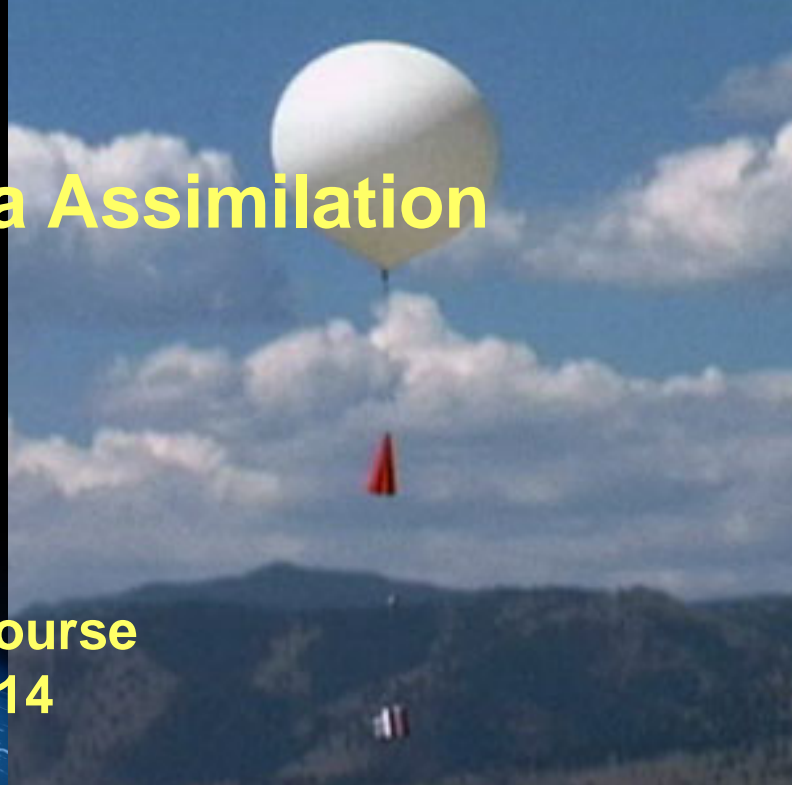# Parametrizations in Data Assimilation

ECMWF Training Course
10-14 March 2014

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(Room 002)

Parametrizations in Data Assimilation

- **Introduction**

- **Why are physical parametrizations needed in data assimilation?**

- **Tangent-linear and adjoint coding**

- **Issues related to physical parametrizations in assimilation**

- **Physical parametrizations in ECMWF's current 4D-Var system**

- **Examples of applications**

- **Summary and conclusions**
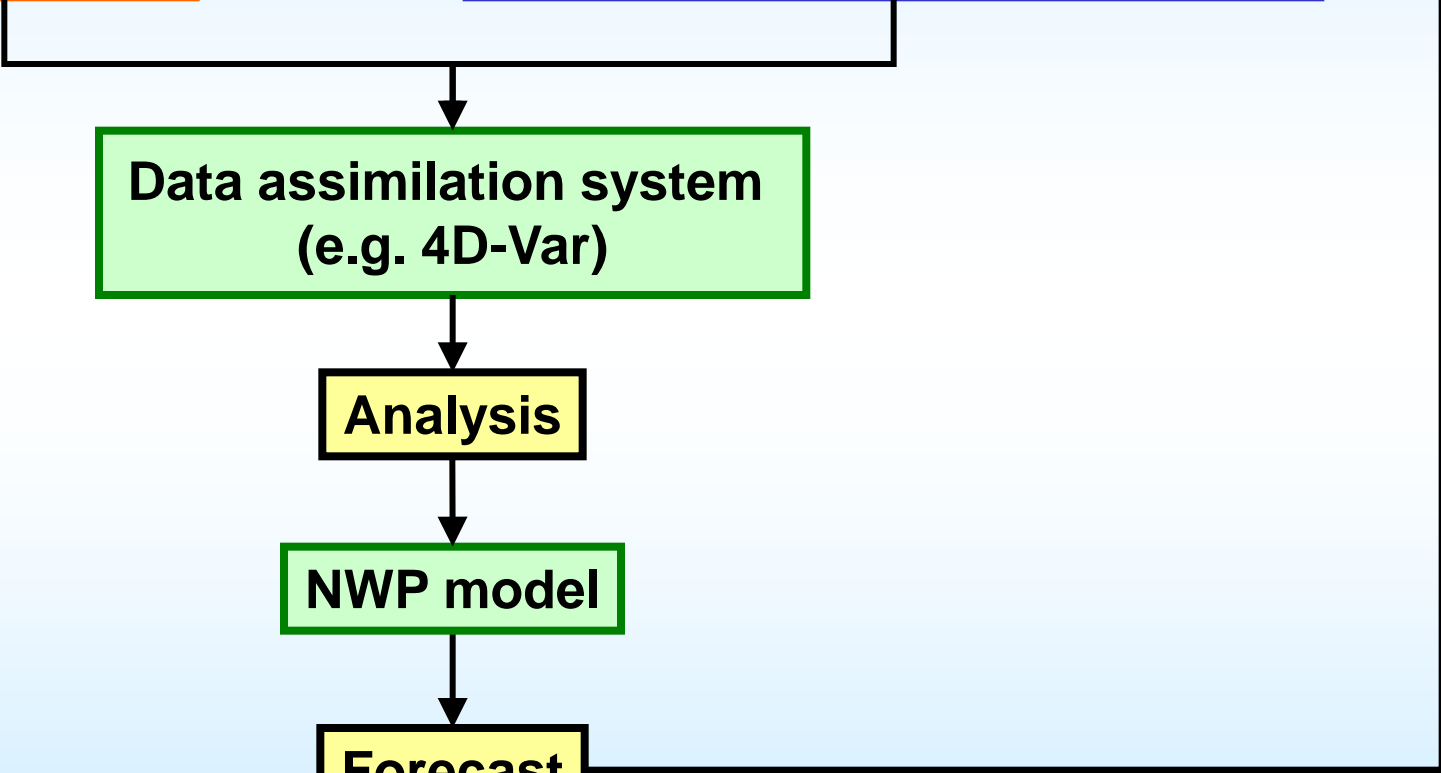
Data assimilation

Observations with errors

a priori **information from model = background state with errors**
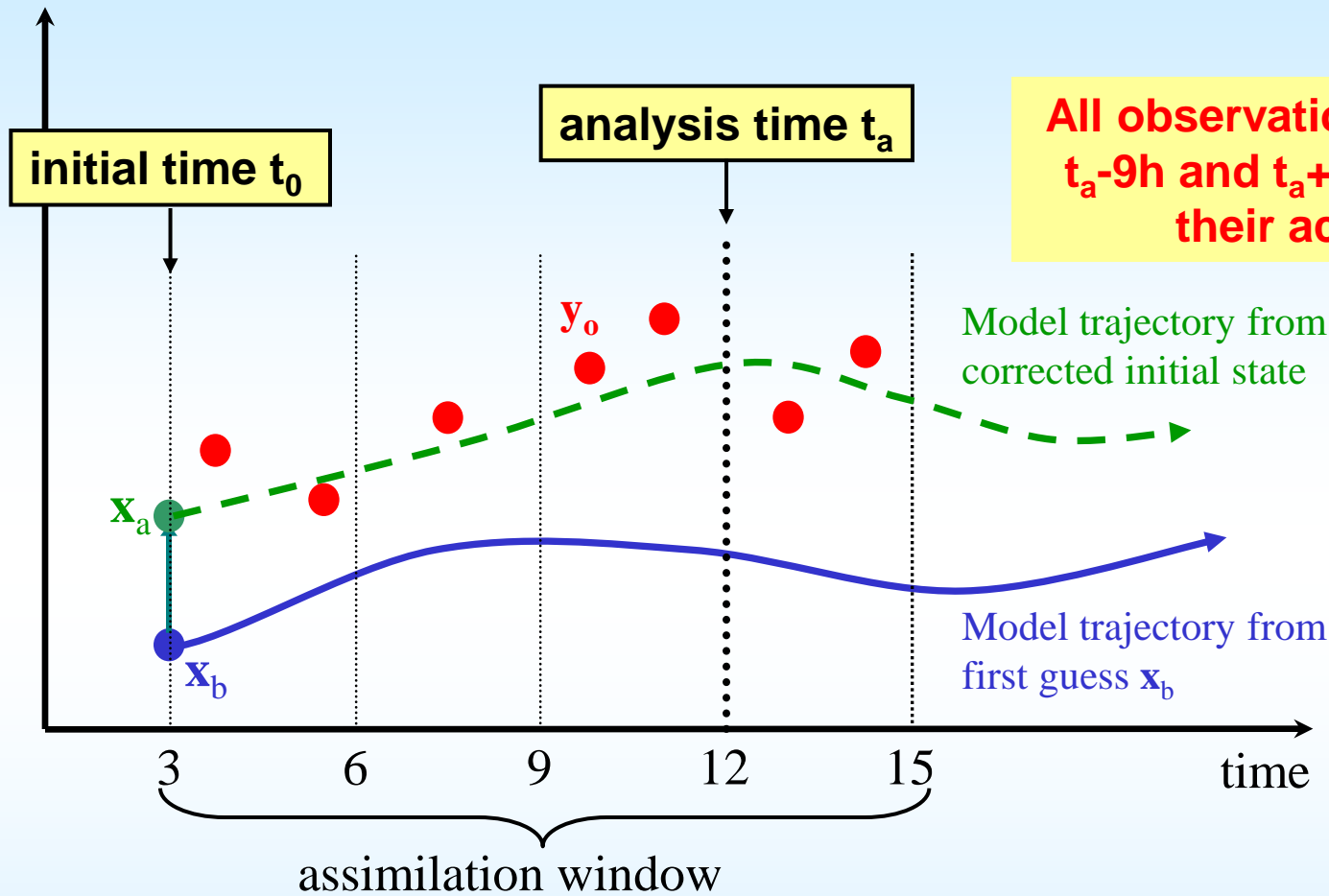
Data assimilation system (e.g. 4D-Var)

Analysis

NWP model

Forecast

4D-Var

model state

initial time t_0

analysis time t_a

All observations y_o between t_a-9h and t_a+3h are valid at their actual time

y_o

Model trajectory from corrected initial state

x_a

x_b

Model trajectory from first guess x_b

3   6   9   12   15   time

assimilation window

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).

