TECHNICAL MEMORANDUM

849

Dry mass versus total mass conservation in the IFS

Sylvie Malardel [1]
Michail Diamantakis [2],
Anna Agusti-Panareda [2],
Johannes Flemming [2]

Research Department

[1] Météo-France, Direction Interrégionale pour l'Océan Indien, Réunion
[2] ECMWF Shinfield Park, Reading, RG2 9AX, UK

June 2019

European Centre for Medium-Range Weather Forecasts
Europäisches Zentrum für mittelfristige Wettervorhersage
Centre européen pour les prévisions météorologiques à moyen terme

Series: ECMWF Technical Memoranda

A full list of ECMWF Publications can be found on our web site under:
http://www.ecmwf.int/en/research/publications

Contact: library@ecmwf.int

Abstract

The continuity equation of the IFS dynamical core assumes that the total atmospheric air mass in the model is conserved. However, in the real atmosphere, there are physical processes that act as sources/sinks of total water. Therefore, while the dry air mass remains constant, the total air mass may change slightly in time. This note aims at clarifying the current state of the IFS with respect to dry mass versus total mass conservation. It also describes an alternative system of equations which conserves dry mass instead of total mass, following an approach that is similar to the one implemented in the Météo-France model ARPEGE. This alternative form of the continuity equation is available in IFS from cycle 46R1. Preliminary testing shows that the impact on IFS forecast skill is small but slightly positive. These changes also imply a modification in tracer advection equation. Tracers in IFS are defined as specific ratios (ratios with respect to moist air density) but "behave" as dry mixing ratios considering that the standard IFS continuity equation assumes that moist rather than dry air is conserved. If an IFS specific ratio is converted to a mixing ratio, its evolution becomes sensitive to the variation of dry air mass which is anti-correlated with the variation of total water. This is very noticeable for carbon tracers such as CO_2, a gas that is very well mixed with its background air. An outcome of the new dry mass conserving continuity formulation is that dry air is no longer anti-correlated with its water content. However, in order to be used by atmospheric composition forecasts modifications will be required to the tracer mass fixers used there. Until this issue is addressed, the recommended option for IFS atmospheric composition forecasts is to keep using the current options for continuity and mass fixers which have been proven to produce good quality results.

1 Introduction

The primitive equations of the IFS model describe the evolution of multi-phase air parcels constituted of "dry air", water vapour, water droplets, rain drops, snow flakes and an ensemble of other gases of negligible concentration which are then considered as "passive" tracers. The prognostic water species are not passive as their mass/weight but also their heat capacities are taken into account in the dynamical core equations.

In the dynamical core equations, the mass of each constituent in an air parcel is conserved and so is the total mass. However, in the physics package, exchanges with the surface through evaporation and precipitation and the corresponding subgrid transport in each vertical column represent sources or sinks of mass of total water in air parcels[1]. As there is no source/sink of dry air in air parcels at the meteorological scales, any change of mass of total water should correspond to the same change in total mass. But it is currently not the case in the IFS equations which always assume that the total mass is conserved inside air parcels. As a consequence, any source/sink of total water in the physics parametrisations is implicitly compensated by a sink/source of dry air.

The non-conservation of dry air in the IFS is already present at the level of the continuous set of equations, i.e. any numerical errors create artificial mass source/sink. Modifying the continuity equation of the IFS for the dry air to be conserved has then an impact on all the other equations. In practice, a lot of formulations in the model have to be revisited.

In the original description of the equations of ARPEGE/IFS (see, for example, Courtier et al, 1991), a mass flux divergence due to precipitation and sub-grid mass transport is present in the continuity equation. However, this term has never been introduced in the IFS physics-dynamics interface routine. At Météo-France, several versions of an option known as "$\delta m = 1$" (NDPSFI=1 in YOMPHY) have been implemented in the IFS/ARPEGE library but none were used operationally. The option NDPSFI=1 ap-

[1] Total water is the sum of all the prognostic solid, liquid or gas water species which are a constituent of the IFS atmosphere.

pears only inside the Météo-France physics/dynamics interface and then can't directly be used with the IFS physics package.

All the tests done at Météo-France with NDPSFI=1 showed a very small effect on the weather forecasts. However, recent developments in the IFS for the forecast and monitoring of air composition highlighted the ambiguity resulting from the approximation made in the continuity equation. For slowly varying tracers such as CO_2, inconsistencies or errors in the treatment of water species in the model was found to be particularly problematic for the assimilation of such tracer observation.

This note aims at clarifying the current state of the IFS with respect to dry mass versus total mass conservation. It also describes an alternative system of equations which conserves dry mass instead of total mass which has been implemented and can be activated in the IFS from CY46R1.

The first section of this note is a reminder of the derivation of the continuity equation used in the ARPEGE/IFS dynamical core. Section 3 exposes the current state of the physics/dynamics coupling for the continuity equation. The equations for a dry mass conserving IFS are derived in section 4. Implementation aspects of this new continuity equation in the IFS model are briefly discussed in section 4.4. The implications for tracer mass fixers is then discussed in section 4.5. Some results from high-resolution forecast experiments are presented in section 4.6. The note ends with a summary and conclusions in section 5.

2 Continuity equation and mass conservation in the IFS dynamical core

2.1 General mass conservation equations for a multi-phase atmosphere with no external source/sink of mass

In the IFS dynamical core, there is no source/sink of mass for any of the constituents j of the air, i.e. the mass of each constituent is supposed to be conserved in any Lagrangian volume:

$$\frac{D(m_j)}{Dt} = 0 \tag{1}$$

where m_j is the mass of constituent j and D/Dt is the Lagrangian time derivative (evolution following air parcels).

Equation (1) can also be written as

$$\frac{D(\rho_j \delta v)}{Dt} = 0 \tag{2}$$

where ρ_j is the density of constituent j in a material volume element δv. Note that if the constituent is a liquid or a solid, the density of this constituent is the ratio of the mass of liquid/solid by the volume of gas (the volume of liquid/solid is neglected with respect to the volume of gas).

From equation (2), we get

$$\delta v \frac{D(\rho_j)}{Dt} + \rho_j \frac{D(\delta v)}{Dt} = 0 \tag{3}$$

From the hypothesis of "continuity" of the fluid (i.e. the fluid behaves as a continuous matter which moves with the wind without creation or loss of mass), we know that a "material" volume δv changes according to the deformation associated to the divergence of the flow:

$$\frac{1}{\delta v} \frac{D(\delta v)}{Dt} = \vec{\nabla}.\vec{u} \tag{4}$$

where $\vec{u}$ is the 3D velocity (note that it is supposed here that all constituents move with the same "resolved" velocity $\vec{u}$).

Combining equation (4) with equation (3) gives:

$$\frac{D(\rho_j)}{Dt} = -\rho_j \vec{\nabla}.\vec{u} \tag{5}$$

Equation (5) is valid for each constituent of the air parcels or for the sum of all the constituents. In the IFS, the constituents which are part of the total mass ρ_t (i.e. constituents which have a contribution to the hydrostatic pressure) are the dry air ρ_d, the water vapour ρ_v, the cloud liquid water ρ_l, the cloud ice ρ_i, the prognostic rain ρ_r and the prognostic snow ρ_s. Other species such as O_3 or CO_2 are treated as *passive* tracers (i.e. an adiabatic simulation with or without such tracer gives bit identical results in terms of wind, thermodynamics variables and surface pressure).

