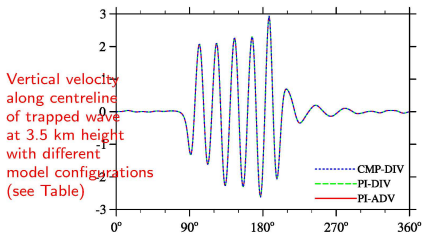
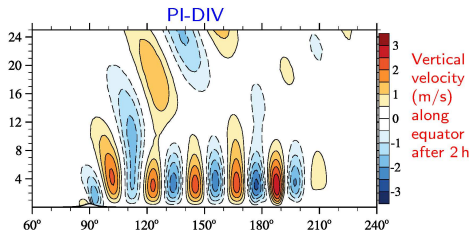
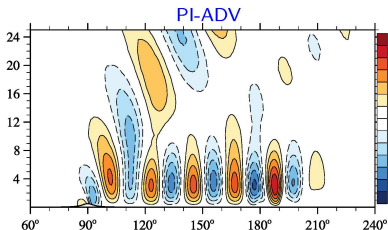
FV-MPDATA solely using face-normal vector components (Kühnlein and Smolarkiewicz, in prep. for JCP):

$$\text{Error} = -\frac{1}{2} |V_j^\perp| \left(\frac{\partial \psi}{\partial r} \right)_{s_j}^* (r_j - r_i) + \frac{1}{2} \delta t \frac{V_j^\perp}{G_j} \{ \nabla \cdot (\mathbf{V}\psi) \}_{s_j}^* + \text{HOT}$$

$$\text{Gauss-divergence theorem: } \int_{\Omega} \nabla \cdot \mathbf{A} = \int_{\partial\Omega} \mathbf{A} \cdot \mathbf{n} = \frac{1}{V_i} \sum_{j=1}^{l(i)} A_j^\perp S_j$$

Finite-volume MPDATA for compressible atmospheric dynamics

Orographically-forced internal gravity waves in sheared ambient flow on small planet (Keller 1994, Wedi & Smolarkiewicz 2009) with octahedral grid O90:

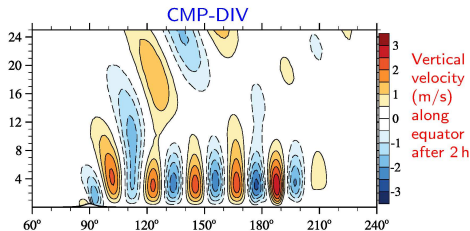
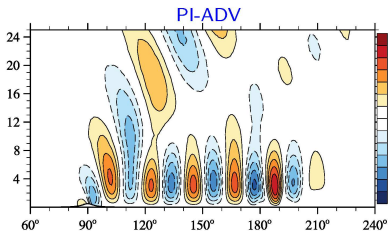


Simulation	Equations	FV-MPDATA
PI-ADV	pseudo-incompressible	established form
PI-DIV	pseudo-incompressible	advanced form
CMP-DIV	fully compressible Euler	advanced form

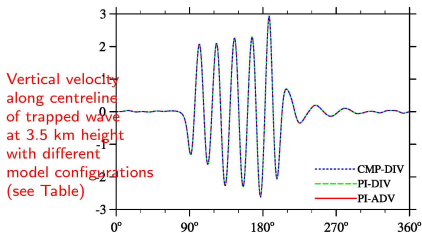
⇒ Proposed FV-MPDATA reproduces reference results of established formulation and enables effective semi-implicit integration of compressible Euler equations on arbitrary meshes

Finite-volume MPDATA for compressible atmospheric dynamics

Orographically-forced internal gravity waves in sheared ambient flow on small planet (Keller 1994, Wedi & Smolarkiewicz 2009) with octahedral grid O90:



Vertical velocity (m/s) along equator after 2 h



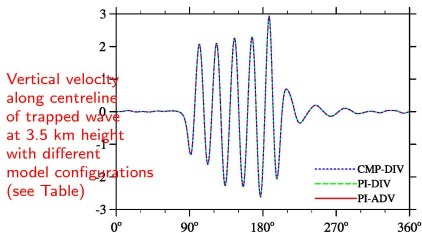
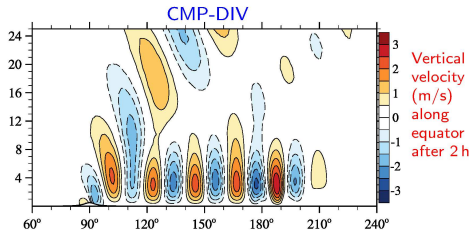
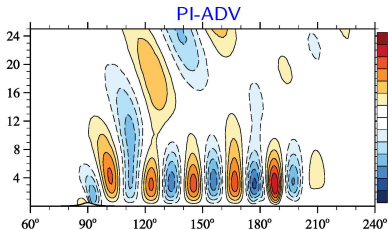
Vertical velocity along centerline of trapped wave at 3.5 km height with different model configurations (see Table)

