Numerics of the Physics and the Physics of Numerics

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1. Introduction
2. Time integration
3. Processes in the ECMWF model
4. Conclusions

Introduction

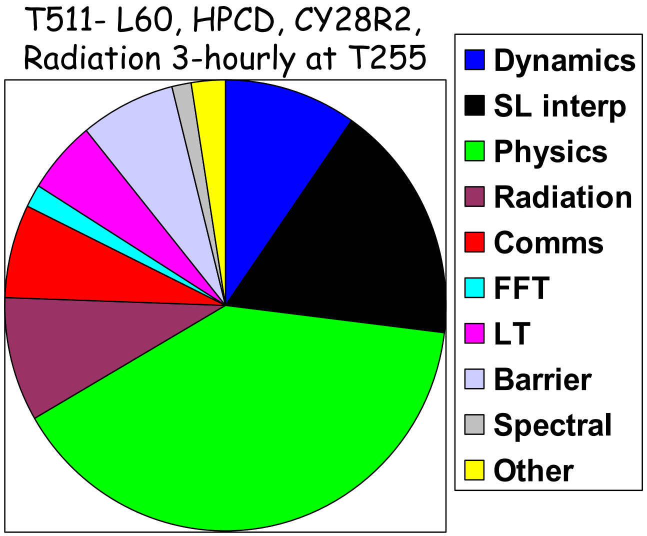
General considerations:

- Parametrization packages have some level of modularity
- Explicit time integration is the preferred option; implicit schemes are used if necessary for stability
- Times steps can be large (in the IFS, 15 minutes for T511 and 1 hour for the seasonal forecasts at T95)
- Vertical resolution is often not sufficient to resolve relevant processes (e.g. sharp inversions, layered clouds)
- Scheme has to be compatible with dynamics; IFS uses 2 time level time integration
- Accuracy of the numerics of parametrization is often ignored and parametrizations are sometimes optimized for a given vertical resolution and time step
- A high level of modularity (i.e. different process are handled independently) is desirable from code maintenance point of view, but not always desirable from numerical point of view

Time stepping

Requirements for time stepping:

1. Stability (requires implicit solution for some processes)
2. Balance (correct steady state for long time steps)
3. Modularity of code
4. Accuracy



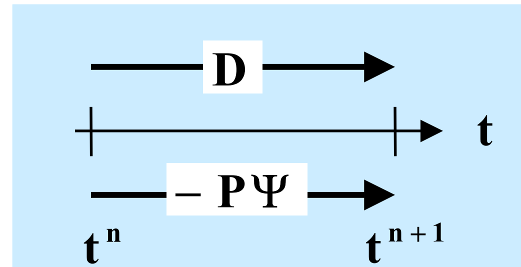
Papers on time stepping of equations with multiple time scales (stiff equations):

Beljaars(1991): Numerical schemes for parametrization (ECMWF seminar)
Browning (1994): Splitting methods for problems with different time scales
Caya et al. (1998): Splitting methods
McDonald (1998): Numerical methods for atmospheric models (ECMWF seminar)
Wedi(1999): Physics dynamics coupling
Sportisse (2000): Operator splitting for stiff problems
Williamson (2002): Sequential-Split versus Parallel-split in the NCAR model
Cullen and Salmand (2003): Predictor-corrector for parametrization
Ropp et al (2003): Time integration of reaction-diffusion equations
Dubal et al. (2004): Parallel versus sequential splitting

Time stepping: Process split / Parallel split

$$\frac{d\Psi}{dt} = D(\Psi) - P(\Psi)\Psi$$

Steady state solution with linear physics (i.e. P=constant): $\psi = \frac{D}{P}$



Different terms are computed independently:

Dynamics (explicit in this example): $\frac{\Psi_D^{n+1} - \Psi^n}{\Delta t} = D(\Psi^n)$

Physics (implicit): $\frac{\Psi_P^{n+1} - \Psi^n}{\Delta t} = -P(\Psi^n)\Psi_P^{n+1} \Rightarrow \frac{\Psi_P^{n+1} - \Psi^n}{\Delta t} = \frac{-P(\Psi^n)\Psi^n}{1 + \Delta t\, P(\Psi^n)}$

Total tendency: $\frac{\Psi^{n+1} - \Psi^n}{\Delta t} = \frac{\Psi_D^{n+1} - \Psi^n}{\Delta t} + \frac{\Psi_P^{n+1} - \Psi^n}{\Delta t} = D(\Psi^n) - \frac{P(\Psi^n)\Psi^n}{1 + \Delta t\, P(\Psi^n)}$

Steady state: $\Psi^n = \frac{D(\Psi^n)\left\{1 + \Delta t\, P(\Psi^n)\right\}}{P(\Psi^n)}$ is time step dependent unless $\Delta t\, P(\Psi^n) << 1$

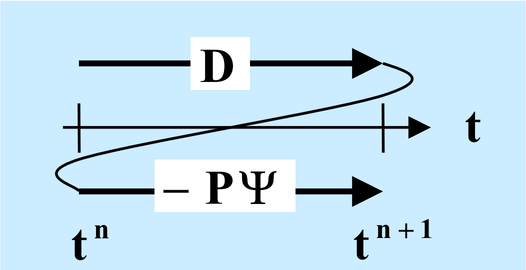
Advantage of process split: Processes can be handled independently!

Time stepping: Time split / Sequential split / Fractional step

$$\frac{d\Psi}{dt} = D(\Psi) - P(\Psi)\Psi$$

Steady state solution with linear physics (i.e. P=constant): $\psi = \frac{D}{P}$

Processes are used incrementally:



Dynamics (explicit in this example):

$$\frac{\Psi^{*} - \Psi^{n}}{\Delta t} = D(\Psi^{n})$$

Physics (implicit) starts from dynamics:

$$\frac{\Psi^{n+1} - \Psi^{*}}{\Delta t} = -P(\Psi^{n})\Psi^{n+1} \quad \text{or} \quad \frac{\Psi^{n+1} - \Psi^{n}}{\Delta t} = D(\Psi^{n}) - P(\Psi^{n})\Psi^{n+1}$$

Total tendency:

$$\frac{\Psi^{n+1} - \Psi^{n}}{\Delta t} = \frac{D(\Psi^{n}) - P(\Psi^{n})\Psi^{n}}{1 + \Delta t\, P(\Psi^{n})}$$

Steady state: $\Psi^{n+1} = \Psi^{n} = \frac{D(\Psi^{n})}{P(\Psi^{n})}$ is correct and independent of time step

Note: **- Nonlinear physics term is at time level n and not at ***
- Implicit process has to be last

Example with sequential split: condensation

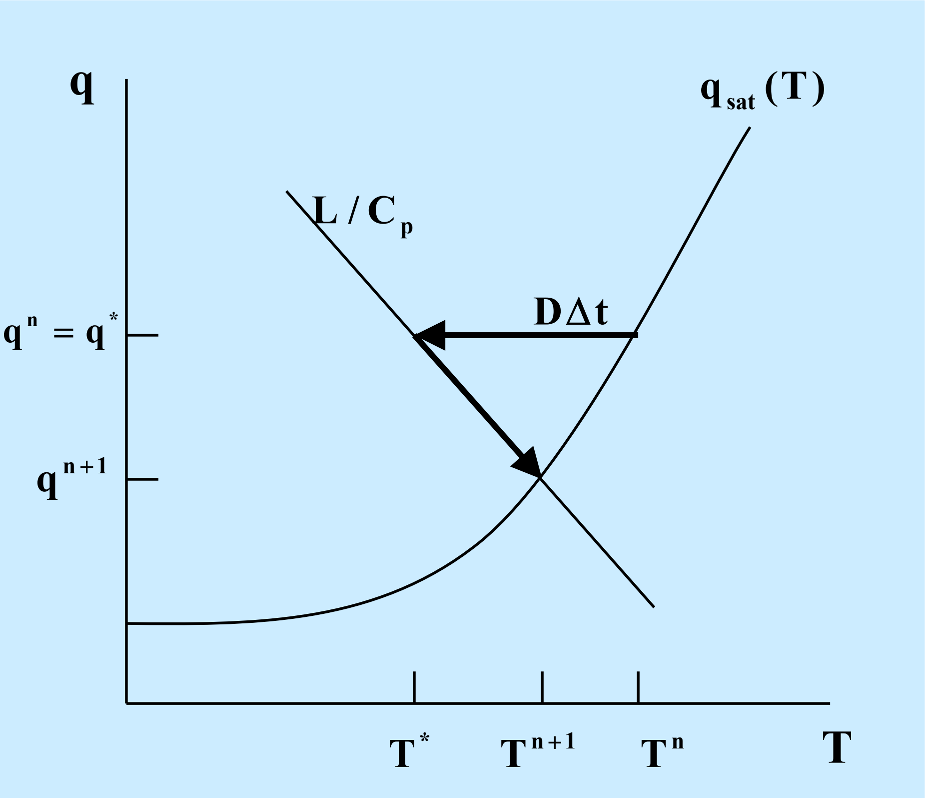
$$\frac{dT}{dt} = D + \frac{L}{C_p} c = D + \frac{L}{C_p} \frac{q - q_{sat}(T)}{\tau}$$

$$\frac{dq}{dt} = -c = -\frac{q - q_{sat}(T)}{\tau}$$

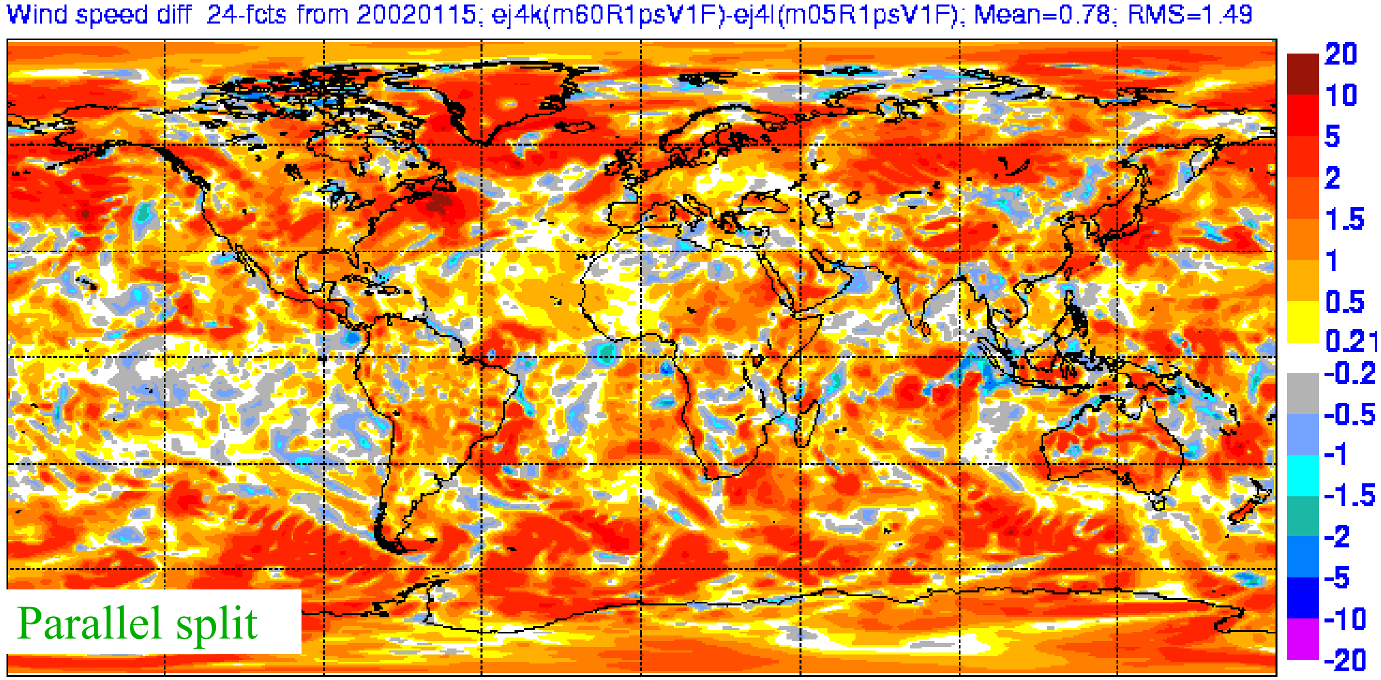
- Assume saturated air
- D is negative e.g. large scale lifting
- q-tendency only from condensation
- Condensation time constant is very small

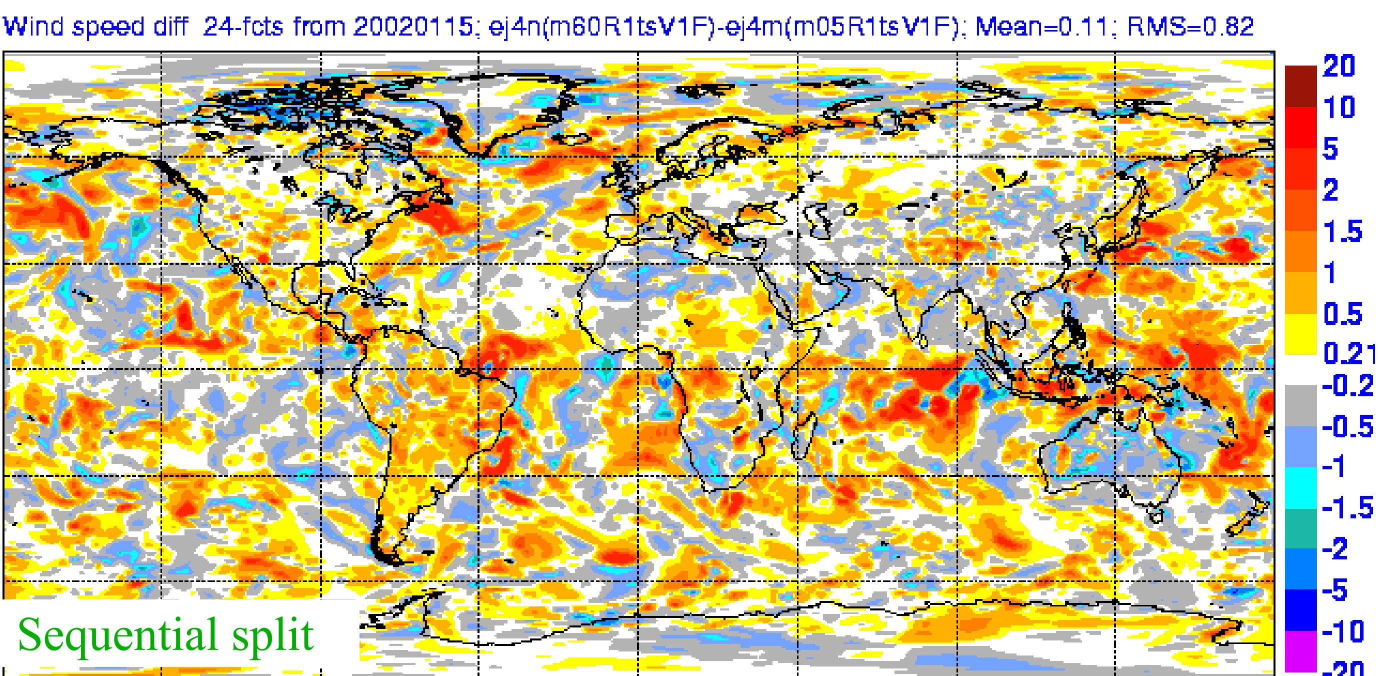
Traditional procedure:

1. Compute T* (after dynamics)
2. Assume $\tau << \Delta t$
3. Set $q^{n+1} = q_{sat}(T^{n+1})$
4. Use $T^{n+1} - T^* = -\left(q^{n+1} - q^*\right) L / C_p$
5. Iterate towards solution



Note: Iterative procedure towards saturation has to be last process; without applying D, condensation will not occur (or only in the next time step)





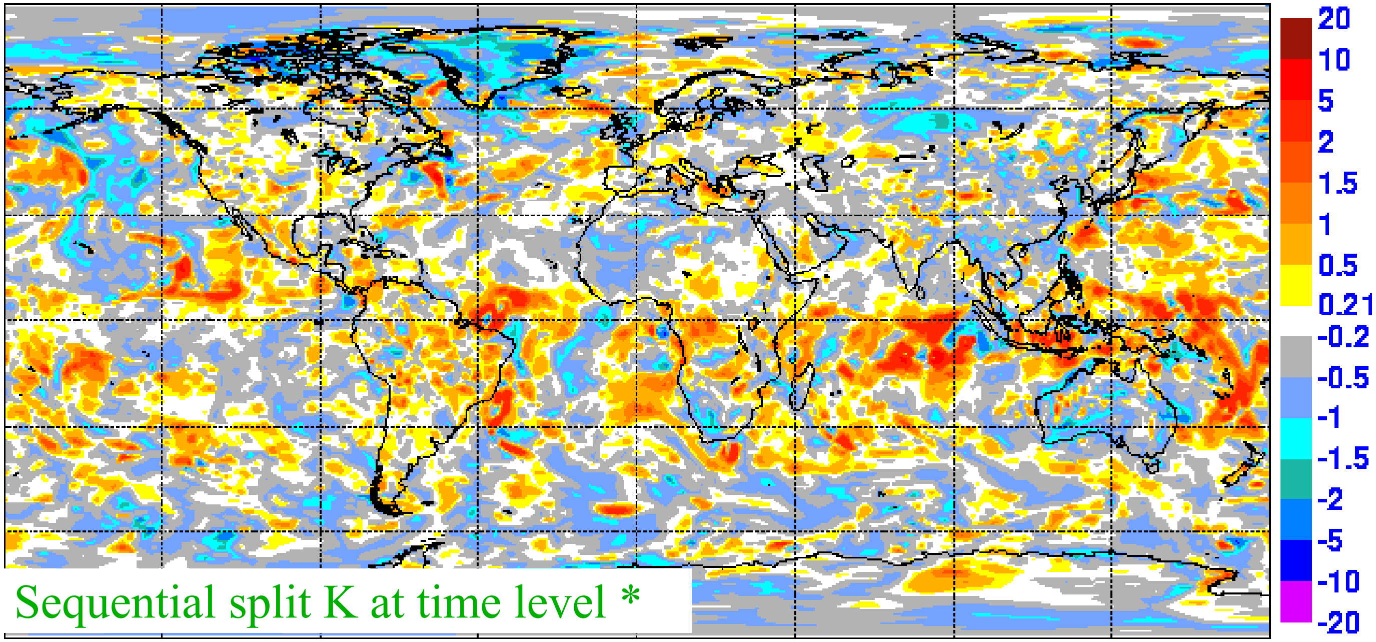
Example with splitting of dynamics and vertical diffusion.

Errors in 10m wind speed (with respect to 5 min time step).

Time step: 60 min
Date: 20020115
Resolution: T159
Forecast: 24 hours

Sequential split guarantees balance between Coriolis term, pressure gradient and turbulent stress divergence.

Wind speed diff 24-fcts from 20020115; ej4x(m60R1btsV1F)-ej4y(m05R1btsV1F); Mean=-0.11; RMS=0.83

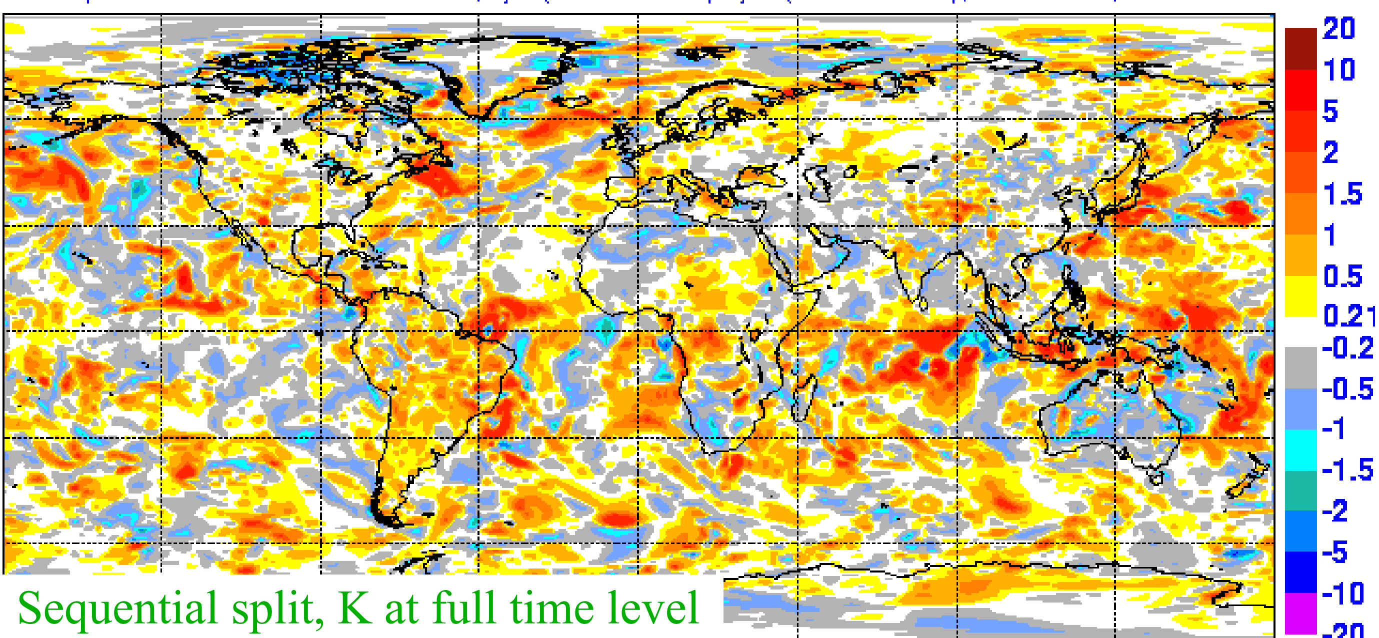


Example with splitting of dynamics and vertical diffusion.

Errors in 10m wind speed (with respect to 5 min time step).

Time step: 60 min
Date: 20020114
Resolution: T159
Forecast: 24 hours

Wind speed diff 24-fcts from 20020115; ej4n(m60R1tsV1F)-ej4m(m05R1tsV1F); Mean=0.11; RMS=0.82



Evaluation of diffusion coefficient at “in between time level” lowers wind speed by 0.2 m/s

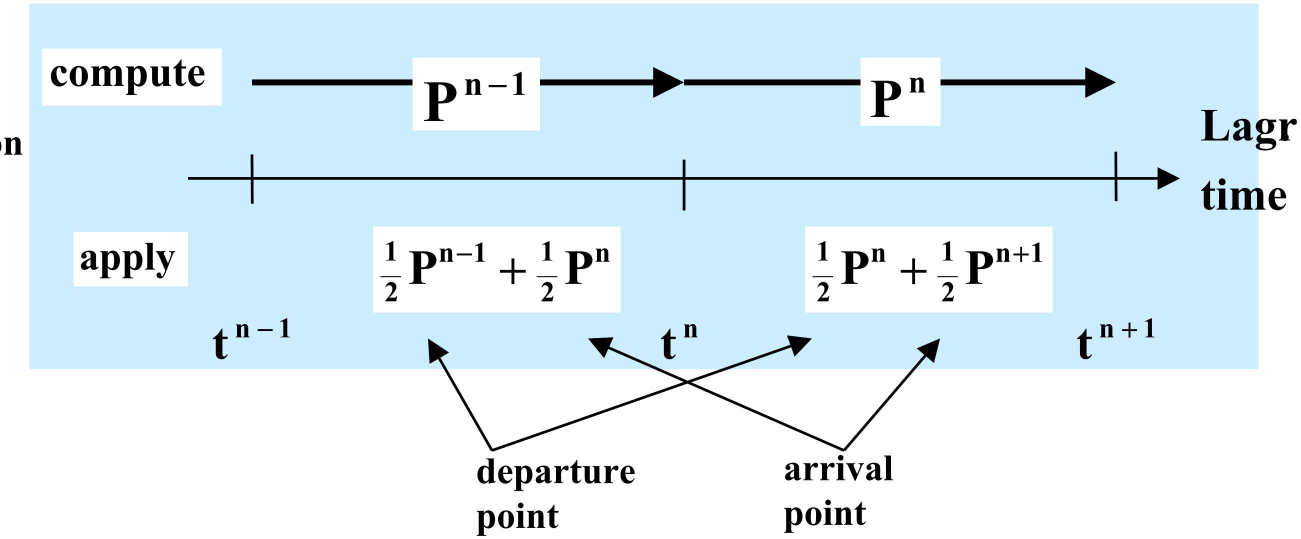
Parallel split versus sequential split: summary

- Some form of splitting is necessary with current parametrizations; "fully unified physics packages" do not exist.
- Parallel split allows for maximum code modularity but steady state solutions are time step dependent if time step is not small compared to time scale of process.
- Sequential split is preferred option
- Order of processes is important:
  1. First: slow explicit processes
  2. Last: fast implicit processes (in principle only one implicit process is allowed)

Towards 2nd order accuracy

$$\frac{d\Psi}{dt} = D + P$$

D : dynamics without advection



Compute physics as an average between departure and arrival points of semi-Lagrangian trajectory

However, some processes are evaluated "implicitly" on the new time level, therefore:

$$\frac{\psi^{n+1} - \psi^{n}}{\Delta t} = D + \frac{1}{2}P^{n+1}_{rad+cnv+cld} + \frac{1}{2}P^{n}_{rad+cnv+cld} + P^{n+1}_{vdf+sgoro}$$

For time level n+1 use ψ^{*} that is as close as possible to the new time level, e.g. for vdf+sgoro as 1st process:

$$\psi^{*} = \psi^{n} + \Delta t\left(D + P^{n}_{rad+cnv+cld} + P^{n+1}_{vdf+sgoro}\right)$$

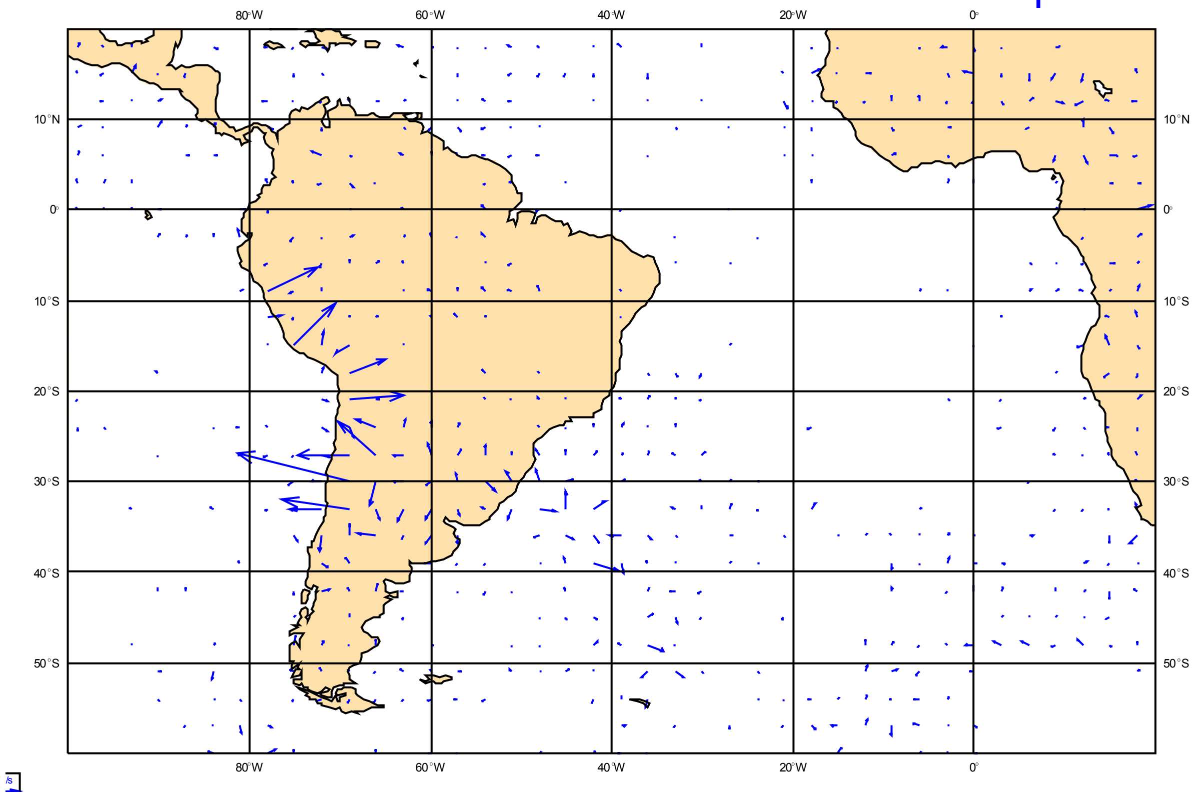
Wedi(1999): The numerical coupling of the physical parametrization to the "dynamical" equations in a forecast model, ECMWF Tech Memo, No 274.