$\delta\mathbf{x}_0 = \mathbf{x}_0 - \mathbf{x^b}_0$ (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.

$$\nabla_{\mathbf{x}_0}J = \mathbf{B}^{-1}\delta\mathbf{x}_0 + \sum_{i=1}^{n}\boxed{\mathbf{M}_i^T[t_i,t_0]}\mathbf{H}_i^T\mathbf{R}_i^{-1}\left(\mathbf{H}_i\mathbf{M}_i\delta\mathbf{x_0} - \mathbf{d}_i\right)$$
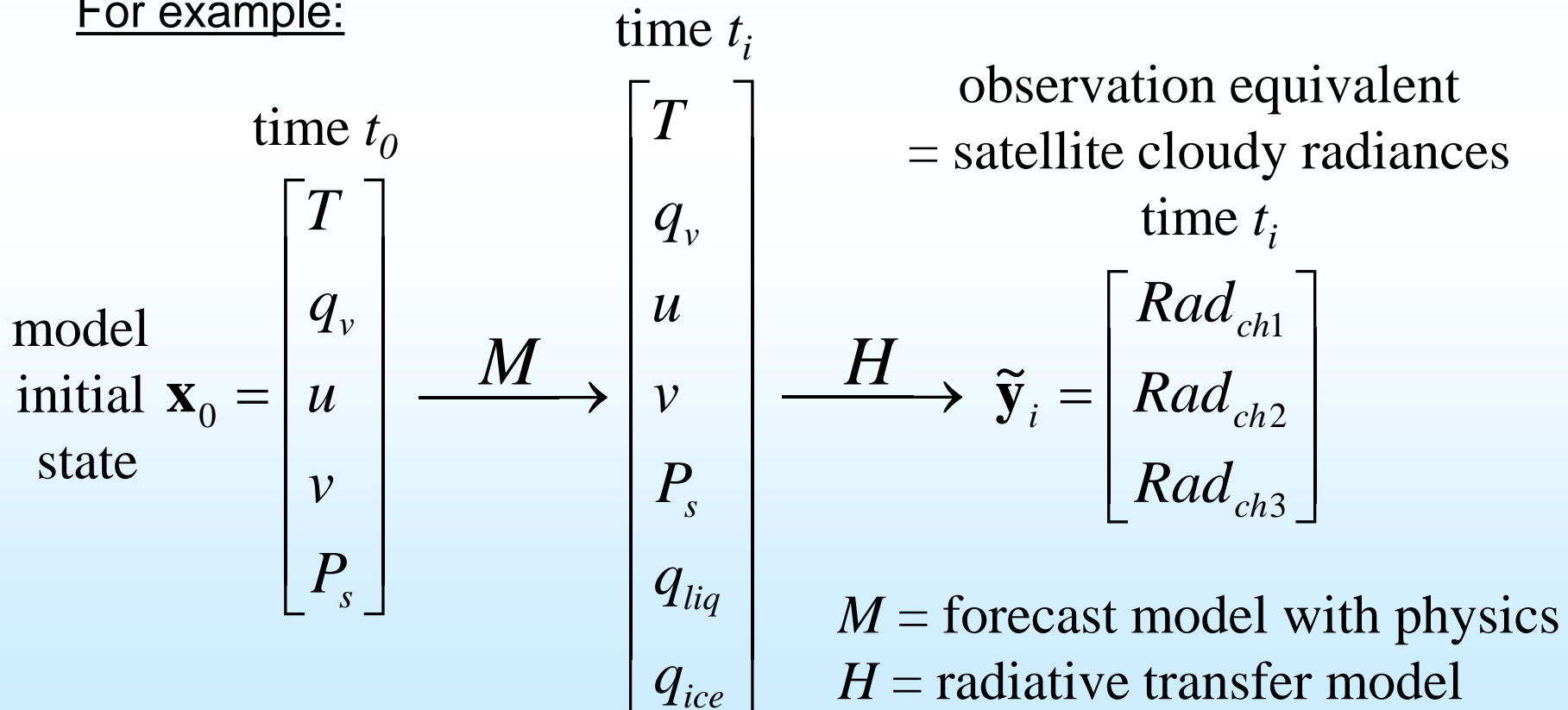
Adjoint of forecast model with <u>simplified</u> linearized physics
(simplified: to reduce computational cost and to avoid non-linear processes)

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:

model initial state

$$\mathbf{x}_0 = \begin{bmatrix} T \\ q_v \\ u \\ v \\ P_s \end{bmatrix}$$

time t_0

$$\xrightarrow{\ M\ }$$

$$\begin{bmatrix} T \\ q_v \\ u \\ v \\ P_s \\ q_{liq} \\ q_{ice} \end{bmatrix}$$

time t_i

$$\xrightarrow{\ H\ }$$

$$\tilde{\mathbf{y}}_i = \begin{bmatrix} Rad_{ch1} \\ Rad_{ch2} \\ Rad_{ch3} \end{bmatrix}$$

observation equivalent = satellite cloudy radiances
time t_i

M = forecast model with physics
H = radiative transfer model

Tangent-linear operators are applied to perturbations:

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

time t_0 \quad\quad\quad time t_i

Adjoint operators are applied to cost function gradient:

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

time t_i \quad\quad\quad time t_0

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
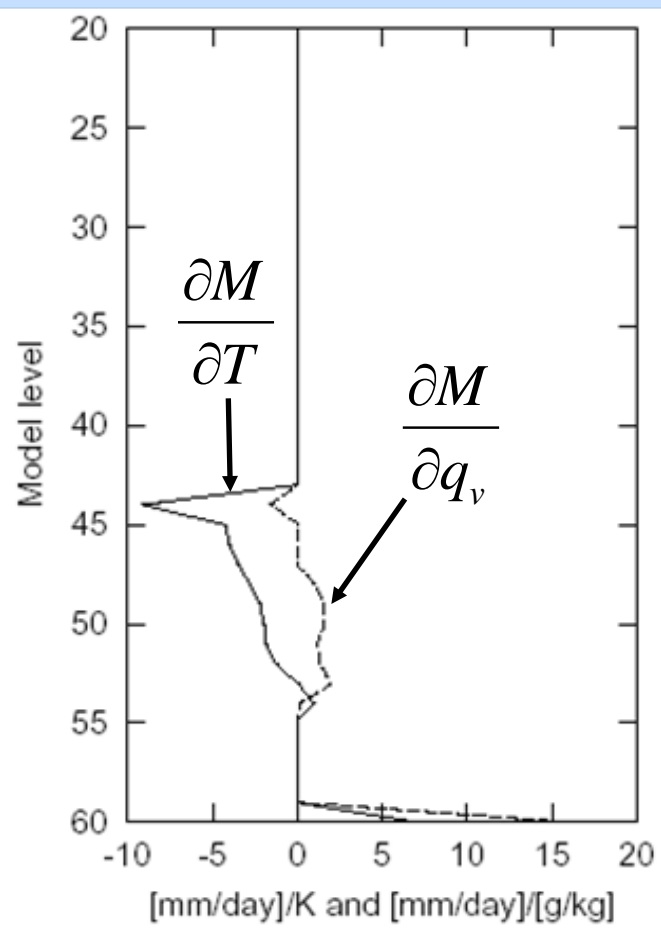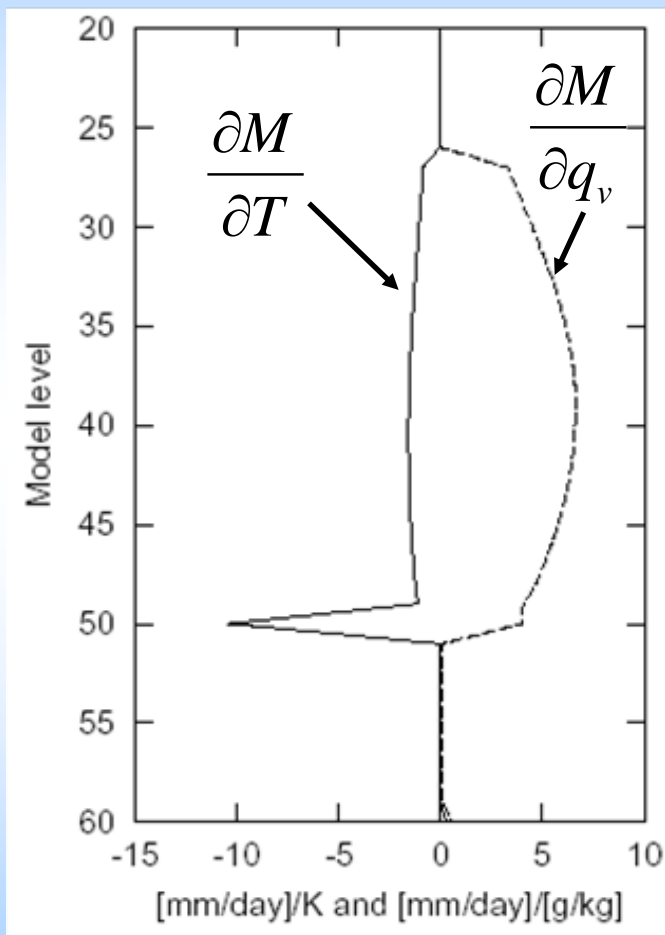
from Marécal and Mahfouf (2002)

Betts-Miller (adjustment scheme)

Tiedtke (ECMWF's oper mass-flux scheme)

- **Taylor formula:**

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

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	0.9993727842790062E+00
0.1E+00	0.9978007454264978E+00
0.1E+01	0.9583066504549524E+00

Perturbation scaling factor

machine precision reached

- adjoint identity:

$$\forall \mathbf{x}, \forall \mathbf{y} \quad < M'.\mathbf{x}, \mathbf{y} >=< \mathbf{x}, \mathbf{M}^*.\mathbf{y} >$$

