Atmospheric tracer transport in the ECMWF model using multiple grids

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PDEs on the Sphere 2019

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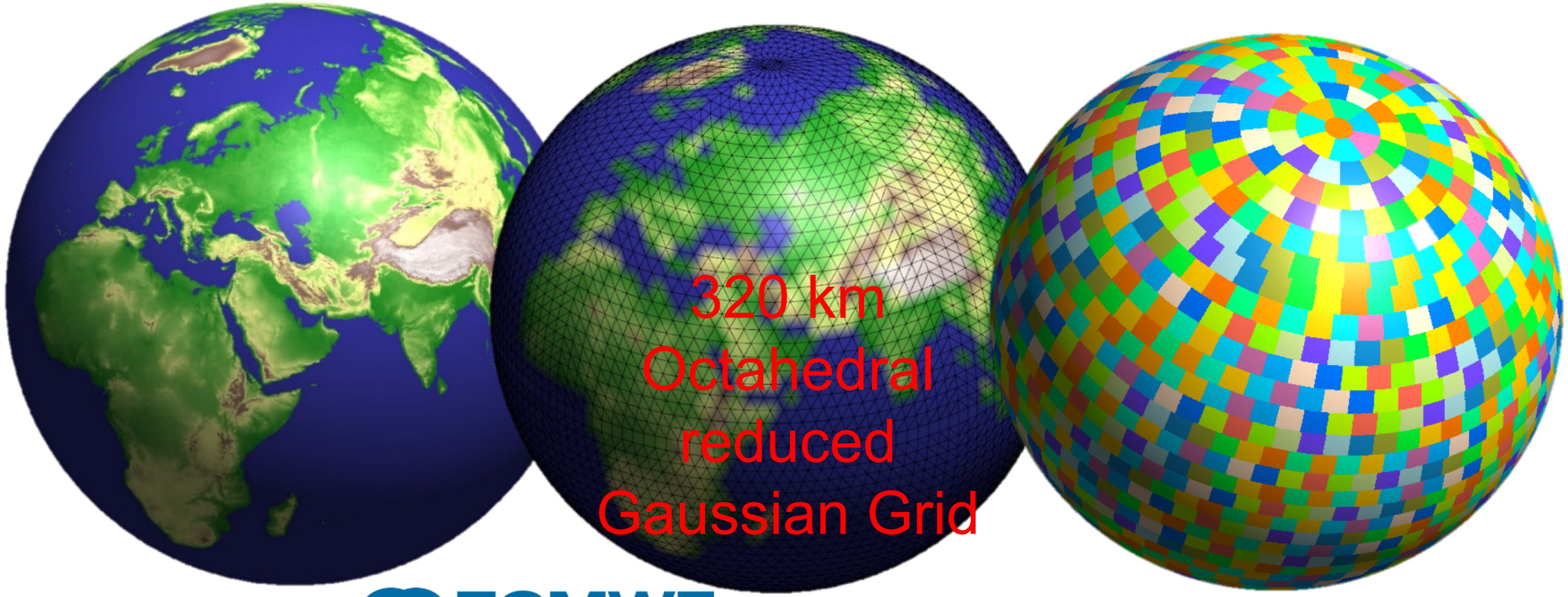
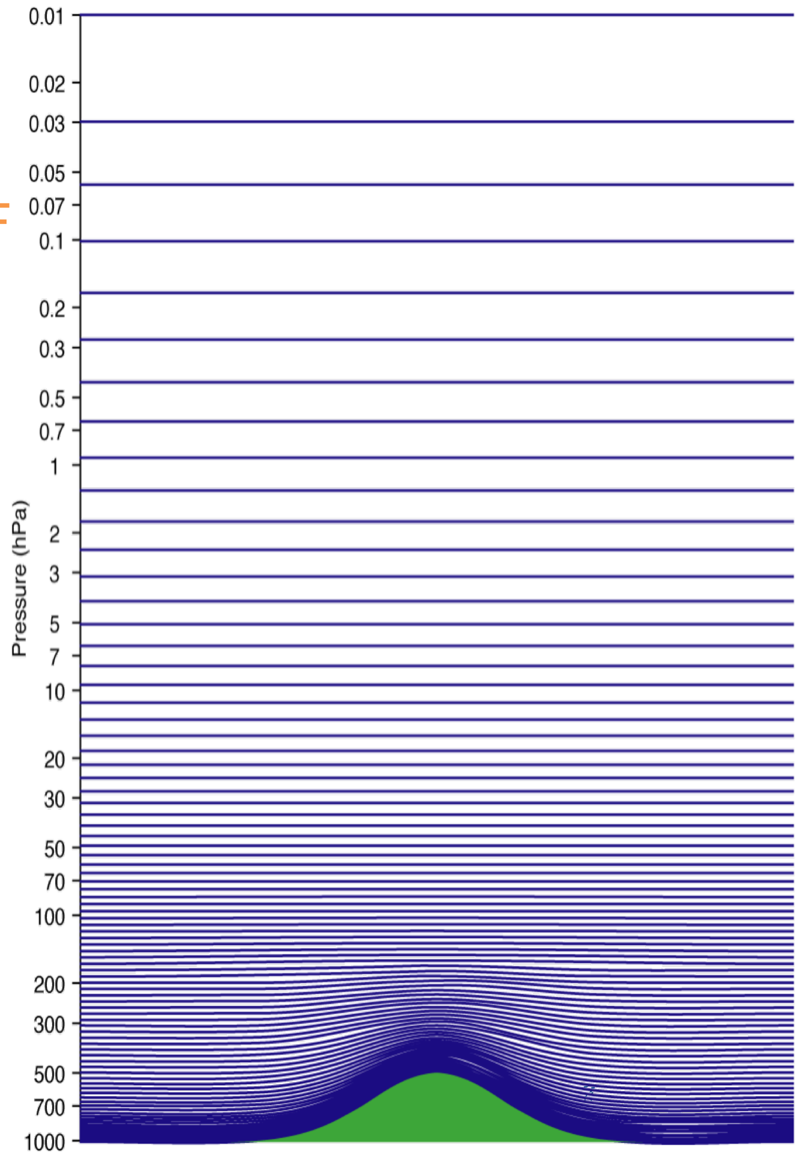
ECMWF

The ECMWF Integrated Forecasting System (IFS)

- Horizontal: *spectral transform on cubic octahedral reduced Gaussian grid*
- Vertical: *pressure based coordinate, finite element discretization*
- *Semi-Lagrangian, semi-implicit timestepping*
- **High resol "deterministic"**: 9 km - 6.6M grid points / 137 levels
- 10 prognostic variables
- Hybrid MPI / OpenMP on 360 CrayXC40 nodes
- 50-member 18km / 91 level **ensemble prediction system**

9 billion DOF





ECMWF model and developments

- IFS current formulation is hydrostatic
  - spectral non-hydrostatic (NH) available - used by ECMWF member states for Limited Area Modelling
- A new scalable (compact stencil) NH dynamical core is developed in ECMWF (IFS-FVM, Kühnlein et al 2019, GMD) based on a finite volume discretization with semi-implicit timestepping
- There is significant effort in infrastructure developments to enhance flexibility of NWP software developments so that the model can run on heterogenous architectures with accelerators
- In-house developed Atlas library (Deconinck et al. 2017, J-CPC) provides flexible data structures for NWP / climate scientific software developments
  - Open-source (Apache 2.0), http://github.com/ecmwf/atlas
  - Modern C++ library implementation with Fortran 2008 (OOP) interfaces → integration in existing models
  - Grid/mesh generation capabilities (supports structured and unstructured, global and regional grids)
  - Mathematical operators: gradient, divergence, Laplacian, spectral transforms on spherical harmonics
  - Data structures and parallelisation routines to support execution on both CPU and GPUs
  - Recently enhanced to support mesh-to-mesh field remapping
  - New dynamical core IFS-FVM is developed in Atlas

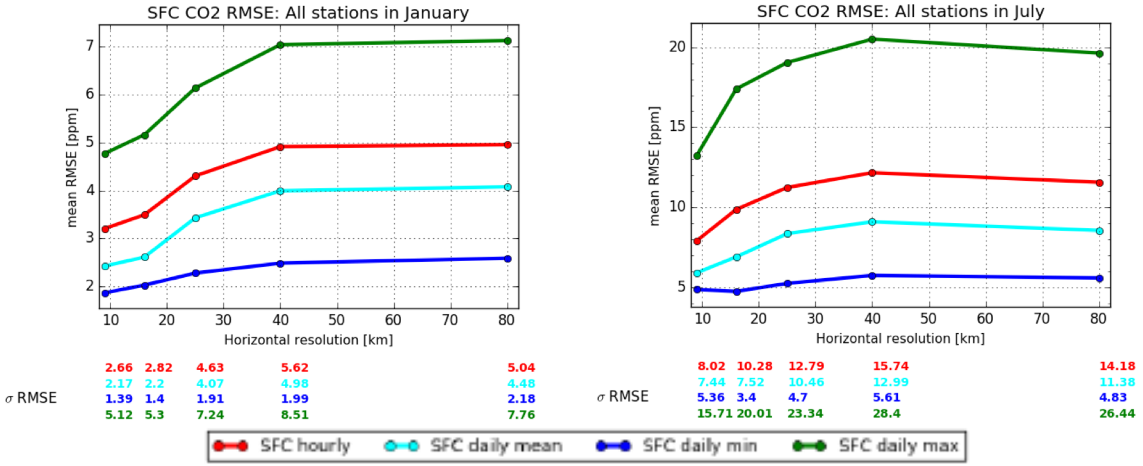
Atmospheric Composition forecasts in IFS