Use of $$\frac{\psi^{n+1}-\psi^{n}}{\Delta t} = D + \frac{1}{2}P^{n+1}_{rad+cnv+cld} + \frac{1}{2}P^{n}_{rad+cnv+cld} + \frac{1}{2}P^{n}_{vdf+sgoro} + \frac{1}{2}P^{n+1}_{vdf+sgoro}$$

Instead of $$\frac{\psi^{n+1}-\psi^{n}}{\Delta t} = D + \frac{1}{2}P^{n+1}_{rad+cnv+cld} + \frac{1}{2}P^{n}_{rad+cnv+cld} + P^{n+1}_{vdf+sgoro}$$

Leads to big wind errors compared to short time step integrations (60 versus 5 minutes)

Level 31 U/V* 8/9/97 12h fc t+6 vt:8/9/1997 18h exp:ztcn



Towards 2nd order accuracy in the IFS

$$\frac{\Psi^{n+1} - \Psi^{n}}{\Delta t} = D + \tfrac{1}{2} P^{n+1} + \tfrac{1}{2} P^{n}$$

In the IFS (CY28R1), "updated" profiles are supplied sequentially to the physics schemes:

$$\begin{aligned} P^{n+1} &= P^{n+1}_{rad}\left(\Psi^{n}\right) \\ &+ P^{n+1}_{vdf+sgoro}\left(\Psi^{n} + \Delta t(D + P^{n+1}_{rad})\right) \\ &+ P^{n+1}_{cnv+cld}\left(\Psi^{n} + \Delta t(D + \tfrac{1}{2} P^{n}_{rad} + \tfrac{1}{2} P^{n+1}_{rad} + P^{n+1}_{vdf+sgoro} + \tfrac{1}{2} P^{n}_{cnv+cld})\right) \end{aligned}$$

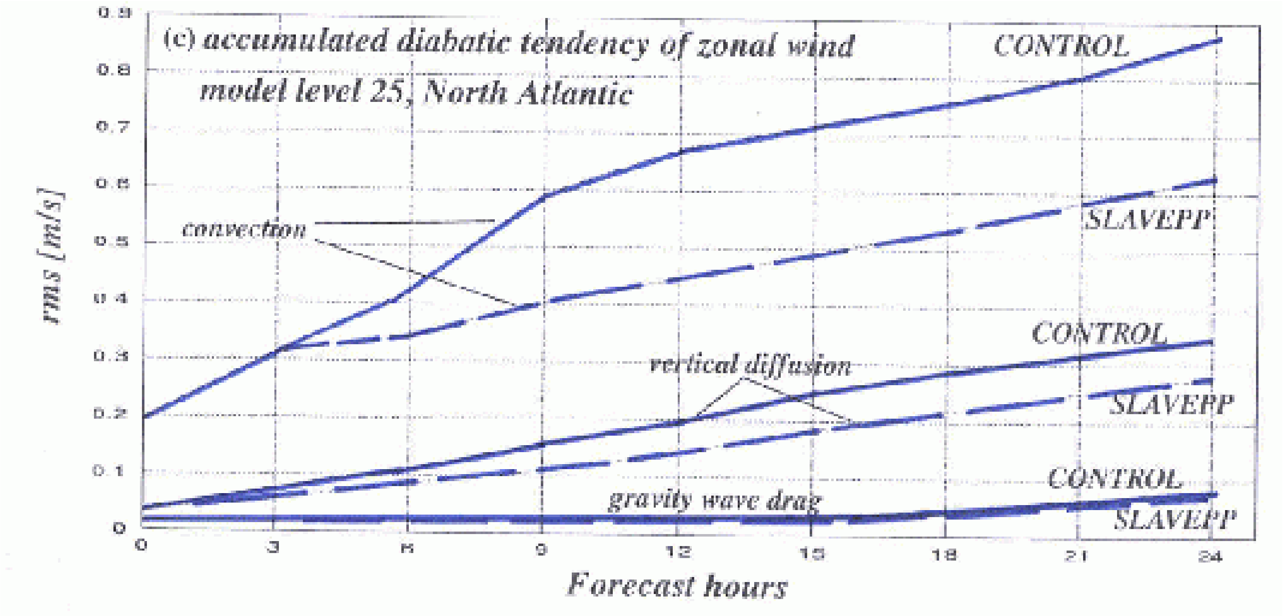
Comments:

♦RAD does not include guess from previous time level (technically difficult because radiation is computed on a low resolution grid)

♦VDF+SGORO does not have guess from CNV+CLD (including these gives unrealistic boundary layers)

♦ CNV+CLD has only half of the tendency from the previous step (empirical choice to maintain sufficient convective activity)

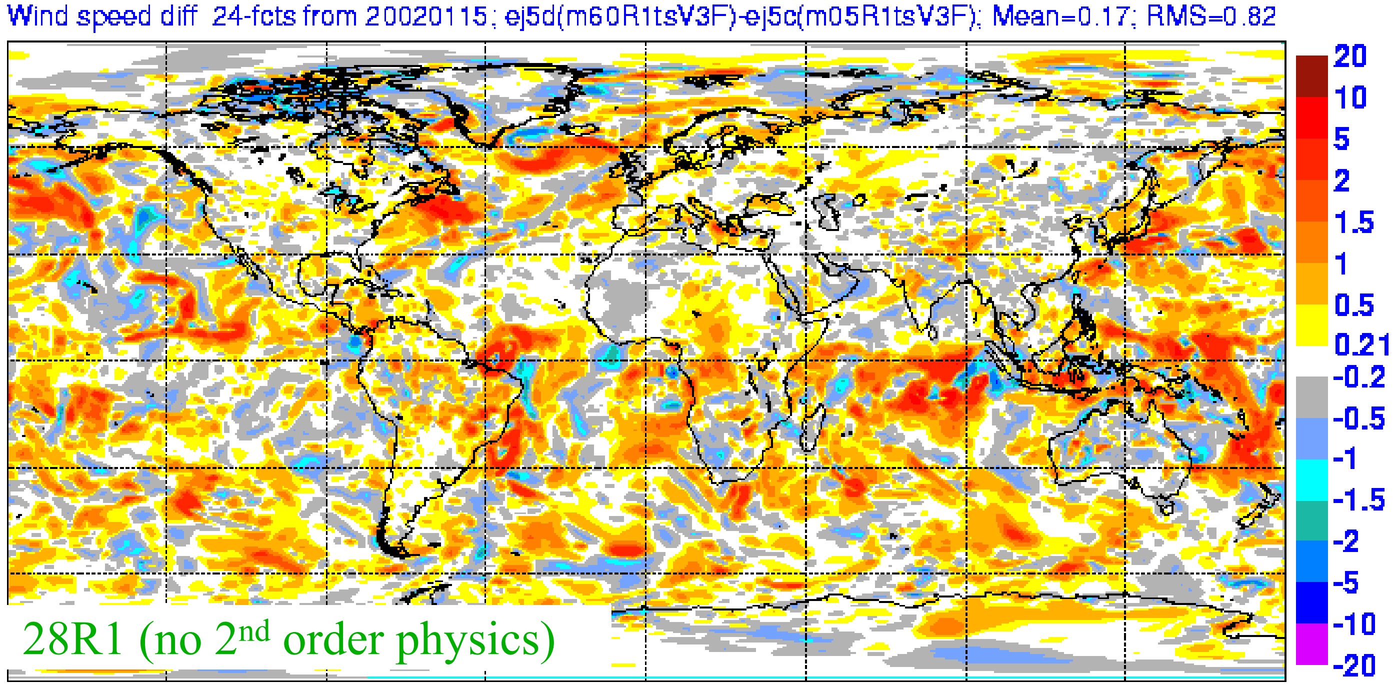
2nd order physics reduces time truncation errors

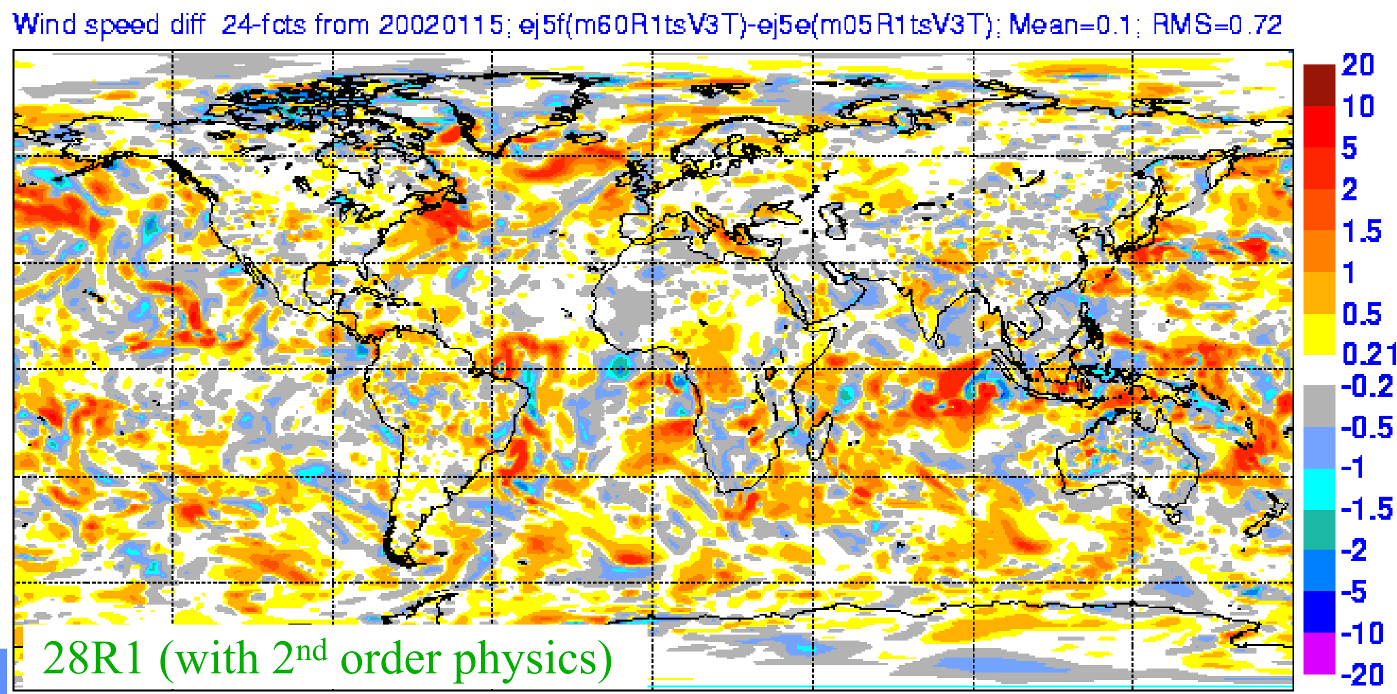


RMS difference of tendencies (cnv, vdf, sgoro) between integration with 60 minute time step and with 5 minute time step. CONTROL uses standard time integration; SLAVEPP uses the 28R1 2nd order physics.

2nd order physics reduces time truncation errors

Wind speed (10 m) difference between integration with 60 minute time step and with 5 minute time step.





Towards 2nd order accuracy in the IFS

$$\frac{\psi^{n+1} - \psi^{n}}{\Delta t} = D + \tfrac{1}{2} P^{n+1} + \tfrac{1}{2} P^{n}$$

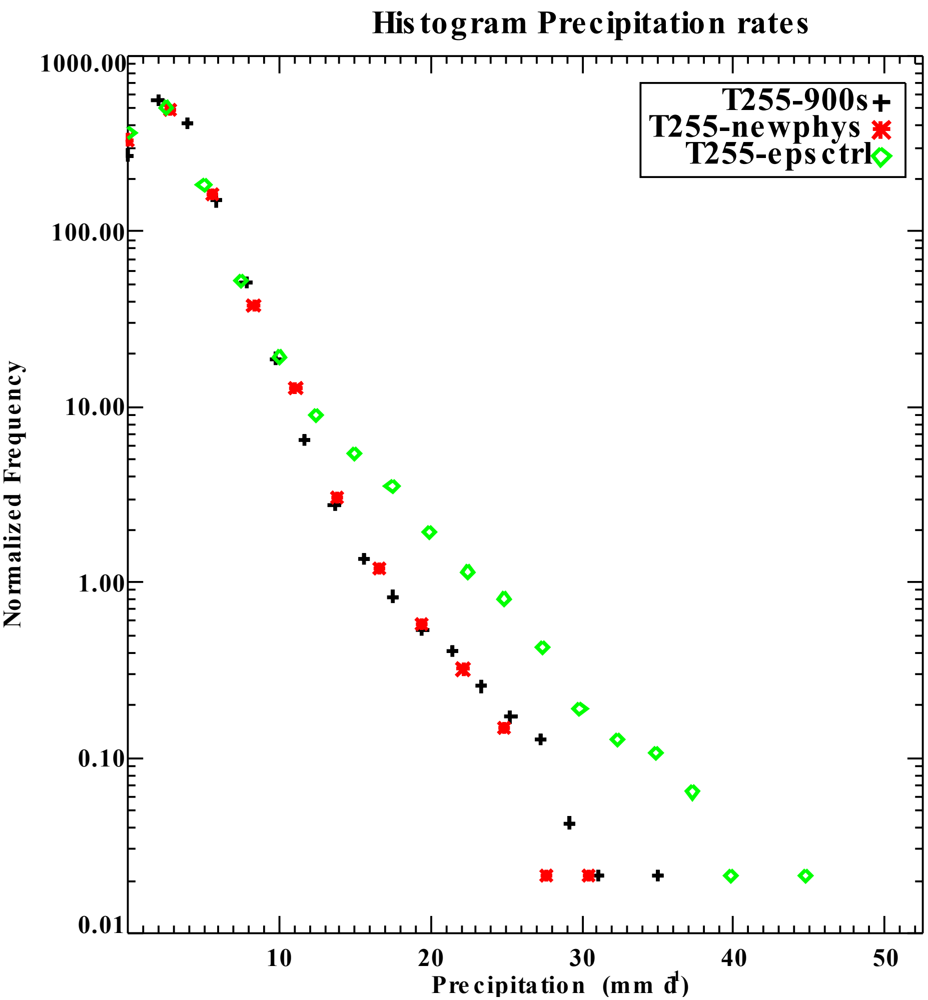
Modification in CY28R3 upgrade (the cloud scheme is also called before the convection to provide a guess of the cloud tendency:

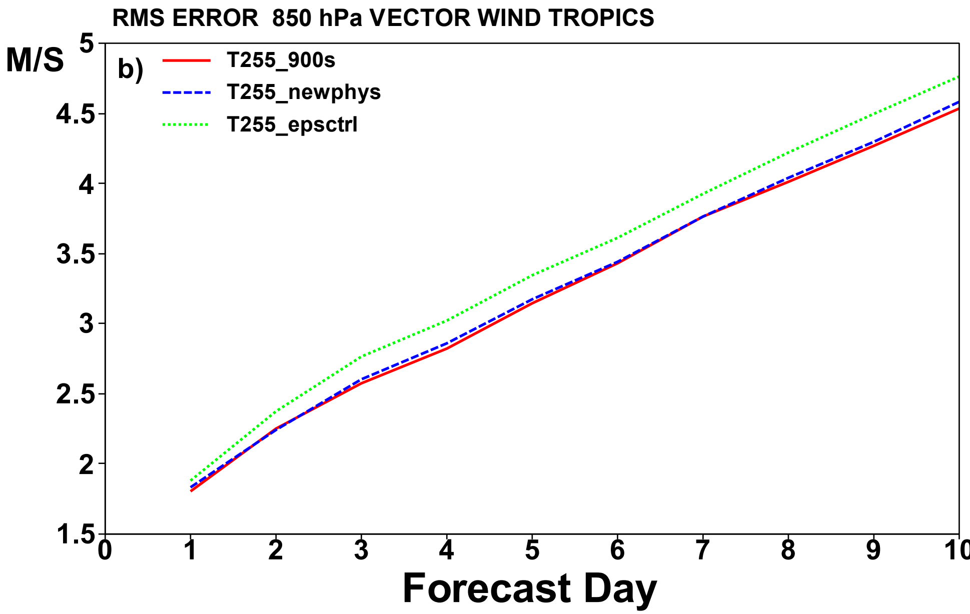
$$\begin{aligned}
P^{n+1} &= P_{rad}^{n+1}\left(\Psi^{n}\right) \\
&+ P_{vdf+sgoro}^{n+1}\left(\Psi^{n} + \Delta t(D + P_{rad}^{n+1})\right) \\
&+ P_{cnv}^{n+1}\left(\Psi^{n} + \Delta t(D + \tfrac{1}{2}P_{rad}^{n} + \tfrac{1}{2}P_{rad}^{n+1} + P_{vdf+sgoro}^{n+1} + \tfrac{1}{2}P_{cldguess}^{n+1})\right) \\
&+ P_{cld}^{n+1}\left(\Psi^{n} + \Delta t(D + \tfrac{1}{2}P_{rad}^{n} + \tfrac{1}{2}P_{rad}^{n+1} + P_{vdf+sgoro}^{n+1} + \tfrac{1}{2}P_{cnv}^{n+1})\right)
\end{aligned}$$

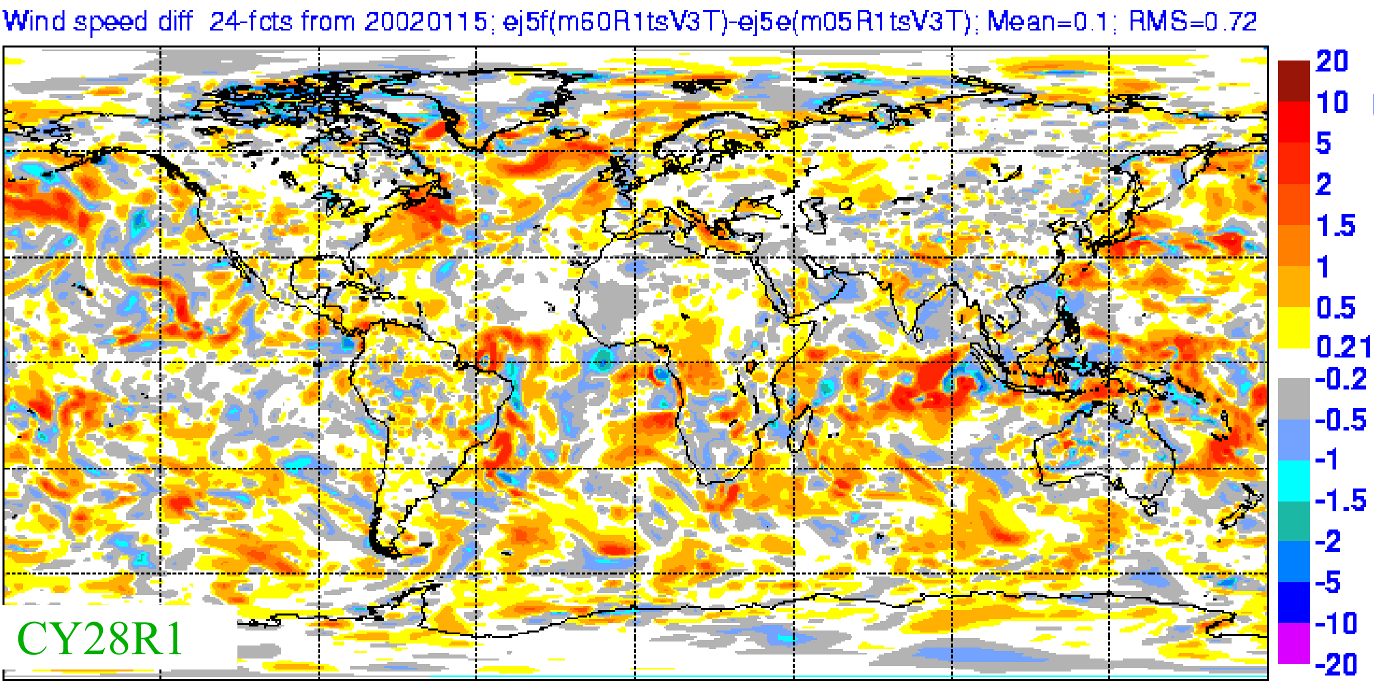
Comments:

♦ The extra call to the cloud scheme before the convection, provides more instability and therefore makes the convection scheme more active

Improvement from CY28R3 time stepping compared to CY28R1



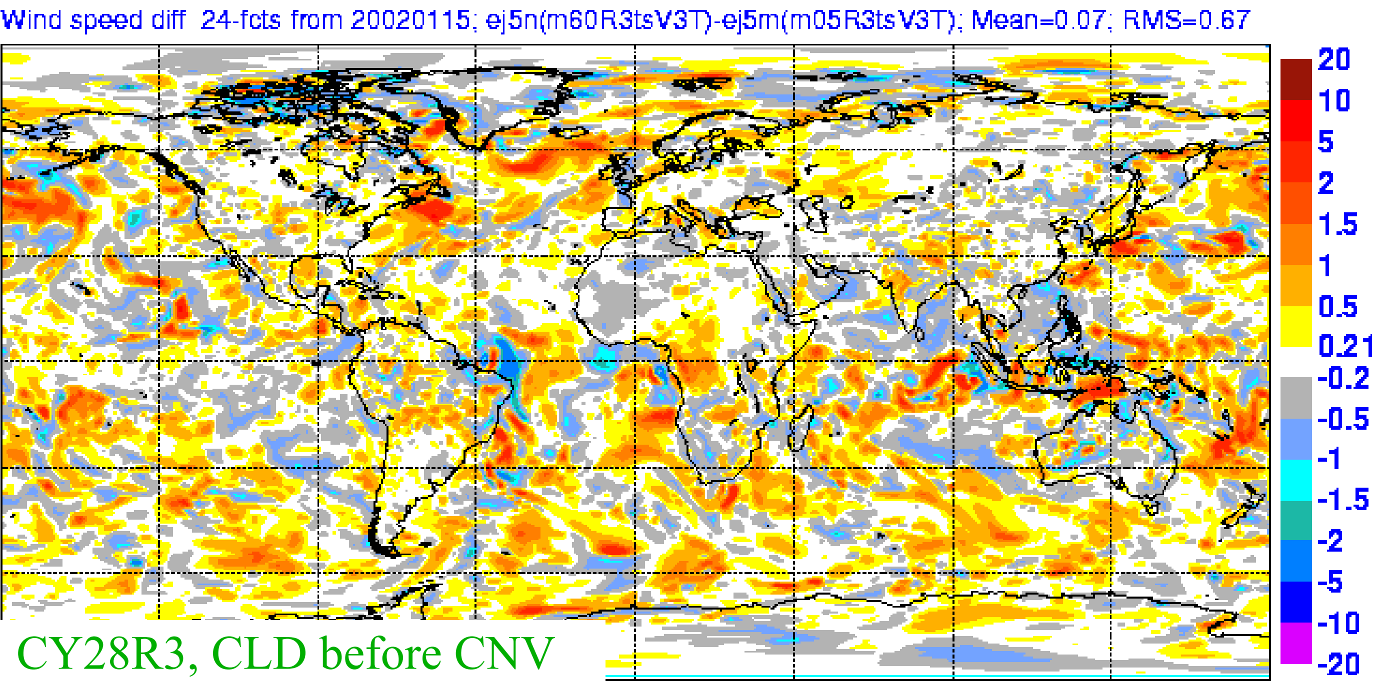




Effect of calling clouds before convection.

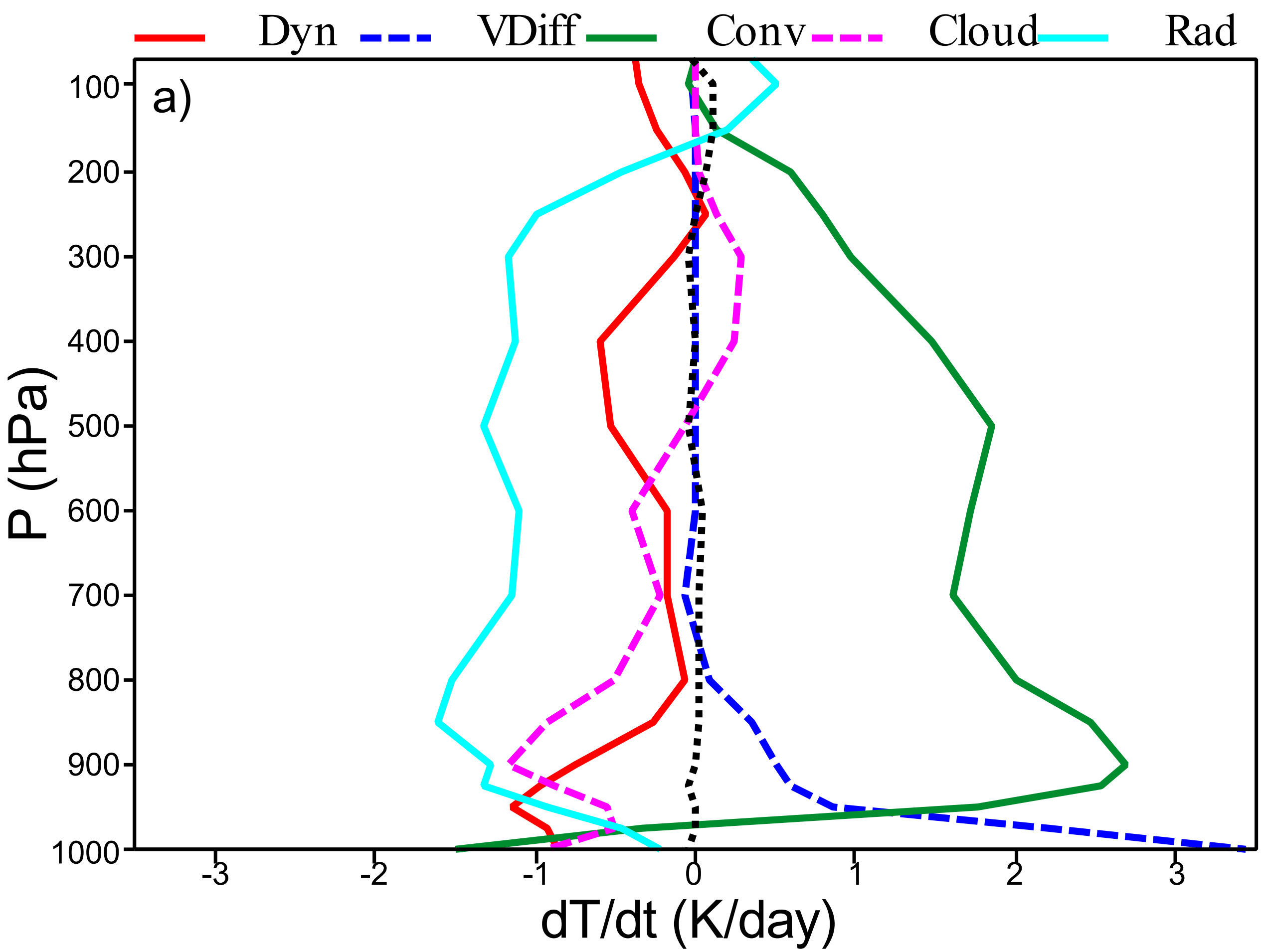
Errors in 10m wind speed (with respect to 5 min time step).

