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

Numerical methods for weather prediction training course
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Content 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
- Weaknesses of the semi-Lagrangian, semi-implicit approach

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
$\mathbf{V}_h$: horizontal momentum
T: temperature
T_v: virtual temperature (used as spectral variable)
q_x: specific humidity, specific ratios for cloud fields and other tracers x, $\delta = c_{pv}/c_{pd}$
Φ: geopotential
p : pressure
$\omega = dp/dt$: diagnostic vertical velocity
P: physics forcing terms

- Primitive equation hydrostatic
- There is non-hydrostatic option available which we use for research purposes but not operational
- Spectral Transform with spherical harmonics basis
- Cubic spline Finite Elements in the vertical
- Timestepping: semi-Lagrangian semi-implicit

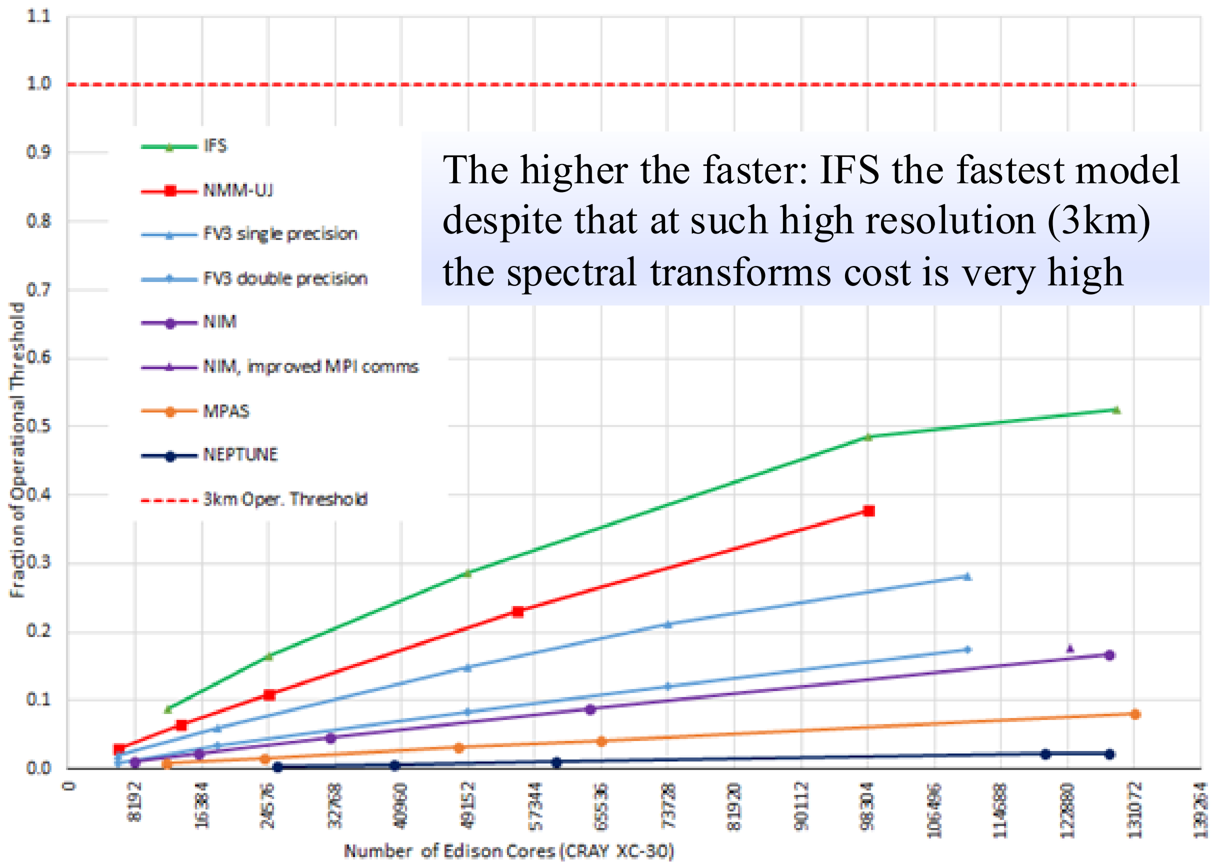
The critical role of time stepping

For operational global weather forecasting an <u>accurate</u> and <u>robust</u> weather model which operates at the <u>lowest possible cost</u> 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 remaining (non-advective) fast forcing terms
    - ➔ No timestep restriction from the integration of "fast forcing" terms such as gravity wave + acoustic terms (present in non-hydrostatic models)
    - ➔ 2nd order accuracy time-stepping + high order spatial discretization

SISL method and efficiency

- Semi-Lagrangian, semi-implicit time integration is very efficient: IFS is the fastest among several global models
- Combined with spectral transform method + Vertical Finite Elements makes it very accurate: IFS produces the best global scores against a range of WMO metrics

