

# Parameterizations in Data Assimilation

(references, summary slides and examples)

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Philippe Lopez

Physical Aspects Section, Research Department, ECMWF  
(Room 002)

**A few references...**

## REFERENCES

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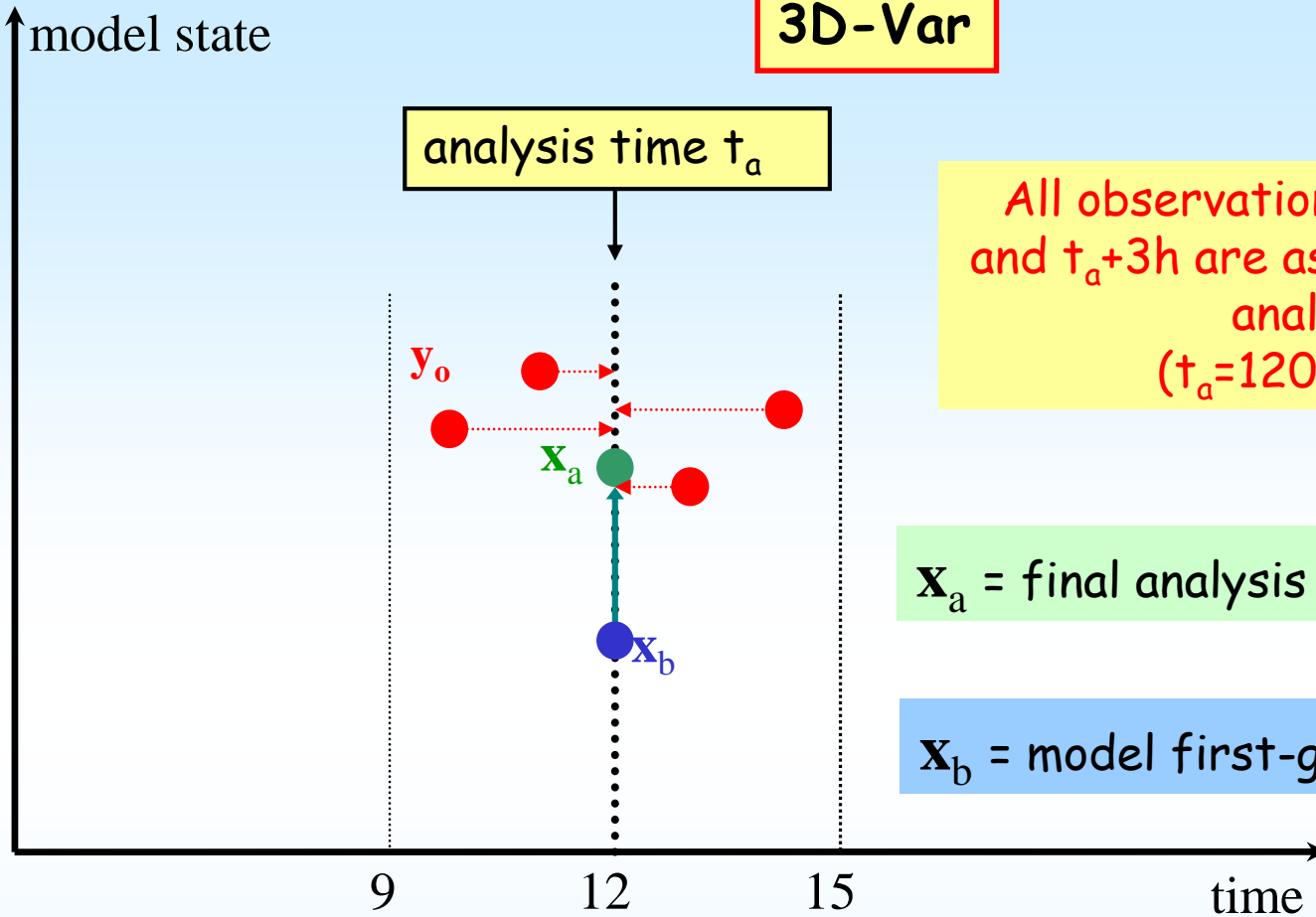
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**A few slides of summary...**