Time step: 60 min
Date: 20020114
Resolution: T159
Forecast: 24 hours



Calling clouds as a "first guess" before convection reduces wind errors in the tropics

Process tendencies averaged between 20S and 20N over a 5-day forecasts



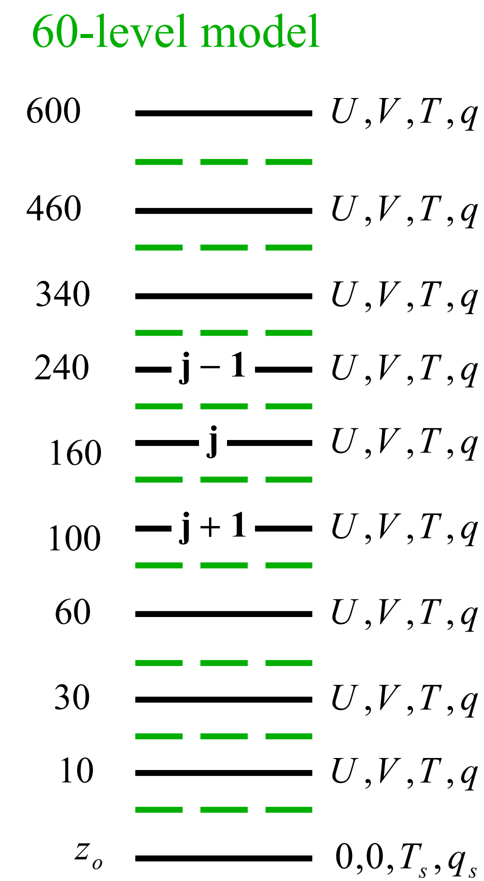
Summary of time stepping procedures for long time steps

- Balance is a important consideration
- Ideal is to do explicit (slow) processes first and to have one implicit solver to take care of the remaining (fast) processes in a time (sequential) split way, i.e. the implicit solver takes the explicit term as part of the forcing
- Convection and clouds have the character of fast (implicit) processes.
- 2nd order time integration is still in its infancy
- Predictor corrector is an option but expensive (Cullen et al. 2002)

Processes in the IFS: Radiation

$$\frac{\partial T}{\partial t} = \frac{g}{C_p}\frac{dF}{dp}$$

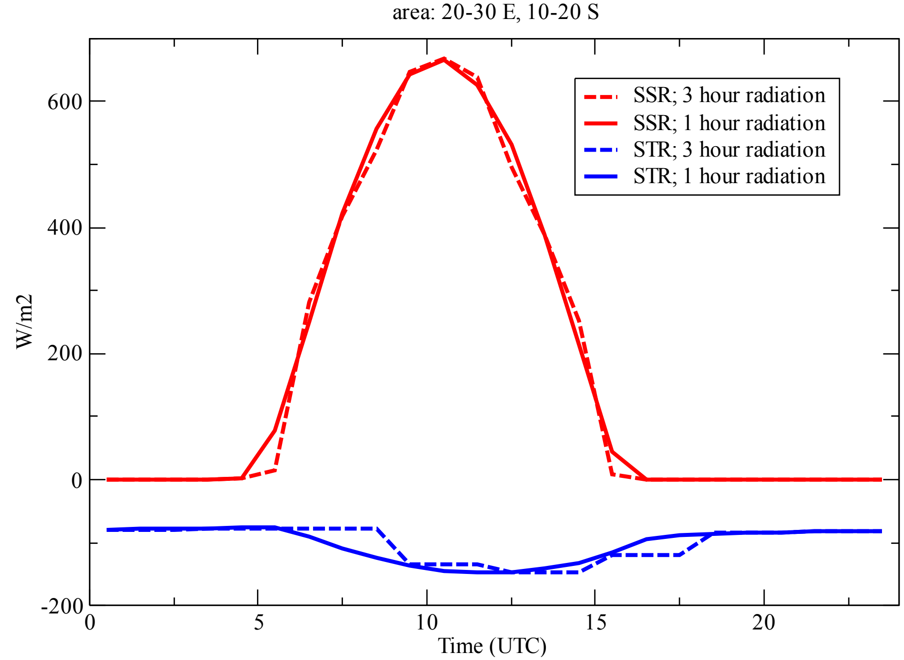
$$\left(\Delta T_j\right)_{rad} = \Delta t \frac{g}{C_p}\frac{F^n_{j+1/2} - F^n_{j-1/2}}{P_{j+1/2} - P_{j-1/2}}$$



- Explicit numerics
- No update from dynamics (appropriate for explicit numerics)
- Low resolution grid for economy (T255 in T511): This can lead to inconsistency between surface radiation and full resolution albedo field which can upset the surface scheme

Processes in the IFS: Radiation

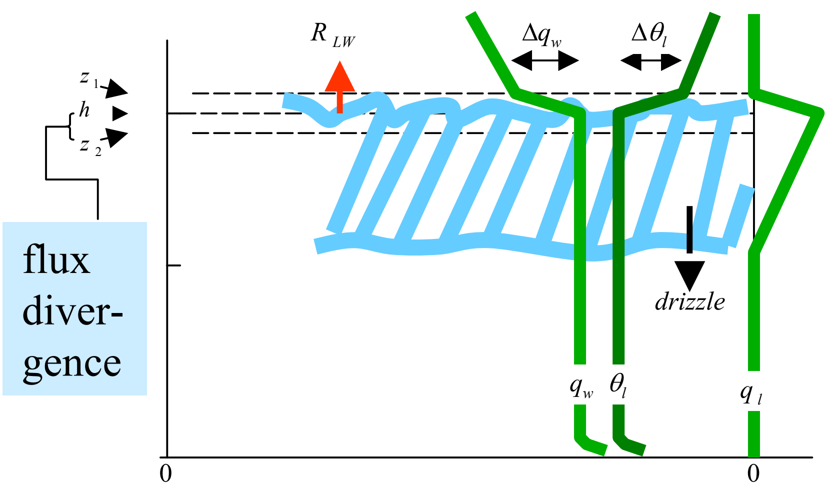
- ♦Full radiation every 3 hours in 28R1 and hourly in 28R3



- ♦Radiative tendency due to cloud top radiative cooling scales with layer depth:

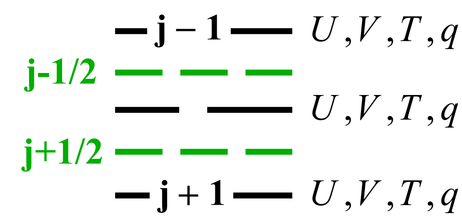
$$\left(\frac{\partial \mathbf{T}}{\partial \mathbf{t}}\right)_{\mathbf{rad}} \approx \frac{\mathbf{g}}{\mathbf{C_p}} \frac{\mathbf{80}}{\mathbf{P_{j+1/2} - P_{j-1/2}}}$$

e.g. 35K/day for a 20hPa layer



Processes in the IFS: Vertical Diffusion

$$\frac{\partial \Psi}{\partial t} = g\frac{dF_{\Psi}}{dp} \qquad F_{\Psi} = K_{\Psi}\rho\frac{d\Psi}{dz}$$



$$\left(\Delta\Psi_j\right)_{vdf} + \left(\Delta\Psi_j\right)_{dyn} + \left(\Delta\Psi_j\right)_{rad} = \Psi_j^{*} - \Psi_j^{n} =$$

$$\frac{\Delta t g}{\Delta p_j}\left(K^{n}_{j+1/2}\frac{\hat{\Psi}_{j+1} - \hat{\Psi}_{j}}{z_{j+1} - z_{j}} - K^{n}_{j-1/2}\frac{\hat{\Psi}_{j} - \hat{\Psi}_{j-1}}{z_{j} - z_{j-1}}\right) + \left(\Delta\Psi_j\right)_{dyn} + \left(\Delta\Psi_j\right)_{rad}$$

$$\hat{\psi} = \alpha\psi^{*} + (1-\alpha)\psi^{n} \qquad \alpha = 1.5$$

- Over-implicit numerics
- Balance with dynamics and radiation
- Specification of similarity profiles in the surface layer (exact finite differencing for a constant flux layer!)
- In the ECMWF model 3 VDF steps are made for every model time step
- Implicit coupling with surface tiles

Processes in the IFS: Vertical Diffusion

Issues:

- Non-linear instability

$$\frac{\partial T(t)}{\partial t} = -KT^P\ T(t) + D(t)$$

$T \equiv$ temperature difference between ground and air

$KT^P \equiv$ exchange coefficient, $K = 10, P = 3$

$D(t) \equiv 1 - \sin(2\pi n \Delta t / 24)$, diurnal cycle

Comments:

- Predictor-corrector does not always give the correct result
- Different options exist, but a large implicitness factor is the more popular and robust option (Kalnay and Kanamitsu, 1988)
- More complicated methods are more expensive (Hammerstrand, 1997)
- Implicitness factor can be made flow dependent (Girard and Delage, 1990)
- Single point diagnostics is not sufficient

$$\frac{T^{n+1} - T^n}{\Delta t} = -K(T^n)^P\left[\alpha T^{n+1} + (1-\alpha)T^n\right] + D^n$$

$\alpha \geq P + 1$, unconditionally stable, over-implicit

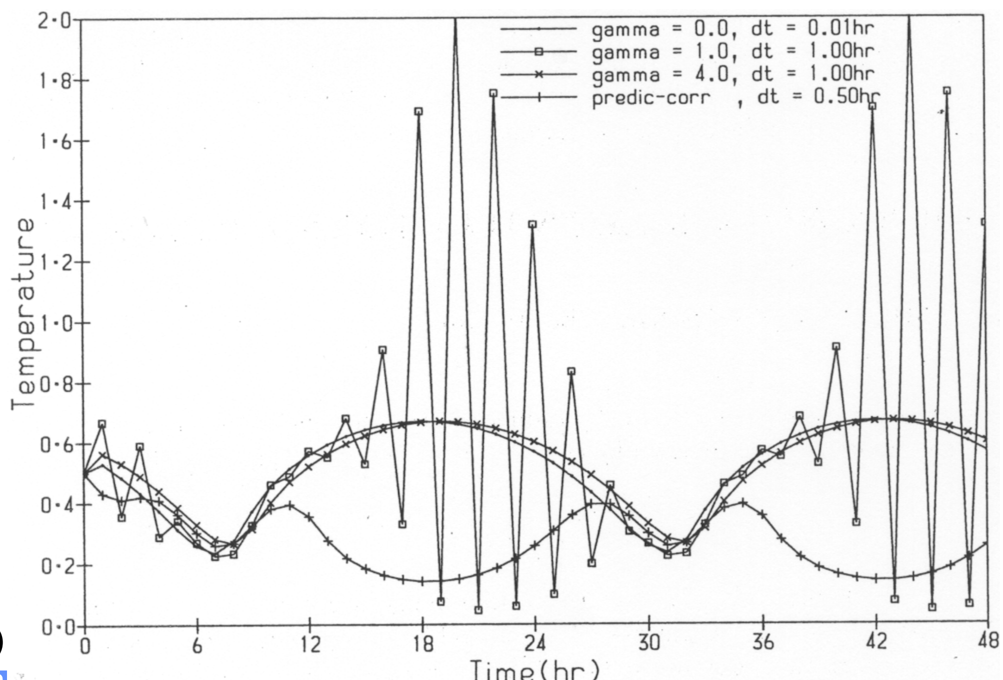
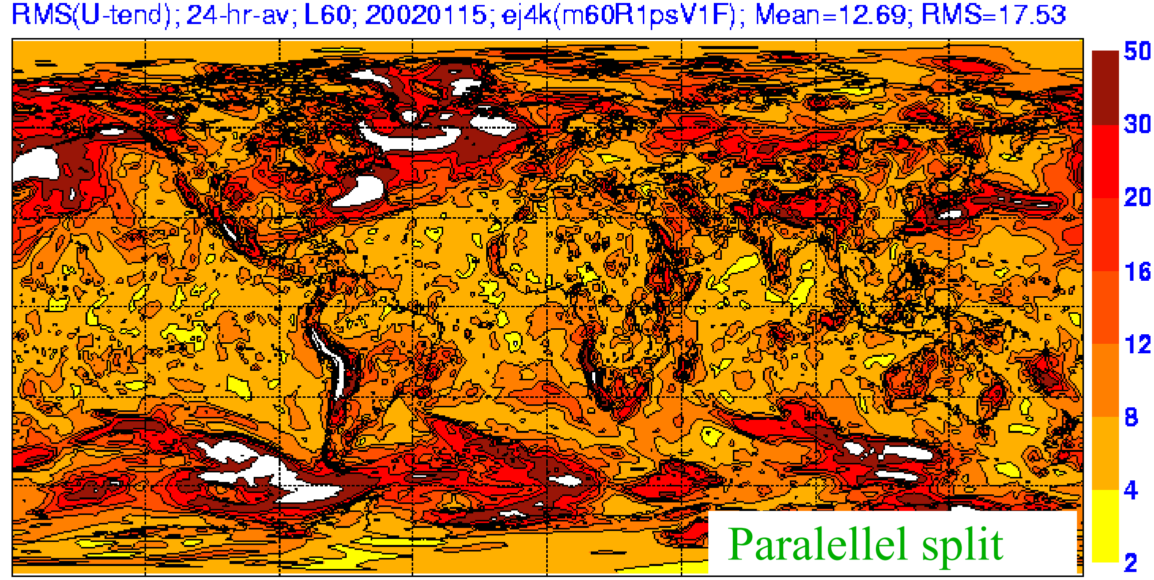


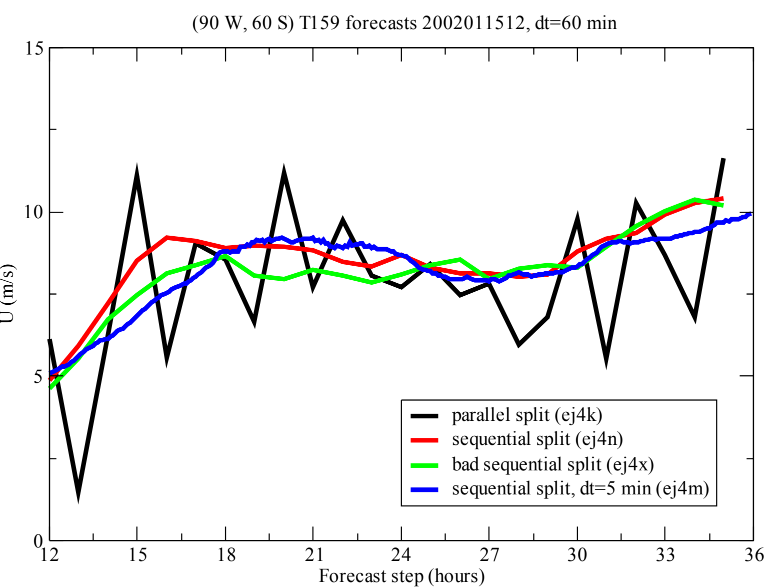
Figure: McDonald (1998)

