Parametrizations in Data Assimilation

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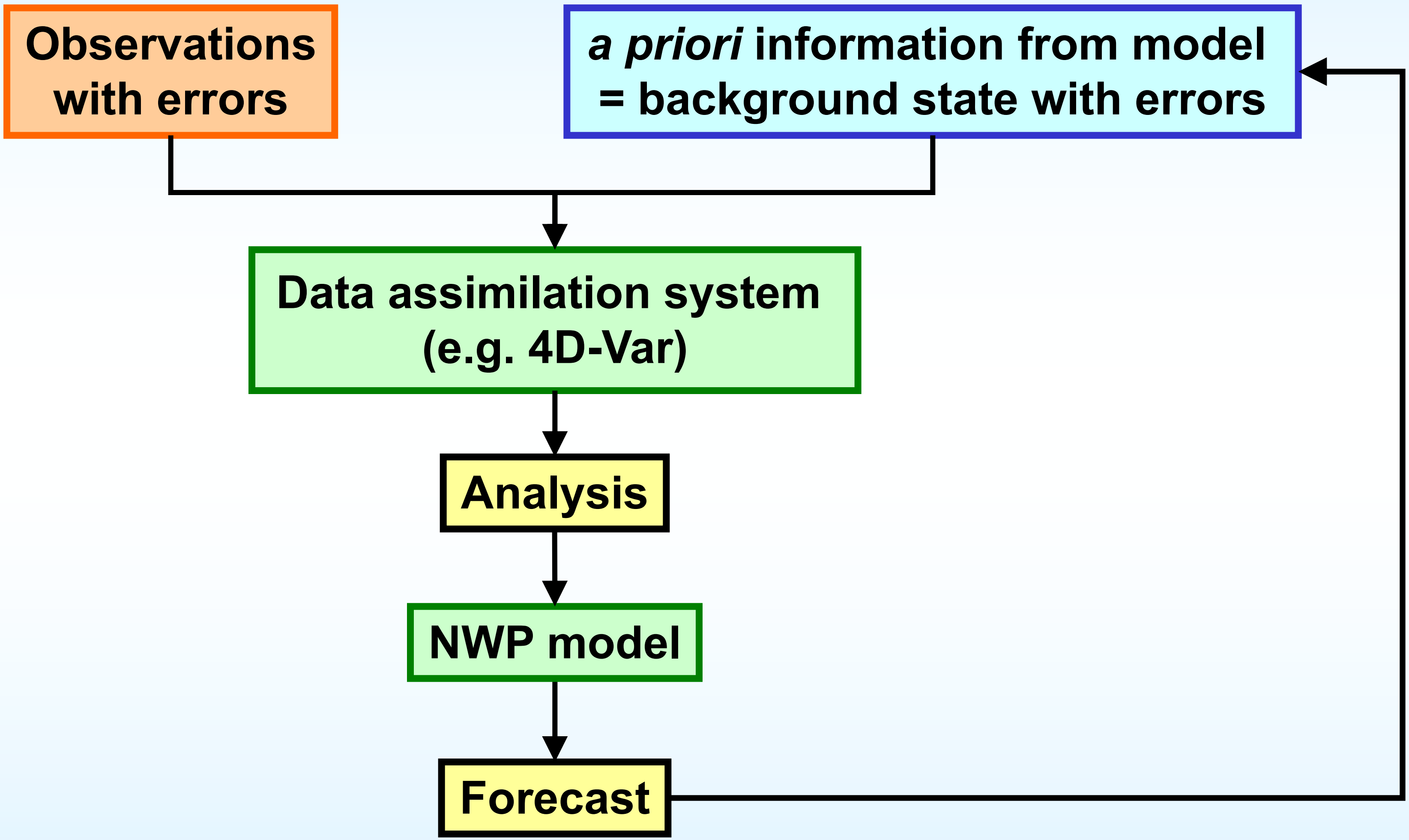
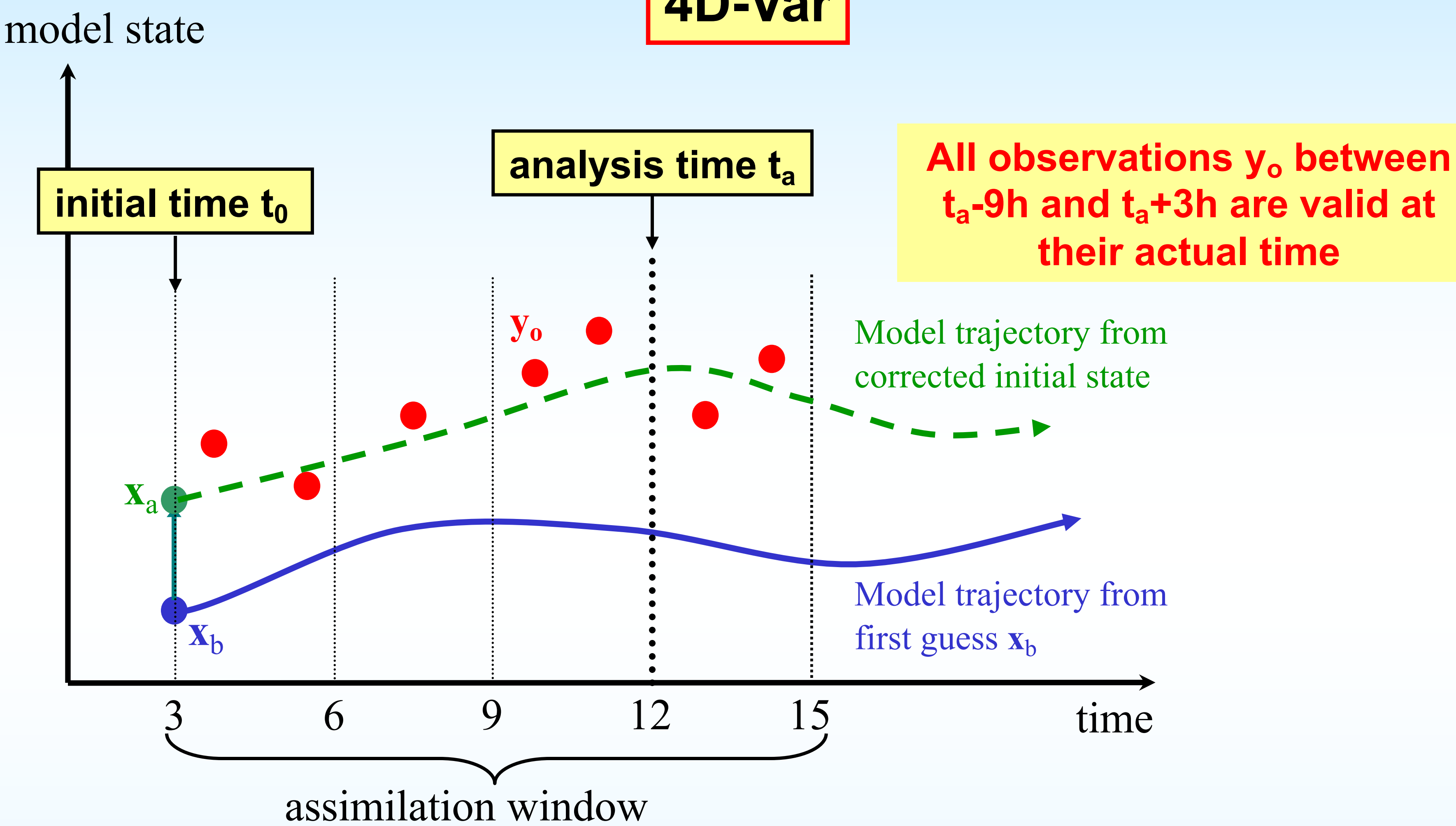
Parametrizations in Data Assimilation

- 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 prospects.

