Emerging finite-volume methods for nonhydrostatic NWP at ECMWF

C. Kühnlein, W. Deconinck, M. Diamantakis, R. Klein, S. Malardel,
Z.P. Piotrowski, P. K. Smolarkiewicz, J. Szmelter, N. P. Wedi

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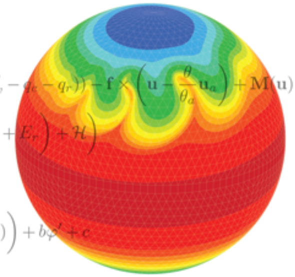
$$\frac{\partial \mathcal{G}\rho}{\partial t} + \nabla\cdot(\mathbf{v}\mathcal{G}\rho) = 0$$

$$\frac{\partial \mathcal{G}\rho\mathbf{u}}{\partial t} + \nabla\cdot(\mathbf{v}\mathcal{G}\rho\mathbf{u}) = \mathcal{G}\rho\left(-\Theta_d\widetilde{\mathbf{G}}\nabla\varphi' - \frac{\mathbf{g}}{\theta_a}(\theta' + \theta_a(\epsilon q_v' - q_c - q_r)) - \mathbf{f}\times\left(\mathbf{u} - \frac{\theta}{\theta_a}\mathbf{u}_a\right) + \mathbf{M}(\mathbf{u}) + \mathbf{D}\right)$$

$$\frac{\partial \mathcal{G}\rho\theta'}{\partial t} + \nabla\cdot(\mathbf{v}\mathcal{G}\rho\theta') = \mathcal{G}\rho\left(-\widetilde{\mathbf{G}}^T\mathbf{u}\cdot\nabla\theta_a - \frac{L}{c_p\pi}\left(\frac{\Delta q_{vs}}{\Delta t} + E_r\right) + \mathcal{H}\right)$$

$$\frac{\partial \mathcal{G}\rho q_k}{\partial t} + \nabla\cdot(\mathbf{v}\mathcal{G}\rho q_k) = \mathcal{G}\rho\mathcal{R}^{q_k}$$

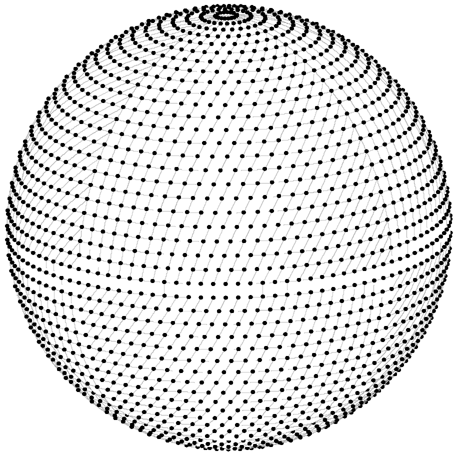
$$\frac{\partial \mathcal{G}\rho\varphi'}{\partial t} + \nabla\cdot(\mathbf{v}\mathcal{G}\rho\varphi') = \mathcal{G}\rho\sum_{\ell=1}^{3}\left(\frac{a_\ell}{\zeta_\ell}\nabla\cdot\zeta_\ell(\check{\mathbf{v}} - \widetilde{\mathbf{G}}^T\mathbf{C}\nabla\varphi')\right) + b\varphi' + c$$

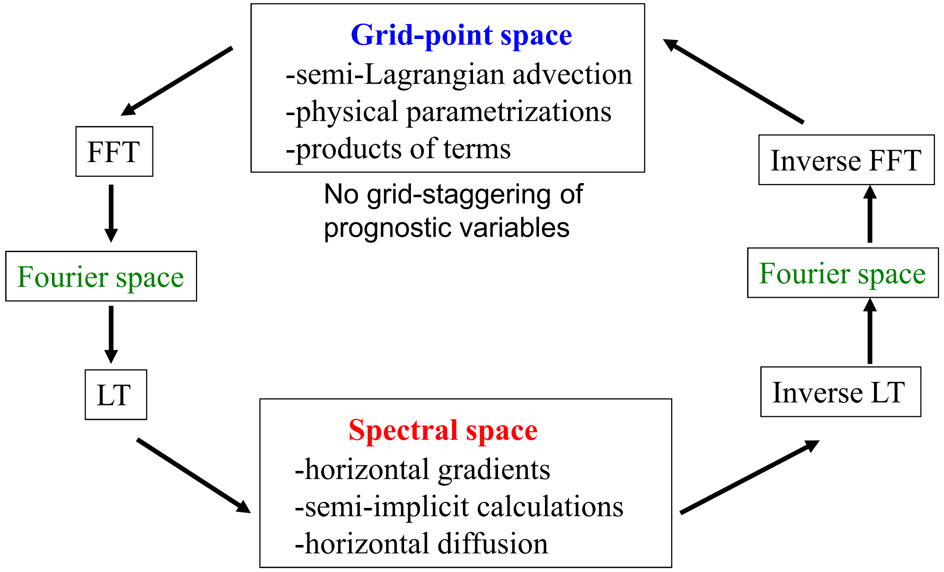


Spectral-transform formulation of IFS

- hydrostatic primitive equations (optionally nonhydrostatic fully compressible equations) in hybrid mass-based vertical coordinate
- spherical-harmonics representation in horizontal
- finite-element integral approximation in vertical
- two-time-level semi-implicit semi-Lagrangian integration scheme
- cubic-octahedral grid (“TCo“)
- coupling to IFS physics using SLAVEPP (Semi-Lagrangian Averaging of Physical Parametrisations)

Nodes of octadedral reduced Gaussian grid





Grid-point space
-semi-Lagrangian advection
-physical parametrizations
-products of terms

No grid-staggering of prognostic variables

FFT

Fourier space

LT

Spectral space
-horizontal gradients
-semi-implicit calculations
-horizontal diffusion

Inverse LT

Fourier space

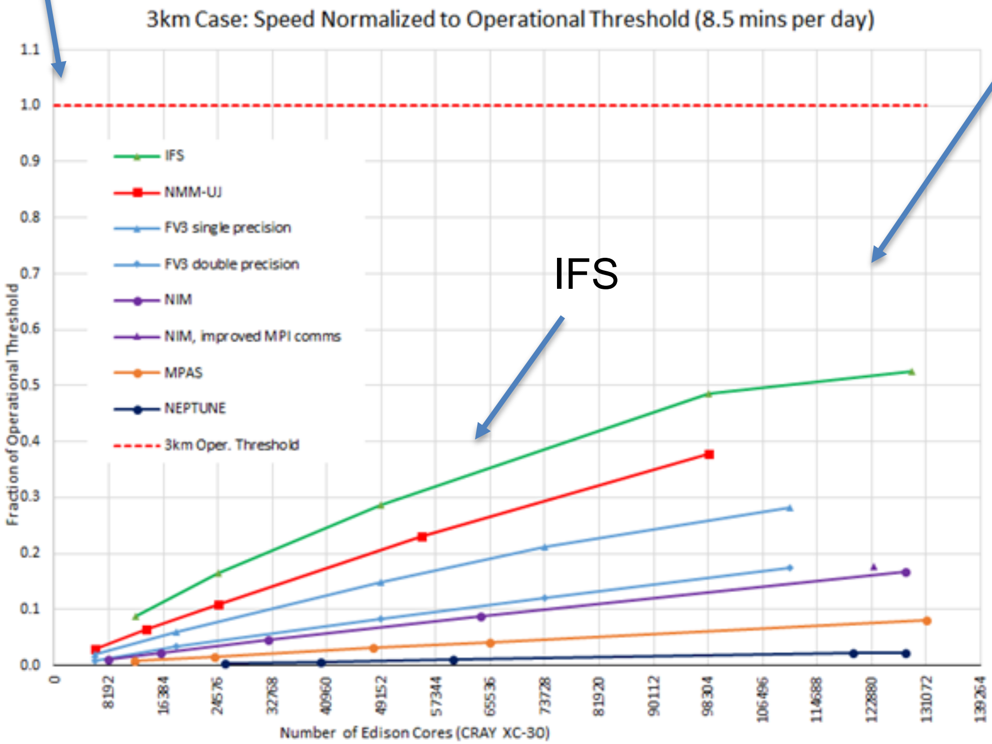
Inverse FFT

$$\psi(\lambda, \varphi) = \sum_{l=0}^{NSMAX} \sum_{-l \leq m \leq l} \psi_{l,m} Y_{l,m}(\lambda, \varphi)$$