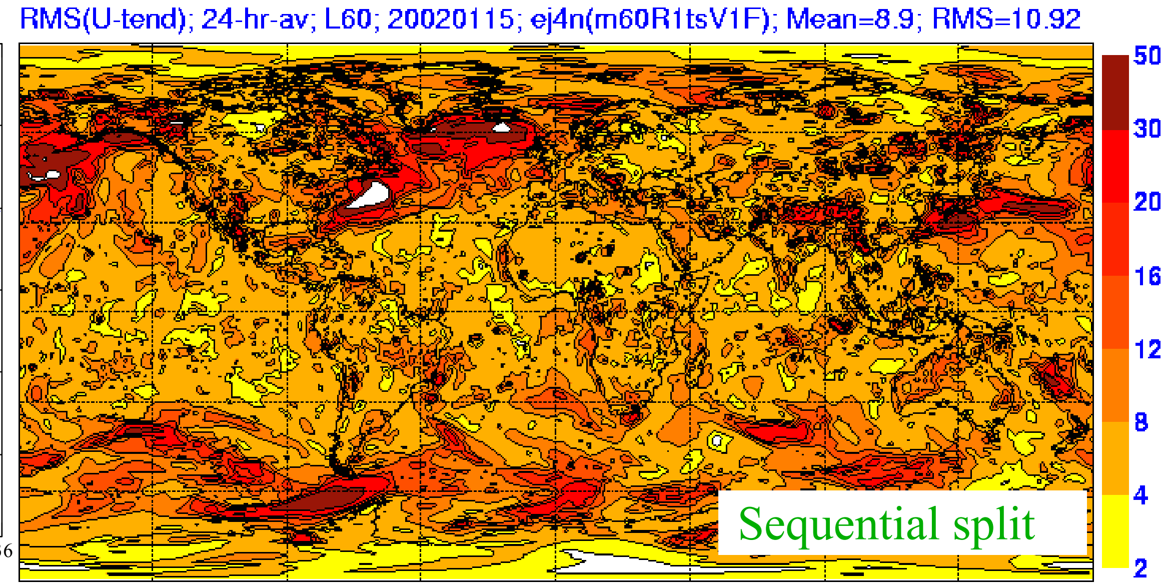
Processes in the IFS: Vertical Diffusion

RMS(dU/dt) (m/s/day) at 10 m level

Time stepping of vertical diffusion affects noise







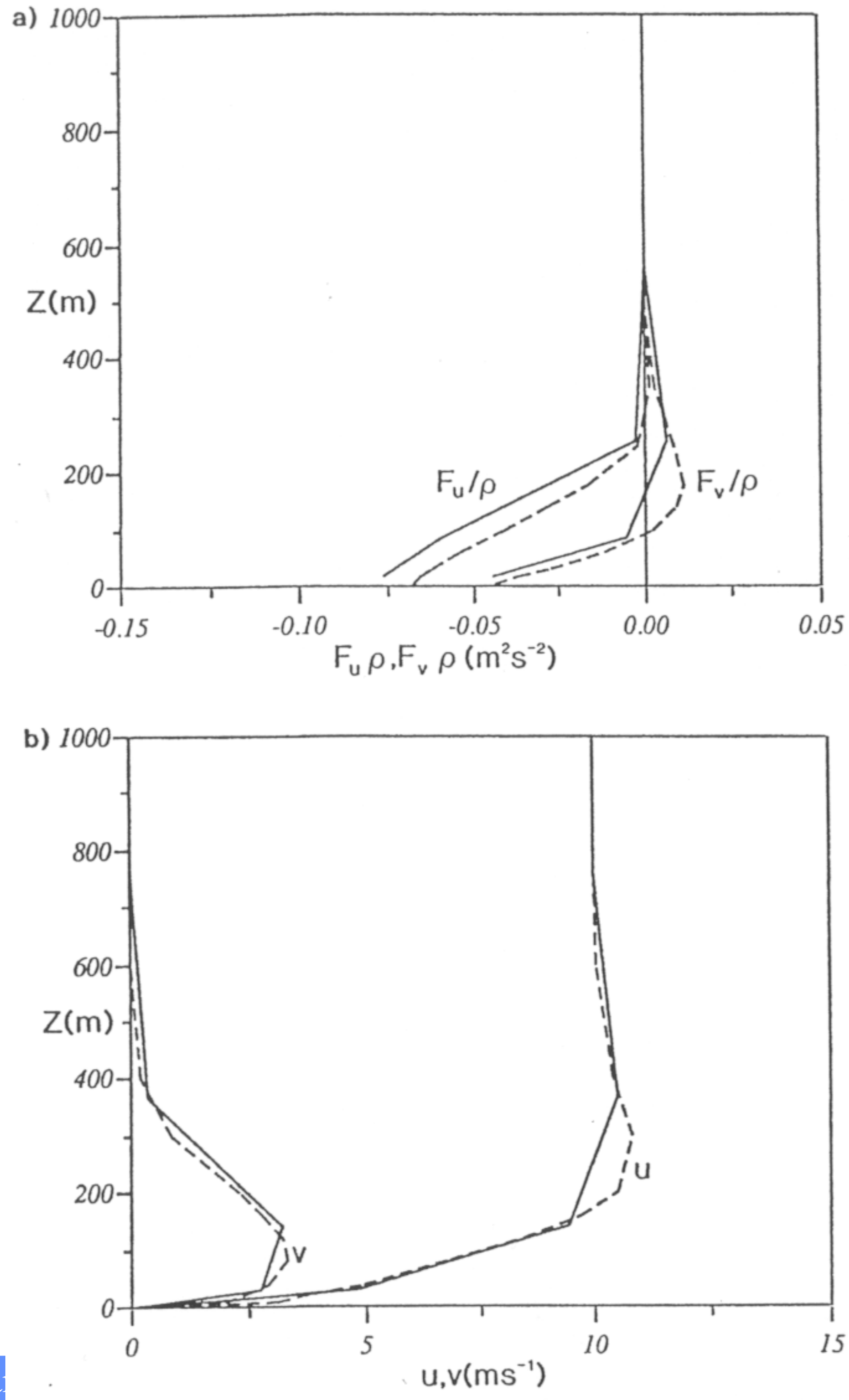
Processes in the IFS: Vertical Diffusion

Issue:

♦Vertical resolution

Comments:

♦In spite of the low number of levels in the stable boundary layer the solution is surprisingly insensitive to resolution



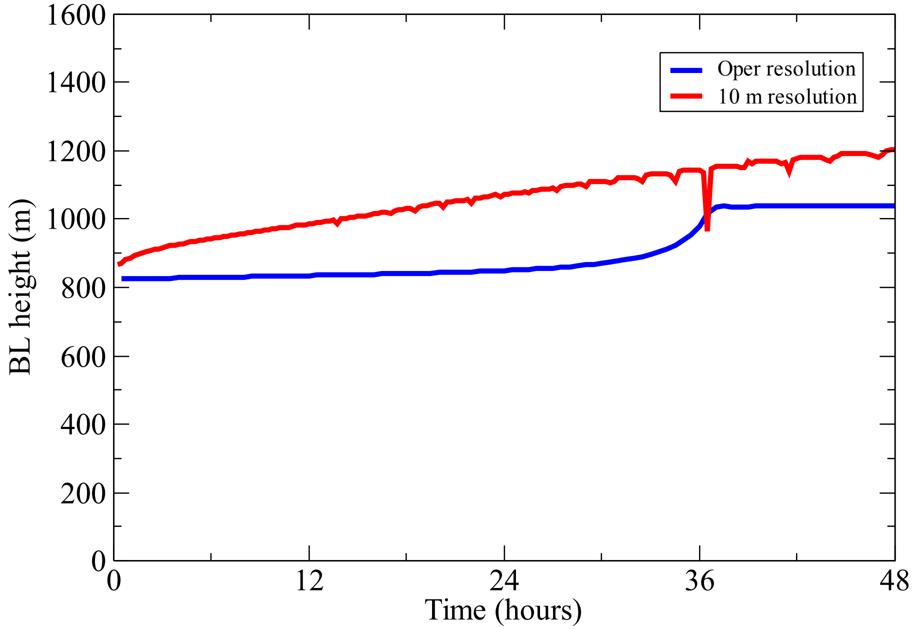
Processes in the IFS: Vertical Diffusion

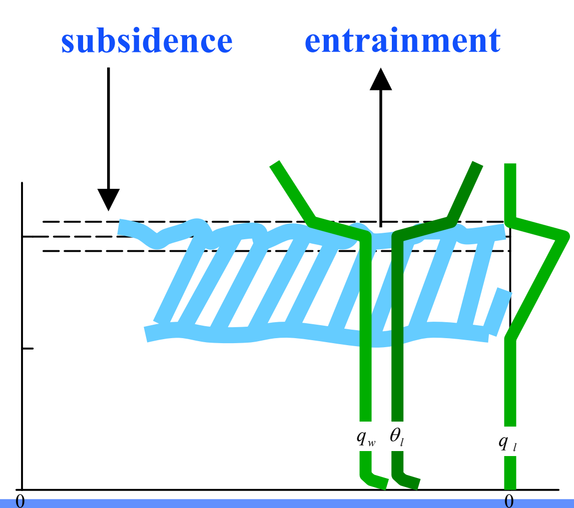
Issues:

- ♦Vertical resolution
- ♦Handling of inversions

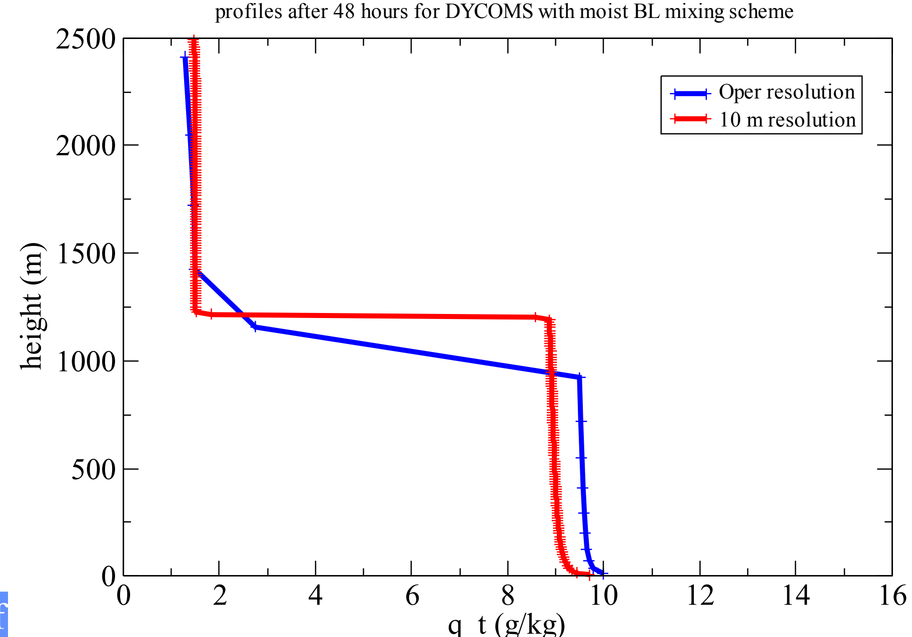
Comments:

♦Mixing through inversions is often in balance with subsidence

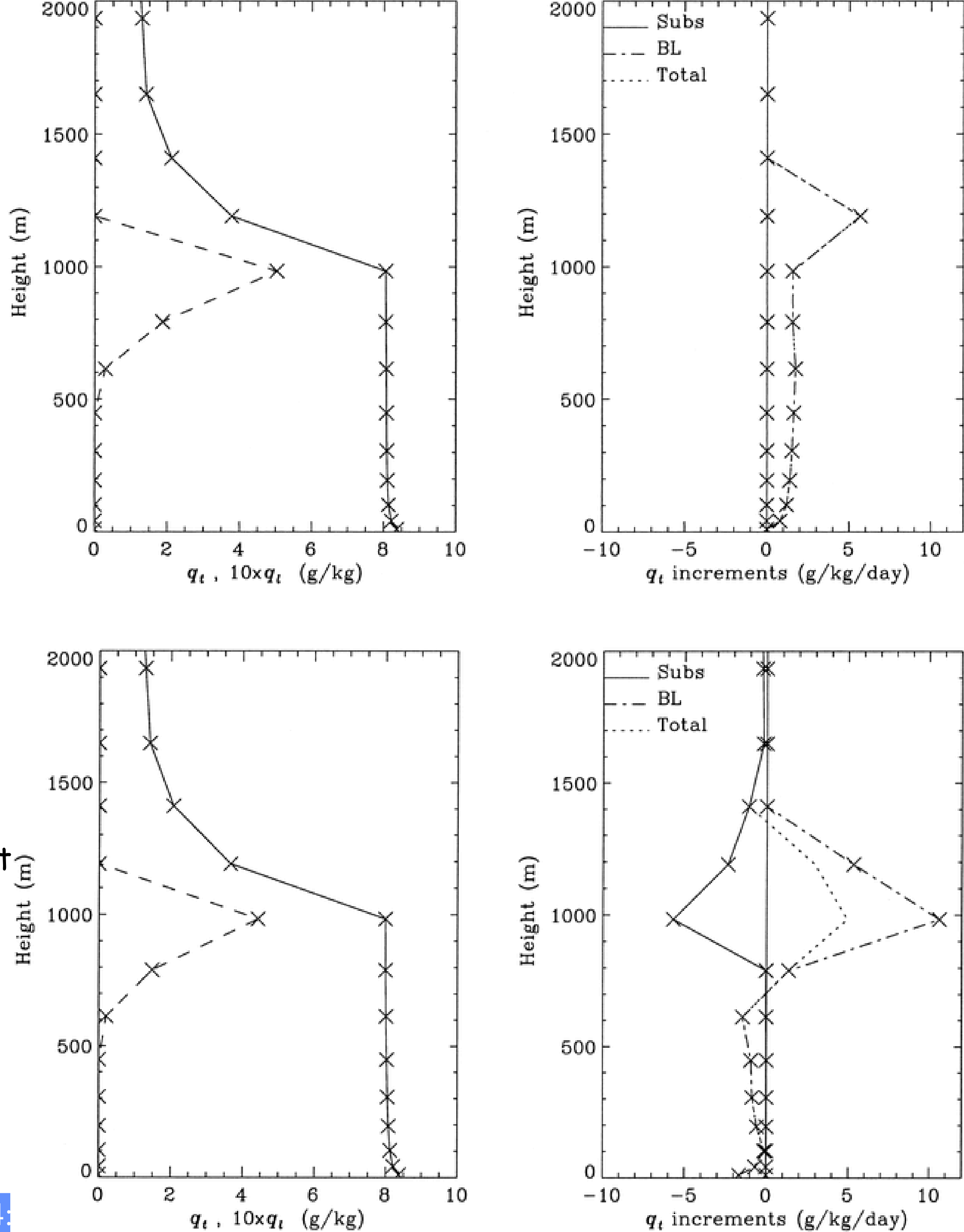




profiles after 48 hours for DYCOMS with moist BL mixing scheme



Inversion numerics



Figures by A. Lock: The numerical representation of entrainment in parametrizations of boundary layer turbulent mixing, MWR, 2001, 129, 1148-1163.