2.2 Continuity equation in η-coordinate

The moist hydrostatic pressure π at each hybrid pressure level η_k of the IFS (see Simmons and Burridge (1981)) is given by

$$\pi(\eta_k) = A(\eta_k) + B(\eta_k)\pi_s \tag{6}$$

where π_s is the moist hydrostatic pressure at the surface. The moist hydrostatic pressure π is related to the total density by[2] :

$$\partial\pi/\partial z = -\rho_t g$$

The ratio of the surface pressure and the gravity, π_s/g, is the total mass per m^2 at the surface (i.e. "total column" of total mass). In the hydrostatic model, the pressure p is supposed to adjust "instantaneously" (i.e. in a characteristic time faster than a time step) to the hydrostatic value. Note that in the non-hydrostatic version of the IFS, π is still used to characterise the hybrid η-levels of the model (equation 6). In this case, the hybrid levels of the non-hydrostatic IFS are mass-based levels rather than pressure-based (Laprise (1992)).

In π-coordinate, the continuity equation (5), when applied to the total mass gives :

$$\frac{\partial u}{\partial x}|_\pi + \frac{\partial v}{\partial y}|_\pi + \frac{\partial \omega}{\partial \pi} = 0 \tag{7}$$

where

$$\omega = \dot{\pi} = \frac{D\pi}{Dt}$$

In η-coordinate, equation (5) becomes :

$$\frac{D(\frac{\partial\pi}{\partial\eta})}{Dt} = -\frac{\partial\pi}{\partial\eta}(\vec{\nabla}_{|\eta}.\vec{V} + \frac{\partial\dot{\eta}}{\partial\eta}) \tag{8}$$

where $\vec{V} = (u,v)$ is the horizontal wind vector.

The Eulerian form of this equation is :

$$\frac{\partial(\frac{\partial\pi}{\partial\eta})}{\partial t} = -\vec{\nabla}_{|\eta}.(\frac{\partial\pi}{\partial\eta}\vec{V}) - \frac{\partial(\dot{\eta}\frac{\partial\pi}{\partial\eta})}{\partial\eta} \tag{9}$$

[2]Note that, in the presence of condensates, the hydrostatic relationship is valid only for the moist hydrostatic pressure and the total mass density. It is not valid for the dry hydrostatic pressure π_d and the density of dry air ρ_d, i.e. $\partial\pi_d/\partial z \neq -\rho_d g$ (see Lauritzen et al., 2018 for more details).

2.3 Eulerian equation for the hydrostatic surface pressure

Equation (9) is integrated along the vertical from the top of the atmosphere ($\eta = 0$, $\dot{\eta}_{(\eta=0)} = 0$) to the surface ($\eta = 1$, $\dot{\eta}_{(\eta=1)} = 0$) to get an equation for the surface pressure π_s.

The hydrostatic pressure in the LHS of (9) is first replaced by its definition on η-levels (equation (6)) :

$$\frac{\partial(\frac{\partial \pi}{\partial \eta})}{\partial t} = \frac{\partial(\frac{\partial A}{\partial \eta})}{\partial t} + \frac{\partial(\frac{\partial (B\pi_s)}{\partial \eta})}{\partial t} = \frac{\partial B}{\partial \eta}\frac{\partial(\pi_s)}{\partial t} \tag{10}$$

Then, equation (10) is integrated along an atmospheric column :

$$\int_{\eta=0}^{\eta=1} \frac{\partial B}{\partial \eta}\frac{\partial \pi_s}{\partial t}\, d\eta = -\int_{\eta=0}^{\eta=1} \vec{\nabla}_{|\eta}.(\frac{\partial \pi}{\partial \eta}\vec{V})d\eta - \underbrace{[\dot{\eta}\frac{\partial \pi}{\partial \eta}]_{\eta=1}}_{=0} + \underbrace{[\dot{\eta}\frac{\partial \pi}{\partial \eta}]_{\eta=0}}_{=0} \tag{11}$$

As π_s is not a function of the vertical and

$$\int_{\eta=0}^{\eta=1} \frac{\partial B}{\partial \eta}\, d\eta = 1 \tag{12}$$

we get :

$$\frac{\partial \pi_s}{\partial t} = -\int_{\eta=0}^{\eta=1} \vec{\nabla}_{|\eta}.(\frac{\partial \pi}{\partial \eta}\vec{V})d\eta = S_{eul} \tag{13}$$

In the IFS, the prognostic variable is not π_s, but $\ln(\pi_s)$. The equation for $\ln(\pi_s)$ is deduced from equation (13) after a division by π_s on both sides:

$$\frac{\partial(\ln(\pi_s))}{\partial t} = \frac{S_{eul}}{\pi_s} \tag{14}$$

Following Ritchie et al. (1994), the discretized version of the Eulerian equation (14) for the logarithm of the surface pressure at a point M at the surface is:

$$\begin{aligned} \ln(\pi_s)^+_M &= \ln(\pi_s)^-_M - \frac{\Delta t}{\pi_s}\sum_{k=1}^{NFLEV} \vec{\nabla}_{|\eta}.(\vec{V}_k \Delta\pi_k) \\ &= \ln(\pi_s)^-_M - \sum_{k=1}^{NFLEV}\left(\frac{1}{\pi_s}D_k\Delta\pi_k + \vec{V}_k.\vec{\nabla}_{|\eta}(\ln(\pi_s))\Delta B_k\right) \\ &= \ln(\pi_s)^-_M + \frac{S_{eul}}{\pi_s} \end{aligned} \tag{15}$$

where D_k, $\vec{V}_k$ are respectively the divergence and the horizontal wind at level k above M and Δt the time step length.

2.4 Equations for $\dot{\eta}$ and ω

$\dot{\eta}$ (generalised vertical velocity in η-coordinate used for the vertical advection in IFS) and $\omega = D\pi/Dt$ (used in the right hand side of T-equation) are diagnostics variables which are computed at each time step. The derivation of the formula used to computed these variables is very similar to the derivation of the evolution of the surface pressure.

In equation (9), the time and η derivatives in the LHS commute:

$$\frac{\partial(\frac{\partial\pi}{\partial t})}{\partial\eta} = -\vec{\nabla}_{|\eta}.(\frac{\partial\pi}{\partial\eta}\vec{V}) - \frac{\partial(\dot{\eta}\frac{\partial\pi}{\partial\eta})}{\partial\eta} \tag{16}$$

Integrating equation (16) from the model top to a level η gives the Eulerian change of hydrostatic pressure at η:

$$\frac{\partial\pi}{\partial t} = -\left[\int_{\eta=0}^{\eta}\vec{\nabla}_{|\eta}.(\frac{\partial\pi}{\partial\eta}\vec{V})d\eta\right] - \dot{\eta}\frac{\partial\pi}{\partial\eta} \tag{17}$$

In order to get an equation for ω, the 3D advection of pressure $\vec{V}.\vec{\nabla}_{|\eta}\pi + \dot{\eta}\partial\pi/\partial\eta$ is added to both the LHS and the right hand side (RHS) of the last equation. The vertical component of the advection cancels with $(-\dot{\eta}\partial\pi/\partial\eta)$ on the RHS of equation (17) to finally give:

$$\omega = \frac{D\pi}{Dt} = -\left[\int_{\eta=0}^{\eta}(\vec{\nabla}_{|\eta}.(\frac{\partial\pi}{\partial\eta}\vec{V})d\eta\right] + \vec{V}.\vec{\nabla}_{|\eta}\pi \tag{18}$$

$\dot{\eta}$ is also computed from equation (17):

$$\dot{\eta}\frac{\partial\pi}{\partial\eta} = -\frac{\partial\pi}{\partial t} - \left[\int_{\eta=0}^{\eta}\vec{\nabla}_{\eta}.(\frac{\partial\pi}{\partial\eta}\vec{V})d\eta\right] \tag{19}$$

The first term in the RHS of this last equation is computed from equation (13):

$$-\frac{\partial\pi}{\partial t} = -B(\eta)\frac{\partial\pi_s}{\partial t} = -B(\eta)S_{eul}.$$

In the IFS, it is the equation for the logarithm of the hydrostatic surface pressure, associated with the definition of the η-levels and the formulations of $\dot{\eta}$ and $\omega = \partial\pi/\partial t$ which ensures together the conservation of total mass and the continuity of the multi-phase fluid in the dynamical core. As shown in this section, the equations for $\ln(\pi_s)$, ω and $\dot{\eta}$ are derived from the same continuity equation for the total mass. For consistency, if the original form of the continuity equation for the total mass is modified, the 3 equations have to be modified consistently.