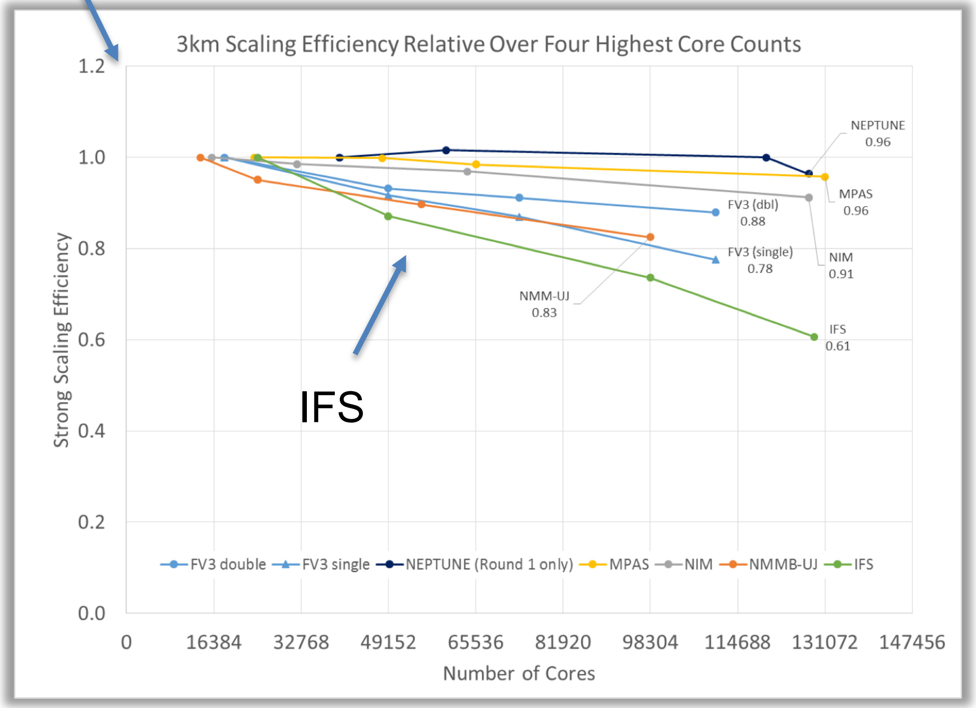
IFS dynamical core performance comparison: time-to-solution at 3km for dry baroclinic instability test case with 10 tracer fields

Operational need!

The higher the better



IFS



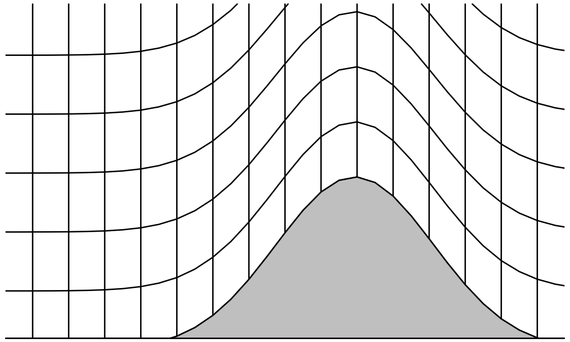
IFS

(adapted from Michalakes et al, NGGPS AVEC report, 2015)

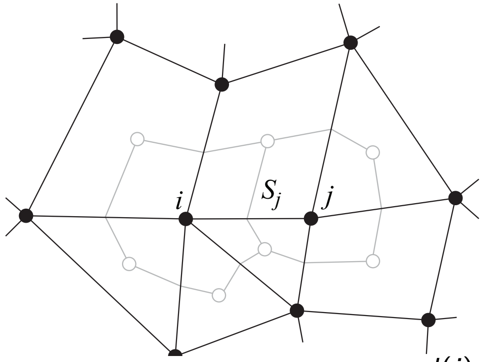
IFS is hydrostatic all other models are nonhydrostatic!

Finite-Volume Module of IFS

- deep-atmosphere nonhydrostatic fully compressible equations in height-based generalised vertical coordinate
- hybrid horizontally-unstructured finite-volume and vertically-structured finite-difference/finite-volume discretisation framework
- two-time-level semi-implicit integration
- nonoscillatory forward-in-time Eulerian advection based on MPDATA methods
- bespoke preconditioned nonsymmetric generalised conjugate residual iterative solvers



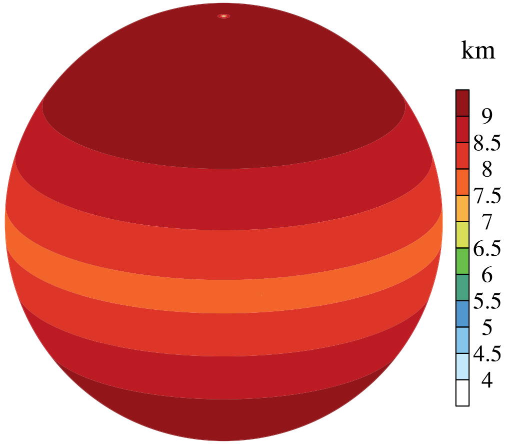
terrain-following coordinate



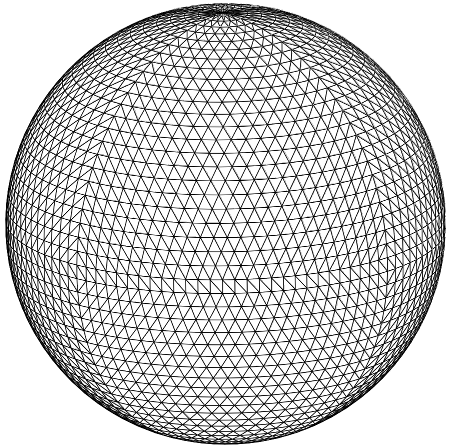
$$\int_\Omega \nabla\cdot\mathbf{A} = \int_{\partial\Omega}\mathbf{A}\cdot\mathbf{n} = \frac{1}{\mathcal{V}_i}\sum_{j=1}^{l(i)} A_j^\perp S_j$$

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

see:
Smolarkiewicz et al. (2016,2017,2018)
Kühnlein and Smolarkiewicz (2017),
Kühnlein et al. (2018)



Dual mesh spacing O1280



Primary FV mesh about nodes of octahedral grid O24

Finite-volume and spectral-transform dynamical core formulations of IFS

IFS-FVM represents an alternative dynamical core formulation to spectral-transform IFS with:

- finite-volume discretisation operating on a compact stencil
- deep-atmosphere nonhydrostatic fully compressible equations in generalised height-based vertical coordinate
- fully conservative and monotone advective transport
- flexible horizontal and vertical meshes
- robustness wrt steep slopes of orography

-> but at the same time IFS-FVM can share important formulation features with the spectral-transform IFS

