The semi-Lagrangian semi-implicit time stepping scheme in the ECMWF model IFS

Numerical methods for weather prediction training course
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Outline of this lecture

- Motivation and benefits of semi-Lagrangian, semi-implicit methods
- A detailed overview of semi-Lagrangian advection (definitions, stability and error analysis, algorithmic details, parallel implementation on spherical geometry domains)
- The semi-implicit time stepping and how it is combined with a semi-Lagrangian method to solve the full set of the ECMWF model prognostic equations
- Conservation aspects in the IFS time stepping

The ECMWF hydrostatic global operational model equation set

$$\frac{D\mathbf{V}_h}{Dt} + f\mathbf{k}\times\mathbf{V}_h + \nabla_h\Phi + R_d T_v \nabla_h \ln p = P_{\mathrm{v}}$$

$$\frac{DT}{Dt} - \frac{\kappa T_v \omega}{(1+(\delta-1)q)\,p} = P_{\mathrm{T}}$$

$$\frac{Dq_x}{Dt} = P_{\mathrm{q}_x}$$

$$\frac{\partial}{\partial t}\left(\frac{\partial p}{\partial \eta}\right) + \nabla_h\cdot\left(\mathbf{V}_h \frac{\partial p}{\partial \eta}\right) + \frac{\partial}{\partial \eta}\left(\dot{\eta}\frac{\partial p}{\partial \eta}\right) = 0$$

$$\Phi = \Phi_s - \int_1^{\eta} R_d T_v \frac{\partial}{\partial \eta}(\ln p)\, d\eta$$

η : hybrid (pressure based) vertical coordinate η∈ [0,1]
V*h: horizontal momentum*
T: temperature
T_v: virtual temperature, $\kappa = R_d / c_{pd}$, $\delta = c_{pv}/c_{pd}$
q_x: specific humidity, specific ratios for cloud fields and other tracers x
Φ: geopotential
p : pressure
ω=dp/dt : diagnostic vertical velocity
P: physics forcing terms

Continuity equation in terms of full (moist) pressure: the model conserves the total (rather than dry) atmospheric mass. Dry mass conserving version research option, ECMF TM 849 2019, Malardel et al.

- Primitive equation hydrostatic
- A **non-hydrostatic** option is available **for research** purposes but not used operationally
- Spectral Transform with spherical harmonics basis
- Cubic spline Finite Elements in the vertical
- Time stepping: semi-Lagrangian semi-implicit

The critical role of time stepping

For operational global weather forecasting an accurate and robust weather model which operates at the lowest possible cost is essential

- Role of time stepping scheme is central into achieving this goal
- Semi-Lagrangian (SL) semi-implicit (SI) method is ideal
  - Unconditionally stable SL advection scheme with small phase speed errors and little numerical dispersion
    - ➔ Large timesteps can be used (no CFL restriction) without accuracy penalty
    - ➔ Multi-tracer efficient
  - Unconditionally stable SI time stepping for the integration of fast forcing terms
    - ➔ No timestep restriction from the integration of “fast forcing” terms (e.g. gravity waves and acoustic terms in non-hydrostatic models)
    - ➔ 2^{nd} order accurate time scheme

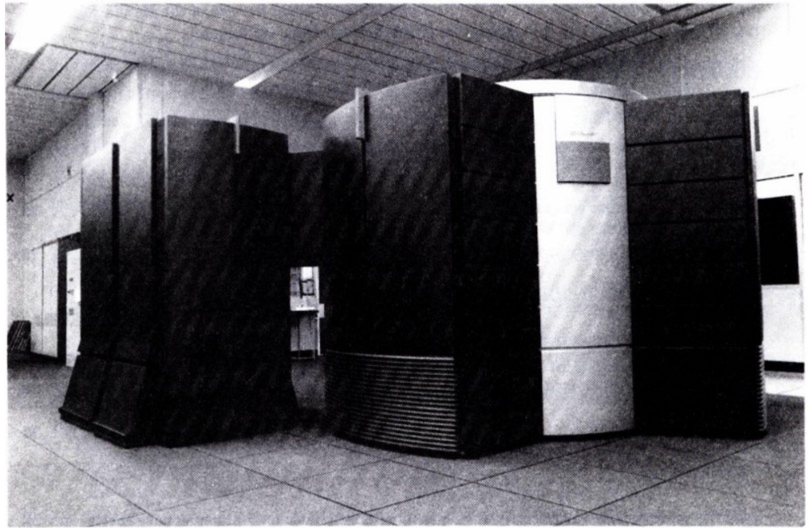
Benefits of spectral transforms combined with SISL

- A spectral SISL scheme like the one in IFS offers additional advantages
  - **Derivative terms** in the equations can be computed **extremely accurately** using analytical formulae
  - The common **"pole singularity" problem** of regular lat-lon grid-point models **does not apply**
  - The derived **3D Helmholtz** elliptic equation can be **decoupled to a set of small dimension** and **computationally cheap** to solve linear systems thanks to the properties of **Spherical Harmonics** (eigenfunctions of the Laplace operator)

- Advancements in algorithms, hardware and software have enabled us to keep running efficiently the spectral transform method at ever increasing resolutions
- ecTrans: a multi-node GPU enabled spectral transform library

History of SISL method at ECMWF

- 1991: IFS was a **spectral semi-implicit** Eulerian model on a full Gaussian grid at T106 horizontal resolution and 19 levels
  - An increase to T231 L31 resolution was planned
  - This upgrade required at least 12 x available CPU power
  - Funding was available for 4 x CPU increase …
- Upgrade was made possible by introducing:
  - A **semi-Lagrangian**, **semi-implicit** scheme on a **reduced Gaussian** grid
  - The new model was 6 x faster!



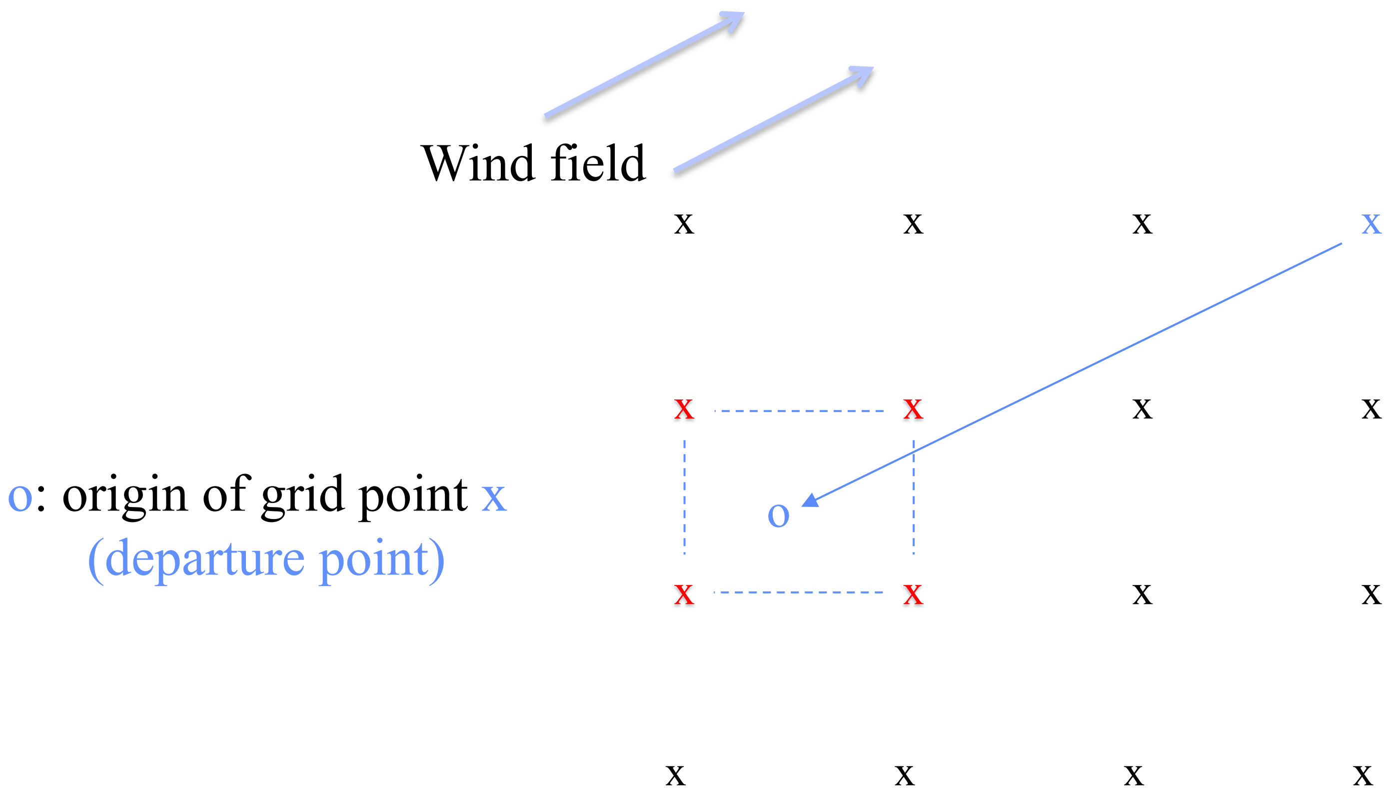
CRAY Y-MP/8: first HPC to run spectral SISL operationally (1992)
Source: ECMWF newsletter 60, Dec 1992

ATOS HPC at Bologna data centre (2022)

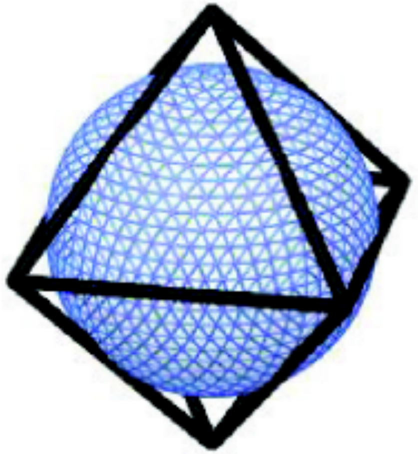
What is a semi-Lagrangian (SL) advection scheme?