2.5 Semi-Lagrangian equation for the hydrostatic surface pressure

A “Lagrangian” form of equation (15) is used in the semi-Lagrangian version of the IFS dynamical core. But as π_s is an integrated quantity, the semi-Lagrangian equation for π_s is not obtained by a simple transfer of the advection from the RHS to the LHS of π_s equation. It has to be reconstructed from the vertical integral of the advection equation of π_s at each η-level k.

The surface pressure is a 2D variable which can be considered as a 3D variable with a constant value along a vertical column. The semi-Lagrangian form of the hydrostatic surface pressure equation results from the vertical integration of semi-Lagrangian equations for the hydrostatic surface pressure at each η_k-level in a model column. As the wind is different for each level k, the semi-Lagrangian trajectories are different for each level, and then the surface pressure of the departure column is different for each level. The computation of the surface pressure in the departure columns involves only 2D trajectories, but the contribution of the RHS which depends on the vertical involves 3D trajectories.

In practice, to get a Lagrangian equation for π_s, the 3D advection is added on both side of equation (13):

$$\frac{\partial \pi_s}{\partial t} + \vec{V}_k.\vec{\nabla}_{|\eta}(\pi_s) + \dot{\eta}\frac{\partial \pi_s}{\partial \eta} = S_{eul} + \vec{V}_k.\vec{\nabla}_{|\eta}(\pi_s) + \dot{\eta}\frac{\partial \pi_s}{\partial \eta} \tag{20}$$

As π_s does not vary along a vertical column, $\partial \pi_s / \partial \eta = 0$. Equation (20) is then multiplied by $\partial B / \partial \eta$ and integrated along the vertical:

$$\int_{\eta=0}^{\eta=1} \left(\frac{D_\eta \pi_s}{Dt}\right)\frac{\partial B}{\partial \eta}\, d\eta = \int_{\eta=0}^{\eta=1} S_{eul}\frac{\partial B}{\partial \eta}\, d\eta + \int_{\eta=0}^{\eta=1} \vec{V}_k.\vec{\nabla}_{|\eta}(\pi_s)\frac{\partial B}{\partial \eta}\, d\eta \tag{21}$$

where $D_\eta \pi_s / Dt$ represent the Lagrangian evolution of π_s along a 2D η-level.

The equation for the logarithm of the surface pressure is finally obtained by a division by π_s on both side.

The discrete semi-Lagrangian equation coded in the IFS is finally:

$$\begin{aligned} \ln(\pi_s)_A^+ = & \sum_{k=1}^{NFLEV} \left(\ln(\pi_s)_{O_k^{2D}}\right) \Delta B_k \\ & + \Delta t \sum_{k=1}^{NFLEV} \left(\frac{S_{eul}}{\pi_s}\right)_{M_k} \Delta B_k \\ & + \Delta t \sum_{k=1}^{NFLEV} \left(\vec{V}_k.\vec{\nabla}_\eta(\ln(\pi_s))\right)_{M_k} \Delta B_k \end{aligned} \tag{22}$$

where $\ln(\pi_s)_A^+$ is the logarithm of surface pressure at the arrival point A at the future time step. The $\ln(\pi_s)_{O_k}^{2D}$ in the first term on the RHS of this equation is the value of the logarithm of the surface pressure at the departure point O_k^{2D} of a 2D trajectory computed with the horizontal wind $\vec{V}_k$. Due to the second-order time discretisation used, the second and third terms of the RHS are computed at the mid-point of the 3D trajectories which have been computed with the 3D wind $\vec{u}_k$[3].

2.6 Equations for specific ratios and mixing ratios

In the IFS, the equation for $\ln(\pi_s)$ controls the conservation of total mass. The continuity equation for each individual constituent j of the air is then reduced to an equation for the proportion of each constituent with respect to the total mass, the specific ratios:

$$q_j = \rho_j / \rho_t.$$

To retrieve the mass of each constituent, both the information given by the total mass continuity equation (equation for $\ln(\pi_s)$) and the equations for the specific ratios are needed.

The equation for the specific ratio q_j in the dynamical core results from the combination of equation (5) applied to the species j and equation (5) applied to the total mass:

$$\frac{Dq_j}{Dt} = 0 \tag{23}$$

[3]In theory, only the third term on the RHS of equation (22) needs a 3D interpolation. In practice, in the IFS, the first term of this RHS is interpolated separately with 2D cubic Lagrange polynomials. The second and third terms are interpolated with linear interpolations. In order to reduce the number of interpolations, both terms are interpolated together in a single 3D interpolation.

2.7 Mass of constituents in a vertical column and global mass

The mass per unit of surface of a constituent j in a vertical column of the model (also called "total column") is given by:

$$M_{j_{col}} = \int_{surf}^{top} \rho_j dz = \int_{surf}^{top} q_j \rho_t dz \tag{24}$$

From the definition of the hydrostatic pressure, we have:

$$d\pi = -\rho_t g dz$$

then,

$$M_{j_{col}} = \sum_{\pi=\pi_s}^{\pi=0} q_j \frac{\Delta\pi}{g} \tag{25}$$

where $\Delta\pi$ is the pressure difference between two half model levels.

For each constituent, the global mass is given by the horizontal integral of the total columns.

3 Continuity equation and mass conservation in the IFS model

3.1 Continuity equation in the IFS

We have seen in the previous section that the processes which are represented by the dynamical core do not change the composition of the air parcels. It is however not the case of the physical parametrisations. Processes such as precipitation or subgrid transports of water species can be a net source/sink of total water in an air parcel.

In the IFS, the continuity equation in the dynamics is not coupled to the physics. The 3D solver of the dynamics always supposes total mass conservation inside air parcels (equation (22)). In the physics package, the parametrisations are coded as independent simplified 1D solvers (vertical column). In these solvers, it is supposed that the hydrostatic pressure in a grid box is not modified by the parametrisations, i.e. there is no net total mass change in a grid box due to the parametrisations in the physics. Such an approximation corresponds to a very simple solution of the continuity equation which imposes that there is no net mass change inside a grid box. As neither the dynamics nor the physics deal with the total mass change due to the change of total water in the physics, any source or sink of total water in a parametrisation is implicitly compensated by an artificial sink or source of dry mass which instantaneously "disappear" or "appear" in the grid box (with the same temperature and momentum than the air in this grid box) in order to maintain a constant hydrostatic pressure. It is important to understand that the change of dry air mass in the IFS and in most NWP models (see Lauritzen et al., 2018 for example) is not explicitly coded in the physics. It is an implied consequence of two hypotheses:

- no physics-dynamics coupling for the continuity equation,
- the "moist" hydrostatic pressure is supposed to be constant in a parametrisation which does not conserve total water locally

3.2 Equation for total water

The equation for the density of total water $\rho_w = \rho_v + \rho_l + \rho_i + \rho_r + \rho_s$ is

$$\frac{D\rho_w}{Dt} = -\rho_w \vec{\nabla}.\vec{u} - \frac{\partial J_w}{\partial z} + \frac{\partial P}{\partial z} \tag{26}$$

where P is the precipitation flux (positive downwards) and $J_w = \overline{\rho_w' w'}$ is the subgrid vertical flux of total water computed by the boundary layer parametrisations and the convection scheme. Note that all the tendencies associated with water phase changes cancel when the equation for the densities of the different water species are summed up into an equation for the total water density; that's why they are not present in equation (26).

