# The IFS dynamical core and its new features in cycle 43r3

### **Michail Diamantakis**

**OpenIFS Workshop 2019** 

University of Reading

17 June 2019





© ECMWF June 24, 2019

### The ECMWF hydrostatic dynamical core equations

Primitive equation model (hydrostatic, shallow atmosphere)

$$\frac{D\mathbf{V}_{h}}{Dt} + f\mathbf{k} \times \mathbf{V}_{h} + \nabla_{h}\Phi + R_{d}T_{v}\nabla_{h}\ln p = P_{v}$$

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

$$\frac{Dq_{x}}{Dt} = P_{q_{x}}$$

$$\frac{Dq_{x}}{Dt} = P_{q_{x}}$$

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

$$\Phi = \Phi_{s} - \int_{1}^{\eta} R_{d}T_{v}\frac{\partial}{\partial \eta} (\ln p) d\eta$$

$$\eta : hybrid vertical coordinate$$

$$V_{h}: horizontal momentum$$

$$T: temperature$$

$$V_{h}: horizontal momentum$$

$$T: temperature (used as spectral variable)$$

$$q_{x}: specific humidity, specific ratios for cloud fields and other tracers x, \ \delta = c_{pv}/c_{pd}$$

$$\Phi: geopotential$$

$$p: pressure$$

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

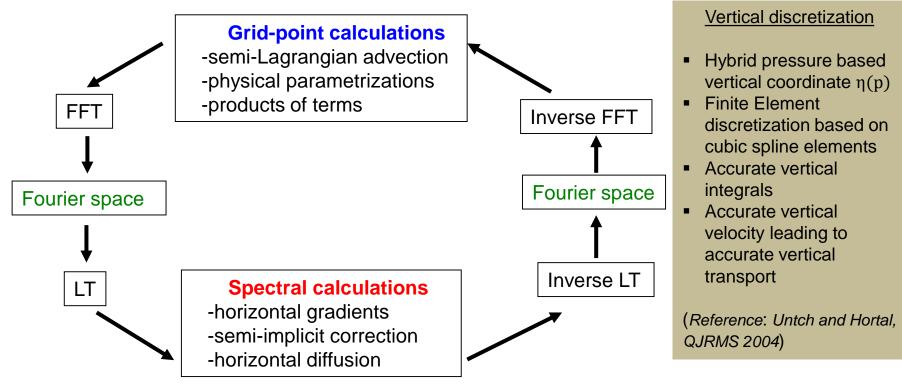
$$P: physics forcing terms$$

Non-hydrostatic, version available but currently not in operational use in ECMWF

How do we solve these equations?



### Solving the equations: spectral transform Semi-implicit semi-Langrangian (SISL) method



FFT: Fast Fourier Transform, LT: Legendre Transform



### **Spectral transform on spherical harmonics**

$$\phi(\lambda,\mu) = \sum_{m=-N}^{N} \sum_{n=|m|}^{N} a_{m,n} Y_{n}^{m}(\lambda,\mu), \quad \mu = \sin \theta \qquad \lambda, \theta: \text{ lon, lat}$$

Associated Legendre Polynomials

$$Y_n^m(\lambda,\mu) = P_{m,n}(\mu)e^{im\lambda}$$

Spherical harmonics:

Analytical derivatives "infinite order of accuracy":

$$(1-\mu^2)\frac{\partial Y_n^m}{\partial \mu} = -n\varepsilon_{m,n+1}Y_{m,n+1} + (n+1)\varepsilon_{m,n}Y_{m,n-1}, \quad \varepsilon_{m,n} = \sqrt{\frac{n^2 - m^2}{4n^2 - 1}}$$

$$\frac{\partial Y_n^m}{\partial \lambda} = im Y_{m,n}$$

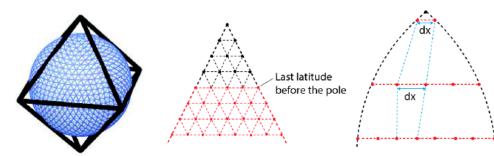
$$\nabla^2 Y_{m,n} = -\frac{n(n+1)}{R^2} Y_{m,n}$$

Earth radius

Spherical harmonics are the eigenfunctions of the Laplace operator => elliptic equations can be solved efficiently due to their simple discrete structure © Important property given that at each timestep the set of equations is reduced to an elliptic equation.



