

# Parametrizations in Data Assimilation

ECMWF Training Course  
14 March 2019

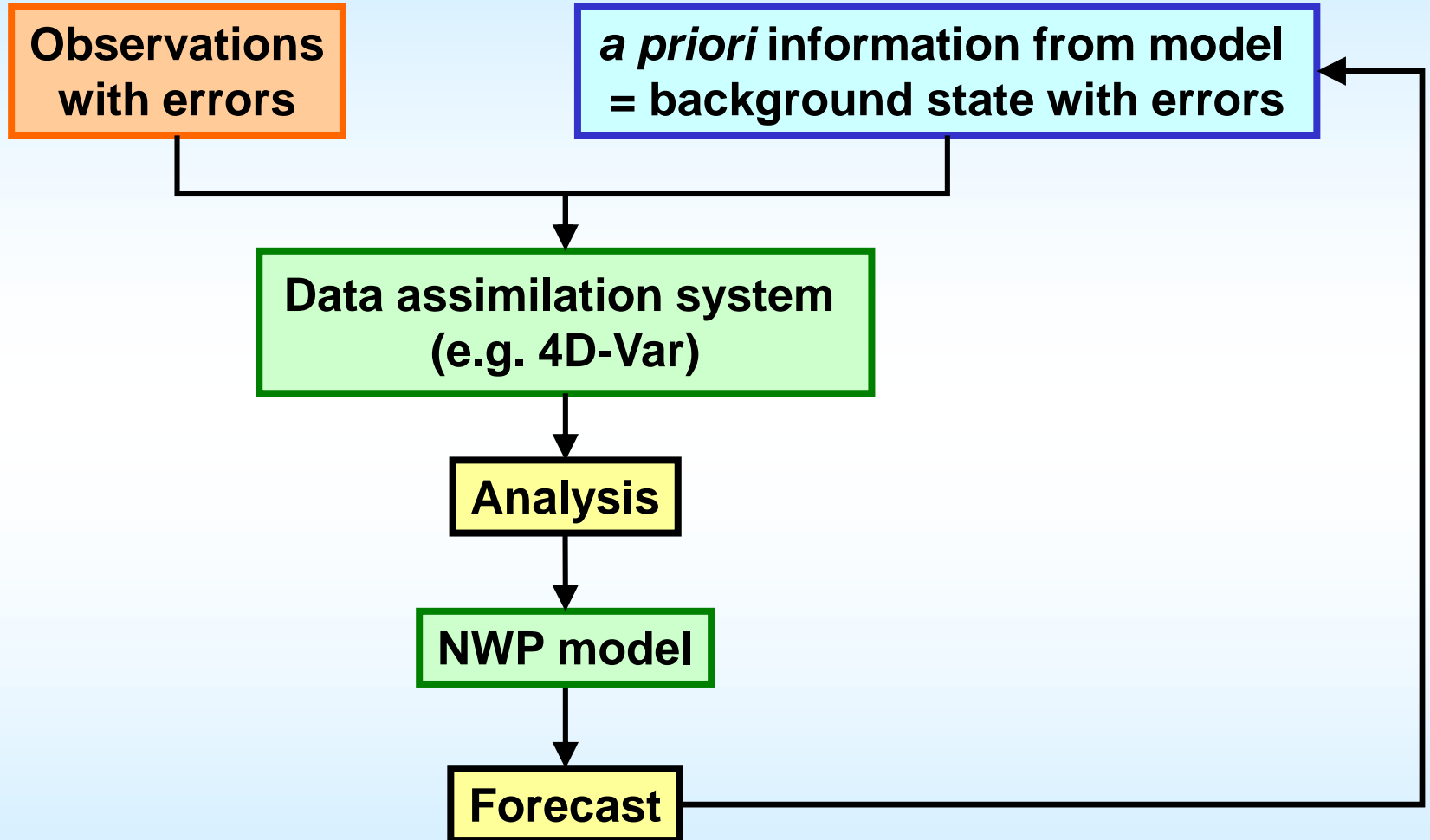


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# Parametrizations in Data Assimilation

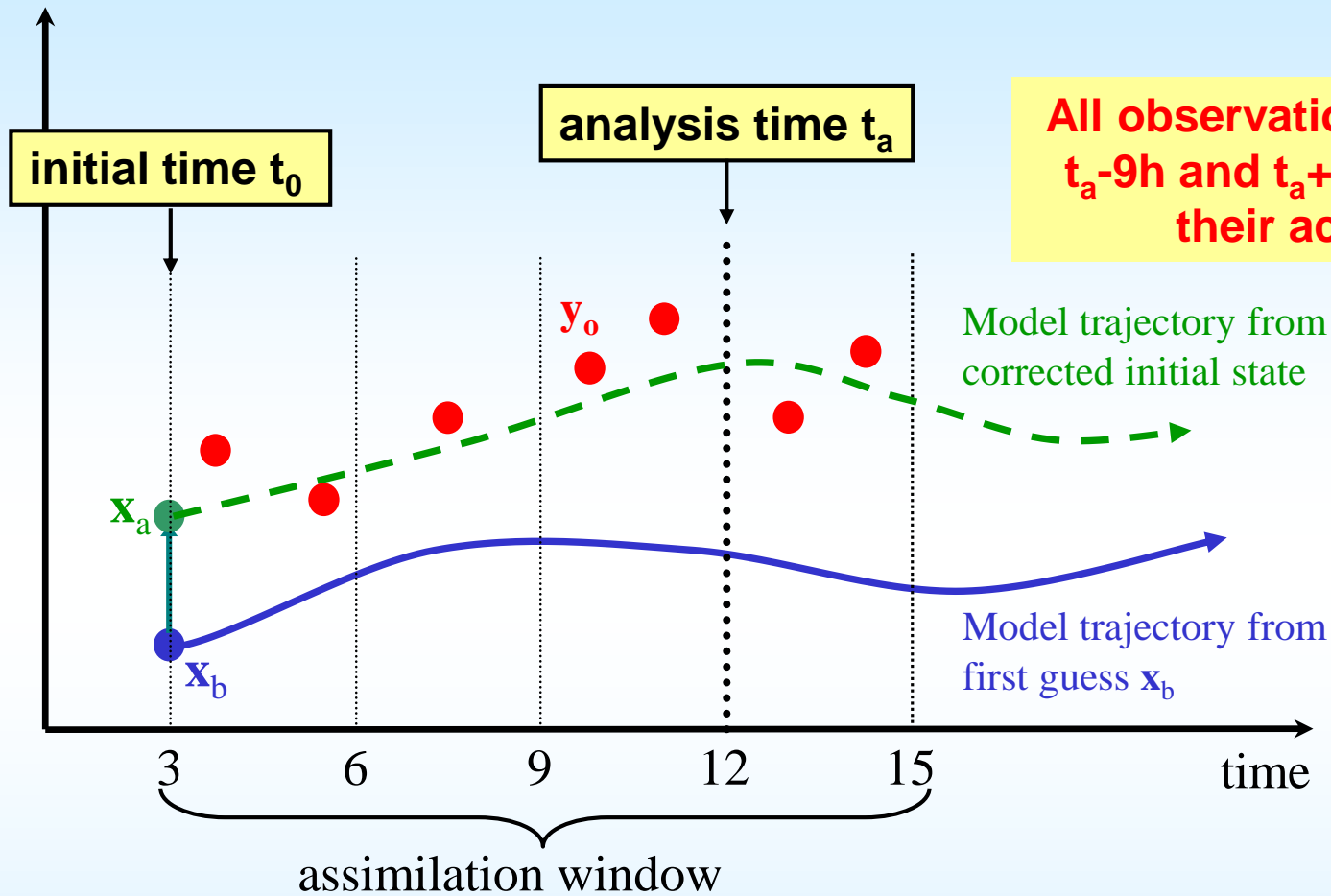
- Introduction
- Why are physical parametrizations needed in data assimilation?
- Tangent-linear and adjoint coding
- Issues related to physical parametrizations in data assimilation
- Physical parametrizations in ECMWF's current 4D-Var system
- Examples of applications
- Summary and conclusions

# Data assimilation



## 4D-Var

model state



4D-Var produces the **analysis** ( $x_a$ ) that minimizes the distance to a set of available **observations** ( $y_o$ ) under the constraint of some ***a priori* background information from the model** ( $x_b$ ) and given the respective errors of observations and model background.

## 4D-Var

Incremental 4D-Var minimizes the following cost function:

$$J = \frac{1}{2} \delta \mathbf{x}_0^T \mathbf{B}^{-1} \delta \mathbf{x}_0 + \frac{1}{2} \sum_{i=1}^n (\mathbf{H}_i \mathbf{M}_i \delta \mathbf{x}_0 - \mathbf{d}_i)^T \mathbf{R}_i^{-1} (\mathbf{H}_i \mathbf{M}_i \delta \mathbf{x}_0 - \mathbf{d}_i)$$

where:  $i$  = time index (inside 4D-Var window, typ. 12h).

$\delta \mathbf{x}_0 = \mathbf{x}_0 - \mathbf{x}^b_0$  (increment).

$\mathbf{H}_i$  = tangent-linear of observation operator.

$\mathbf{M}_i$  = tangent-linear of forecast model ( $t_0 \rightarrow t_i$ ).

$\mathbf{d}_i = \mathbf{y}^o_i - H_i(M_i[\mathbf{x}^b_0])$  (innovation vector).

$\mathbf{B}$  = background error covariance matrix.