- Daily produced atmospheric composition forecasts (CAMS: Copernicus Atmospheric Monitoring System) require the transport of many tracers
  - Greenhouse gases (2), aerosols (12), chemical tracers (60)
- Available advection schemes for tracers in IFS:
  - *the semi-Lagrangian scheme - computationally very efficient as it can advect multiple tracers at small computational overhead, but … it does not conserve mass*
  - *Emerging alternative: the MPDATA scheme in the new (at development stage) dynamical core IFS-FVM which is locally (and globally) conserving but obeys a CFL timestep restriction*
- With recently introduced Atlas multiple-grids feature in IFS:
  - It is possible to run selected model processes at a separate grid that could be at lower resolution
  - A prototype has been implemented for **tracer advection** which due to its object oriented design naturally leads to a flexible "plug-in and test" development system for tracer transport schemes in IFS
  - Ultimate goal is to simulate **chemistry** at a low resolution grid as this is the most expensive process by far

Resolution and atmospheric composition forecasts

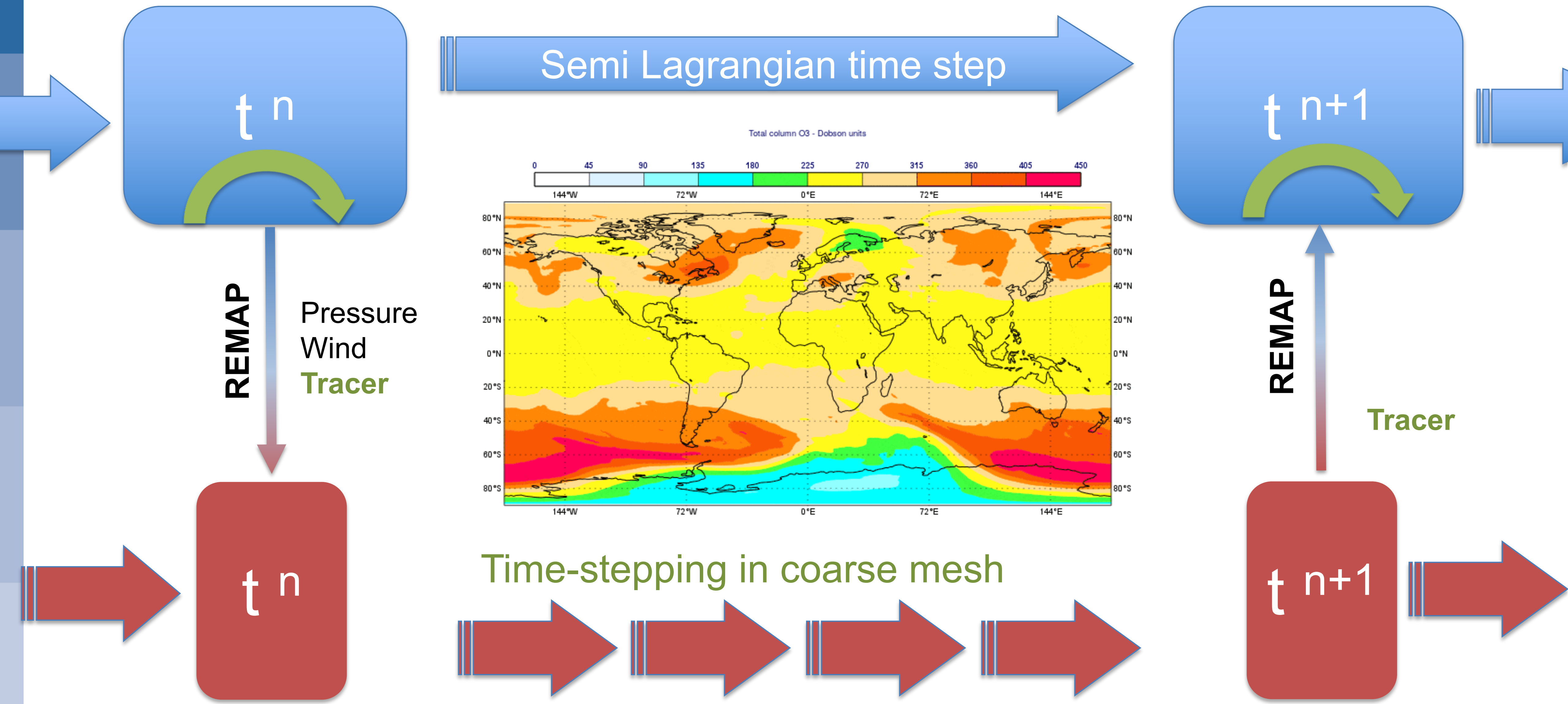
- Resolution improves atmospheric composition forecasts (Agusti-Panareda et al, ACPD 2019 under review)
  - Greenhouse gases (CO2, CH4) (passive) forecasts run at 9km resolution – high resolution improves results

Near surface CO2 mean RMSE reduction with increasing resolution across different timescales (average from 51 stations)
Left: January 2015
Right: July 2015



  - Global mass conservation is **essential** for long-lived tracers such as CO2, CH4
    - Mass conservation error from the IFS SL scheme is corrected by a sophisticated & highly tuned global mass fixer based on the MWR 2002 Bermejo & Conde scheme (Diamantakis & Agusti-Panareda ECMWF Tech Memo 2017)
    - Simple mass fixers may produce unwanted hemispheric gradients in tracer concentration (Agusti-Panareda et al, GMD 2016)
  - Inherently locally mass conserving scheme is desirable, especially for chemically active tracers
  - Chemically active tracer forecasts run at 50km resolution – it is desirable but unaffordable to increase much further resolution (high computational cost of chemistry): an alternative cost effective way to do it is to use the high resolution model to provide the meteorological forcing but simulate the tracer on a coarse grid

Demo: ozone transport at 32km grid forced by winds from a 18km model



Remapping using linear interpolation (cubic available soon)

Using Atlas multiple grids to interface MPDATA with spectral IFS for tracer advection

MPDATA finite volume transport equation solver of FVM could be used for tracer transport in IFS?

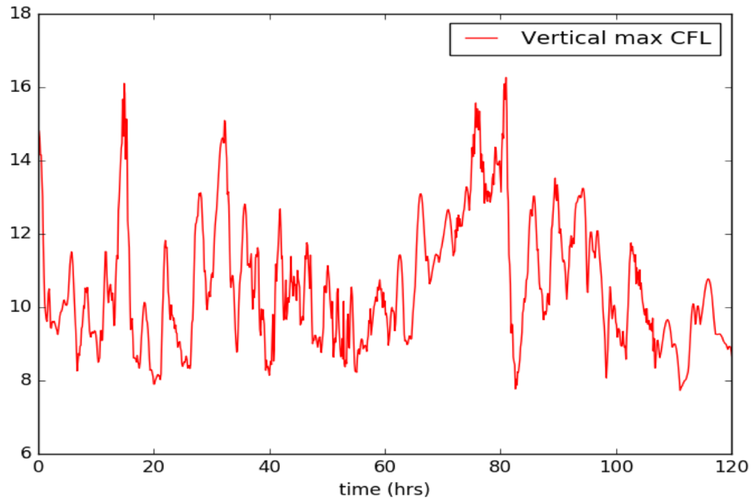
$$\frac{\partial J\rho_d}{\partial t} + \nabla\cdot(\mathbf{v}J\rho_d) = 0,$$

$$\frac{\partial J\rho_d m_x}{\partial t} + \nabla\cdot(\mathbf{v}J\rho_d m_x) = 0, \qquad m_x = \rho_x / \rho_d$$

Eqns solved by MPDATA (Kühnlein & Smolarkiewicz JCP 2017)
J: *coordinate transformation Jacobian*
v: contravariant velocity
ρ_d, ρ_x: dry air and tracer density