# 3D-Var



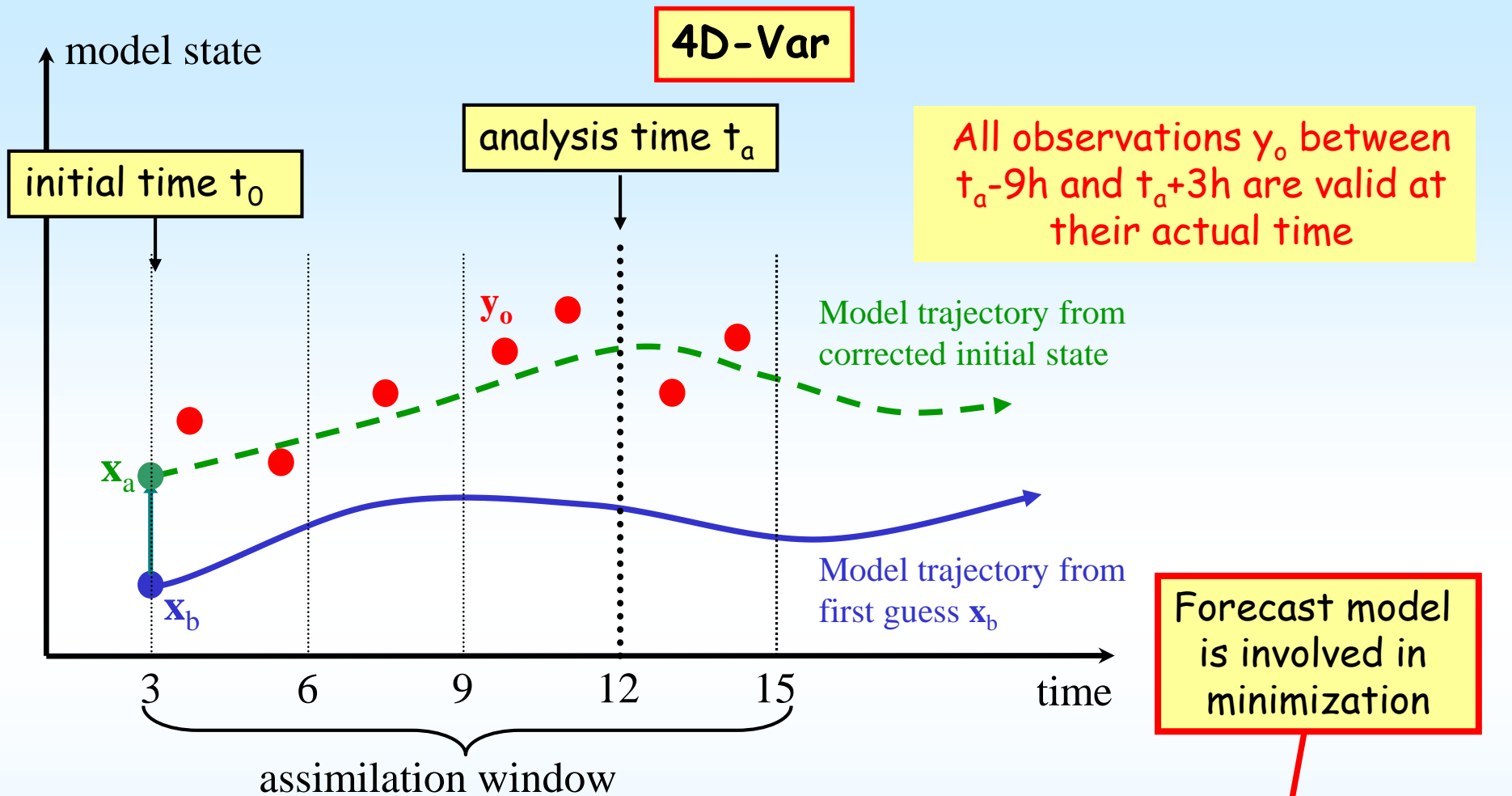
All observations  $y_o$  between  $t_a-3h$  and  $t_a+3h$  are assumed to be valid at analysis time ( $t_a=1200$  UTC here)

$\mathbf{x}_a$  = final analysis

$\mathbf{x}_b$  = model first-guess

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

$$\Leftrightarrow \nabla_{\mathbf{x}} J = \mathbf{B}^{-1} (\mathbf{x} - \mathbf{x}_b) + \mathbf{H}^T \mathbf{R}^{-1} (H(\mathbf{x}) - \mathbf{y}_o) = 0$$