< F(X) , Y > = -.13765102625251640000E-01
< X , F*(Y) > = -.13765102625251680000E-01
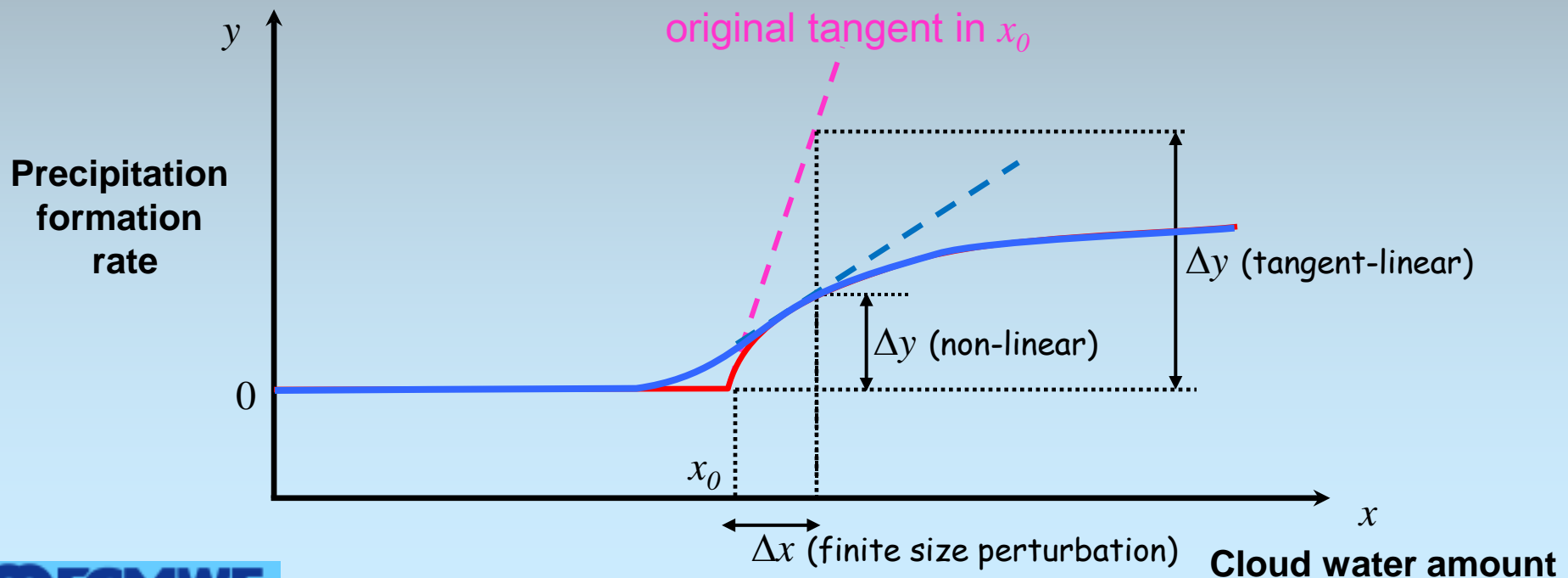
ratio of norms = 1.00000000000000005

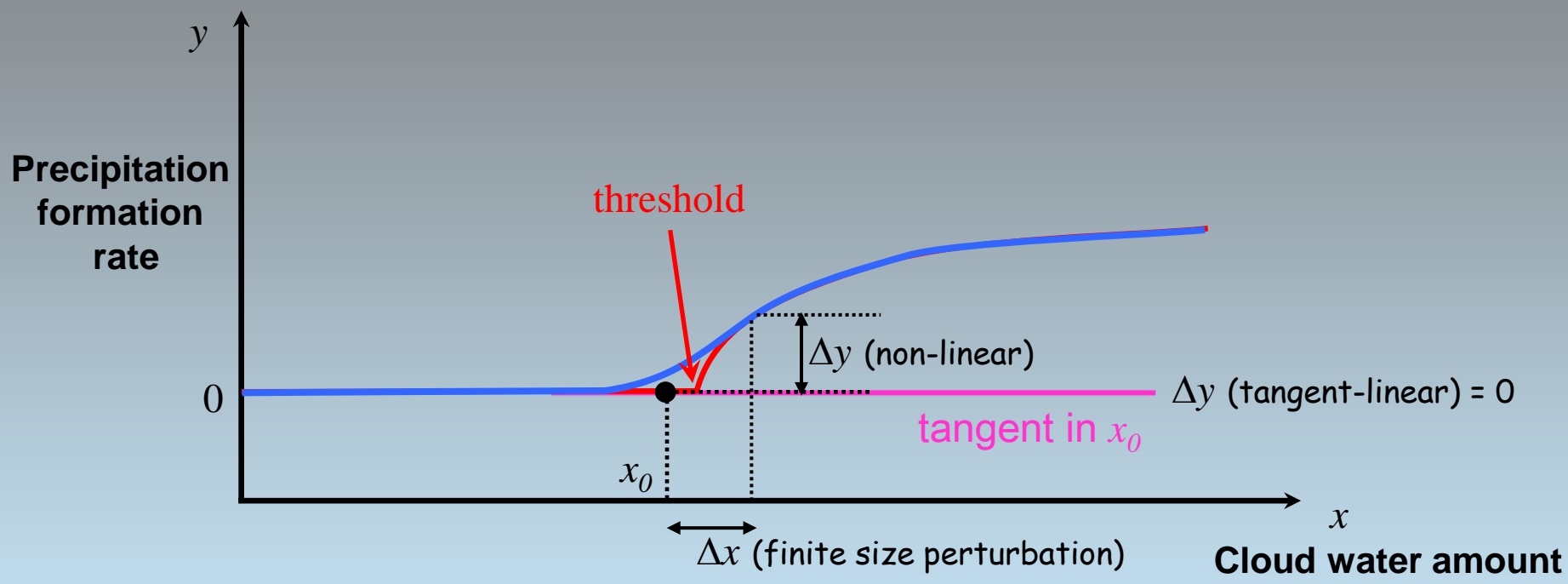THE DIFFERENCE IS 11.351 TIMES THE ZERO OF THE MACHINE

The adjoint test should be correct at the level of machine precision (i.e. 13 to 15 digits, typically).
If not, something is still wrong somewhere in the code!

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.**

original tangent in x_0

y

Precipitation formation rate

Δy (tangent-linear)

Δy (non-linear)

0

x_0

x

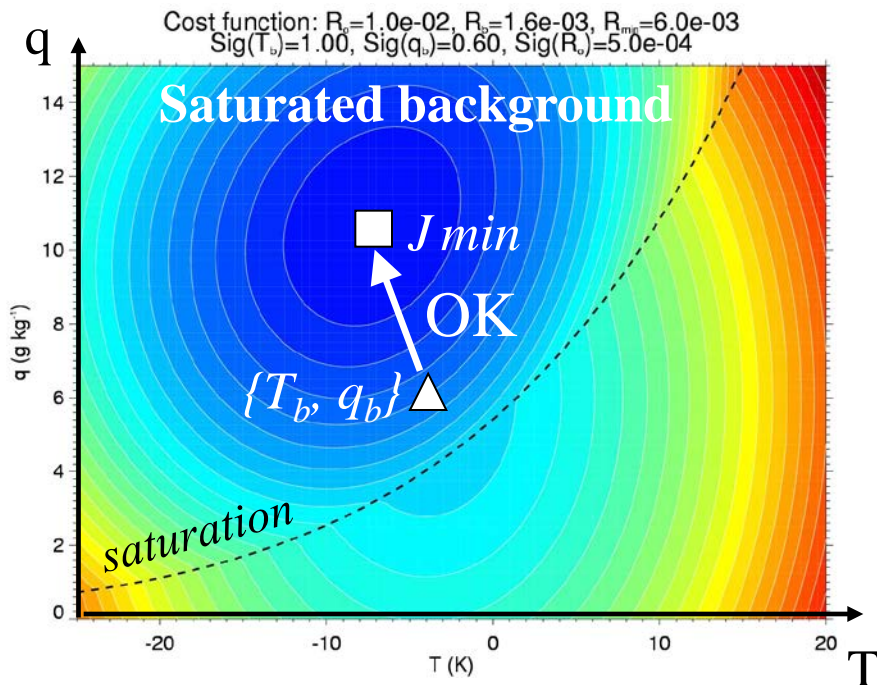Δx (finite size perturbation)

Cloud water amount

ECMWF

Illustration of discontinuity effect on cost function shape:

Model background = $\{T_b, q_b\}$; Observation = RR_{obs}
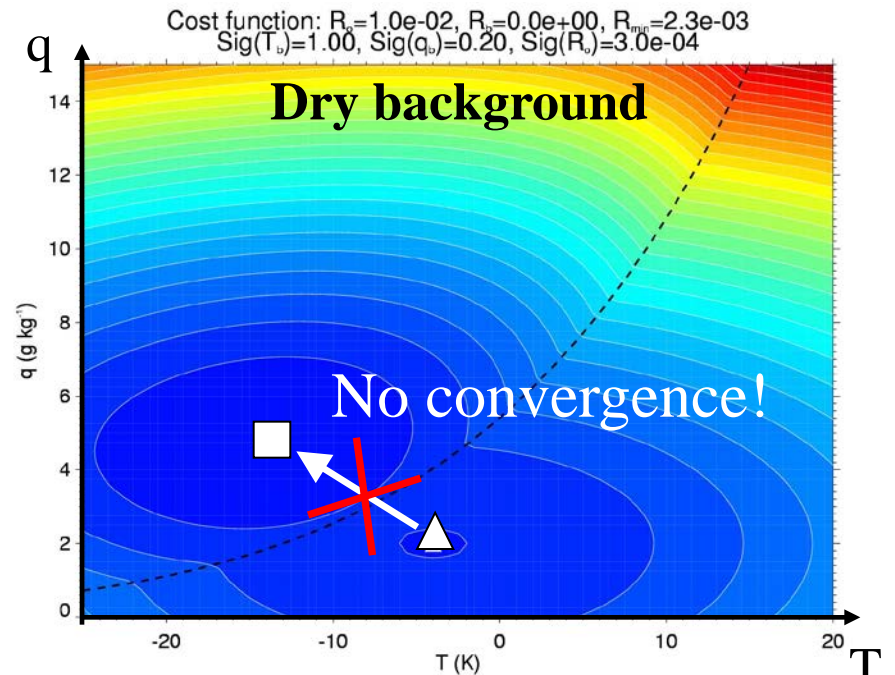
Simple parametrization of rain rate:

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

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

Single minimum of cost function   Several local minima of cost function

REGULARIZATION OF VERTICAL DIFFUSION SCHEME

- perturbation of the exchange coefficients is neglected, $K' = 0$ *(Mahfouf, 1999)*

  (*exchange coefficient K is given by* $K = l^2 \left\| \frac{\partial \mathbf{V}}{\partial z} \right\| f(Ri)$)