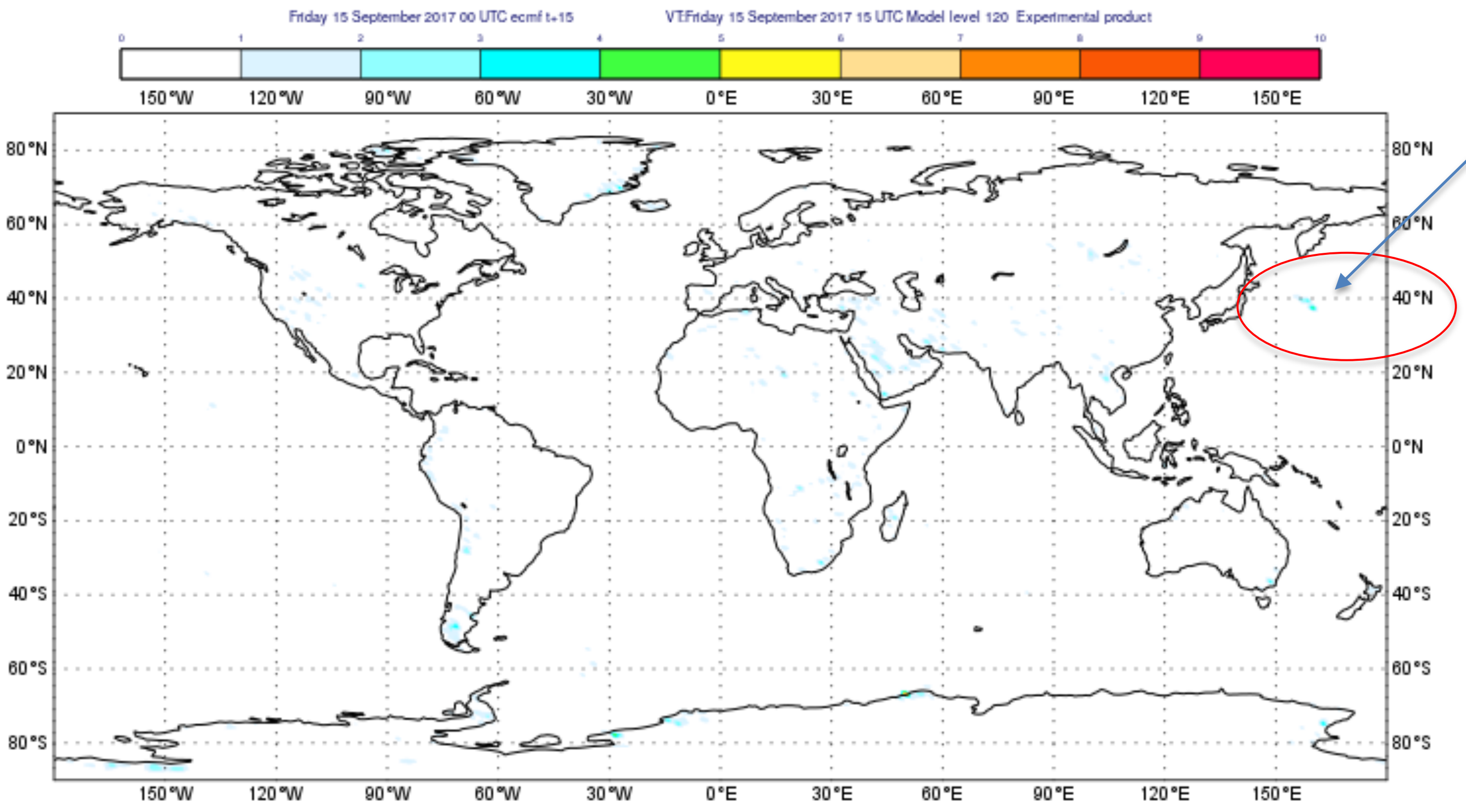
Invoked at each model timestep [t,t+Δt] driven by IFS winds

- MPDATA obeys a CFL≤1 limit
  - *Spectral SISL-IFS Δt is too long: k sub-steps where k determined by max CFL*
- MPDATA code uses a height based vertical coordinate while IFS uses a pressure-based coordinate
  - MPDATA vertical levels are derived by IFS geopotential height levels
- MPDATA obeys a flux-form continuity equation and must advect consistently density and mixing ratio
  - *IFS continuity is expressed in terms of pressure - it does not explicitly compute density but at each new step diagnoses density by IFS pressure*
- *MPDATA is locally + globally mass conserving, however:*
  - *It may not conserve globally in IFS because global mass of tracer is computed with respect to the IFS density which obeys a SISL discretization of the continuity equation.*
- *Because of the above issues MPDATA may not perform at standards matching those achieved in its "native" FVM dynamical core. Can it produce a realistic solution?*



IFS max CFL in the vertical (9km, Δt =450s)

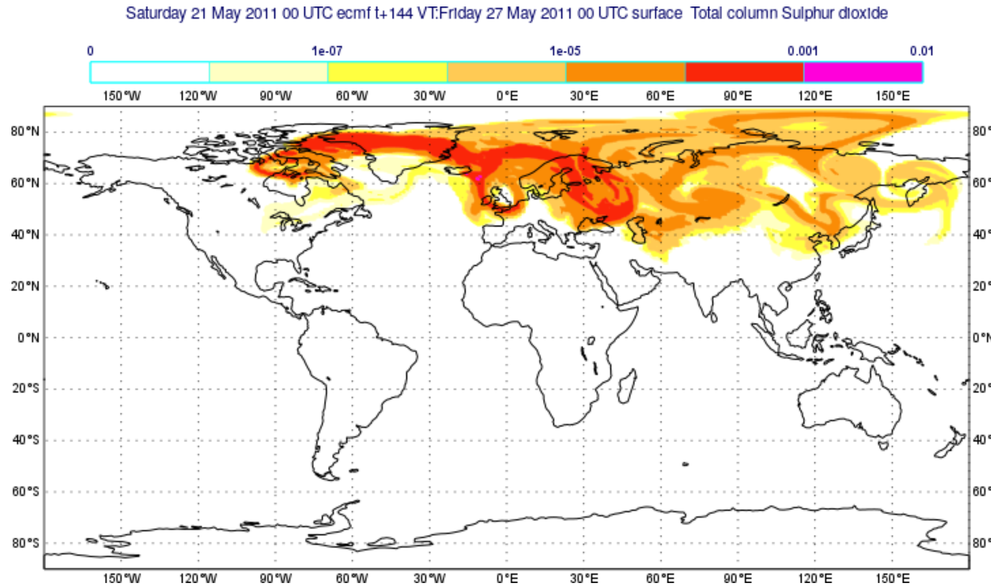
Max CFL number: model level 120 ~ 900hPa



Max CFL=16 (tropical cyclone)

Vast majority of gridpoints have a very small vertical CFL number <1

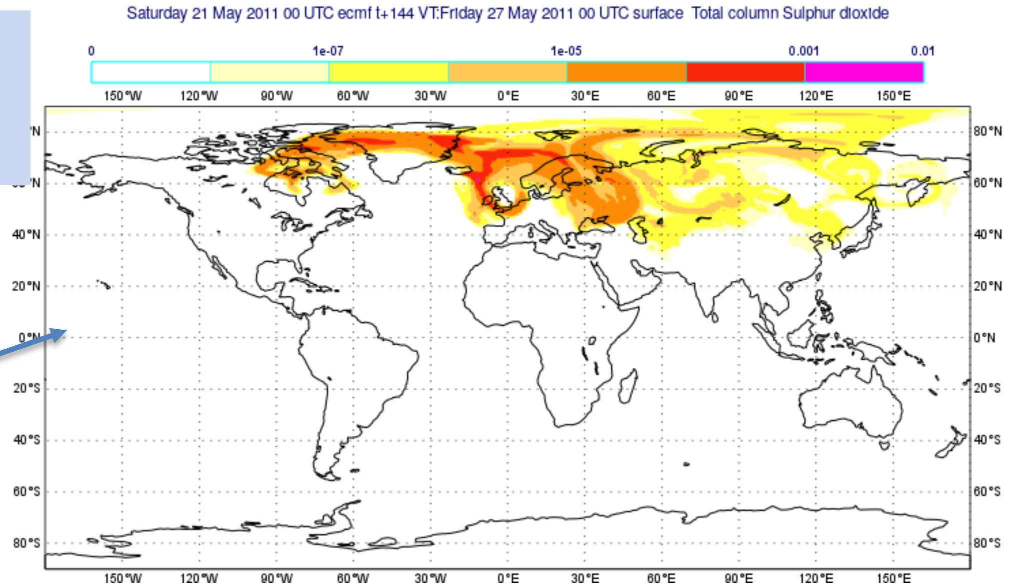
Plug-in and test: SL vs MPDATA multiple grid simulation of volcanic plume