- Advection (movement of air, moisture, heat, momentum) is a fundamental process in a weather prediction model
- A SL scheme is a numerical technique for solving advection type PDEs which applies *Lagrangian* “thinking” on grid-point models:
  - For all discrete fluid elements (parcels) the corresponding upstream points (“backward” trajectories) are computed
    - ➔ SL assumes that by the end of each time-step each air parcel arrives at a grid-point location but the location where its trajectory started (departure point) is unknown and must be found.
  - Gradually evolved from schemes introduced in the ’50s, ’60s,’70s (Wiin-Nielsen, Krishnamurti, Sawyer, Leith, Purnel)

Semi-Lagrangian advection in a picture



Octahedral Gaussian grid (see a new grid for IFS ECMWF newsletter 146, Malardel et al) : the grid that IFS uses since cycle 41r2 (2015)

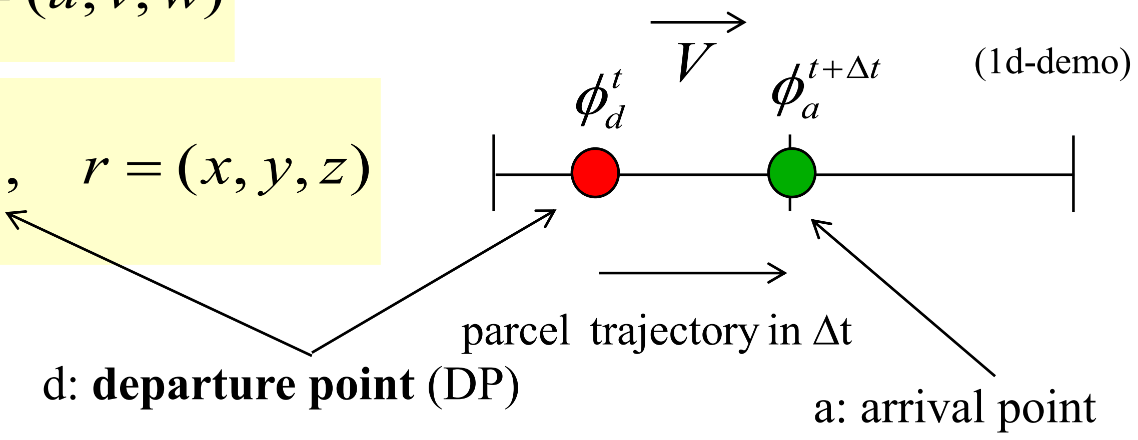


The SL solution of the advection equation

Passive advection of the tracer mixing ratio $\phi = \rho_\phi / \rho$ ($\Leftrightarrow$ air density + tracer density advection) in Cartesian coordinates:

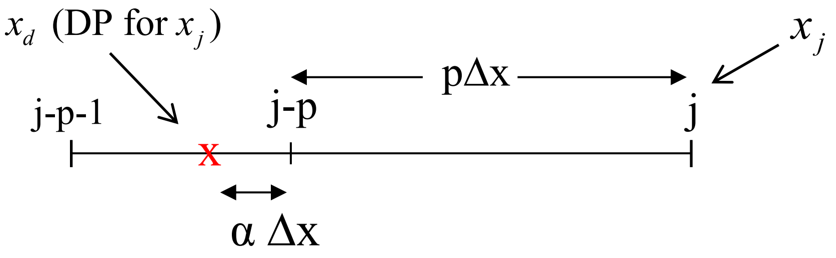
$$\frac{D\phi}{Dt} \equiv \frac{\partial \phi}{\partial t} + V \cdot \nabla \phi = 0, \qquad V = (u, v, w)$$

$$\int_{(r_d,t)}^{(r_a,t+\Delta t)} \frac{D\phi}{Dt} Dt = 0 \Rightarrow \phi_a^{t+\Delta t} = \phi_d^t, \qquad r = (x, y, z)$$



- Solution at t+Δt is obtained by finding the DP location and interpolating the available (defined at time t) grid-point values of ϕ at the DP
- Advection term $V \cdot \nabla \phi$ is not explicitly computed – it is absorbed by the Lagrangian derivative: nonlinear advection problem is reduced to DP search and interpolation!

Unconditional stability (Bates & McDonald MWR 82)



$$\frac{D\phi}{Dt} \equiv \frac{\partial \phi}{\partial t} + u_0 \frac{\partial \phi}{\partial x} = 0$$ (constant wind)

Departure to arrival pt distance: $x_j - x_d = u_0 \Delta t = (p+\alpha)\Delta x$ p: integer

Von Neuman stability analysis: $\phi_j^n = \phi_0 \lambda^n e^{ikj\Delta x}$

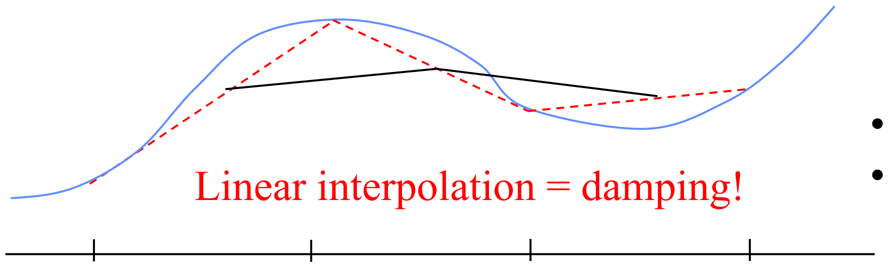
$$\phi_j^{n+1} = \phi_d^n = (1-\alpha)\phi_{j-p}^n + \alpha \phi_{j-p-1}^n, \quad \alpha = \frac{x_{j-p} - x_d}{\Delta x} \longrightarrow \lambda = \left[1 - \alpha\left(1 - e^{-ik\Delta x}\right)\right] e^{-ipk\Delta x}$$

Amplification factor: $|\lambda|^2 = 1 - 2\alpha(1-\alpha)[1-\cos(k\Delta x)]$

$|\lambda| \le 1$ if $0 \le \alpha \le 1$
(interpolation from two nearest points)

NOTE: when p=0 => α is the CFL number => SL with linear interpolation is essentially Eulerian upstream differencing!

$$R = \frac{discr\ freq}{anal\ freq} = \frac{1}{(p+\alpha)k\Delta x}\left[pk\Delta x + \tan^{-1}\left(\frac{a \sin k\Delta x}{1 - a(1-\cos k\Delta x)}\right)\right]$$



- No phase error when DP coincides with gridpoint (R=1)
- Small phase error for large CFL

SL algorithm when winds are constant

Use SL method to solve:

$$\frac{D\phi}{Dt} = 0, \quad V \equiv V_0 = (u_0, v_0, w_0).$$

At the beginning of each step advected variable values ϕ_j^t are available on the computational grid. To compute next time step solution:

- Compute departure point (DP) location:

$$r_{d,j} = r_j - V_0 \Delta t, \quad r = (x, y, z)$$

- Using field values at nearest points surrounding $r_{d,j}$ interpolate variable ϕ_j^t to obtain solution at future time $t + \Delta t$ i.e.

$$\phi_j^{t+\Delta t} = \phi_d^t \equiv I(\phi_j^t)\Big|_{r_d}, \quad I: \quad \text{interpolation operator}$$

Accurate calculation of DP and an accurate interpolation scheme are essential! For accuracy, more sophisticated method required for the DP search in real atmospheric (non-constant wind) flows

Departure point search in real atmospheric flows: SETTLS

Assume straight line trajectories within a time step. Perform a **2nd order Taylor expansion of an arrival (grid) point to its departure point**:

Stable Extrapolation Two Time Level Scheme (Hortal, QJRMS 2002)

$$r_a(t+\Delta t) = r_d(t) + \Delta t \cdot \left(\frac{Dr}{Dt}\right)_d^t + \frac{\Delta t^2}{2} \cdot \left(\frac{D^2 r}{Dt^2}\right)_{AV}$$

AV: average value along SL trajectory

$$\left(\frac{Dr}{Dt}\right)_d^t = V_d(t), \qquad \left(\frac{D^2 r}{Dt^2}\right)_{AV} = \left(\frac{DV}{Dt}\right)_{AV} \approx \frac{V_a(t) - V_d(t-\Delta t)}{\Delta t}$$

Hence,

$$r_a(t+\Delta t) \approx r_d(t) + \frac{\Delta t}{2} \cdot \left(V_a(t) + \{2V(t) - V(t-\Delta t)\}_d\right)$$

Therefore DP can be computed by iterative sequence:

$$r_d^{(0)} = r_a - \Delta t V(r_a, t)$$

$$r_d^{(k)} = r_a - \frac{\Delta t}{2} \cdot \left(V_a(t) + \{2V(t) - V(t-\Delta t)\}\Big|_{r_d^{(k-1)}}\right) \qquad k = 1, 2, \ldots K$$

Interpolate at $r_d^{(k-1)}$ In the IFS: K=2 (was 4 until cy48r1)

For convergence of iterative scheme trajectories should not cross. This is equivalent with the Lipschitz condition (see MWR 2016, Diamantakis & Magnusson)

$$\Delta t \left|\partial V / \partial r\right| < 1$$

which is less restrictive than CFL for atmospheric flows

Benefits of SETTLS

- SETTLS has better stability than the classic **2nd order mid-point scheme below**:

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

$$r_d^{(k)} = r_a - \Delta t \cdot \left\{ \underbrace{\frac{3}{2}V(t) - \frac{1}{2}V(t-\Delta t)}_{\approx V(t+\Delta t/2)} \right\}_{\frac{r_d^{(k-1)}+r_a}{2}} \qquad k = 1, 2, \ldots K$$

"Functional" or "fixed-point" iteration

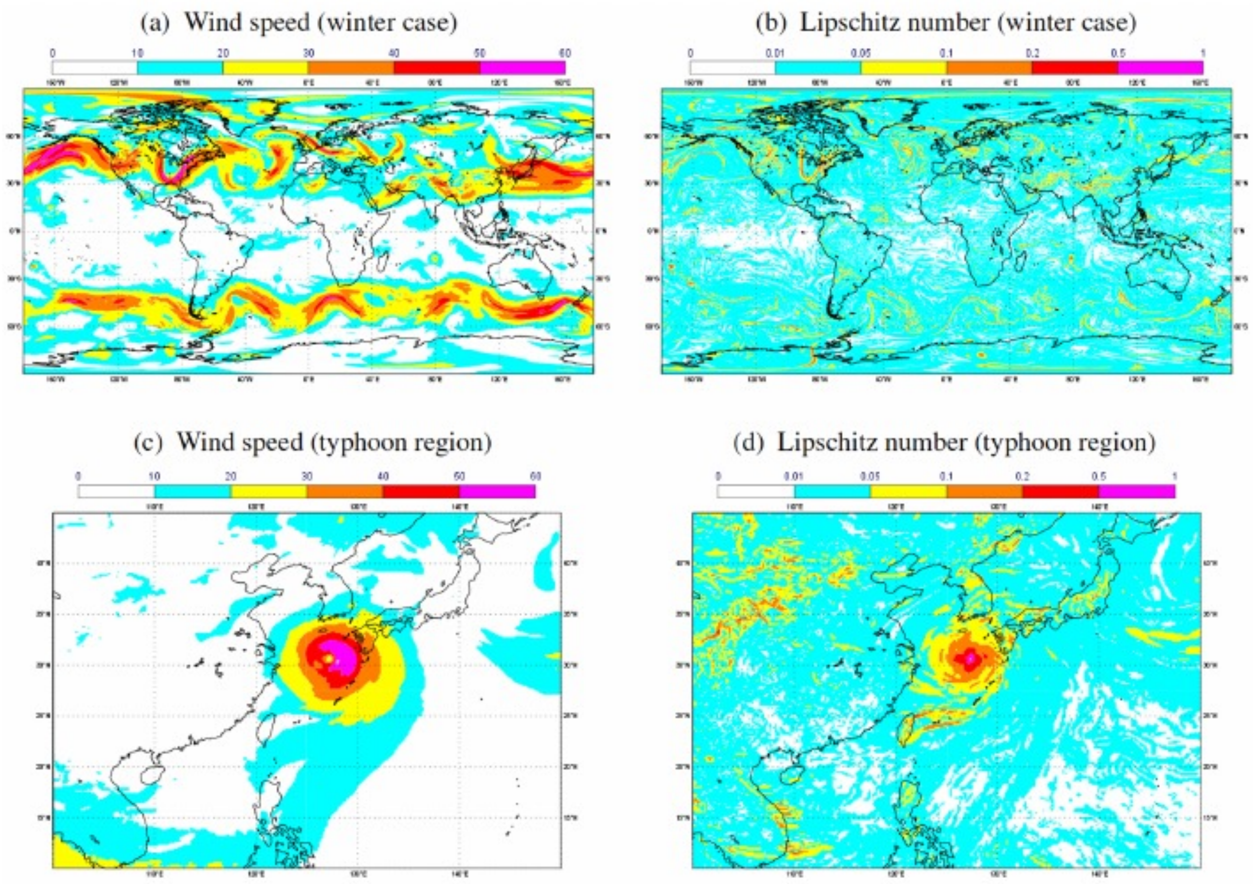
Interpolate to midpoint estimate

- In general, such iterative schemes converge if the Lipschitz number < 1

$$L \equiv \Delta t \left\| \frac{\partial \mathbf{V}}{\partial \mathbf{r}} \right\| \qquad \text{Lipschitz (deformational Courant) number}$$

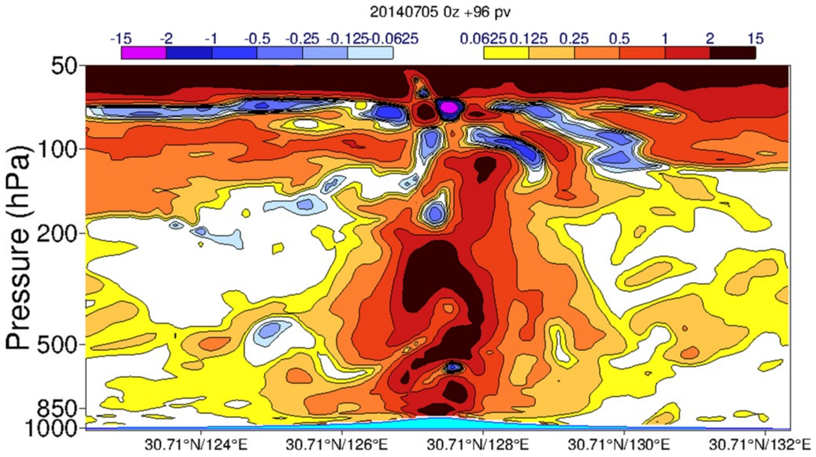
- $L < 1$ is a sufficient condition for convergence
- L is an upper bound of the rate of convergence

Lipschitz numbers in IFS forecasts

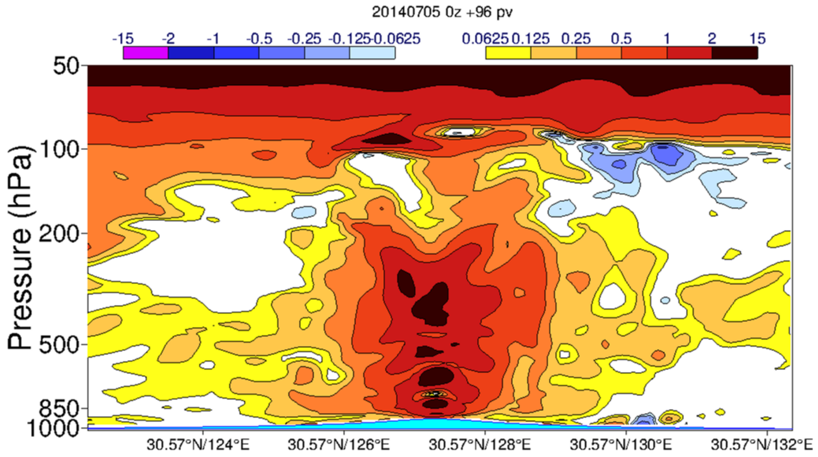


(a), (b): 00UTC 10 January 2014, t+48hrs fc at 500hPa. (c), (d): 00UTC 5 July 2014 t+96 hrs fc at 850hPa

Side-effects of non-converging DP iterations

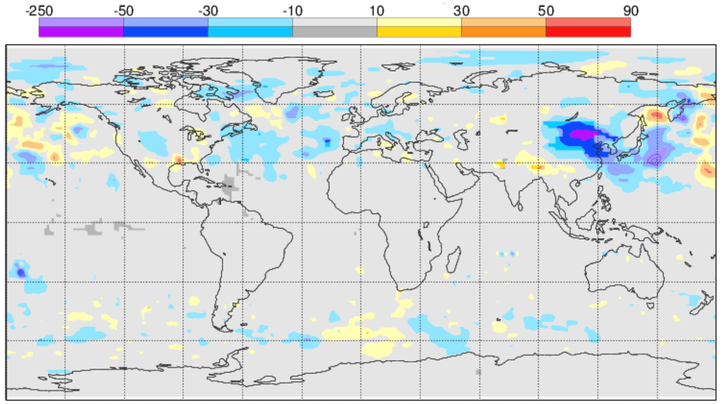


DP iterations haven't converged: **3 –iterations** with **old scheme**



DP iterations have converged: **5-iterations** with **old scheme** or **3-iterations** with **new scheme**

- **Pre IFS software cycle 48r1**: **5 DP iterations** needed for sufficient convergence (Diamantakis & Magnusson, MWR2016 doi:10.1175/MWR-D-15-0432.1)
- **From cycle 48r1:** fast convergence in **3 iterations** starting from previous timestep DPs (Diamantakis & Vana, QJRMS 2021, https://doi.org/10.1002/qj.4224)



Root Mean Square Error difference for the geopotential height when DP iterations have not sufficiently converged

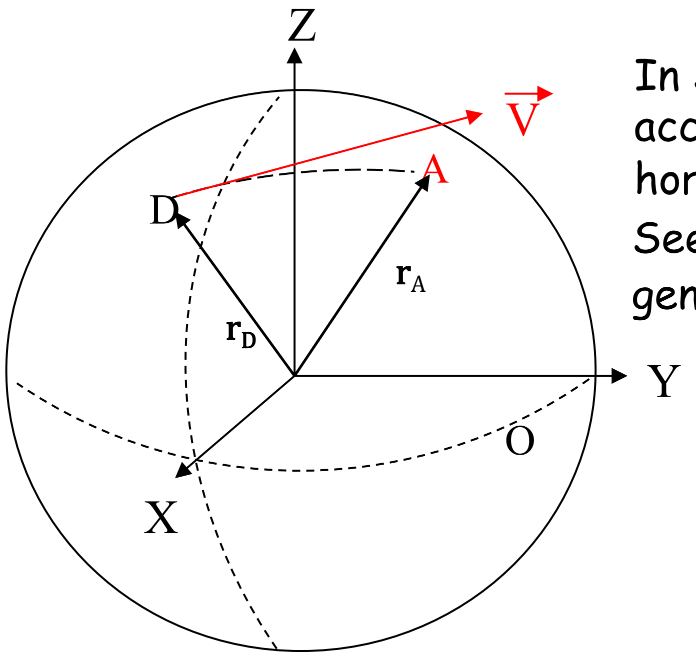
SL advection on the sphere in cycle 48r1+

To compute DP on the sphere:

1. Transform horizontal velocities (u,v) in a geocentric Cartesian system (X, Y, Z)
2. Apply SETTLS algorithm to compute $r_d = (X_d, Y_d, Z_d, \eta_d)$
3. Compute lon/lat of DP from (X_d, Y_d, Z_d) ⟶ $\lambda_d = ATAN2(Y_d, X_d)$

$$\theta_d = \arcsin \frac{Z_d}{\sqrt{X_d^2 + Y_d^2 + Z_d^2}}$$

Details of the implementation on the IFS terrain following coordinate in: Diamantakis & Vana QJRMS 2021 10.1002/qj.4224.