$\mathbf{R}_i$  = observation error covariance matrix.

$$\nabla_{\delta \mathbf{x}_0} J = \mathbf{B}^{-1} \delta \mathbf{x}_0 + \sum_{i=1}^n \mathbf{M}_i^T [t_i, t_0] \mathbf{H}_i^T \mathbf{R}_i^{-1} (\mathbf{H}_i \mathbf{M}_i \delta \mathbf{x}_0 - \mathbf{d}_i)$$

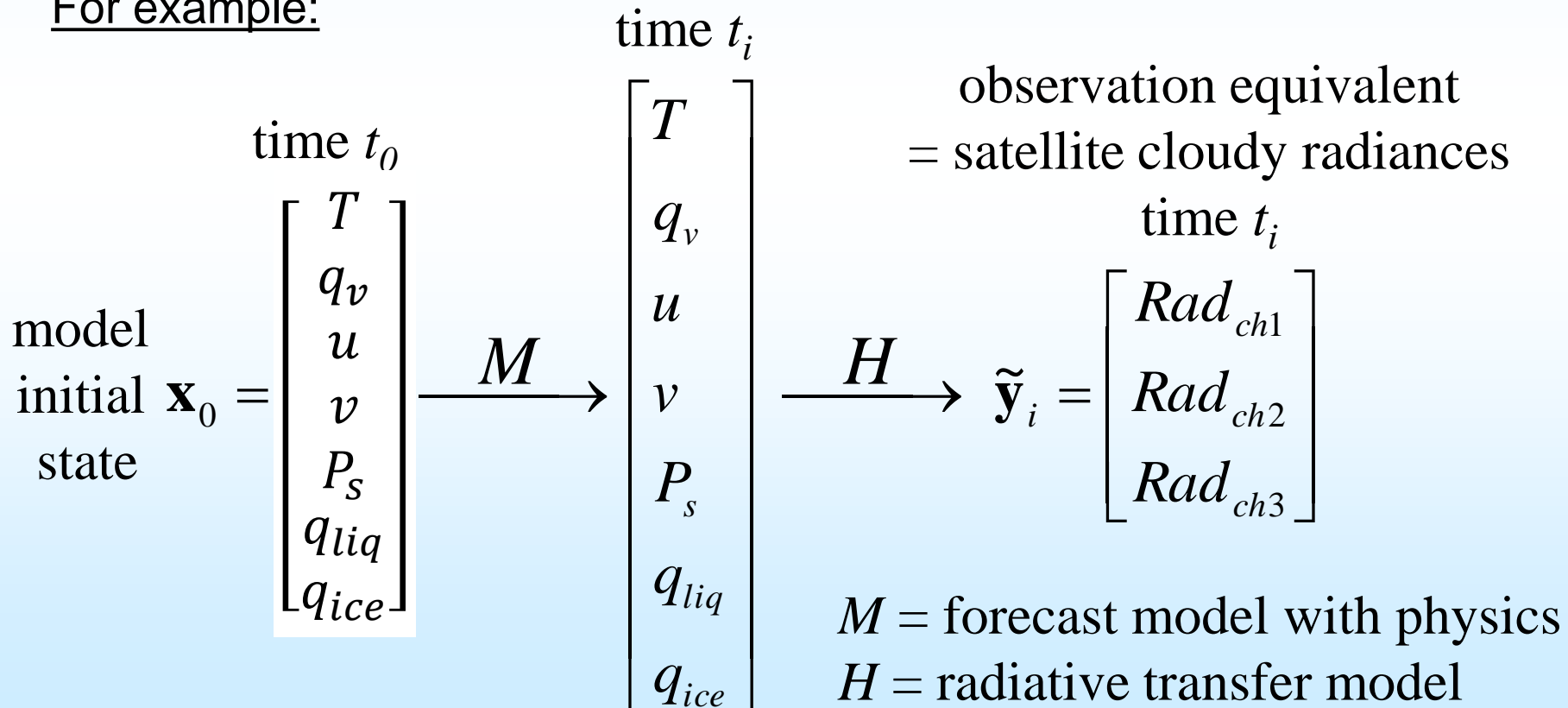
Adjoint of forecast model with simplified linearized physics  
(simplified: to reduce computational cost and to avoid non-linear processes)

# Why do we need physical parametrizations in DA?

## Physical parametrizations are needed in data assimilation:

- 1) To evolve the model state in time during the 4D-Var assimilation,
- 2) To convert the model state variables to observed equivalents,  
→ so that obs–model differences can be computed at obs time.

For example:



# Why do we need physical parametrizations in DA?

Tangent-linear operators are applied to perturbations:

$$\begin{array}{ccc}
 \text{time } t_0 & & \text{time } t_i \\
 \delta \mathbf{x}_0 = \begin{bmatrix} \delta T \\ \delta q_v \\ \delta u \\ \delta v \\ \delta P_s \end{bmatrix} & \xrightarrow{\mathbf{M}[t_0, t_i]} & \begin{bmatrix} \delta T \\ \delta q_v \\ \delta u \\ \delta v \\ \delta P_s \\ \delta q_{liq} \\ \delta q_{ice} \end{bmatrix} & \xrightarrow{\mathbf{H}} & \delta \tilde{\mathbf{y}}_i = \begin{bmatrix} \delta Rad_{ch1} \\ \delta Rad_{ch2} \\ \delta Rad_{ch3} \end{bmatrix} \\
 & & \text{diagnostic variables} & & 
 \end{array}$$

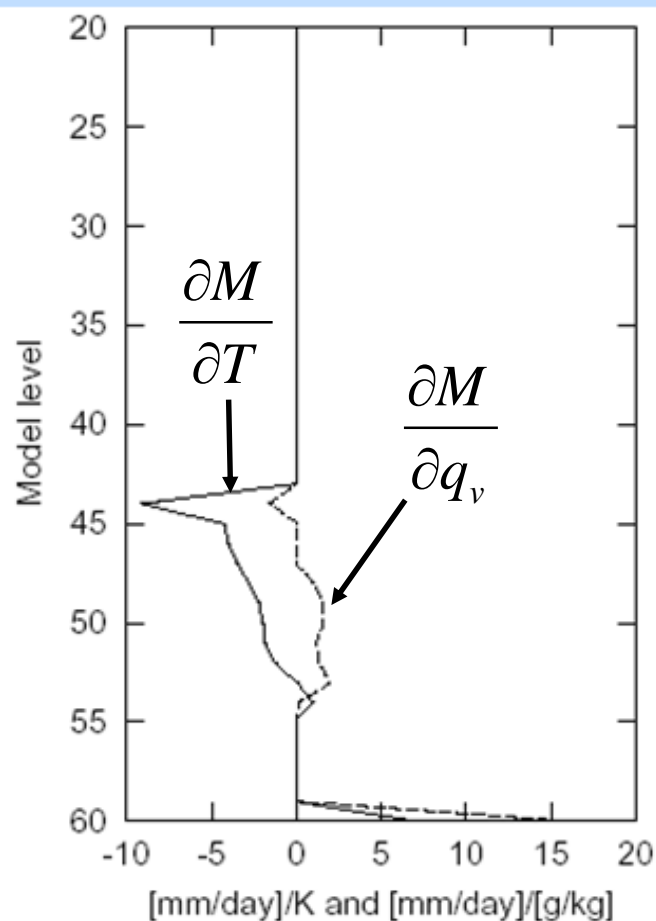
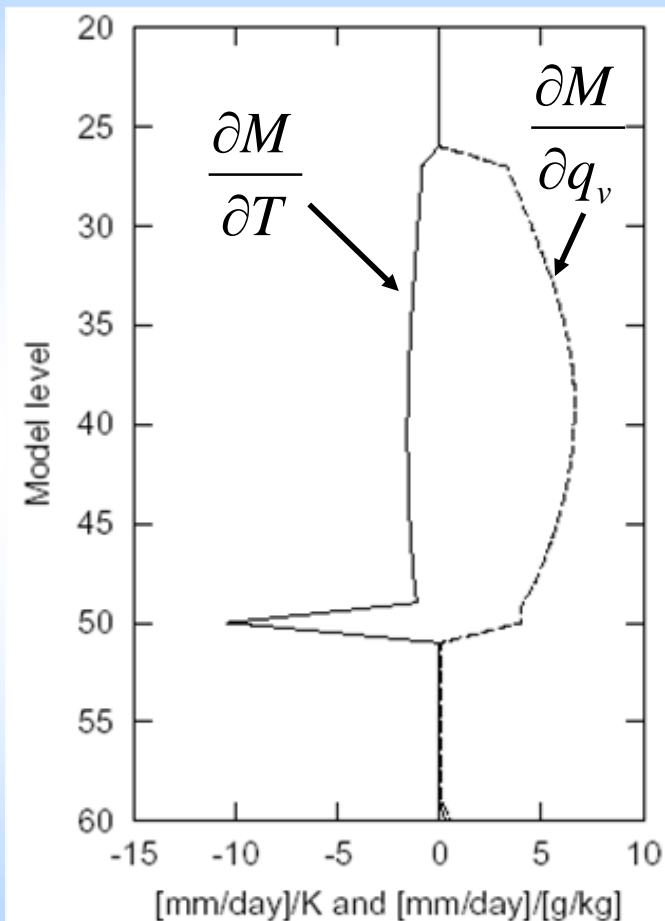
Adjoint operators are applied to cost function gradient:

$$\begin{array}{ccc}
 \text{time } t_i & & \text{time } t_0 \\
 \nabla_{\tilde{\mathbf{y}}_i} J_o = \begin{bmatrix} \partial J_o / \partial Rad_{ch1} \\ \partial J_o / \partial Rad_{ch2} \\ \partial J_o / \partial Rad_{ch3} \end{bmatrix} & \xrightarrow{\mathbf{H}^T} & \begin{bmatrix} \partial J_o / \partial T \\ \partial J_o / \partial q_v \\ \partial J_o / \partial u \\ \partial J_o / \partial v \\ \partial J_o / \partial P_s \\ \partial J_o / \partial q_{liq} \\ \partial J_o / \partial q_{ice} \end{bmatrix} & \xrightarrow{\mathbf{M}^T[t_i, t_0]} & \nabla_{\delta \mathbf{x}_0} J_o = \begin{bmatrix} \partial J_o / \partial T \\ \partial J_o / \partial q_v \\ \partial J_o / \partial u \\ \partial J_o / \partial v \\ \partial J_o / \partial P_s \end{bmatrix}
 \end{array}$$

# The choice of physical parametrizations will affect the results of 4D-Var

$M$ : input = model state  $(T, q_v) \rightarrow$  output = surface convective rainfall rate

Jacobians of surface rainfall rate w.r.t.  $T$  and  $q_v$



from Marécal and Mahfouf (2002)

Betts-Miller (adjustment scheme)

Tiedtke (ECMWF's operational mass-flux scheme)



## A glimpse of tangent-linear and adjoint coding

- Simplified nonlinear code:  $Z = a / X^2 + b Y \log(W)$
- Tangent-linear code:  $\delta Z = -(2 a / X^3) \delta X + b \log(W) \delta Y + (b Y / W) \delta W$
- Adjoint code:  
 $\delta X^* = 0$   
 $\delta Y^* = 0$   
 $\delta W^* = 0$   
  
 $\delta X^* = \delta X^* - (2 a / X^3) \delta Z^*$   
 $\delta Y^* = \delta Y^* + b \log(W) \delta Z^*$   
 $\delta W^* = \delta W^* + (b Y / W) \delta Z^*$   
  
 $\delta Z^* = 0$

## Testing the tangent-linear code

The correctness of the tangent-linear model must be assessed by checking that the first-order Taylor approximation is valid:

$$\forall \delta \mathbf{x} \quad \lim_{\lambda \rightarrow 0} \frac{M(\mathbf{x} + \lambda \delta \mathbf{x}) - M(\mathbf{x})}{\lambda \mathbf{M} \delta \mathbf{x}} = 1$$

Example of output from a successful tangent-linear test:

	$\lambda$	RATIO	
<b>Tiny perturbations</b>	0.1E-09	0.9994875881543574E+00	} Machine precision reached
	0.1E-08	0.9999477148855701E+00	
	0.1E-07	0.9999949234236705E+00	
	0.1E-06	0.9999993501022509E+00	
	0.1E-05	0.9999999496119013E+00	
	0.1E-04	0.99999995111338369E+00	↑ Improvement when perturbation size decreases
	0.1E-03	0.9999953179193711E+00	
	0.1E-02	0.9999724488345042E+00	
	0.1E-01	0.9998727842790062E+00	
	0.1E+00	0.9978007454264978E+00	
<b>Larger perturbations</b>	0.1E+01	0.9583066504549524E+00	

## Testing the adjoint code

The correctness of the adjoint model needs to be assessed by checking that it satisfies the mathematical relationship:

$$\forall \delta \mathbf{x}, \delta \mathbf{y} \quad \langle \mathbf{M} \delta \mathbf{x}, \delta \mathbf{y} \rangle = \langle \delta \mathbf{x}, \mathbf{M}^T \delta \mathbf{y} \rangle$$

where  $\mathbf{M}$  is the tangent-linear model and  $\mathbf{M}^T$  is the adjoint model.