Data assimilation



4D-Var



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:

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

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

$\delta\mathbf{x_0} = \mathbf{x_0} - \mathbf{x^b}_\mathbf{0}$ (increment).

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

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

$\mathbf{d}_i = \mathbf{y^o}_i - H_i(M_i[\mathbf{x^b}_\mathbf{0}])$ (innovation vector).

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

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

$$\nabla_{\delta\mathbf{x}_0} J = \mathbf{B}^{-1}\,\delta\mathbf{x}_0 + \sum_{i=1}^{n}\mathbf{M}_i^T[t_i,t_0]\mathbf{H}_i^T\mathbf{R}_i^{-1}\left(\mathbf{H}_i\mathbf{M}_i\delta\mathbf{x_0} - \mathbf{d}_i\right)$$

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:

$$\text{model initial state } \mathbf{x}_0 = \underset{\text{time } t_0}{\begin{bmatrix} T \\ q_v \\ u \\ v \\ P_s \\ q_{liq} \\ q_{ice} \end{bmatrix}} \xrightarrow{M} \underset{\text{time } t_i}{\begin{bmatrix} T \\ q_v \\ u \\ v \\ P_s \\ q_{liq} \\ q_{ice} \end{bmatrix}} \xrightarrow{H} \tilde{\mathbf{y}}_i = \begin{bmatrix} Rad_{ch1} \\ Rad_{ch2} \\ Rad_{ch3} \end{bmatrix}$$

observation equivalent = satellite cloudy radiances time t_i

M = forecast model with physics

H = radiative transfer model

Why do we need physical parametrizations in DA?

Tangent-linear operators are applied to perturbations:

time t_0 → time t_i

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

diagnostic variables (δq_{liq}, δq_{ice})

Adjoint operators are applied to cost function gradient:

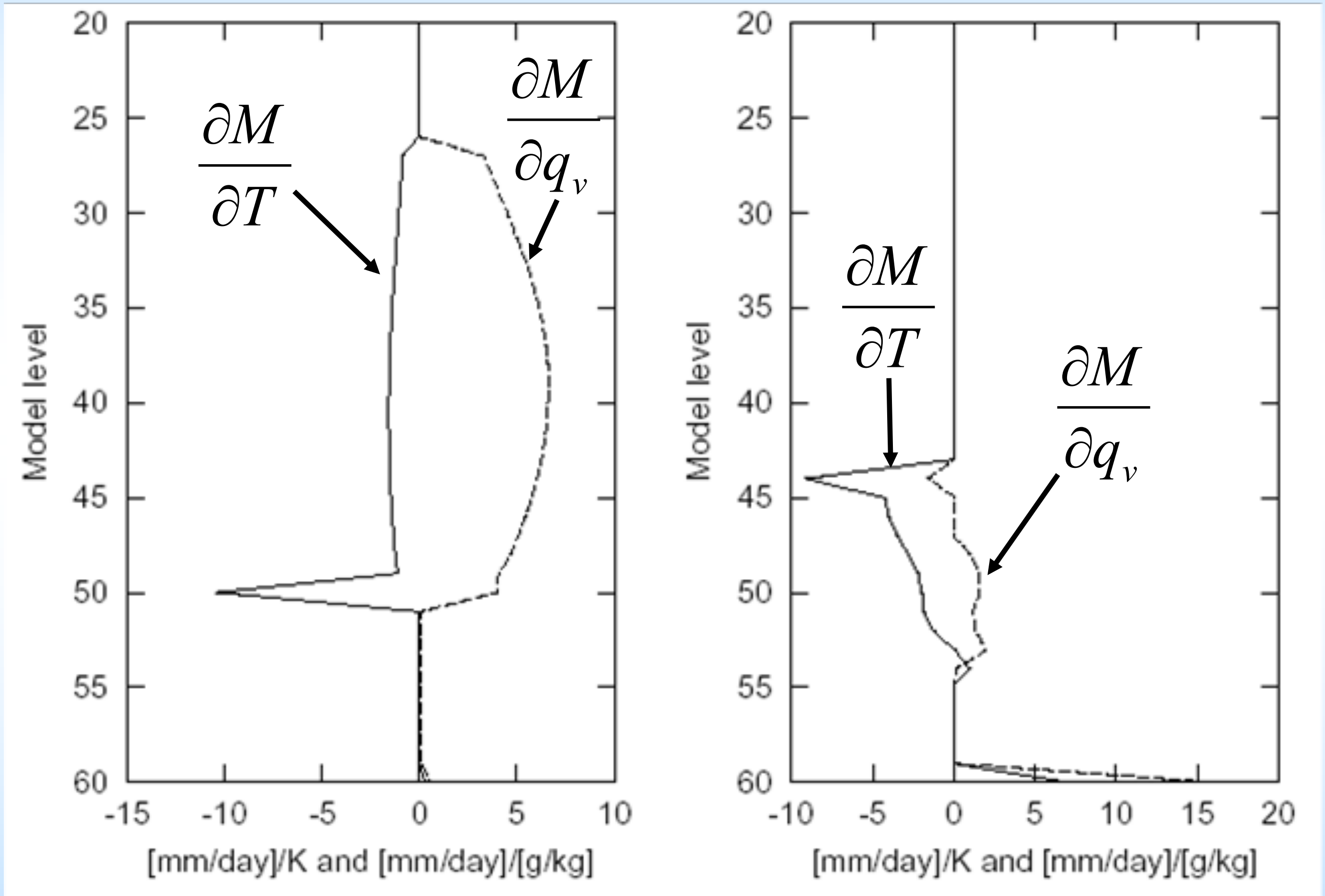
time t_i → time t_0

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

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

M: input = model state (T, q_v) → 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 oper 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:** $\delta Z = -(2a / X^3)\,\delta X + b \log(W)\,\delta Y + (b\,Y / W)\,\delta W$

- **Adjoint code:**

$$\delta X^* = 0$$
$$\delta Y^* = 0$$
$$\delta W^* = 0$$

$$\delta X^* = \delta X^* - (2a / X^3)\,\delta Z^*$$
$$\delta Y^* = \delta Y^* + b \log(W)\,\delta Z^*$$
$$\delta W^* = \delta W^* + (b\,Y / W)\,\delta Z^*$$

$$\delta Z^* = 0$$

The adjoint can be obtained through transposition of the tangent-linear operator, by manual line-by-line coding, or using an automatic adjoint coding software (but latter code will usually not be optimized).

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:

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

Example of output from a successful tangent-linear test:

Tiny perturbations

λ	RATIO
0.1E-09	0.9994875881543574E+00
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	0.9999996111338369E+00
0.1E-03	0.9999953179193711E+00
0.1E-02	0.9999724488345042E+00
0.1E-01	0.9998727842790062E+00
0.1E+00	0.9978007454264978E+00
0.1E+01	0.9683066504549524E+00

Larger perturbations

Machine precision reached

Improvement when perturbation size decreases

Testing the adjoint code

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

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

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

Example of output from a successful adjoint test:

$$<\mathbf{M}\,\delta\mathbf{x}, \qquad \delta\mathbf{y}> = -0.13765102625164\text{E-}01$$

$$< \qquad \delta\mathbf{x}, \mathbf{M}^T\delta\mathbf{y}> = -0.13765102625168\text{E-}01$$

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)!