- original computation of the Richardson number Ri

  $Ri = \frac{g}{c_p T} \frac{\frac{\partial s}{\partial z}}{\left\| \frac{\partial \vec{v}}{\partial z} \right\|^2}$ modified as
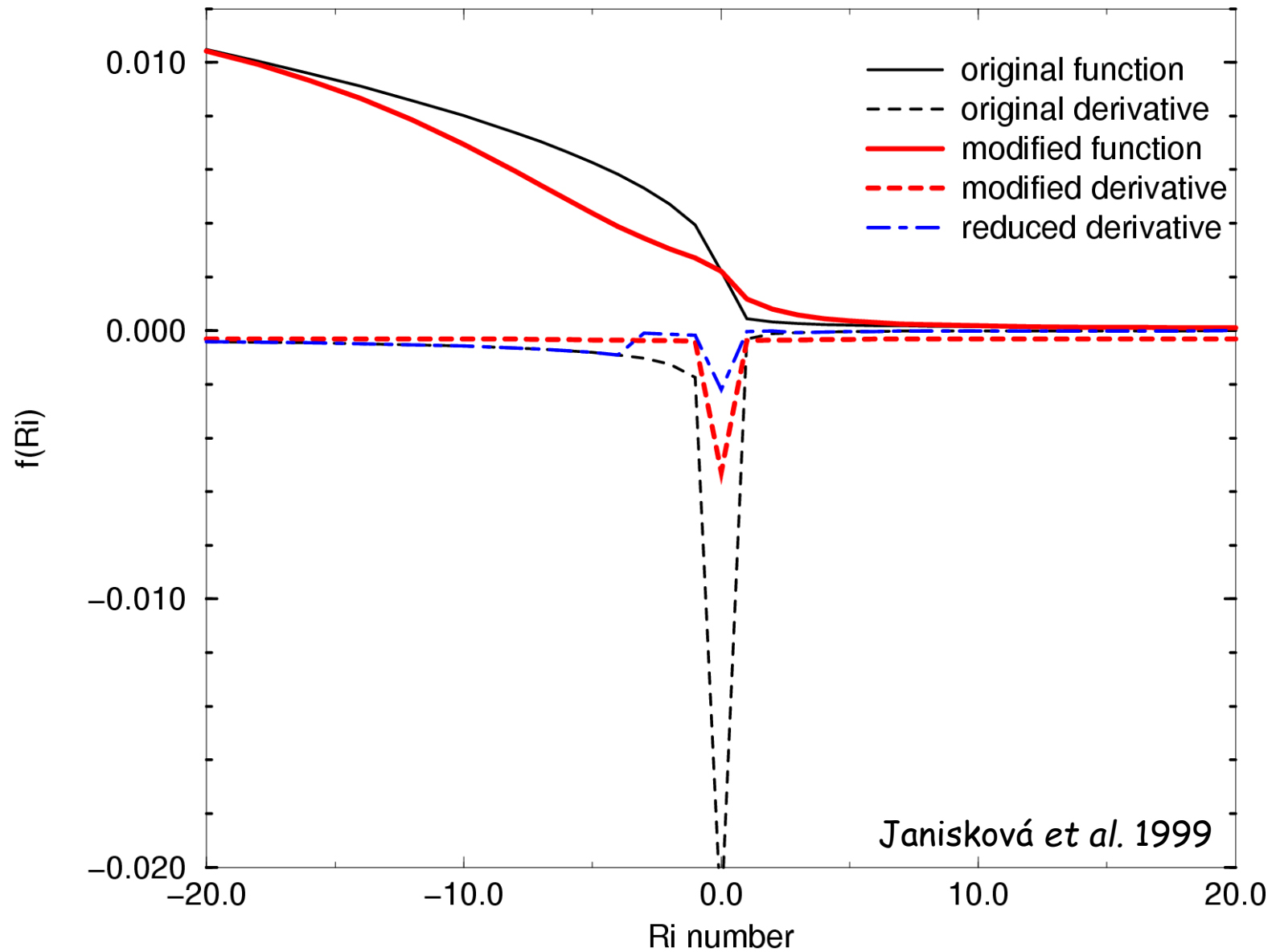
  $$\boxed{Ri' = \frac{g}{c_p T} \frac{\frac{\partial s}{\partial z}}{\| \frac{\partial \vec{v}}{\partial z} \|^2 + c}}$$
  with a time constant $c = \frac{a}{(\Delta t_{phys})^2}$

  where Δt_{phys} is the physical time step

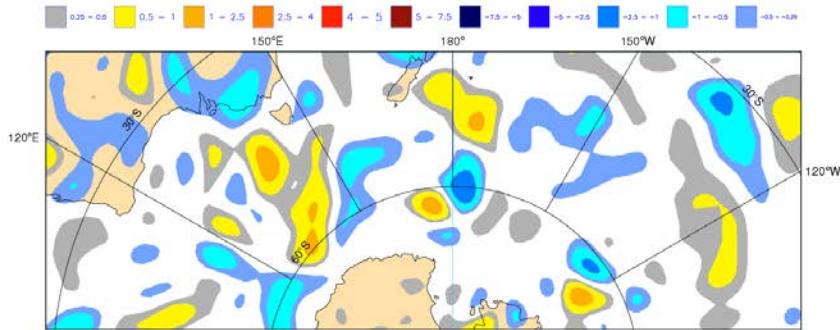 a is a tuning parameter of the regularization step

- reducing a derivative $f(Ri)$ by a factor 10 in the central part (around the point of singularity) - *(Janisková et al., 1999)*

function of the Richardson number f(Ri)
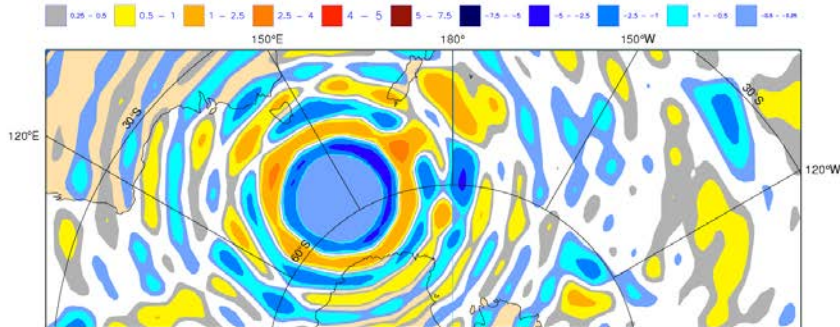
Janisková *et al.* 1999

Importance of regularization to prevent instabilities in tangent-linear model
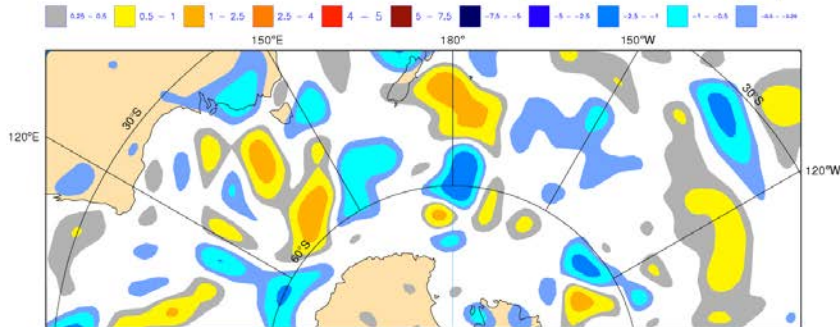

lv31 T 1999-06-15 12h fc t+24 (NL reference)

lv31 T 1999-06-15 12h fc t+24 (TL with K'.ne. 0)

lv31 T 1999-06-15 12h fc t+24 (TL with K' .eq. 0)

Evolution of temperature increments (24-hour forecast) with the tangent linear model using different approaches for the exchange coefficient K in the vertical diffusion scheme.
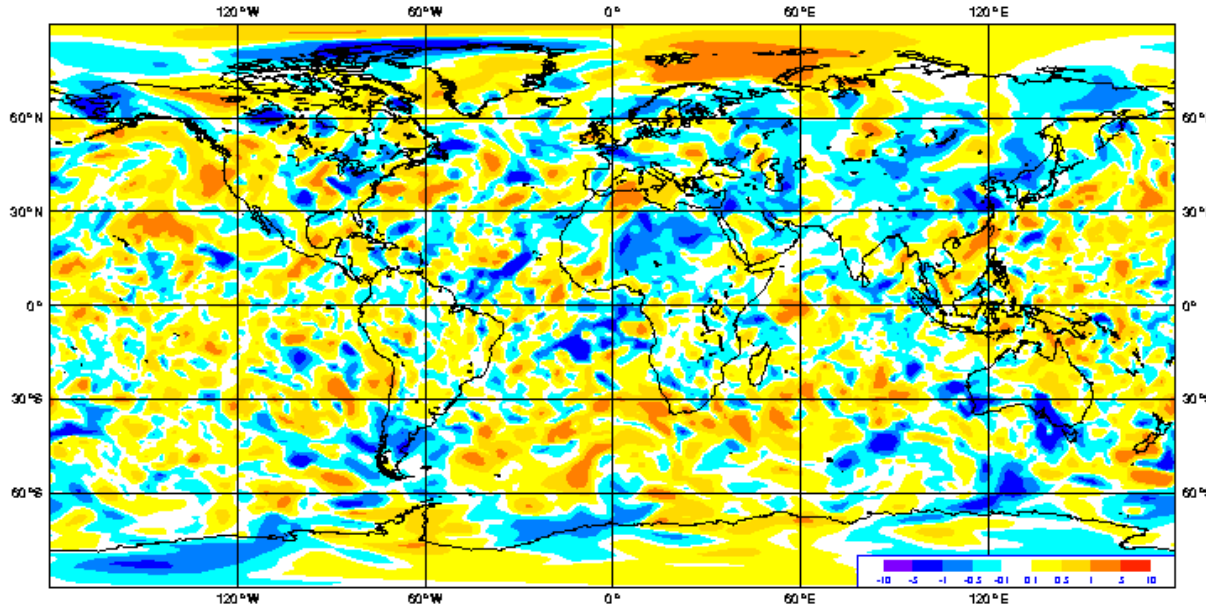
Perturbations of K included in TL

Perturbations of K set to zero in TL

Importance of regularization to prevent instabilities in tangent-linear model

Thursday 15 March 2001 12UTC ECMWF Forecast t+12 VT: Friday 16 March 2001 00UTC Model Level 48 **Temperature

Thursday 15 March 2001 12UTC ECMWF Forecast t+12 VT: Friday 16 March 2001 00UTC Model Level 48 **Temperature

12-hour ECMWF model integration (T159 L60)

Temperature on level 48 (approx. 850 hPa)

