Overview of dynamical core numerical method developments at ECMWF

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Many thanks to Numerical Methods team colleagues who provided input for this talk

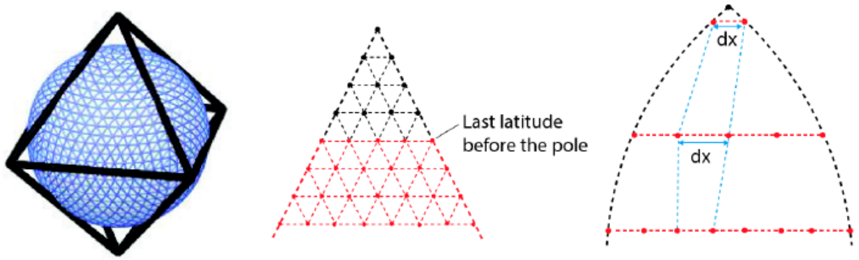
41st EWGLAM and 26th SRNWP meeting

Sofia 2019

ECMWF EUROPEAN CENTRE FOR MEDIUM-RANGE WEATHER FORECASTS

Spectral transform with semi-implicit semi-Langrangian (SISL) time-stepping

Grid-point computations (cubic grid)
- unconditionally stable SL advection
- physical parametrizations
- products of terms



FFT

Fourier space

LT

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

Inverse LT

Fourier space

Inverse FFT

FFT: Fast Fourier Transform, LT: Legendre Transform

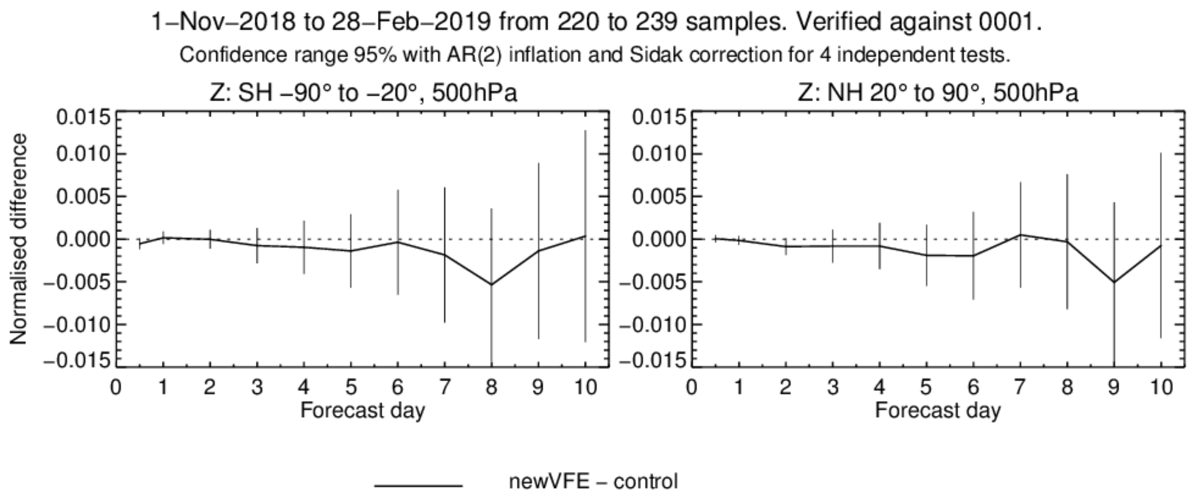
Vertical discretization

- Hybrid pressure based vertical coordinate $\eta(p)$
- Finite Element discretization based on cubic spline elements
- Accurate vertical integrations with noticeable positive impact in the stratosphere

(*Untch and Hortal, QJRMS 2004*)

New VFE for H/NH in IFS in collaboration with member states

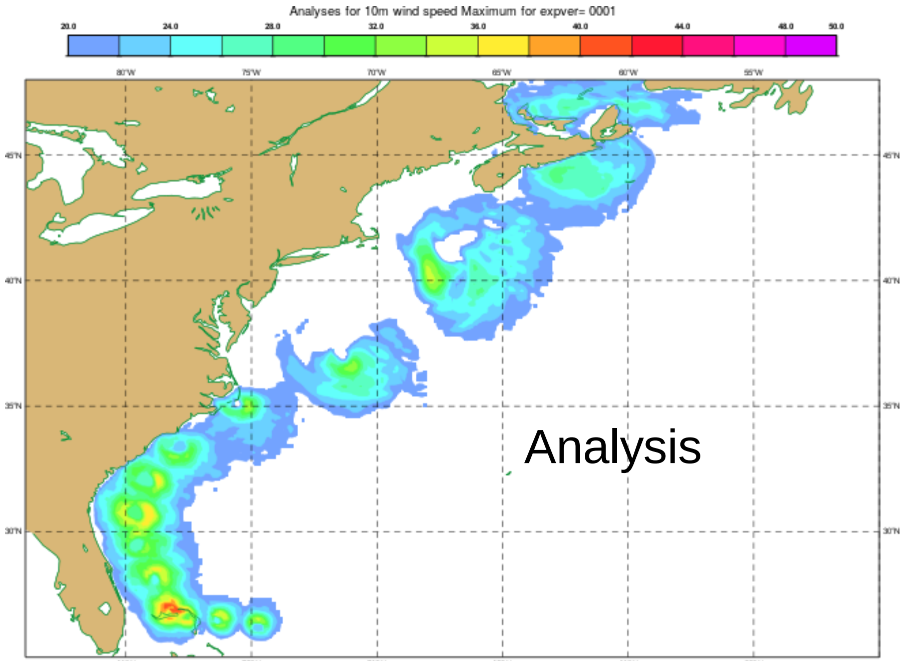
- *Hydrostatic-IFS: Finite Element discretization in the vertical (VFE)*
- *NH-IFS: Finite Difference vertical discretization (applying FE to NH not straightforward due to C1 constraint)*
- *New VFE (Vivoda, Smolikova, Simarro MWR 2018) overcomes "C1 condition" restriction at the price of a small computational overhead:*
  - *A single code base for a unified H & NH version that is stable and can have order of up to 12*
  - *Allows use of single precision in high order*
  - *Having the same discretization for both H and NH model will allow use of same numerics and "fair" straightforward comparisons between the two formulations*