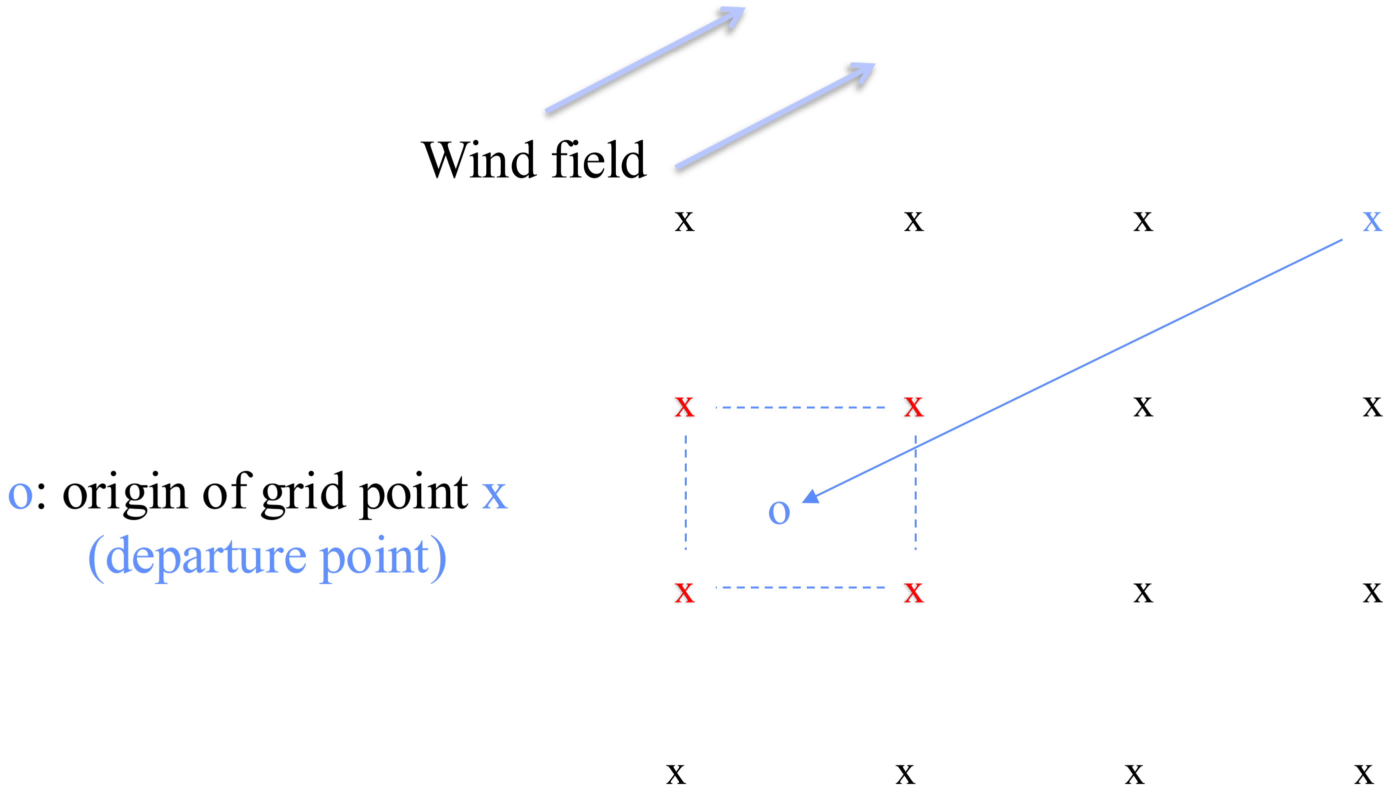


- *An example of IFS computational performance at approximately 3km resolution on a dry baroclinic wave case with tracers, adapted from Michalakes et al, NGGPS AVEC report, **2015***
- *Different "candidate US global models" were compared to IFS*

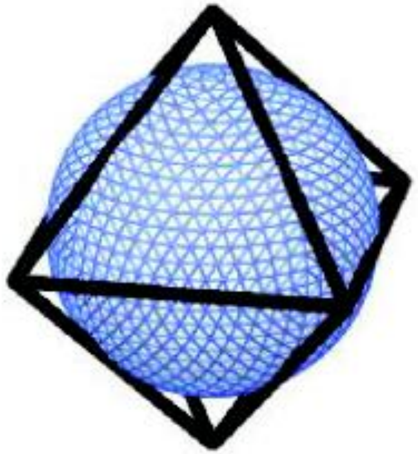
What is a semi-Lagrangian (SL) advection scheme?

- Advection (movement of air, its constituents such as 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)



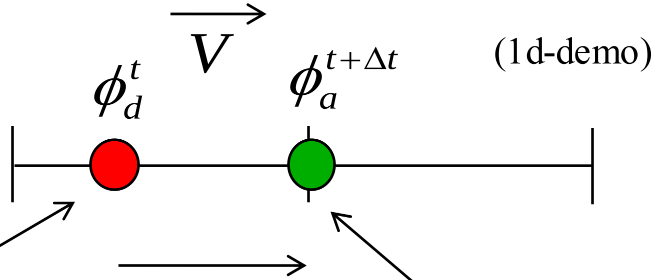
The SL solution of the advection equation

Tracer mixing ratio $\phi = \rho_\phi / \rho$ passive advection equation (equiv. with tracer continuity eqn):

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

At time t parcel is at d and at t +Δt arrives at a grid-point

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



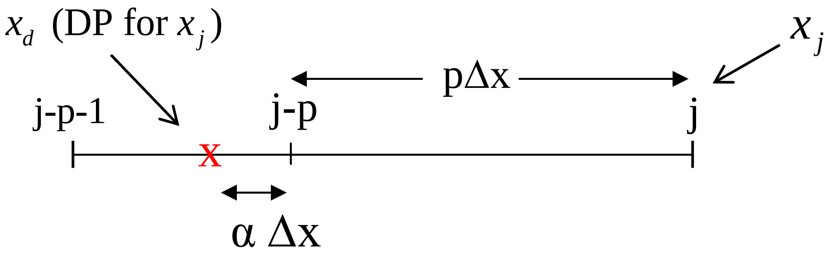
This is the known result: $\phi(r, t+\Delta t) = \phi(r - \Delta t V, t)$

d: **departure point** (DP)

a: arrival point

- Solution at t+Δt is obtained by finding the DP location and interpolating the available (defined at time t) grid-point ϕ values 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 (displacement): $x_j - x_d = u_0 \Delta t = (p+\alpha)\Delta x$ p: integer

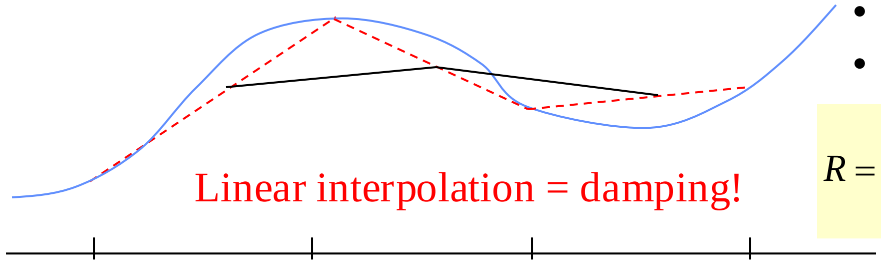
Von Neuman stability analysis assumes: $\phi_j^n = \phi_0 \lambda^n e^{ikj\Delta x}$

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

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

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

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



- No phase error when DP coincides with gridpoint
- Small phase error for large CFL

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

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

Consider that air parcels move in time in straight line trajectories. Perform a 2nd order Taylor expansion of an arrival (grid) point to its departure point:

Stable Extrapolation Two Time Level Scheme

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

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 (Hortal, QJRMS 2002) is an improvement of the **2nd order mid-point scheme below**:

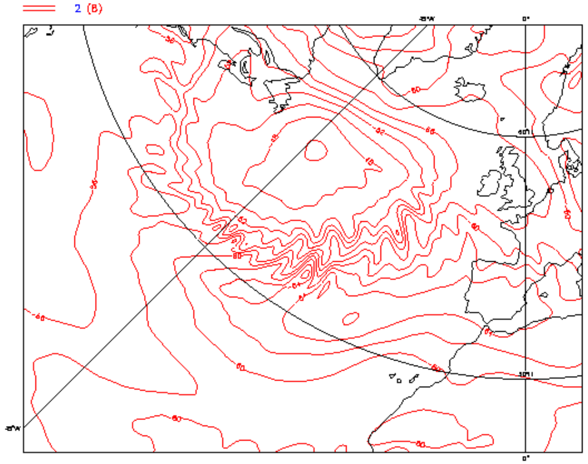
$$r_d^{(0)} = r_a - \Delta t V\left(r_a, t\right)$$

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

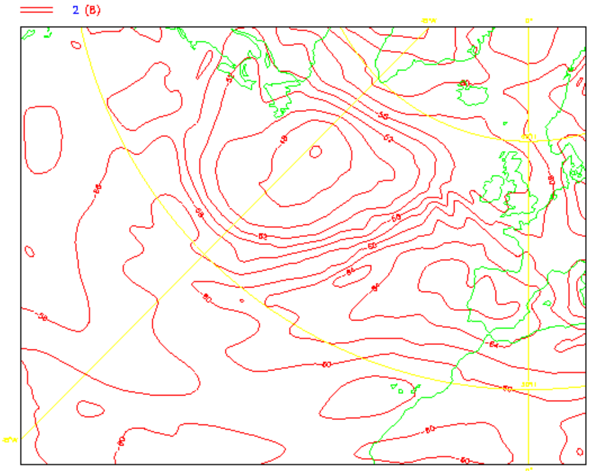
A familiar method: "Functional" or "fixed-point" iteration

Interpolate to midpoint estimate

- SETTLS improved stability eliminates noise in upper troposphere. Recent comparisons also confirm that is overall better



T forecast 200 hP (from 1997/01/04)

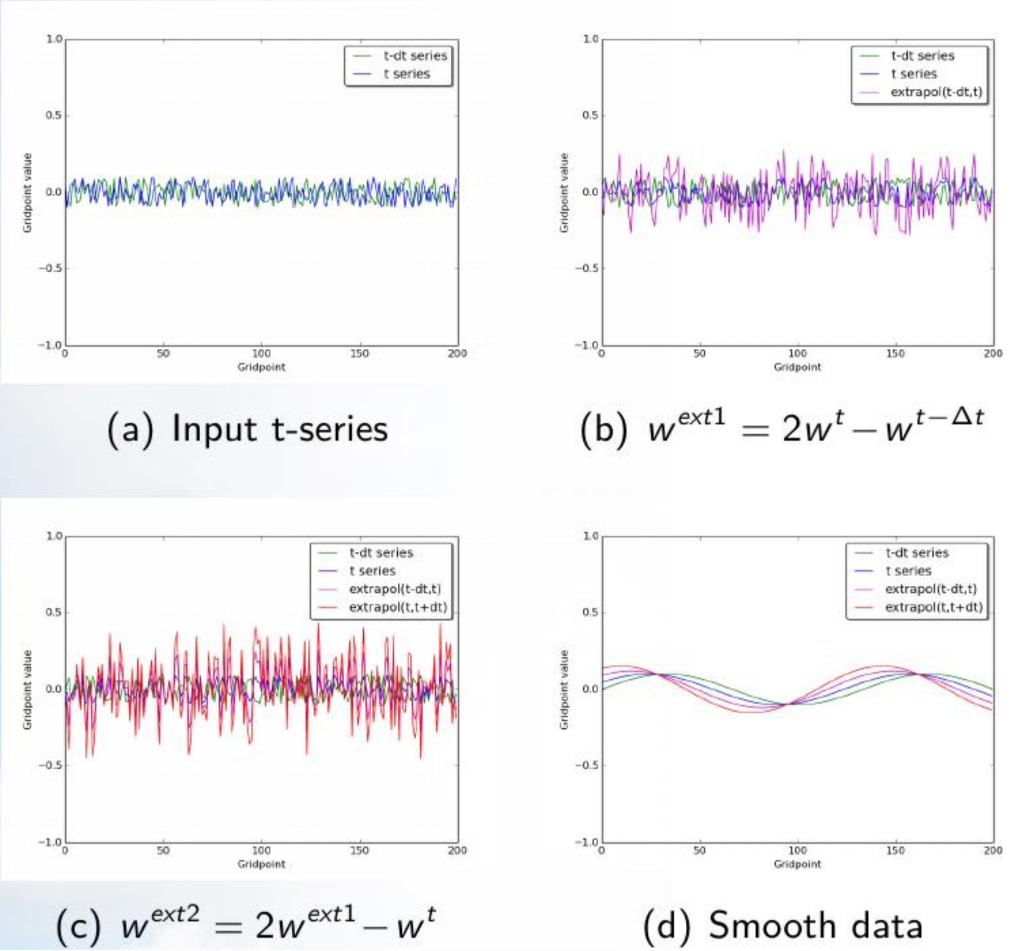


ECMWF

SETTLS adjustment for stratospheric warming predictions

- In “Sudden Stratospheric Warmings” noise is seen in upper stratosphere and model underpredicts the temperature
- Time extrapolation of Vertical velocity in SETTLS is the culprit
- 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

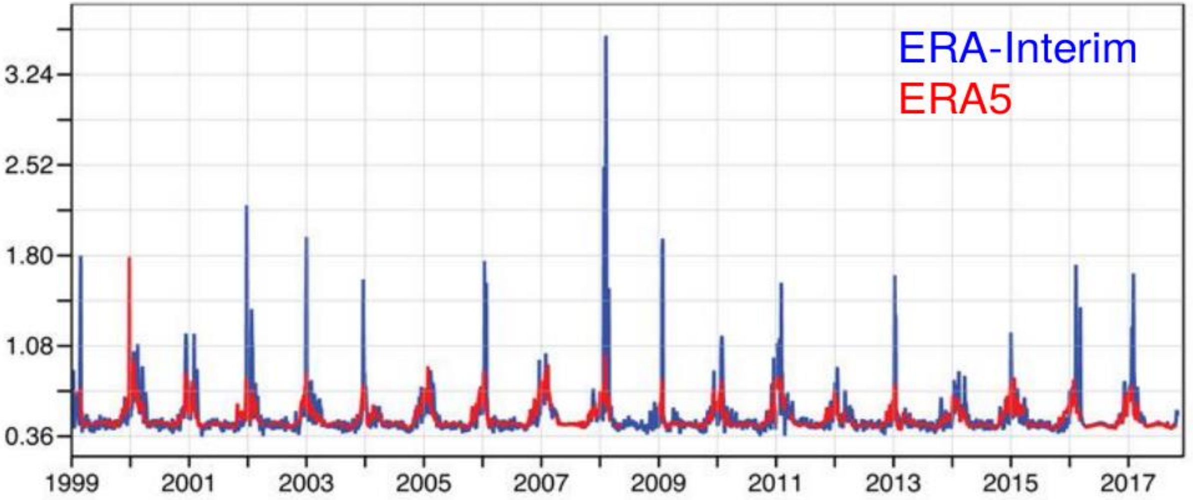
(b) $w^{ext1} = 2w^{t} - w^{t-\Delta t}$