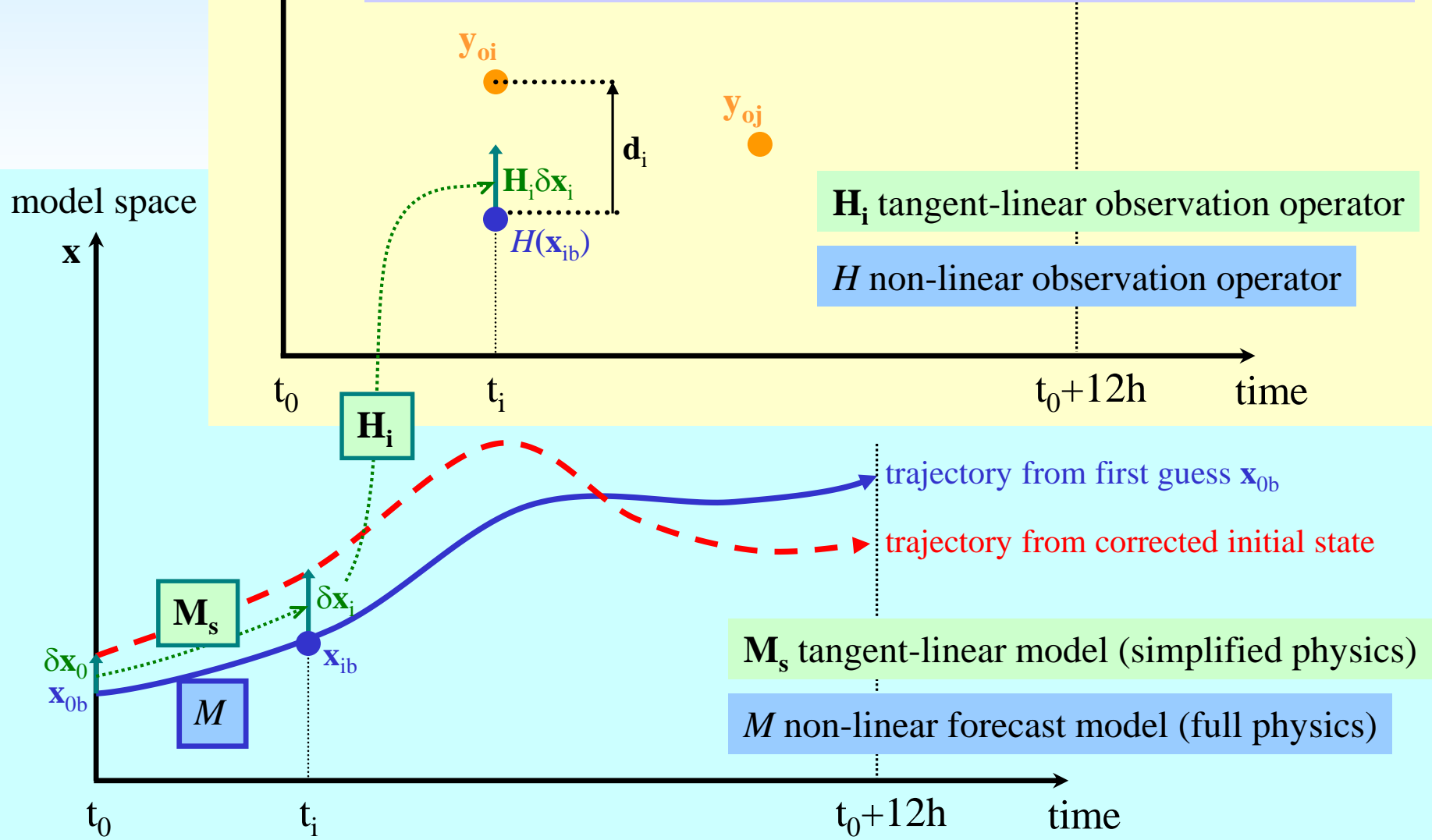
$$\min J = \frac{1}{2} (\mathbf{x}_0 - \mathbf{x}_b)^T \mathbf{B}^{-1} (\mathbf{x}_0 - \mathbf{x}_b) + \sum_{i=0}^n \mathbf{M}^T [t_i, t_0] \mathbf{H}_i^T \mathbf{R}_i^{-1} (H_i(M[\mathbf{x}_0]) - \mathbf{y}_{oi})$$

$$\Leftrightarrow \nabla_{\mathbf{x}} J = \mathbf{B}^{-1} (\mathbf{x}_0 - \mathbf{x}_b) + \sum_{i=0}^n \mathbf{M}^T [t_i, t_0] \mathbf{H}_i^T \mathbf{R}_i^{-1} (H_i(M[\mathbf{x}_0]) - \mathbf{y}_{oi}) = 0$$