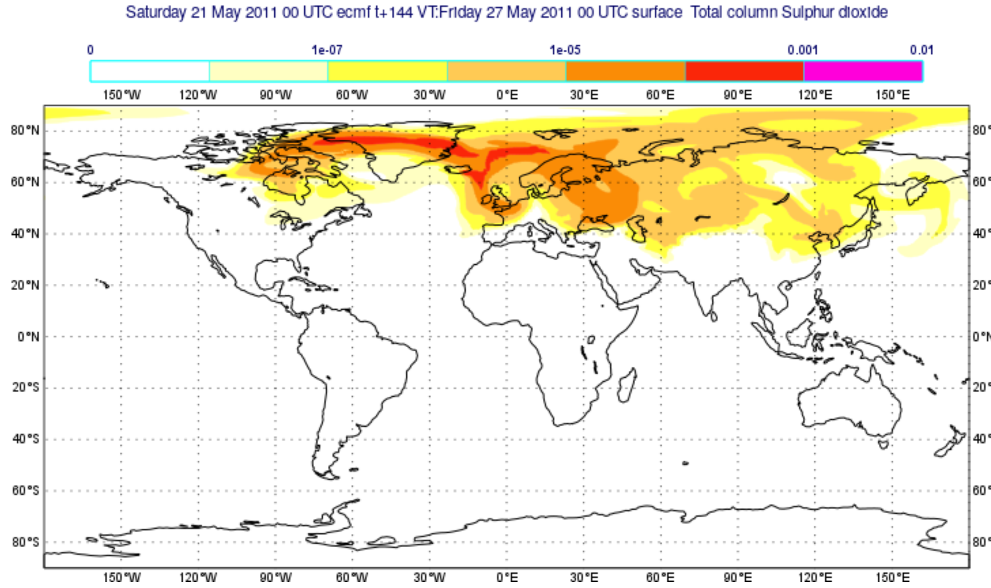


t+6 days total column SO2 (18km res)

SL

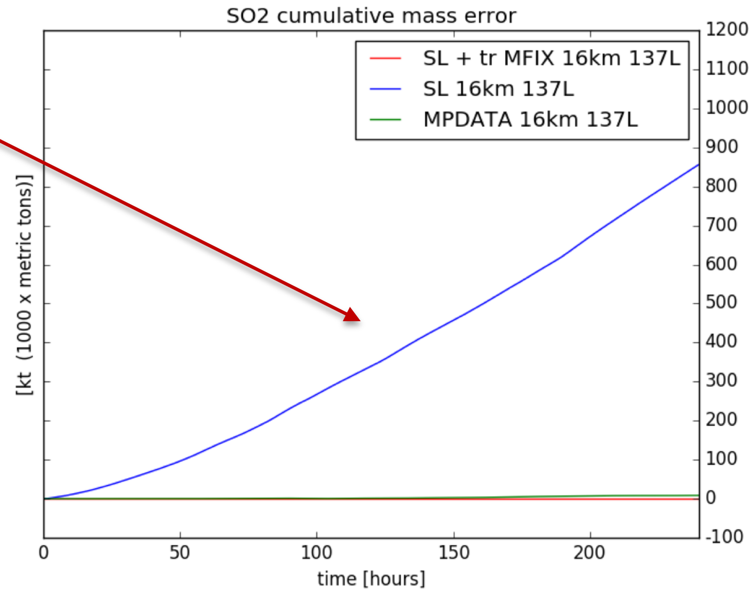
SL + fixer



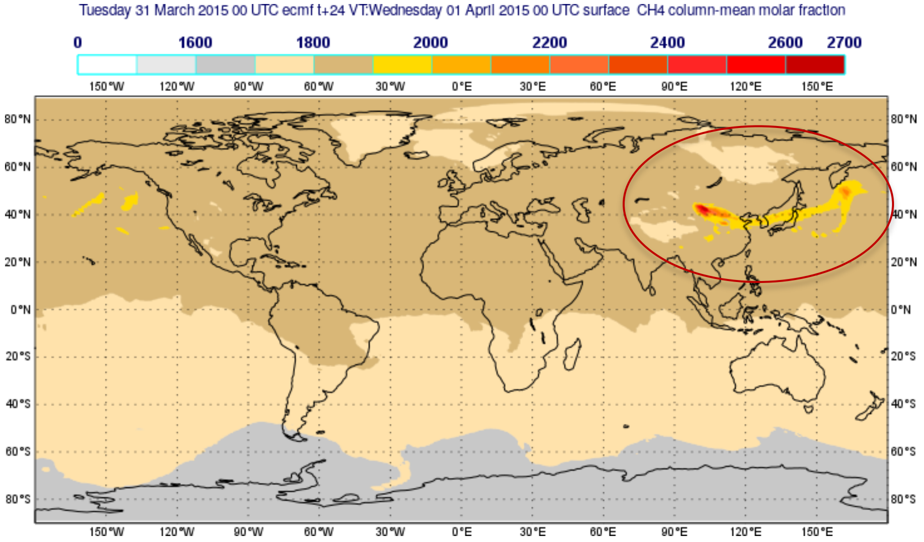


MPDATA

- Without mass fixer SL advection accumulates tracer mass conservation error
- MPDATA shows very good global mass conservation even measured “unfairly” wrt IFS density

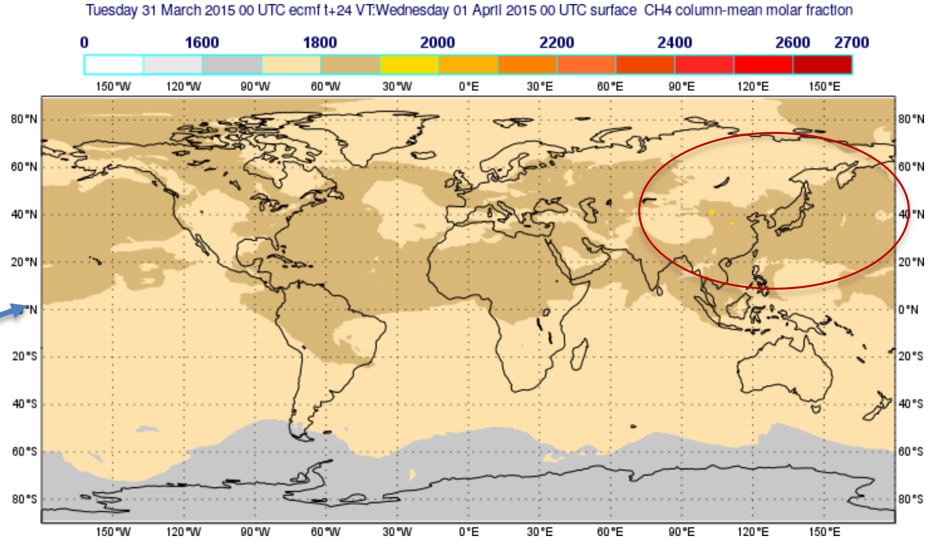


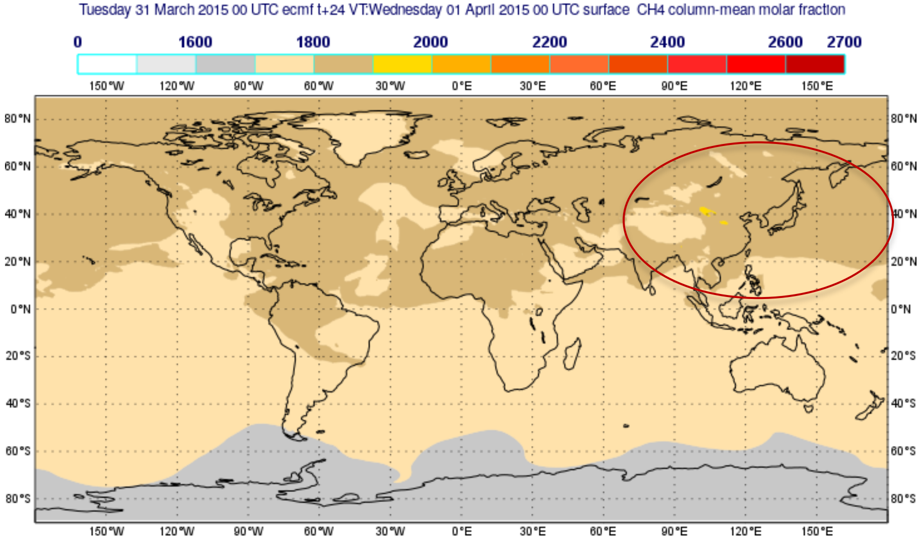
Plug-in and test: SL vs MPDATA multiple grid simulation for CH4



Total column CH4 after 90 days (18km res)