Model aspect	IFS-FVM	IFS-ST	IFS-ST (NH option)
Equation system	fully compressible	hydrostatic primitive	fully compressible
Prognostic variables	$\rho_d, u, v, w, \theta', r_v, r_l, r_r, r_i, r_s$	$p_s, u, v, T_v, q_v, q_l, q_r, q_i, q_s$	$\pi_s, u, v, d_4, T_v, q_v, q_l, q_r, q_i, q_s$
Horizontal coordinates	λ, ϕ (lon-lat)	λ, ϕ (lon-lat)	λ, ϕ (lon-lat)
Vertical coordinate	generalized height	hybrid η-pressure	hybrid η-pressure
Horizontal discretization	unstructured finite-volume (FV)	spectral-transform (ST)	spectral-transform (ST)
Vertical discretization	structured FD/FV	structured FE	structured FD/FE
Horizontal staggering	co-located	co-located	co-located
Vertical staggering	co-located	co-located	co-located/Lorenz
Horizontal grid	octahedral Gaussian/arbitrary	octahedral Gaussian	octahedral Gaussian
Time-stepping scheme	2-TL SI	2-TL constant-coefficient SI	2-TL constant-coefficient SI
Advection	conservative FV Eulerian	non-conservative SL	non-conservative SL

Atlas infrastructure developments: a library for NWP and Climate

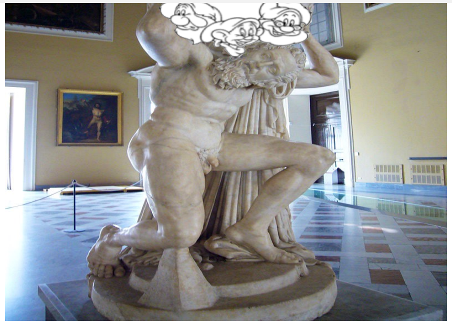
- Atlas (Deconinck et al, 2017) provides flexible data structures, grid/mesh generation capabilities and mathematical operators for NWP and climate modelling software developments in a parallel HPC computing environment

- It has been recently developed and incorporated in IFS and has been the basis for new developments including a new dynamical core based on Finite Volume discretization

- Open source
- C++ or Fortran interface
- It supports developments on:
    - structured grids
    - unstructured hybrid meshes
- Parallel mesh generation
- Mesh to mesh interpolation
- Mathematical operators (nabla etc) for Finite Volume and high order DG discretizations
- Accelerator (GPU) capable

```
grid = atlas_Grid(“O1280”) ! Create O1280 octahedral Gaussian grid
meshgenerator = atlas_MeshGenerator(“structured”)
mesh = meshgenerator%generate(grid)   ! Generate mesh from grid
method = atlas_fvm_Method(mesh)       ! Setup finite volume method
nabla  = atlas_Nabla(method)          ! Create FVM nabla operator

call nabla%gradient(scalarfield, gradientfield) ! Compute  gradient
```



Finite-Volume Module of IFS: Moist-precipitating nonhydrostatic fully compressible equations

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

$$\frac{\partial \mathcal{G}\rho_d\mathbf{u}}{\partial t} + \nabla\cdot(\mathbf{v}\mathcal{G}\rho_d\mathbf{u}) = \mathcal{G}\rho_d\left[-\theta_\rho\widetilde{\mathbf{G}}\nabla\varphi' + \mathbf{g}\mathcal{B} - \mathbf{f}\times\left(\mathbf{u}-\frac{\theta_\rho}{\theta_{\rho a}}\mathbf{u}_a\right) + \mathcal{M}' + \boldsymbol{P}^{\mathbf{u}}\right]\ ,$$

$$\frac{\partial \mathcal{G}\rho_d\theta'}{\partial t} + \nabla\cdot\left(\mathbf{v}\mathcal{G}\rho_d\,\theta'\right) = \mathcal{G}\rho_d\left[-\widetilde{\mathbf{G}}^T\mathbf{u}\cdot\nabla\theta_a + P^{\theta'}\right]\ ,$$

$$\frac{\partial \mathcal{G}\rho_d r_k}{\partial t} + \nabla\cdot(\mathbf{v}\mathcal{G}\rho_d\ r_k) = \mathcal{G}\rho_d P^{r_k} \qquad \text{where} \quad r_k = r_v\,,\, r_l\,,\, r_r\,,\, r_i\,,\, r_s\ ,$$

Kühnlein et al. 2018

$$\frac{\partial \mathcal{G}\rho_d\ \Lambda_a}{\partial t} + \nabla\cdot(\mathbf{v}\mathcal{G}\rho_d\ \Lambda_a) = \mathcal{G}\rho_d P^{\Lambda_a}\ ,$$

$$\varphi' = c_{pd}\left[\left(\frac{R_d}{p_0}\rho_d\,\theta\,(1+r_v/\varepsilon)\right)^{R_d/c_{vd}} - \pi_a\right]\ .$$

with:

$$\mathbf{v} = \widetilde{\mathbf{G}}^T\mathbf{u}\ , \qquad \theta_\rho = \frac{\theta\,(1+r_v/\varepsilon)}{(1+r_t)}\ , \qquad \varepsilon = \frac{R_d}{R_v}\ , \qquad \theta' = \theta - \theta_a\ ,$$

$$\mathcal{B} = 1 - \frac{\theta_\rho}{\theta_{\rho a}} = 1 - \frac{\vartheta}{\theta_{\rho a}}\left(\theta_a + \theta'\right)\ , \qquad \vartheta \equiv \frac{1+r_v/\varepsilon}{1+r_t}\ , \qquad r_t = \sum_k r_k = r_v + r_l + r_r + r_i + r_s\ .$$

Finite-Volume Module of IFS: Semi-implicit integration

Generalized transport equation:

$$\frac{\partial G\Psi}{\partial t} + \nabla \cdot (\mathbf{V}\Psi) = G\left(\mathcal{R}^{\Psi} + P^{\Psi}\right)$$

NFT template integration scheme:

$$\Psi_{\mathbf{i}}^{n+1} = \mathcal{A}_{\mathbf{i}}(\widetilde{\Psi}, \mathbf{V}^{n+1/2}, G^{n}, G^{n+1}, \delta t) + b^{\Psi}\,\delta t\,\mathcal{R}^{\Psi}|_{\mathbf{i}}^{n+1} \equiv \widehat{\Psi}_{\mathbf{i}} + b^{\Psi}\,\delta t\,\mathcal{R}^{\Psi}|_{\mathbf{i}}^{n+1}$$

where

$$\widetilde{\Psi} = \Psi^{n} + a^{\Psi}\,\delta t\,\mathcal{R}^{\Psi}|^{n} + \delta t\,P^{\Psi}|^{n}$$

and

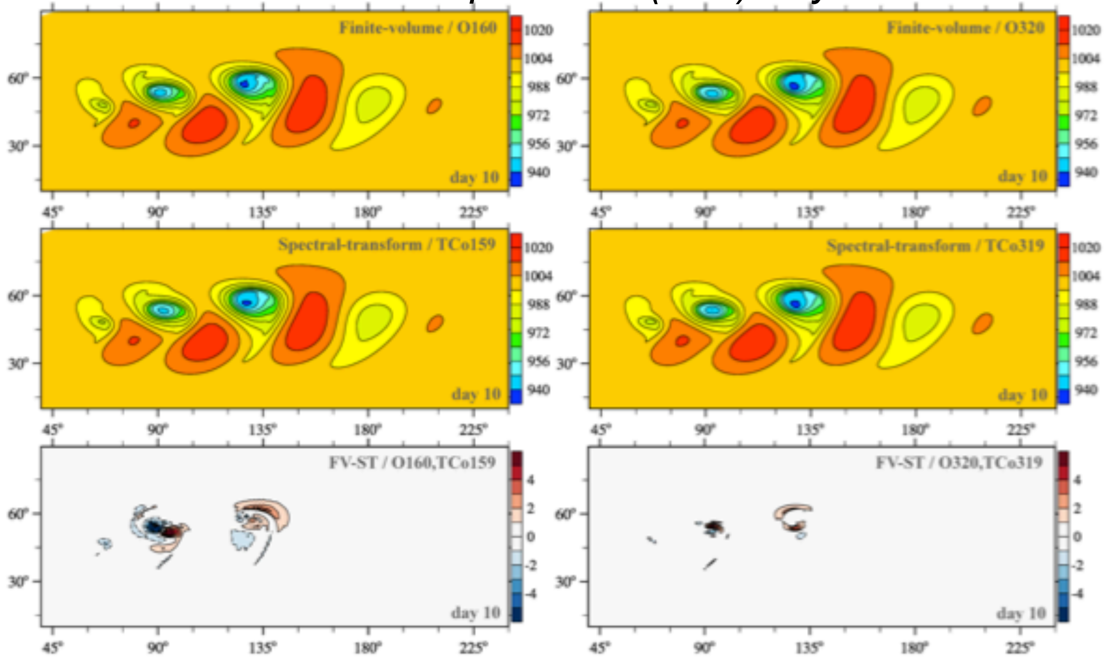
$$P^{\Psi}|^{n} = P^{\Psi}(t_{phys}, \Delta t_{phys}) \text{ where } \Delta t_{phys} = N_s \delta t \quad \text{and} \quad (N_s = 1, 2, 3, ..)$$