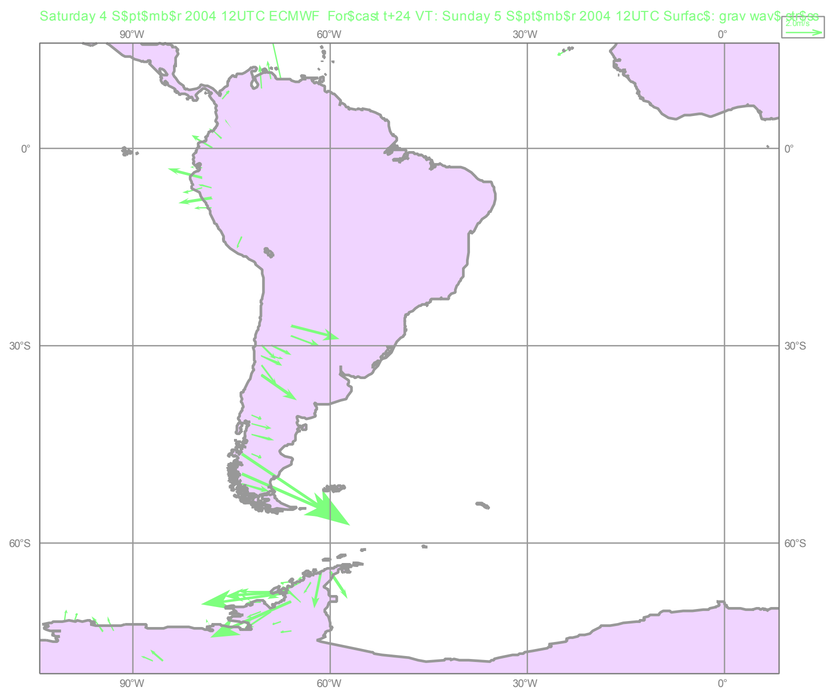
See also:

Grenier and Bretherton (2001): MWR, 129, 357-377.

Lenderink and Holtslag (2000): MWR, 128,244-258.

Processes in the IFS: Subgrid orography

- Low level blocking + gravity wave drag
- Low level tendencies can be very large on isolated points
- Good balance would benefit from simultaneous solution of vertical diffusion and subgrid orography with the same tri-diagonal solver



Processes in the IFS: Convection

$$\frac{\partial \Psi}{\partial t} = g \frac{d}{dp}\left[M_u\left(\Psi_u - \Psi\right)\right] + S$$

$$\left(\Delta \Psi_j\right)_{cnv} = \frac{\Delta t g}{\Delta p_j}\Big[(M_u \Psi_u)_{j+1/2} - (M_u \Psi_u)_{j-1/2} - \left(M_u\right)_{j+1/2}\Psi_j + \left(M_u\right)_{j-1/2}\Psi_{j-1}\Big] + S_j$$

- Upwind differencing in vertical
- Mass flux limiter to prevent instability
- Shallow convection is closed by assuming balance of moist static energy between dynamics, vertical diffusion and convection in subcloud layer i.e. the convection scheme needs surface fluxes from vertical diffusion as input
- For deep convection cloud base mass flux is based on CAPE reduction over a specified relaxation time (1 hour for low resolution to 15 minutes at high resolution, which is close to the time step)
- Subcloud layer fluxes are specified as a linear profile with zero at the surface

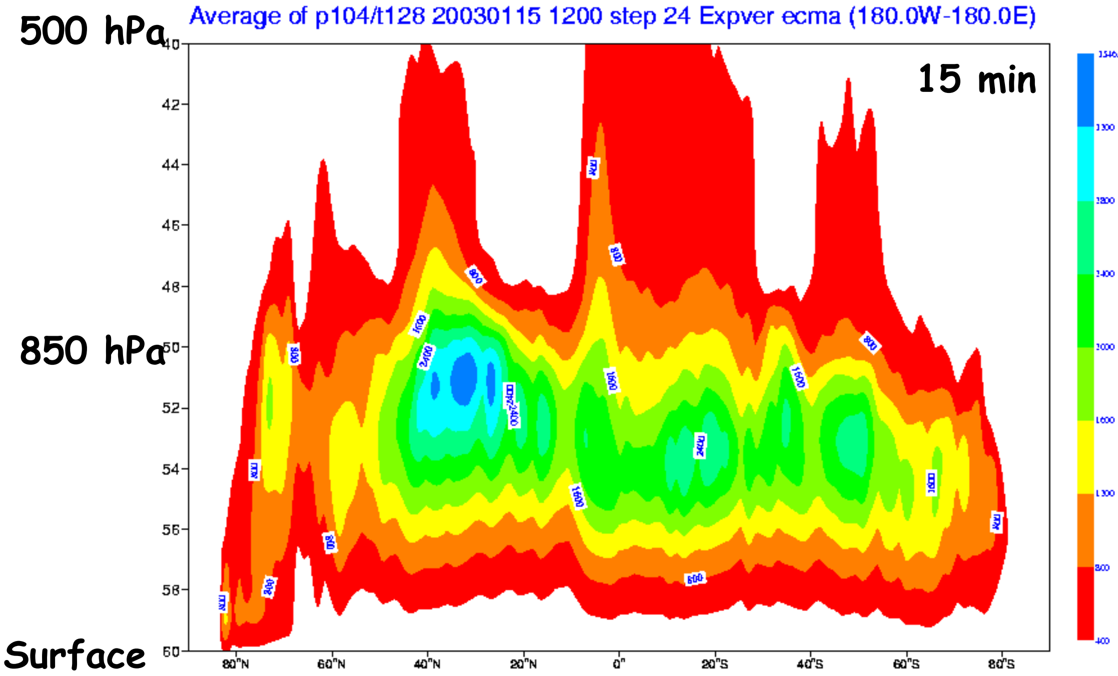
Processes in the IFS: Convection

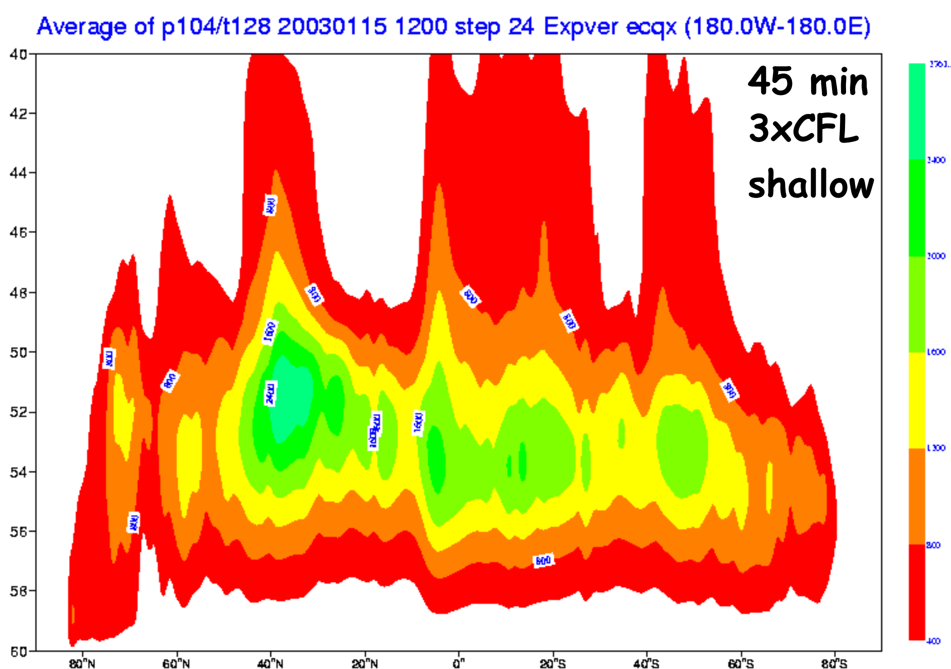
Issues:

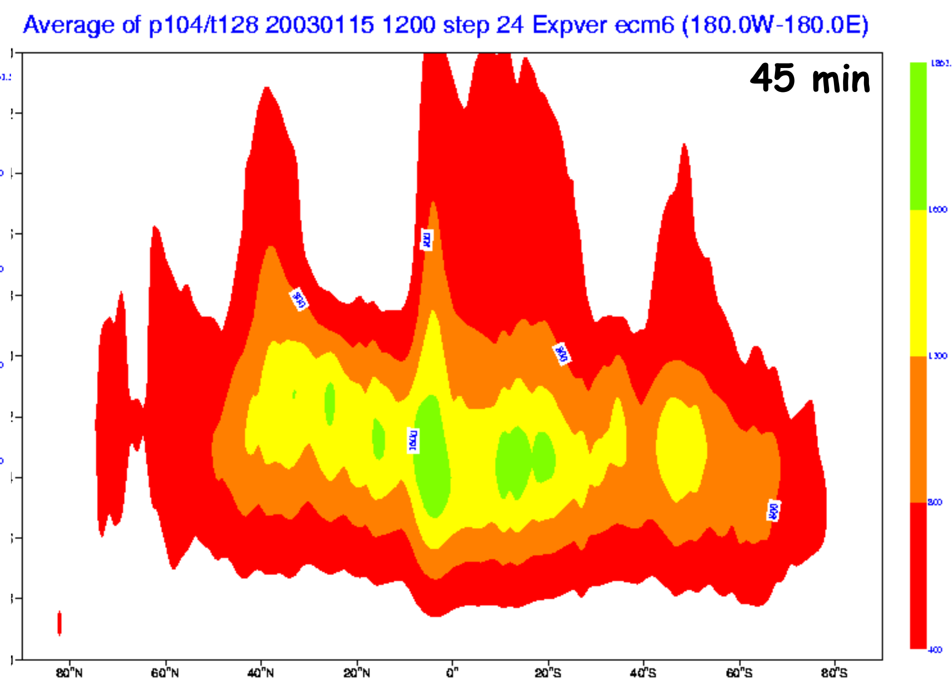
- Mass flux limiter introduces time step dependency with high vertical resolution
- Implicit formulation is desirable, but specification of linear flux profile below cloud base turns out to be essential to balance fluxes from vertical diffusion scheme
- Input profile is crucial for convection triggering and for CAPE diagnosis
- Should convection be seen as a slow process that can be handled with explicit numerics or as a fast process that needs implicit numerics?
- Which are the critical processes that balance convection? (dynamics, radiation, vertical diffusion, clouds)

Mass flux limiter in convection

T255 24-hour zonally averaged updraught mass flux (cnt. int.: 400 kg/m2/day).







Processes in the IFS: Clouds

$$\frac{\partial \ell}{\partial t} = S_{cnv} + S_{vdf} + S_{strat} - E_{cld} - G_{prec} - \frac{1}{\rho}\frac{\partial}{\partial z}\rho(\overline{w'l'})_{entr}$$

$$\frac{\partial a}{\partial t} = \delta a_{cnv} + \delta a_{vdf} + \delta a_{strat} - \delta a_{evap}$$

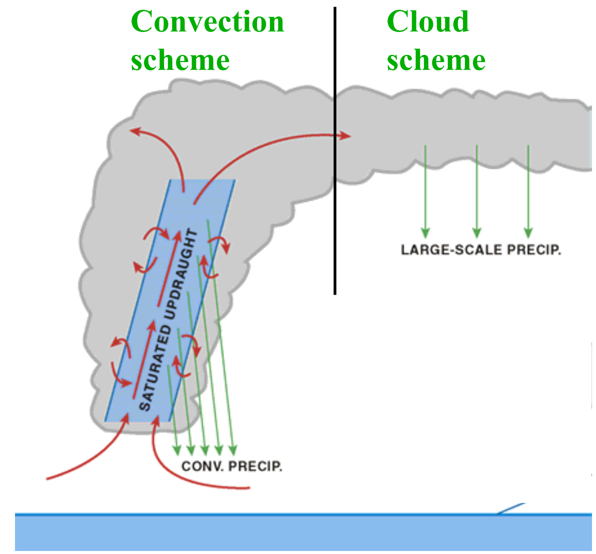
Equations are written (level by level) as:

$$\frac{\partial \ell}{\partial t} = C - D\ell$$

$$\frac{\partial a}{\partial t} = A - Ba$$

with A,B,C,D from processes, e.g. vertical motion, convective detrainment, precipitation, turbulence, cloud erosion. An exponential solution over single time step is used to integrate in time.