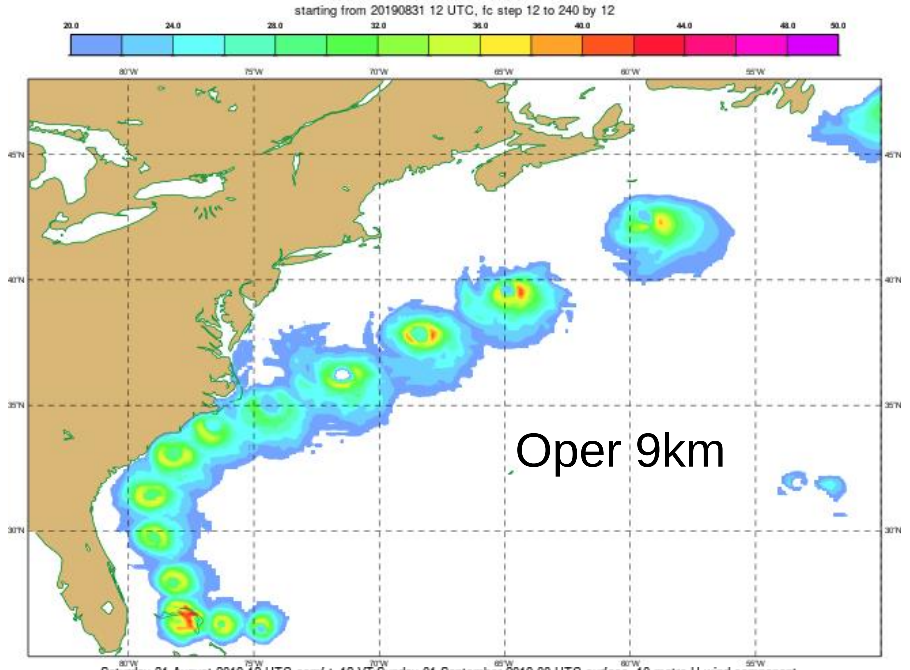


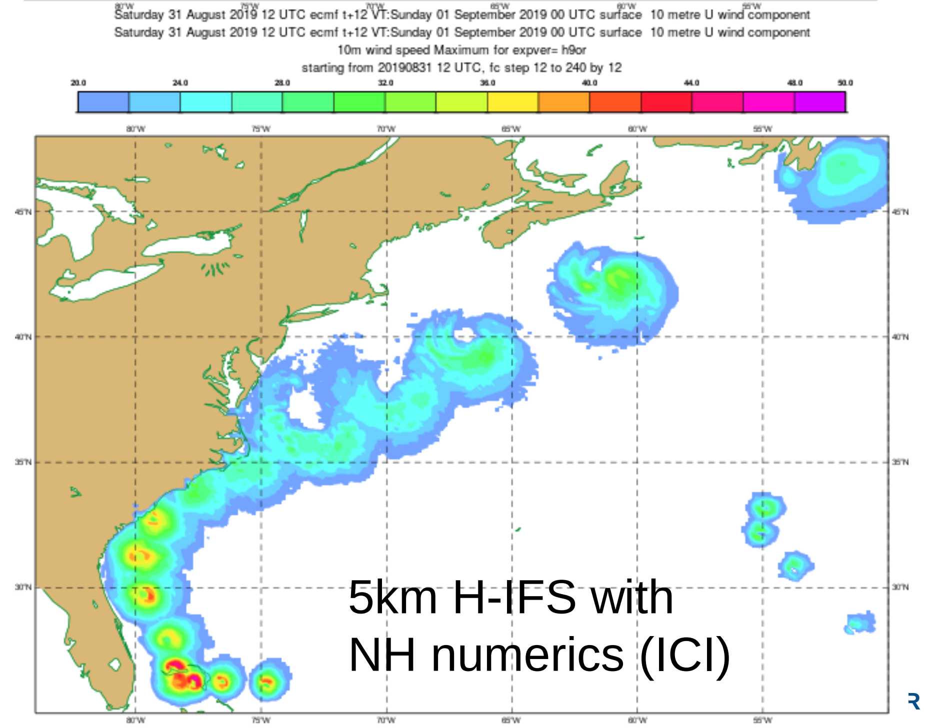
Many thanks to J. Vivoda (SHMU) who visited ECMWF to couple this new VFE scheme with the global spectral IFS

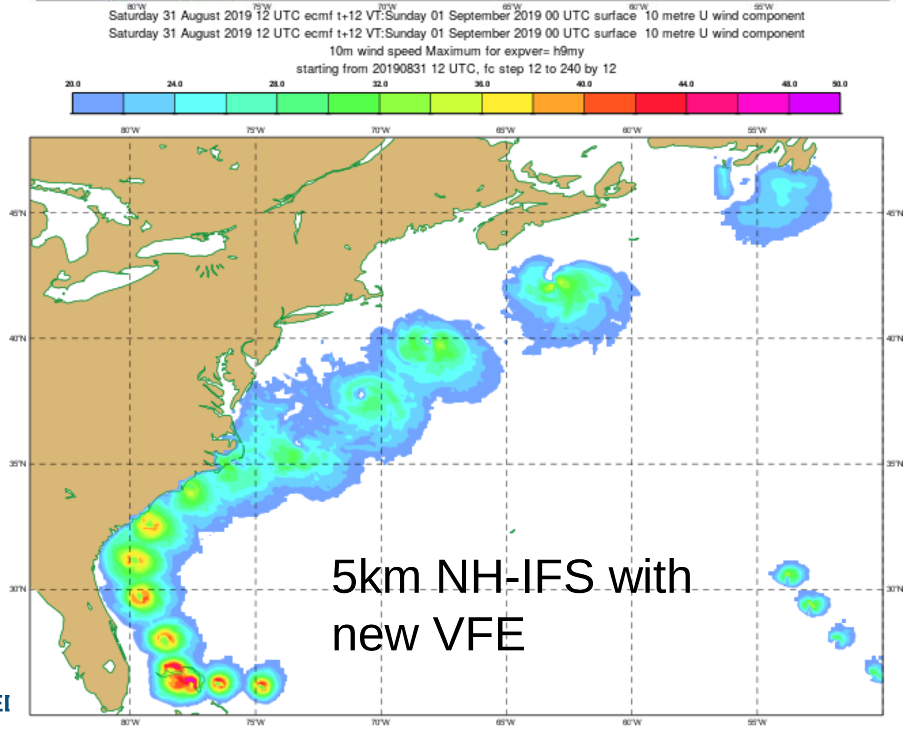
New VFE compared with current scheme in the hydrostatic model:

- Same cost
- Neutral scores
- High order VFE gave neutral scores
- At 30km res temperature RMSE reduces in the stratosphere (but note resolution dependence of IFS temperature biases)
- New VFE could be adopted and replace current one (future work)









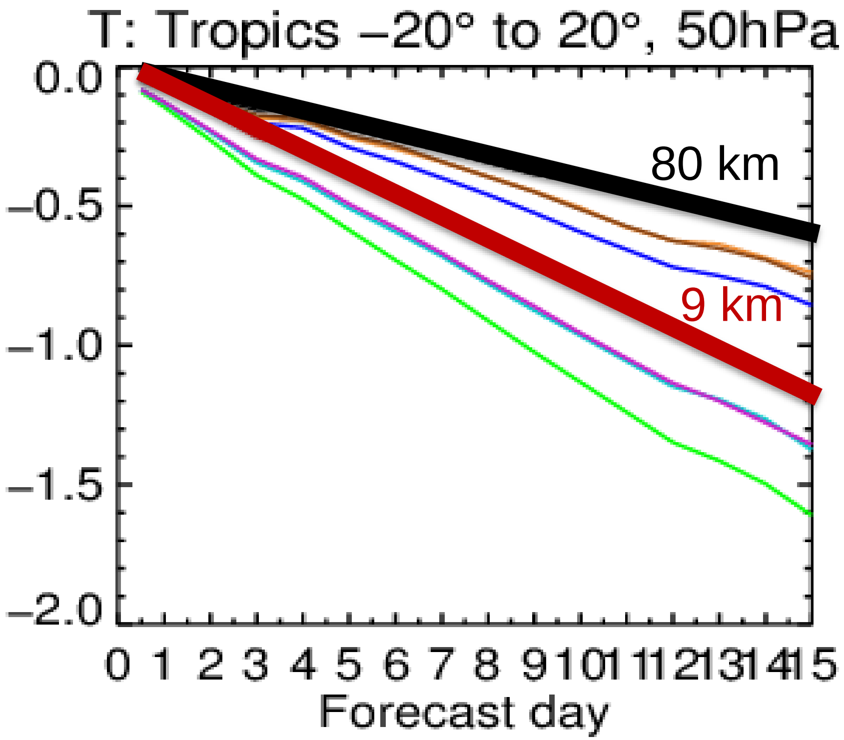
Hurricane Dorian forecast initialised from 31-08-2019 operational analysis

- H and NH give same track and intensity
- Track appears slightly improved at 5km resolution

Horizontal resolution sensitivity of temperature biases

Stratosphere cools in the global mean with increase **in horizontal resolution** → biases **worse** in the lower- to mid- stratosphere with increase in horizontal resolution. Affects all forecast ranges, from medium to seasonal *(Polichtchouk et al ECMWF TM 847)*.