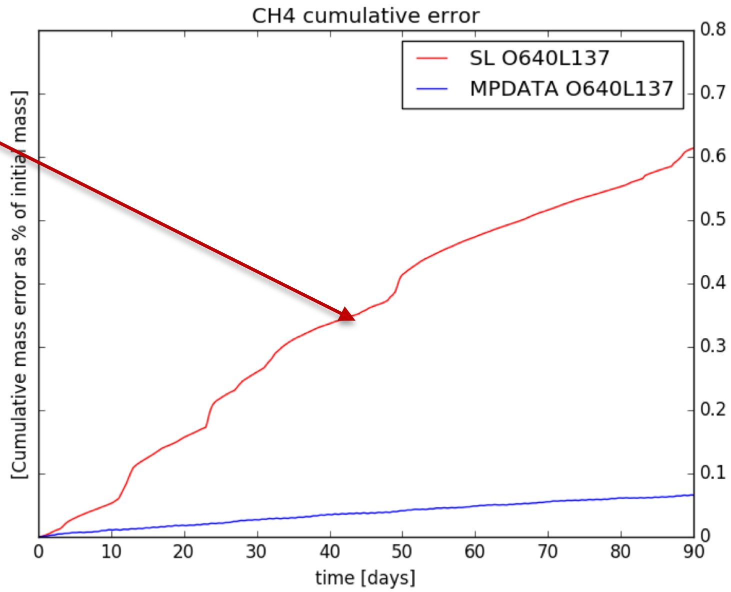
SL + fixer



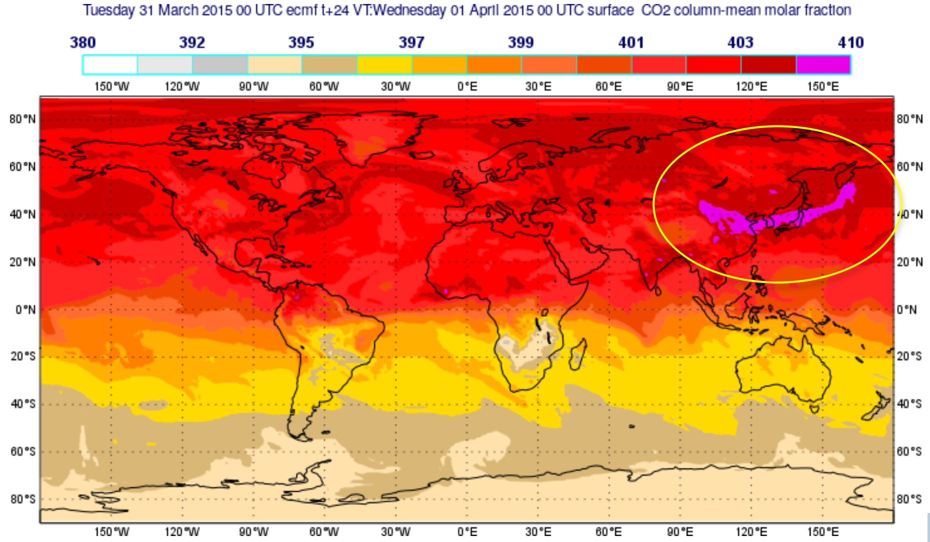


- Without mass fixer SL advection accumulates tracer mass cons error
- MPDATA global mass conservation error measured wrt IFS density is much smaller!

MPDATA

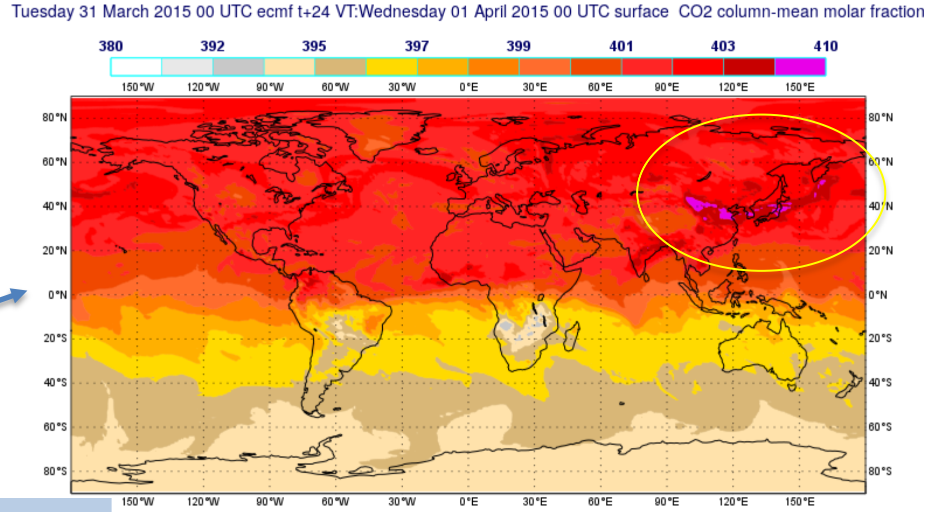


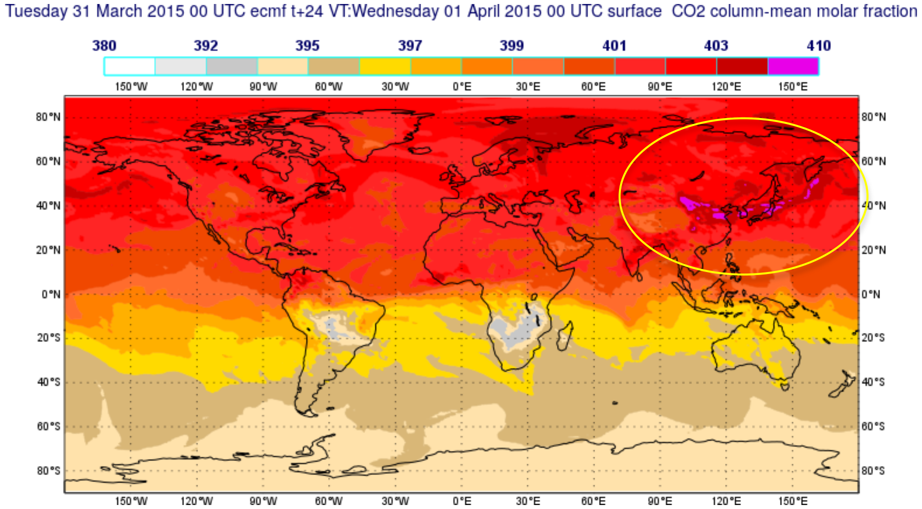
Plug-in and test: SL vs MPDATA multiple grid simulation for CO2



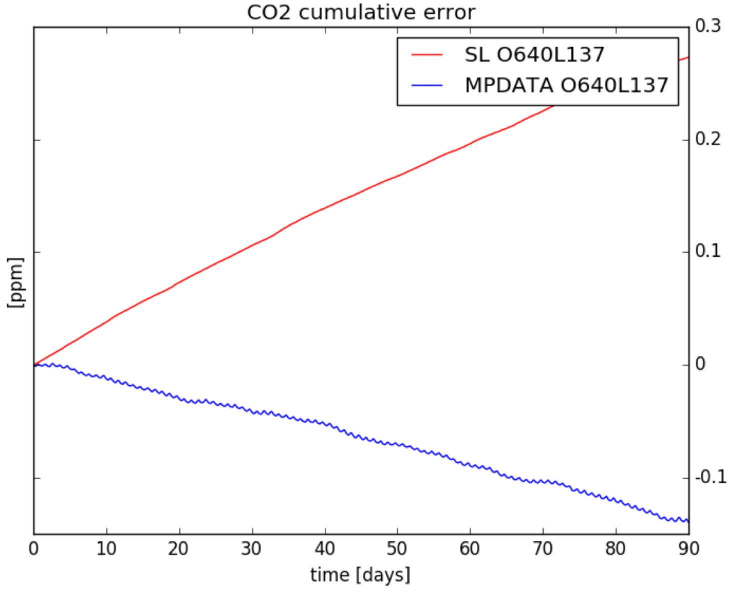
Total column CO2 after 90 days (18km res)

SL + fixer





- MPDATA is better than pure SL in the emission zone and comparable with SL + BC fixer
- MPDATA global mass conservation error doesn't reduce as much as in CH4 – it is very sensitive to background air conservation



Plug-in and test: McGregor’s SL scheme (MWR 1993) on water species (tracers)

Multiple-grid advection IFS code includes a SL option with:

- Standard iterative algorithm for computing the DP
- Non-iterative scheme based on McGregor’s Taylor series scheme: *attractive as an alternative for reducing computational and communication cost at high resolution*

SL advection of tracer

$$\phi_j^n = \phi_{D(j)}^n, \quad j = 1, \ldots, N \quad D(j): \text{ departure point (DP) for gridpoint j}$$

DP calculation with SETTLS iterative scheme (Hortal, QJRMS 2002). In Cartesian coordinates is written:

$$r_D^{(0)} = r_A - \Delta t V\left(r_A, t\right)$$

$$r_D^{(k)} = r_A - \frac{\Delta t}{2} \cdot \left(V_A(t) + \left\{ 2V(t) - V(t - \Delta t) \right\} \Big|_{r_D^{(k-1)}} \right) \quad k = 1, 2, \ldots$$