Simulation	Equations	FV-MPDATA
PI-ADV	pseudo-incompressible	established form
PI-DIV	pseudo-incompressible	advanced form
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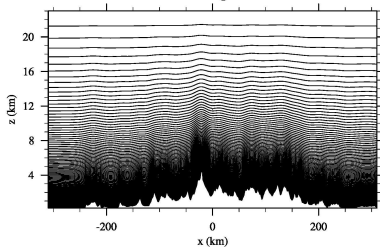


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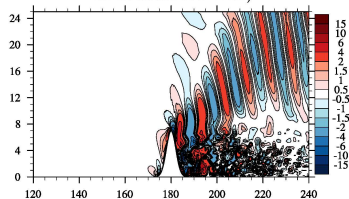
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Vertical discretisation and incorporation of orography in FVM

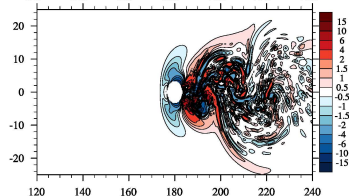
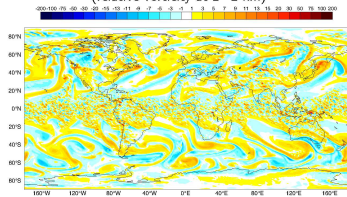
Generalised terrain-following vertical coordinate



stratified flow past steep orography with maximum slope $\sim 70^\circ$ on small planet
(vertical velocity in m/s, lon-height section at lat=0, lon-lat section at $z=2$ km)

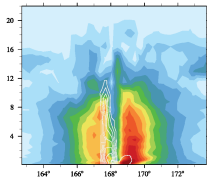
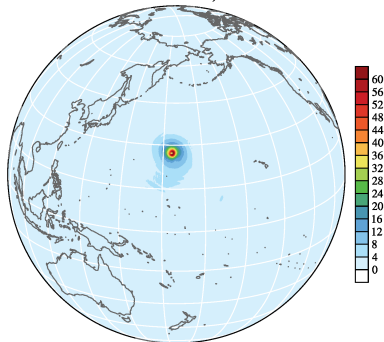


Held-Suarez benchmark N640 (16 km) with realistic IFS orography at day 90
(relative vorticity at $z=2$ km)

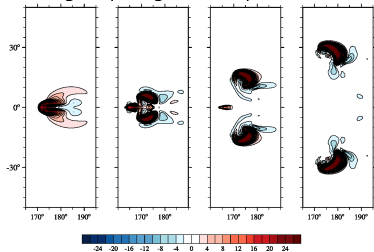


⇒ robust and efficient handling of steep orography

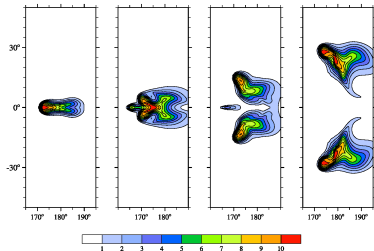
Tropical cyclone with FVM at day 10 ($\Delta_h = 0.25^\circ$):



Supercell evolution (0.5, 1, 1.5, 2h) with FVM at 500 m grid spacing on small planet:



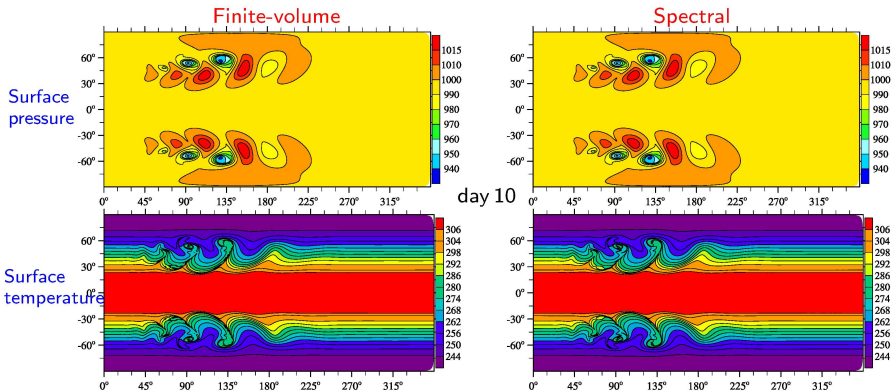
Vertical velocity (m/s) at 5 km



Rainwater (g/kg) at 5 km

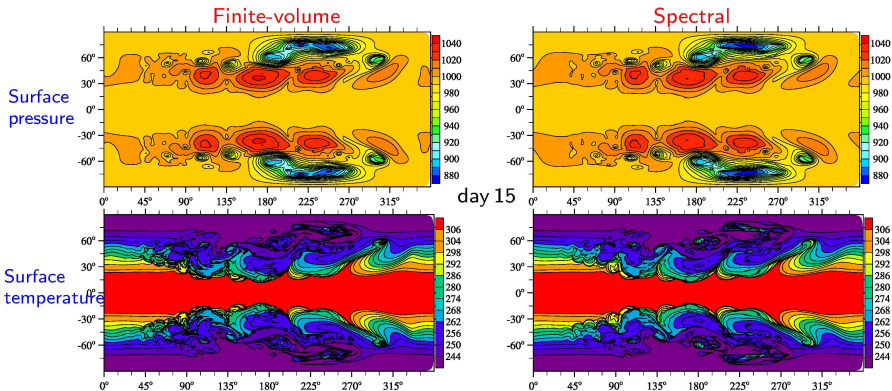
→ FVM with simplified cloud microphysics and PBL parametrisations

Dry baroclinic instability, FVM (O640) versus the spectral IFS (T_{co639}):

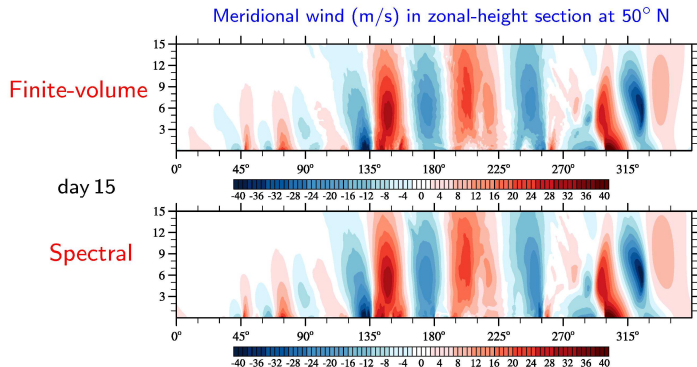


Finite-volume versus spectral solutions in the IFS

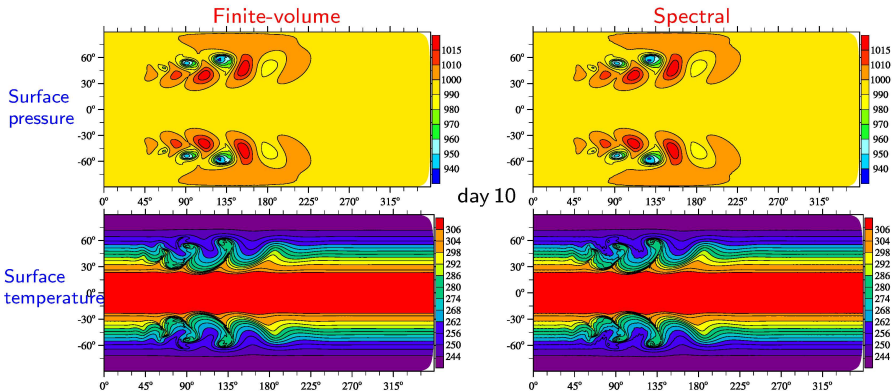
Dry baroclinic instability, FVM (O640) versus the spectral IFS (T_{co}639):