Resolved dynamics the culprit. Forecasts with no physical parametrizations, show the same horizontal resolution.



Verification against analysis

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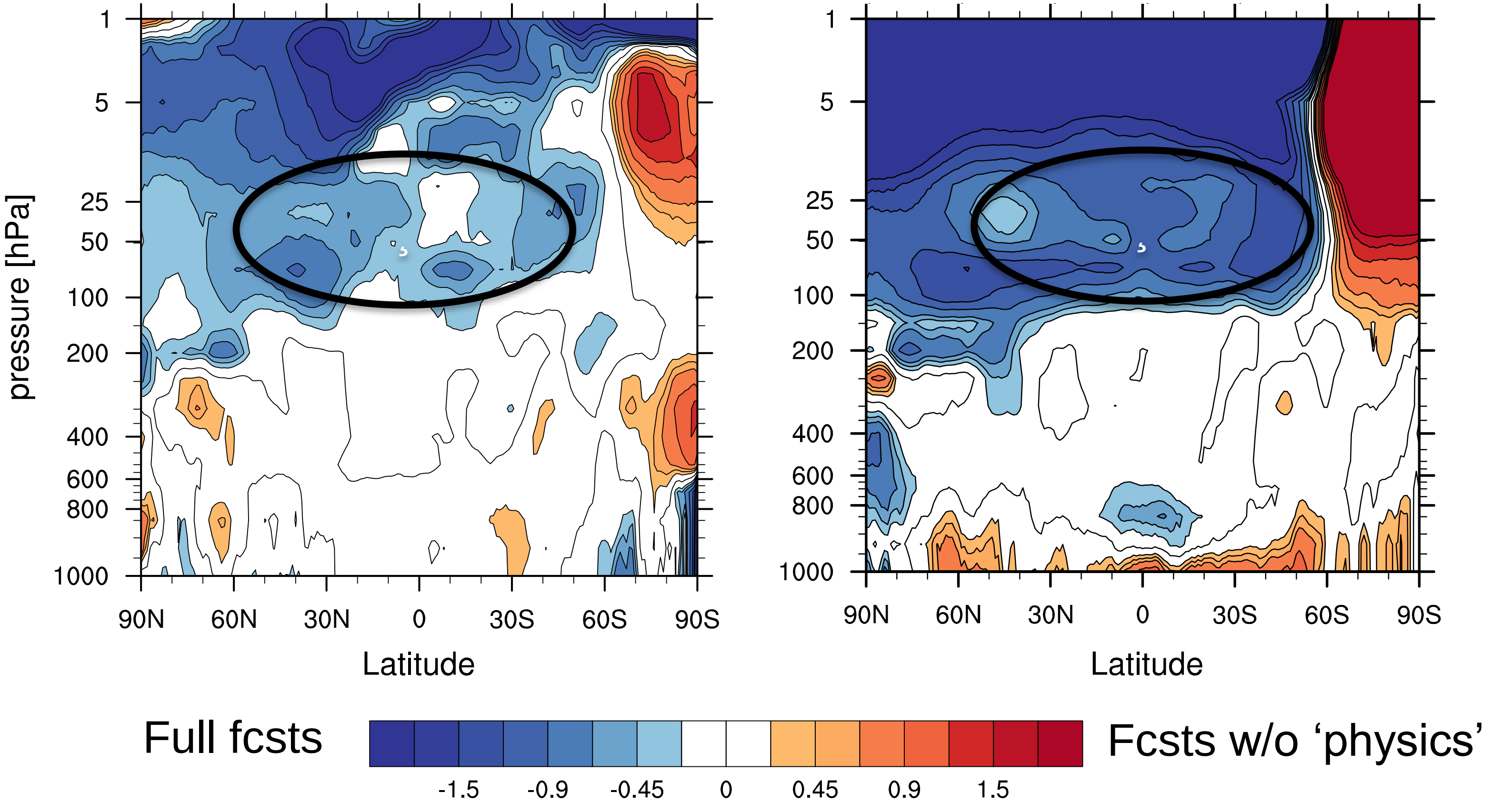
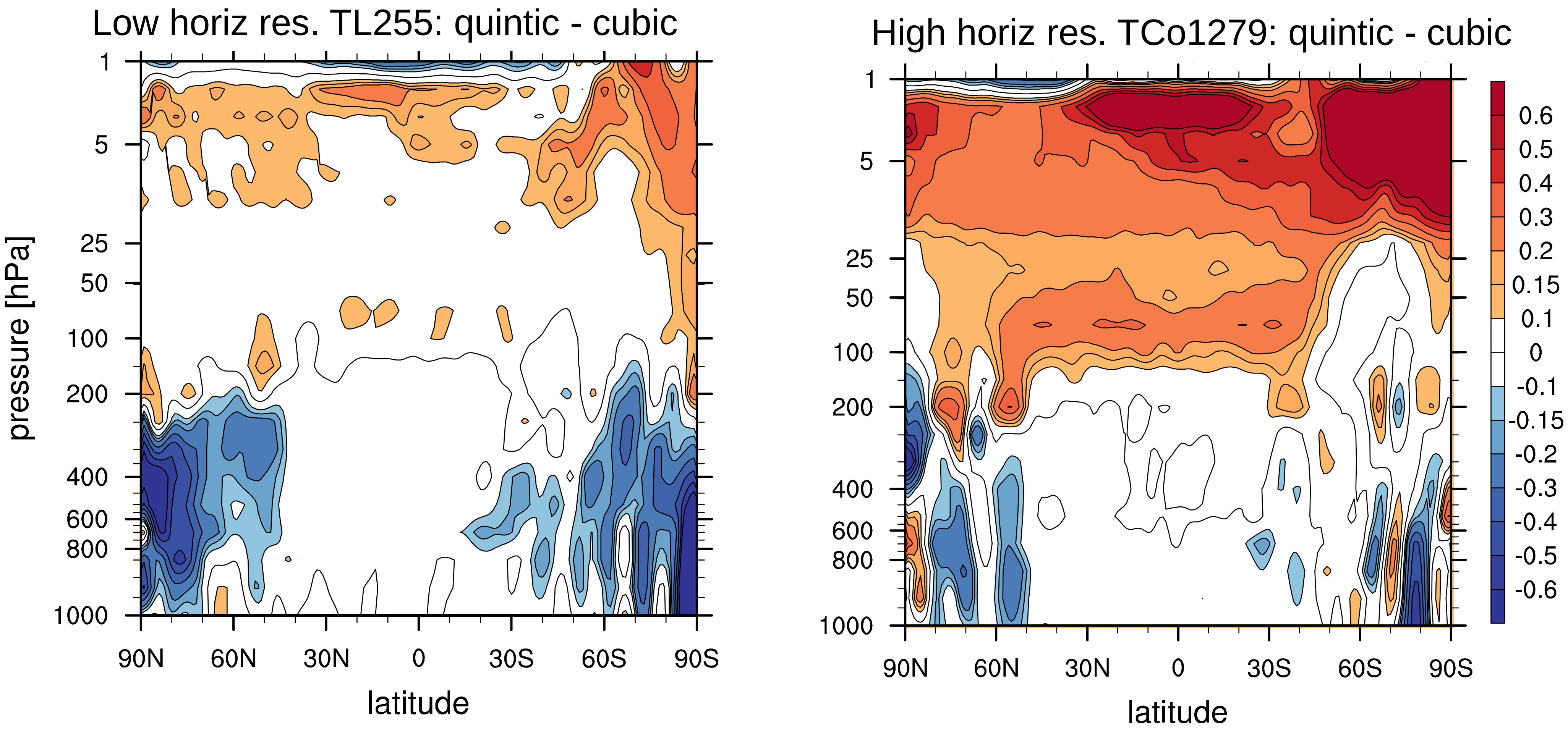
T [K]: 9 - 80km 10day fc for July



Higher order vertical semi-Lagrangian (SL) interpolation

Does improving accuracy of vertical semi-Lagrangian advection help?