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

(d) Smooth data

Much better representation of Sudden Stratospheric Warming events, due to changes in the Semi-Langrangian scheme (*Diamantakis, 2014*)

NH winter SSWs

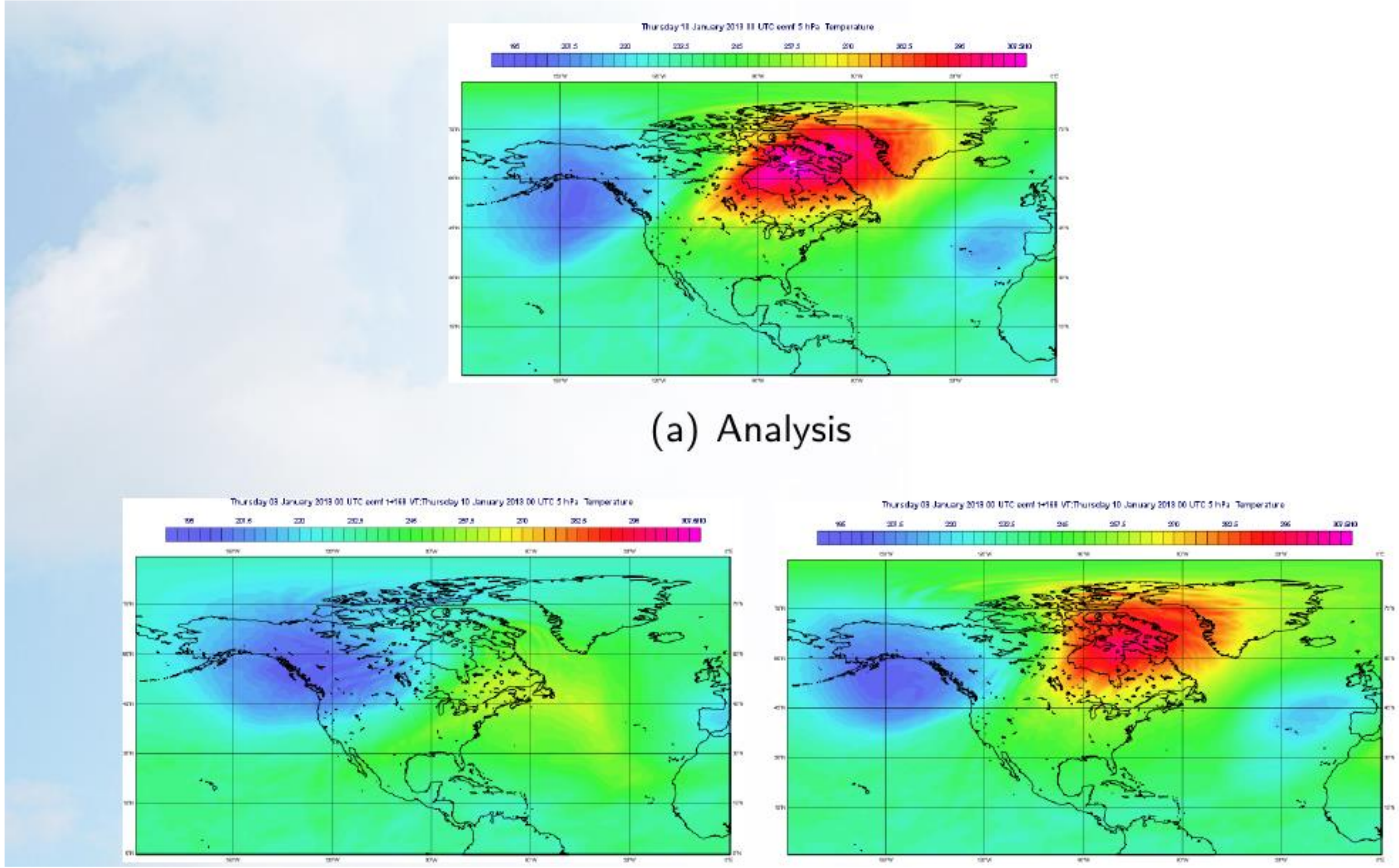


Standard deviation of MW radiances observed vs simulated temperature fields of ERA-Interim (blue) and ERA5 (red) using satellite channel (noaa15) peaking around 5hpa.