Kühnlein et al. 2018

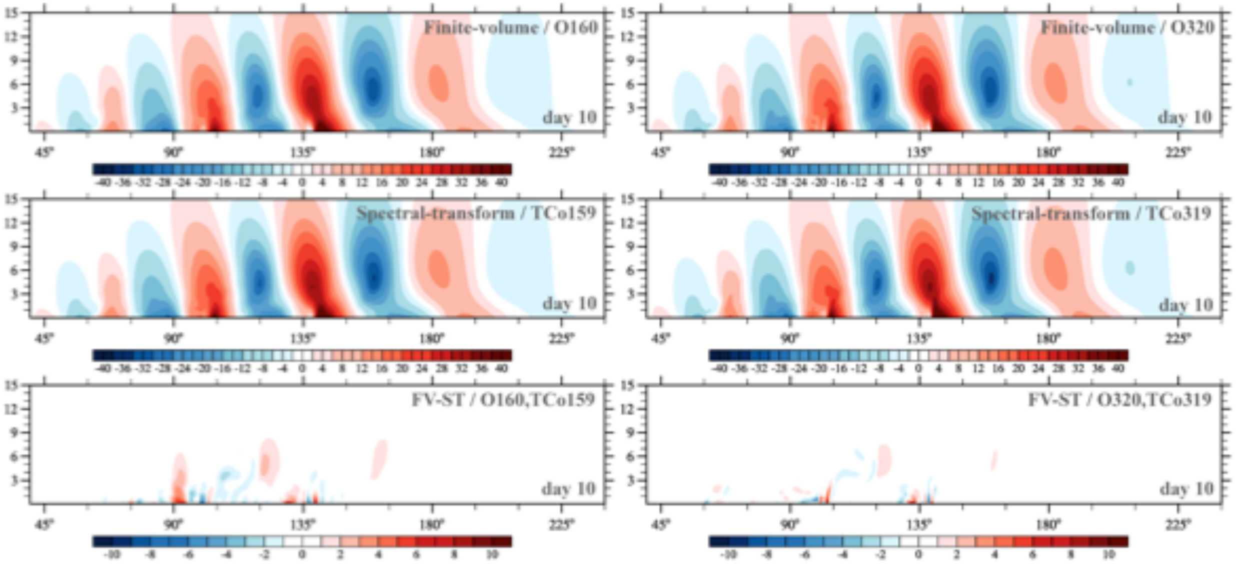
Prognostic variable	Ψ	$\mathbf{V}$	G	a^{Ψ}	b^{Ψ}
Dry density	ρ_d	$\mathbf{v}\mathcal{G}$	$\mathcal{G}$	-	-
Zonal physical velocity	u	$\mathbf{v}\mathcal{G}\rho_d$	$\mathcal{G}\rho_d$	0.5	0.5
Meridional physical velocity	v	$\mathbf{v}\mathcal{G}\rho_d$	$\mathcal{G}\rho_d$	0.5	0.5
Vertical physical velocity	w	$\mathbf{v}\mathcal{G}\rho_d$	$\mathcal{G}\rho_d$	0.5	0.5
Potential temperature perturbation	θ'	$\mathbf{v}\mathcal{G}\rho_d$	$\mathcal{G}\rho_d$	0.5	0.5
Water vapor mixing ratio	r_v	$\mathbf{v}\mathcal{G}\rho_d$	$\mathcal{G}\rho_d$	-	-
Liquid water mixing ratio	r_l	$\mathbf{v}\mathcal{G}\rho_d$	$\mathcal{G}\rho_d$	-	-
Rain water mixing ratio	r_r	$\mathbf{v}\mathcal{G}\rho_d$	$\mathcal{G}\rho_d$	-	-
Ice mixing ratio	r_i	$\mathbf{v}\mathcal{G}\rho_d$	$\mathcal{G}\rho_d$	-	-
Snow mixing ratio	r_s	$\mathbf{v}\mathcal{G}\rho_d$	$\mathcal{G}\rho_d$	-	-
Cloud fraction	Λ_a	$\mathbf{v}\mathcal{G}\rho_d$	$\mathcal{G}\rho_d$	-	-
Exner pressure perturbation	φ'	$\mathbf{v}\mathcal{G}\rho_d$	$\mathcal{G}\rho_d$	0	1.0