Going from **3rd to 5th** order vertical interpolation helps → Stratosphere warms with higher order interpolation at high horizontal resolution.



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Slide courtesy of Inna Polichtchouk

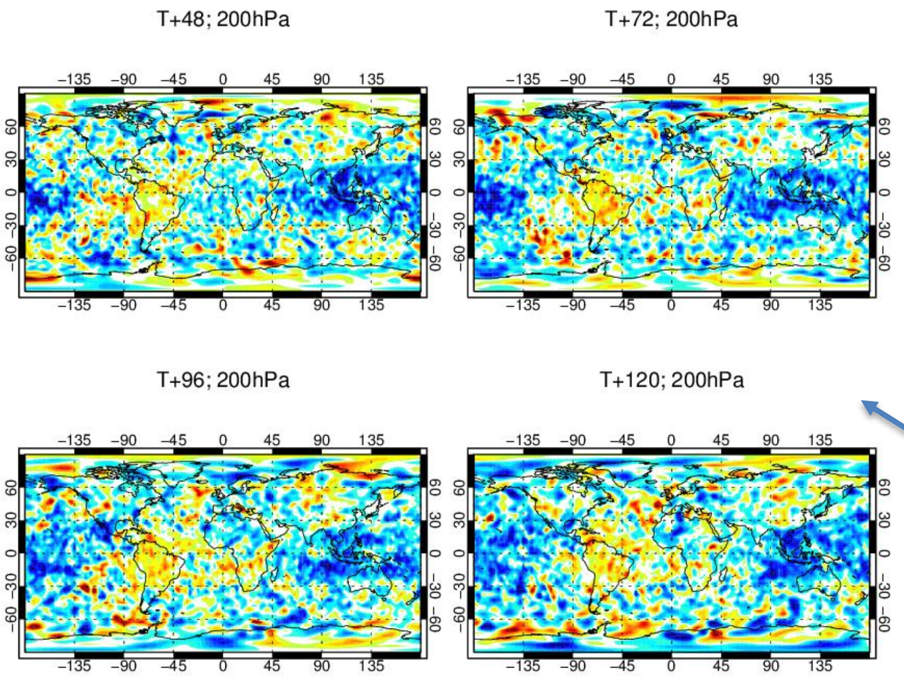
High order departure point calculation scheme option for CY47R1

Available in 47r1 (implemented by F. Vana)

Lobato IIIA Runge-Kutta for DP: similar properties as Crank-Nicolson but higher order

- 4th order
- A-stable
- Symmetric
- Requires solution of two implicit stages which is done iteratively as the SETTLS scheme (but twice more expensive)

0	0	0	0
1/2	5/24	1/3	−1/24
1	1/6	2/3	1/6
	1/6	2/3	1/6



Initialise with an explicit method and then iterate:

$$\mathbf{r}_M^{(l)} = \mathbf{r}_A - \frac{\Delta t}{24}\left[5\mathbf{V}^{t+\Delta t}(\mathbf{r}_A) + 8\mathbf{V}^{t+\Delta t/2}(\mathbf{r}_M^{(l-1)}) - \mathbf{V}^{t}(\mathbf{r}_D^{(l-1)})\right]$$

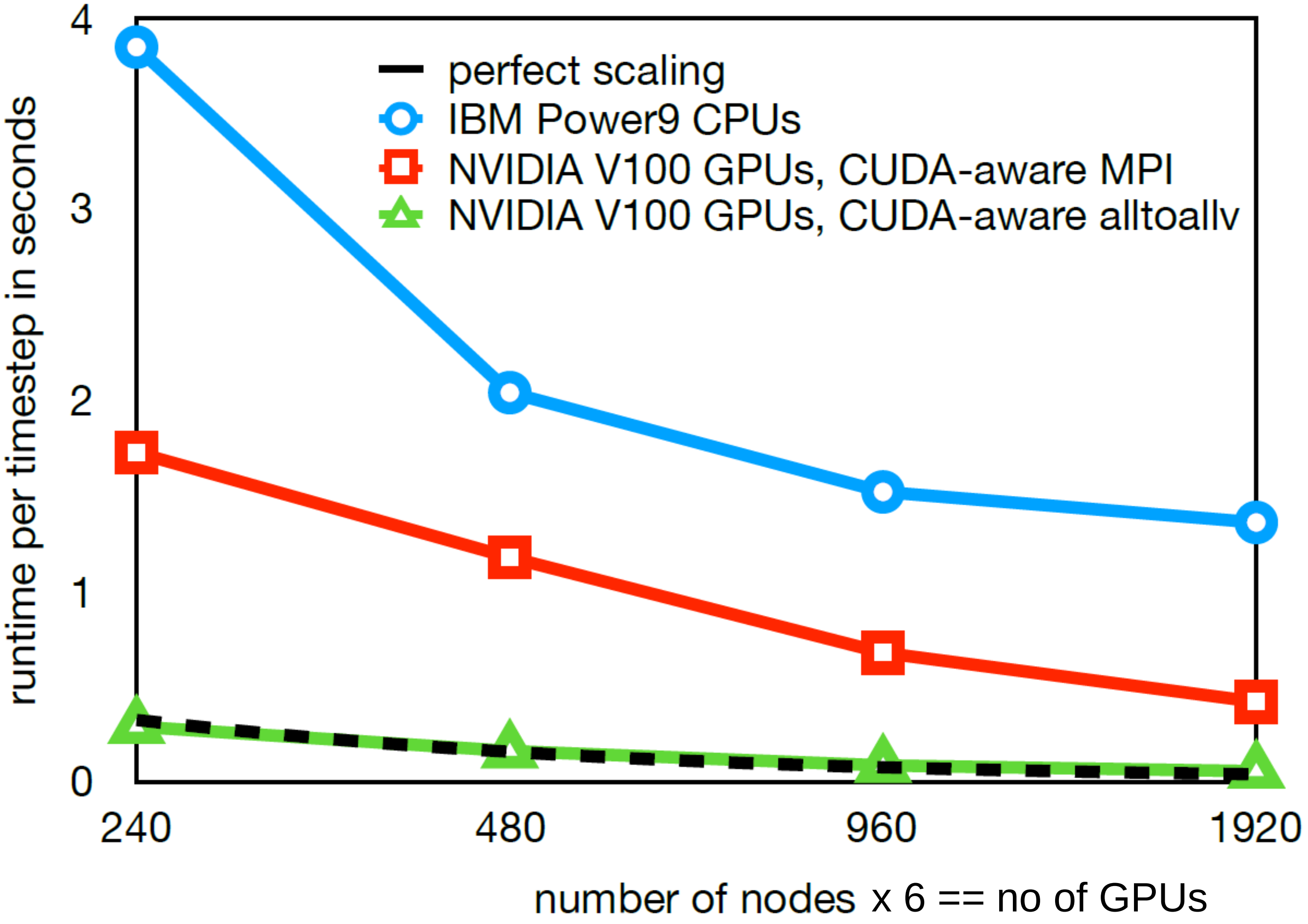
$$\mathbf{r}_D^{(l)} = \mathbf{r}_A - \frac{\Delta t}{6}\left[\mathbf{V}^{t+\Delta t}(\mathbf{r}_A) + 4\mathbf{V}^{t+\Delta t/2}(\mathbf{r}_M^{(l)}) + \mathbf{V}^{t}(\mathbf{r}_D^{(l-1)})\right], \qquad \ell = 1, 2, \ldots$$

- RK4 with quadratic wind interpolation (at M, D) in above iterations
- Research experiments at ~30km res are overall neutral but show some improvement at 200 hPa temperature
- Extra cost ~ 10% mainly due to quadratic wind interpolation

Optimizing spectral transforms on GPUs: results from stand alone dwarf

- At high resolution the communication and overall computational cost of spectral transforms rises considerably
- At 2.5km resolution, the time-step must be less than 1s to fit operational requirements including communication cost of the transpositions

Slide courtesy of Andreas Mueller based on optimizations by Alan Gray (NVIDIA)



This research used resources of the Oak Ridge Leadership Computing Facility, which is a DOE office of Science User Facility supported under contract DE-AC05-00OR22725.