Processes in the IFS: Clouds



Example of convective detrainment and ice fallout

$$\frac{\partial \ell}{\partial t} = \mathbf{C} - \mathbf{D}\,\ell$$

$$\frac{\partial \ell}{\partial t} = \frac{1}{\rho}\mathbf{D}_{up}(\ell_u - \ell) - \rho g w_{ice}\frac{\partial \ell}{\partial p}, \text{ with } w_{ice} = c_1 \ell^{c_2}$$

$$\text{for level } j: \quad \mathbf{C} = \frac{1}{\rho_j}\mathbf{D}_{up,j}(\ell_{u,j} - \ell_j) - \rho_{j-1} g w_{ice,j-1}\frac{\ell_{j-1}}{\Delta p_{j-1}}$$

$$: \quad \mathbf{D} = -\rho_j g w_{ice,j}\frac{1}{\Delta p_j}$$

Comments:

♦Detrainment source term has to be part of the implicit time integration of ice fallout for proper balance (sequential splitting)

♦Ice fallout needs to be computed at full time level

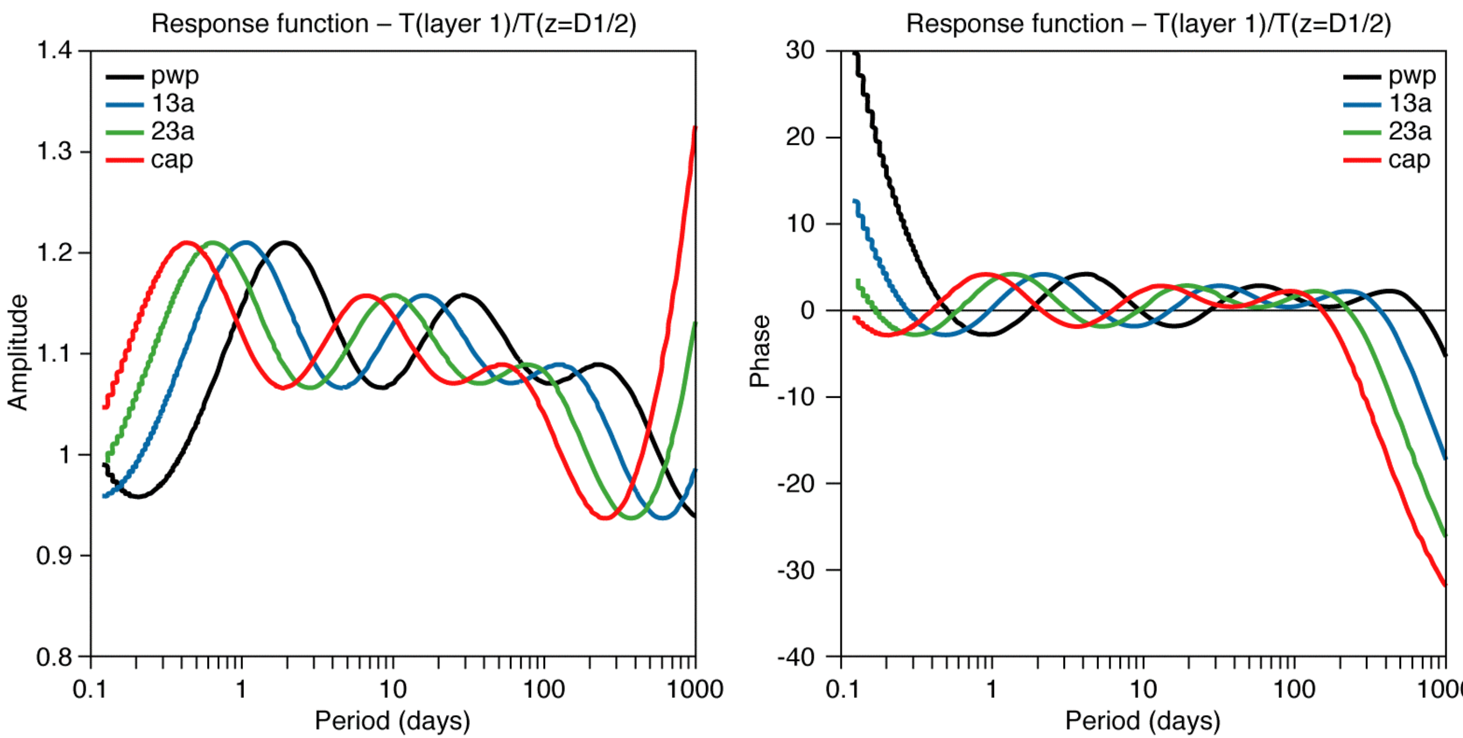
Processes in the IFS: Land surface (TESSEL)

Non-linear diffusion equations for temperature and soil water:

$$C_s \frac{\partial T}{\partial t} = K_T \frac{\partial^2 T}{\partial z^2}$$

Soil numerics:

- ♦Implicit solution as vertical diffusion with implicitness factor equal to 1.
- ♦Crude vertical discretization to cover time scale from hours to one year.
- ♦Layer depths: 0.07, 0.21, 0.72 and 1.89 m



Processes in the IFS: Coupling of TESSEL to the atmosphere (Best coupler)[1]

Coupling includes skin layer with instantaneously responding skin temperature for each tile.

$$\mathbf{H} = \rho C_H^n |\vec{U}| (S_l^{n+1} - S_{sk}^{n+1}), \quad S = C_p T + gz$$

$$\mathbf{E} = \rho C_Q^n |\vec{U}| \beta (q_l^{n+1} - \alpha q_{sat}(T_{sk}^{n+1}))$$

Eliminate T_{sk} by linearizing and using the surface energy balance equation (i.e. derive Penman /Monteith equation):

$$R_{sw} + R_{lw} + H + LE = \Lambda (T_{sk}^{n+1} - T_s)$$

The result is two linear relations between lowest model level variables and fluxes with tile dependent coefficients D

$$H = D_{H1} S_l^{n+1} + D_{H2} q_l^{n+1} + D_{H3}$$

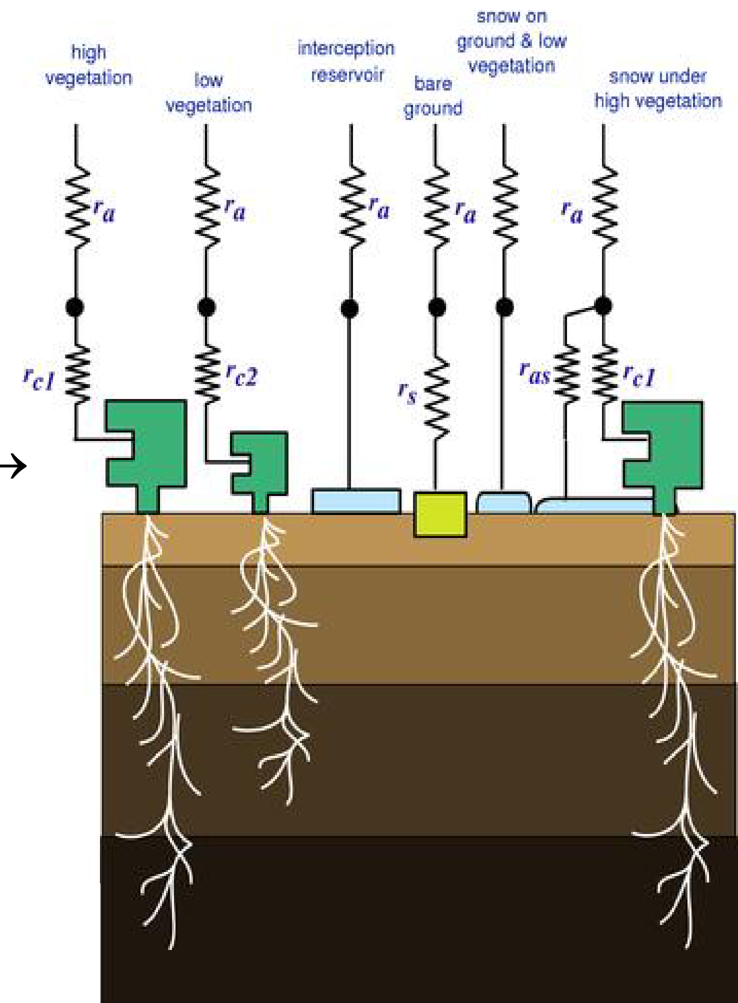
$$E = D_{E1} S_l^{n+1} + D_{E2} q_l^{n+1} + D_{E3}$$

[1])Best et al. (2004): A proposed structure for coupling tiled surfaces with the planetary boundary layer, JHM

Land surface tiles:

- High vegetation
- Low vegetation
- Wet surface
- Bare ground
- Exposed snow
- Snow under vegetation

$T_{sk} \rightarrow$



Processes in the IFS: Coupling of TESSEL to the atmosphere (Best coupler)[1]

Averaging of fluxes over tiles, by averaging coefficients:

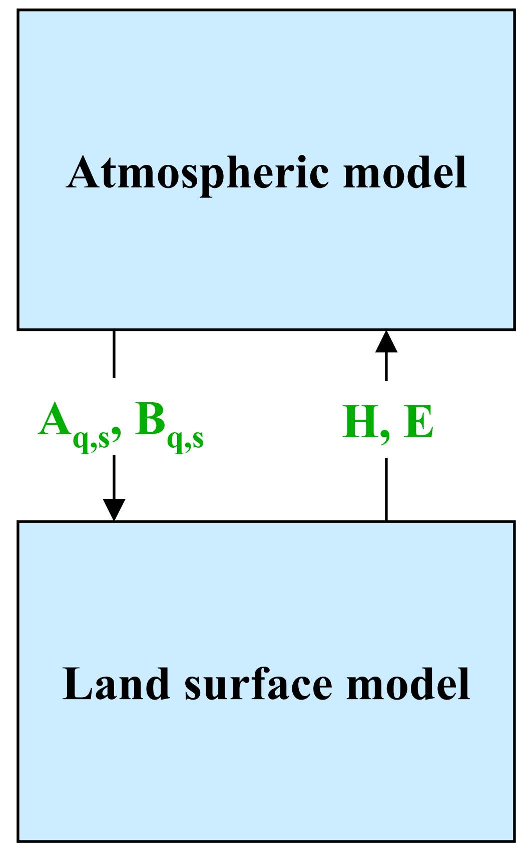
$$\overline{H} = S_l^{n+1} \sum_i \nu^i D_{H1}^i + q_l^{n+1} \sum_i \nu^i D_{H2}^i + \sum_i \nu^i D_{H3}^i$$

$$\overline{E} = S_l^{n+1} \sum_i \nu^i D_{E1}^i + q_l^{n+1} \sum_i \nu^i D_{E2}^i + \sum_i \nu^i D_{E3}^i$$

Combine with result of downward elimination of tri-diagonal matrix for vertical diffusion:

$$S_l^{n+1} = A_S \overline{H} + B_S$$

$$q_l^{n+1} = A_q \overline{E} + B_q$$

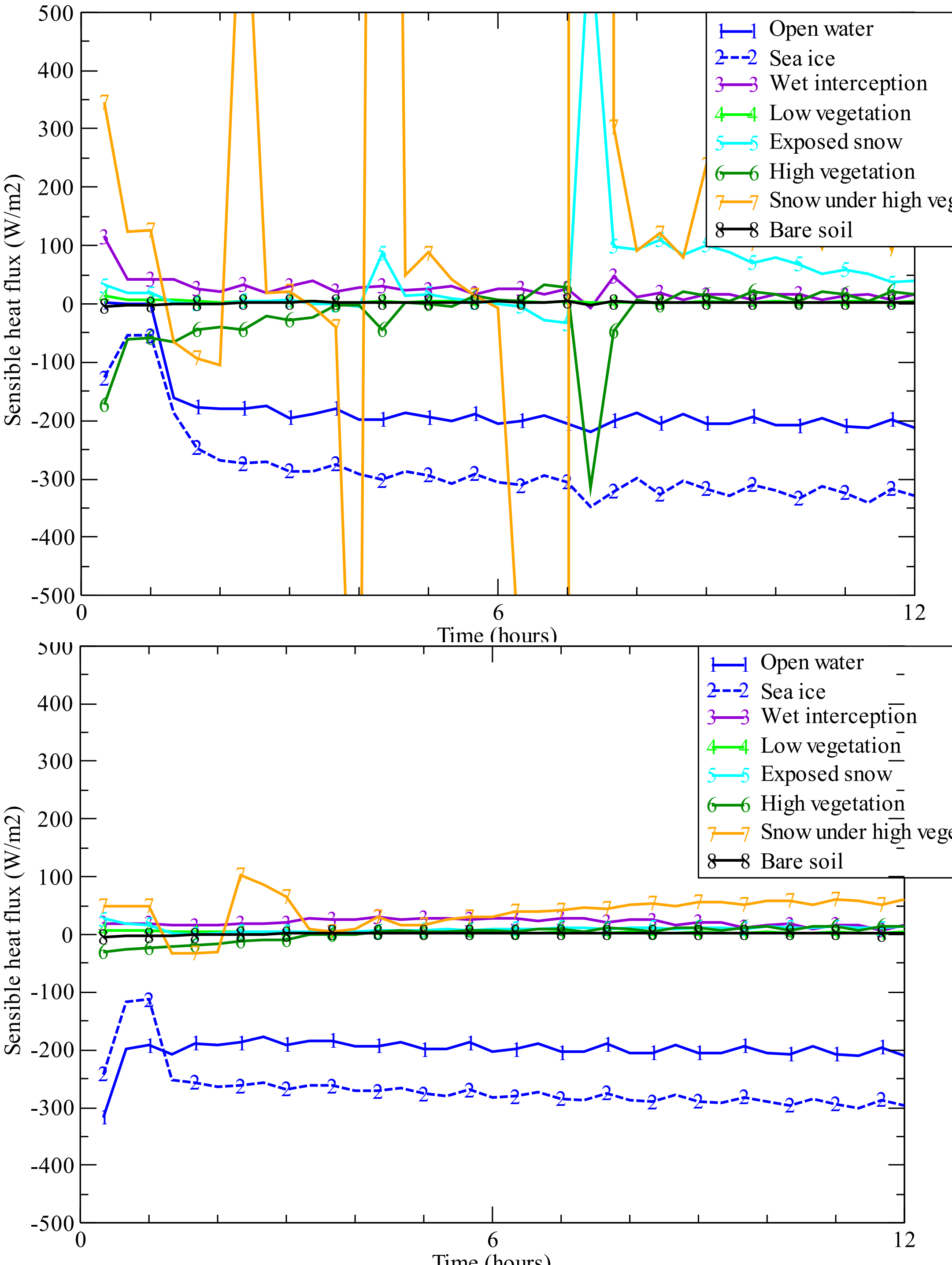


Comments:

- The atmospheric surface layer is part of the LSM
- All the tile dependent parameters are part of the LSM

[1)]Best et al. (2004): A proposed structure for coupling tiled surfaces with the planetary boundary layer, JHM

Coupling of TESSEL to the atmosphere (Best coupler)[1]



Fractions

1: 0.0
2: 0.0
3: 0.53
4: 0.04
5: 0.00
6: 0.37
7: 0.00
8: 0.06

Conclusions

- The physics of a process and its coupling to other processes is important from the numerical point of view
- Splitting is major issue
- Sequential split with slow process first and a single fast implicit process is preferred option
- Unification of fast processes is desirable (e.g. BL, subgrid orography and shallow convection)
- Balance is important
- 2nd order physics in ECMWF model should be reformulated considering convection and clouds as implicit processes
- Different processes have different problems e.g.:

    convection needs implicit numerics at high vertical resolution,

    microphysics is fast and therefore difficult,

    vertical diffusion is noisy.