Finite-Volume Module of IFS: dry adiabatic dynamics

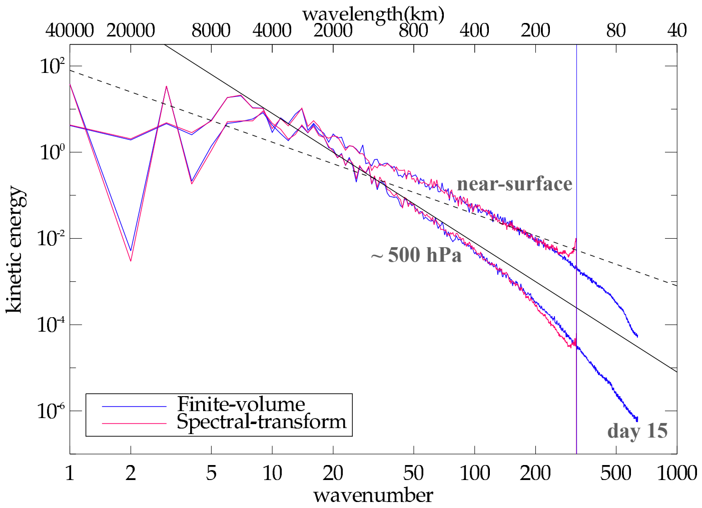
surface pressure (hPa) day 10

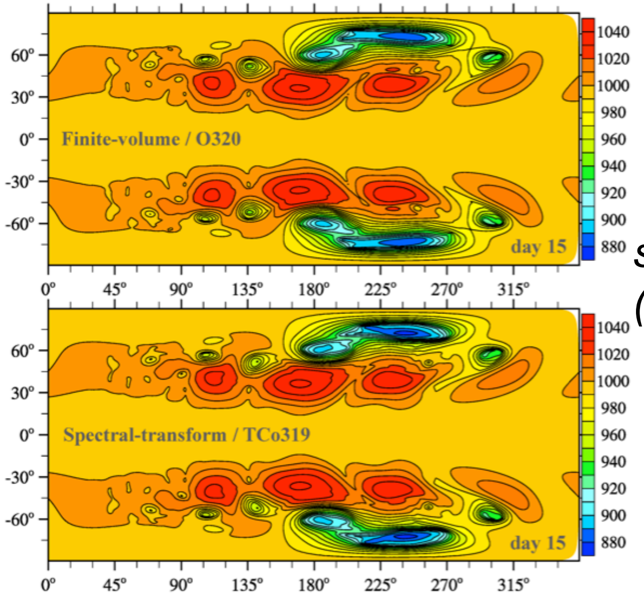


meridional wind (m/s) at 50N day 10



KE spectra

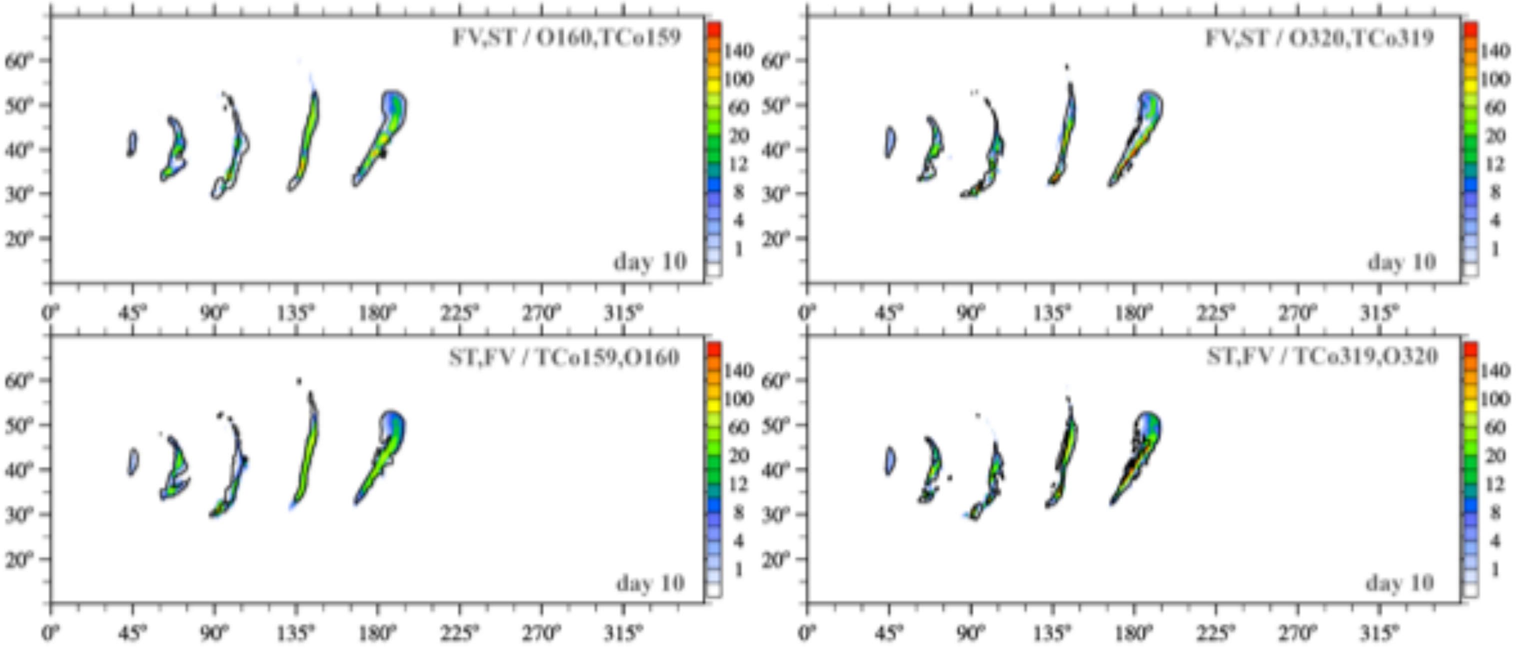




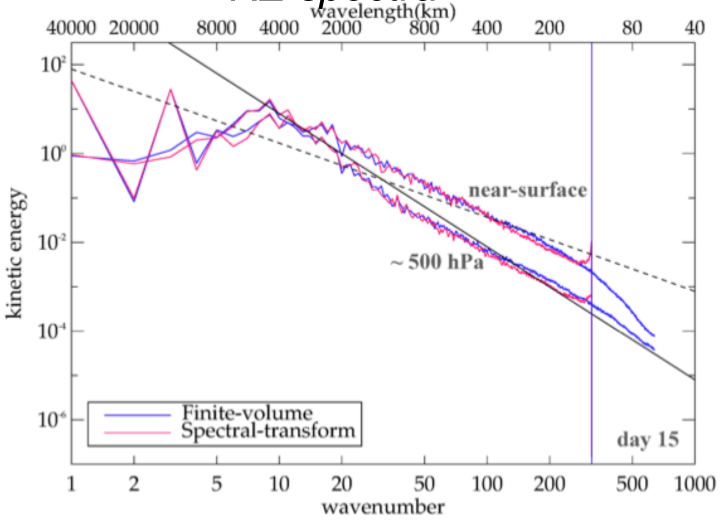
surface pressure (hPa) day 15

Finite-Volume Module of IFS: moist-precipitating dynamics and coupling to IFS physical parametrisations

precipitation rate (mm/day)