When equation (26) is combined with equation (5) applied to the total mass, we get:

$$\frac{Dq_w}{Dt} = \frac{1}{\rho_t}\left(-\frac{\partial J_w}{\partial z} + \frac{\partial P}{\partial z}\right) = S_w \tag{27}$$

3.3 Evolution of dry air

In the IFS, there is no equation for dry air. The evolution of the mass of dry air is deduced from the difference between the evolution of the total mass and the evolution of the mass of total water.

$$\frac{D\rho_d}{Dt} = -\rho_t \vec{\nabla}.\vec{u} - \left[-\rho_w \vec{\nabla}.\vec{u} - \frac{\partial J_w}{\partial z} + \frac{\partial P}{\partial z}\right] = -\rho_d \vec{\nabla}.\vec{u} + \frac{\partial J_w}{\partial z} - \frac{\partial P}{\partial z} \tag{28}$$

or

$$\frac{Dq_d}{Dt} = -\frac{Dq_w}{Dt} = -\frac{1}{\rho_t}\left(-\frac{\partial J_w}{\partial z} + \frac{\partial P}{\partial z}\right) = -S_w \tag{29}$$

As the sources/sinks of total mass are not included in the continuity equation of the IFS, artificial (non-physical) sinks/sources of mass of dry air compensate for the sources/sinks of mass of total water. This behaviour is illustrated on figure 1 which shows the evolution of the global means of total mass and dry mass for a year long run at TL255. In such long runs, a mass fixer is activated for the total mass in order to correct numerical errors which are mainly coming from the semi-Lagrangian advection. Fixing the total mass in this case is consistent with the assumption made for the conservation of total mass in the full model. Note that the amplitude of the error made on the dry mass budget at TL255 is about one order of magnitude smaller compared to the error made on the total mass if the global mass fixer is not activated (figure 2). With a cubic grid, the numerical errors for the total mass are significantly reduced (figure 2). The importance of the assumption that the IFS conserves total mass instead of dry mass becomes then more visible.

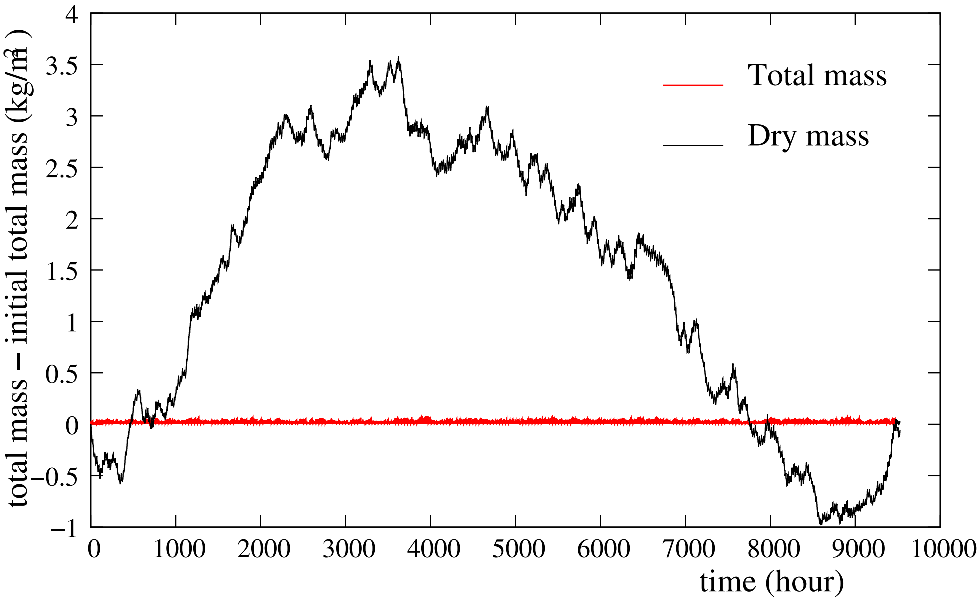

Figure 1: Difference between the global mean of mass (kg/m^2) and the initial value as a function of time for a one year long forecasts at TL255 resolution with the IFS CY45r1. For this simulation, a spectral mass fixer is applied to the total mass every 24 hours in order to correct numerical errors. The red curve shows the evolution of the total mass, the black curve the evolution of the dry mass.

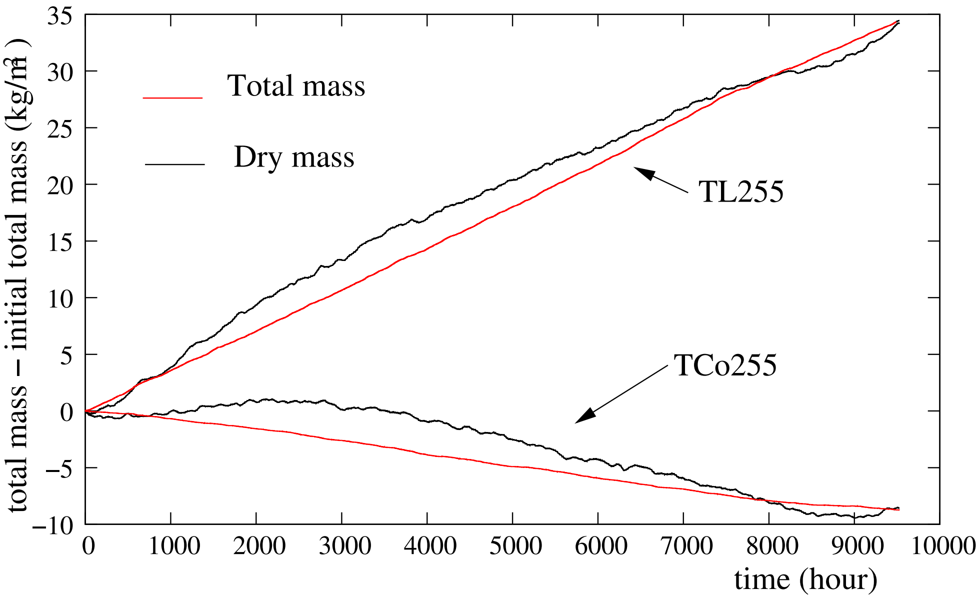

Figure 2: Difference between the global mean of mass (kg/m^2) and the initial value as a function of time for a one year long forecast at TL255 and at TCo255 for simulation without global mass fixer. Total mass evolution in red, dry mass evolution in black.

3.4 Equations for the tracers

Tracers may have their own parametrised sources/sinks in the physics parametrisation:

$$\frac{D\rho_c}{Dt} = -\rho_c \vec{\nabla}.\vec{u} + \rho_t S_c \tag{30}$$

where S_c is the source/sink of mass of tracer in kg per kg of total mass per second.