# Incremental 4D-Var

$$J = \frac{1}{2} \delta \mathbf{x}_0^T \mathbf{B}^{-1} \delta \mathbf{x}_0 + \frac{1}{2} \sum_{i=0}^n (\mathbf{H}_i(\delta \mathbf{x}_i) - \mathbf{d}_i)^T \mathbf{R}_i^{-1} (\mathbf{H}_i(\delta \mathbf{x}_i) - \mathbf{d}_i)$$





## Summary

- Variational data assimilation relies on some essential assumptions:
  - Gaussian and unbiased model background and observation errors,
  - Quasi-linearity of all operators involved ( $H, M$ ).
- Given some background fields and a very large set of asynchronous observations available within a certain time window (6 or 12h-long), 4D-Var searches the statistically optimal initial model state  $\mathbf{x}_0$  that minimizes the cost function:

$$J(\mathbf{x}_0) = J_b(\mathbf{x}_0) + J_o(HM(\mathbf{x}_0))$$

- The calculation of  $\nabla_{\mathbf{x}_0} J$  requires the coding of tangent-linear and adjoint versions of the observation operator  $H$  and of the full nonlinear forecast model  $M$  (including physical parameterizations).
- The tangent-linear and adjoint forecast models,  $\mathbf{M}$  and  $\mathbf{M}^T$ , are usually based on a simplified version of the full nonlinear model,  $M$ , to reduce computational cost in the iterative minimization and to avoid nonlinearities.

## Summary

- The aim of data assimilation is to produce a statistically optimal model state (the **analysis**) which can be used to initialize a forecast model.
- In variational DA, this is achieved by minimizing a **cost function**,  $J$ , that measures the distance to the **model background** and **observations**, weighted by their respective **error statistics**.

In 3D-Var:

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

- **Parameterizations** are needed during the minimization to convert the model control variables ( $T, q, u, v, P_s$ ) into observed equivalents (e.g. reflectivities, radiances,...) ("**observation operator**"  $H$ ).
- Fundamental assumptions:
  - **Background and observation errors** are **Gaussian** and **unbiased**.
  - Observation operator  $H$  is **not too non-linear**.

## Summary

- The aim of a data assimilation system is to produce a statistically optimal model state (the **analysis**) that can be used to initialize a forecast model.
- In variational DA this is achieved by minimizing iteratively a **cost function** ( $J$ ) that measures the distance to the **model background** and **observations**, weighted by their respective **error statistics** (**Gaussian** and **unbiased**).
- **Parameterizations** are needed during the minimization to:
  - convert the model variables ( $T, q, u, v, P_s$ ) into observed equivalents (e.g. reflectivities, radiances,...) (observation operator  $H$ ),
  - evolve the model state from analysis time to observation time (4D-Var).
- The **tangent-linear** and **adjoint** versions of these usually **simplified** parameterizations must be coded, **tested**, and some **regularization** is usually needed to eliminate **discontinuities/non-linearities**.
- The **adjoint** version of the parameterizations is needed to compute the gradient of the cost function with respect to the initial model state,  $\mathbf{x}$ :

$$\nabla_{\mathbf{x}_0} J = \mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}_b) + \mathbf{M}[t_i, t_0]^T \mathbf{H}^T \nabla_{\mathbf{y}} J_o \quad \text{with} \quad \nabla_{\mathbf{y}} J_o = \mathbf{R}^{-1}(H(\mathbf{x}) - \mathbf{y}_o)$$

**A few examples and exercises...**

## A simple analysis problem

### Exercise

- 6-hour forecast of 2m temperature produced by the model:  
 $\mathbf{x}_b$  with a standard deviation of forecast error  $\sigma_b$
- observation of 2m temperature:  
 $\mathbf{y}_o$  with a standard deviation of observation error  $\sigma_o$
- The best estimate of the 2m temperature (analysis) minimizes the departure from the model first-guess and from the observation according to their relative accuracies:

$$\mathcal{J}(\mathbf{x}) = \frac{1}{2} \left( \frac{\mathbf{x} - \mathbf{x}_b}{\sigma_b} \right)^2 + \frac{1}{2} \left( \frac{\mathbf{x} - \mathbf{y}_o}{\sigma_o} \right)^2$$