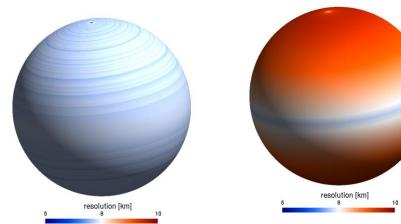
# Improved accuracy, efficiency and scalability with octahedral reduced cubic A-grid



Collignon projection on the sphere:  $Nlati = 4 \times i + 16$ , i = 1, ..., N

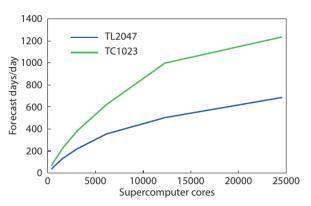
Benefits of cubic octahedral grid compared with old linear grid:

- Improved effective resolution
- · Improved mass conservation
- Improved efficiency and scalability (higher gridpoint resolution, same spectral truncation)



Latitudinal variation of resolution for standard cubic grid and octahedral cubic grid

Reference: "A new grid for the IFS" ECMWF newsletter 146, Winter 2015-2016, Malardel et al

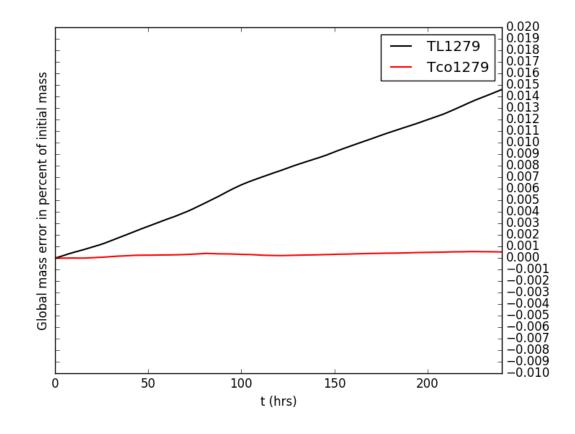


Above: cubic versus linear grid run at same gridpoint resolution. Plotted: forecast days / day per number of cores. Note that at high number of cores the rate achieved with a cubic grid is twice as large as the one by the linear!



### Improvement in mass conservation with octahedral grid

- Global mass conservation error is reduced by a factor of 30
  - No need to use de-aliasing in pressure gradient term, less numerical diffusion and improved accuracy



# Virtues of semi-implicit semi-Lagrangian techniques

Semi-Lagrangian (SL) semi-implicit (SI) technique is ideal for global NWP – stable, efficient and accurate integration of the governing equations

- Unconditionally stable SL advection scheme having small phase speed errors with little numerical dispersion
  - ✓ No CFL restriction in timestep!
- Unconditionally stable SI time stepping for the integration of fast changing forcing terms
  - No timestep restriction from the integration of "fast forcing" terms such as gravity wave + acoustic terms (present in non-hydrostatic models)

# What is a semi-Lagrangian advection scheme?

Semi-Lagrangian method is a numerical technique for solving advection type PDEs which applies *Lagrangian* "thinking" on gridpoint models:

- Resembles a "backward" Lagrangian method: for every discrete element (parcel) of the fluid a "backward" trajectory is computed
- This means that, at each time-step the final location of a moving parcel is known (it is a grid-point) and the location that its trajectory started (departure point) must be found
- As this computation is repeated at each timestep the grid is not allowed to deform

## **History of semi-Lagrangian method in IFS**

- The ECMWF model IFS (Integrated Forecast System) has been operating since 1979
- Until the beginning of 1991 IFS is 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 only due to switching to:
  - ♦ A semi-Lagrangian scheme on a reduced Gaussian grid
  - The new model was 6 x faster!

### The SL solution of the advection equation

Consider passive tracer linear advection equation:

$$\frac{D\phi}{Dt} \equiv \frac{\partial\phi}{\partial t} + V \cdot \nabla\phi = 0, \quad V = (u, v, w)$$
  
At time t parcel is at d and at t + $\Delta t$  arrives at a grid-point  $\phi_d^t \quad V \quad \phi_a^{t+\Delta t}$  (1d-demo)  
 $\int_{(r_a,t+\Delta t)}^{(r_a,t+\Delta t)} \frac{D\phi}{Dt} Dt = 0 \Rightarrow \phi_a^{t+\Delta t} = \phi_d^t, \quad r = (x, y, z)$   
parcel trajectory in  $\Delta t$   
d: departure point (DP) a: arrival point

- Finding the "departure point" is an essential part of the technique:
  - ♦ Solution at t+∆t is obtained by 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 (advection problem is reduced to interpolation)

## **DP** calculation in **IFS** and **NWP** models

In atmospheric flows wind field changes in space and time

To find departure points, solve equation:

 $\frac{Dr}{Dt} = V(r,t)$  where r, V the position and wind vector

Second order mid-point rule was used in early versions of IFS:

$$\int_{t}^{t+\Delta t} Dr = \int_{t}^{t+\Delta t} V(r,t)Dt \Rightarrow r_{a}^{t+\Delta t} - r_{d}^{t} = \int_{t}^{t+\Delta t} V(r,t)dt \approx \Delta t V(r_{M}, t + \Delta t / 2)$$
  
Trajectory midpoint

Can obtain V at forward time  $t+\Delta t/2$ explicitly using extrapolation such as:  $V(t+\Delta t)$ 

$$V(t + \Delta t / 2) = \frac{3}{2}V(t) - \frac{1}{2}V(t - \Delta t)$$

To tackle implicitness departure point is computed iteratively

The scheme used currently in IFS is called SETTLS

### SETTLS: Stable Extrapolation Two Time Level Scheme

Taylor expansion to second order:

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

AV: average value along SL trajectory

$$\left(\frac{Dr}{Dt}\right)_{d}^{t} = V_{d}\left(t\right), \quad \left(\frac{D^{2}r}{Dt^{2}}\right)_{AV} = \left(\frac{DV}{Dt}\right)_{AV} \approx \frac{V_{a}(t) - V_{d}(t - \Delta t)}{\Delta t}$$

Hence,

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

Therefore DP can be computed by iterative sequence:

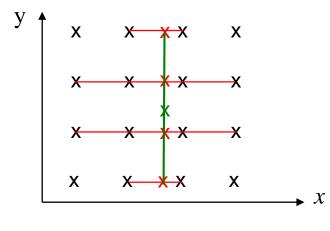
Reference: Hortal QJRMS 2002, doi:10.1002/qj.200212858314

### **Interpolation in the IFS semi-Lagrangian scheme**

After computing the departure points we need to:

• Interpolate the advected field to the DP to obtain:  $\varphi^{t+\Delta t} = \varphi_d^t$ Interpolation must use (for stability) neighbouring to d.p. gridpoints ECMWF model uses <u>quasi-monotone</u> <u>quasi-cubic</u> Lagrange interpolation

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

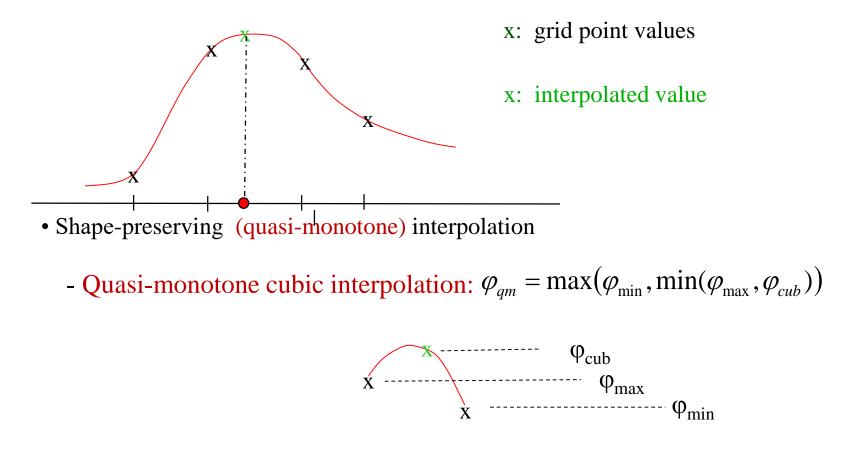


*Number of 1D cubic interpolations in 2D: 5 =>3D: 21* (64pt stencil)

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)

### **Shape-preserving (locally monotonic) interpolation**

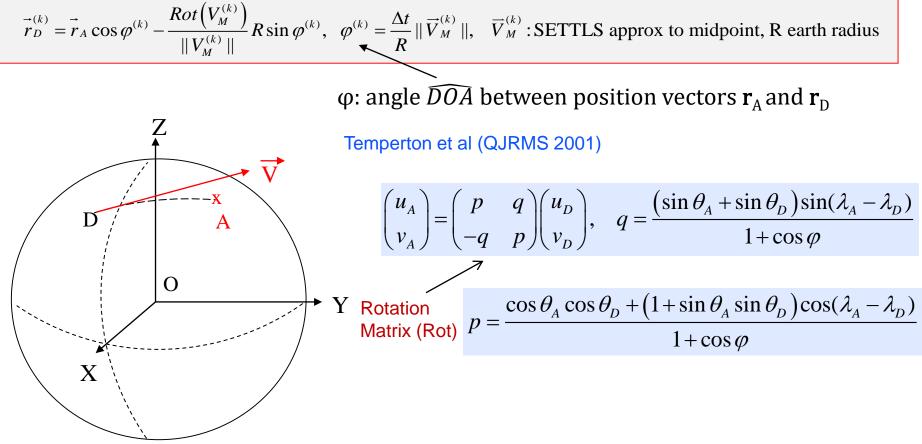
• Creation of "artificial" maxima /minima



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

### **SL advection on the sphere**

- A semi-Lagrangian trajectory from D to A is an arc of a great circle
- When computing the DP we need to account for the impact of the Earth curvature to the wind vector that transports a parcel from D to A
- Apply rotation operator from D to A to take into account Earth's curvature in DP iterations:



### **Do SL iterations always converge?**

- SETTLS scheme for computing the departure point is iterative
- Its convergence depends on Lipschitz number magnitude. Let r<sub>D</sub>, r<sub>D</sub><sup>[v]</sup> the converged solution and an estimate at iteration number v. Then:

$$\|\mathbf{r}_{\mathbf{D}} - \mathbf{r}_{\mathbf{D}}^{[\nu]}\| \le L^{\nu-1} \|\mathbf{r}_{\mathbf{D}} - \mathbf{r}_{\mathbf{D}}^{[1]}\|, \quad \nu = 2, 3, \dots, \nu_{max}$$

or

$$\|\mathbf{r}_{\mathbf{D}}^{[\nu]} - \mathbf{r}_{\mathbf{D}}^{[\nu-1]}\| \le L \|\mathbf{r}_{\mathbf{D}}^{[\nu-1]} - \mathbf{r}_{\mathbf{D}}^{[\nu-2]}\|, \quad \nu = 2, 3..., \nu_{max}$$

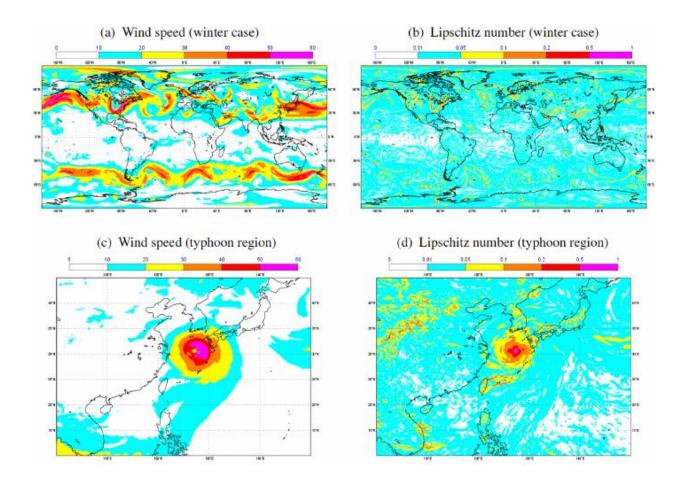
 $L \equiv \Delta t \| \frac{\partial \mathbf{V}}{\partial \mathbf{r}} \| \qquad \text{Lipschitz (deformational Courant) number}$ 

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

### What happens in IFS?

Reference: Diamantakis & Magnusson MWR2016 doi:10.1175/MWR-D-15-0432.1

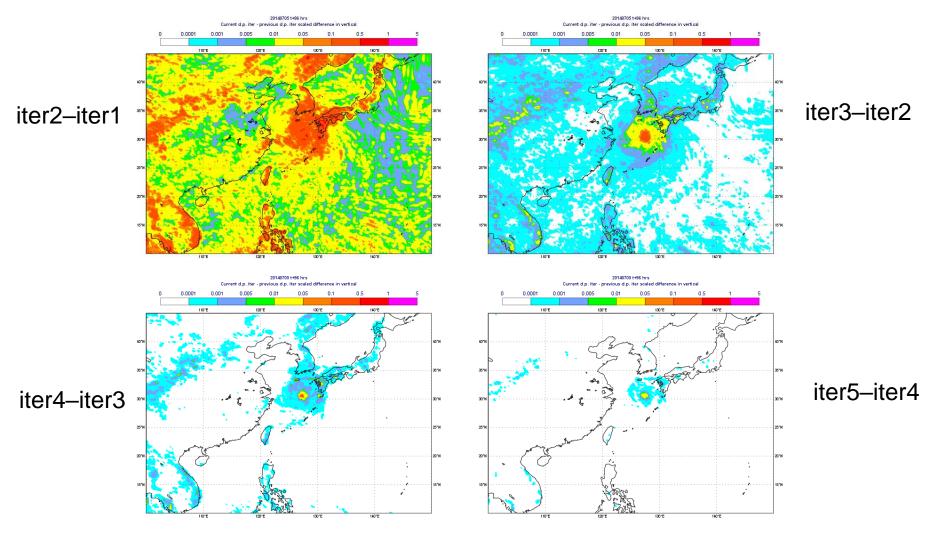
### **Lipschitz numbers in IFS forecasts**



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

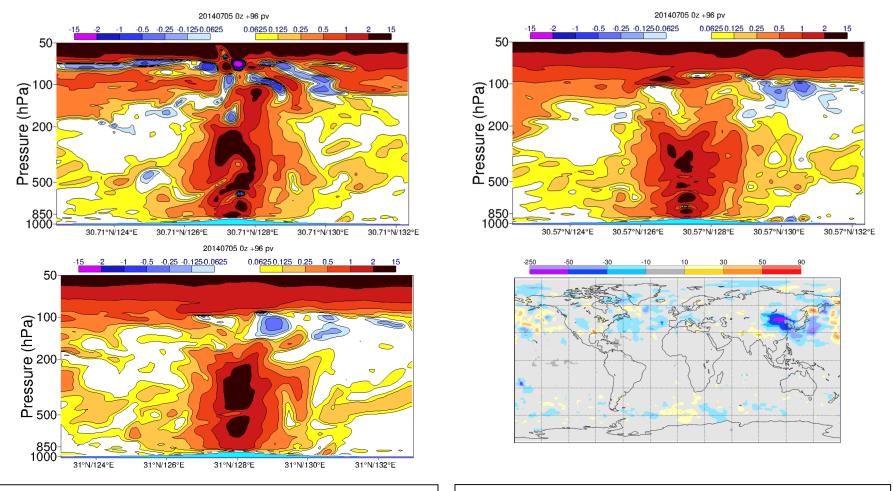
### **DP convergence in typhoon Neoguri**