T. McNally, A. Simmons

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

Major SSW January 2013

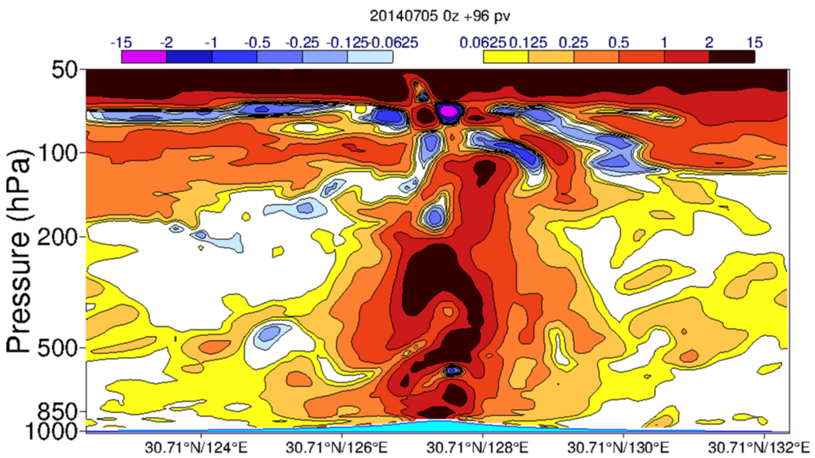


Original SETTLS t+7day

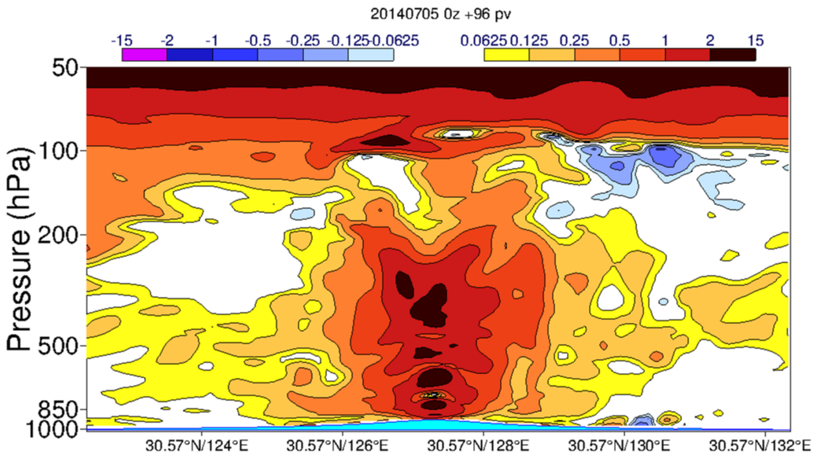
Improved SETTLS switching off 2nd order time-extrapolation in regions of oscillations: t+7days

Side-effects of non-converging DP iterations

- Due to very long timesteps, DP iteration convergence is slow in areas of strong winds & high shear. Non-convergence: "noise" in TCs or forecast skill loss (Diamantakis & Magnusson, MWR 2016)

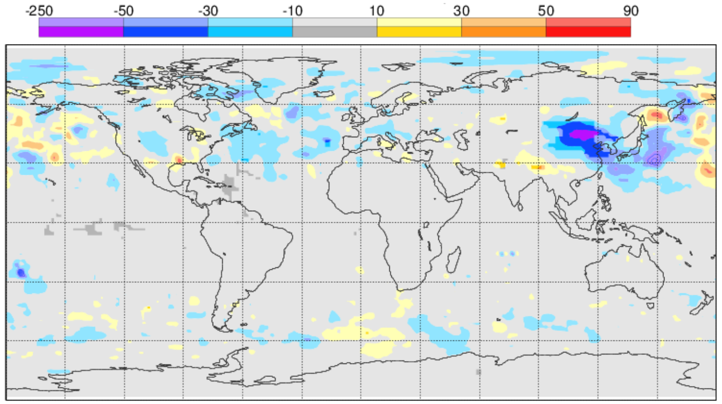


DP iterations haven't converged



DP converged with additional iterations

- Before cy48r1: 5 DP iterations needed for sufficient convergence
- Cycle 48r1: fast convergence in 3 iterations starting from previous timestep DPs (Diamantakis & Vana, QJRMS 2021)



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

ECMWF

Semi-Lagrangian advection on the sphere

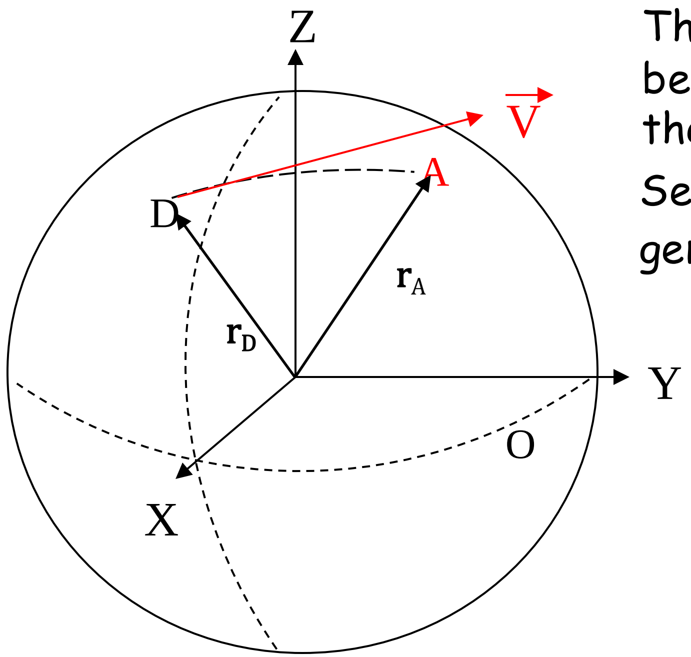
To compute DP on the sphere:

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) ⟶ $\lambda_d = ATAN2(Y_d, X_d)$

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

η_d is computed from SETTLS formula and iterated together with (X_d, Y_d, Z_d)

Details of the implementation, geometrical subtleties, cost benefits and how to deal with terrain following coordinates also in: Diamantakis & Vana QJRMS 2021 10.1002/qj.4224.



The Earth's curvature means that vector quantities transported from D to A must be rotated to account for curvature effects: multiply with a "rotation matrix" R(V) the interpolated to D vector quantities

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 $\mathbf{r}_D$)

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

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

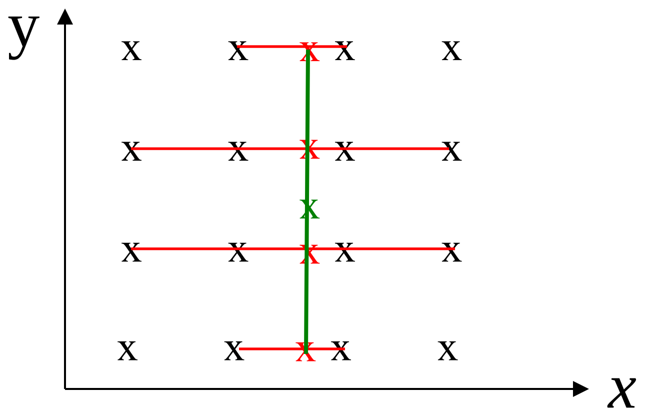
Interpolation in the IFS semi-Lagrangian scheme

After computing the departure points we need to:

- *Interpolate the advected field to the DP*
- *Interpolation must use the gridpoints that lie in the neighbourhood of the DP*
- *Weights are computed only once: same weights for all tracers (multi-tracer efficient)*

ECMWF model uses quasi-monotone quasi-cubic Lagrange interpolation (quintic in the vertical for temperature, specific humidity)