Since the analysis  $\mathbf{x}_a$  minimizes the cost function, then

$$\frac{\partial \mathcal{J}}{\partial \mathbf{x}}(\mathbf{x}_a) = 0$$

Analysis state can be written as:

$$\mathbf{x}_a = \mathbf{x}_b + \alpha(\mathbf{y}_o - \mathbf{x}_b)$$

## A simple analysis problem

### Exercise

- **Problem:**

- Find the coefficient  $\alpha$ .
- Show that the variance of the analysis error is:

$$\frac{1}{\sigma_a^2} = \frac{1}{\sigma_b^2} + \frac{1}{\sigma_o^2}$$

(Note:  $\sigma_o^2 = \overline{(\mathbf{x} - \mathbf{x}_t)^2}$ , where  $\mathbf{x}_t$  is the unknown true state).

## A simple analysis problem

### Solution

- Since the analysis  $\mathbf{x}_a$  minimizes the cost function, then

$$\frac{\partial \mathcal{J}}{\partial \mathbf{x}}(\mathbf{x}_a) = 0$$

$$\frac{\partial \mathcal{J}}{\partial \mathbf{x}} = \frac{\mathbf{x} - \mathbf{x}_b}{\sigma_b^2} + \frac{\mathbf{x} - \mathbf{y}_o}{\sigma_o^2} = 0$$

$$\frac{\mathbf{x}\sigma_o^2 - \mathbf{x}_b\sigma_o^2 + \mathbf{x}\sigma_b^2 - \mathbf{y}_o\sigma_b^2}{\sigma_b^2\sigma_o^2} = 0$$

$$(*) \quad \mathbf{x}(\sigma_o^2 + \sigma_b^2) = \mathbf{x}_b\sigma_o^2 + \mathbf{y}_o\sigma_b^2$$

$$\mathbf{x} = \frac{\mathbf{x}_b\sigma_o^2 + \mathbf{y}_o\sigma_b^2 - \mathbf{x}_b\sigma_b^2 + \mathbf{x}_b\sigma_b^2}{\sigma_o^2 + \sigma_b^2}$$

$$\mathbf{x} = \frac{\mathbf{x}_b(\sigma_o^2 + \sigma_b^2) + \sigma_b^2(\mathbf{y}_o - \mathbf{x}_b)}{\sigma_o^2 + \sigma_b^2}$$

$$\mathbf{x} = \mathbf{x}_b + \frac{\sigma_b^2}{\sigma_o^2 + \sigma_b^2}(\mathbf{y}_o - \mathbf{x}_b)$$

$\alpha$

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## A simple analysis problem

### Solution

- Analysis error:  
starting from equation (\*) one gets

$$\begin{aligned} \mathbf{x}_a &= \mathbf{x}_b \frac{\sigma_o^2}{\sigma_o^2 + \sigma_b^2} + \mathbf{y}_o \frac{\sigma_b^2}{\sigma_o^2 + \sigma_b^2} \\ \mathbf{x}_a - \mathbf{x}_t &= (\mathbf{x}_b - \mathbf{x}_t) \frac{\sigma_o^2}{\sigma_o^2 + \sigma_b^2} + (\mathbf{y}_o - \mathbf{x}_t) \frac{\sigma_b^2}{\sigma_o^2 + \sigma_b^2} \\ \overline{(\mathbf{x}_a - \mathbf{x}_t)^2} &= \overline{(\mathbf{x}_b - \mathbf{x}_t)^2} \frac{\sigma_o^4}{(\sigma_o^2 + \sigma_b^2)^2} + \overline{(\mathbf{y}_o - \mathbf{x}_t)^2} \frac{\sigma_b^4}{(\sigma_o^2 + \sigma_b^2)^2} \\ &\quad + \overline{(\mathbf{x}_b - \mathbf{x}_t)(\mathbf{y}_o - \mathbf{x}_t)} \frac{\sigma_o^2 \sigma_b^2}{(\sigma_o^2 + \sigma_b^2)^2} \end{aligned}$$