Testing the adjoint code

At ECMWF, the adjoint is tested for multiple dates and configurations of the linearized physics → tabulated number of common digits:

AD test, exper ca**
TL399 L137 +12, cy47r1, 20 members

Number of matching digits

Members \ Physics configurations	1	2	3	4	5	6	7	8	9	10
20	7	7	13	10	13	12	11	14	11	12
19	8	8	13	11	14	13	14	14	13	12
18	9	9	13	10	13	11	11	12	11	11
17	13	13	13	13	10	13	13	12	12	14
16	9	9	14	11	13	14	15	15	14	9
15	10	10	15	11	15	14	14	13	14	14
14	11	11	14	13	14	14	14	15	15	12
13	10	10	14	12	14	15	14	15	14	13
12	9	9	14	10	14	13	13	14	12	12
11	9	9	14	11	13	12	11	14	12	13
10	9	9	11	10	10	12	14	12	13	12
9	8	8	14	10	14	12	11	14	12	11
8	8	8	14	9	14	13	9	14	13	13
7	9	9	15	11	15	13	12	14	13	13
6	10	10	12	10	12	10	12	12	10	12
5	9	9	13	10	13	11	12	13	11	12
4	10	10	14	12	13	13	13	15	13	12
3	10	10	15	11	14	12	13	14	13	12
2	9	9	14	11	14	12	13	15	12	12
1	10	10	13	11	13	11	11	13	11	14

AD test, exper au**
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Members \ Physics configurations	1	2	3	4	5	6	7	8	9	10
20	11	11	13	13	13	13	13	14	13	12
19	14	14	13	14	14	14	14	13	13	14
18	12	13	12	12	12	12	12	13	12	12
17	12	12	12	13	12	13	13	13	14	13
16	11	11	14	12	15	15	14	15	14	11
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9	14	14	13	13	14	14	13	12	13	13
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7	12	13	14	13	14	14	14	14	15	12
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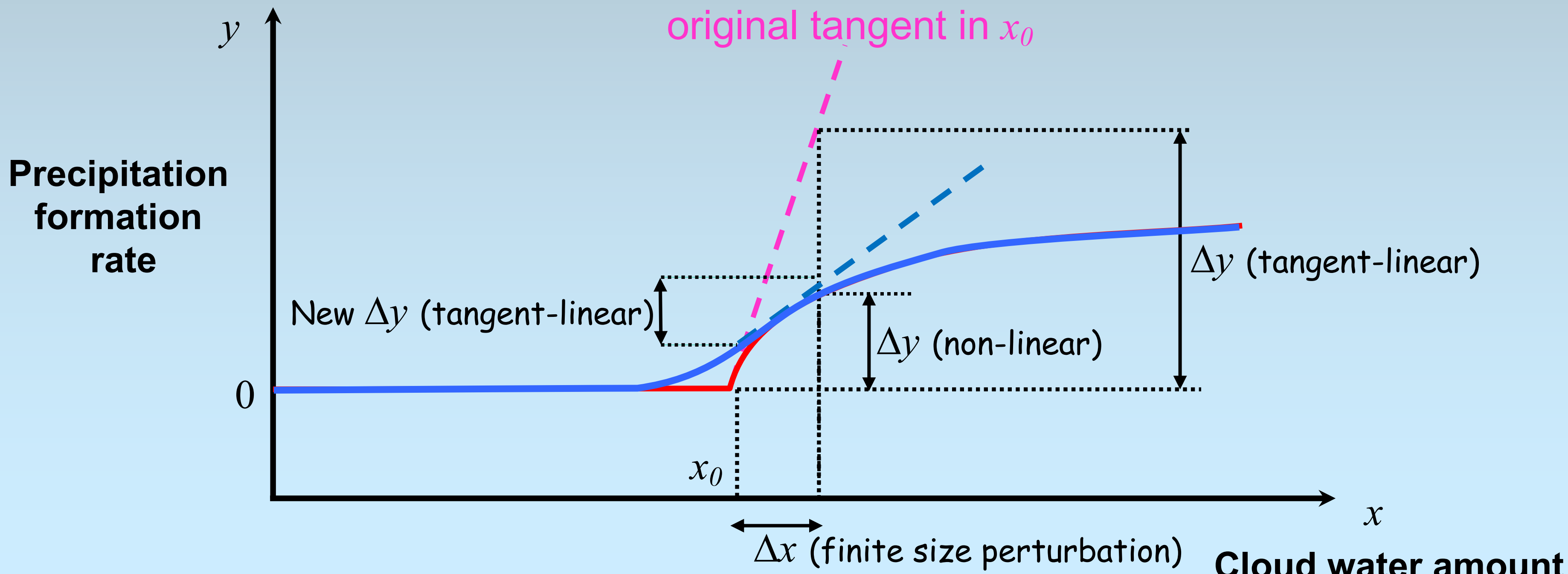
3	12	12	14	14	14	15	15	13	14	13
2	13	13	14	12	15	15	13	15	14	13
1	13	13	13	15	13	13	13	13	12	13

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.**



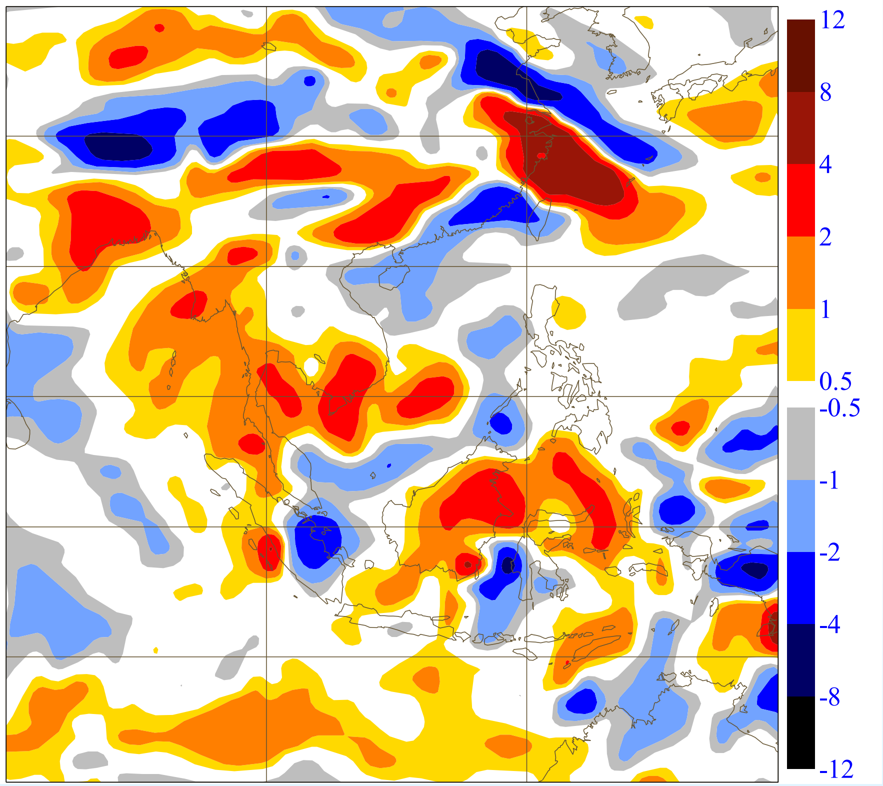
ECMWF

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.