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



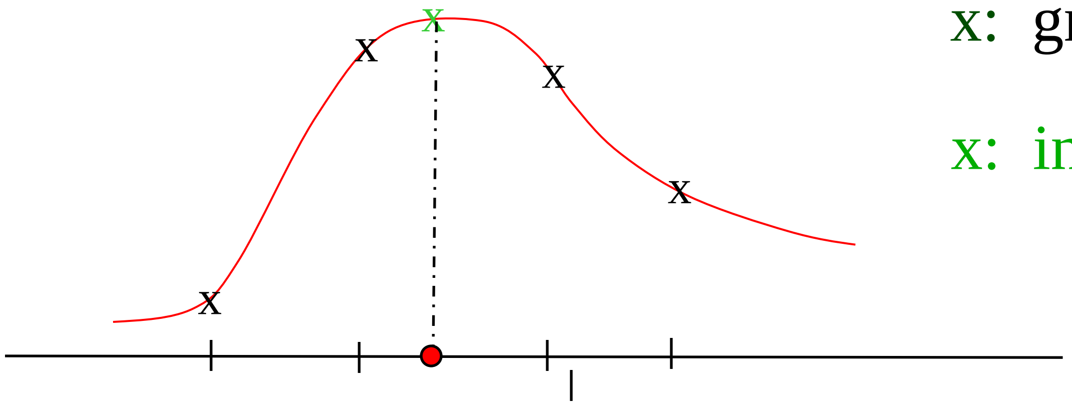
Number of 1D cubic interpolations in 2D: 5 =>3D: 21 (64pt stencil)

To save computations: use *cubic interpolation only for nearest neighbour rows and linear interpolation remaining rows. "quasi-cubic interpolation": 3*cubic+2*linear* interpolations in 2D

*7*cubic+10*linear* in 3D (32 pt stencil)

Limiter for shape-preserving (locally monotonic) interpolation

- Creation of "artificial" maxima /minima

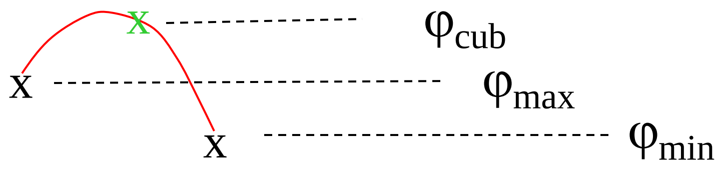


x: grid point values

x: interpolated value

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

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



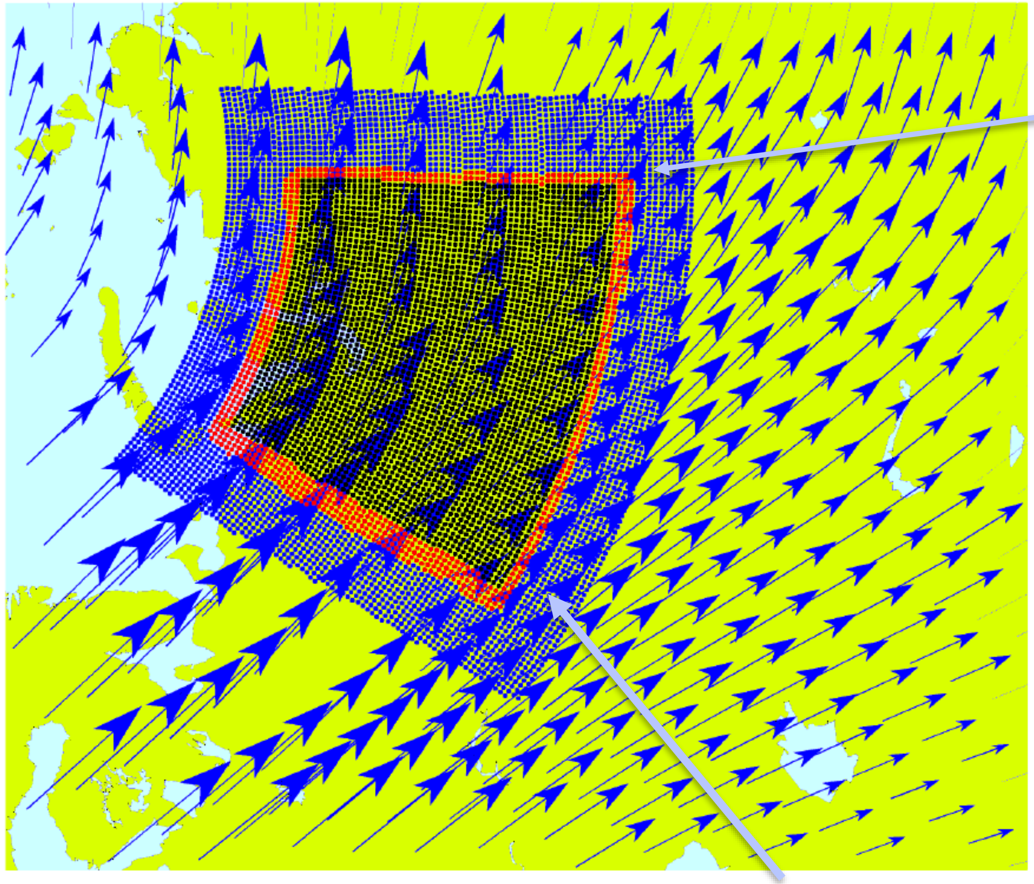
- Alternative: Spline or Hermite interpolation (not used in IFS operationally)

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

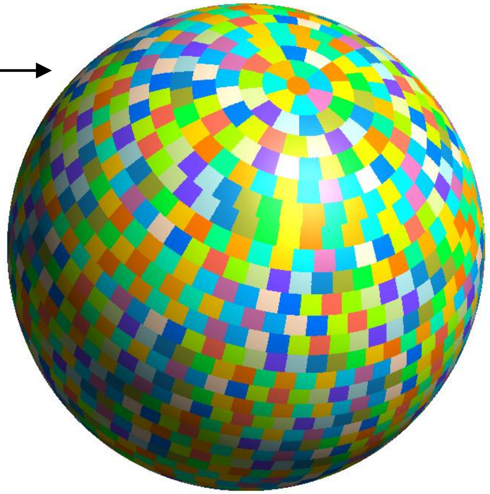
Parallel implementation

Interpolation at the DP near the edges of MPI domains requires data from 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: interpolation at the departure point

Subscript is omitted when variables are defined 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

The Helmholtz equation

- The previous system contains several discretized equations each applied over the globel at each vertical level (huge system!)
- In IFS system is reduced to a single elliptic equation with constant coefficients which can be solved with a fast and accurate direct solver in spectral space ☺
  - *Eliminate prognostic variables to derive Helmholtz equation in terms of horizontal wind divergence*
  - *"Back-substitute" to update remaining prognostic variables*
  - *The Helmholtz solver exploits spherical Harmonics properties resulting to a very cheap direct solver!*
  - *Having a cheap solver + being able to use large Δt (due to unconditional stability and good dispersion properties of SISL) explains why IFS is a very computationally efficient model*