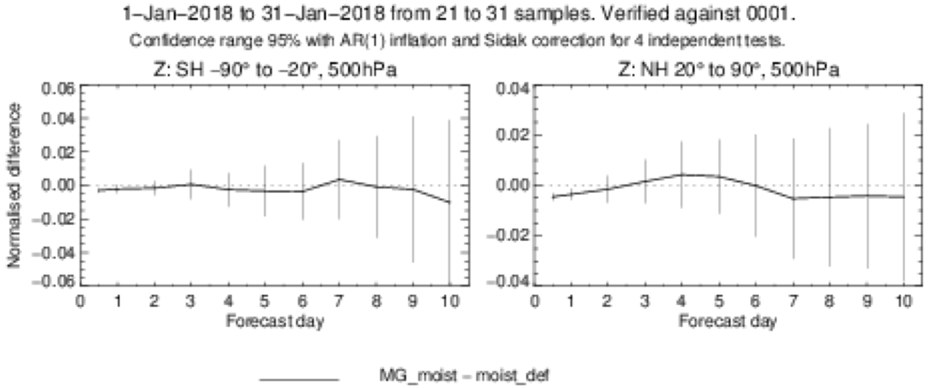
DP calculation with McGregor scheme:

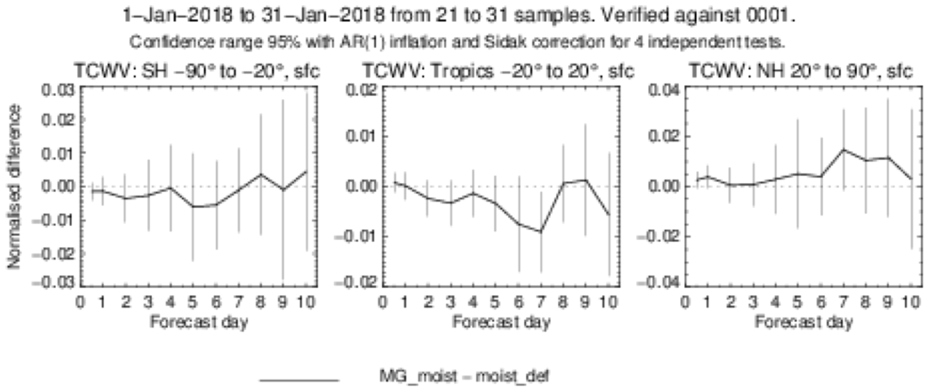
$$\mathbf{r}_D(t) = \mathbf{r}_A(t + \Delta t) + \sum_{k=1}^{p} \frac{(-\Delta t)^k}{k!} \frac{d^k \mathbf{r}_A}{dt}(t + \Delta t), \quad \mathbf{V}^{t+\Delta t/2} \cdot \nabla = \frac{u^{t+\Delta t/2}}{a \cos\theta} \frac{\partial}{\partial \lambda} + \frac{v^{t+\Delta t/2}}{a} \frac{\partial}{\partial \theta}$$

$$\frac{d\mathbf{r}_A}{dt}(t + \Delta t) \approx \mathbf{V}^{t+\Delta t/2} \cdot \nabla (X, Y, Z)_A = \left(u \sin\lambda - v \cos\lambda \sin\theta, u \cos\lambda - v \sin\lambda \sin\theta, v \cos\theta \right)_A$$

$$\frac{d^k \mathbf{r}_A}{dt} = \frac{d}{dt}\left(\frac{d^{k-1} \mathbf{r}_A}{dt} \right) \approx \mathbf{V}^{t+\Delta t/2} \cdot \nabla \left(\frac{d^{k-1} \mathbf{r}_A}{dt} \right)$$

In current implementation of McGregor’s SL k=2. Is 2nd order algorithm sufficiently accurate?

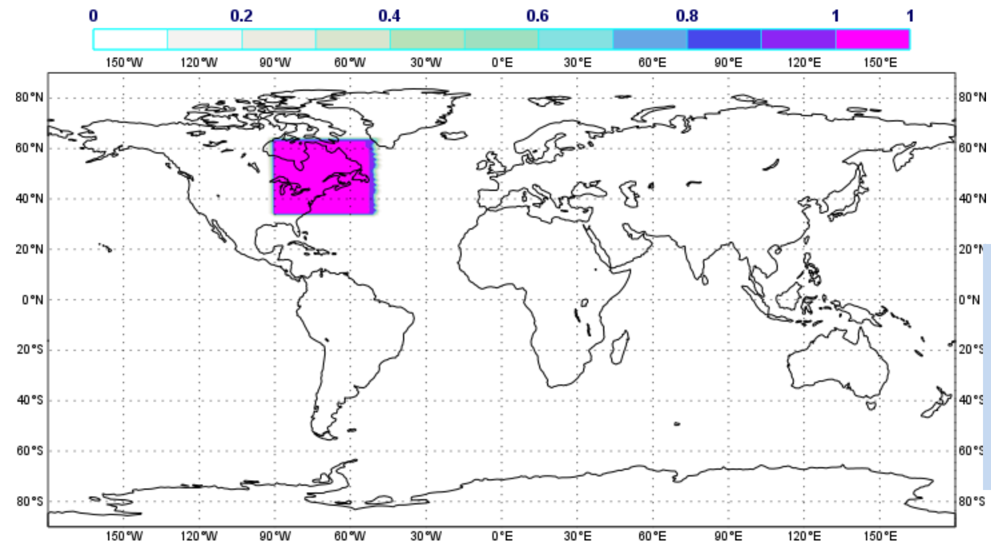




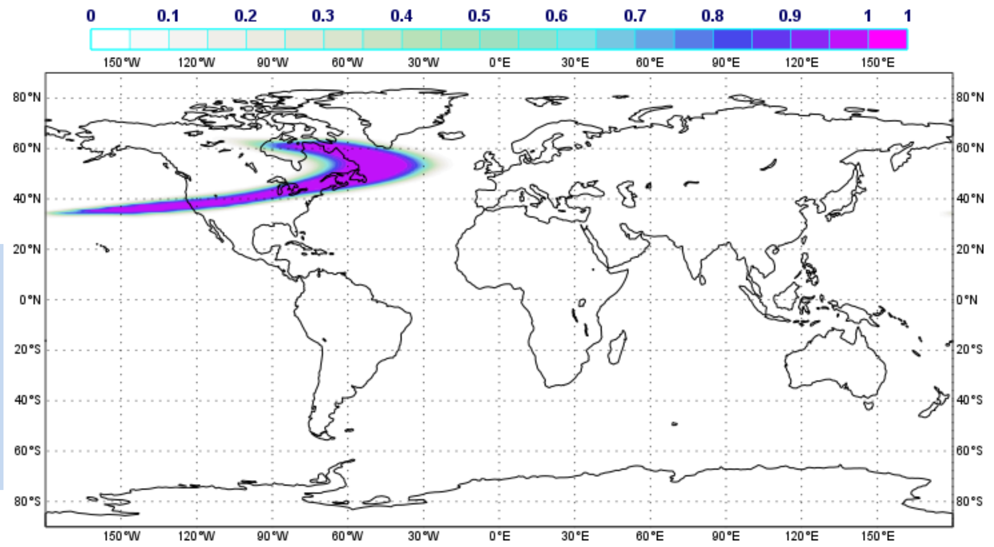
RMSE difference for 32km res forecasts (31 cases): McGregor scheme for 6 moist tracers - default iterative SL advection scheme.
Very neutral in terms of accuracy + more efficient

Plug-in and test: low res dry baroclinic-instability with tracer with different schemes