- Model level near 850 hPa / 16km resolution
- Distance of two successive DP iterations scaled by gridlength
- Faster convergence when timestep reduced (not shown)



## **Revision of number of iterations in 41r2**

Lack of adequate convergence became more noticeable at 9km res and that prompted increase from 3 to 5 iterations

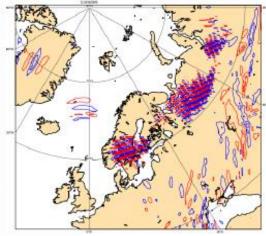


Tropical Cyclone PV x-section with 3, 5 and 5 with <sup>1</sup>/<sub>2</sub> timestep departure point iterations

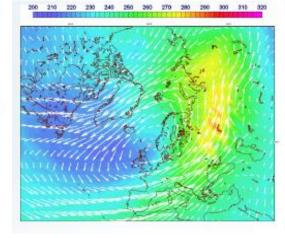
RMSE of geopotential reduction by improved convergence of DP iteration

### **Numerical noise in upper stratosphere**

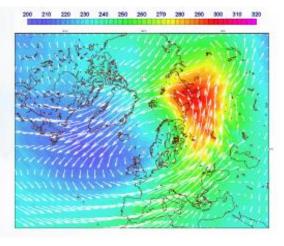
- In "Sudden Stratospheric Warming" events noise is often seen in upper stratosphere and model underpredicts the temperature there
- The origin of the noise is the time extrapolation used in SETTLS
- IFS 41r1: noise reduction & accuracy improvement with change in the vertical part of 2<sup>nd</sup> order SETTLS i.e.
  - switch to a non-extrapolating 1<sup>st</sup> order version when sudden changes in vertical velocities occur in two consecutive timesteps (Reference: M. Diamantakis, ECMWF newsletter No.141 Autumn 2014)



noisy divergence

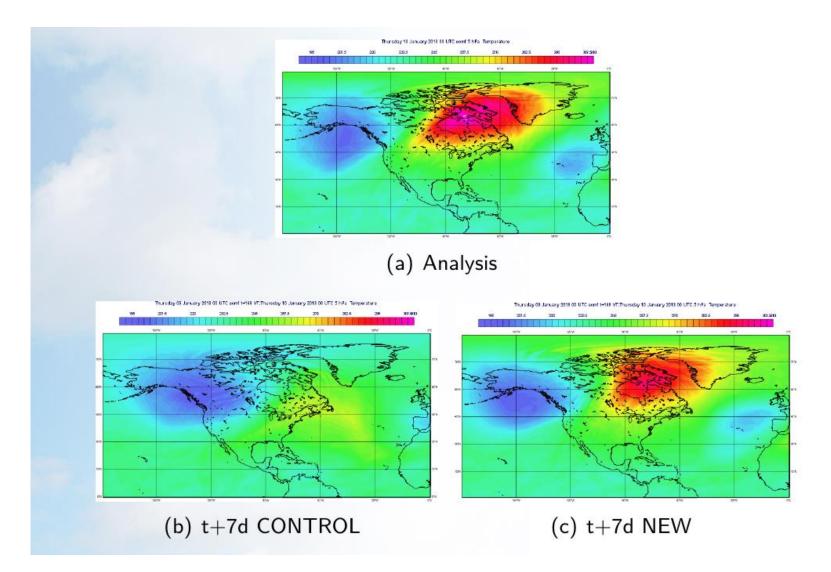


24hrs forecast: weak warming TTLS



no noise + "correct" warming (cycle 41r1) (revised vertical scheme)

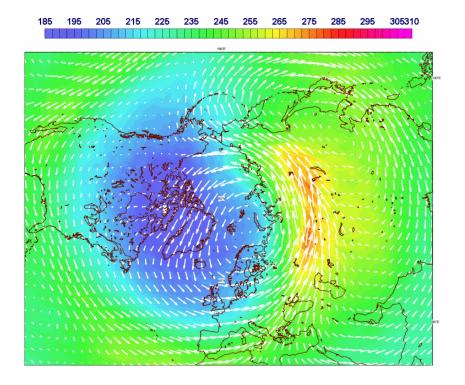
### **Major SSW January 2013**



Original (CONTROL) versus revised (NEW) SETTLS scheme

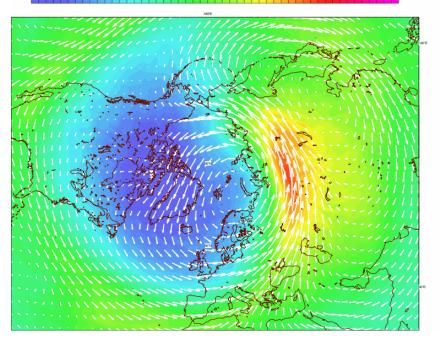
## **SSW case January 2013: Analysis animation**