Application to the IFS Hydrostatic Primitive Equation set

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

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

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

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

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

SL continuity derived from Eulerian equation

BCs: $\dot{\eta}(1) = 0, \dot{\eta}(0) = 0$

$$\frac{\partial}{\partial t}\left(\frac{\partial p}{\partial \eta}\right) + \nabla_h \cdot (\mathbf{V}_h \frac{\partial p}{\partial \eta}) + \frac{\partial}{\partial \eta}\left(\dot{\eta}\frac{\partial p}{\partial \eta}\right) = 0 \overset{\int_0^1 ...d\eta}{\Rightarrow}$$

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

Term is further simplified using vertical coordinate definition: $p=A(\eta)+B(\eta)p_s$

Linearise fast nonlinear terms of this equation set:

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

nonlinear but slow changing ($\Re$) — linear but fast changing (LX)

Deriving Helmholtz equation

- For simplicity assume dry dynamics ($T=T_v$)
- Also assume that Coriolis terms are incorporated in V_h (advective form): $\boldsymbol{X} = \boldsymbol{V}_h + 2\Omega \times \boldsymbol{r}$
- Having defined L, R we may write the 2nd order semi-implicit time discretization as:

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

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)

[in IFS **α=1/2** (Crank-Nicolson), however, off-centring i.e. 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:

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

- Matrix Γ can be diagonalised (before timestepping starts) and decoupled to its vertical eigenmodes solving cheaply the above system for each (m,n) => Computationally Efficient!
- Once divergence D at new time level is found the remaining fields can be computed through back-substitution

ECMWF

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

↓

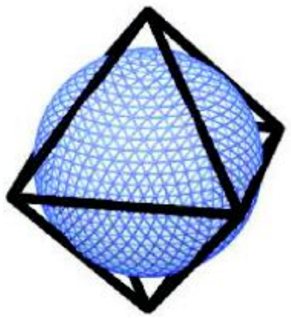
- **Solve Helmholtz** problem
- **Update** main **prognostic** variables
- **Add** horizontal **diffusion**

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



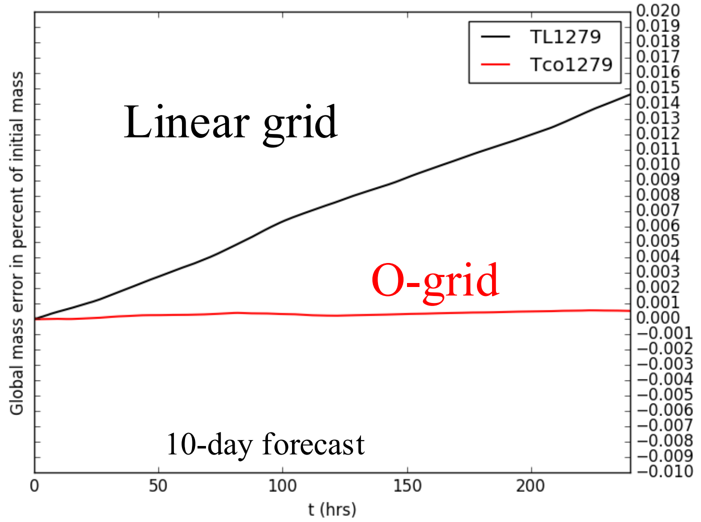
Octahedral grid

FFT: Fast Fourier Transform, LT: Legendre Transform

Mass conservation in semi-Lagrangian advection

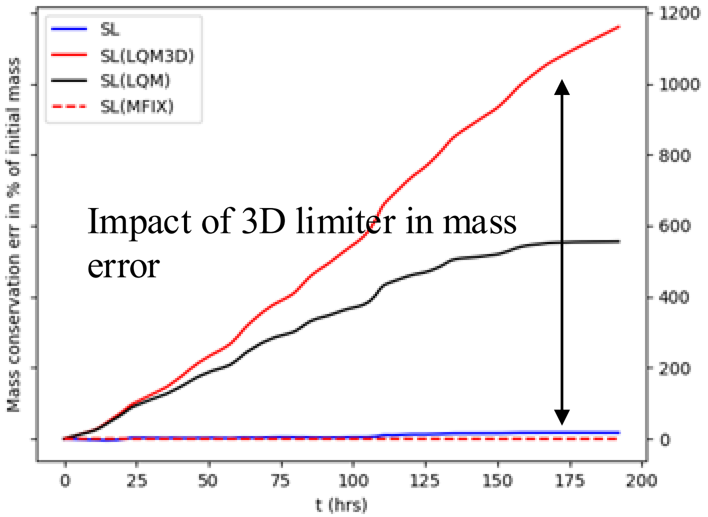
Mass conservation: important for atmospheric composition forecasts, for long range forecasts, climate and overall for high-resolutions

- SISL time-stepping does not conserve mass, energy, momentum
- Why? (i) continuity expressed in non-conservation form (ii) interpolation introduces global conservation errors
- Mass conservation error depends on the characteristics of the transported variable:
    - Small error for smooth tracers and total mass of air
    - Large error for localised tracers with large gradients. Monotone limiters amplify cons errors!
    - Region matters: tracer near the surface exhibit larger conservation errors (boundary condition issue)



