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

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The ECMWF hydrostatic dynamical core equations

- Primitive equation model (hydrostatic, shallow atmosphere)

\[
\frac{DV}{Dt} + f k \times V_h + \nabla_h \phi + R_v T_v \nabla_h \ln p = P_v
\]

\[
\frac{DT}{Dt} - \frac{\kappa T_v \omega}{(1 + (\delta - 1)q) p} = P_T
\]

\[
\frac{Dq_x}{Dt} = P_{q_x}
\]

\[
\frac{\partial}{\partial t} \left( \frac{\partial p}{\partial \eta} \right) + \nabla_h \cdot \left( V_h \frac{\partial p}{\partial \eta} \right) + \frac{\partial}{\partial \eta} \left( \hat{\eta} \frac{\partial p}{\partial \eta} \right) = 0
\]

\[
\Phi = \Phi_s - \int_{1}^{\eta} R_v T_v \frac{\partial}{\partial \eta} (\ln p) d\eta
\]

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

How do we solve these equations?

\( \eta \): hybrid vertical coordinate

\( V_h \): horizontal momentum

\( T \): temperature

\( T_v \): virtual temperature (used as spectral variable)

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

\( \Phi \): geopotential

\( p \): pressure

\( \omega = dp/dt \): diagnostic vertical velocity

\( P \): physics forcing terms
Solving the equations: spectral transform Semi-implicit semi-Langrangian (SISL) method

**Grid-point calculations**
- semi-Lagrangian advection
- physical parametrizations
- products of terms

**Spectral calculations**
- horizontal gradients
- semi-implicit correction
- horizontal diffusion

FFT: Fast Fourier Transform, LT: Legendre Transform

**Vertical discretization**
- Hybrid pressure based vertical coordinate $\eta(p)$
- Finite Element discretization based on cubic spline elements
- Accurate vertical integrals
- Accurate vertical velocity leading to accurate vertical transport

*Reference: Untch and Hortal, QJRMS 2004*
Spectral transform on spherical harmonics

\[ \phi(\lambda, \mu) = \sum_{m=-N}^{N} \sum_{n=|m|}^{N} a_{m,n} Y^m_n(\lambda, \mu), \quad \mu = \sin \theta \]

\( \lambda, \theta: \text{lon, lat} \)

Spherical harmonics:

\[ Y^m_n(\lambda, \mu) = P_{m,n}(\mu)e^{im\lambda} \]

Associated Legendre Polynomials

Analytical derivatives “infinite order of accuracy”:

\[ (1-\mu^2) \frac{\partial Y^m_n}{\partial \mu} = -n \varepsilon_{m,n+1} Y_{m,n+1} + (n+1) \varepsilon_{m,n} Y_{m,n-1}, \quad \varepsilon_{m,n} = \sqrt{\frac{n^2 - m^2}{4n^2 - 1}} \]

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: $N_{lati} = 4 \times i + 16, \ i = 1, \ldots, N$

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)

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!

Reference: “A new grid for the IFS” ECMWF newsletter 146, Winter 2015-2016, Malardel et al
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 grid-point 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 + Δt arrives at a grid-point a:

\[
\int_{(r_d, t)}^{(r_a, t+\Delta t)} \frac{D\phi}{Dt} \, Dt = 0 \implies \phi_a^{t+\Delta t} = \phi_d^t, \quad r = (x, y, z)
\]

Finding the “departure point” is an essential part of the technique:

- Solution at t+Δt is obtained by interpolating the available (defined at time t) grid-point \( \phi \)-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:

\[
\frac{Dr}{Dt} = V(r, t) \quad \text{where } r, V \text{ the position and wind vector}
\]

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

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

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

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

♦ To tackle implicitness departure point is computed iteratively

♦ The scheme used currently in IFS is called SETTtls


**SETTLS: Stable Extrapolation Two Time Level Scheme**

Taylor expansion to second order:

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

AV: average value along SL trajectory

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

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:

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

\[
r_d^{(k)} = r_a - \frac{\Delta t}{2} \cdot \left( V_a(t) + \left\{ 2V(t) - V(t - \Delta t) \right\}_d \right) \bigg|_{r_d^{(k-1)}} \quad k = 1, 2, \ldots K
\]

Interpolation in the IFS semi-Lagrangian scheme

After computing the departure points we need to:
• Interpolate the advected field to the DP to obtain: \( \phi^{t+\Delta t} = \phi_d^t \)

Interpolation must use (for stability) neighbouring to d.p. gridpoints
ECMWF model uses quasi-monotone quasi-cubic Lagrange interpolation

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

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

• Shape-preserving (quasi-monotone) interpolation

  - Quasi-monotone cubic interpolation: \( \varphi_{qm} = \max(\varphi_{\text{min}}, \min(\varphi_{\text{max}}, \varphi_{\text{cub}})) \)

  - 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:

\[
\begin{align*}
r_D^{(k)} &= r_A \cos \varphi^{(k)} - \frac{\text{Rot} \left( V_M^{(k)} \right)}{\| V_M^{(k)} \|} R \sin \varphi^{(k)}, \\
\varphi^{(k)} &= \frac{\Delta t}{R} \| V_M^{(k)} \|, \quad V_M^{(k)} : \text{SEITLSS approx to midpoint, R earth radius}
\end{align*}
\]

\[\varphi: \text{angle } \overrightarrow{DOA} \text{ between position vectors } r_A \text{ and } r_D\]

Temperton et al (QJRMS 2001)

\[
\begin{pmatrix} u_A \\ v_A \end{pmatrix} = \begin{pmatrix} p & q \\ -q & p \end{pmatrix} \begin{pmatrix} u_D \\ v_D \end{pmatrix}, \quad q = \frac{\sin \theta_A + \sin \theta_D}{1 + \cos \varphi} \sin(\lambda_A - \lambda_D)
\]

\[
p = \frac{\cos \theta_A \cos \theta_D + (1 + \sin \theta_A \sin \theta_D) \cos(\lambda_A - \lambda_D)}{1 + \cos \varphi}
\]
Do SL iterations always converge?