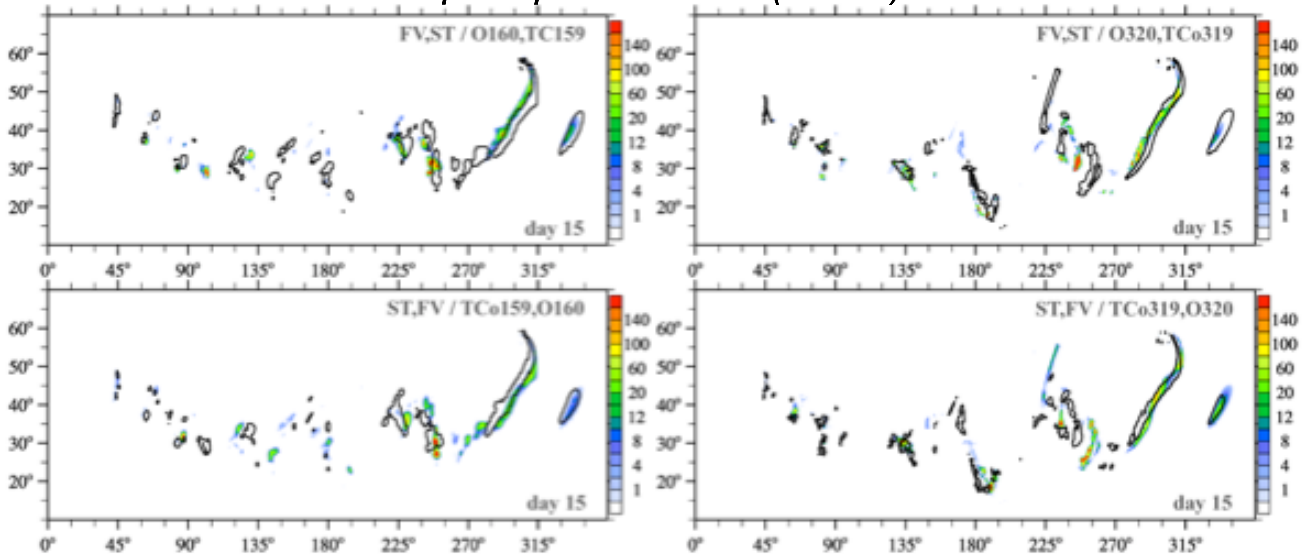
KE spectra



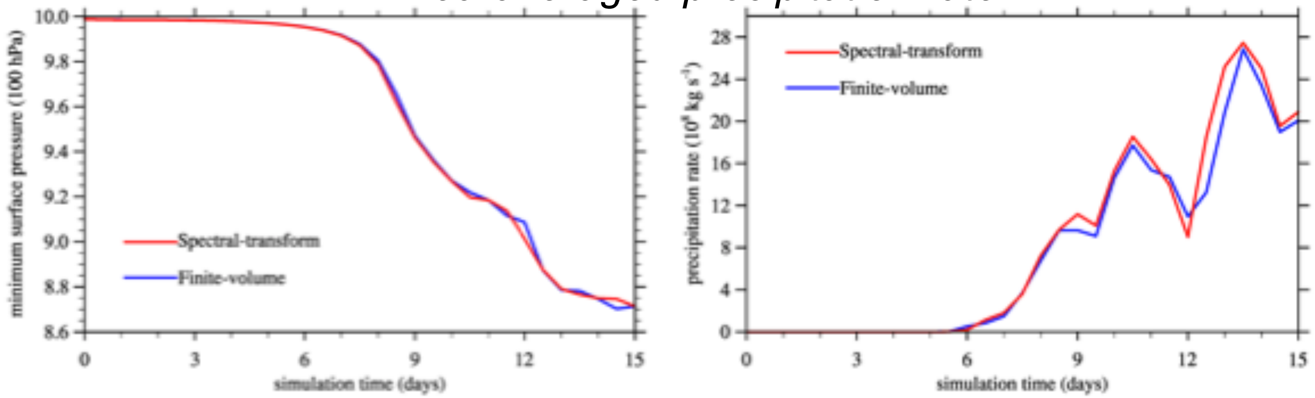
- IFS-FVM with comprehensive moist-precipitating dynamics and coupled to IFS cloud parametrisation by means of a generic interface with optional subcycling (Kühnlein et al. 2018)
- Ongoing research couples IFS-FVM to full IFS physics parametrisation package

Finite-Volume Module of IFS: moist-precipitating dynamics and coupling to IFS physical parametrisations

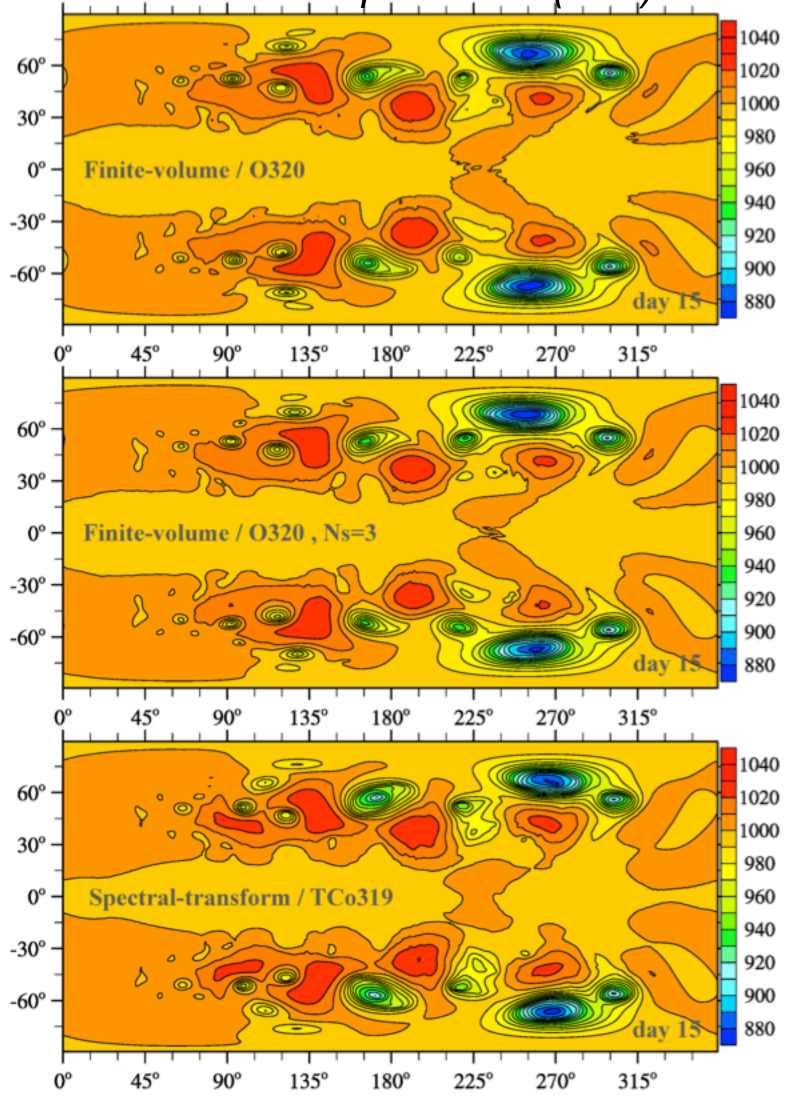
precipitation rate (mm/h)



Area-averaged precipitation rate



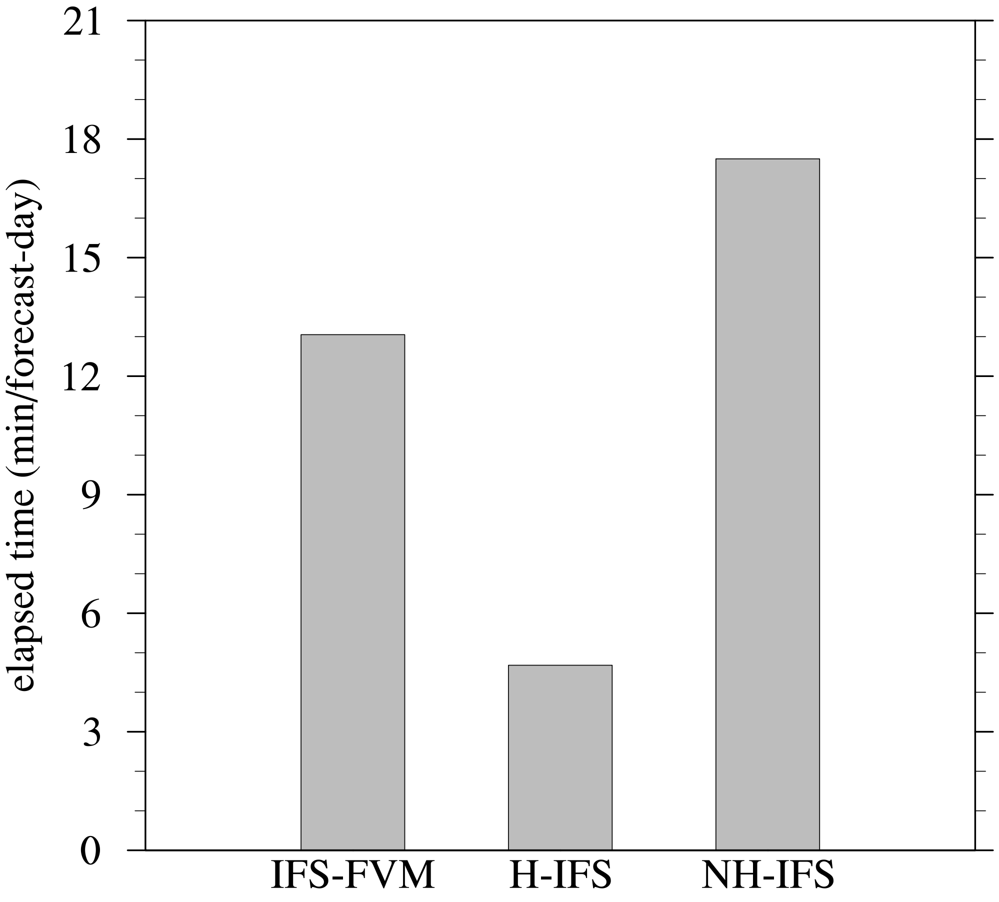
surface pressure (hPa)