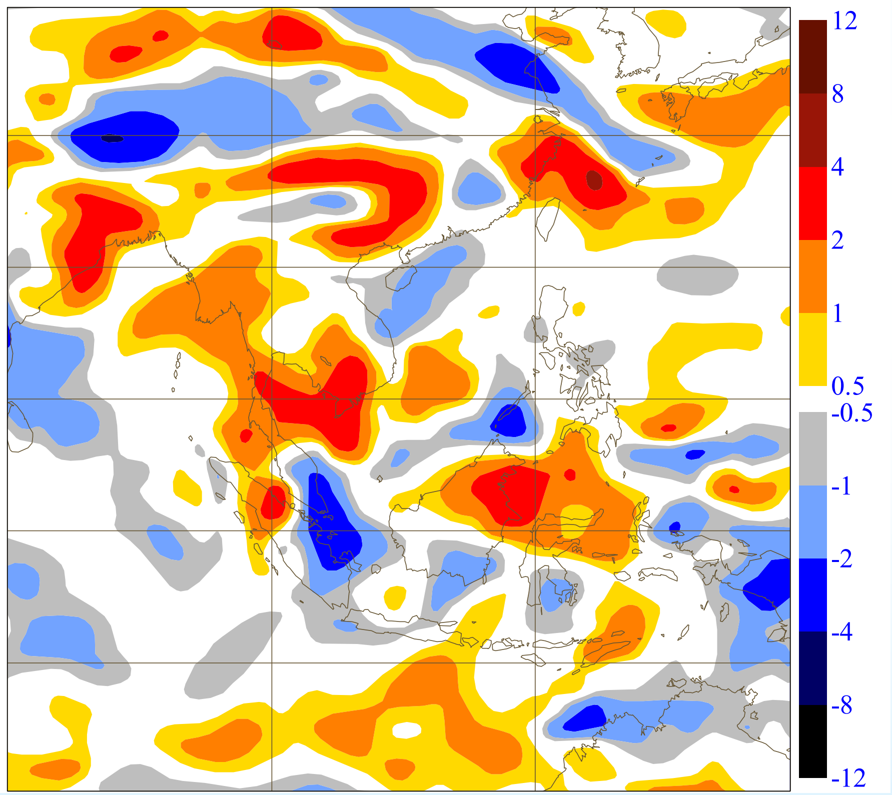
Nonlinear finite difference:

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



from M. Janisková

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



with perturbation reduction in autoconversion

ECMWF

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:

$$M(\mathbf{x}_{an}) - M(\mathbf{x}_{bg}) \leftrightarrow \mathbf{M}(\underbrace{\mathbf{x}_{an} - \mathbf{x}_{bg}})$$

typical size of 4D-Var analysis increments

Diagnostics:

- mean absolute errors: $\varepsilon = \overline{\left| \left[M(\mathbf{x}_{an}) - M(\mathbf{x}_{bg}) \right] - \mathbf{M}(\mathbf{x}_{an} - \mathbf{x}_{bg}) \right|}$
- relative error change: $\dfrac{\varepsilon_{\mathrm{EXP}} - \varepsilon_{\mathrm{REF}}}{\varepsilon_{\mathrm{REF}}} \times 100\%$ (improvement if < 0)
- here: REF = adiabatic run (i.e. no physical parametrizations in tangent-linear)

Impact of linearized physics on tangent-linear approximation

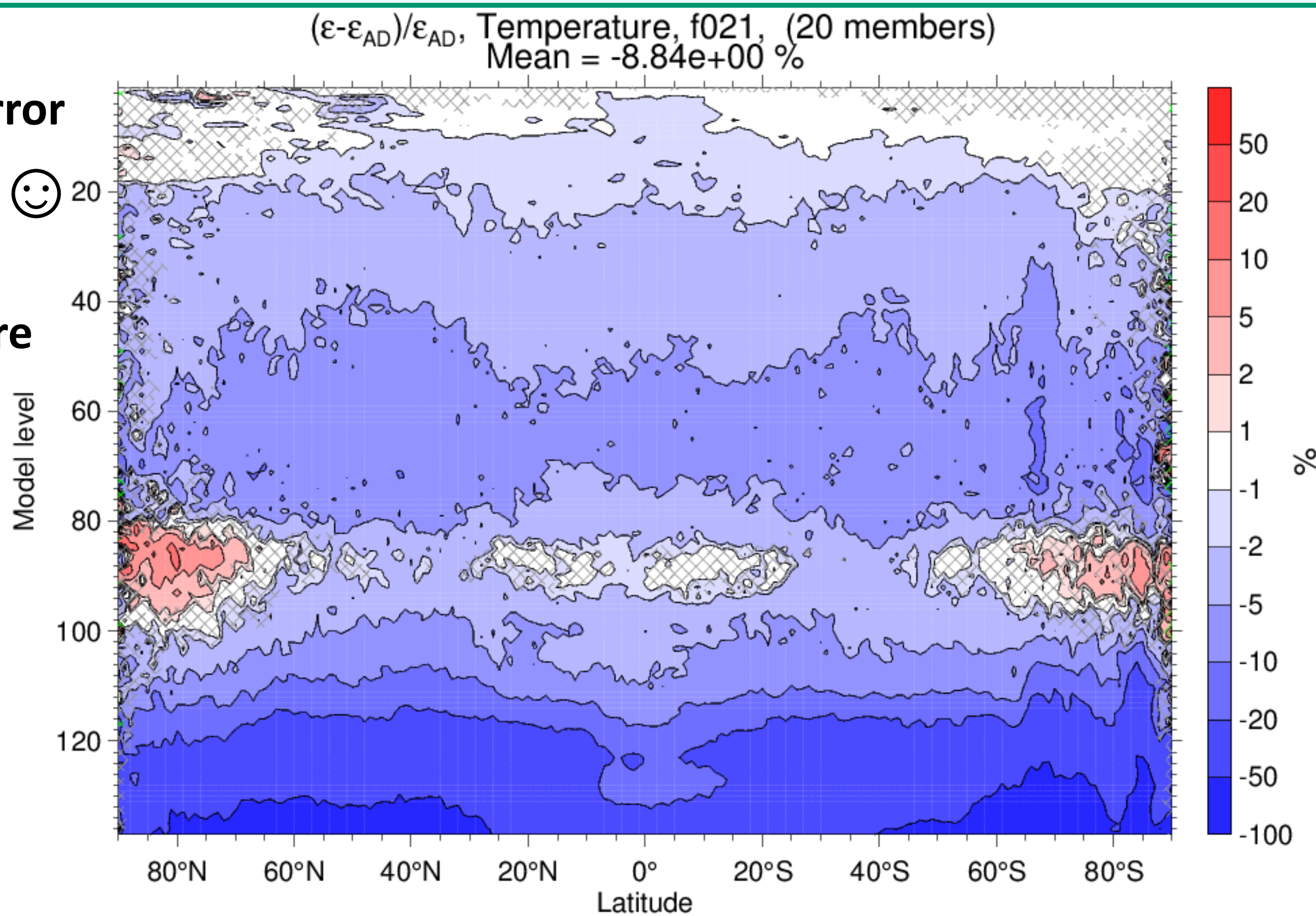
Zonal mean cross-section of change in TL error when TL includes:

VDIF + orog. GWD + SURF

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

Blue = TL error reduction = ☺

Temperature



Impact of linearized physics on tangent-linear approximation

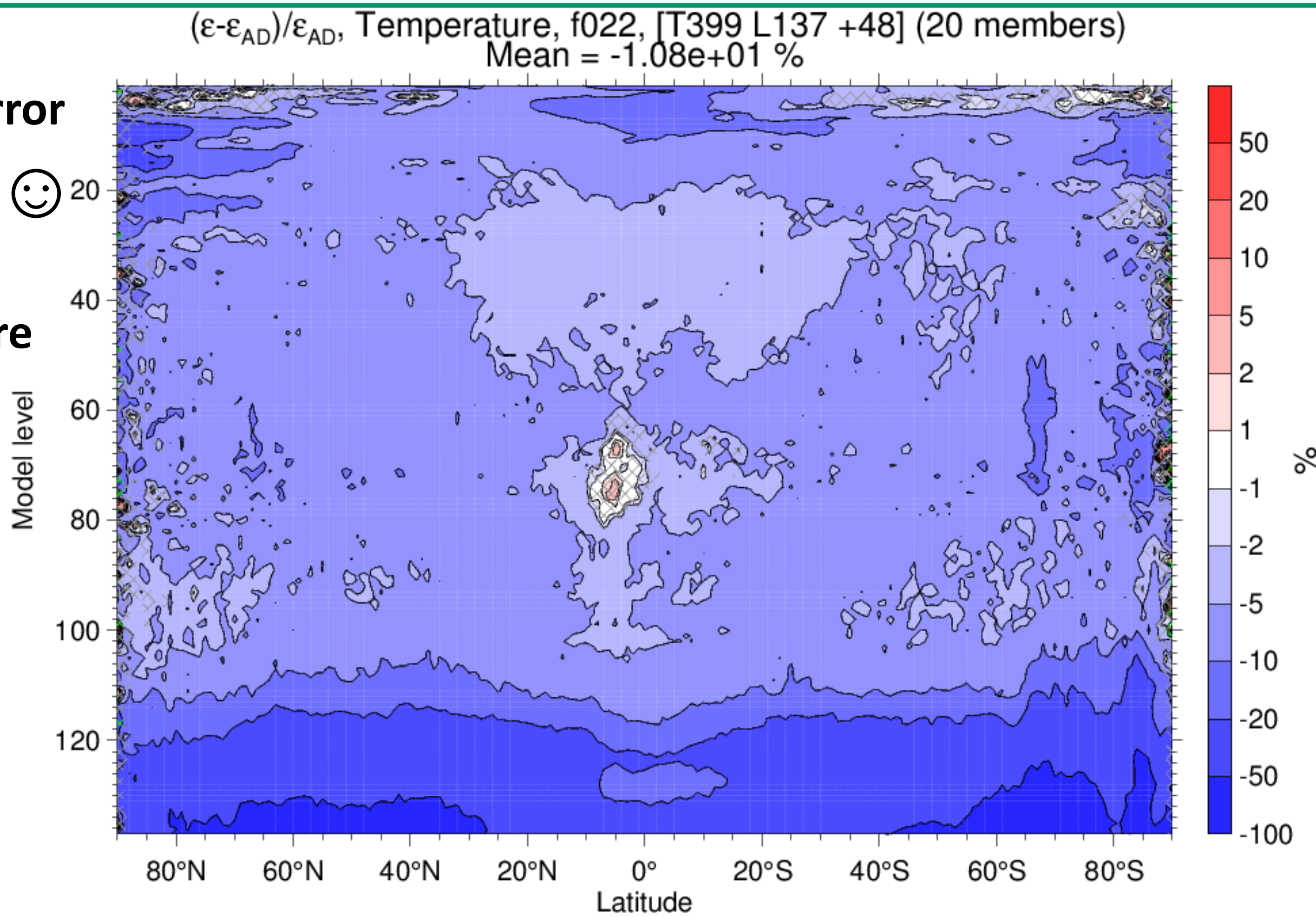
Zonal mean cross-section of change in TL error when TL includes:

VDIF + orog. GWD + SURF + RAD

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

Blue = TL error reduction = ☺

Temperature



Impact of linearized physics on tangent-linear approximation

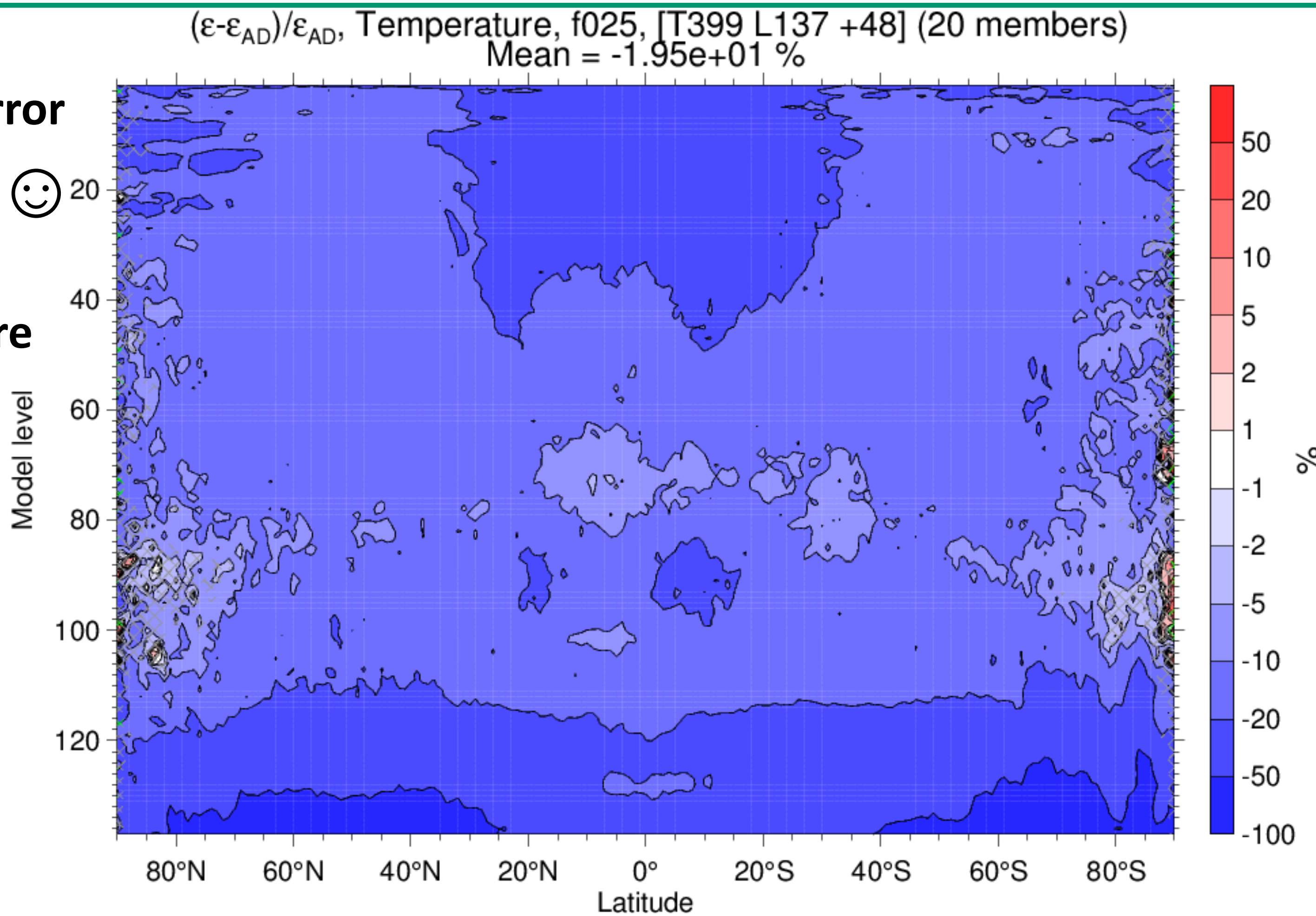
Zonal mean cross-section of change in TL error when TL includes:

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

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

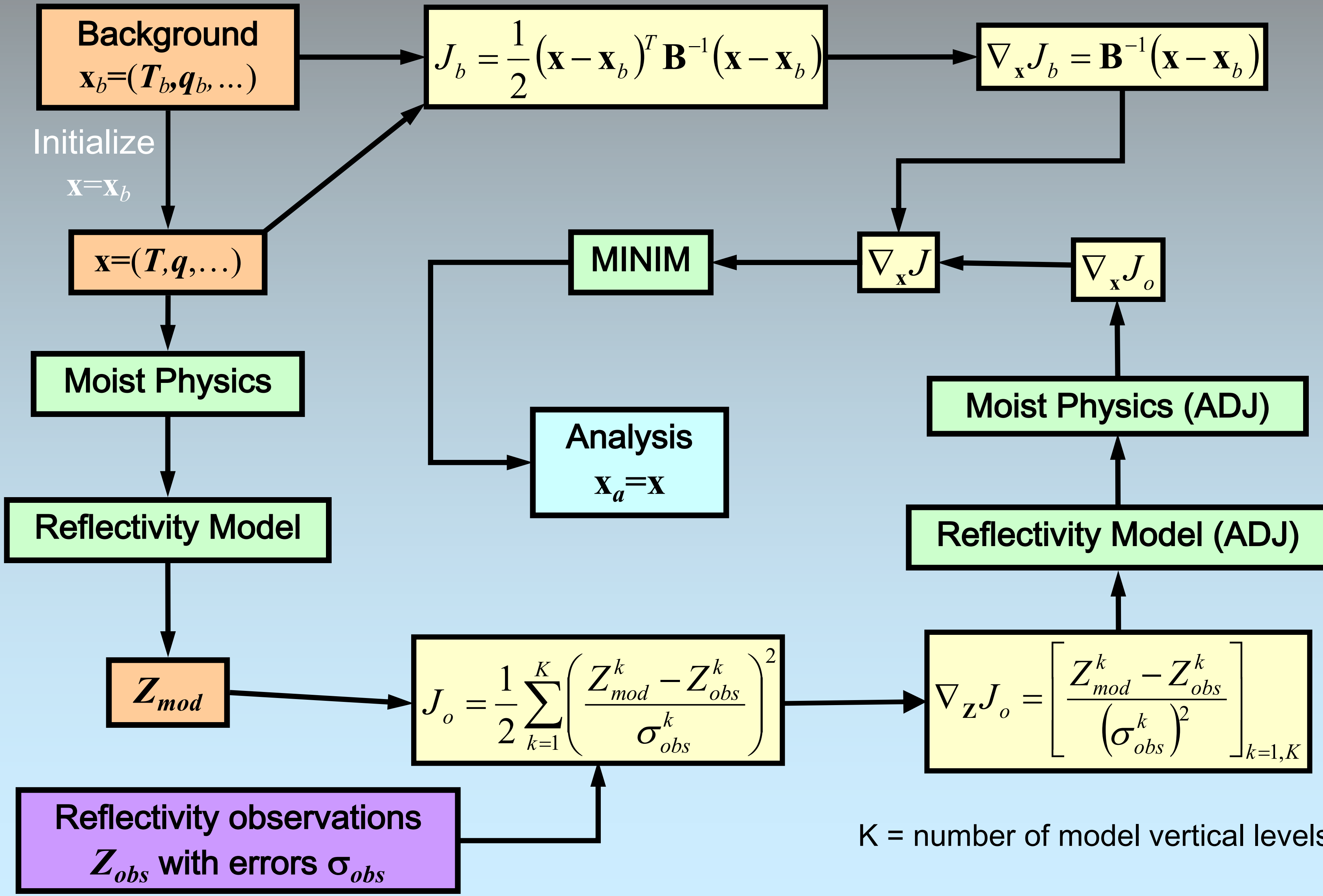
Blue = TL error reduction = ☺

Temperature



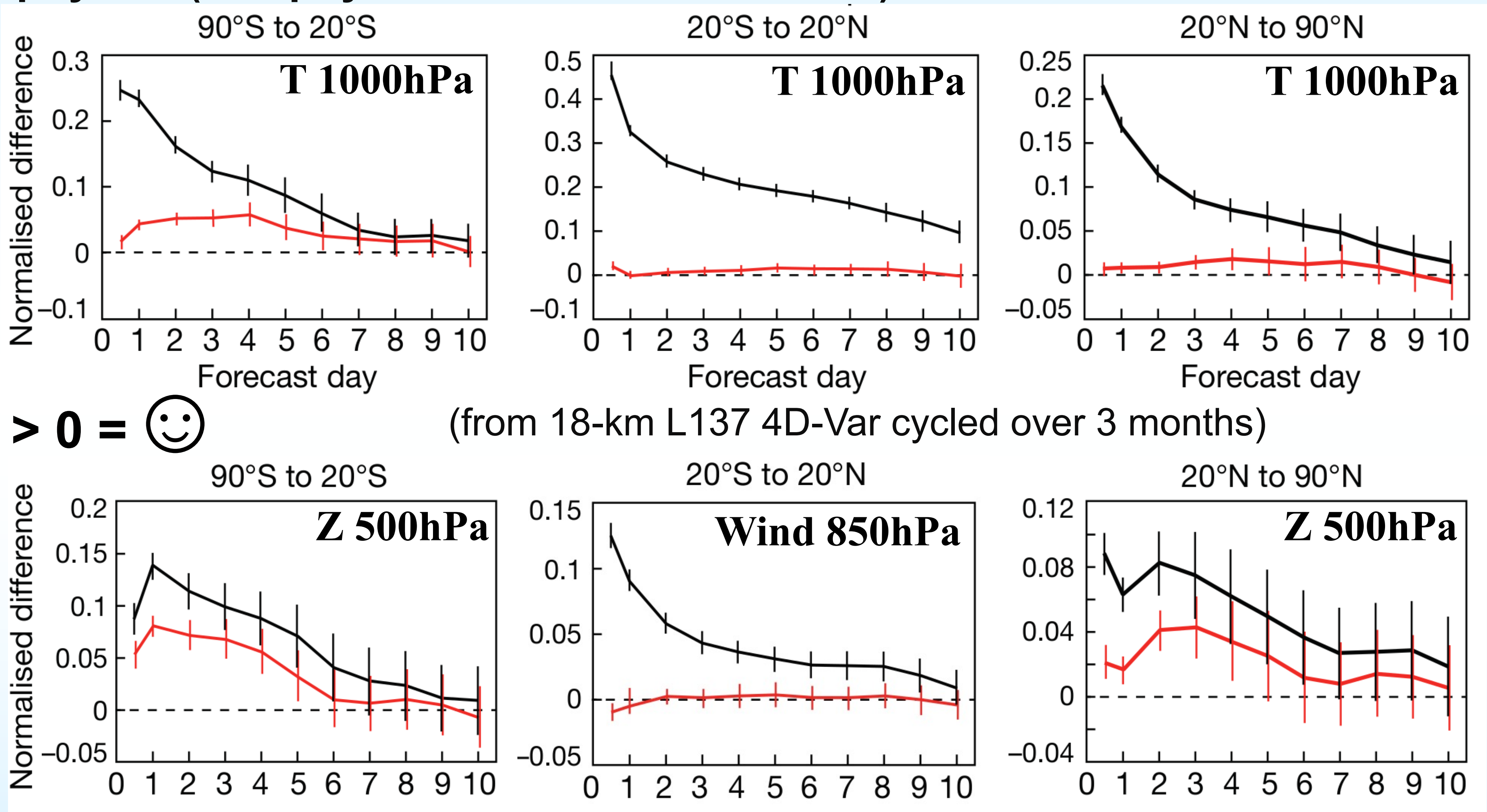
Applications

1D-Var with radar reflectivity profiles



Impact of linearized physics on analyses and forecasts

Relative change in forecast RMS error due to the inclusion of linearized physics (and physics-related observations) in 4D-Var assimilation.



Black line: impact of physics-related obs + linearized physics.

Red line: impact of physics-related obs.

Janisková and Lopez (2023)

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:

$$J = \frac{1}{2}(\mathbf{x}-\mathbf{x}_b)^T \mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}_b) + \frac{1}{2}(\mathbf{p}-\mathbf{p}_b)^T \mathbf{B}_{\mathbf{p}}^{-1}(\mathbf{p}-\mathbf{p}_b)$$

$$+\frac{1}{2}\left(H(\mathbf{x},\mathbf{p})-\mathbf{y}_o\right)^T \mathbf{R}^{-1}\left(H(\mathbf{x},\mathbf{p})-\mathbf{y}_o\right)$$

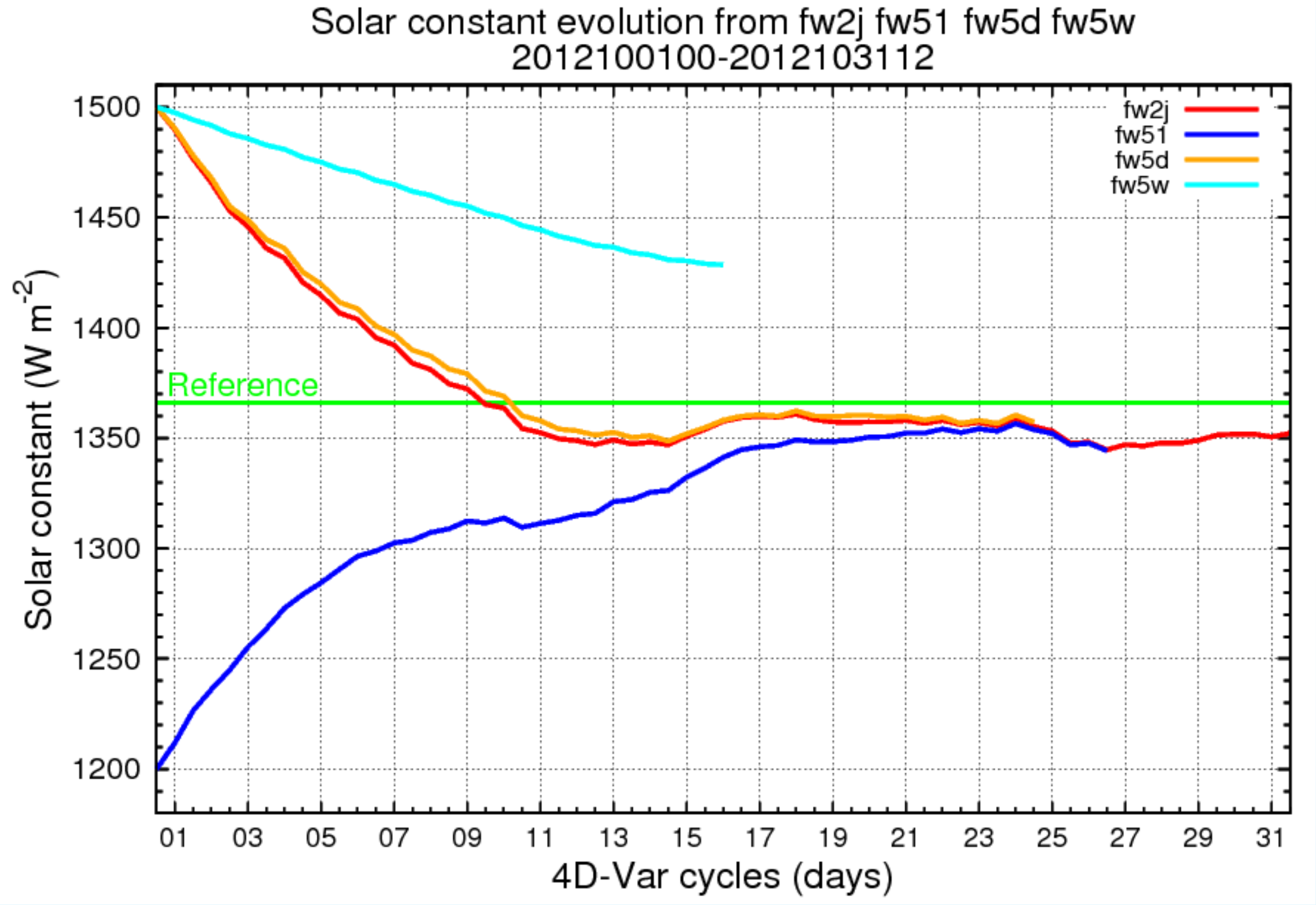
Limitations: Only parameters that are present in both the forecast model and the linearized simplified physics (TL & AD) can be treated in this way.

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

Parameters to be optimized need to be well-constrained by observations.

Physics parameter optimization: an example.