- SETTLS scheme for computing the departure point is iterative
- Its convergence depends on Lipschitz number magnitude. Let $r_D, r_D^{[\nu]}$ the converged solution and an estimate at iteration number $\nu$. Then:

$$
\|r_D - r_D^{[\nu]}\| \leq L^{\nu-1}\|r_D - r_D^{[1]}\|, \quad \nu = 2, 3, \ldots, \nu_{max}
$$

or

$$
\|r_D^{[\nu]} - r_D^{[\nu-1]}\| \leq L\|r_D^{[\nu-1]} - r_D^{[\nu-2]}\|, \quad \nu = 2, 3 \ldots, \nu_{max}
$$

$L \equiv \Delta t\|\frac{\partial V}{\partial r}\|$ 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?

Lipschitz numbers in IFS forecasts

(a) Wind speed (winter case)
(b) Lipschitz number (winter case)

(c) Wind speed (typhoon region)
(d) Lipschitz number (typhoon region)

(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 ½ 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\textsuperscript{nd} order SETTLS i.e.
  - switch to a non-extrapolating 1\textsuperscript{st} order version when sudden changes in vertical velocities occur in two consecutive timesteps (Reference: M. Diamantakis, ECMWF newsletter No.141 Autumn 2014)

![Images showing noisy divergence, weak warming, and corrected warming with SETTLS](image)
Major SSW January 2013

(a) Analysis

(b) t+7d CONTROL  

(c) t+7d NEW

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

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

Revised in the vertical SETTLS extrapolation for DP calculation
Combining SL with SI scheme to solve the governing equations

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

\[
\frac{DX}{Dt} = F(X) \Rightarrow X_{a}^{t+\Delta t} - X_{d}^{t} = \frac{\Delta t}{2} \left(F_{d}^{t} + F_{a}^{t+\Delta t}\right), \quad X = (X_1, X_1, \ldots, X_m)
\]

\(d\): interpolate to departure point

Split F and linearize fast nonlinear terms to simplify solution:

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

With previous splitting the two-time-level, 2nd 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

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

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 $\Delta t$ (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:

\[
\left(I - \alpha^2 \Delta t^2 \left(\gamma \tau + R_d T_{\text{ref}} \nu \right) \nabla_h^2 \right) D^{t+\Delta t} = D^* - \alpha \Delta t \nabla_h^2 \left(\gamma T^* + R_d T_{\text{ref}} P^* \right)
\]

[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: \(\Gamma \equiv \alpha^2 \Delta t^2 \left(\gamma \tau + R_d T_{\text{ref}} \nu \right)\), \(\mathfrak{R} = D^* - \alpha \Delta t \nabla_h^2 \left(\gamma T^* + R_d T_{\text{ref}} P^* \right)\)

\[
\left(I - \Gamma \nabla_h^2 \right) D^{t+\Delta t} = \mathfrak{R}
\]

Matrix \(\Gamma\) couples all vertical levels

Decouple equations by diagonalizing \(\Gamma\) and solving in spectral space

\[
\Gamma = Q^{-1} \Lambda Q, \quad \tilde{D}^{t+\Delta t} = Q D^{t+\Delta t}, \quad \tilde{\mathfrak{R}} = Q \mathfrak{R} \Rightarrow \left(I - \Lambda \nabla_h^2 \right) \tilde{D}^{t+\Delta t} = \tilde{\mathfrak{R}}, \quad \Lambda = \left(\lambda_i \right)
\]

\[
(I - \lambda_i \nabla_h^2) \tilde{D}^{t+\Delta t}_{(i)} = \tilde{\mathfrak{R}}_{(i)}, \quad \tilde{D} \equiv (\tilde{D})^m_n, \quad \tilde{\mathfrak{R}} \equiv (\tilde{\mathfrak{R}})^m_n, \quad \nabla^2 (\tilde{D})^m_n = -\frac{n(n+1)}{r_0^2} (\tilde{D})^m_n
\]

- The above equation is further simplified to the form which can be easily solved exactly for each \(i\)
- Once divergence \(D\) at new time level is found the remaining fields can be computed through back-substitution

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 $t+\Delta t$ 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 $t+\Delta t$. 
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

\[
\phi_{jk} = \phi_{jk}^* - \lambda w_{jk}
\]

\[
\lambda = \frac{\delta M}{\sum_{j=1}^{N} \sum_{k=1}^{K} A_j w_{jk} \frac{\Delta p_{jk}^*}{g}}
\]

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

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

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

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

\(\phi^L\): 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

CH4 synoptic variability: 25 to 29th of March 2010
Average total column CH4 [ppb]

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.

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