Mass errors as percent of initial mass

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



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

IFS 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

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

Corrected tracer mixing ratio

Tracer mixing ratio after advection

Lagrange multiplier

M total mass for tracer ϕ

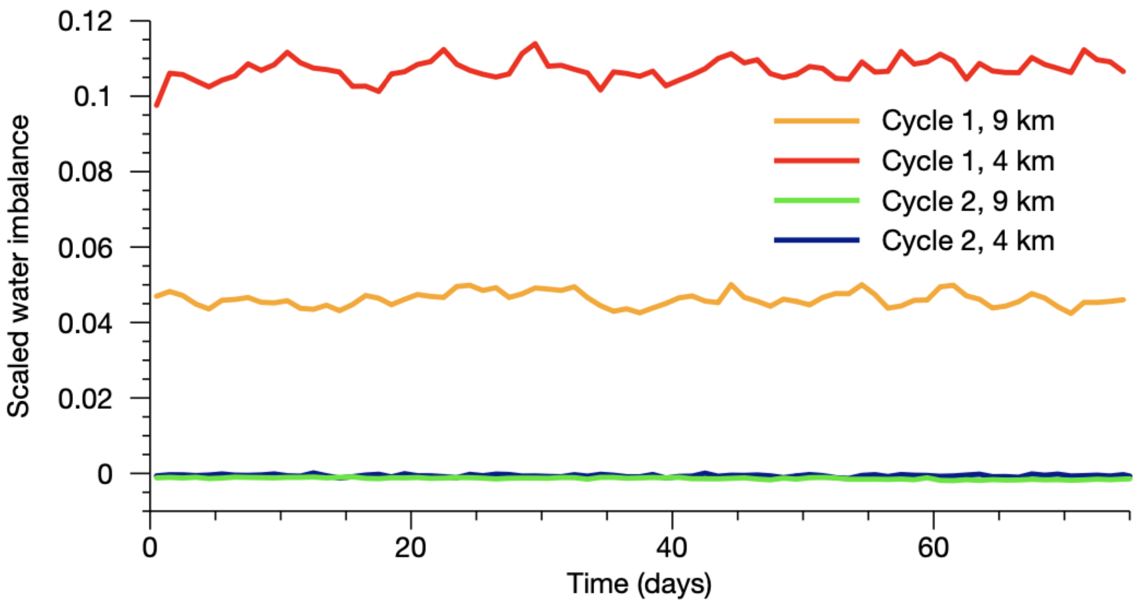
δM: mass conservation error in a timestep after SL advection

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

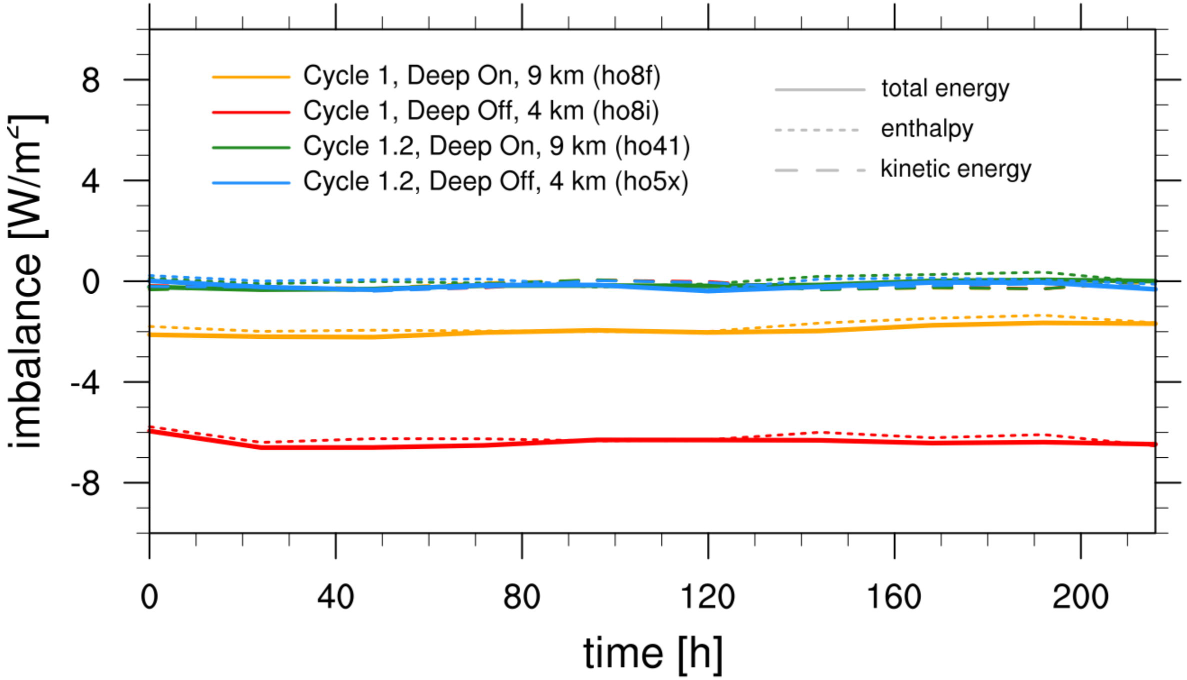
Fixing water leakage in IFS

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 runs

Summary of limitations of the SISL approach

- Unconditionally stable and multi-tracer efficient but not formally conserving
  - In long integrations mass drifts and needs to be "fixed"
  - In IFS mass fixers are used for individual tracers and surface pressure in long simulations
  - Inherently conserving SL options have been developed in some models (e.g. SLICE in ENDGame, CSLAM in CAM-SE, SL-AV models). With the very large timesteps used in IFS such options may not be absolutely stable
- Scalability issues as resolution increases:
  - ECMWF spectral IFS: high global communication cost of spectral transforms (transpositions) + scalability/memory scalability of SL (very large halos to be filled, see GMD 11, 3409-3426, 2018)

Some references cited here and further relevant ones

- Diamantakis & Vana (QJRMS 2021): "A fast converging and concise algorithm for computing the departure points in semi-Lagrangian weather and climate models"
- ECMWF Tech Memo 819 2017: "A positive definite tracer mass fixer for high-resolution weather and atmospheric composition forecasts"
- 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"
- Staniforth & Cote (MWR 1990): "Semi Lagrangian schemes for Atmospheric models"
- Temperton, Hortal, Simmons (QJRMS 2001): "A two-time-level SL global spectral model"

IFS SI time stepping and stability

- In the non-hydrostatic IFS, extrapolations in SISL can be unstable: A non-extrapolating **ICI** (Iterative Centred Implicit scheme) is used
- Predictor gives a first approximation $X^{+(0)} \sim X^{t+\Delta t}$. Crank-Nicolson type corrector iterations evaluate nonlinear residual terms R=M-L based on latest estimate of $X^{t+\Delta t}$:

$$\text{Predictor:}\ \frac{X^{+(0)} - X^{t}_{d(0)}}{\Delta t} = \frac{1}{2}\left[\Re\left(X^{t}\right)+\Re\left(X^{t}_{d}\right)\right]+\frac{1}{2}\left[L^{+(0)}+L^{t}_{d(0)}\right]$$

$$\text{Corrector:}\ \frac{X^{+(i)} - X^{t}_{d(i)}}{\Delta t} = \frac{1}{2}\left[\Re\left(X^{+(i-1)}\right)+\Re\left(X^{t}_{d(i)}\right)\right]+\frac{1}{2}\left[L^{+(i)}+L^{t}_{d(i)}\right],\ i=1,2,\ldots,K$$

K=1 suffices

- For stability, non-hydrostatic IFS requires a linearisation constant temperature T* reference state for acoustic terms such that T*<Tref, Tref reference temperature for gravity wave terms used also in hydrostatic (see paper by P. Benard et al QJRMS 2010, Vol 136, p155)