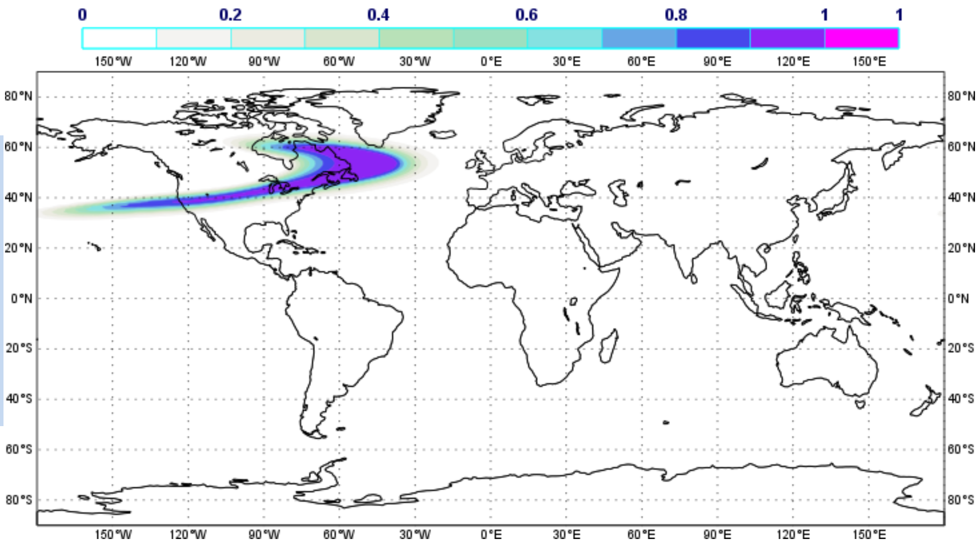
Tracer at t=0



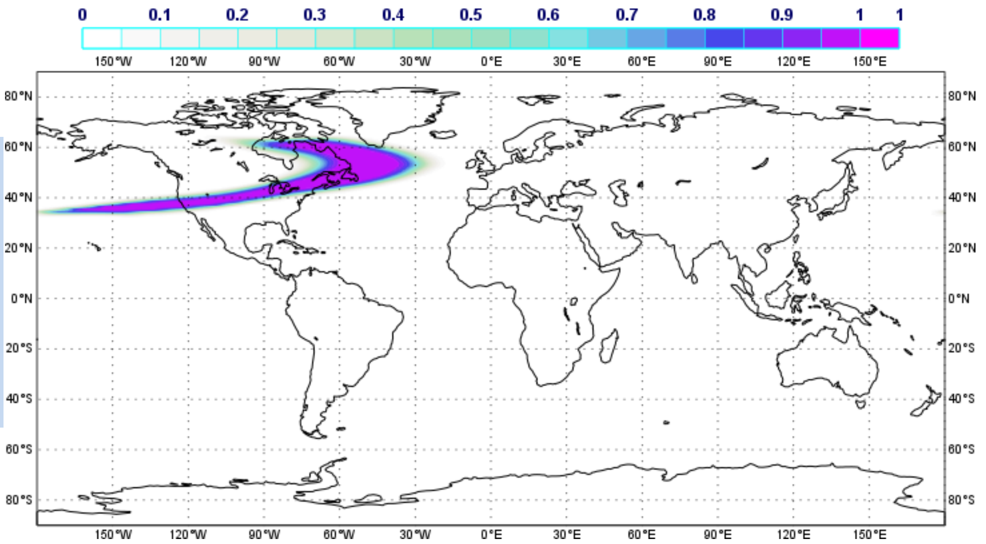
Tracer at t+240hrs / **SL** advec at model lev 30 ~35hPa