When combined with the current IFS equation for the total density (equation (5) applied to total mass), we get:

$$\frac{Dq_c}{Dt} = S_c \tag{31}$$

The total mass of a tracer can be retrieved from formulae (25).

Figure 3 shows the evolution of the ratios between the total mass of CO_2 and the global integral of total mass (red curve) or the global integral of dry air (green curve) in a one year integration using mass fixers for the total mass and for the tracers and no source/sink for the tracers. It confirms that, in the current IFS, the ratio between the total mass of CO_2 and the total mass is conserved when the mass fixers are switched on. However, the ratio between the total mass of CO_2 and the mass of dry air is not conserved. Such a nonphysical behaviour directly results from the approximation made in the current IFS concerning the conservation of total mass. It creates an ambiguity when observations made with respect to dry mass have to be assimilated or are used for validation in atmospheric composition applications.

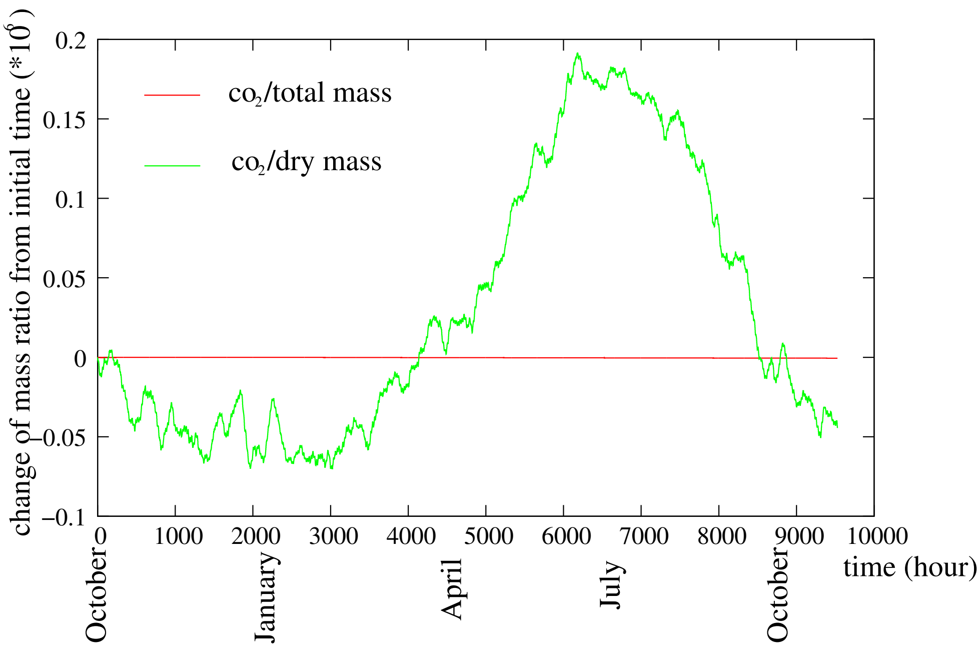

Figure 3: Evolution of the ratio between the mass of CO_2 ($\times 10^6$) and the total mass of air (red line) or the dry mass (green line) with respect to the initial ratios as a function of time for a one year forecast at TL255 resolution with global mass fixer for the total mass and for the CO_2.

4 Towards a dry mass conserving IFS

In the real atmosphere, dry mass is conserved inside air parcels and the variations of the total mass follow the variations of total water.

In this section we explain how the continuity equation of the dynamics can be coupled to the physics via the total water tendency computed in the physics for the IFS to formally conserve dry mass instead of total mass. In this case, the continuity equation of the IFS remains an equation for the total mass (i.e. "moist" hydrostatic pressure) unlike the solution proposed by Lauritzen et al. (2018) for CAM-SE.

4.1 New equations for the total mass

As there is no source of dry air in air parcel, the equation for the density of dry air has to be:

$$\frac{D\rho_d}{Dt} = -\rho_d \vec{\nabla}.\vec{u} \tag{32}$$

The equation for the evolution of total water (26), combined to equation (32) gives a new equation for the density of total mass which assures the conservation of dry air:

$$\frac{D\rho_t}{Dt} = \frac{D\rho_d}{Dt} + \frac{D\rho_w}{Dt} = -\rho_t \vec{\nabla}.\vec{u} + \rho_t S_w \tag{33}$$

This equation shows that the physics parametrisations "break" the continuity of the fluid as they allow source/sink of mass which are not explained by the mass advection by the "resolved" velocity $\vec{u}$. In other words, the dynamics sees such a change of mass, as if mass is injected in or sucked from air parcels "by a syringe". The dynamics will however react to this mass change which will induce a local circulation to readjust the mass distribution.

The different steps presented in section 2 to transform the equation for the density of total mass in z-coordinates into an equation for the logarithm of surface pressure in η-coordinates have to be applied to the new continuity equation (33).

The equation for the generalised density $\partial\pi/\partial\eta$ in η-coordinates becomes :

$$\frac{D(\frac{\partial\pi}{\partial\eta})}{Dt} = \frac{\partial\pi}{\partial\eta}\left(-\vec{\nabla}_{|\eta}.\vec{V} - \frac{\partial\dot{\eta}}{\partial\eta} + S_w\right). \tag{34}$$

The Eulerian form of this equation is:

$$\frac{\partial(\frac{\partial\pi}{\partial\eta})}{\partial t} = -\vec{\nabla}_{|\eta}.(\frac{\partial\pi}{\partial\eta}\vec{V}) - \frac{\partial(\dot{\eta}\frac{\partial\pi}{\partial\eta})}{\partial\eta} + \frac{\partial\pi}{\partial\eta}S_w \tag{35}$$

After integration along a vertical, we get a new equation for π_s which replaces equation (13) if dry mass is to be conserved:

$$\frac{\partial\pi_s}{\partial t} = \underbrace{-\int_{\eta=0}^{\eta=1}\vec{\nabla}_{|\eta}.(\frac{\partial\pi}{\partial\eta}\vec{V})d\eta}_{S_{eul}} + \int_{\pi=0}^{\pi=\pi_s} S_w d\pi \tag{36}$$

The new equation for ω is obtained from the vertical integration of equation (35):

$$\omega = -\left[\int_{\eta=0}^{\eta}(\vec{\nabla}_{|\eta}.(\frac{\partial\pi}{\partial\eta}\vec{V})d\eta\right] + \vec{V}.\vec{\nabla}_{|\eta}\pi + \int_{\pi=0}^{\pi} S_w d\pi \tag{37}$$

The new $\dot{\eta}$ is also computed from equation (35):

$$\dot{\eta}\frac{\partial \pi}{\partial \eta} = -\frac{\partial \pi}{\partial t} - \left[\int_{\eta=0}^{\eta} \vec{\nabla}_{\eta}.(\frac{\partial \pi}{\partial \eta}\vec{V})d\eta\right] + \int_{\pi=0}^{\pi} S_w d\pi \tag{38}$$

with $\partial \pi/\partial t = -B(\eta)\partial \pi_s/\partial t$ given by equation (36).

4.2 New equations for tracers

The equation for the density of tracer (30) is not affected by the change of continuity equation. However, the equation for the ratio of mass of tracer with respect to total mass is affected. The combination of equation (30) with the new equation (33) gives:

$$\frac{Dq_c}{Dt} = -q_c S_w + S_c. \tag{39}$$

With this new continuity equation, q_c changes if there are sources/sinks of tracer and/or if there is a change of total mass unlike in the current IFS where q_c can change only if there are sources/sinks of tracer as the total mass is supposed to be conserved (equation (31)).