T analysis at 5hPa: 1 to 14 Jan 2013



# Original SETTLS extrapolation for DP calculation

185 195 205 215 225 235 245 255 265 275 285 295 30531



# Revised in the vertical SETTLS extrapolation for DP calculation

GPSRO and other obs confirm that this is analysis represents better the truth



# Combining SL with SI scheme to solve the governing equations

2<sup>nd</sup> order SISL discretization (Crank-Nicolson) applied to m prognostic eqn:

$$\frac{DX}{Dt} = F(X) \Longrightarrow X_a^{t+\Delta t} - X_d^t = \frac{\Delta t}{2} \left( F_d^t + F_a^{t+\Delta t} \right), \quad X = \left( X_1, X_1, \dots, X_m \right)$$

d: interpolate to departure point

Wind comp, temperature etc

Split F and linearize fast nonlinear terms to simplify solution:

Let  $L(X) = A \cdot X$ ,  $N = F - L(X) \Longrightarrow F = N + L(X)$ 

With previous splitting the two-time-level, 2<sup>nd</sup> order IFS discretization becomes (Temperton et al, QJRMS 2001) :

$$X_{a}^{t+\Delta t} - X_{d}^{t} = \frac{\Delta t}{2} \left( L_{d}^{t} + L_{a}^{t+\Delta t} \right) + \frac{\Delta t}{2} \left( N_{d}^{t+\Delta t/2} + N_{a}^{t+\Delta t/2} \right)$$

 $N^{t+\Delta t/2}$  changes slowly and can be computed "explicitly" by SETTLS extrapolation

$$N^{t+\Delta t/2} = \frac{1}{2} \left( N^{t} + \left\{ 2N^{t} - N^{t-\Delta t} \right\}_{d} \right)$$

all right-hand side terms are given

## **The Helmholtz equation**

We have m prognostic equations that are expensive to solve

Instead of solving the whole coupled system, with analytical manipulations we can eliminate its variables in terms of horizontal wind divergence deriving a single elliptic (Helmholtz) equation. Once this is solved all prognostic variables can be updated through "back-substitution".

- In the IFS the resulting Helmholtz equation has constant coefficients and is solved in spectral space very accurately and efficiently using spherical Harmonics properties
- Having a cheap solver + being able to use large ∆t (due to unconditional stability and good dispersion properties of SISL) explains why IFS is computationally a very efficient model.



### **Solving Helmholtz equation**

Eliminate variables we derive a Helmholtz equation wrt to D:

$$\left(\underline{\underline{I}} - \alpha^2 \Delta t^2 (\underbrace{\underline{\gamma}}_{\underline{\underline{\tau}}} + R_d T_{ref} \underbrace{\underline{\nu}}_{p}) \nabla_h^2\right) D^{t+\Delta t} = D^* - \alpha \Delta t \nabla_h^2 (\underbrace{\underline{\gamma}}_{\underline{\underline{\tau}}} T^* + R_d T_{ref} P^*)$$

[in the presented discretization I have assumed  $\alpha = 1/2$  (Crank-Nicolson), however, off-centring i.e. using  $\alpha$ -value slightly >0.5 (0.55) is often used by some models to control unwanted oscillations]

Define: 
$$\underline{\Gamma} \equiv \alpha^2 \Delta t^2 \Big( \underbrace{\gamma}_{\underline{\tau}} \underbrace{\tau}_{\underline{\tau}} + R_d T_r \underbrace{\nu}_{\underline{\tau}} \Big), \Re = D^* - \alpha \Delta t \nabla_h^2 (\underbrace{\gamma}_{\underline{\tau}} \underbrace{\tau}_{\underline{\tau}} + R_d T_r P^*)$$
$$(I - \Gamma \nabla_h^2) D^{t + \Delta t} = \Re \quad \text{Matrix } \Gamma \text{ couples all vertical levels}$$

Decouple equations by diagonalizing  $\Gamma$  and solving in spectral space

$$\underline{\underline{\Gamma}} = Q^{-1}\underline{\underline{\Lambda}}Q, \quad \tilde{D}^{t+\Delta t} = QD^{t+\Delta t}, \quad \tilde{\mathfrak{R}} = Q\mathfrak{R} \Longrightarrow \left(\underline{\underline{I}} - \underline{\underline{\Lambda}}\nabla_{h}^{2}\right)\tilde{D}^{t+\Delta t} = \tilde{\mathfrak{R}}, \quad \underline{\underline{\Lambda}} = \left(\lambda_{i}\right)$$

$$\left(I - \lambda_i \nabla_h^2\right) \tilde{D}_{(i)}^{t+\Delta t} = \tilde{\Re}_{(i)}, \ \tilde{D} \equiv \left(\tilde{D}\right)_n^m, \ \tilde{\Re} \equiv \left(\tilde{\Re}\right)_n^m, \quad \nabla^2 \left(\tilde{D}\right)_n^m = -\frac{n(n+1)}{r_0} \left(\tilde{D}\right)_n^m$$