IFS-FVM main features

Finite-volume (uniformly second-order accurate in space-time)

Deep-atmosphere nonhydrostatic fully compressible equations in perturbation form

Fully conservative and monotone advective transport

Shares important properties with IFS-ST (co-located, octahedral grid, physical parametrisations,..)

FVM numerical framework is flexible (curvilinear coordinates, mesh, time-stepping, governing equations, domain)

"Light" communication overhead due to local stencils as opposed to global com heavy IFS-ST

FVM uses Atlas library (parallel data structures, mesh generator, memory management,…), which will greatly facilitate adaptation to future HPC systems

FVM so far delivered at least similar solution/forecast quality to IFS-ST on standard test and shows potential for high computational efficiency

Governing fully compressible NH IFS-FVM equations

Flux-form fully compressible eqns with moist precipitation processes and IFS phys parametrizations (Kühnlein et al. GMD 2019):

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

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

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

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

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

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

with:

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

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

$\mathcal{G}$: coordinate transformation Jacobian

v: contravariant velocity

θ': potential temperature perturbation from an ambient state a

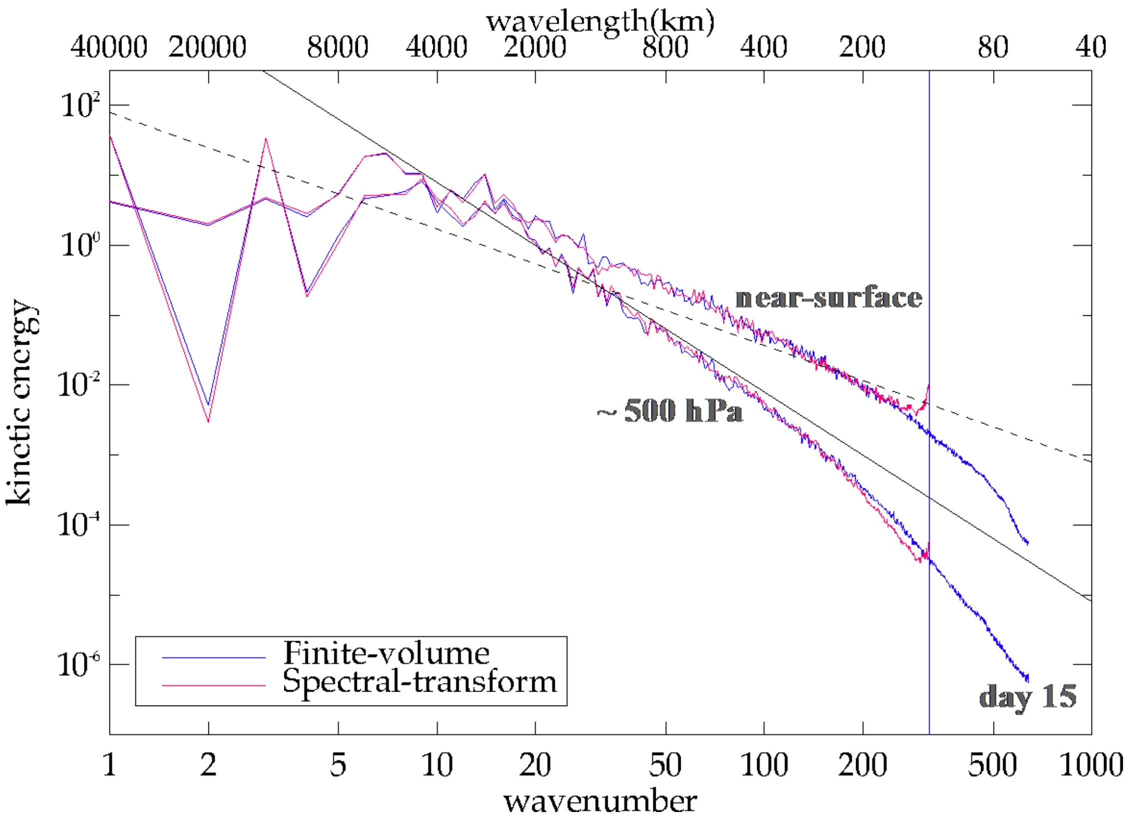
φ': Exner pressure perturbation from an ambient state a