In the current IFS, the specific ratios "behave" as mixing ratios because they are defined as a ratio with respect to a quantity, the total mass, which is supposed to be constant. If a mixing ratio (ratio with respect to dry air) is computed from an IFS specific ratio, its evolution is affected by the variation of dry air mass which is anti-correlated with the variation of total water. With the modified continuity equation, mixing ratios vary only if there is a change of mass of tracer.

In practice, the impact of the non-conservation of dry mass is small compared to the conservation errors in the semi-Lagrangian scheme. The spurious correlation in the current IFS between the evolution of total water and the evolution of tracer is seen only if mass fixers are used for the total mass and the mass of tracers. In the modified system, the conservative quantity becomes the dry mass and the mass fixers need to be adapted to the new continuity equation (see discussion in section 4.5).

4.3 New equations for other specific variables

In the hydrostatic IFS, the other prognostic variables are the horizontal wind $\vec{V} = (U, V)$ (or vorticity/divergence in spectral space) and the temperature (or the virtual temperature in spectral space). The equations for both the horizontal wind and the temperature are written in "advection" and "barycentric" form, i.e. the total mass continuity equation has been combined with the flux form equations for momentum and enthalpy. When the total mass continuity equation is modified, these two equations should, in principle, be modified too. But these modifications have been neglected in the first implementation of the coupling between the continuity equation and the physics in CY46R1 of the IFS.

4.4 Implementation in CY46R1 of the IFS

The equations described in the previous section can be implemented in the current IFS with a minimal set of changes if the prognostic continuity equation remains an equation for the total mass. Changing the prognostic continuity equation into an equation for the dry mass (i.e."dry" hydrostatic pressure, see Lauritzen et al., 2018) would result in a major revision of the entire IFS system.

In the IFS, the coupling with the physics parametrisations is done in grid-point space, after the explicit dynamics (i.e. after the computation of the explicit guess for the RHS and semi-Lagrangian advection) and before the semi-implicit correction of the RHS which is computed at the end of each time step in spectral space.

Because of the structure of the physics interface in the IFS, the physics mass tendencies can't be used to update consistently the surface pressure, ω and $\dot{\eta}$ at the same time step. It is however possible to store the physics tendencies of total water S_w and update the surface pressure, ω and $\dot{\eta}$ at the beginning of the next time step before the semi-Lagrangian advection. With such a solution, the future state of the model (stored in IFS variables GMVT1, GFLT1) still sees compensating dry air fluxes momentarily in the semi-implicit. But it will be corrected at the beginning of the next time step.

In practice, the change of total water S_w due to physics is computed in subroutine CPQTUV at the end of the physics computation. It is then stored as a 3D grid-point field (new GFL array PHYCTY) until the beginning of the next time step. S_w is then used in the grid point dynamics, in the routine which computes S_{eul}, ω and $\dot{\eta}$ (GPCTY). In CY46R1, in order to activate the new continuity equation which ensures dry mass conservation, the following namelist options are required:

```
&NAMDYN
LNODRYFLX=true
/
&NAMGFL
YPHYCTY_NL%%LGP=true,
YPHYCTY_NL%%IGRBCODE=241,
/
&NAMFPC
NFP3DFS=1,
MFP3DFS(:)=241,
/
```

The above grib code setting is required as the new GFL PHYCTY doesn't have yet a dedicated grib code (241 is just an example of a grib code which can be borrowed). The term S_w is stored in GFL array PHYCTY and can be output on model or pressure level if the grib code is present in NAMFPC.

4.5 Interaction with the mass fixers

Several types of mass fixers are available in the IFS model in order to compensate for numerical errors. They have to be revisited for consistency with the hypothesis of conservation of dry mass instead of total mass.

4.5.1 Global spectral mass fixers

In spectral space, the spectral coefficient for $n = 0$ gives the mean of the logarithm of the moist hydrostatic surface pressure. Keeping this coefficient constant imposes global total mass conservation (option LMASCOR=T, LMASDRY=F). If the dry mass is to be conserved, an approximate correction is computed in grid point space where the water species are available and the correction is applied in spectral space to the $n = 0$ spectral coefficient of the logarithm of the hydrostatic surface pressure (option LMAS-

COR=T, LMASDRY=T). From CY46R1, the computation of the correction if LMASDRY=T has been modified to take into account all the prognostic water species, not only the water vapour.

With the current IFS, total mass conservation is supposed at the level of the equations. It is then the total mass which has to be fixed from numerical error (LMASCOR=T, LMASDRY=F).

But, with the new continuity equation, it is the dry mass which has to be fixed (LMASCOR=T, LMASDRY=T).

Figure 4 show the evolution of the global mean of total mass and dry mass with the new continuity equation in one year simulation at TL255 with and without global dry mass fixer. When no mass fixer is applied, the dry mass increases linearly with time and it is now the total mass which follows the evolution of total water in the atmosphere. When the global dry mass fixer is turned on, the dry mass is conserved and the total mass varies with the total water annual cycle.

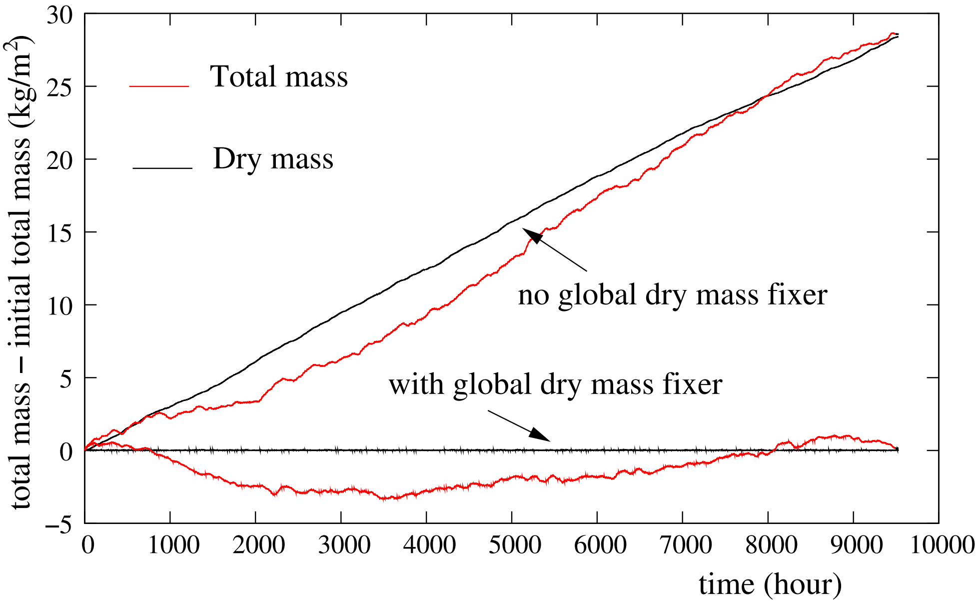

Figure 4: Difference between the global mean of mass (kg/m^2) and the initial value as a function of time for a one year long forecasts at TL255 resolution with the modified continuity equation in the IFS with and without global dry mass fixer. The red curves show the evolution of the total mass, the black curves the evolution of the dry mass.