Example of output from a successful adjoint test:

$$\begin{aligned} \langle \mathbf{M} \delta \mathbf{x}, \delta \mathbf{y} \rangle &= -0.13765102625164\text{E-}01 \\ \langle \delta \mathbf{x}, \mathbf{M}^T \delta \mathbf{y} \rangle &= -0.13765102625168\text{E-}01 \end{aligned}$$

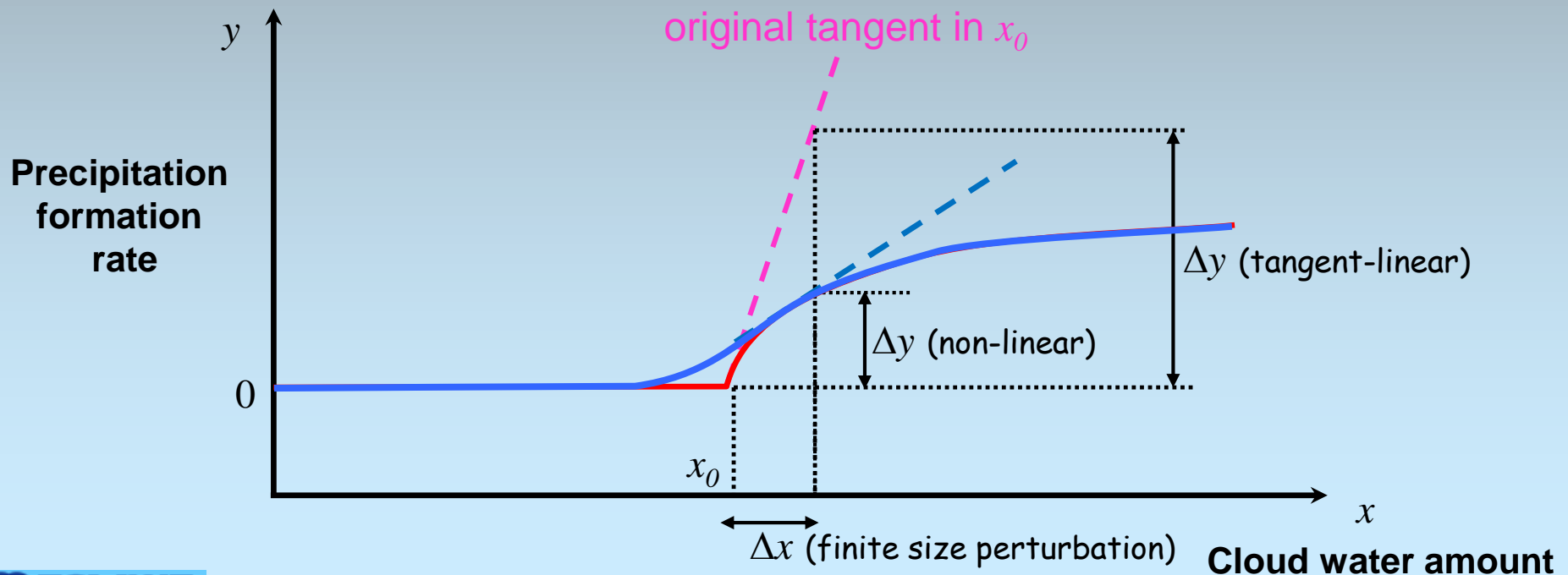
The difference is 11.351 times the zero of the machine

The adjoint test should be correct at the level of machine precision (e.g. at least 11 identical digits for a 12h global integration of the IFS at 50 km resolution).

Otherwise there must be a bug in the code (or in the test itself)!

## Linearity assumption

- Variational assimilation is based on the strong assumption that the analysis is performed in a **(quasi-)linear** framework.
  - However, in the case of physical processes, strong non-linearities can occur in the presence of discontinuous/non-differentiable processes (e.g. **switches or thresholds** in cloud water and precipitation formation).
- “Regularization” needs to be applied: **smoothing of functions, reduction of some perturbations.**



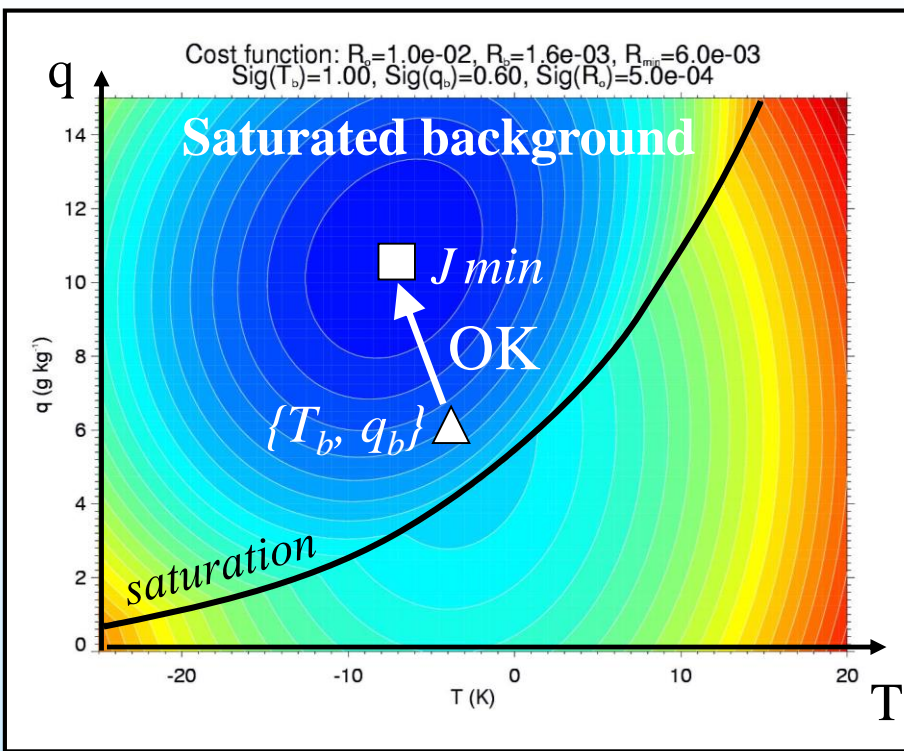
# Illustration of discontinuity effect on cost function shape:

Model background =  $\{T_b, q_b\}$ ; Observation =  $RR_{obs}$

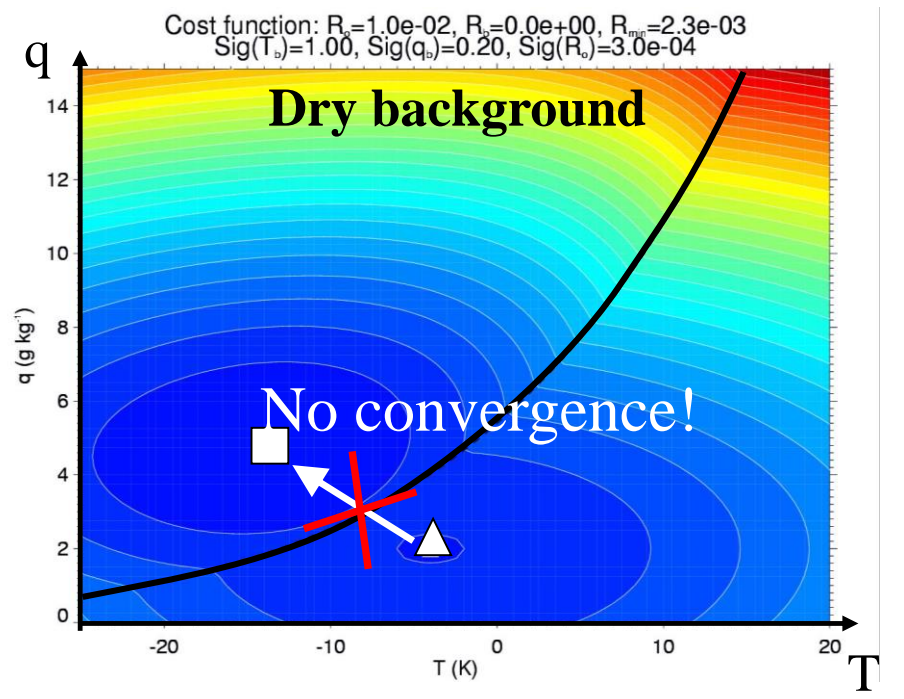
Simple parametrization of rain rate:

$$RR = \begin{cases} \alpha \{q - q_{sat}(T)\} & \text{if } q > q_{sat}(T), \\ 0 & \text{otherwise} \end{cases}$$

$$J = \frac{1}{2} \left( \frac{T - T_b}{\sigma_T} \right)^2 + \frac{1}{2} \left( \frac{q - q_b}{\sigma_q} \right)^2 + \frac{1}{2} \left( \frac{\alpha[q - q_{sat}(T)] - RR_{obs}}{\sigma_{RR_{obs}}} \right)^2$$



Single minimum of cost function



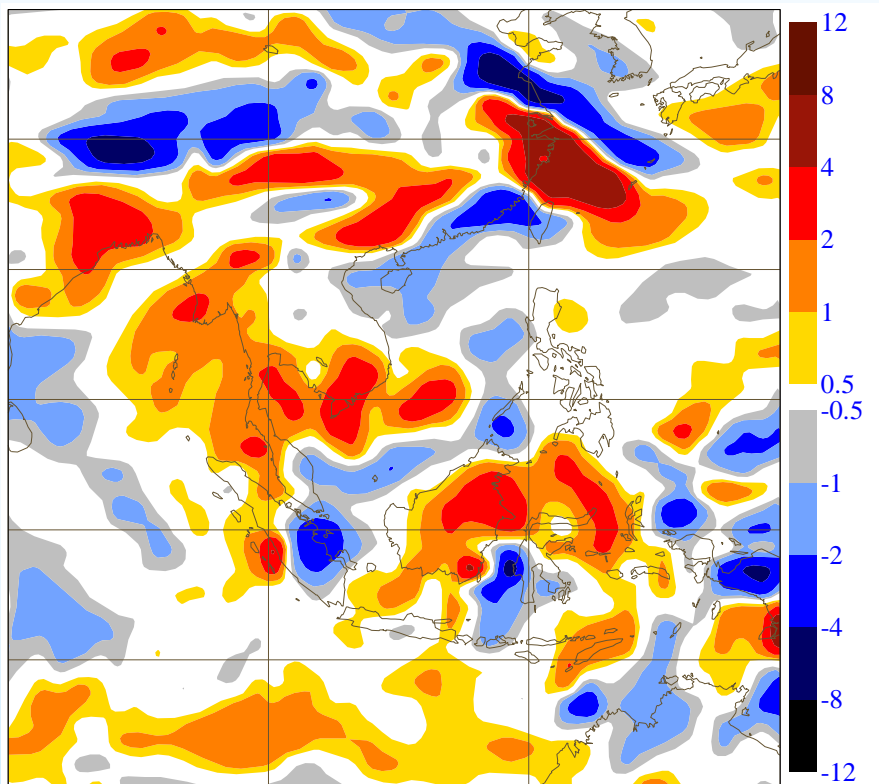
Several local minima of cost function

An example of spurious TL noise caused by a threshold in the autoconversion formulation of the large-scale cloud scheme.