Finite difference between two non-linear model integrations

Corresponding perturbations evolved with tangent-linear model

No regularization in convection scheme

Importance of regularization to prevent instabilities in tangent-linear model

Thursday 15 March 2001 12UTC ECMWF Forecast t+12 VT: Friday 16 March 2001 00UTC Model Level 48 **Temperature
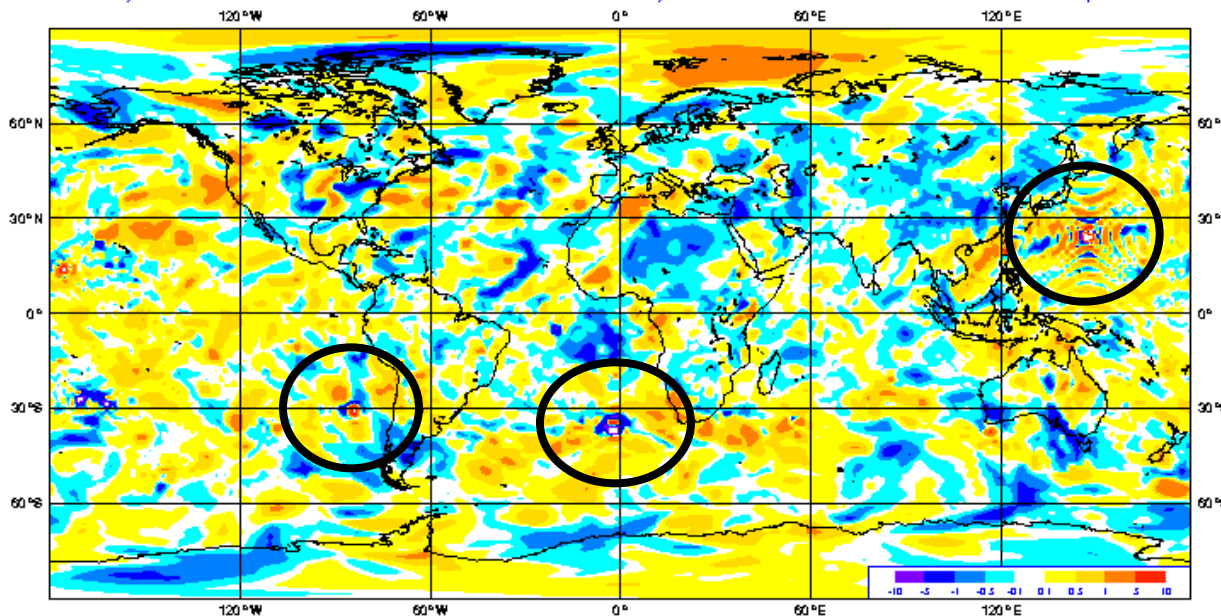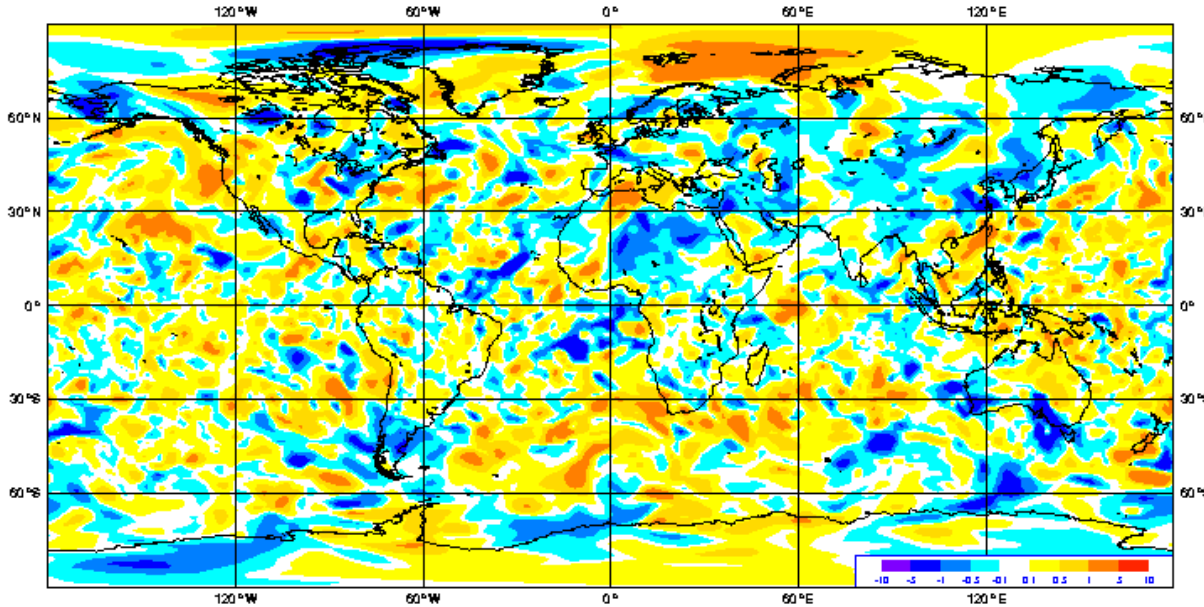

12-hour ECMWF model integration (T159 L60)
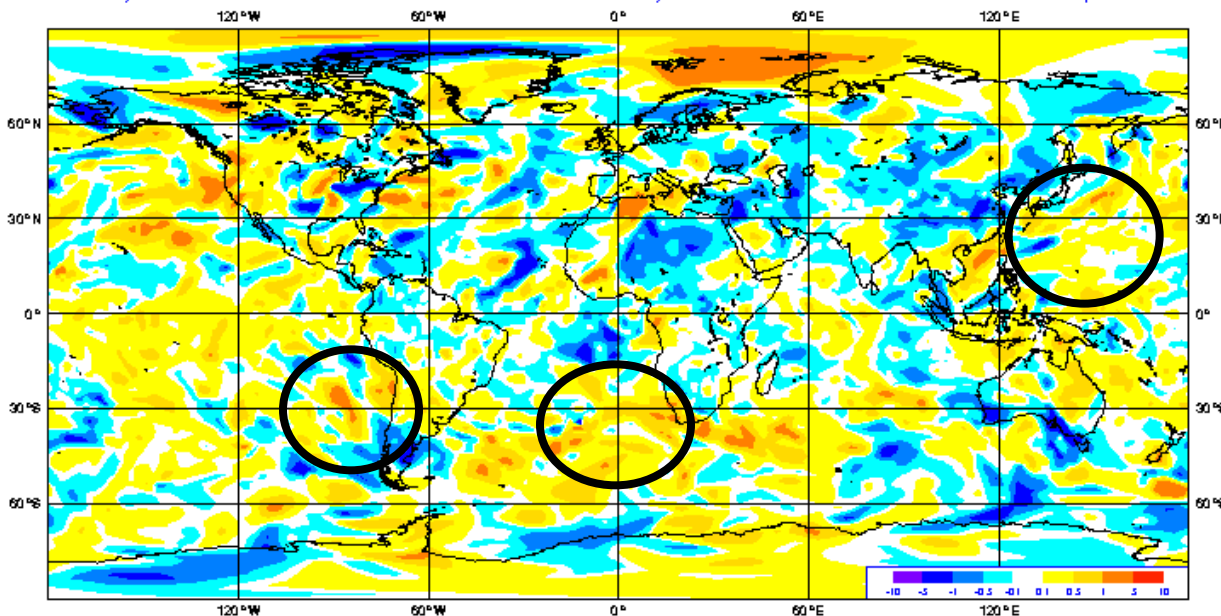
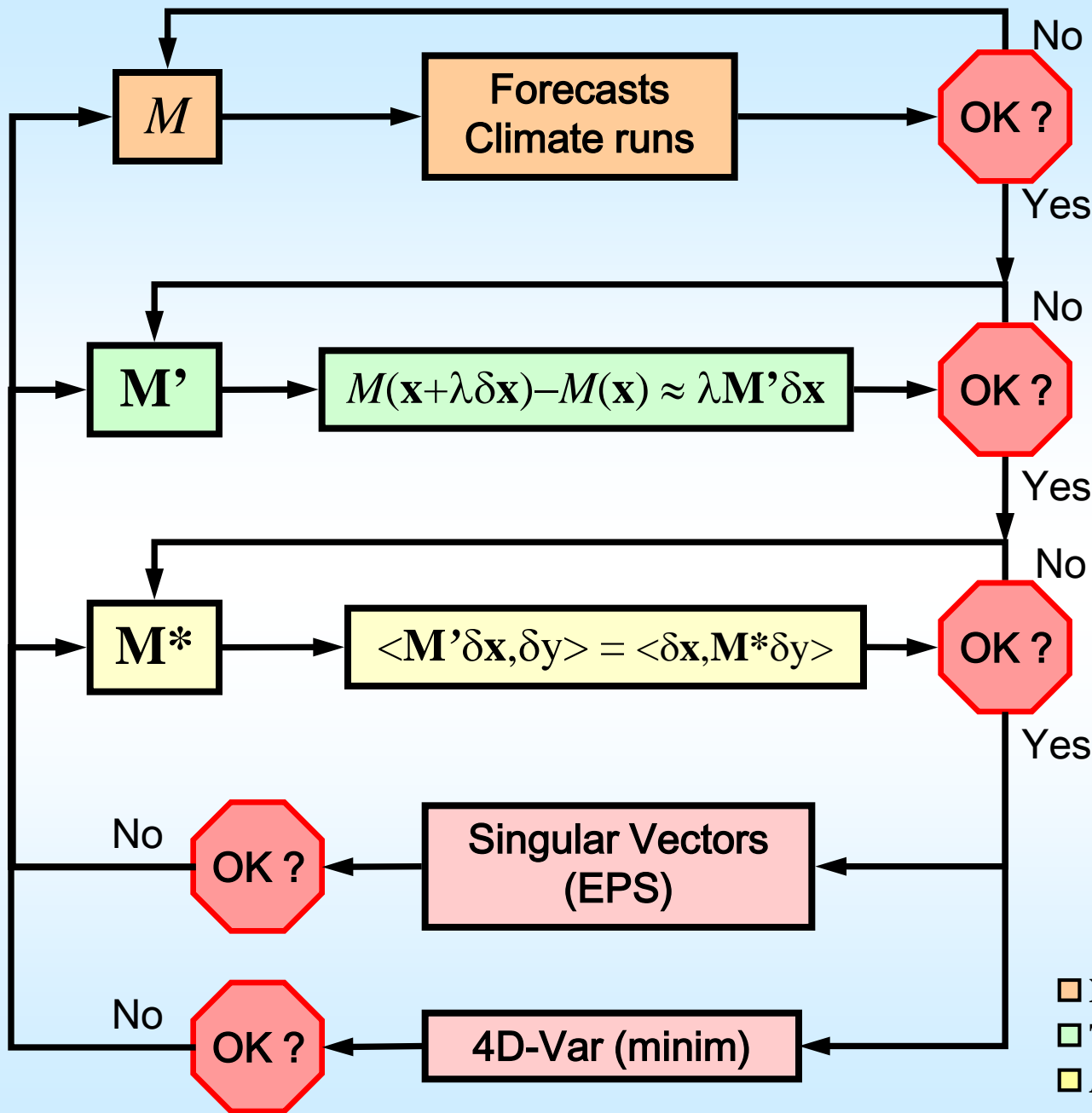Temperature on level 48 (approx. 850 hPa)

Finite difference between two non-linear model integrations

Thursday 15 March 2001 12UTC ECMWF Forecast t+12 VT: Friday 16 March 2001 00UTC Model Level 48 **Temperature

Corresponding perturbations evolved with tangent-linear model

Regularization in convection scheme (buoyancy & updraught velocity reduced perturb.)

Timing:

Pure coding
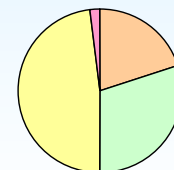
Debugging and testing
(incl. regularization)

M

Forecasts
Climate runs

OK ?

No

Yes

M'

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

OK ?

No

Yes

M*

$\langle\mathbf{M'}\delta\mathbf{x},\delta y\rangle = \langle\delta\mathbf{x},\mathbf{M}^*\delta y\rangle$

OK ?