M' : contains metric forces

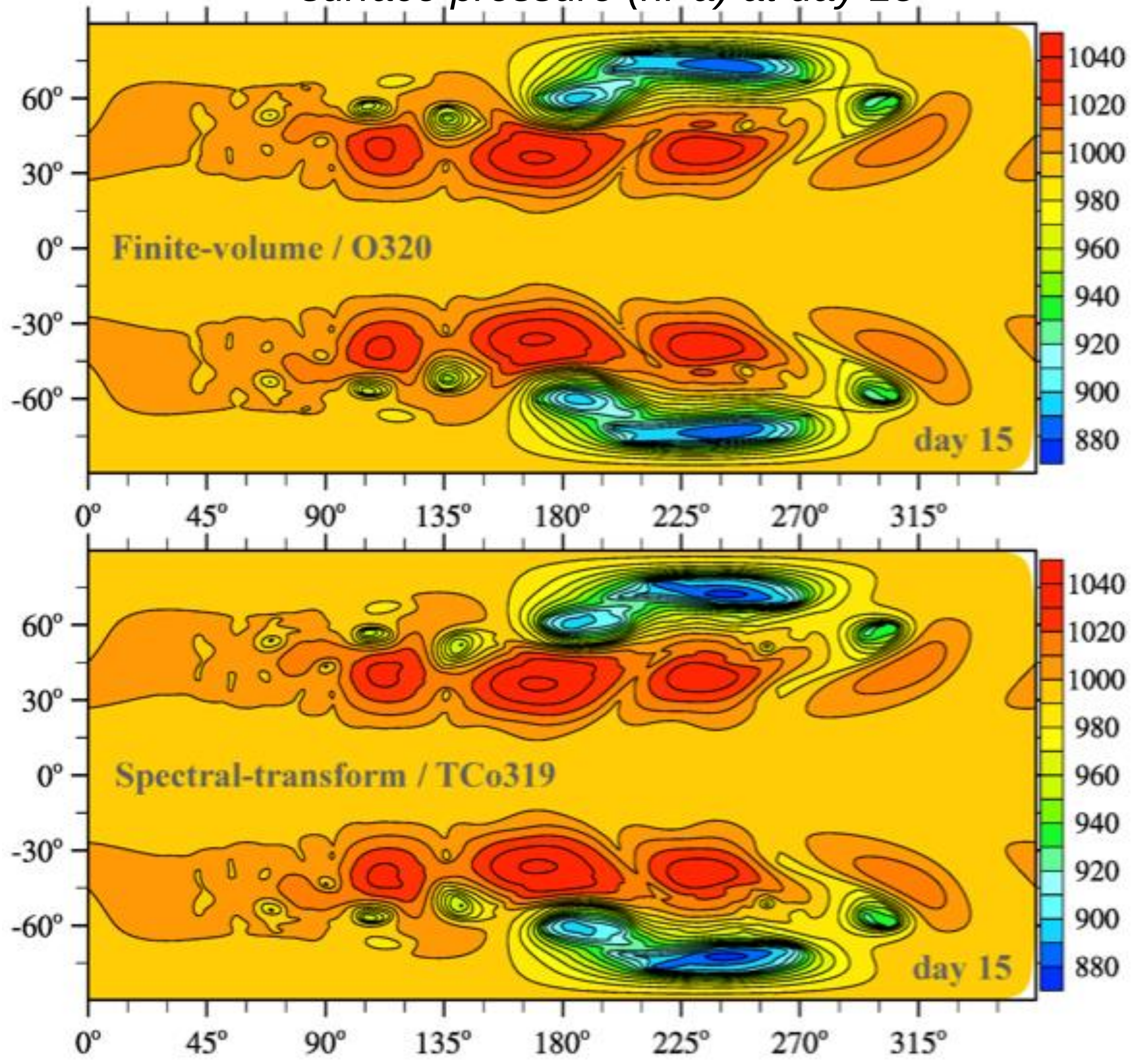
r_k : moist species mixing ratios

IFS-FVM comparison to hydrostatic IFS-ST: dry adiabatic dynamics

KE spectra with O320/TCo319 at day 15



surface pressure (hPa) at day 15



32km

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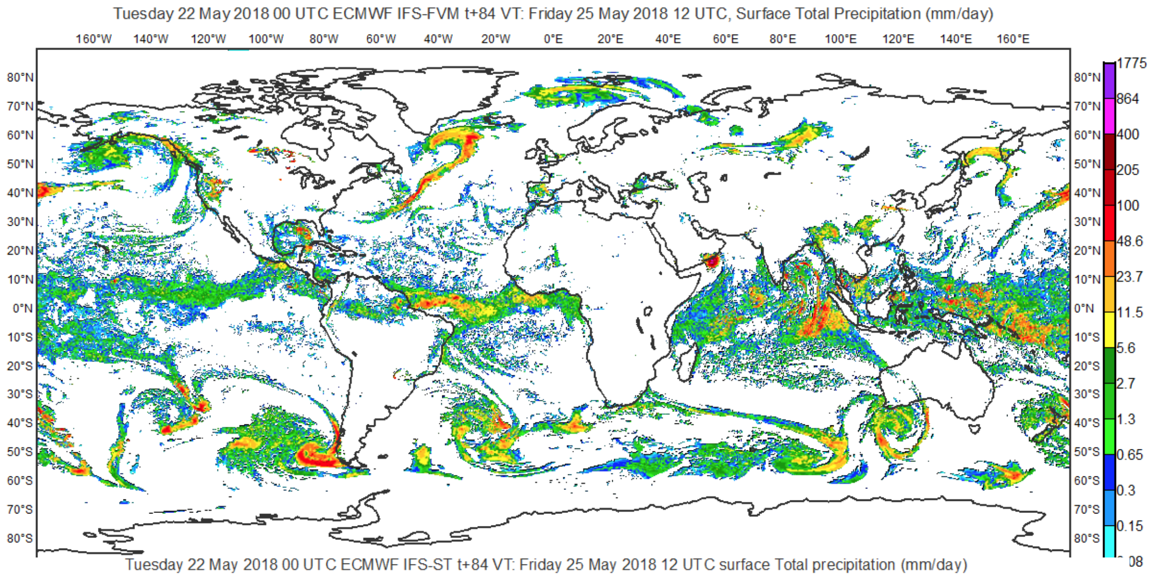
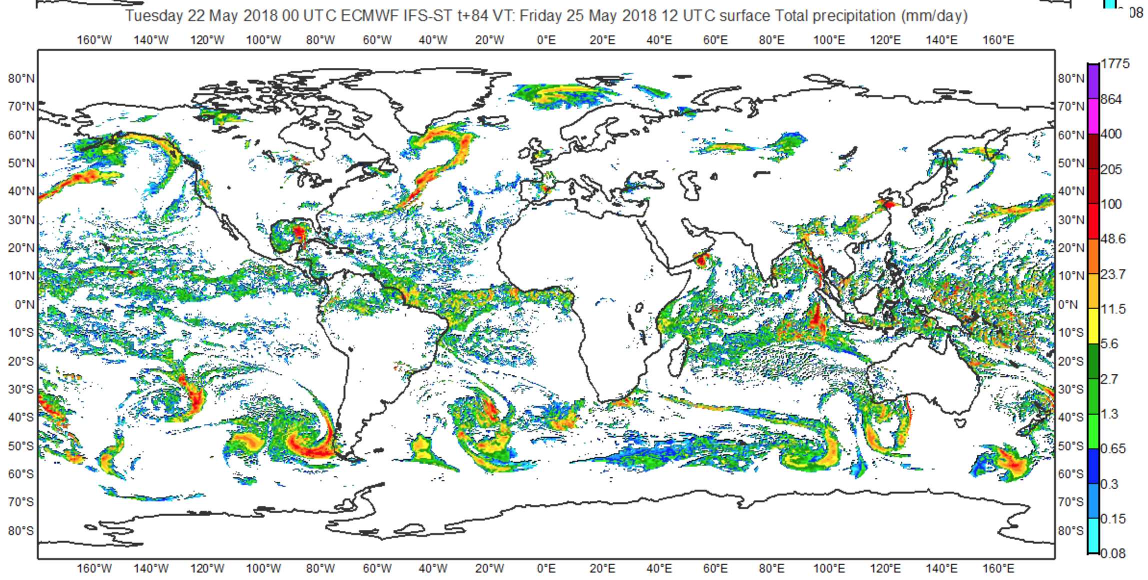
First IFS-FVM real weather forecasts experiments from ECMWF analysis



IFS-FVM

Same initial conditions and physics with operational IFS-ST are used



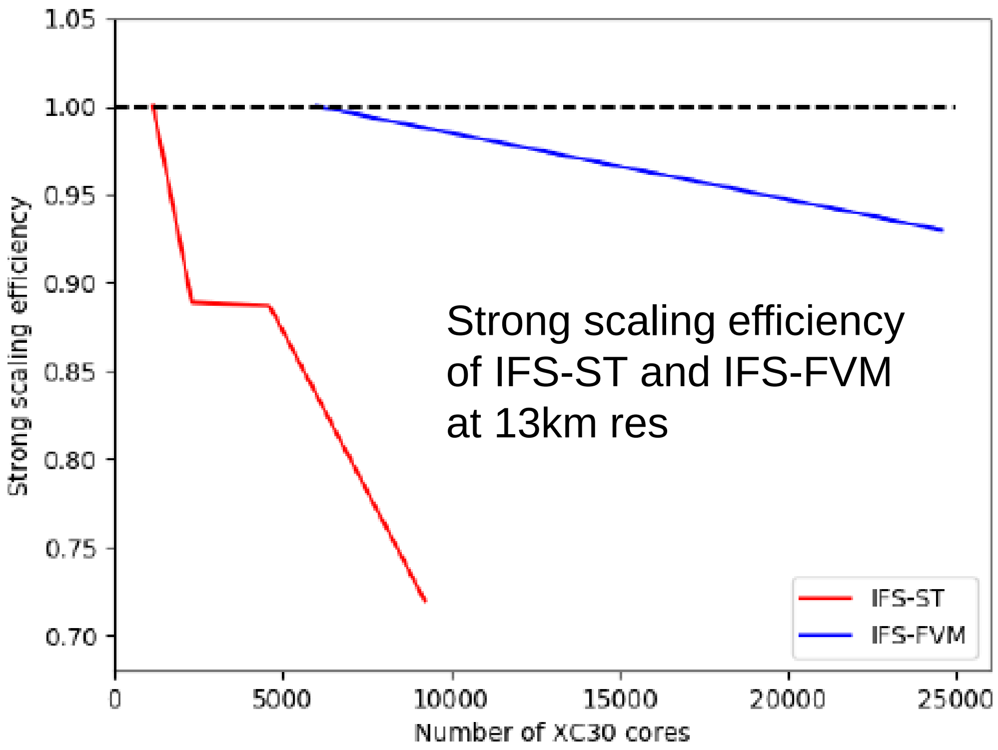
Stratiform+convective surface precipitation rate (mm/day) at t+84h using O640(18km)/L62