~700 hPa zonal wind increments [m/s] from 12h model integration.

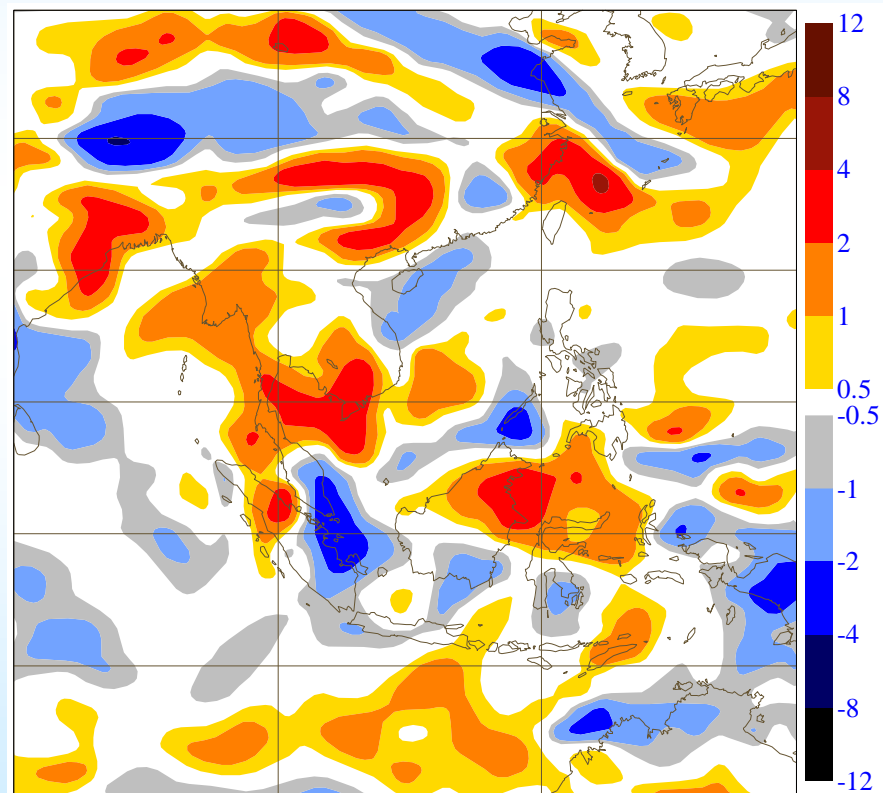
Nonlinear finite difference:

$$M(\mathbf{x}+\delta\mathbf{x}) - M(\mathbf{x})$$

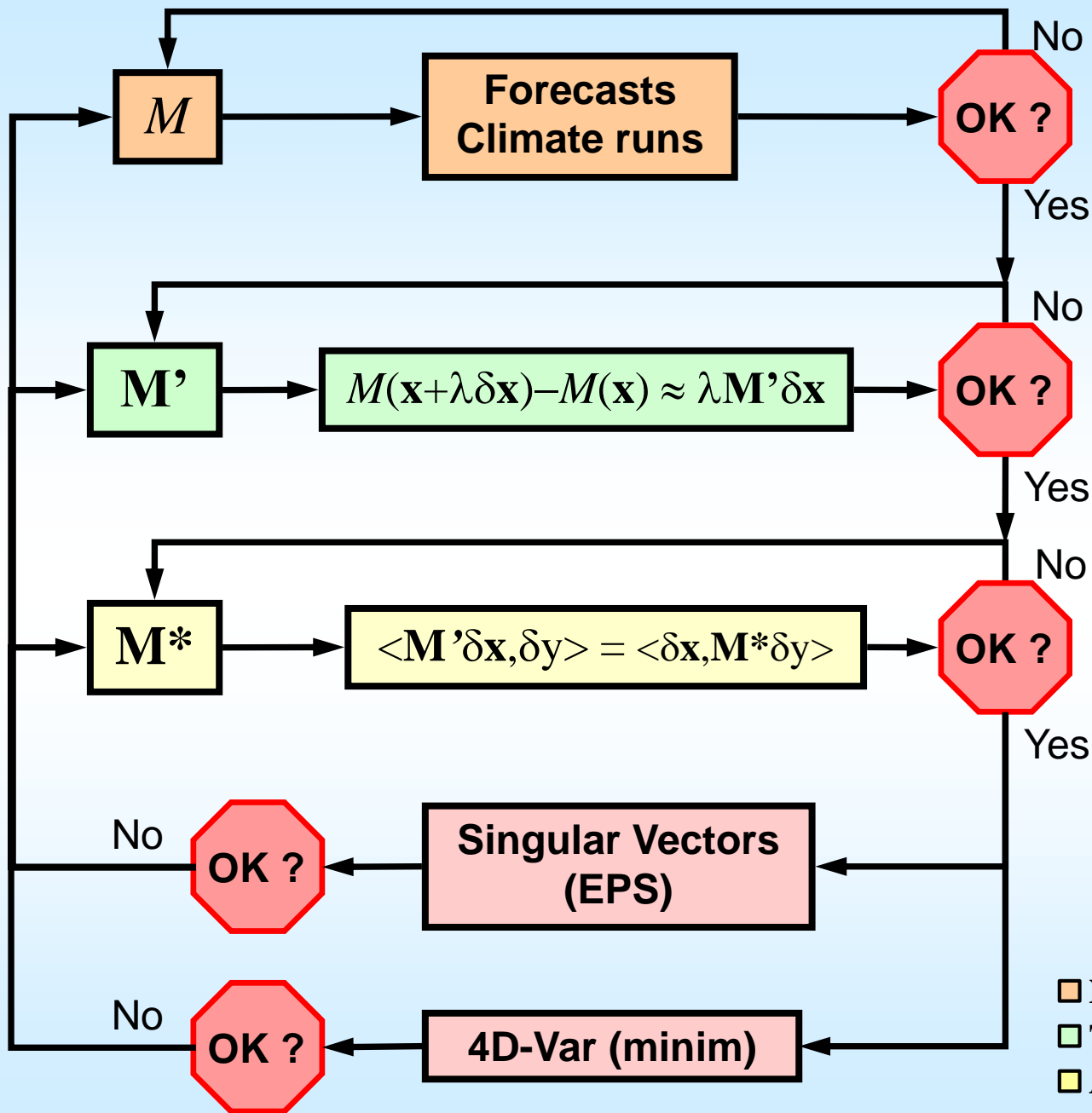


from M. Janisková

Tangent-linear integration:  $M\delta\mathbf{x}$

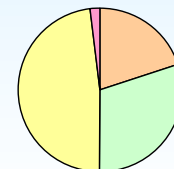


with perturbation reduction in autoconversion

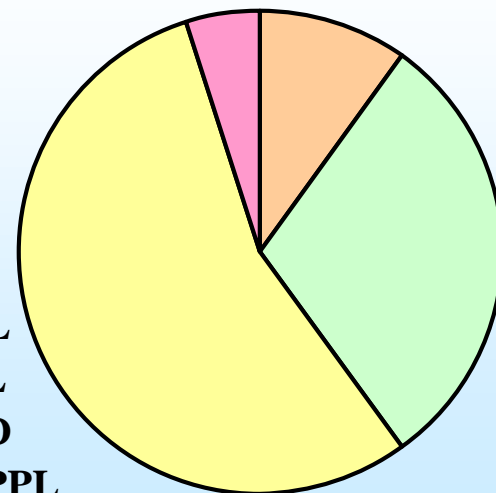


### Timing:

Pure coding



Debugging and testing  
(incl. regularization)



- NL
- TL
- AD
- APPL

## ECMWF operational LP package (operational 4D-Var)

Currently used in ECMWF operational 4D-Var minimizations (main simplifications with respect to the full non-linear versions are highlighted **in red**):

- **Large-scale condensation scheme:** [Tompkins and Janisková 2004]
  - based on a uniform PDF to describe subgrid-scale fluctuations of total water.
  - melting of snow included.
  - precipitation evaporation included.
  - **reduction of cloud fraction perturbation and in autoconversion of cloud into rain.**
- **Convection scheme:** [Lopez and Moreau 2005]
  - mass-flux approach [Tiedtke 1989].
  - deep convection (CAPE closure) and shallow convection (q-convergence) are treated.
  - perturbations of all convective quantities are included.
  - coupling with cloud scheme through detrainment of liquid water from updraught.
  - **some perturbations (buoyancy, initial updraught vertical velocity) are reduced.**
- **Radiation:** TL and AD of longwave and shortwave radiation available [Janisková et al. 2002]
  - **shortwave:** based on Morcrette (1991), **only 2 spectral intervals** (instead of 6 in non-linear version).
  - **longwave:** based on Morcrette (1989), **called every 2 hours only.**



## ECMWF operational LP package (operational 4D-Var)

- Vertical diffusion:

- mixing in the surface and planetary boundary layers,
- based on K-theory and Blackadar mixing length,
- exchange coefficients based on *Louis et al. [1982]*, near surface,
- Monin-Obukhov higher up,
- mixed layer parametrization and PBL top entrainment recently added.
- **Perturbations of exchange coefficients are smoothed (esp. near the surface).**

- Orographic gravity wave drag: [*Mahfouf 1999*]

- subgrid-scale orographic effects [*Lott and Miller 1997*],
- **only low-level blocking part is used.**

- Non-orographic gravity wave drag: [*Oor et al. 2010*]

- isotropic spectrum of non-orographic gravity waves [*Scinocca 2003*],
- **Perturbations of output wind tendencies below 200 hPa reset to zero.**

- RTTOV is employed to simulate radiances at individual frequencies (infrared, longwave and microwave, with cloud and precipitation effects included) to compute model–satellite departures in observation space.