Results for IFS-FVM coupled to IFS cloud parametrisation

Finite-Volume Module of IFS: computational efficiency

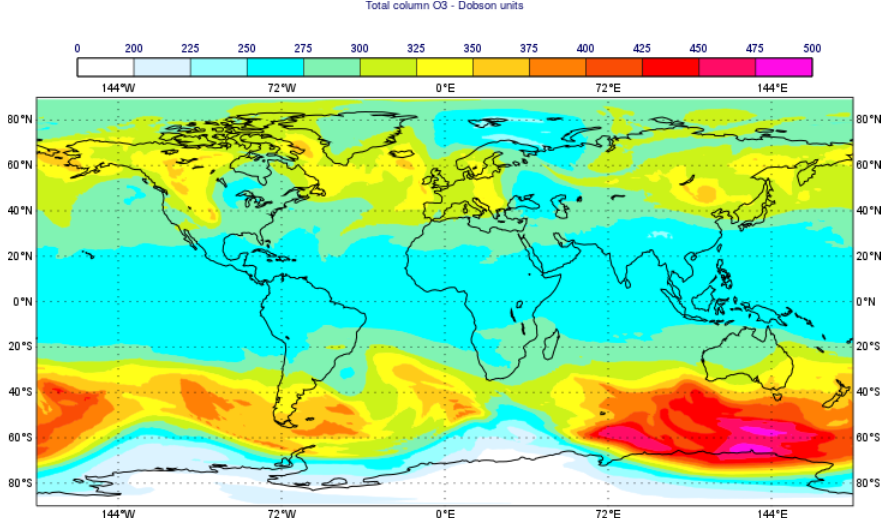
- IFS-FVM substantially improved in terms of computational efficiency (Kühnlein et al. 2018)
- improvement result of various developments, e.g. horizontal-vertical split advection scheme, preconditioning of elliptic solver, variable time step, coding implementation (cache, latency,…)
- IFS-FVM already faster then the nonhydrostatic spectral-transform IFS
- IFS-FVM still slower than the hydrostatic spectral-transform IFS, but gradually getting closer
- IFS-FVM is becoming competitive to current operational formulation while using local discretisation (and smaller time steps)



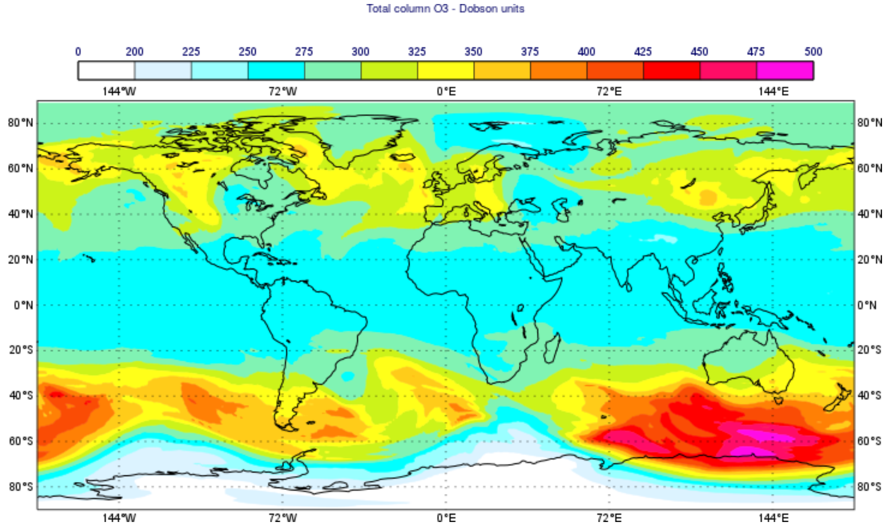
O1280/TCo1279 and L137 dry dycore on 350 nodes of ECMWF's Cray XC40

Atlas application in IFS: tracer transport on multiple meshes (SL versus MPDATA Finite Volume scheme)

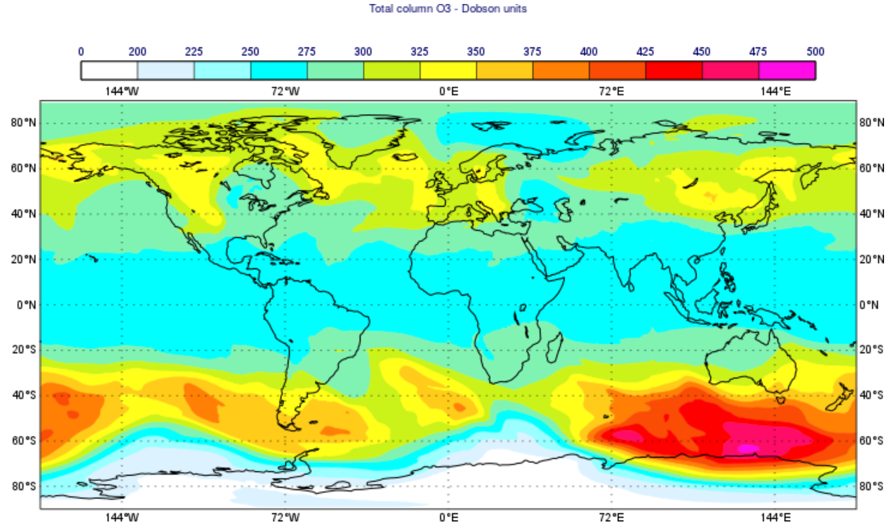
IFS-SL O3 advection at 9km grid



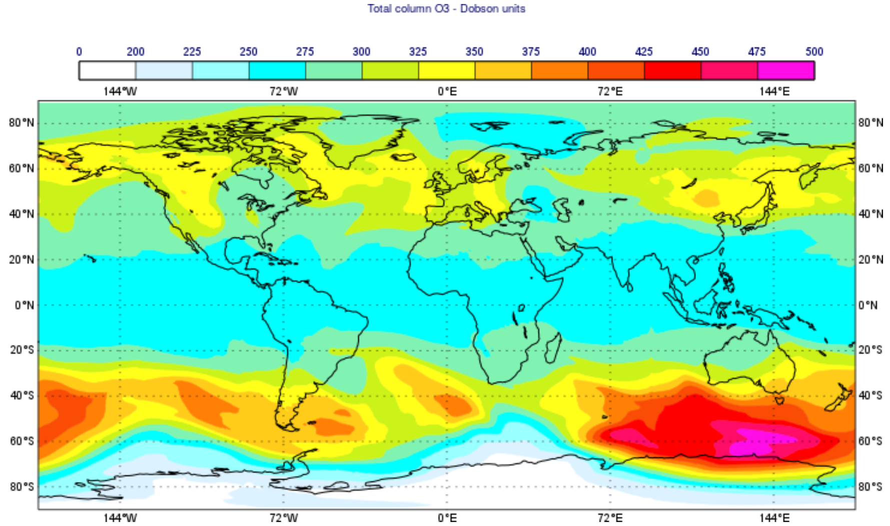
IFS-MPDATA O3 advection at 9km grid



IFS-Atlas-SL O3 advection at 25km grid



IFS-MPDATA O3 advection at 25km grid



- Model resolution of experiments 9km
- Atlas implementation of advection scheme(s) can run on a separate mesh driven by IFS winds
- The Atlas mesh can have same or lower resolution but the forcing (winds) are at model res (9km) and interpolated if necessary
- Choice of SL or finite volume (mass conserving) MPDATA scheme
- Currently only linear mesh-to-mesh interpolation available