No

Yes

Singular Vectors
(EPS)

OK ?

No

4D-Var (minim)

OK ?

No
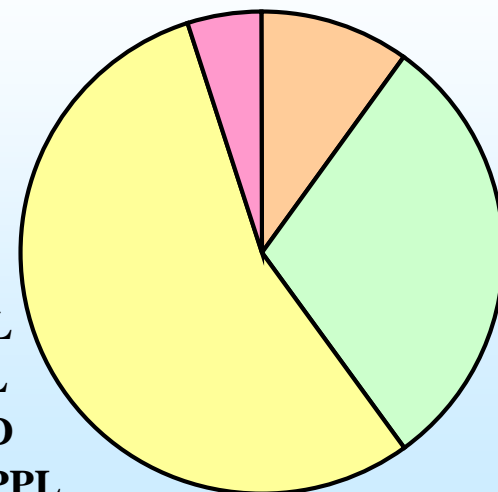
☐ **NL**
☐ **TL**
☐ **AD**
☐ **APPL**

A short list of existing LP packages used in operational DA

- **Tsuyuki (1996):** Kuo-type convection and large-scale condensation schemes (FSU 4D-Var).

- **Mahfouf (1999):** full set of simplified physical parametrizations (gravity wave drag currently used in ECMWF operational 4D-Var and EPS).

- **Janisková et al. (1999):** full set of simplified physical parametrizations (Météo-France operational 4D-Var).

- **Janisková et al. (2002):** linearized radiation (ECMWF 4D-Var).

- **Lopez (2002):** simplified large-scale condensation and precipitation scheme (Météo-France).

- **Tompkins and Janisková (2004):** simplified large-scale condensation and precipitation scheme (ECMWF).

- **Lopez and Moreau (2005):** simplified mass-flux convection scheme (ECMWF).

- **Mahfouf (2005):** simplified Kuo-type convection scheme (Environment Canada).

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 regul. 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

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

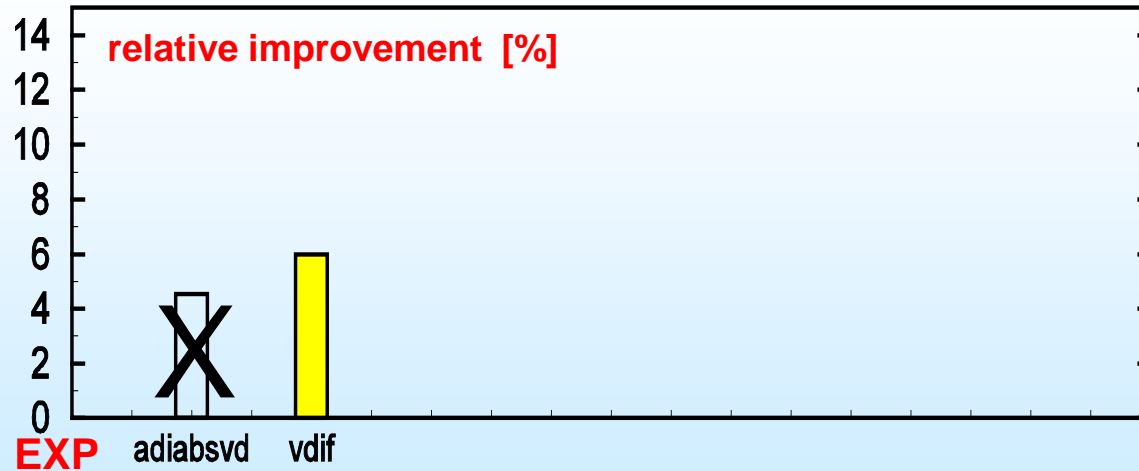- here: REF = adiabatic run (i.e. no physical parametrizations in tangent-linear)

Temperature

$\varepsilon_{EXP} - \varepsilon_{REF}$

REF = ADIAB

relative improvement [%]

14
12
10
8
6
4
2
0

EXP   adiabsvd   vdif

Impact of dry + moist physical processes

$\varepsilon_{EXP} - \varepsilon_{REF}$

relative improvement [%]

14
12
10
8
6
4
2
0

EXP adiabsvd vdif + gwd + radold + lsp + conv
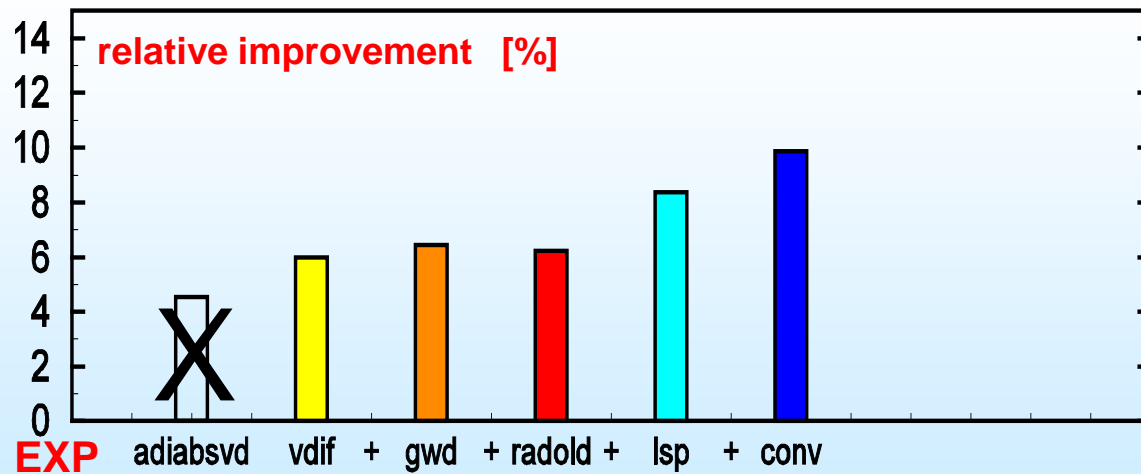
Impact of all physical processes (including new moist physics & radiation)

$\varepsilon_{EXP} - \varepsilon_{REF}$

relative improvement [%]

EXP	adiabsvd	vdif +	gwd	+ radold +	lsp	+ conv	+radnew	+ cl_new	+conv_new
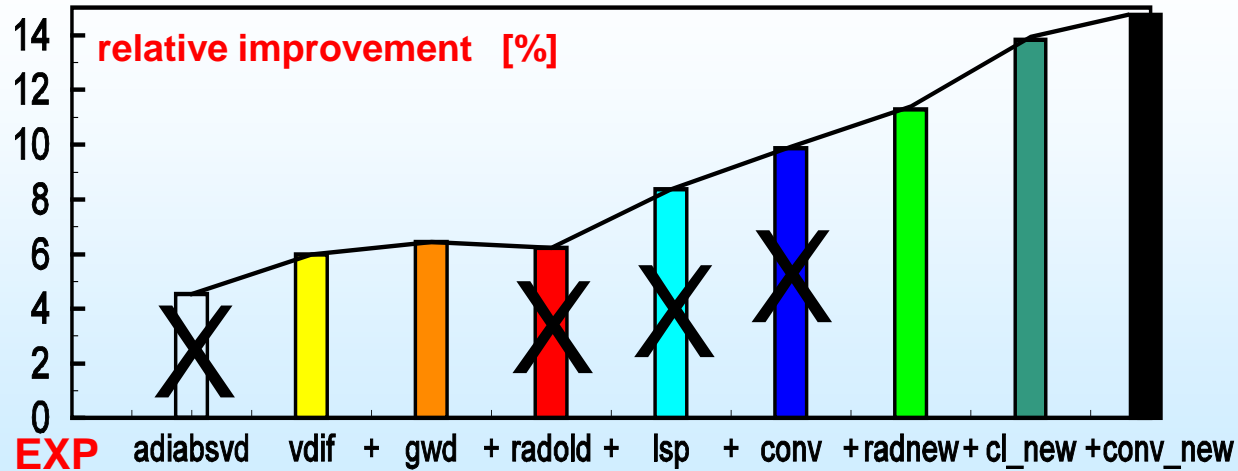
Applications

1D-Var with radar reflectivity profiles

Background $\mathbf{x}_b = (T_b, q_b, \ldots)$

Initialize $\mathbf{x} = \mathbf{x}_b$

$\mathbf{x} = (T, q, \ldots)$

$$J_b = \frac{1}{2}(\mathbf{x} - \mathbf{x}_b)^T \mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}_b)$$

$$\nabla_\mathbf{x} J_b = \mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}_b)$$

no

$\nabla_\mathbf{x} J \approx 0 ?$

MINIM

$\nabla_\mathbf{x} J$

$\nabla_\mathbf{x} J_o$

yes

Analysis $\mathbf{x}_a = \mathbf{x}$

Moist Physics

Moist Physics (ADJ)

Reflectivity Model

Reflectivity Model (ADJ)

Z_{mod}

$$J_o = \frac{1}{2}\sum_{k=1}^{K}\left(\frac{Z_{mod}^k - Z_{obs}^k}{\sigma_{obs}^k}\right)^2$$

$$\nabla_\mathbf{z} J_o = \left[\frac{Z_{mod}^k - Z_{obs}^k}{\left(\sigma_{obs}^k\right)^2}\right]_{k=1,K}$$