# Impact of linearized physics on tangent-linear approximation

## Comparison:

Finite difference of two NL integrations  $\leftrightarrow$  TL evolution of initial perturbations

Examination of the accuracy of the linearization for typical analysis increments:

$$M(\mathbf{x}_{an}) - M(\mathbf{x}_{bg}) \leftrightarrow \mathbf{M}(\underbrace{\mathbf{x}_{an} - \mathbf{x}_{bg}}_{\text{typical size of 4D-Var analysis increments}})$$

## Diagnostics:

- mean absolute errors:

$$\varepsilon = \left| \left[ M(\mathbf{x}_{an}) - M(\mathbf{x}_{bg}) \right] - \mathbf{M}(\mathbf{x}_{an} - \mathbf{x}_{bg}) \right|$$

- relative error change:

$$\frac{\varepsilon_{\text{EXP}} - \varepsilon_{\text{REF}}}{\varepsilon_{\text{REF}}} \times 100\% \quad (\text{improvement if } < 0)$$

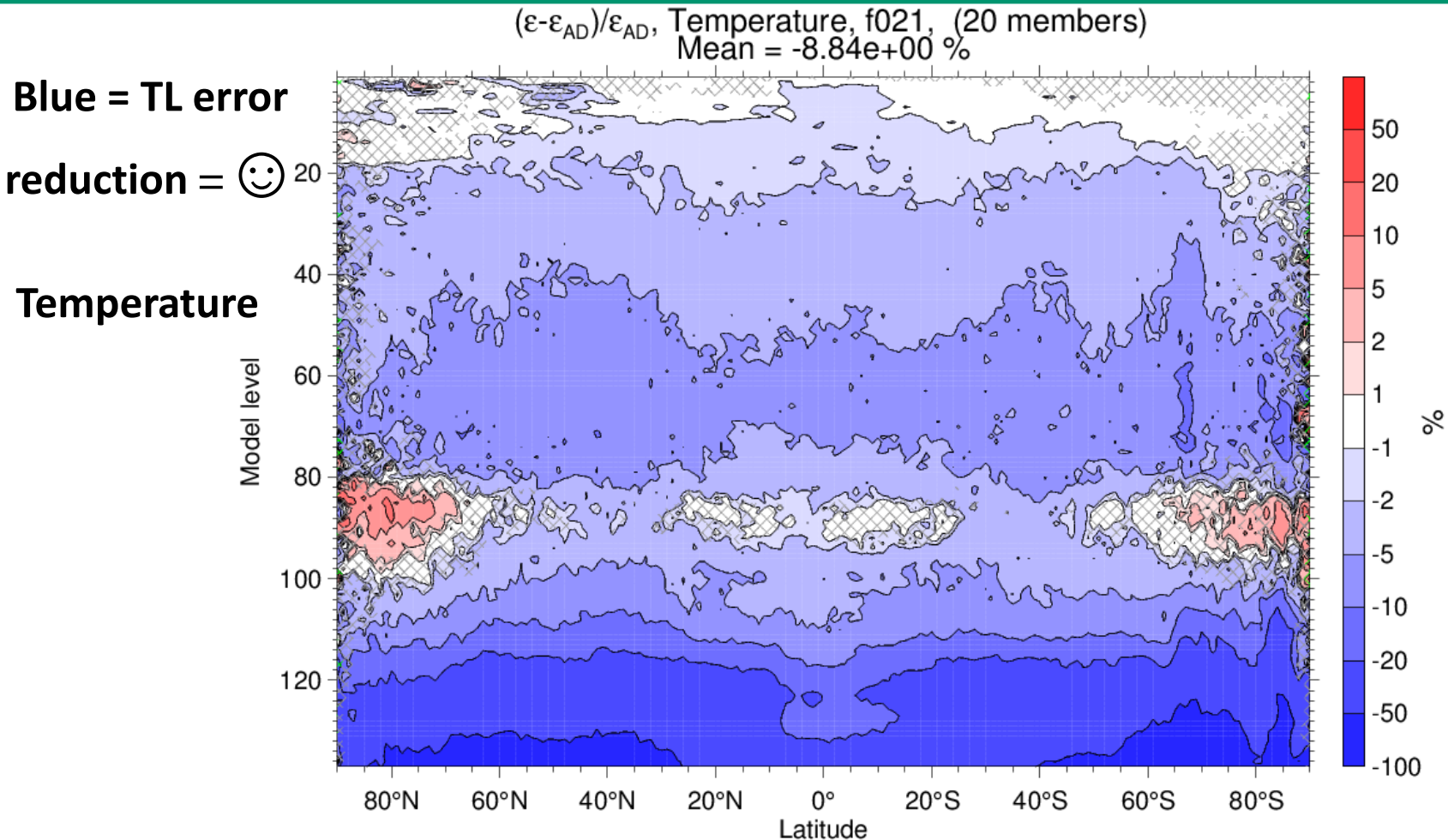
- here: REF = adiabatic run (i.e. no physical parametrizations in tangent-linear)

# Impact of linearized physics on tangent-linear approximation

Zonal mean cross-section of change in TL error when TL includes:

**VDIF + orog. GWD + SURF**

**Relative to adiabatic TL run (50-km resol.; 20 runs; after 12h integr.).**



# Impact of linearized physics on tangent-linear approximation

Zonal mean cross-section of change in TL error when TL includes:

**VDIF + orog. GWD + SURF + RAD**

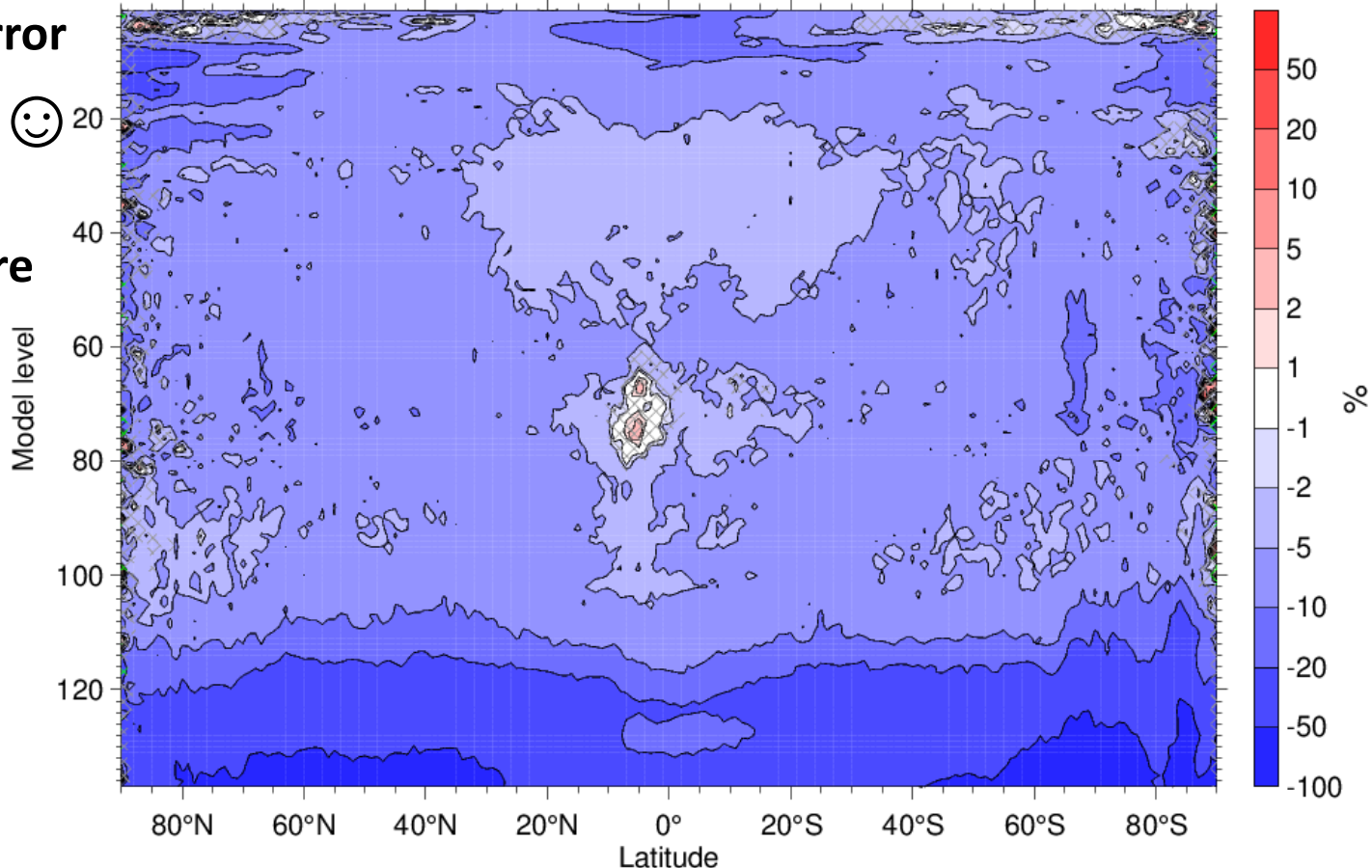
**Relative to adiabatic TL run (50-km resol.; 20 runs; after 12h integr.).**

$(\varepsilon - \varepsilon_{AD}) / \varepsilon_{AD}$ , Temperature, f022, [T399 L137 +48] (20 members)  
Mean =  $-1.08 \times 10^1$  %

Blue = TL error

reduction = 😊

Temperature



# Impact of linearized physics on tangent-linear approximation

Zonal mean cross-section of change in TL error when TL includes:

VDIF + orog. GWD + SURF + RAD + non-orog GWD + moist physics

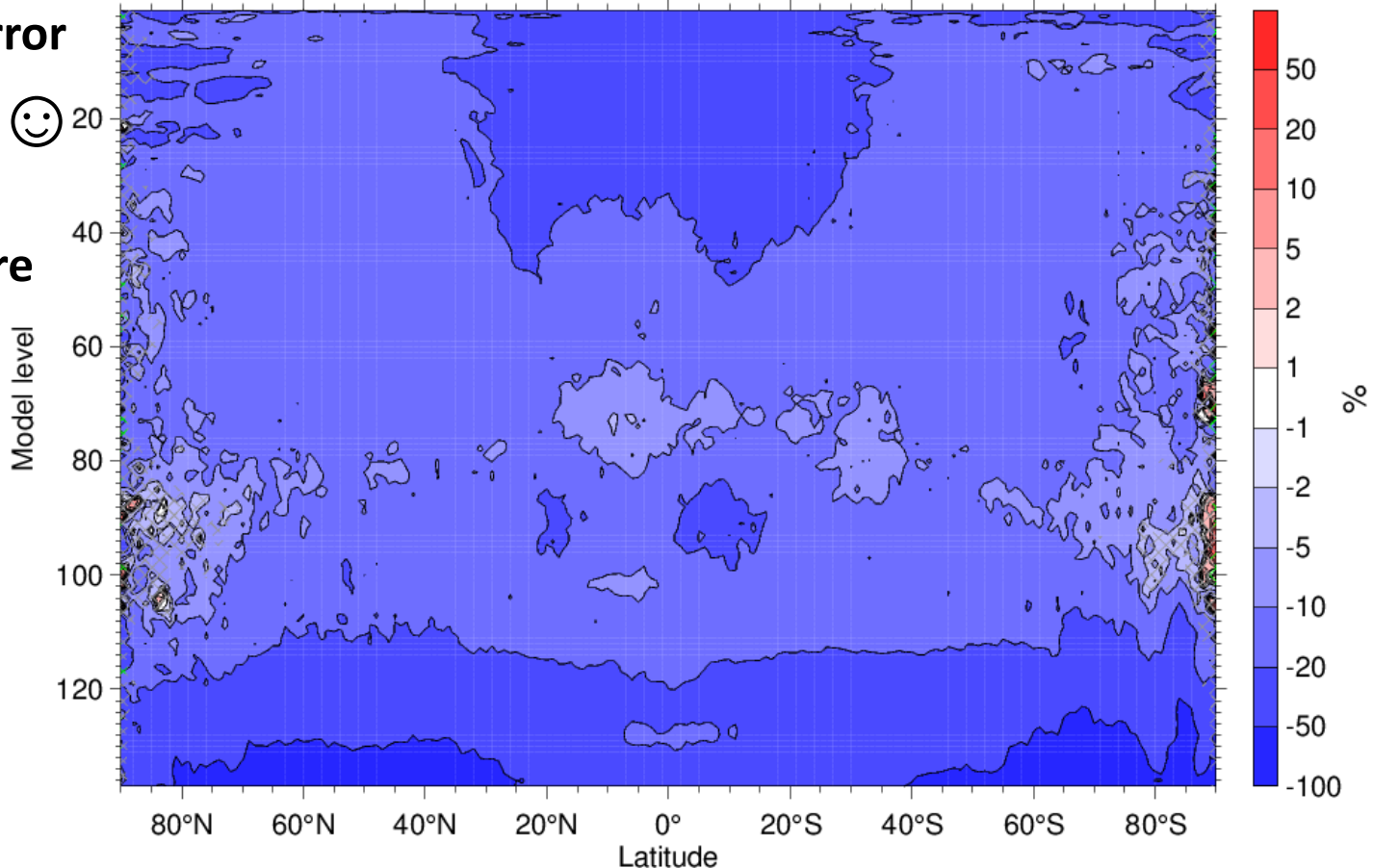
Relative to adiabatic TL run (50-km resol.; 20 runs; after 12h integr.).

$(\epsilon - \epsilon_{AD})/\epsilon_{AD}$ , Temperature, f025, [T399 L137 +48] (20 members)  
Mean =  $-1.95e+01$  %

Blue = TL error

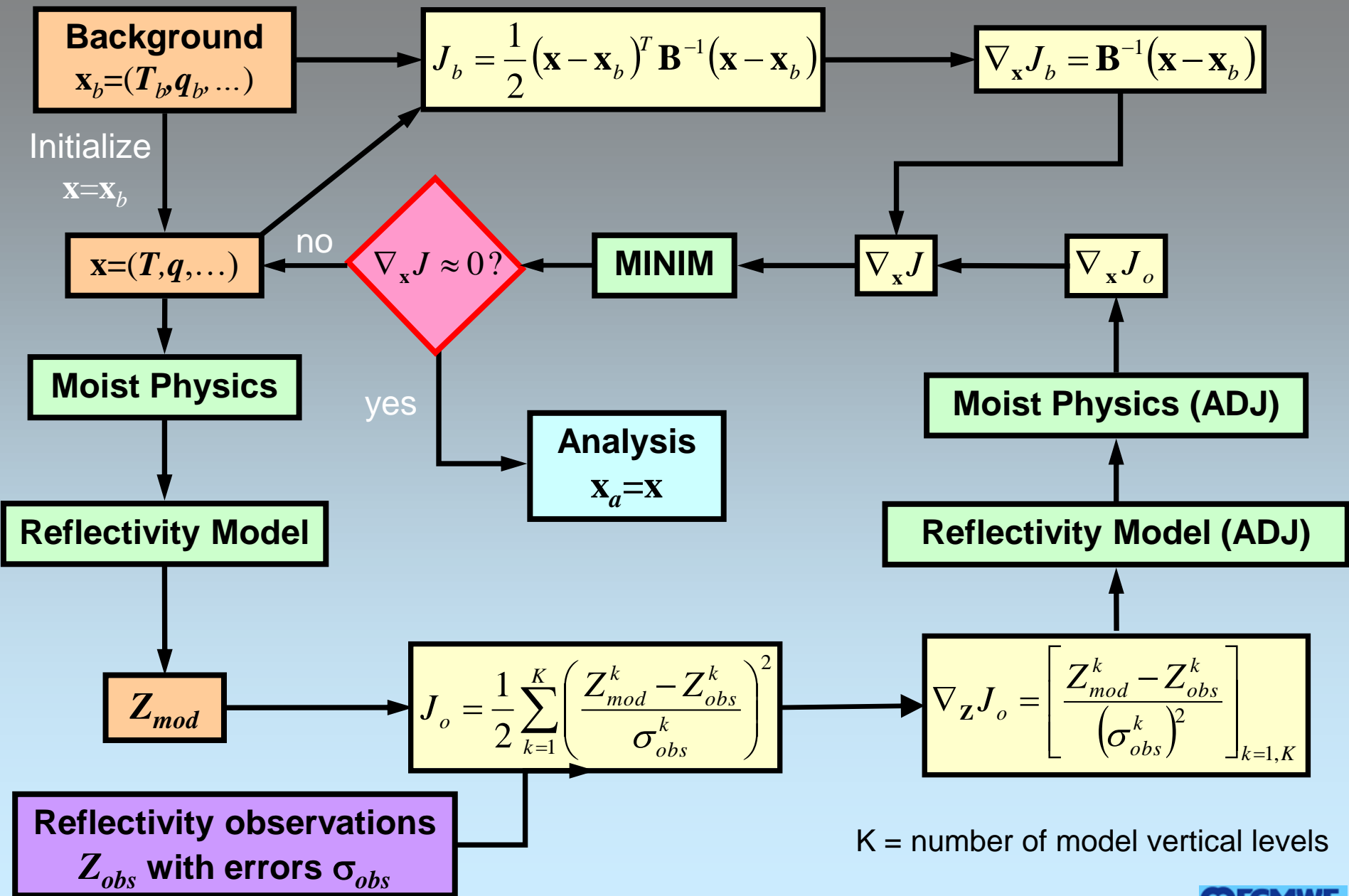
reduction = 😊

Temperature



# *Applications*

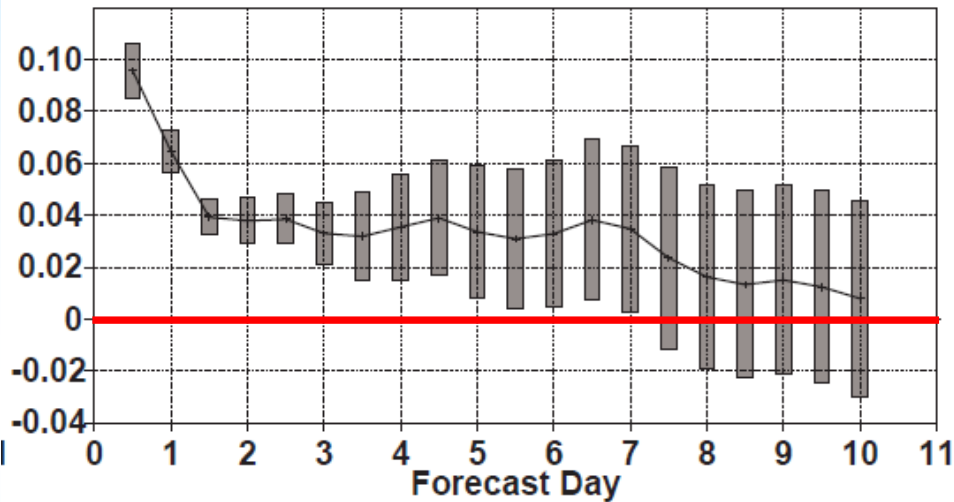
# 1D-Var with radar reflectivity profiles



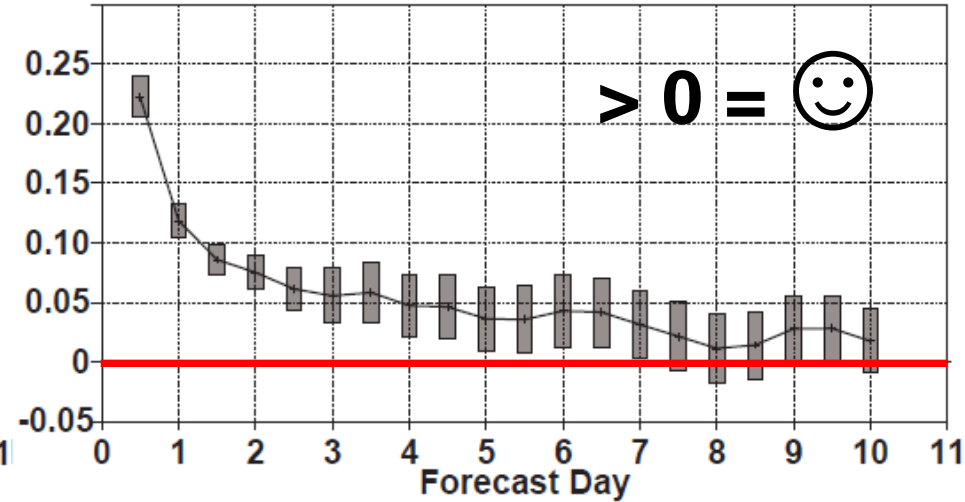
# Impact of ECMWF linearized physics on forecast scores

Comparison of two T511 L91 4D-Var 3-month experiments with & without full linearized physics: Relative change in forecast anomaly correlation.