Since background and observation errors are assumed to be uncorrelated:

$$Cov(\mathbf{x}_b, \mathbf{y}_o) = \overline{(\mathbf{x}_b - \mathbf{x}_t)(\mathbf{y}_o - \mathbf{x}_t)} = 0$$

which gives

$$\begin{aligned} \sigma_a^2 &= \frac{\sigma_b^2 \sigma_o^4}{(\sigma_o^2 + \sigma_b^2)^2} + \frac{\sigma_b^4 \sigma_o^2}{(\sigma_o^2 + \sigma_b^2)^2} \\ \sigma_a^2 &= \frac{\sigma_b^2 \sigma_o^2}{\sigma_o^2 + \sigma_b^2} \iff \boxed{\frac{1}{\sigma_a^2} = \frac{1}{\sigma_b^2} + \frac{1}{\sigma_o^2}} \end{aligned}$$



## 1D-Var assimilation of physical fluxes

### Example

- observation operator = physical parametrization
  - example: thermal radiation at the surface (*Brunt, 1934*)

$$R_L = \sigma T^4 (a + b\sqrt{e})$$

where  $T$  is the screen level temperature and  $e$  is the water vapour pressure

- model temperature and humidity ( $T_b, e_b$ ) can be modified to better match an observation of thermal radiation  $R_{L_o}$
- the optimal values of  $T$  and  $e$  minimize the following cost function:

$$\mathcal{J}(T, e) = \frac{1}{2} \left( \frac{T - T_b}{\sigma_{T_b}} \right)^2 + \frac{1}{2} \left( \frac{e - e_b}{\sigma_{e_b}} \right)^2 + \frac{1}{2} \left( \frac{R_L - R_{L_o}}{\sigma_o} \right)^2$$

gradient of the cost function:

$$\frac{\partial \mathcal{J}}{\partial T} = \frac{T - T_b}{\sigma_{T_b}^2} + \frac{\partial R_L}{\partial T} \left( \frac{R_L - R_{L_o}}{\sigma_o^2} \right)$$

$$\frac{\partial \mathcal{J}}{\partial e} = \frac{e - e_b}{\sigma_{e_b}^2} + \frac{\partial R_L}{\partial e} \left( \frac{R_L - R_{L_o}}{\sigma_o^2} \right)$$

## 1D-Var assimilation of physical fluxes

### Example

- tangent-linear operator:

$$\delta R_L = \left( \frac{\partial R_L}{\partial T} \quad \frac{\partial R_L}{\partial e} \right) \cdot \begin{pmatrix} \delta T \\ \delta e \end{pmatrix}$$

- adjoint of the tangent-linear operator:

$$\left( \frac{\partial J_o}{\partial T} \quad \frac{\partial J_o}{\partial e} \right) = \begin{pmatrix} \frac{\partial R_L}{\partial T} \\ \frac{\partial R_L}{\partial e} \end{pmatrix} \cdot \begin{pmatrix} \frac{\partial J_o}{\partial R_L} \end{pmatrix}$$

with  $\frac{\partial R_L}{\partial T} = 4\sigma T^3(a + b\sqrt{e})$  and  $\frac{\partial R_L}{\partial e} = \frac{b\sigma T^4}{2\sqrt{e}}$

## EXERCISE 2

- write tangent linear (TL) and adjoint (AD) code of the following non-linear (NL) code (FORTRAN 90)

```
SUBROUTINE Longwave_Radiation (EA, TA, RL)

! Longwave radiation at the surface (RL in Watts/m2)
! Empirical expression from Brunt (1934) depending upon
! TA = air temperature (K)
! EA = water vapour pressure (hPa)
!
! Non-linear routine
! -----

IMPLICIT NONE
REAL , INTENT(IN)  :: EA, TA
REAL , INTENT(OUT) :: RL
REAL , PARAMETER  :: A=0.75, B=0.003
REAL , PARAMETER  :: SIGMA=5.67E-8
REAL              :: ZEMIS

ZEMIS = A+B*SQRT(EA)
RL     = ZEMIS*SIGMA*TA**4

END SUBROUTINE Longwave_Radiation
```