Reflectivity observations Z_{obs} with errors σ_{obs}

K = number of model vertical levels

1D-Var with TRMM/Precipitation Radar data
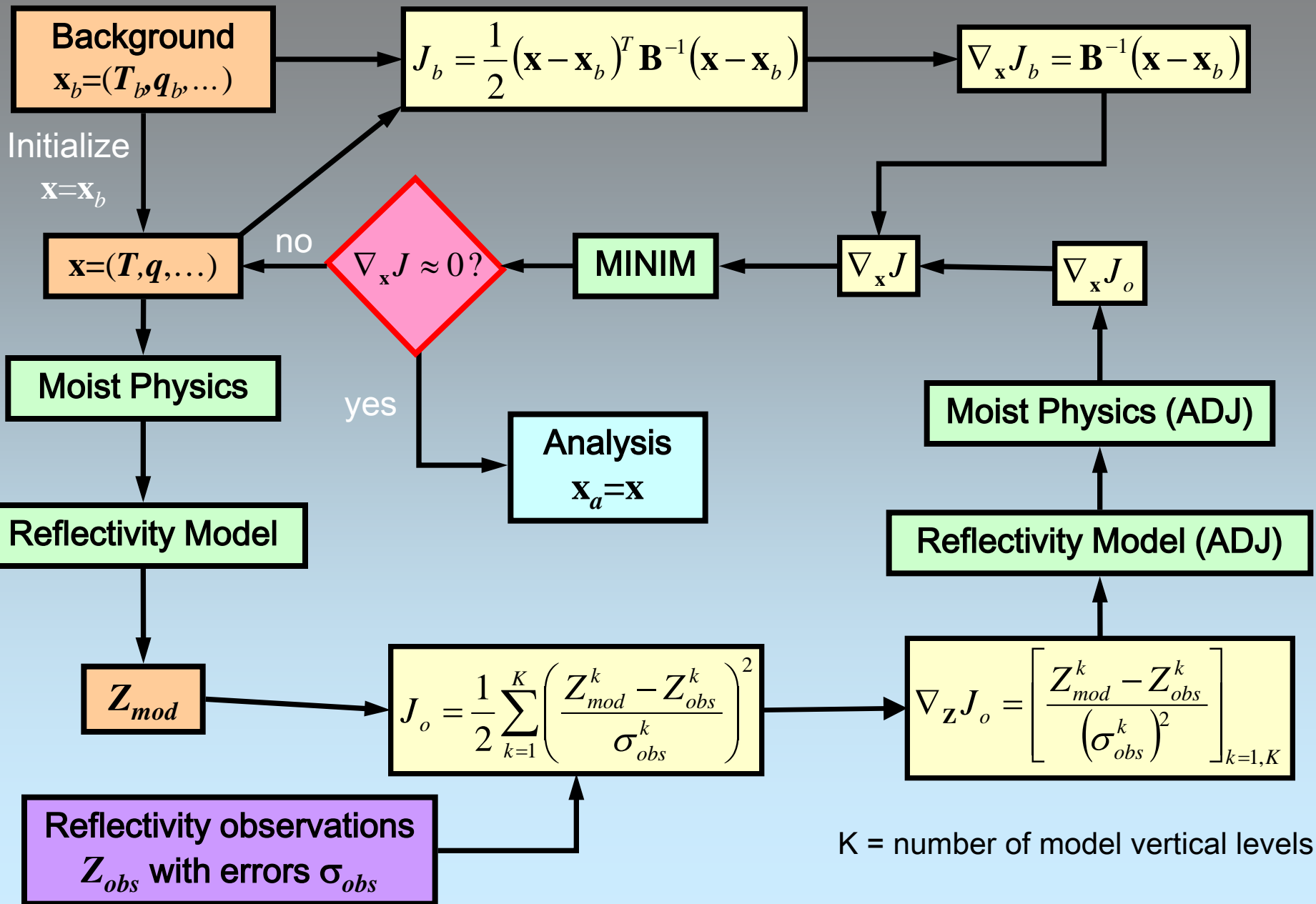
Tropical Cyclone Zoe (26 December 2002 @1200 UTC; Southwest Pacific)

AQUA MODIS image

TRMM Precipitation Radar

Cross-section

TRMM-PR swath

1D-Var with TRMM/Precipitation Radar data
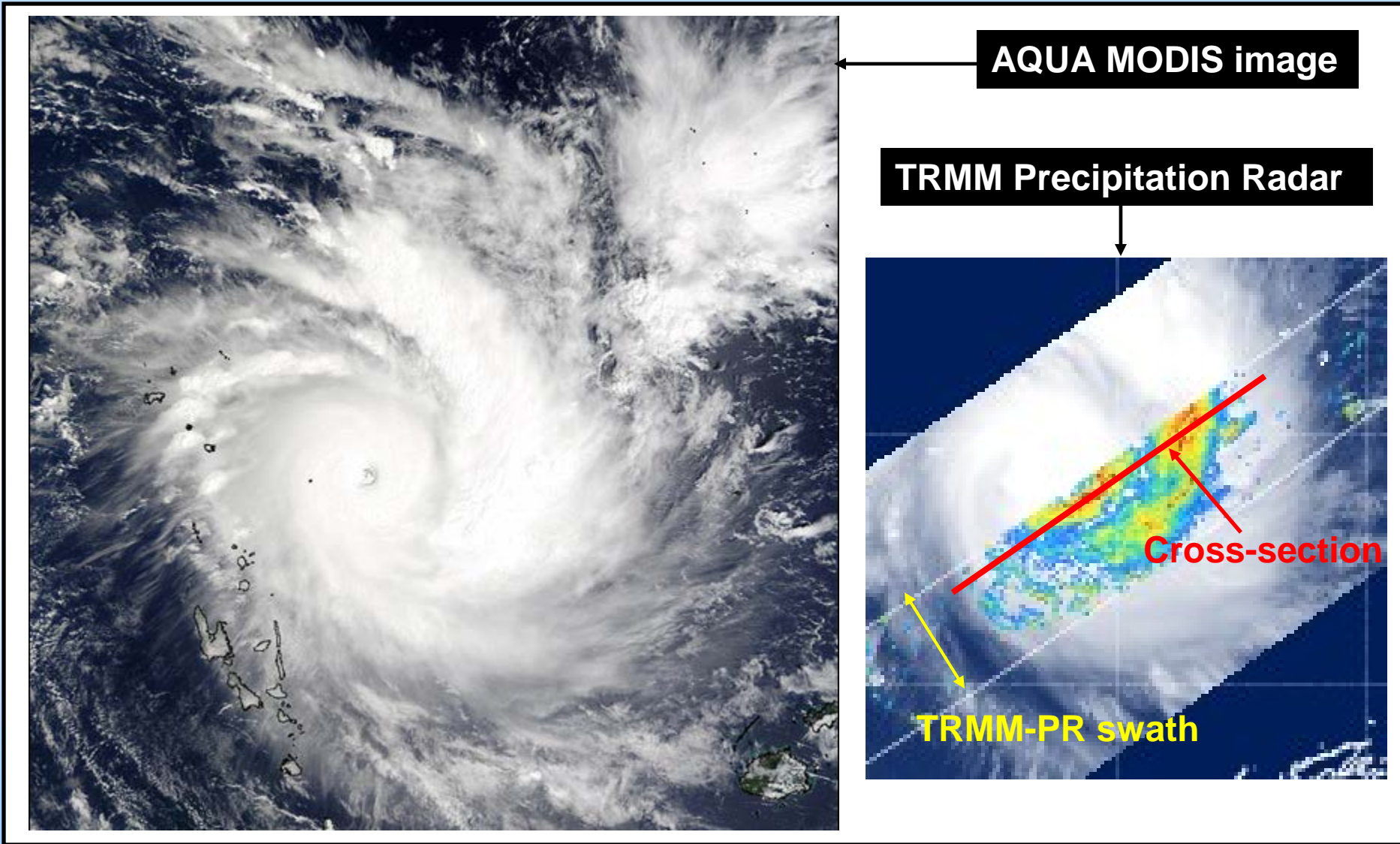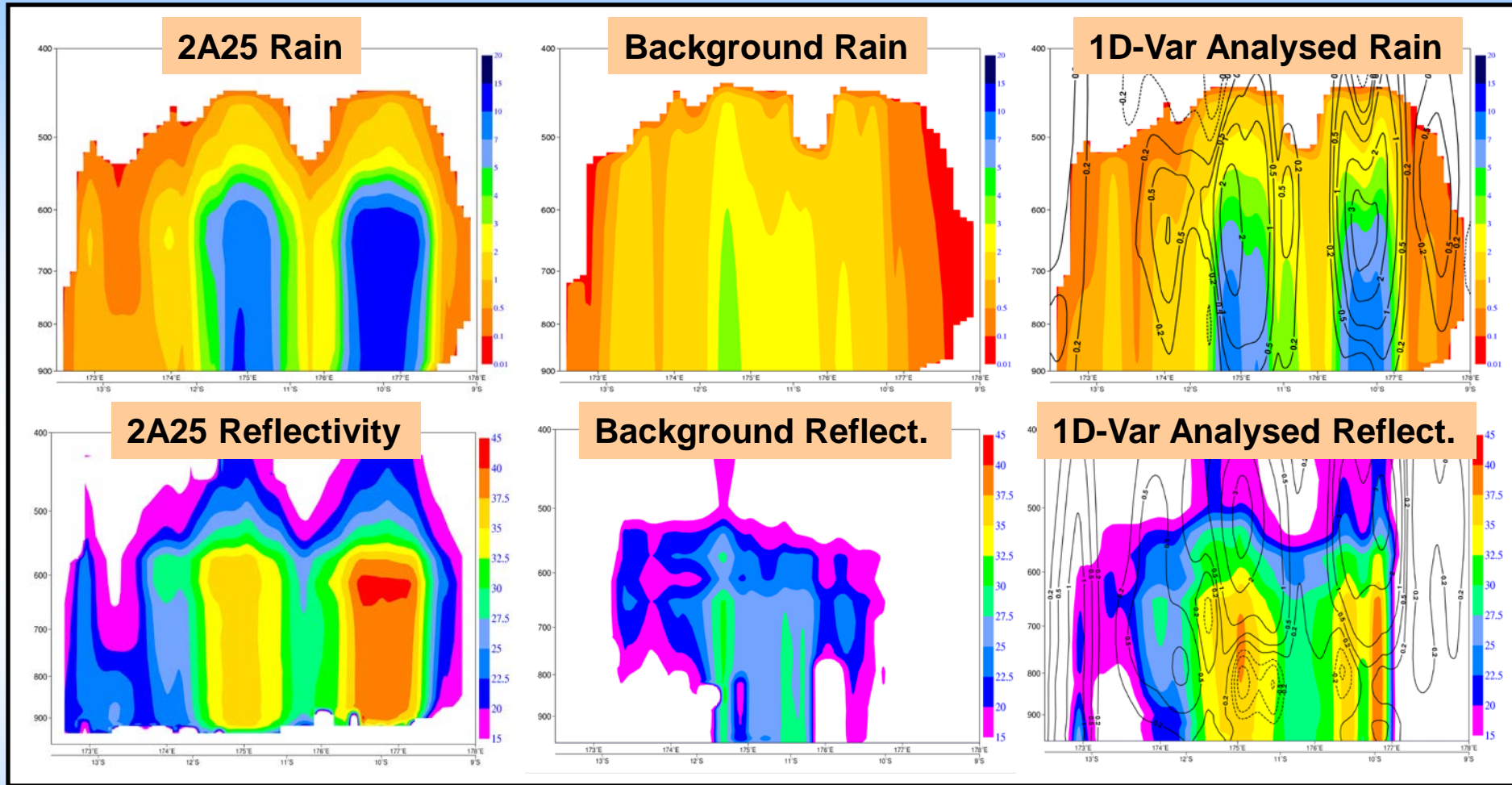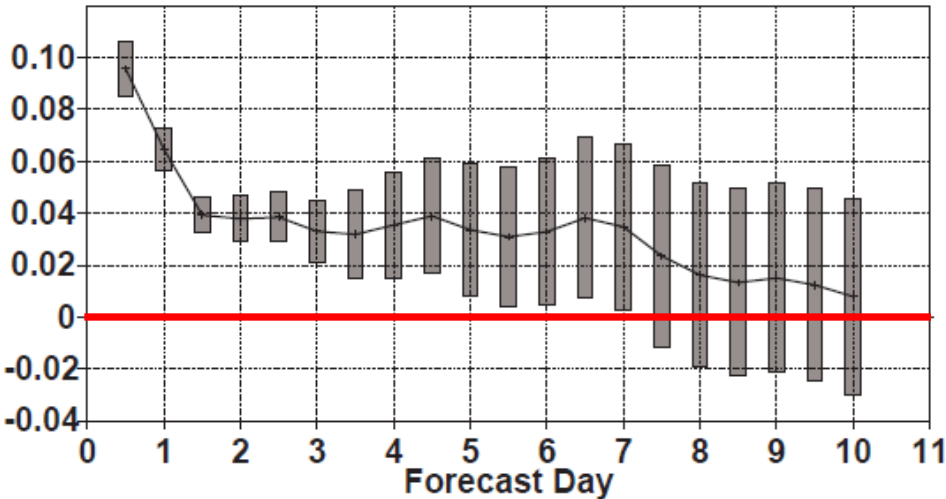

Tropical Cyclone Zoe (26 December 2002 @1200 UTC)

Vertical cross-section of rain rates (top, mm h^{-1}) and reflectivities (bottom, dBZ): observed (left), background (middle), and analyzed (right).