In **SL transport**, **vector** quantities **transported** from **D** to **A must be rotated** to account for curvature effects: multiply with a "rotation matrix" R the interpolated horizontal wind vector at D

See Temperton et al QJRMS 2001, Staniforth et al QJRMS 2010 (provides general formula independent of φ=angle $\widehat{DOA}$ between position vectors $\mathbf{r}_A$ and $\mathbf{r}_D$)

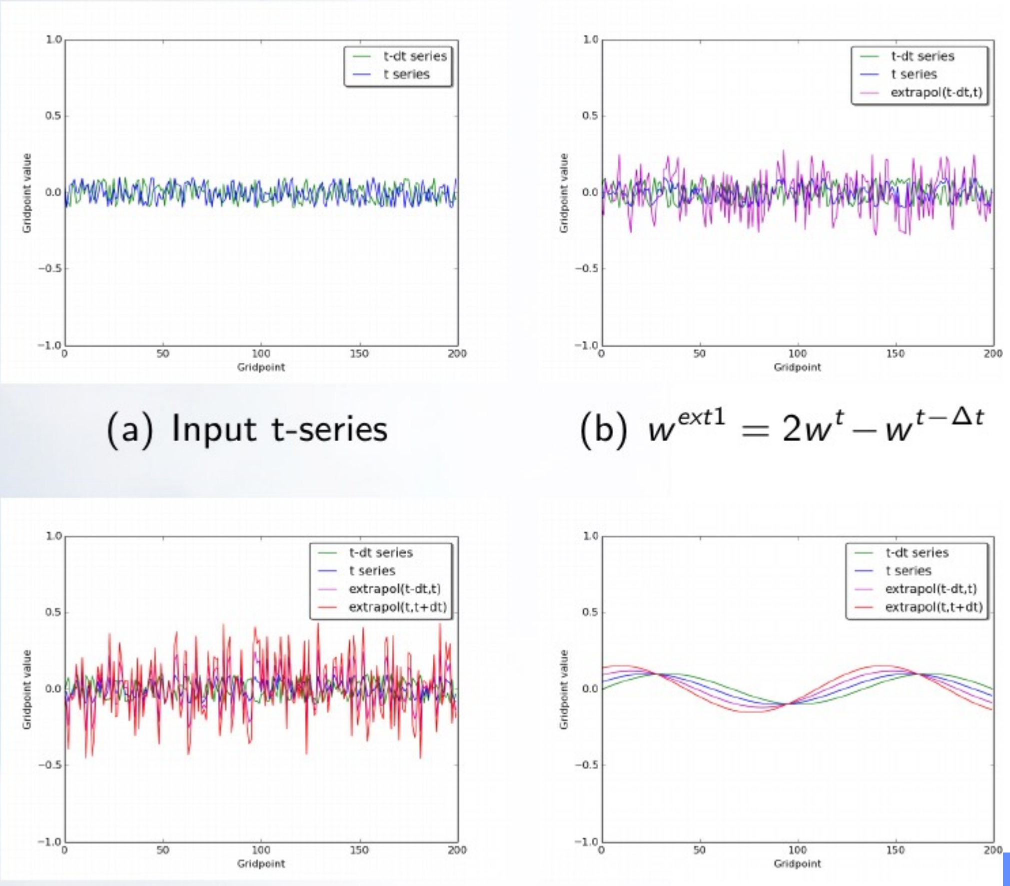
$$\begin{pmatrix} u_A \\ v_A \end{pmatrix} = \underbrace{\begin{pmatrix} p & q \\ -q & p \end{pmatrix}}_{R(V_D):\ rotation\ matrix} \begin{pmatrix} u_D \\ v_D \end{pmatrix}, \quad q = \frac{(\sin\theta_A + \sin\theta_D)\sin(\lambda_A - \lambda_D)}{1+\cos\varphi}$$

$$p = \frac{\cos\theta_A \cos\theta_D + (1+\sin\theta_A \sin\theta_D)\cos(\lambda_A - \lambda_D)}{1+\cos\varphi}$$

SETTLS adjustment for stratospheric warming predictions

- In "Sudden Stratospheric Warmings" noise is seen in upper stratosphere and model underpredicts the temperature
- Noise due to time extrapolation of vertical velocity in SETTLS
- Solution: use non-extrapolating 1st order scheme for gridpoints with sudden changes in vertical velocity in 2 consecutive steps

Impact of SETTLS time-extrapolation on noisy and smooth data



(a) Input t-series

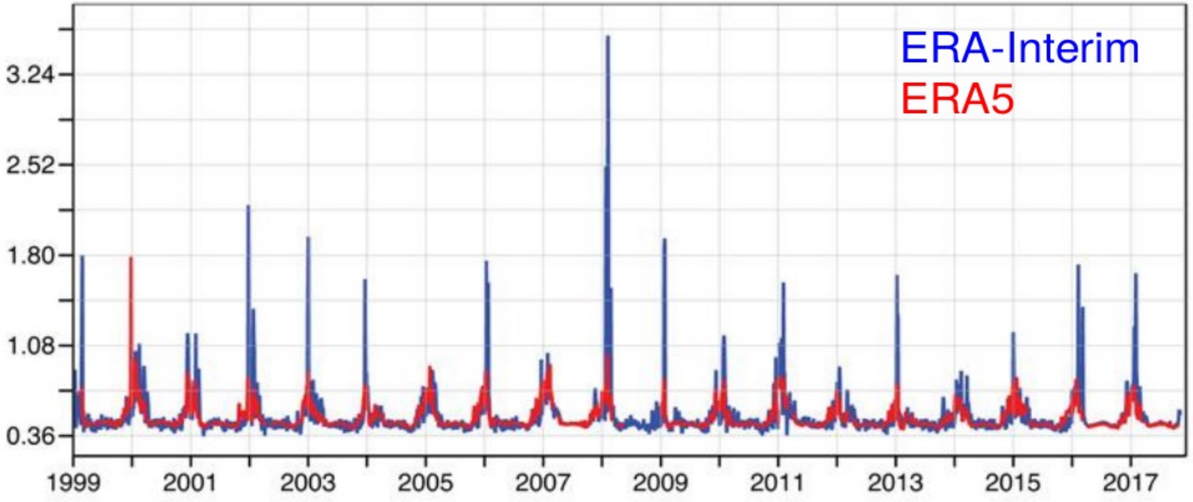
(b) $w^{ext1} = 2w^t - w^{t-\Delta t}$

(c) $w^{ext2} = 2w^{ext1} - w^t$

(d) Smooth data

Much better representation of SSW due to SETTLS improvements

NH winter SSWs

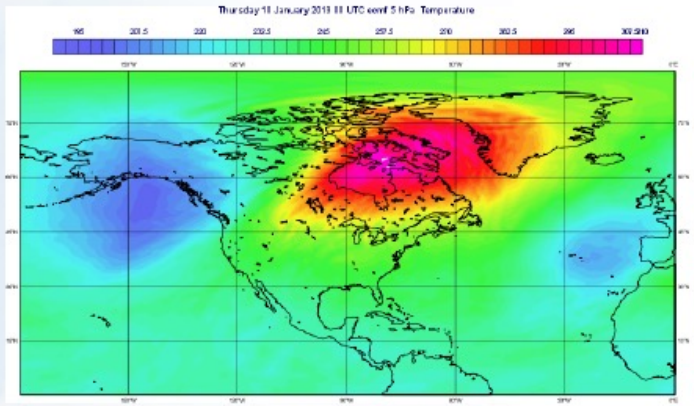


Standard deviation of MW radiances observed vs simulated temperature fields of ERA-Interim (blue) and ERA5 (red) using satellite channel (noaa15) peaking around 5hpa.