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



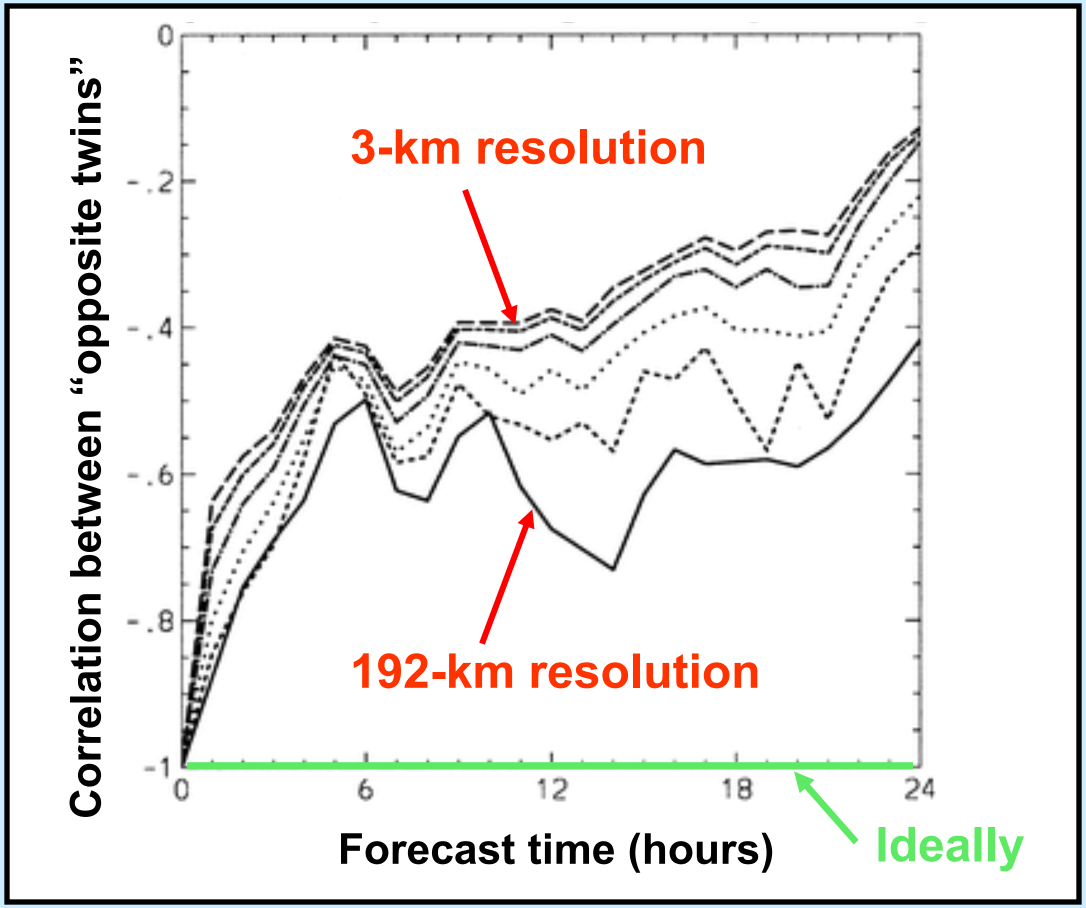
Observations used in 4D-Var manage to constraint the solar constant back to its correct value after 2 weeks or so.

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.

Linearity

☺



→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 validity of the linear hypothesis degrades with increasing resolution and integration length.

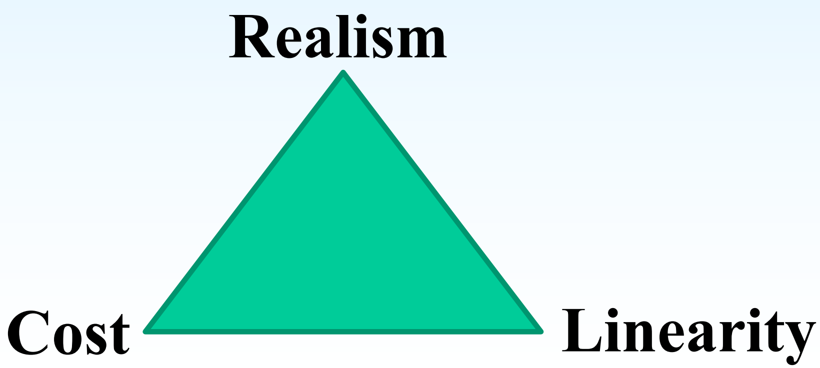
2) Technical:

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:

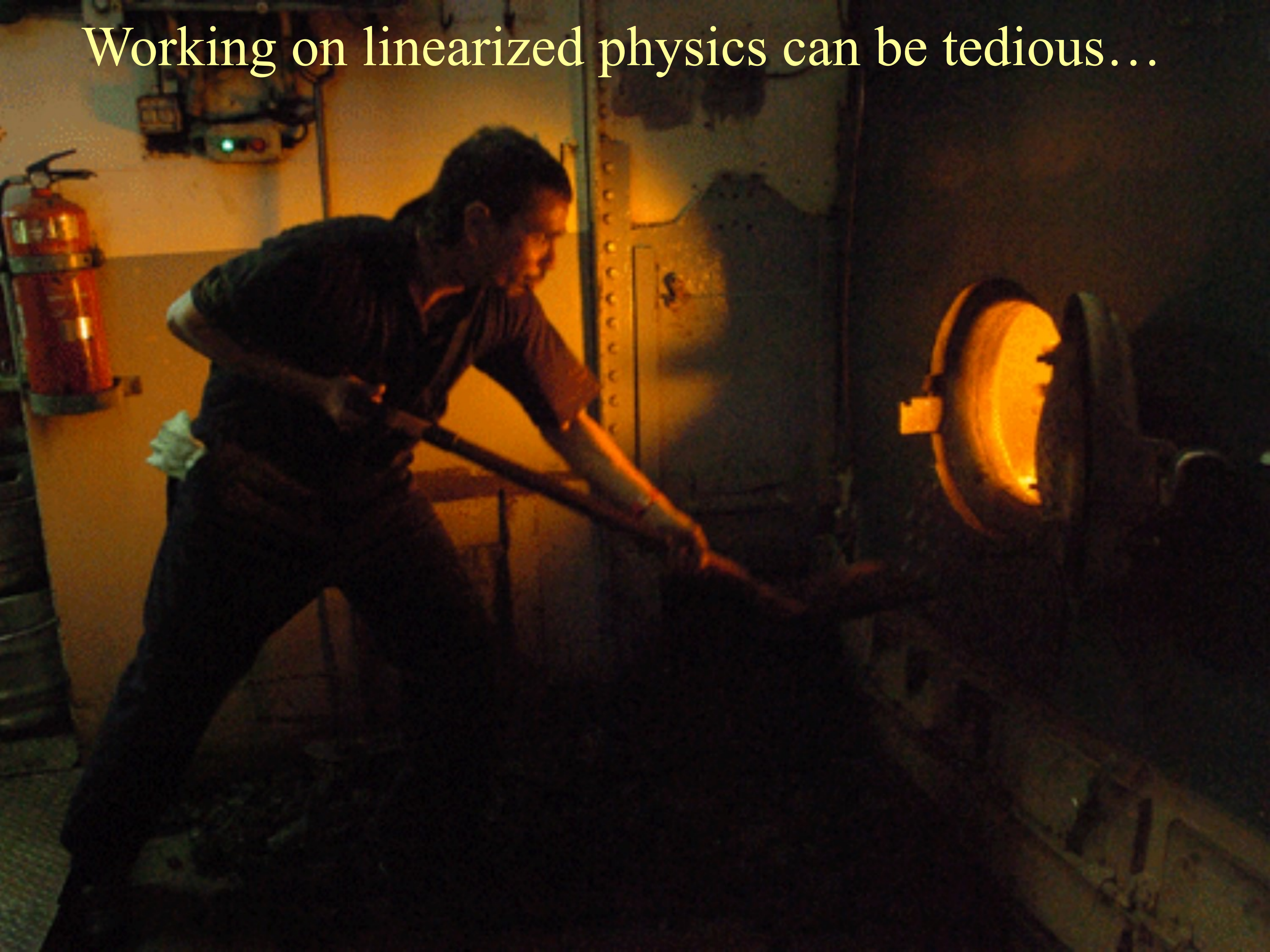


- Alternative data assimilation methods exist that do not require the development of linearized code, but so far none of them has been able to outperform 4D-Var, especially in global models:

  → 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 can 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).**

- **If the current 4D-Var becomes too expensive at very-high resolution, Artificial Intelligence might offer a solution by replacing some of the physical parametrizations with much cheaper equivalents (e.g., based on neural networks). But this is still ongoing research…**

Thank you!

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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 $\mathbf{H}^{\mathrm{T}}$:

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