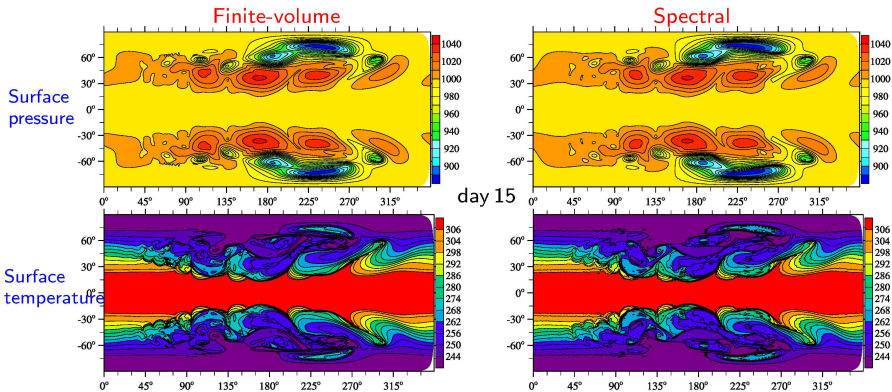
Dry baroclinic instability, FVM (O640) versus the spectral IFS ($T_{co}639$):



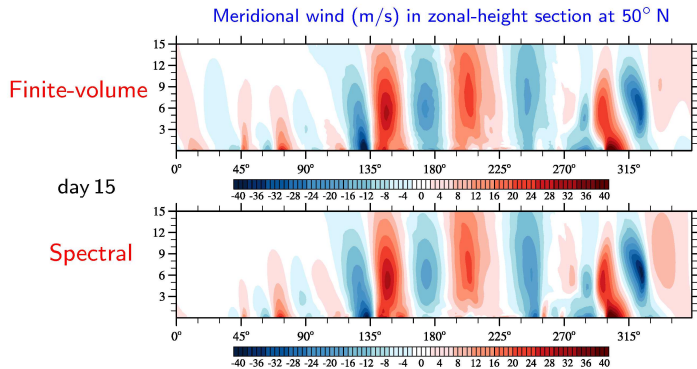
Dry baroclinic instability, FVM (O160) versus the spectral IFS (T_{co159}):

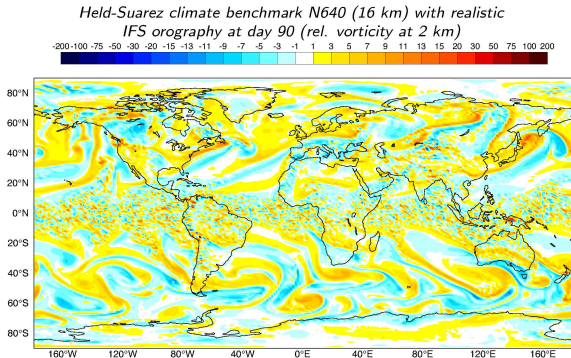


Dry baroclinic instability, FVM (O160) versus the spectral IFS (T_{co}159):



Dry baroclinic instability, FVM (O160) versus the spectral IFS (T_{co159}):





Outlook:

- Efficiency at high resolution and extreme scaling (→ ESCAPE)
- Comprehensive comparison of FVM with spectral IFS
- Towards more realism (Initial conditions, parametrisations,...)

TECHNICAL MEMORANDUM

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The modelling infrastructure of the Integrated Forecasting System: Recent advances and future challenges

N.P. Wedi, P. Bauer, W. Deconinck, M. Diamantakis, M. Hamrud, C. Kühnlein, S. Malardel, K. Mogensen, G. Mozdzyński, P.K. Smolarkiewicz


Research Department

November 2015

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A finite-volume module for simulating global all-scale atmospheric flows

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ABSTRACT

The paper documents the development of a global multidimensional finite-volume module designed to enhance an established spectral-coefficient based numerical weather prediction (NWP) model. The module adheres to NWP standards, with formalization of the governing equations based on the classical meteorological latitude-longitude spherical framework. In the horizontal, a bicubic structured mesh with near-volumes both about the reduced Gaussian grid of the existing NWP model circumvents the numerical stiffness in the polar regions of the spherical framework. All dependent variables are co-located, accommodating both spectral-coefficients and grid-point solutions at the same physical location. In the vertical, a uniform finite-difference discretization facilitates the solution of viscous elliptic problems in thin spherical shells, while the generality of the physical vertical coordinate is delegated to generalised continuous transformations between computational and physical space. The newly developed module assumes the compressible Euler equations as default, but includes reduced-coupled PDEs as an option. Furthermore, it employs semi-implicit forward-in-time integrators of the governing PDE systems, akin to but more general than those used in the NWP model. The module shares the equal region parallelization scheme with the NWP model, with multiple layers of parallelization hybridizing MPI tasks and OpenMP threads. The efficacy of the developed nonhydrostatic module is illustrated with benchmarks of idealized global weather.