4.5.2 Mass fixer for individual constituents

In the IFS, several mass fixers have been implemented mainly to restore mass conservation in the semi-Lagrangian advection of individual constituents of the atmosphere (see Diamantakis and Flemming, 2014; Diamantakis and Agusti-Panareda, 2017). Experiments have shown that for long-lived tracers such as greenhouse gases, it is important to fix the pressure after advection and before applying the mass fixer for the individual tracers, so that the total atmospheric mass remains constant. The reason is that even a small mass conservation error in the total atmospheric mass can lead to a systematic accumulation of the tracer mass conservation error with time as explained by Agusti-Panareda et al. (2017).

The implementation of individual constituent mass fixers becomes more complicated with the new continuity equation because the prognostic quantity, the total mass, is not a conservative quantity any more.

It means that the conservative quantity which is now the dry mass needs to be deduced from two independently advected non-conservative quantities, the total mass and the total water. Both are affected with numerical error in the semi-Lagrangian, but, as they are not conservative (source/sink coming from physics), it is more problematic to fix them. Therefore, in the current cycle 46R1, when the modified continuity equation is activated the IFS tracer mass fixers cannot be applied correctly. Addressing these tracer mass conservation issues will be the subject of a future investigation.

4.6 Validation

The meteorological impact of these changes have been assessed comparing a 10-day forecast experiment that uses the new formulation against an experiment that uses the operational forecast formulation. The horizontal resolution of the experiments is 9km (Tco1279 grid) and the standard 137 vertical level set is used. They are initialised from the 00 UTC Long Window 4D-VAR (LWDA) operational analysis and are validated against this analysis. The forecast period tested is 18/08/2017 to 30/09/2017. For each experiment, a separate forecast is run on each day. During this forecast period, intense hurricane activity was observed in the North Atlantic area.

While verification results from these experiments show a small impact overall, there are also some noticeable differences. These are mostly positive in terms of skill:

- There is a reduction in the mean error of the Mean Sea Level (MSL) pressure in the extra-tropics as it is illustrated in figure 5. Furthermore, linked with this reduction of the MSL pressure bias, there is a small but statistically significant reduction of approximately 1% in Root Mean Square Error (RMSE) of the MSL pressure in the southern hemisphere.
- A small reduction in the RMSE of temperature in the tropics and the southern hemisphere most noticeable in the layer 700 to 500 hPa.
- A small reduction in the RMSE of geopotential height in the southern hemisphere. A similar one in the northern hemisphere but only in the short range. The Anomaly Correlation Coefficient (ACC) also shows a similar positive response.
- The vector wind component RMSE reduces in the North Atlantic basin and along the southern storm track troposphere, mostly in the first 5-6 days of the forecast.
- A reduction of 1% in relative humidity RMSE at very low tropospheric levels.
- Results for total column water, cloud cover are neutral.

The impact of the two continuity formulations on three major North Atlantic Hurricane forecasts has also been examined: Harvey, Irma and Maria. Results from 5 forecasts in total have been analysed: 2 for Maria, 2 for Irma and 1 for Harvey. In most of these forecasts the impact seen on hurricane track, core pressure, maximum wind, minimum pressure - max wind relationship, radius to maximum wind and total precipitation is small. However, the 00 UTC 17/09/2017 Maria forecast with the new continuity shows a better agreement with observations in the core pressure and the radius to maximum wind (see figure 6). There is also some difference in the total precipitation between the two experiments but at this stage we are unable to say if this difference is an improvement or deterioration due to lack of a verifying data set. Furthermore, the forecast track for Hurricane Harvey appears to be closer to observations from day 5 and beyond in the forecast experiment that uses the new continuity (not shown here). These results suggest that a more detailed investigation is needed in order to establish whether there is a systematic measurable impact on tropical cyclone cases. Furthermore, it is more likely that any impact may be more visible at higher resolutions.

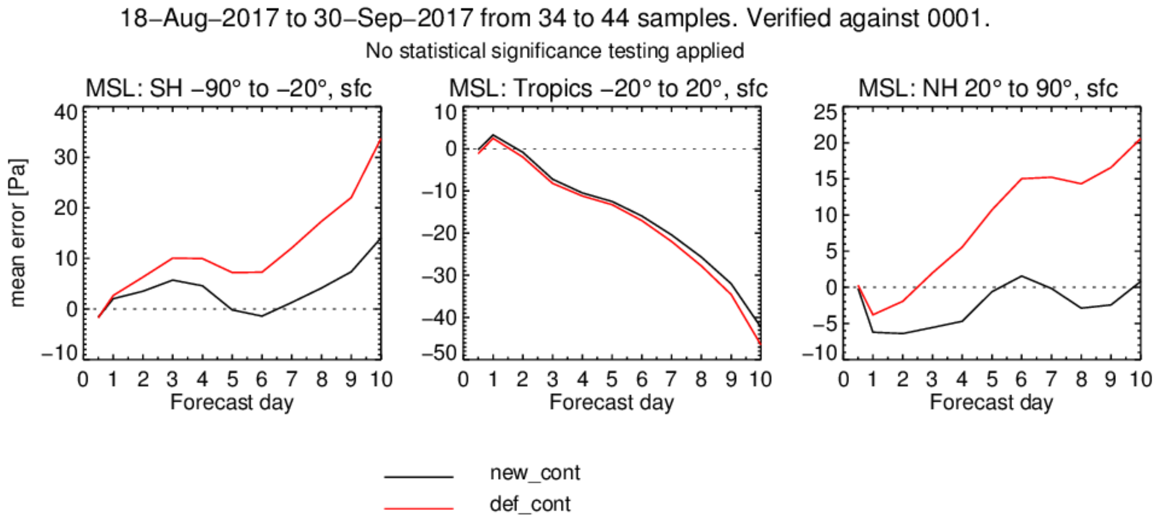

Figure 5: MSL pressure mean error of a 10-day forecast experiment using the new continuity (black line) compared with a control experiment that uses the default continuity (red line). Both forecast experiments have run starting from the same set of initial dates that cover the period from 18/08/2017 to 30/09/2017.

5 Conclusions

In the IFS dynamical core, mass conservation comes from the equation of moist hydrostatic surface pressure, the definition of the hybrid levels η and the computation of the corresponding generalised vertical velocity $\dot{\eta}$. The complete set of IFS equations is written consistently with a continuity equation which controls the conservation of the total mass of multi-phase air parcels composed of dry air, water vapour and several categories of water condensates which are both dynamically and thermodynamically active (water loading of air parcel by the condensates, moist heat capacities etc). Air parcels also contain passive tracers which are transported by the flow but whose composition is small enough to be neglected in the equations for the other prognostic variables of the IFS.

The dynamical core is coupled to a set of parametrisations in the physics package which can be seen as individual 1D solvers. Such simple solvers are usually based on a simplifying assumption in terms of mass redistribution. In fact they are usually not designed to solve mass redistribution inside vertical columns as this would require a re-computation in the physics of quantities such as $\dot{\eta}$ followed by a vertical advection. However, some of the parametrised physical processes, are a source or a sink of total water in air parcels (precipitation, subgrid transport). Therefore, there should be a net mass redistribution resulting from these processes.