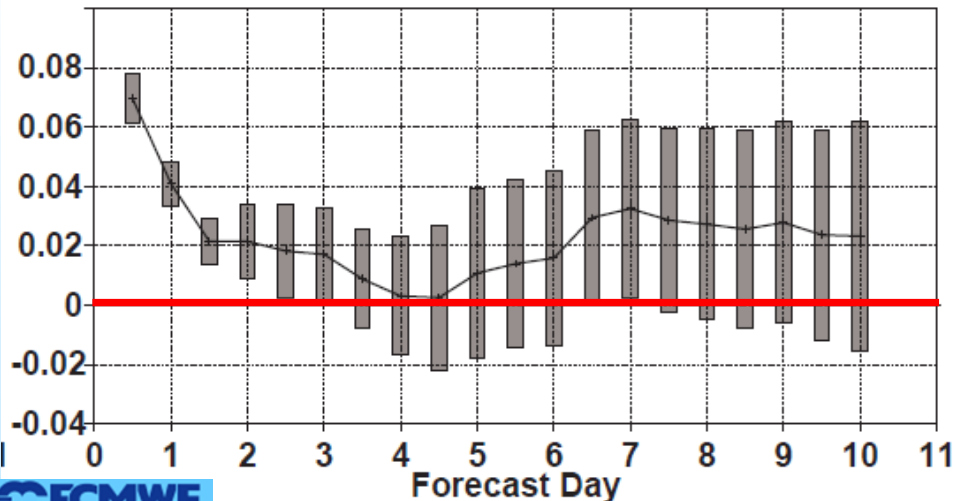
NHem: 700hPa temperature - Anomaly correlation



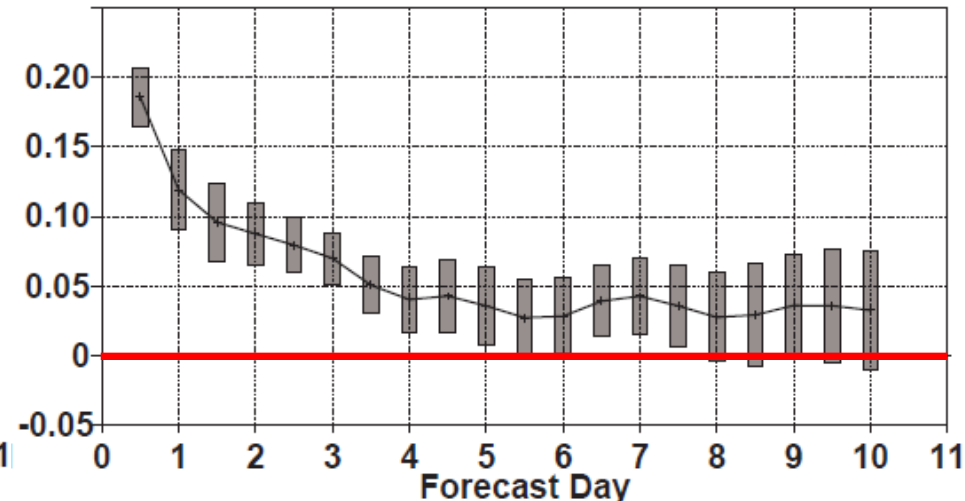
NHem: 200hPa vector wind - Anomaly correlation



SHem: 700hPa temperature - Anomaly correlation



SHem: 200hPa vector wind - Anomaly correlation





## Physics parameter optimization

**Idea:** It might be feasible to optimize the values of parameters used in the physical schemes with the variational data assimilation approach.

This would require to include the parameter(s) in the control vector of the 4D-Var data assimilation system:

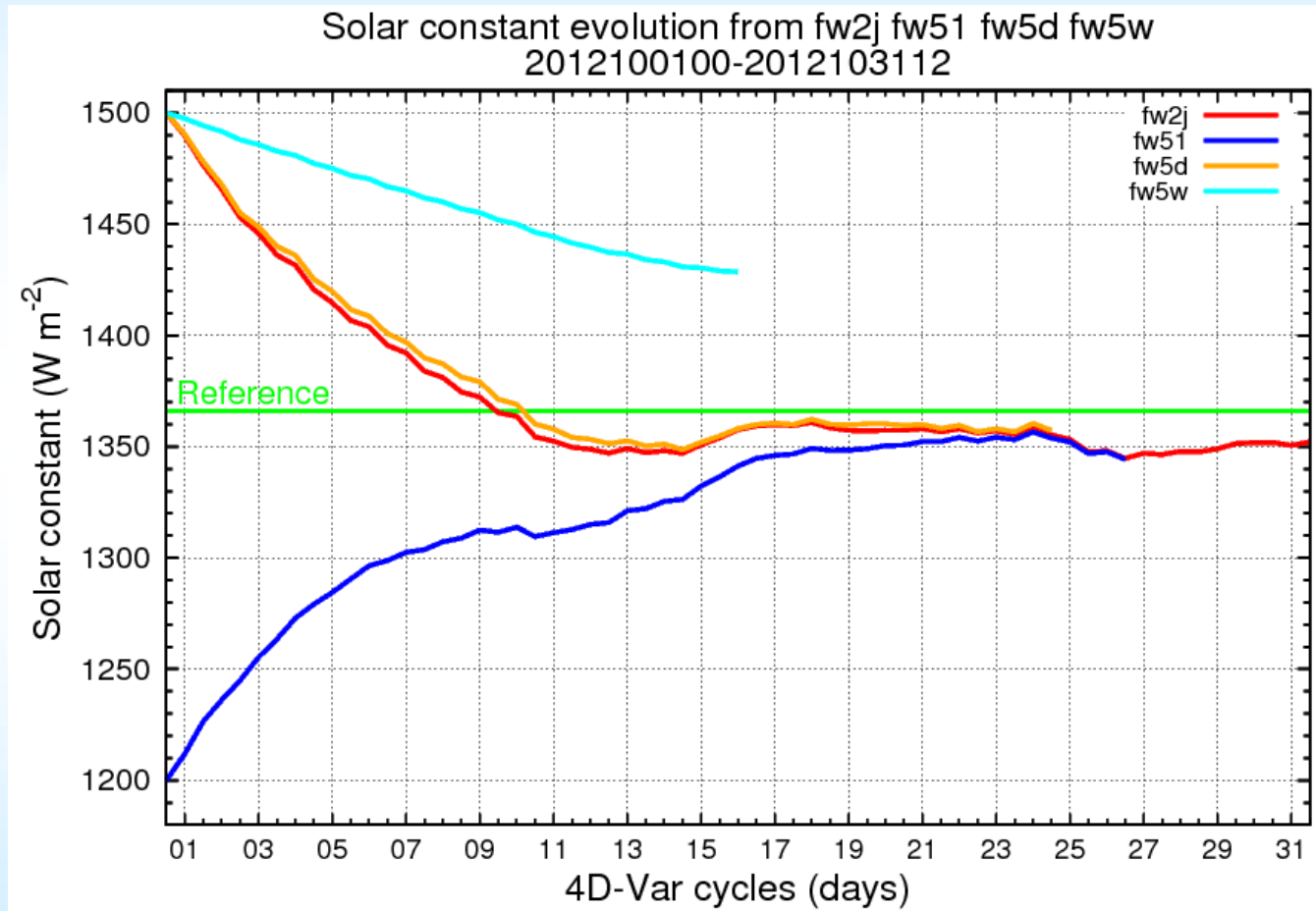
$$J = \frac{1}{2} (\mathbf{x} - \mathbf{x}_b)^T \mathbf{B}^{-1} (\mathbf{x} - \mathbf{x}_b) + \frac{1}{2} (\mathbf{p} - \mathbf{p}_b)^T \mathbf{B}_p^{-1} (\mathbf{p} - \mathbf{p}_b) + \frac{1}{2} (H(\mathbf{x}, \mathbf{p}) - \mathbf{y}_o)^T \mathbf{R}^{-1} (H(\mathbf{x}, \mathbf{p}) - \mathbf{y}_o)$$

**Limitations:** Only parameters that are present in both the forecast model and the linearized simplified physics (TL & AD) can be treated in this way.

Discrepancies between the full non-linear physics and the TL & AD physics (used in the minimization of  $J$ ) might lead to sub-optimal results.

# Physics parameter optimization: an example.

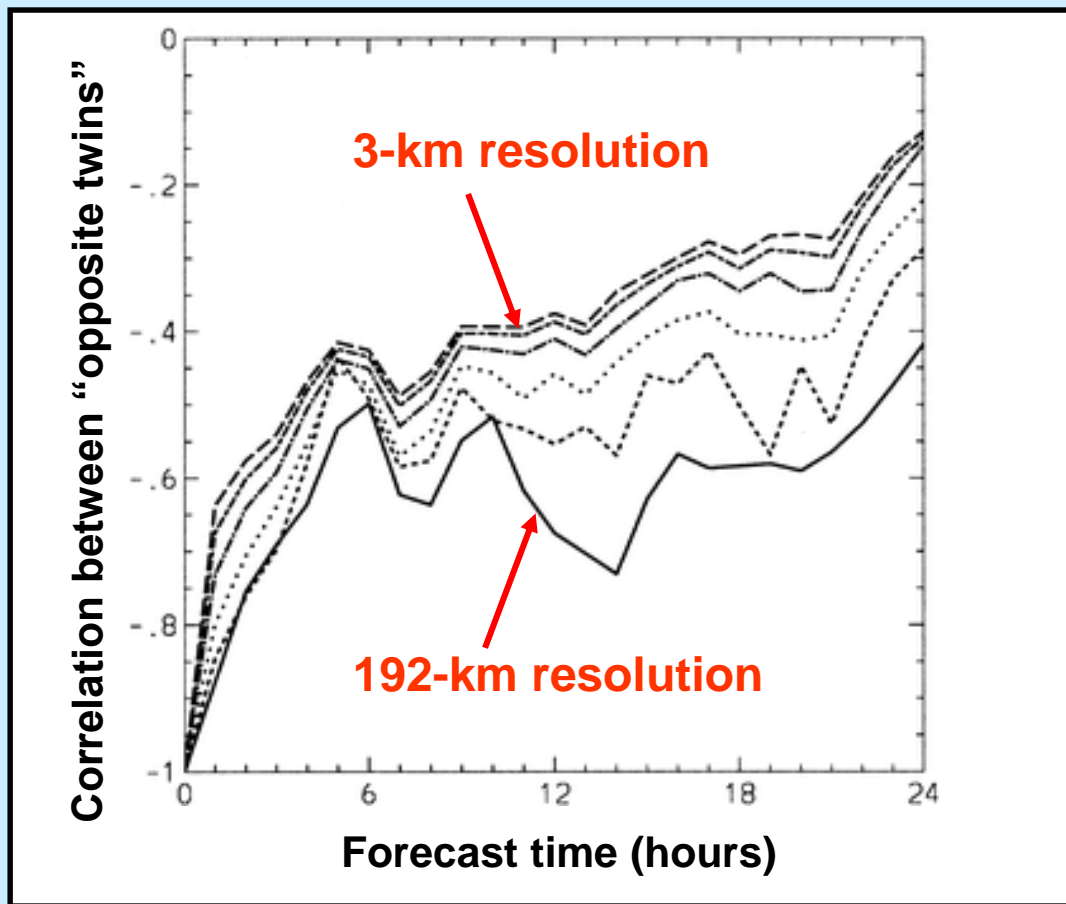
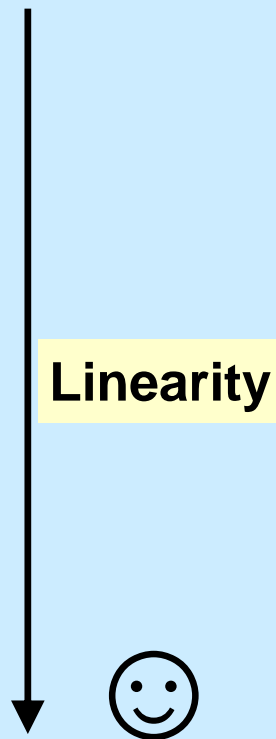
**Application:** Solar constant ( $1366 \text{ W/m}^2$ ) taken as the parameter to be optimized in 4D-Var (starting from either  $1500$  or  $1200 \text{ W/m}^2$ ).