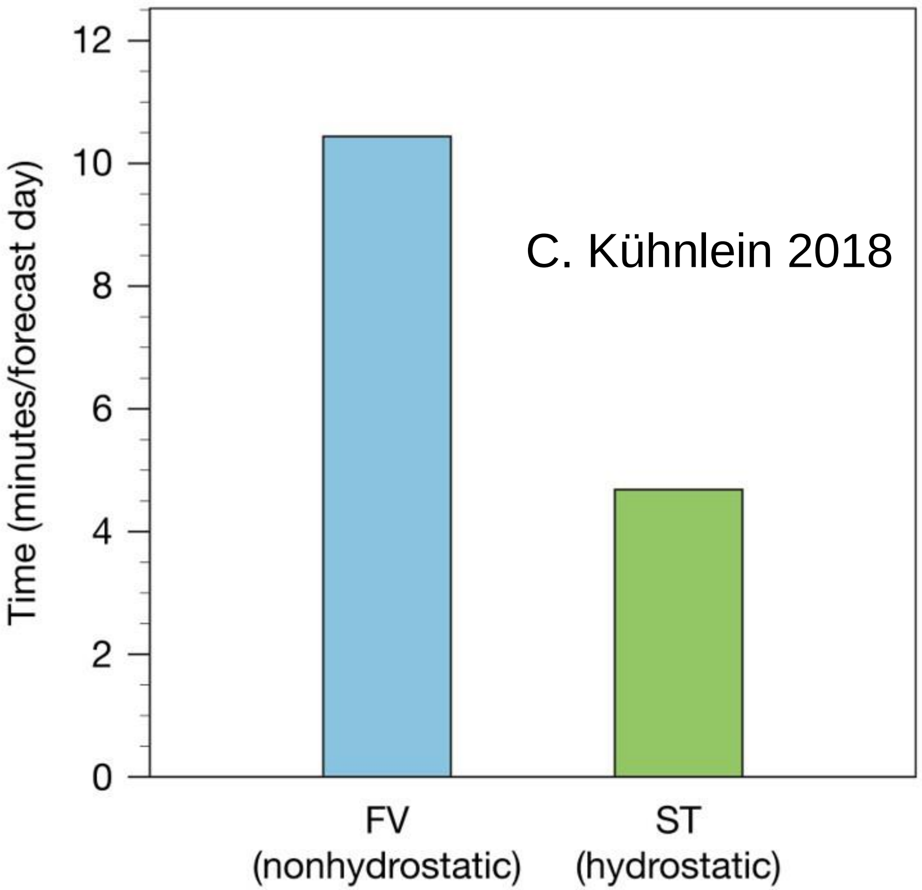
IFS-ST

Slide courtesy of C. Kühnlein

Snapshot of computational efficiency: IFS-FVM vs IFS-ST

- Dry baroclinic instability experiments in identical configuration O1280/TCo1279 (9km) with L137
- Time steps of IFS-FVM were a factor of 6-7 smaller than IFS-ST
- IFS-FVM factor 2 slower than hydrostatic IFS-ST
- IFS-FVM faster than nonhydrostatic IFS-ST