- The above equation is further simplified to the form  $\left(1+\lambda_i \frac{n(n+1)}{r_o^2}\right)\widetilde{D}_{(i)}^{+\lambda_i} = \widetilde{\Re}_{(i)}^{+\lambda_i}$
- Once divergence D at new time level is found the remaining fields can be computed through back-substitution

Reference: Ritchie et al, MWR 1995 Vol 123 p. 489

## **NH-IFS: SI time stepping and stability**

- The global non-hydrostatic IFS is more sensitive to explicit (using extrapolation) integration of the non-linear terms: instabilities occur
- An iterative approach can be used to avoid extrapolation and improve stability allowing long timesteps as in the hydrostatic:
  - ♦ ICI: Iterative Centred Implicit
  - It works like predictor-corrector but dynamics become twice as expensive:
    - → First predict state of prognostic variables at t+∆t using a 1st order scheme that doesn't require extrapolation
    - → Recompute solution using the "predicted" values for those right hand side semi-implicit terms that must be computed at t+∆t

### **Limitations of the SISL approach**

- Not formally conserving
  - In long integrations mass drifts and needs to be "fixed"
  - In IFS mass fixers are used for individual tracers and pressure (total mass of air) in long simulations
- Scalability issues as resolution increases:
  - ECMWF spectral IFS: high global communication cost of spectral transforms + scalability/memory scalability of SL (very large halos to be filled, see GMD 11, 3409-3426, 2018)
  - Regular lat/lon gridpoint models: too much resolution near the poles (slow convergence for implicit solvers + large communication MPI overhead )

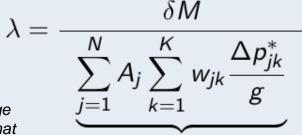
## Improved tracer Mass fixer in 43r3 (carbon tracers)

A modified version of Bermejo & Conde mass fixer implemented in IFS is applied to CO2, CH4 in atmospheric composition forecasts

$$\underbrace{\phi_{jk} = \phi_{jk}^* - \lambda w_{jk}}_{k}$$

j,k: horizontal, vertical index

Correction obtained using a Lagrange multiplier approach which ensures that the global norm of the difference from the original field is minimum



-,  $\delta M = M(\phi_{\chi}^*) - M(\phi_{\chi}^n)$ 

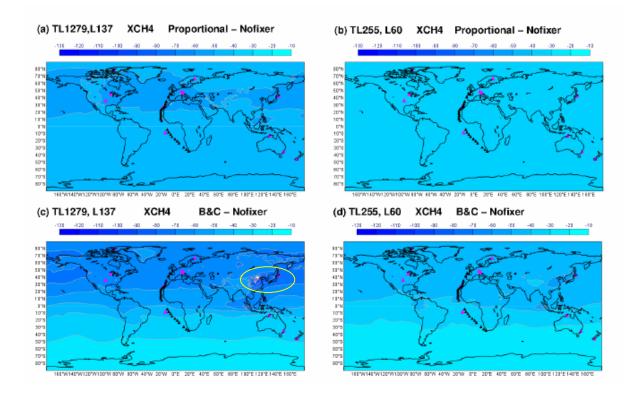
where  $M(\phi_{\chi})$ : total mass of  $\phi_{\chi}$ ,  $\phi^*$ : interpolated field to the DP (cubic Lagrange),  $p^*$ : pressure field after advection and  $w_{jk}$  such that mass fixer active mostly in areas where interpolation error is larger

$$w_{jk} = \max\left[0, sgn(\delta M) sgn\left(\phi_{jk}^* - \phi_{jk}^L
ight) \left|\phi_{jk}^* - \phi_{jk}^L
ight|^eta m_{jk}
ight]$$

 $\phi^{L}$ : linearly interpolated field to the DP,  $\beta = 2$  (species dependent parameter),  $m_{jk} \approx$  gridbox mass

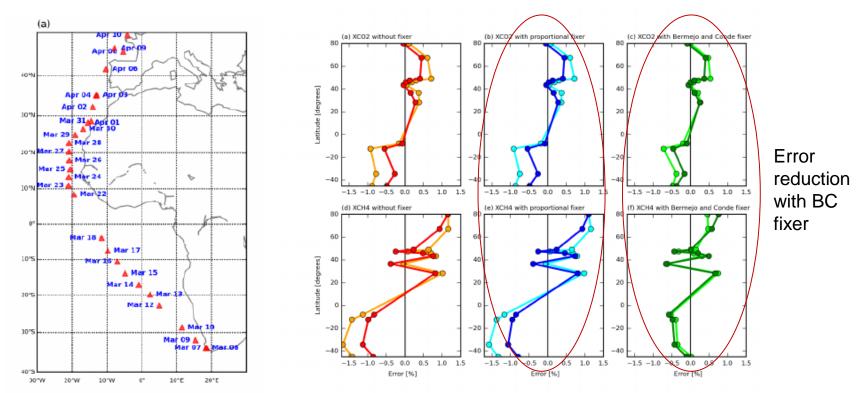
### Reference: Diamantakis & Agusti-Panareda ECMWF Tech Memo 819, 2017