Observations used in 4D-Var manage to constraint the solar constant back to its correct value after 2 weeks or so.

# Influence of time and resolution on linearity assumption in physics

Results from ensemble runs with the MC2 model (3 km resolution) over the Alps, from *Walser et al. (2004)*.  
Comparison of a pair of “opposite twin” experiments.



→ The validity of the linear assumption for precipitation quickly drops in the first hours of the forecast, especially at higher resolution.

## Summary and prospects (1)

- **Linearized physical parameterizations have become essential components of variational data assimilation systems:**
  - **Better representation of the evolution of the atmospheric state during the minimization of the cost function (via the adjoint model integration).**
  - **Extraction of information from observations that are strongly affected by physical processes (e.g. by clouds or precipitation).**
- **However, there are some limitations to the LP approach:**
  - 1) **Theoretical:**

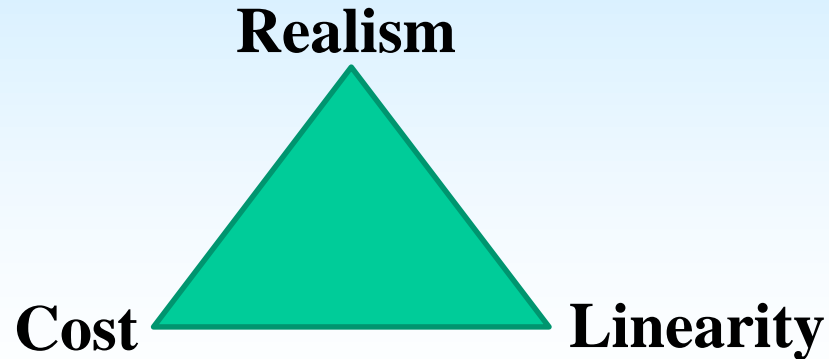
The domain of validity of the linear hypothesis shrinks with increasing resolution and integration length.
  - 2) **Technical:**

Linearized models require sustained & time-consuming attention:

    - **Testing tangent-linear approximation and adjoint code.**
    - **Regularizations / simplifications to eliminate any source of instability.**
    - **Revisions to ensure good match with reference non-linear forecast model.**

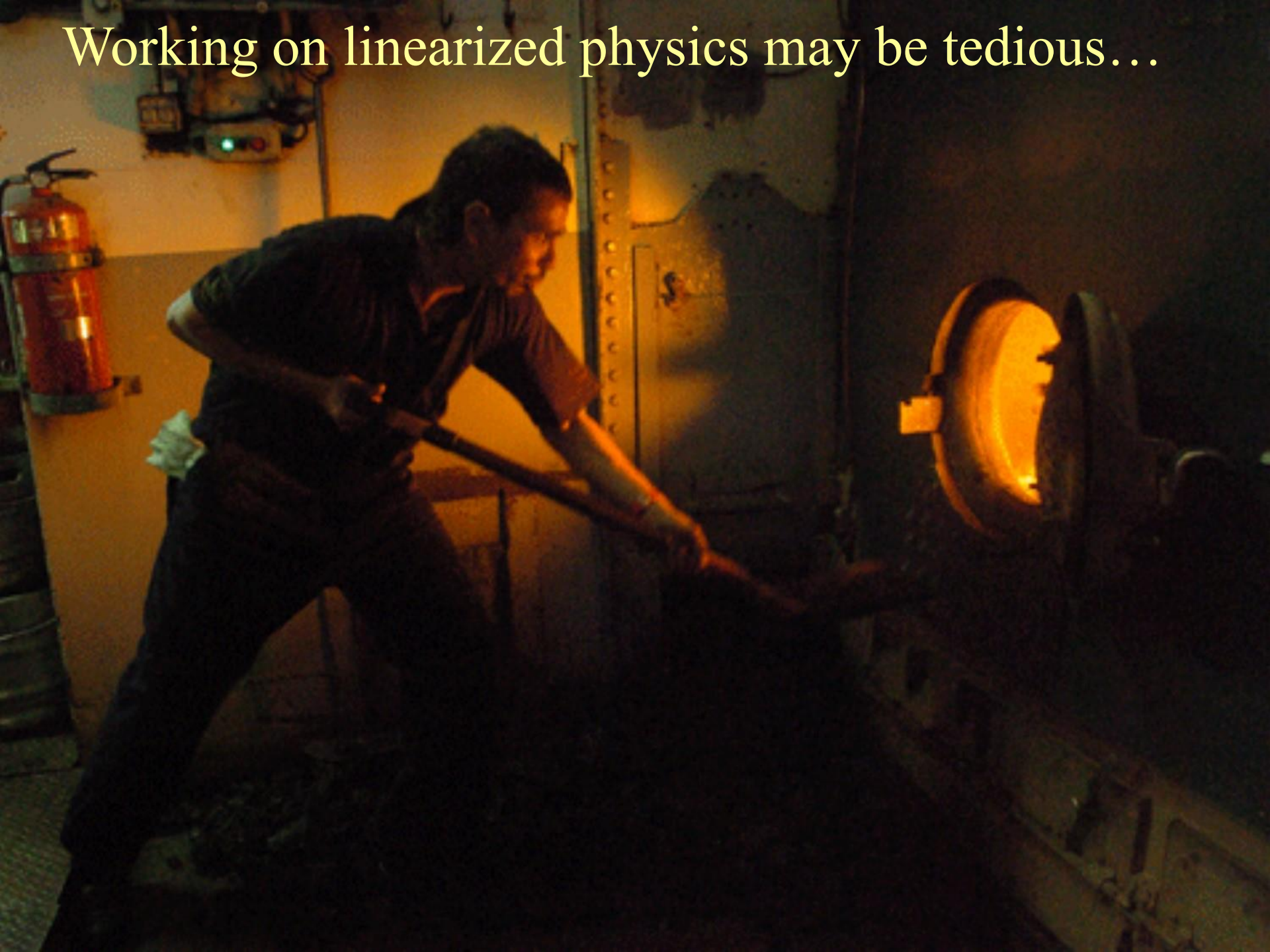
## Summary and prospects (2)

- In practice, it all comes down to achieving the best compromise between:



- Alternative data assimilation methods exist that do not require the development of linearized code, but so far none of them has been able to outperform 4D-Var, especially in global models:
  - Ensemble Kalman Filter (EnKF; still relies on the linearity assumption),
  - Particle filters (difficult to implement for high-dimensional problems).
- So what is the future of LP?

Working on linearized physics may be tedious...



...but it is for the greater good.



## Summary and prospects (3)

- Eventually, it might become impractical or even impossible to make LP work efficiently at resolutions of a few kilometres, even if the linearity constraint can be relaxed (e.g. by using shorter 4D-Var window or weak-constraint 4D-Var).



*Thank you!*



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Marécal, V., and J.-F. Mahfouf, 2003, *Quarterly Journal of the Royal Meteorological Society*, **129**, 3137-3160.

Example of observation operator  $H$  (radiative transfer model):

$$\mathbf{x} = \begin{bmatrix} T_1 \\ \vdots \\ T_n \\ q_1 \\ \vdots \\ q_n \end{bmatrix} \xrightarrow{H} \mathbf{y} = \begin{bmatrix} Rad_{ch1} \\ Rad_{ch2} \\ Rad_{ch3} \end{bmatrix}$$

Tangent-linear operator  $\mathbf{H}$ :

$$\mathbf{H} = \begin{bmatrix} \frac{\partial Rad_{ch1}}{\partial T_1} & \cdots & \frac{\partial Rad_{ch1}}{\partial T_n} & \frac{\partial Rad_{ch1}}{\partial q_1} & \cdots & \frac{\partial Rad_{ch1}}{\partial q_n} \\ \frac{\partial Rad_{ch2}}{\partial T_1} & \cdots & \frac{\partial Rad_{ch2}}{\partial T_n} & \frac{\partial Rad_{ch2}}{\partial q_1} & \cdots & \frac{\partial Rad_{ch2}}{\partial q_n} \\ \frac{\partial Rad_{ch3}}{\partial T_1} & \cdots & \frac{\partial Rad_{ch3}}{\partial T_n} & \frac{\partial Rad_{ch3}}{\partial q_1} & \cdots & \frac{\partial Rad_{ch3}}{\partial q_n} \end{bmatrix}$$

Adjoint operator  $\mathbf{H}^T$ :

$$\mathbf{H}^T = \begin{bmatrix} \frac{\partial Rad_{ch1}}{\partial T_1} & \frac{\partial Rad_{ch2}}{\partial T_1} & \frac{\partial Rad_{ch3}}{\partial T_1} \\ \vdots & \vdots & \vdots \\ \frac{\partial Rad_{ch1}}{\partial T_n} & \frac{\partial Rad_{ch2}}{\partial T_n} & \frac{\partial Rad_{ch3}}{\partial T_n} \\ \frac{\partial Rad_{ch1}}{\partial q_1} & \frac{\partial Rad_{ch2}}{\partial q_1} & \frac{\partial Rad_{ch3}}{\partial q_1} \\ \vdots & \vdots & \vdots \\ \frac{\partial Rad_{ch1}}{\partial q_n} & \frac{\partial Rad_{ch2}}{\partial q_n} & \frac{\partial Rad_{ch3}}{\partial q_n} \end{bmatrix}$$