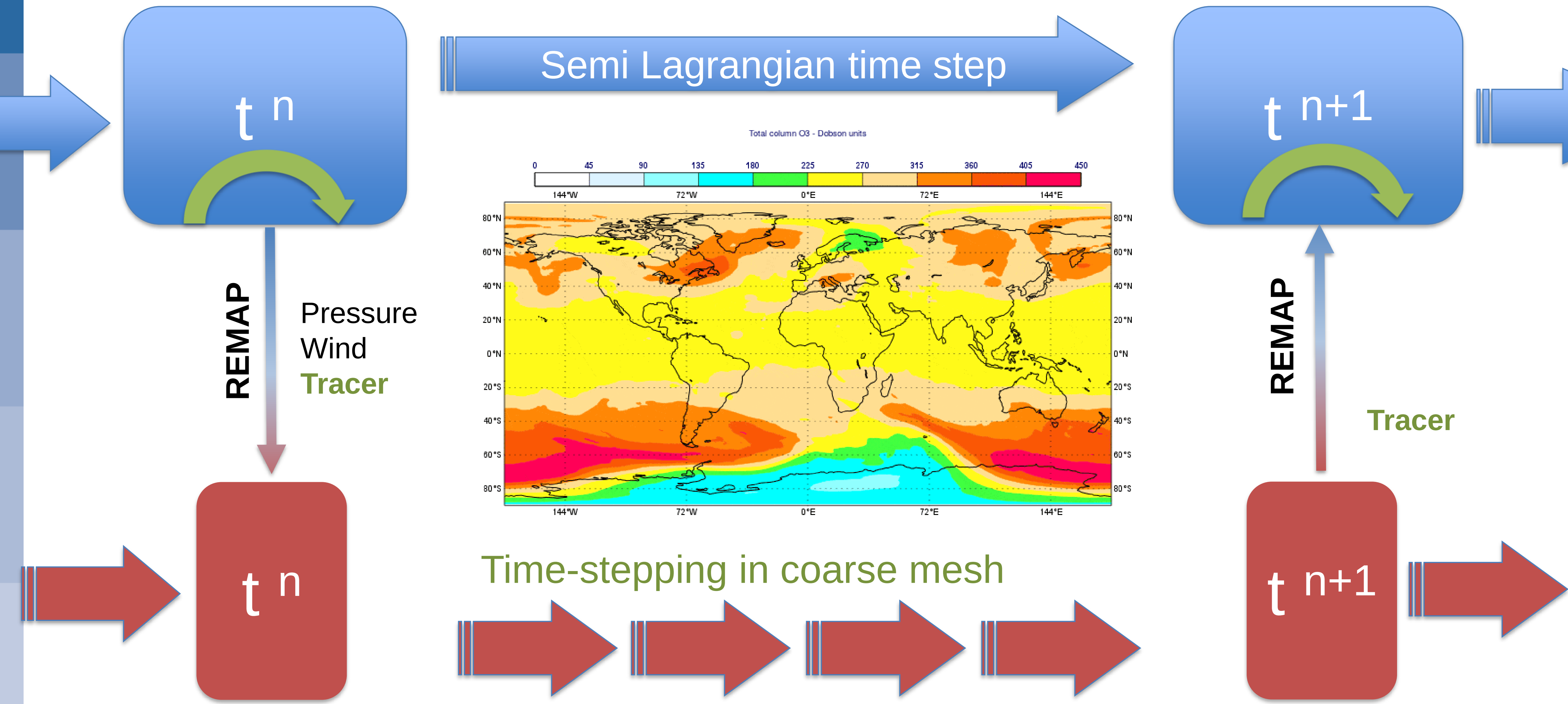


O1280/TCo1279 with L137 dry dycore on 350 nodes of ECMWF‘s Cray XC40

Atlas and multiple grids

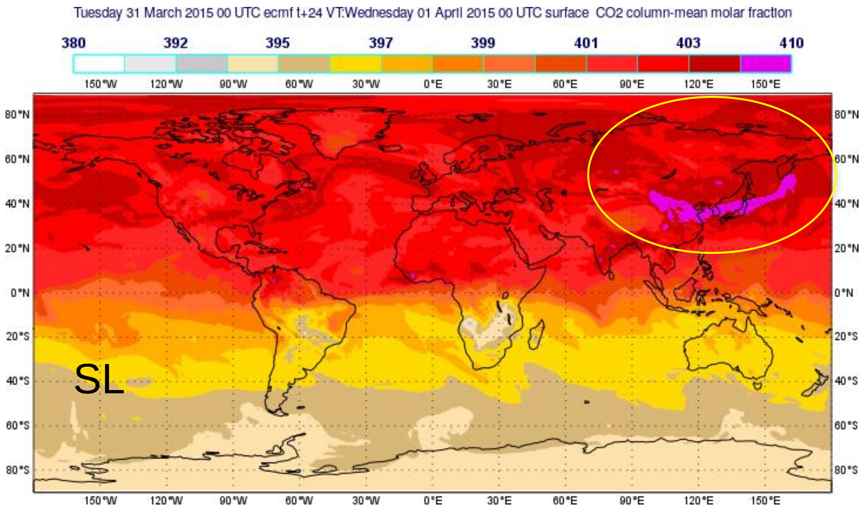
- Atlas (Deconinck et al, 2017):
  - provides flexible data structures, grid/mesh generation capabilities
  - mathematical operators for NWP & climate modelling software developments in a parallel HPC environment
  - *Accelerator ready:* functionality to facilitate computation on GPU hosts
- It is the basis for new developments:
  - FVM dynamical core developed in Atlas
  - *Underpins work to produce an IFS version which can seamlessly run on either traditional CPU or heterogenous with accelerators (GPUs) architectures*
  - Using its newly developed multiple grids feature allows to combine in a “non-intrusive” way different tracer transport schemes (dynamical core components)
  - In 46R1 we have developed a prototype for testing tracer transport driven by IFS winds using MPDATA (transport scheme of FVM) or SL advection at a mesh which may have same or different resolution. Eventually the aim of this work is to run expensive processes such as chemistry at a lower resolution grid

Transport on multiple grids: ozone transport at 32km grid forced by winds from a 18km model

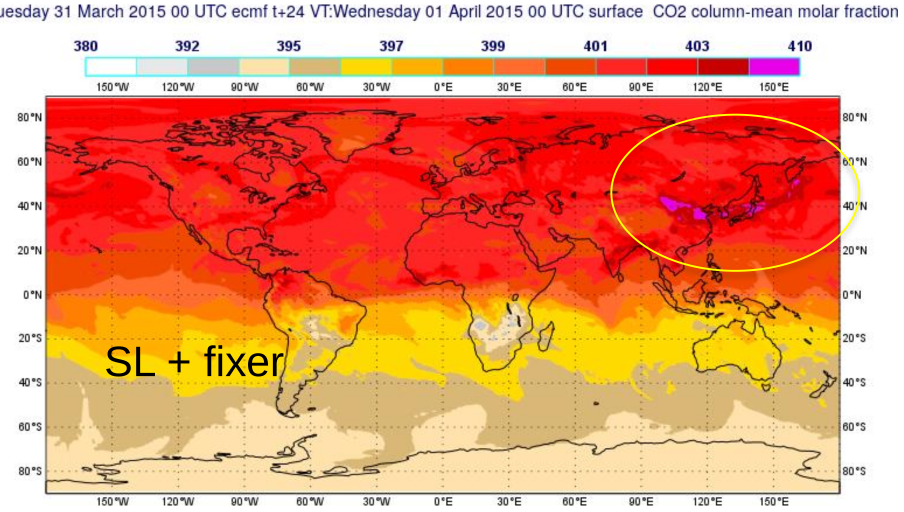


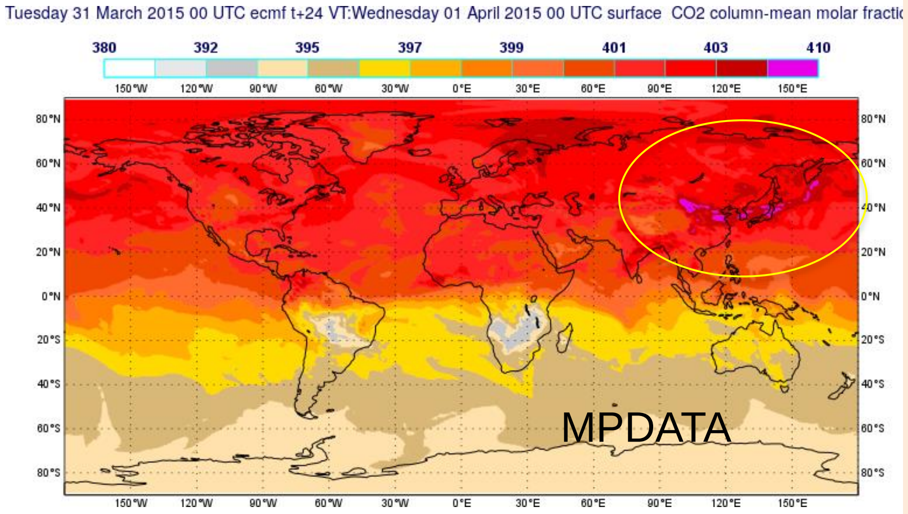
Remapping using linear or cubic interpolation (animation courtesy of W. Deconinck)

IFS with MPDATA CO2 tracer transport (Atlas multiple same resolution grids)



Total column CO2 after 90 days (18km res)

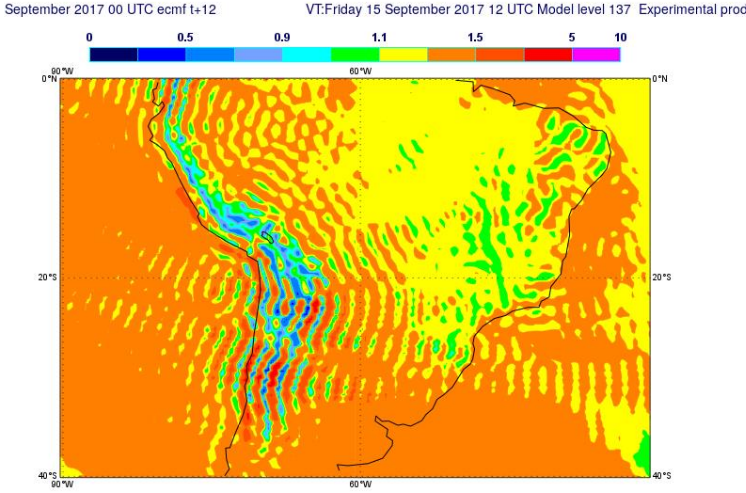




- Locally mass conserving MPDATA is driven by IFS winds and sub-stepped in IFS (CFL restriction)

Outstanding issues IFS-ST-MPDATA:

- *MPDATA operates on height levels derived from spectral IFS*
- *Spectral ripples from forcing fields contaminate MPDATA BCs with noise in steep orography (not an issue for FVM which uses consistently a FV discretization)*



MPDATA advected air density lowest level

Summary

- ECMWF maintains and continues performance optimisation and development of both hydrostatic & non-hydrostatic dynamical cores in close collaboration with member state and industrial partners
- Development of a new dynamical core based on Finite Volume discretization is progressing well:
  - Promising scientific results
  - Good scalability and efficiency
- Work to investigate Discontinuous Galerkin SL has begun with funding from ESCAPE-2
- Atlas NWP library:
  - “Bedrock” of new developments
  - Allows combining elements of different dynamical cores under a unified code as demonstrated by multiple grids case

Thank you for your attention!