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1. Introduction

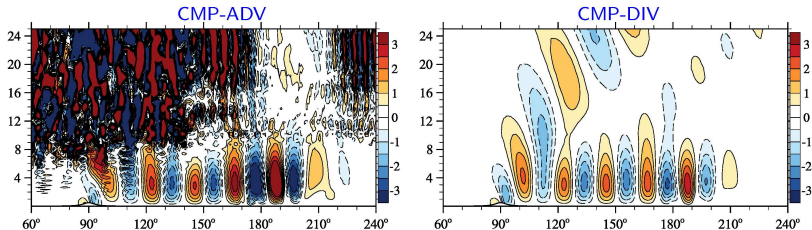
Numerical weather prediction (NWP) has achieved high proficiency over the past 50 years. This owes much to advances in computer hardware, observational networks and data assimilation techniques as well as numerical methods for integrating hydrostatic primitive equations (HPE). One particular numerical approach embraced widely by NWP combines semi-implicit time stepping with semi-Lagrangian advection (SIL) and with spectral-transform spatial discretization of the governing HPE [46]. The SIL time stepping enables integrations with Courant numbers of the fluid flow and wave motions much larger than unity, whereas the spectral-transform discretization facilitates the efficient solution of elliptic equations induced by the SIL approach. Moreover, it circumvents the computational expense of the latitude-longitude (lat-lon) co-

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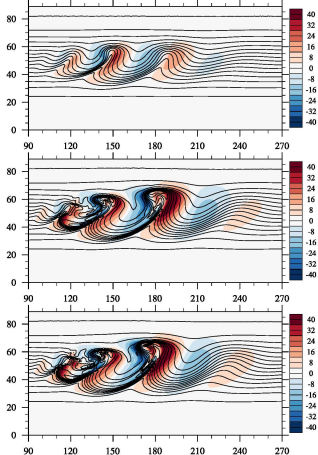
Finite-volume MPDATA for compressible atmospheric dynamics

Orographically-forced internal gravity waves in sheared ambient flow on small planet (Keller 1994, Wedi & Smolarkiewicz 2009) with octahedral grid O90:



Options for 3D governing equations in FVM

Baroclinic instability (Jablonowski and Williamson, 2006) with FVM (from top: anelastic, pseudo-incompressible, compressible)



→ Generic nonhydrostatic formulation with consistent options:

- ★ fully compressible Euler equations (default)
- ★ pseudo-incompressible (Durran, JAS 1989)
- ★ anelastic (Lipps and Hemler, JAS 1982)

$$\frac{\partial \mathcal{G}_\varrho}{\partial t} + \nabla \cdot (\mathbf{v} \mathcal{G}_\varrho) = 0$$

$$\frac{\partial \mathcal{G}_\varrho \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{v} \mathcal{G}_\varrho \mathbf{u}) = -\mathcal{G}_\varrho \left(\Theta \tilde{\mathbf{G}} \nabla \varphi' + \mathbf{g} \Upsilon_B \frac{\theta'}{\theta_b} + \mathbf{f} \times (\mathbf{u} - \Upsilon_C \mathbf{u}_a) + \mathbf{M} \right)$$

$$\frac{\partial \mathcal{G}_\varrho \theta'}{\partial t} + \nabla \cdot (\mathbf{v} \mathcal{G}_\varrho \theta') = -\mathcal{G}_\varrho (\tilde{\mathbf{G}}^T \mathbf{u} \cdot \nabla \theta_a)$$

with optional coefficients:

$$\varrho := \left[\rho(\mathbf{x}, t), \rho_b \frac{\theta_b(z)}{\theta_0}, \rho_b(z) \right], \quad \varphi' := [c_p \theta_0 \pi', c_p \theta_0 \pi', c_p \theta_b \pi']$$

$$\Theta := \left[\frac{\theta}{\theta_0}, \frac{\theta}{\theta_0}, 1 \right], \quad \Upsilon_B := \left[\frac{\theta_b(z)}{\theta_a(\mathbf{x})}, \frac{\theta_b(z)}{\theta_a(\mathbf{x})}, 1 \right], \quad \Upsilon_C := \left[\frac{\theta}{\theta_a(\mathbf{x})}, \frac{\theta}{\theta_a(\mathbf{x})}, 1 \right]$$