## "Proportional" versus Bermejo and Conde mass fixer



Difference in mean XCH4 [ppb] between: (a,b) the simulations using the proportional mass fixer and the simulation without mass fixer at high and low resolution respectively; and likewise (c,d) the simulation with Bermejo and Conde (B&C) and the simulation without mass fixer. Period: 7/03/16-10/04/16

### Validation against CO2 observations



Latitudinal monthly mean error (%) distribution at different resolutions for (a-c) XCO2 and (d-f) XCH4 with respect to the observed distribution. Dark colours: low resolution, Light: high resolution. See *GMD 10, 2017, "Improving the inter-hemispheric gradient of total column atmospheric CO2 and CH4 …"* 

### Modelling atmospheric CH4 in the ECMWF Integrated Forecasting system

 $CH_4$  synoptic variability: 25 to 29<sup>th</sup> of March 2010

Average total column CH<sub>4</sub> [ppb]

# 20100325 00 UTC 1817.4 788.6 1785.0





### TRANSPORT

High resolution IFS (16km, L137)

#### SURFACE FLUXES

- Anthropogenic : EDGARv4.2 2008
- Near-real-time GFAS biomass burning
- Climatologies for other fluxes

#### CHEMISTRY Monthly mean loss rate climatology



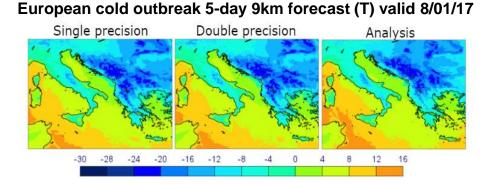
## Code efficiency improvement: A single precision IFS

A single precision version of IFS has been developed

Efficiency gain for uncoupled (atmos) model 40%

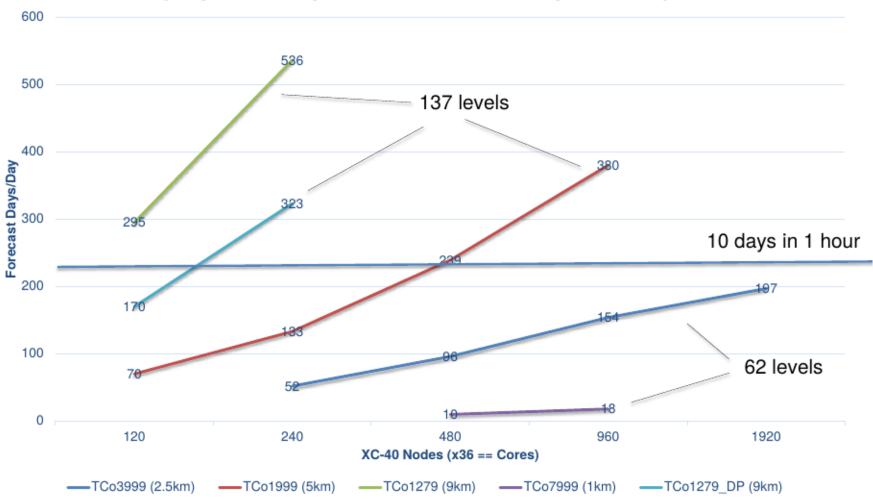
Neutral in terms of forecast skill for a range of different resolutions compared with double precision version

Some deterioration in terms of mass conservation (mostly due to single precision spectral transform package) but at acceptable levels for NWP forecasts: use of mass (pressure) fixer eliminates geopotential biases Total Mass change in a 10-day fc with SP, DP (new cubic and old linear grid)



DM(t)/M(t0 Tco1279 single precision TL1279 double precision 0.02 Tco1279 double precision 0.01 0.00 Cco1279 L137 -0.01 -0.02 50 100 150 200 250 fc hours

Reference: Vana et al, MWR 2017 doi: 10.1175/MWR-D-16-0228.1



### IFS single precision performance – Atmosphere only (no I/O)

# Summary

• IFS relies on an efficient and accurate dynamical core that we constantly improve

• 43r3 compared with 40r1 (earlier version that OpenIFS was based) has some noticeable differences:

- A new grid that improves further the accuracy and efficiency of the model
- Improvements in the semi-Lagrangian scheme
- Improvements in air mass conservation and tracer mass conservation
- Option to run faster in single precision at the same level of accuracy as double precision

While we continue improving the spectral dynamical core we also develop a new compact stencil Finite Volume core that scales well at massively parallel architectures and conserves mass.

### Thank you for your attention!