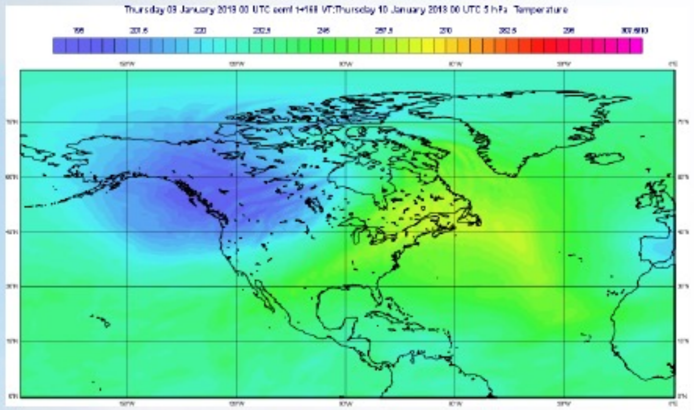
T. McNally, A. Simmons

Reference: "Improving ECMWF forecasts of sudden stratospheric warmings", ECMWF newsletter No.141 Autumn 2014

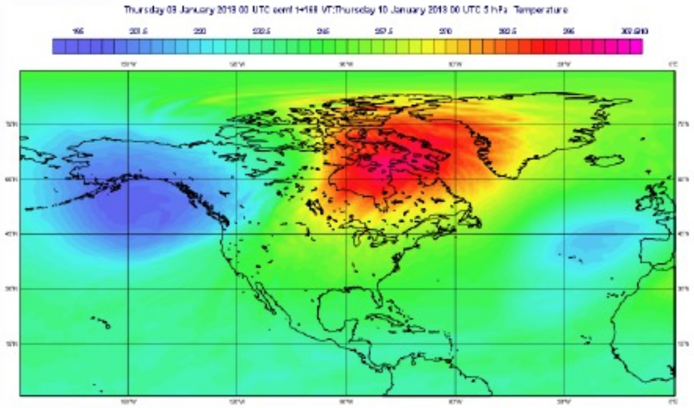
Major SSW January 2013



(a) Analysis



Original SETTLS t+7day



Improved SETTLS switching off 2nd order time-extrapolation in regions of oscillations: t+7days

Interpolation in the IFS semi-Lagrangian scheme

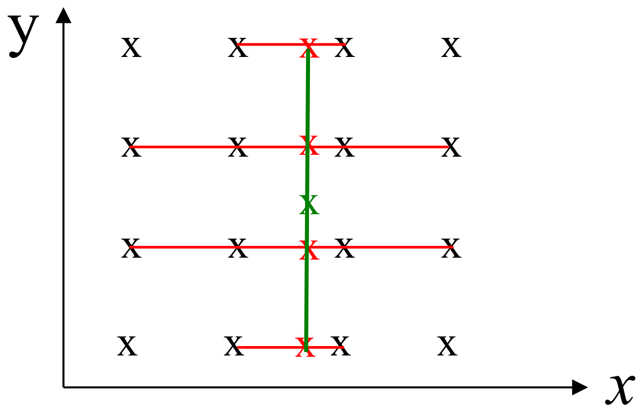
After computing the departure points we need to:

- ***Interpolate** the advected field at the **DP** using neighbouring gridpoints*
- ***Interpolation weights** are **computed once per time step** and are the same for all advected variables**: multi-tracer efficient scheme***

ECMWF model uses quasi-monotone quasi-cubic Lagrange interpolation (quintic in the vertical for temperature, specific humidity ref Policthchouk et al ECMWF newsletter 163)

Cubic Lagrange interpolation: $$\phi(x) = \sum_{i=1}^{4} w_i(x)\phi_i \;,\; w_i(x) = \frac{\prod_{k\neq i}^{4}(x - x_k)}{\prod_{k\neq i}^{4}(x_i - x_k)}$$

Faster alternative currently investigated: sweep-quadratic interpolation GMD 17, 2024



Fully cubic interpolation:

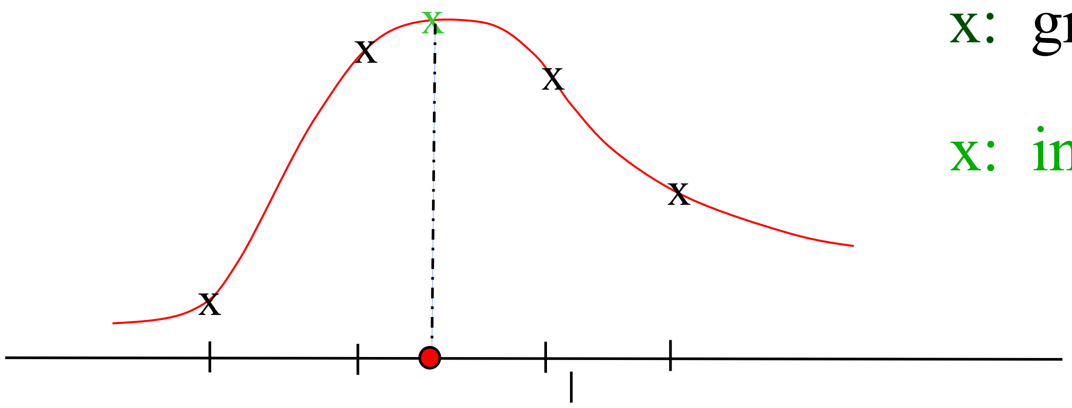
- **5 cubic interpolations in 2D**
- **21 in 3D (64pt stencil)**

Quasi-cubic interpolation reduces computational cost maintaining accuracy:

- **3*cubic+2*linear interpolations in 2D**
- **7*cubic+10*linear in 3D (32 pt stencil)**
  - Cubic interpolation at nearest to the departure point rows
  - Linear interpolation for remaining rows

Limiter for shape-preserving (locally monotonic) interpolation

- Creation of “artificial” maxima /minima

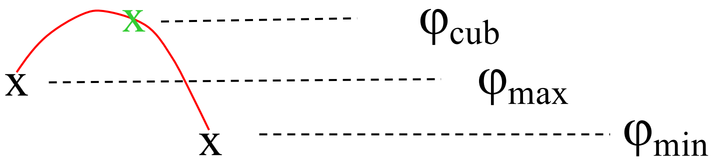


x: grid point values

x: interpolated value

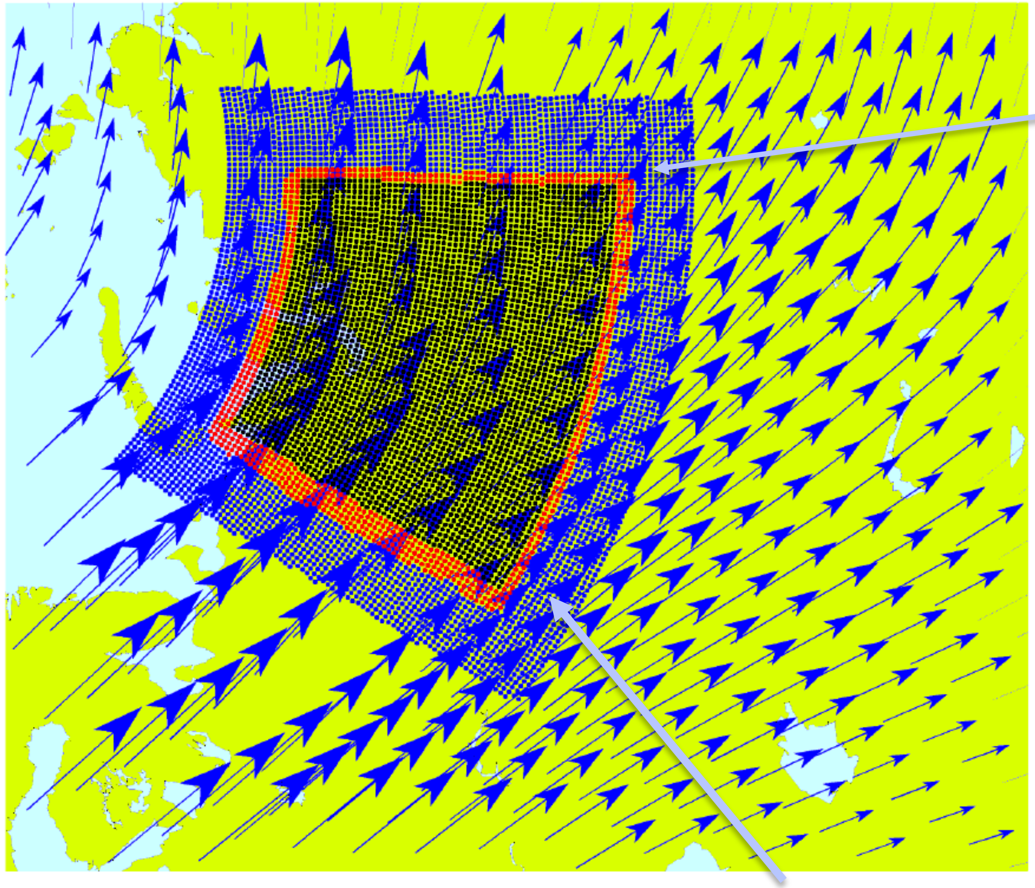
- Shape-preserving (quasi-monotone) cubic interpolation QMSL scheme (Bermejo & Staniforth, MWR 1992)

$$\varphi_{qm} = \max\left(\varphi_{\min}, \min\left(\varphi_{\max}, \varphi_{cub}\right)\right)$$



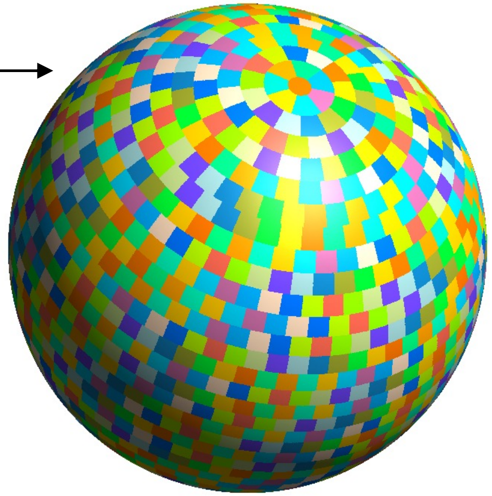
Parallel implementation

Interpolation at the DP near the edges of MPI domains requires data from a neighbouring domain (note that DP may lie at a different domain)