T+7days total column ozone forecast field

ESCAPE project and NWP & Climate Dwarfs

This project is funded
by the European Union

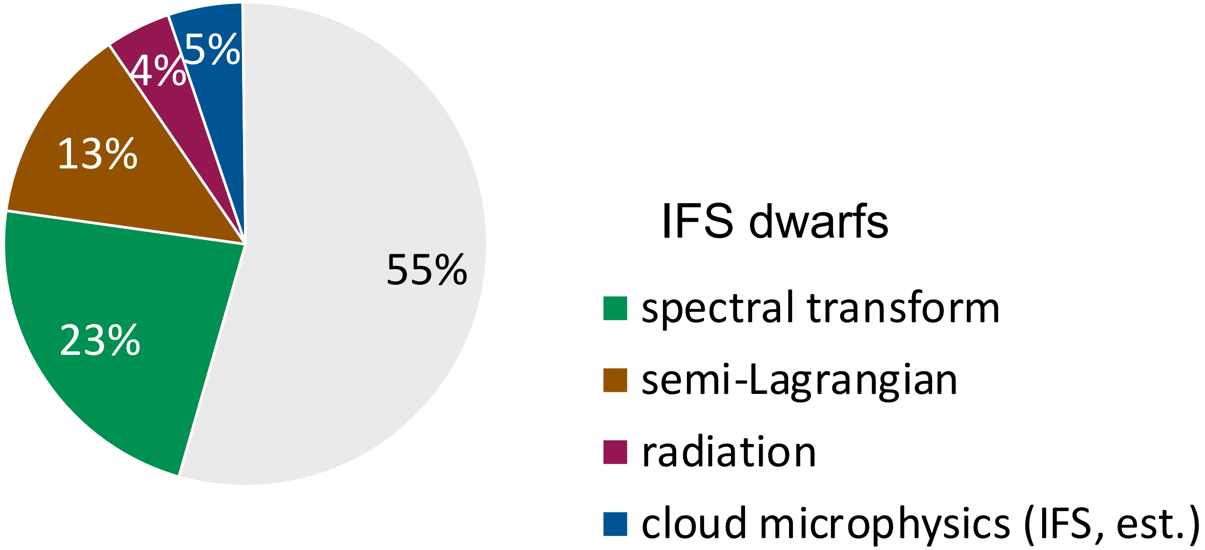
Energy efficient SCalable Algorithms for weather Prediction at Exascale

Disassemble global NWP model → **Extract, redesign key components "Dwarfs"** … **Optimize for energy efficiency on new hardware** … **Reassemble global NWP model**

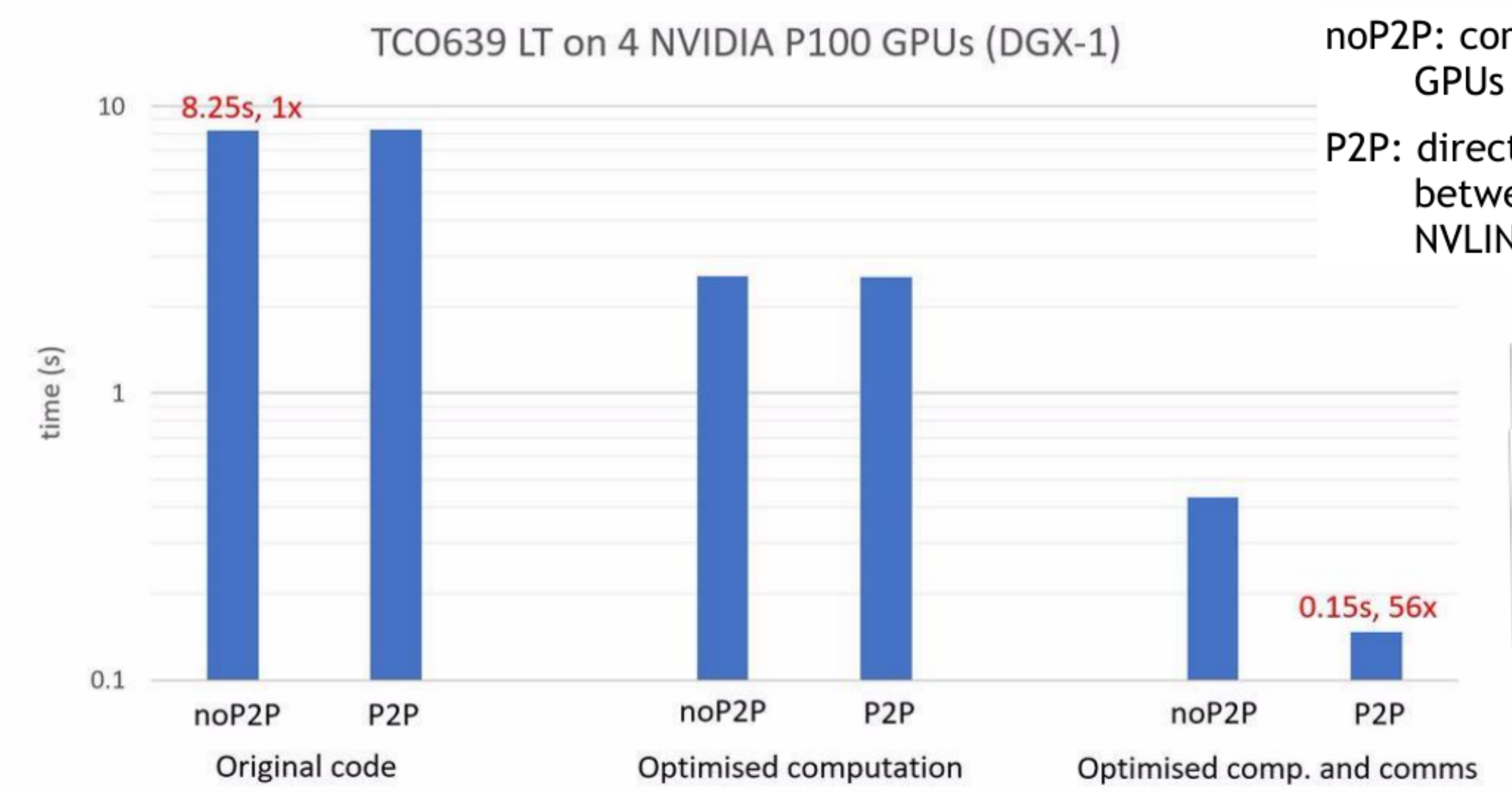
Weather & Climate Dwarfs encapsulate basic algorithmic motifs by breaking down numerical weather prediction legacy codes into key functional components - in analogy to the Berkeley Dwarfs.

Weather & Climate Dwarfs are distinctly motivated by the requirement to maximise computing performance, energy consumption, as well as time-and-cost-to-solution.

Time share of different IFS components as a percent of total run time



Can the spectral transform method overcome its efficiency limitations? GPU optimisations by NVIDIA



noP2P: communication between GPUs through host CPU

P2P: direct communication between GPUs through NVLINK

- 56x speedup for Legendre transform
- 23x speedup for entire spectral transform

figure: courtesy of Alan Gray, Peter Messmer (NVIDIA)

References

Smolarkiewicz P. K., C. Kühnlein, N. P. Wedi, A discrete framework for consistent integrations of soundproof and compressible PDEs of atmospheric dynamics., J. Comput. Phys., 2014.

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

Kühnlein C., P.K. Smolarkiewicz, An unstructured-mesh finite-volume MPDATA for compressible atmospheric dynamics. J. Comput. Phys. 2017.

Deconinck W., P. Bauer, M. Diamantakis, M. Hamrud, C. Kühnlein, G. Mengaldo, P. Marciel, T. Quintino, B. Raoult, P. K. Smolarkiewicz, N. P. Wedi, Atlas: The ECMWF framework to flexible numerical weather and climate modelling., 2017.

Smolarkiewicz P. K., C. Kühnlein, N. P. Wedi, Semi-implicit integrations of perturbation equations for all-scale atmospheric dynamics, J. Comput. Phys., 2018.

Kühnlein C., W. Deconinck, R. Klein, S. Malardel, Z.P. Piotrowski, P.K. Smolarkiewicz, J. Szmelter, N.P. Wedi, FVM 1.0: A nonhydrostatic finite-volume formulation for IFS, submitted to GMD.