Tracer at t+240hrs / **MPDATA** advec at model lev 30~35hPa

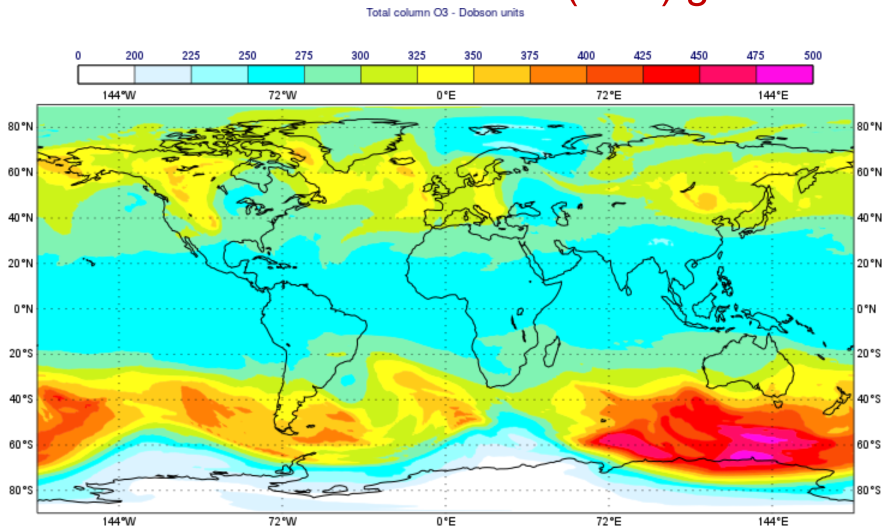


Tracer at t+240hrs / **McGregor SL** advec at model lev30 ~35hPa

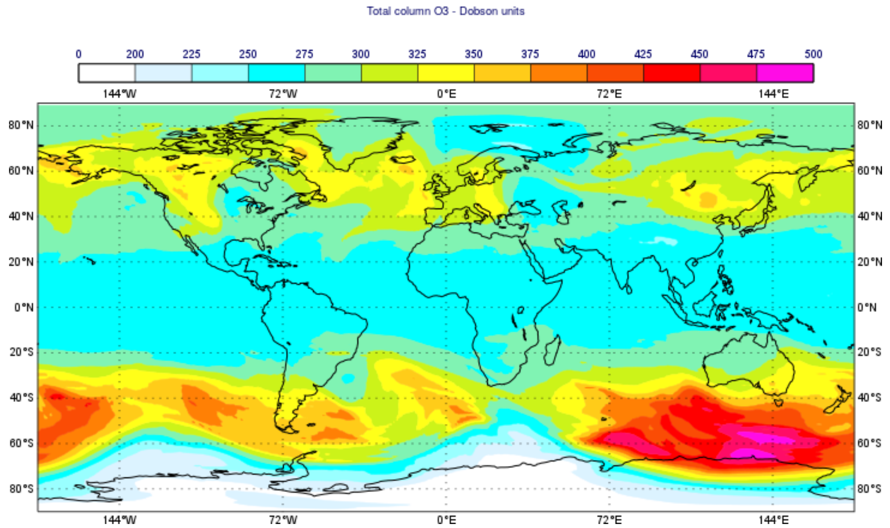


Plug-in and test: Ozone transport on multiple grids using different schemes

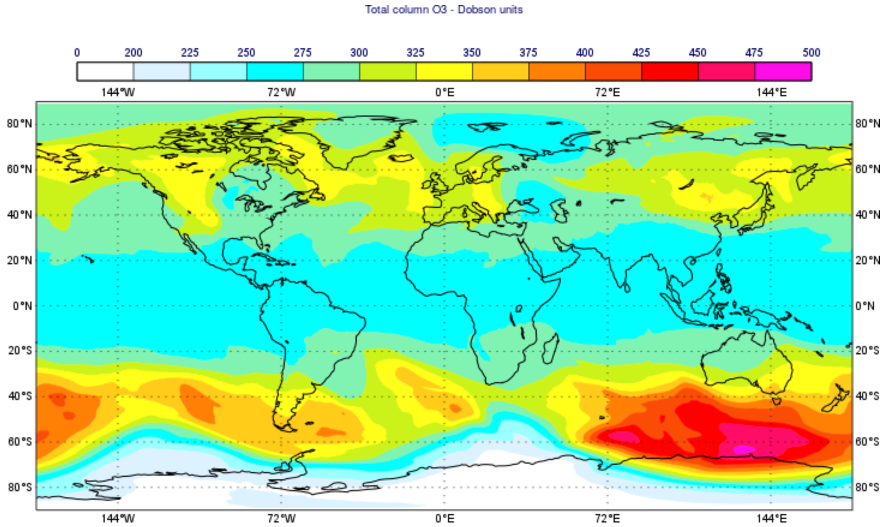
SL O3 advection at same (9km) grid



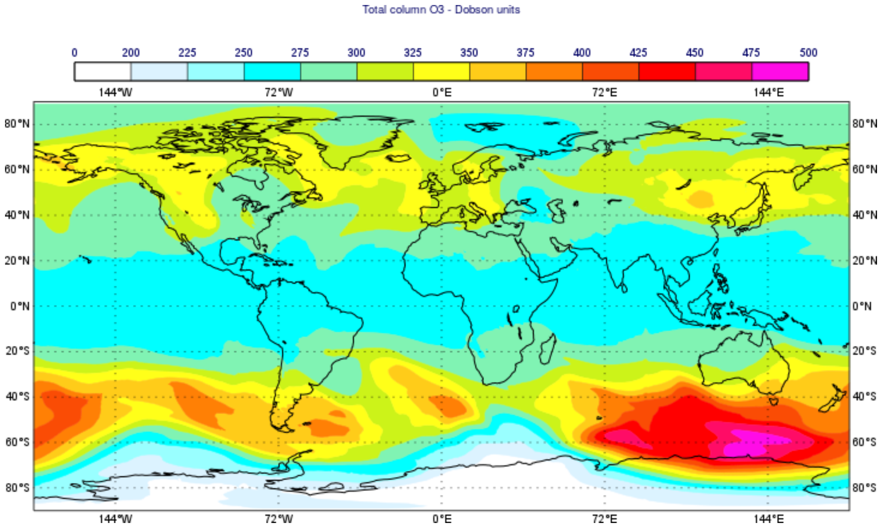
MPDATA O3 advection at same (9km) grid



SL O3 advection at coarse (25km) grid



MPDATA O3 advection at coarse (25km) grid

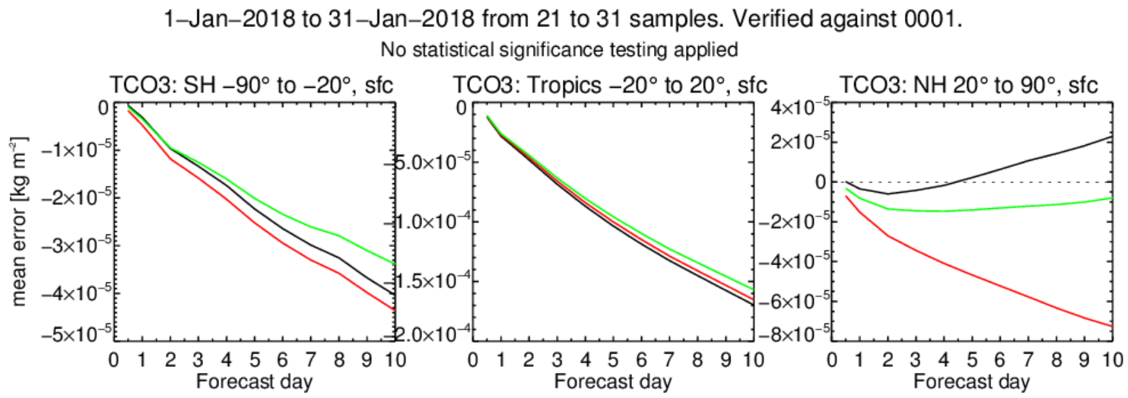


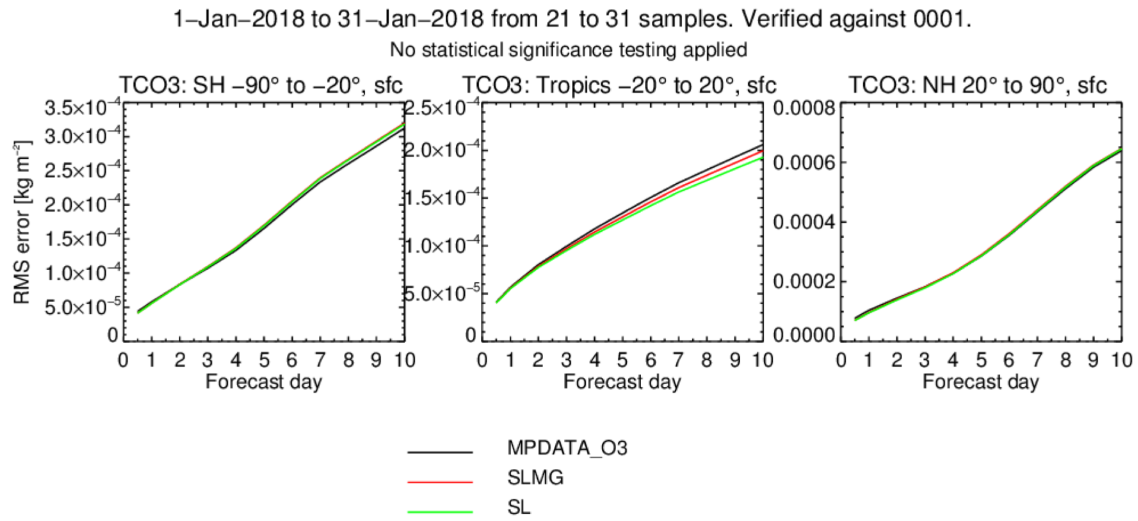
- “Meteorological forcing” at 9km with Ozone advected at a separate grid driven by IFS winds
- Currently only linear mesh-to-mesh interpolation tested

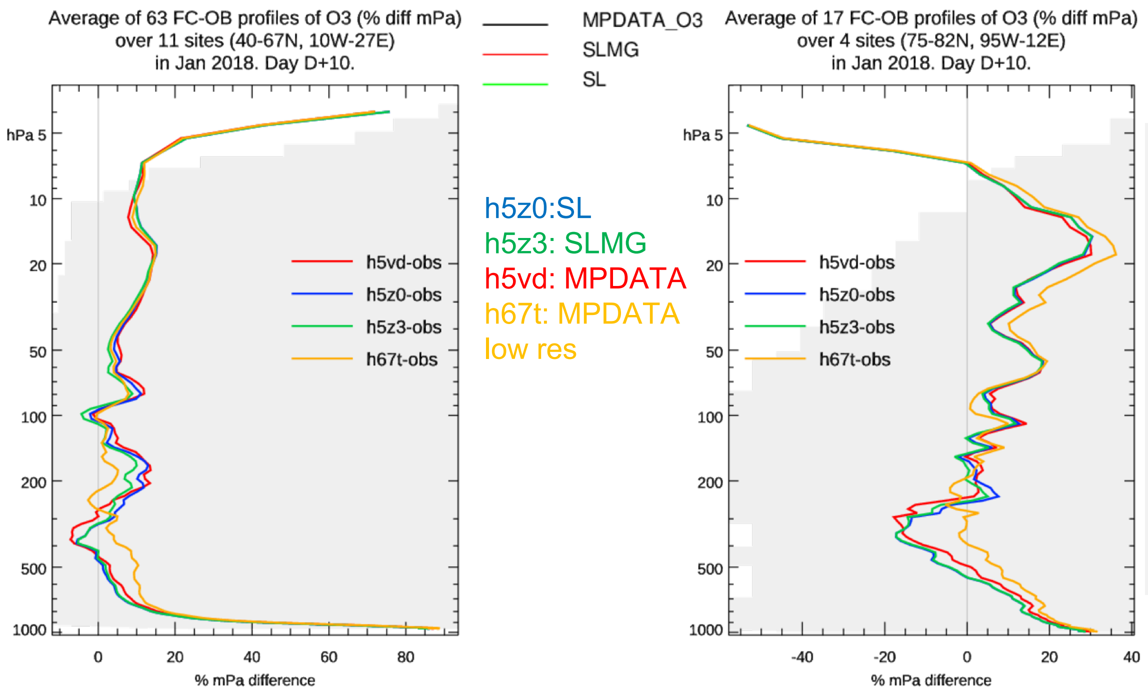
T+7days total column ozone (Dobson units) forecast field

ECMWF

Total column O3 errors from 25km forecasts (31 winter cases, different schemes) with chemistry

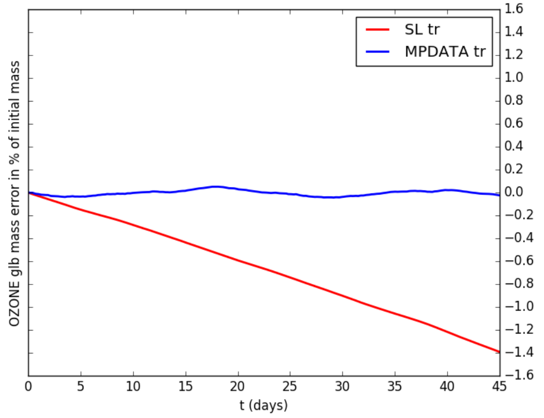






h5z0:SL
h5z3: SLMG
h5vd: MPDATA
h67t: MPDATA low res

- MPDATA
  - Overall, results are comparable. Larger differences in the troposphere
- McGregor-SL:
  - Root Mean Sq Err is nearly identical at the extra-tropics slightly worse in the tropics. Enhances an existing negative bias in the northern hemisphere



Global mass conservation error for O3 in a single free (no chemistry) 45-days run. Comparison between MPDATA/SL

Summary and future work

- IFS with Atlas has the capability to perform simulations using multiple grids and resolutions
- This approach has been applied and tested for the advection problem - it enables to interface and test advection schemes easily providing a useful tool for analysing performance of numerical schemes
- An advantage of this tool is that it provides an integrated environment for testing with the option of using idealised or real forecast cases. Tests on two newly implemented schemes showed:
  - *Despite formulation inconsistencies between IFS model and MPDATA as well as other limitations in current implementation, it produces a similar solution with the SL scheme in passive (without meteorological feedback) tracer advection problems but with clearly better conservation. CO2 tracer global conservation error is dominated by background air conservation error and for this reason MPDATA appears "less conservative" there but still better than pure SL advection*
  - McGregor's SL scheme tested on moist tracers and ozone produced neutral results in terms of accuracy
- Future work:
  - Improve MPDATA implementation as a tracer transport scheme in spectral IFS: vertical coordinate, time-stepping aspects, computational efficiency, conservation and inconsistencies
  - High order and conservative remapping algorithms
  - Investigate impact of using lower resolution grid and investigate further McGregor's scheme
- Ultimately we wish to extend this work to chemistry …