Blue: Halo region

Equal region domain decomposition + MPI and openMP parallel



Halo width for MPI assumes a maximum wind speed larger than the ones observed in the atmosphere e.g. 250m/s

Two levels of communication:

- Entire wind halo filled for the DP iterations
- When the DP is known then only a smaller sub-region around the DP needs to be filled
- No need to fetch data from remote processors at the expense of extra memory use

Combining semi-Lagrangian with semi-implicit (SI) time stepping

- A nonlinear system of m-prognostic equations must be solved:

$$\frac{DX}{Dt} = M(X), \quad X = (X_1, X_2, \ldots, X_m)$$

e.g. X=(u,v,T,p,q,…)

- Integrate along SL trajectory using a "trapezoidal" 2nd order approximation to obtain semi-implicit (Crank-Nicolson) scheme:

$$X^{t+\Delta t} - X_d^t = \int_t^{t+\Delta t} M(X)dt \Rightarrow X^{t+\Delta t} - X_d^t = \frac{\Delta t}{2}\left(M_d^t + M^{t+\Delta t}\right)$$

Subscript d denotes interpolation at the departure point

Subscript is omitted when variables are at arrival (grid) points

- Use isothermal reference profiles to linearise the "fast" terms of the right-hand side M and split them to a linear and a residual part:

$$\Re = M - L$$

R: nonlinear residual terms; these are changing slowly and can be integrated explicitly

L:"Fast linearized" (e.g. GW) terms. These must be integrated implicitly for stability

IFS-SISL for NWP prognostic equations

With splitting in fast linear and slow nonlinear residual terms the two-time-level, 2nd order IFS discretization (Temperton et al, QJRMS 2001) becomes:

$$\frac{X^{t+\Delta t} - X_d^t}{\Delta t} = \frac{1}{2}\left(L_d^t + L^{t+\Delta t}\right) + \frac{1}{2}\overbrace{\left(\Re_d^{t+\Delta t/2} + \Re^{t+\Delta t/2}\right)}^{\text{time-extrapolated nonlinear res}}$$

terms interpolated at the DP

The 2nd right hand side term in brackets is an extrapolation & approximation (space/time) at the trajectory mid-point i.e. $\approx \Re_M^{t+\Delta t/2}$ and can be substituted by the SETTLS expansion:

$$\Re_M^{t+\Delta t/2} = \Re_d^t + \frac{\Delta t}{2}\left(\frac{d\Re}{dt}\right)_{AV} \approx \Re_d^t + \frac{\Delta t}{2}\frac{\Re^t - \Re_d^{t-\Delta t}}{\Delta t}$$

Re-arranging terms, yields the familiar SETTLS formula resulting in a 2nd order discretization scheme

$$\frac{X^{t+\Delta t} - X_d^t}{\Delta t} = \frac{1}{2}\left(L_d^t + L^{t+\Delta t}\right) + \Re_M^{t+\Delta t/2}, \qquad \Re_M^{t+\Delta t/2} = \frac{1}{2}\left(\Re^t + \left\{2\Re^t - \Re^{t-\Delta t}\right\}_d\right)$$

all right-hand side terms are given

Helmholtz equation

- Elimination of variables in the semi-implicit discretized equations, leads to a single **Helmholtz elliptic equation** in terms of horizontal wind divergence
- Helmholtz equation is solved in spectral space at the end of each timestep
- Constant reference profiles ⇨ constant coefficient **Helmholtz equation**
- Using spherical Harmonics properties Helmholtz equation can be solved very cheaply with a direct diagonal solver (or 5-diagonal when Coriolis terms are implicit)
  - Having a cheap Helmholtz solver + being able to use large Δt (due to unconditional stability and good dispersion properties of SISL) contributes to high computational efficiency
- Remaining prognostic variables are computed with back substitution

Application to the IFS Hydrostatic model

$$\frac{D\mathbf{V}_h}{Dt} + f\mathbf{k}\times\mathbf{V}_h + \nabla_h\Phi + R_d T_v \nabla_h \ln p = P_{\mathrm{v}}$$

$$\frac{DT}{Dt} - \frac{\kappa T_v \omega}{\left(1+(\delta-1)q\right)p} = P_{\mathrm{T}}, \qquad \frac{Dq_x}{Dt} = P_{\mathrm{q}_x}$$

$$\frac{D}{Dt}(\ln p_s) = \mathbf{V}_h \cdot \nabla_h (\ln p_s) - \frac{1}{p_s}\int_0^1 \nabla_h \cdot (\mathbf{V}_h \frac{\partial p}{\partial \eta}) d\eta$$

$$\Phi = \Phi_s - \int_1^\eta R_d T_v \frac{\partial}{\partial \eta}(\ln p)\, d\eta$$

η : terrain following (pressured based) vertical coordinate

V_h : horizontal momentum $\mathbf{V}_h = (u, v)$

∇_h : horizontal gradient

T_v: virtual temperature

q_x: humidity and moist tracers, $\delta = c_{pv}/c_{pd}$

Φ: geopotential

p, p_s : pressure, surface pressure

$\omega = dp/dt$: diagnostic vertical velocity

P: physics forcing terms

Identify fast nonlinear terms of this equation set and linearise equations:

$$\frac{DX}{Dt} = M(X), \quad \Re \equiv M(X) - LX, \quad X = \mathbf{V}_h, T, \ln p_s$$

nonlinear but slow changing — linear but fast changing

Deriving Helmholtz equation

- For simplicity assume dry dynamics ($T=T_v$)
- Also assume that **Coriolis terms are incorporated in V_h** (advective form): $\boldsymbol{X} = \boldsymbol{V}_h + 2\Omega\times\boldsymbol{r}$

$$\frac{X^{t+\Delta t} - X_d^t}{\Delta t} = 0.5\left(L_d^t + L^{t+\Delta t}\right) + \Re_M^{t+\Delta t/2}$$

Note: following convention terms without subscript are assumed to be on a grid-point

$$X^{t+\Delta t} - 0.5\Delta t L^{t+\Delta t} = \underbrace{X_d^t + 0.5\Delta t L_d^t + \Delta t\, \Re_M^{t+\Delta t/2}}_{\equiv X^*\ (known\ part)}$$

$$L \equiv -\nabla_h(\underline{\underline{\gamma}}\, T + R_d T_{ref} \ln p_s), -\underline{\underline{\tau}} D, -\underline{\underline{\nu}} D \quad \text{for } X = D, T, \ln p_s$$

Linearised terms for different equations

$$D^{t+\Delta t} + 0.5\Delta t \nabla_h^2\left(\underline{\underline{\gamma}} T^{t+\Delta t} + R_d T_{ref} \ln p_s^{t+\Delta t}\right) = D^*$$

$$T^{t+\Delta t} + 0.5\Delta t\, \underline{\underline{\tau}} D^{t+\Delta t} = T^*$$

$$\ln p_s^{t+\Delta t} + 0.5\Delta t\, \underline{\underline{\nu}} D^{t+\Delta t} = P^*$$

Momentum equation in terms of divergence D has been derived by applying the $\nabla\cdot$ operator in horizontal momentum component discrete equation

T_{ref} : constant temperature reference profile

$\underline{\underline{\gamma}}, \underline{\underline{\tau}}, \underline{\underline{\nu}}$: operators defined in Ritchie et al MWR vol 123, 1995

D : horizontal divergence

T, $\ln p_s$ can now be eliminated deriving a single elliptic equation in terms of D

Solving Helmholtz equation in spectral space

Prognostic variables are eliminated to derive a Helmholtz equation wrt to D in **spectral space**:

$$\left(\underline{\underline{I}} - \alpha^2 \Delta t^2 (\underline{\underline{\gamma}}\,\underline{\underline{\tau}} + R_d T_{ref} \underline{\underline{\nu}}) \nabla_h^2 \right) D^{t+\Delta t} = RHS$$

RHS contains all known terms (at time t)

[**α=1/2** (Crank-Nicolson), using **α**-value slightly >0.5 is often used by other models to control unwanted oscillations]

Define: $\underline{\underline{\Gamma}} \equiv \alpha^2 \Delta t^2 \left(\underline{\underline{\gamma}}\,\underline{\underline{\tau}} + R_d T_r \underline{\underline{\nu}} \right) \Longrightarrow \left(\underline{\underline{I}} - \underline{\underline{\Gamma}}\, \nabla_h{}^2 \right) D^{t+\Delta t} = RHS$

- Γ is constant in time, depends on the vertical discretization and couples all vertical levels
- In a spectral model, the Laplacian operator can be substituted analytically using properties of spherical harmonics:

$$\nabla^2 D_n^m = -\frac{n(n+1)}{r_0} D_n^m \Longrightarrow \left(\underline{\underline{I}} + \frac{n(n+1)}{r_o{}^2} \underline{\underline{\Gamma}} \right) D_n^m = B_n^m$$

(B is the RHS – known right hand side)

- The above system has a diagonal structure and can be easily solved for each (m,n) => Computationally Efficient!
- Once divergence D at new time level is found the remaining fields can be computed through back-substitution

A simplified overview of IFS time-stepping

Transform from **Spectral->Gridpoint** space

↓

1. **Compute R.H.S. terms** of equations at time t
2. Call **radiation** scheme (currently every 1 hr) and store output
3. **SL advection**: compute DP / interpolate at DP (advected variables and eqn RHS terms) / update variables adding advection tendencies
4. **Call physics updating tendencies** each time.