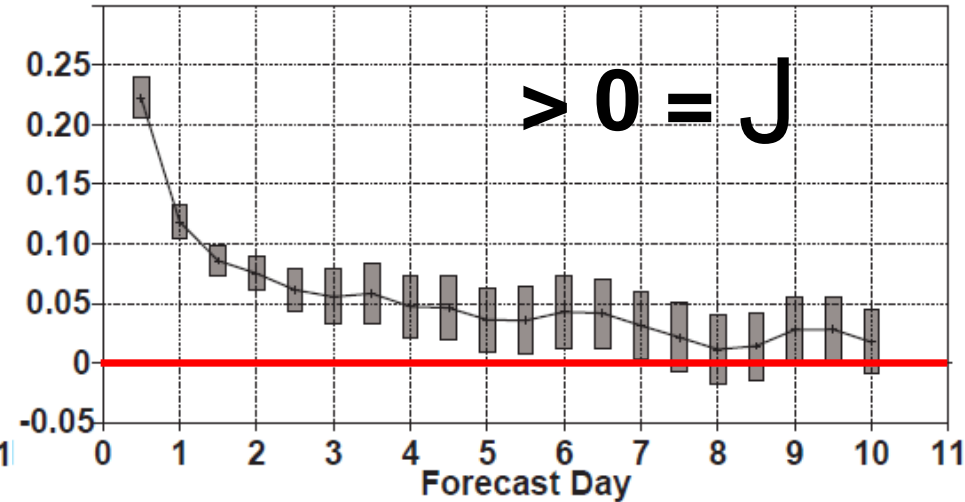Black isolines on right panels = 1D-Var specific humidity increments.

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.
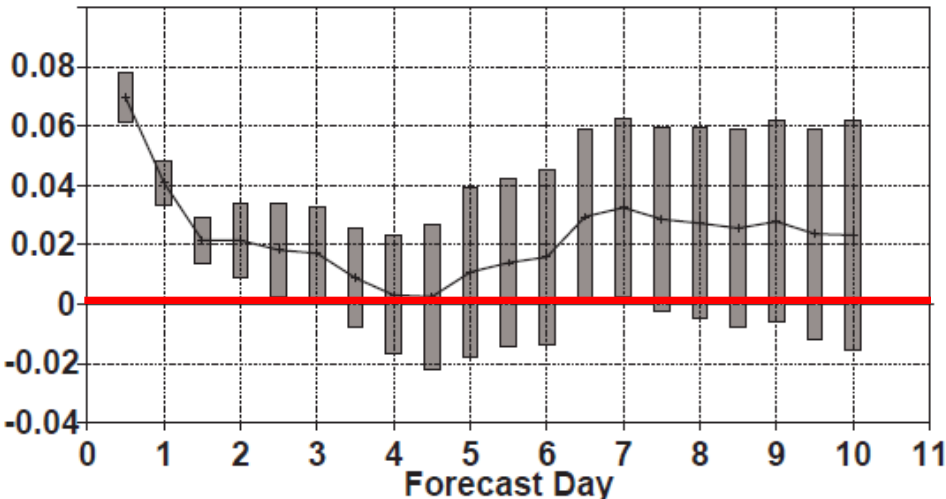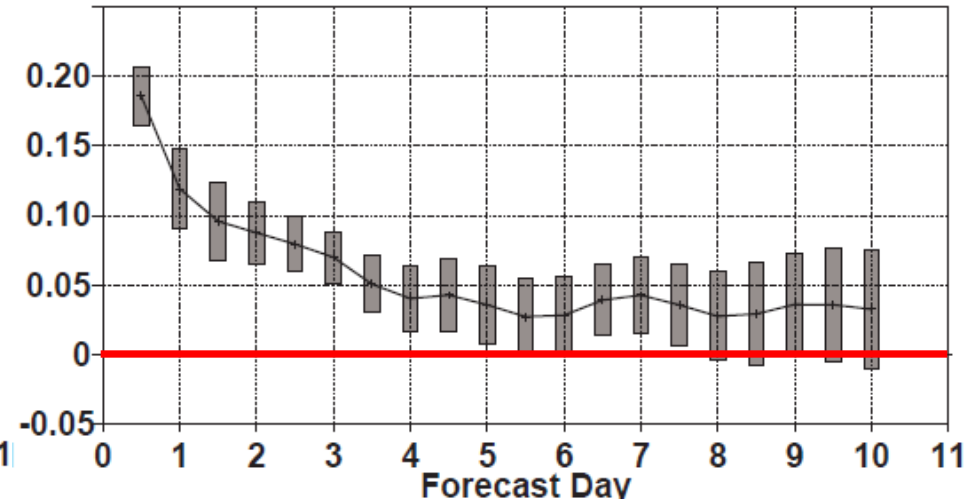
Physics parameter optimization (new research)

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 data assimilation system (4D-Var, for instance):

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

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

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.

ECMWF

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.

L

Linearity

J
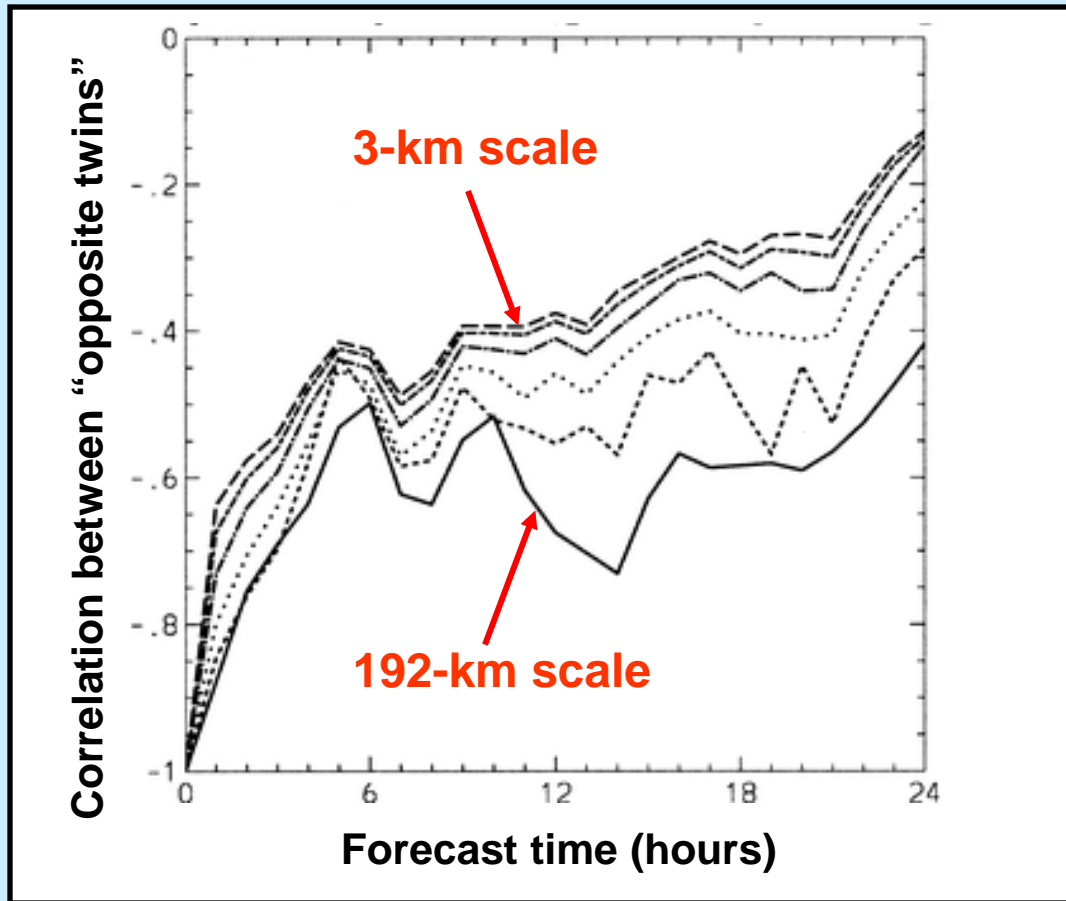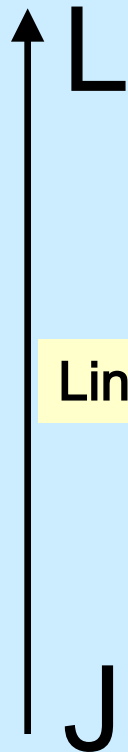
→The validity of the linear assumption for precipitation quickly drops in the first hours of the forecast, especially for smaller scales.

General conclusions

- **Physical parametrizations have become important components in variational data assimilation systems because they allow:**
- the comparison of the model state with observations (forward model),
- the minimization of the cost function (tangent-linear and adjoint models).

- **However, their linearized versions (tangent-linear and adjoint) require some special attention (regularizations/simplifications) in order to eliminate or smooth possible discontinuities and non-differentiability of the physical processes they represent.**

- **This is particularly true for the assimilation of observations related to precipitation, clouds and soil moisture.**

- **Developing new simplified parametrizations for data assimilation requires:**
  - Compromise between realism, linearity and computational cost,
  - Validation of simplified forward code against observations,
  - Comparison to full non-linear code used in forecast mode (4D-Var trajectory),
  - Numerical tests of tangent-linear and adjoint codes for small perturbations,
  - Validity of the linear hypothesis for perturbations with larger size (typical of analysis increments) → no spurious perturbation growth.
  - Successful convergence of 4D-Var minimizations.

Thank you!

Example of observation operator H (radiative transfer model):

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

and its tangent-linear operator $\mathbf{H}$:

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

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