In the IFS physics, it is supposed that the moist hydrostatic pressure in each grid box is unchanged by the parametrisations and there is no coupling between the physics and the continuity equation (i.e. prognostic equation for the moist surface pressure and for the computation of $\dot{\eta}$). Such an absence of physics-dynamics coupling for the mass means that the IFS always conserve total mass inside air parcels even if physics modify the total water inside these air parcels. An implied consequence is then that

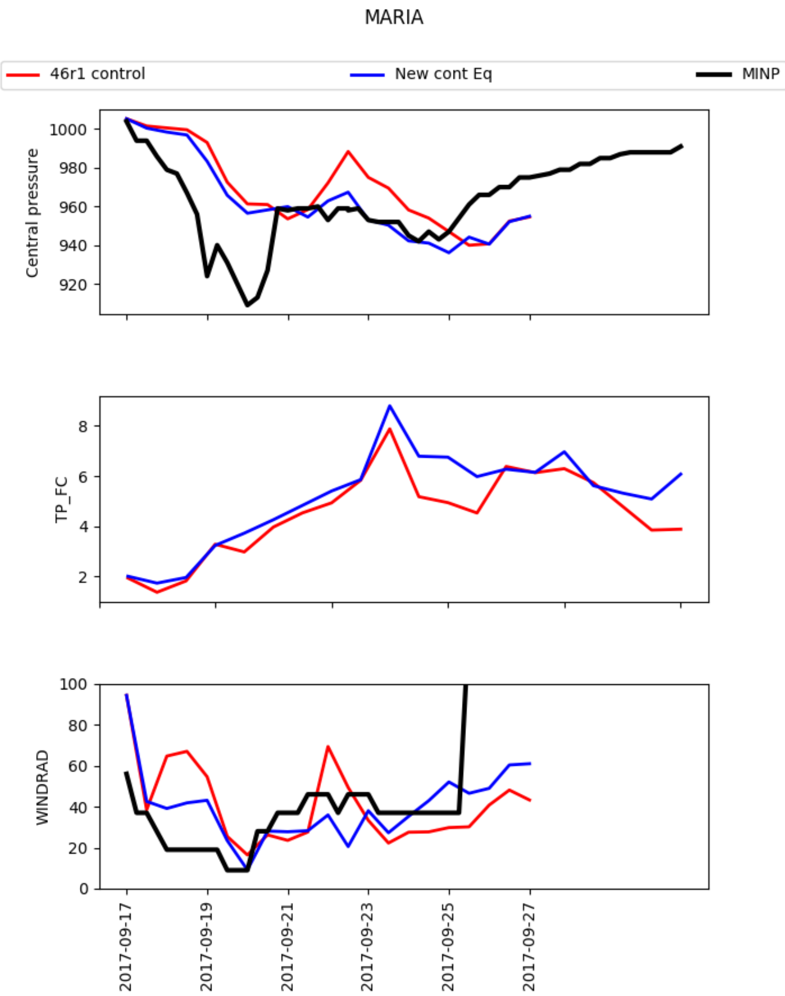

Figure 6: Core pressure (top row), integrated total precipitation within 150 km from the core centre since previous evaluated step (middle row) and radius to maximum wind speed in metres (bottom row) for Hurricane Maria forecast initialised from 00 UTC 17/09/2017 IFS LWDA analysis. Red line: experiment with standard (operational) continuity formulation. Blue line: experiment with new formulation. Black line: "Best track" observations.

artificial sources/sinks of dry air compensate for the sinks/sources of total water. This is a problem for atmospheric composition. The ambiguity in the definition of the ratios of mass of tracers such as CO_2 with respect to total mass (specific ratios) or dry mass (mixing ratios) may introduce a spurious evolution of the tracer concentration which is anti-correlated with the evolution of total water in the atmosphere. Such nonphysical evolution is masking the intrinsic evolution of the tracer concentration.

A new coupling between the continuity equation and the physics via the total water tendencies produced by the physics package has been implemented and tested in IFS (from CY46R1). Thanks to the modified continuity equation, dry mass is formally conserved by the IFS instead of total mass. Also, the global mass fixers had to be reformulated to fix the dry mass instead of the total mass when the modified equation is used.

With this new formulation, total mass (i.e. moist hydrostatic pressure) remains the prognostic variable in the model and the reference for the definition of the vertical levels unlike the solution which has been implemented by Lauritzen et al. (2018) in CAM-SE. Furthermore, with this new formulation mixing ratios vary only if there is a change of mass of tracer. This is a desirable behaviour, however, at this stage this new model development cannot be used for atmospheric composition forecasts as it is incompatible with the existing implementation of tracer mass fixers used there. Until this issue is addressed, the recommended option for carbon tracers is to keep using the standard IFS continuity which has also been proven to produce good quality results.

Validation experiments show that the new formulation has a small positive impact in IFS forecasts which is more noticeable in MSL pressure. Testing at longer periods and different seasons will be necessary to establish the significance of this finding. Likewise, further testing will be necessary in order to establish if there is a benefit for tropical cyclones and if this is more obvious at resolutions higher than the ones currently used operationally by the ECMWF model IFS.

The coupling between the physical parametrisations and the continuity equation which has been implemented to ensure dry mass conservation instead of total mass can be generalised to any other source/sink of mass generated by physical parametrisations. It has recently been used to couple the deep convection scheme and the IFS dynamics via the divergence of mass flux (Malardel and Bechtold, 2019). In this case, the subsiding and the horizontal branches of the convective overturning circulation which are necessary to close the mass budget associated with a convective updraught are taken over by the 3D solver of the dynamics whereas, in a traditional scheme, the compensating subsidence is computed in the same 1D column as the subgrid updraught by the convection scheme. In the grey zone of convection, a better 3D representation of the convective overturning is expected to help a seamless representation of deep convection in the model. However, with the modified convection scheme, the control of the convective stabilisation is still driven by the formulation of the mass flux. Other assumptions will have to be revisited to improve the transition from fully parametrised to fully resolved deep convection at horizontal resolution in the grey zone of convection.

References

A. Agusti-Panareda, M. Diamantakis, Victor Bayona, Friedrich Klappenbach, and Andre Butz. Improving the inter-hemispheric gradient of total column atmospheric co2 and ch4 in simulations with the ECMWF semi-lagrangian atmospheric global model. *GMD*, 10:1–18, 2017.

M. Diamantakis and A. Agusti-Panareda. A positive definite tracer mass fixer for high resolution weather and atmospheric composition forecasts. Technical Report 819, ECMWF, 2017.

M. Diamantakis and J. Flemming. Global mass fixer algorithms for conservative tracer transport in the ECMWF model. *GMD*, 7:965–979, 2014.

R. Laprise. The euler equations of motion with hydrostatic pressure as an independent variable. *Mon. Wea. Rev.*, 120:197207, 1992.

P. H. Lauritzen, R. D. Nair, A. R. Herrington, P. Callaghan, S. Goldhaber, J. M. Dennis, J. T. Bacmeister, B. E. Eaton, C. M. Zarzycki, M. A. Taylor, P. A. Illrich, T. Dubos, A. Gettelman, R. B. Neale, B. Bobbins, K. A. Reed, C. Hannay, B. Medeiros, J. J. Benedict, and J. J. Tribbia. Ncar release of cam-se in cesm2.0: A reformulation of the spectral element dynamical core in dry-mass vertical coordinates with comprehensive treatment of condensates and energy. *Journal of Advances in Modeling Earth Systems*, 10:15371570, 2018.

S. Malardel and P. Bechtold. The coupling of deep convection with the resolved flow via the divergence of mass flux in the ifs. *Quart. J. Meteor. Soc.*, 2019. (in revision).

H. Ritchie, C. Temperton, A.J. Simmons, M. Hortal, T. Davies, D. Dent, and M. Hamrud. Implementation of the semi-lagrangian method in a high resolution version of the ecmwf forecast model. Technical Report 72, ECMWF, 1994. 68 pp.

A. J. Simmons and D. M. Burridge. An energy and angular-momentum conserving vertical finite-difference scheme and hybrid vertical coordinates. *Mon. Wea. Rev.*, 109:758766, 1981.