↓

Transform from **Gridpoint-> Spectral** space

↓

- **Solve Helmholtz** problem
- **Update** main **prognostic** variables
- **Add** horizontal **diffusion**

Grid-point space
- SL advection
- parametrizations
- products of NL terms

FFT

Fourier space

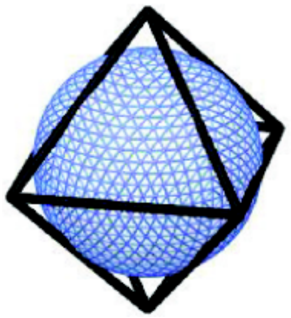
LT

Spectral space
- horizontal gradients
- SI calculations
- horizontal diffusion

Inverse LT

Fourier space

Inverse FFT



Octahedral grid

FFT: Fast Fourier Transform, LT: Legendre Transform

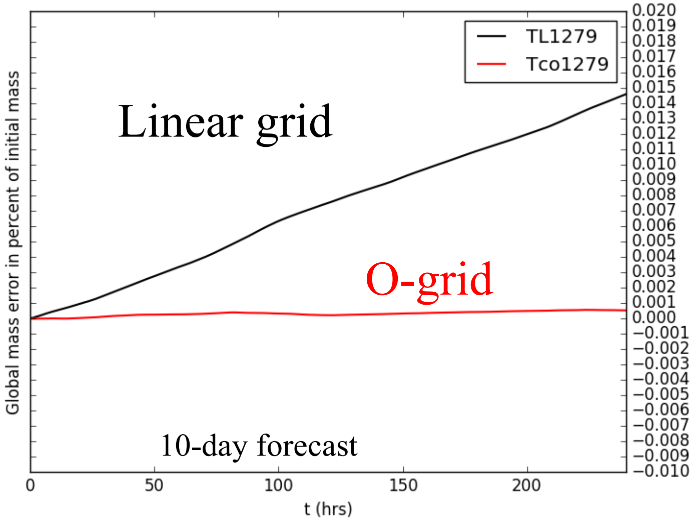
A note on SL and its truncation error

- Falcone, Feretti SIAM J. 1998: *the leading order truncation error term for a SL method applied to a 1D constant wind advection equation with an interpolation formula of order p on a grid with constant spacing Δx and an order k time-integration method with timestep Δt for the DP is* $O\left(\Delta t^k + (\Delta x)^{p+1}/\Delta t\right)$
- Resolution refinement and timestep reduction should be applied simultaneously rather than separately to improve accuracy
  - small Δt improves the accuracy of the DP calculation
  - However, with unnecessarily short Δt too many interpolations and therefore more diffusion from them
  - Smaller Δx reduces spatial truncation errors
  - $\Delta t, \Delta x$ ratio must be adjusted together to optimize accuracy

Mass conservation in semi-Lagrangian advection

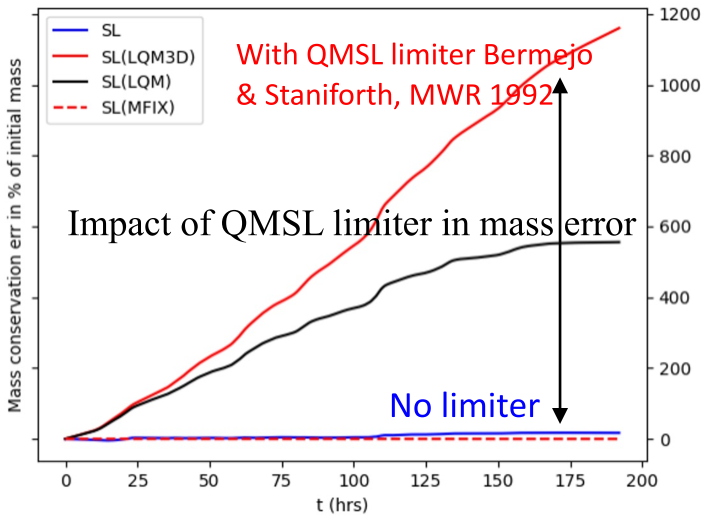
Mass conservation: important for atmospheric composition forecasts, for long range forecasts, climate and overall for high-resolutions

- Semi-Lagrangian time-stepping does not conserve mass, energy, momentum
- Why? (i) continuity expressed in non-conservation form (ii) interpolation errors
- Mass conservation errors depend on the characteristics of the transported variable:
  - Small for smooth tracers and total mass of air
  - Large for localised tracers with large gradients: **monotone interpolation limiters amplify** cons errors!
  - Tracers flowing near the surface exhibit larger conservation errors (stronger vertical advection and boundary condition influence)



With O-grid **total air** mass conservation error is very small in double precision

Mass errors as percent of initial mass

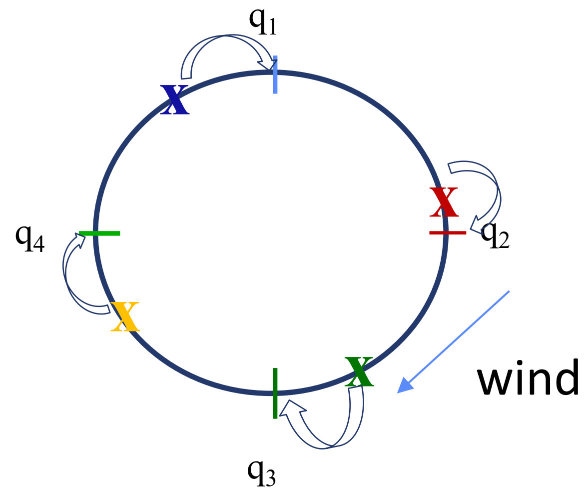


Case study: artificial discontinuous tracer 4x5 degrees rectangle placed on the near surface level near Shanghai:

- Large mass conservation error growth in time
- Monotone limiter greatly amplifies those

Why SL does not conserve? A simple 1D demo

$$q=\frac{\rho_t}{\rho},\ \Delta x=const,\ m=q\rho\Delta x$$



x: a departure point associated with grid-point

For a uniform grid and non-divergent constant wind flow the SL method without limiter can conserve a tracer mass if the background air density does not change but not in the general case

Case A: constant wind on uniform grid (departure point distances from grid-points are equal which results into constant interpolation SL weights on each grid cell)

$$q_j^{n+1}=(1-\alpha)\,q_j^n+\alpha q_{j-1}^n,\qquad q_0=q_N,\ N=4$$

$$M^{n+1}=\sum_{j=1}^{N}q_j^{n+1}\rho\,\Delta x=\sum_{j=1}^{N}\left[(1-\alpha)\,q_j^n+\alpha q_{j-1}^n\right]\rho\,\Delta x=\sum_{j=1}^{N}q_j^n\rho\,\Delta x=M^n$$

Case B: non-constant wind or non-uniform grid (variable departure point distances)

$$q_j^{n+1}=\left(1-\alpha_j\right)q_j^n+\alpha_j q_{j-1}^n,\qquad q_0=q_N$$

$$M^{n+1}=\sum_{j=1}^{N}q_j^{n+1}\rho\,\Delta x=\sum_{j=1}^{N}\left[\left(1-\alpha_j\right)q_j^n+\alpha_j q_{j-1}^n\right]\rho\,\Delta x$$

Conservation error

$$=\sum_{j=1}^{N}q_j^n\rho\,\Delta x+\sum_{j=1}^{N}\left[\alpha_j\left(q_j^n-q_{j-1}^n\right)\right]\rho\,\Delta x=M^n+\sum_{j=1}^{N}\left[\alpha_j\left(q_j^n-q_{j-1}^n\right)\right]\rho\,\Delta x$$

Enforcing conservation with mass fixers

- A simple mass fixer (rescaling) is applied on surface pressure field to keep air mass constant in time
- A tracer mass fixer is also applied on water tracers, GHG gases, aerosols
  - The tracer mass fixer used is a locally weighted scheme (ECMWF TM 819, 2017 Diamantakis & Agusti-Panareda, scheme based on Bermejo & Conde MWR 2002) which gives more skilful tracer concentration predictions apart of correcting their global mass error

$$\phi_{jk} = \phi_{jk}^{adv} - \lambda w_{jk}, \quad \lambda = \frac{\delta M}{\underbrace{\sum_j A_j \sum_k w_{jk} \frac{\Delta p_{jk}^{adv}}{g}}_{\text{mass integral}}}, \quad \delta M = M\left(\phi_\chi^{adv}\right) - M\left(\phi_\chi^n\right)$$

Corrected tracer mixing ratio (ϕ_{jk})

Tracer mixing ratio after advection (ϕ_{jk}^{adv})

Lagrange multiplier (λ)

M total mass for tracer ϕ

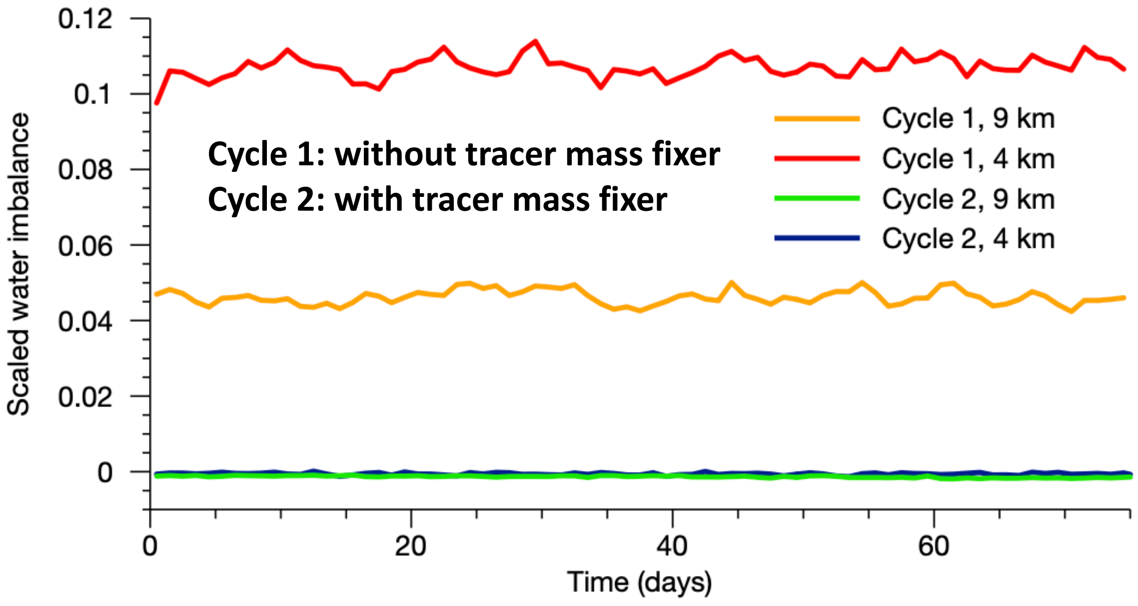
δM: mass conservation error in a timestep after SL advection

w_{jk} is a weight that depends on the sign of δM, it is proportional to the interpolation truncation error and the mass content of grid-box that corresponds to jk

Correction computed by the mass fixer is the solution of a constrained optimization problem that ensures that its global norm is minimized subject to the constraint that global mass remains constant

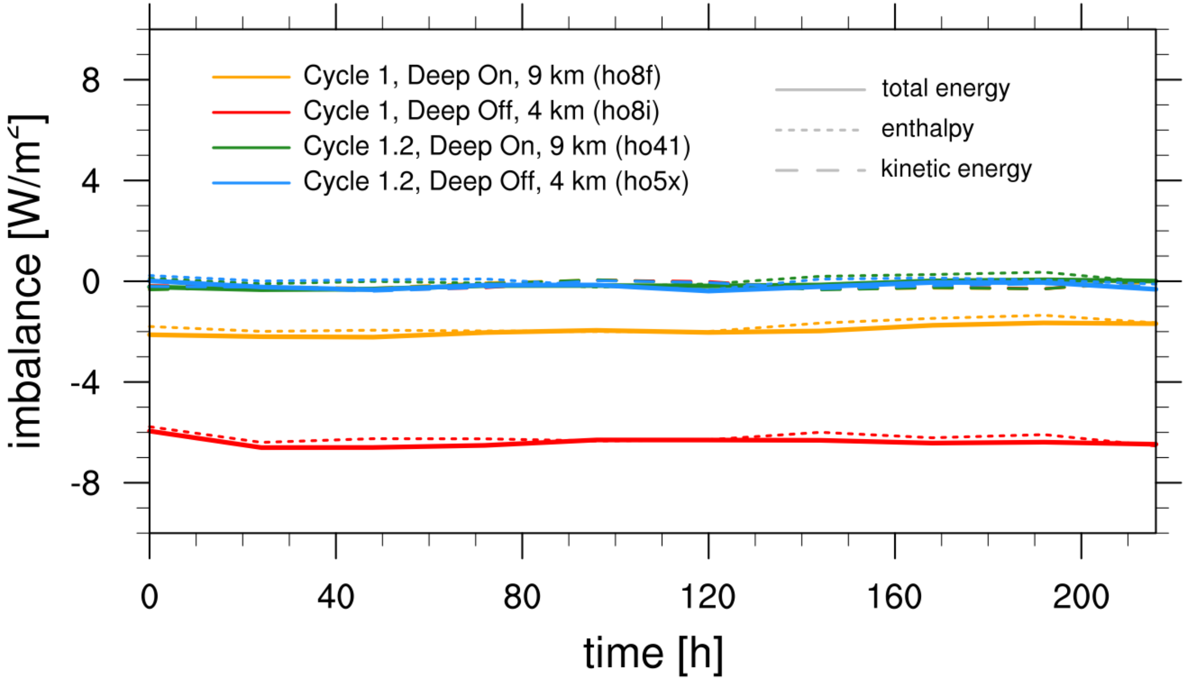
Fixing water leakage in IFS

Mass fixer on moist tracers (humidity, clouds): improvement in precipitation scores and overall skill of ENS forecasts



Total water conservation error as a fraction of total precipitation in long integrations

- 10% surplus is reduced to nearly 0% with tracer mass fixer



Total Energy leakage reduction with fixer:
2 W/m2 -> -0.15 (deep conv on)
6 W/m2 -> -0.32 (deep conv off)

Reference: ECMWF newsletter 172, p14

Plots and diagnostics by Tobias Becker from **nextGEMS project** runs

CATRINE = Carbon Atmospheric Tracer Research to Improve Numerical schemes and Evaluation

Funded by the European Union

CATRINE
Carbon Atmospheric Tracer Research to Improve Numerics and Evaluation

- HE project supporting CO2MVS (inversions of greenhouse gases)
- **Focus** on **numerical schemes + evaluation**
  - Development of case studies & diagnostics to understand origin & evolution of mass conservation errors in IFS SL advection
  - Design / implementation of improved algorithms and analysis of their impact on conservation & transport accuracy

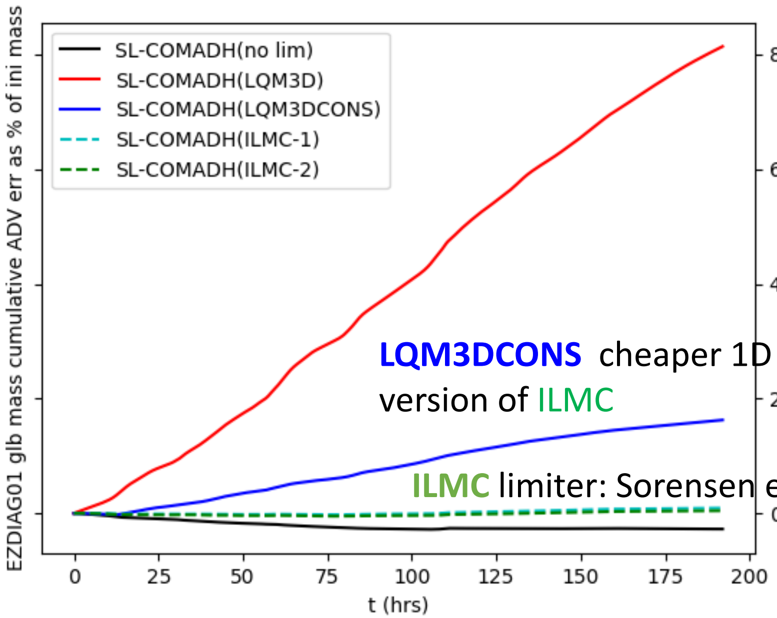
Project reports with detailed information on SL advection transport scheme evaluation and improvements:

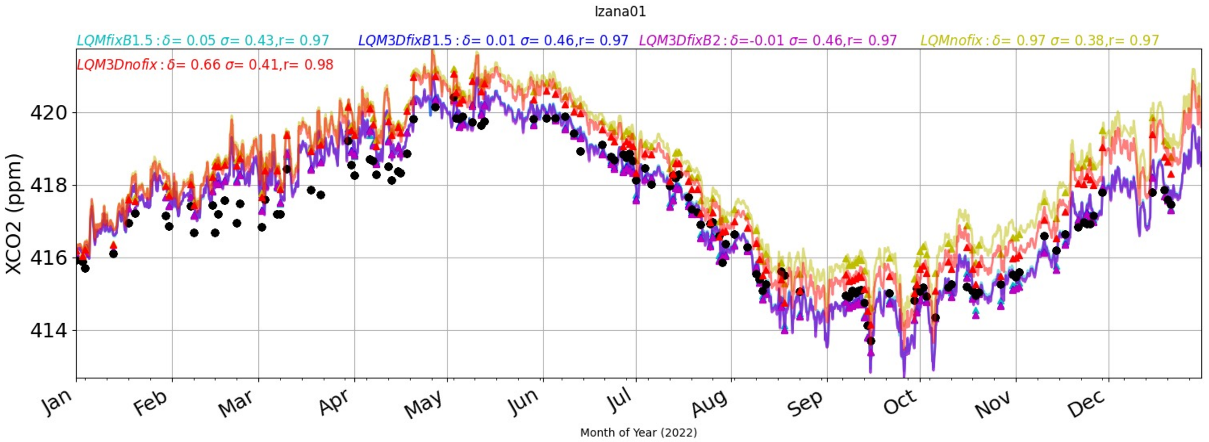
https://www.catrine-project.eu/sites/default/files/2025-04/CATRINE-D1-1-V1.1.pdf

https://www.catrine-project.eu/sites/default/files/2025-06/CATRINE-D1-2-V1.0.pdf

Case study: artificial tracer initialized at the near surface level

Reduction of conservation error by ~ O(100) due to **conservative limiter**





Simulated time-series of CO_2 concentration versus observations at Izana site using CATRINE optimized fluxes (plot courtesy of A. Agusti-Panareda). **Conservation improves CO_2 simulation accuracy.** Mass fixer (purple, blue) compared to run without mass fixer (yellow, red)

Some references cited here and further relevant ones

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- Diamantakis & Magnusson (MWR 2016): “Sensitivity of the ECMWF Model to Semi-Lagrangian Departure Point Iterations ”
- S. Fletcher book: *Semi-Lagrangian Advection Methods and Their Applications in Geoscience* (2020)
- Hortal (QJRMS 2002): “The development and testing of a new two-time level semi-Lagrangian scheme (SETTLS) in the ECMWF model”
- Ritchie et al (MWR 1995): “Implementation of the Semi-Lagrangian Method in a High-Resolution version of the ECMWF forecast model”
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- Temperton,Hortal,Simmons (QJRMS 2001): “A two-time-level SL global spectral model”