---

## EXERCISE 2 - solution

- tangent linear code

```
SUBROUTINE Longwave_Radiation_TL (EA5, TA5, RL5, EA, TA, RL)
```

```
! Longwave radiation at the surface (RL in Watts/m2)
! Empirical expression from Brunt (1934) depending upon
! TA = air temperature (K)
! EA = water vapour pressure (hPa)
!
! Tangent-linear routine
! -----
```

```
IMPLICIT NONE
```

```
REAL , INTENT(IN)  :: EA5, TA5      ! Trajectory
REAL , INTENT(OUT) :: RL5          ! Trajectory
REAL , INTENT(IN)  :: EA, TA       ! Perturbation
REAL , INTENT(OUT) :: RL           ! Perturbation
REAL , PARAMETER   :: A=0.75, B=0.003
REAL , PARAMETER   :: SIGMA=5.67E-8
REAL               :: ZEMIS5, ZEMIS
```

```
ZEMIS5 = A+B*SQRT(EA5)
ZEMIS  = B/(2.*SQRT(EA5))*EA
RL5    = ZEMIS5*SIGMA*TA5**4
RL     = ZEMIS *SIGMA*TA5**4 + 4.*ZEMIS5*SIGMA*TA5**3*TA
```

```
END SUBROUTINE Longwave_Radiation_TL
```



---

## EXERCISE 2 - solution

- adjoint code

```
SUBROUTINE Longwave_Radiation_AD (EA5, TA5, RL5, EA, TA, RL)

! Longwave radiation at the surface (RL in Watts/m2)
! Empirical expression from Brunt (1934) depending upon
! TA = air temperature (K)
! EA = water vapour pressure (hPa)
!
! Adjoint routine
! -----

IMPLICIT NONE
REAL , INTENT(IN)  :: EA5, TA5      ! Trajectory
REAL , INTENT(OUT) :: RL5          ! Trajectory
REAL , INTENT(IN)  :: EA, TA       ! Perturbation
REAL , INTENT(OUT) :: RL           ! Perturbation
REAL , PARAMETER  :: A=0.75, B=0.003
REAL , PARAMETER  :: SIGMA=5.67E-8
REAL              :: ZEMIS5, ZEMIS

! Trajectory computations

ZEMIS5 = A+B*SQRT(EA5)
RL5    = ZEMIS5*SIGMA*TA5**4

! Initialization of local variables
```



---

ZEMIS = 0.

! Adjoint computation

TA = TA + 4.\*ZEMIS5\*SIGMA\*TA5\*\*3\*RL

ZEMIS = ZEMIS + SIGMA\*TA5\*\*4\*RL

RL = 0.

EA = EA + B/(2.\*SQRT(EA5))\*ZEMIS

ZEMIS = 0.

END SUBROUTINE Longwave\_Radiation\_AD

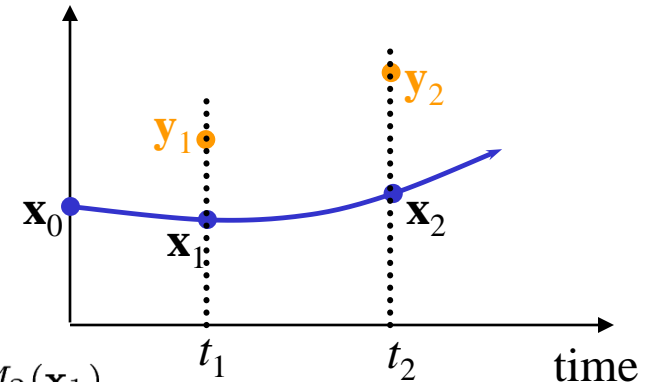


## A simple 4D-Var analysis problem

### Exercise

- Observations  $\mathbf{y}_1$  and  $\mathbf{y}_2$  at time  $t_1$  and  $t_2$
- Model first guess  $\mathbf{x}_1$  and  $\mathbf{x}_2$  at time  $t_1$  and  $t_2$
- Time evolution from the initial time  $t_0$ :

$$\mathbf{x}_1 = M_1(\mathbf{x}_0) \quad \text{and} \quad \mathbf{x}_2 = M_2(\mathbf{x}_1)$$



- Cost function:

$$\mathcal{J}(\mathbf{x}_0) = \frac{1}{2} \left( \frac{\mathbf{x}_1 - \mathbf{y}_1}{\sigma_1} \right)^2 + \frac{1}{2} \left( \frac{\mathbf{x}_2 - \mathbf{y}_2}{\sigma_2} \right)^2 = \mathcal{J}_1 + \mathcal{J}_2$$

- **Problem:**

Estimate the gradient of  $\mathcal{J}$  with respect to the initial state  $\mathbf{x}_0$ .

---

## A simple 4D-Var analysis problem

### Solution

- At time  $t_2$ :

$$\frac{\partial \mathcal{J}_2}{\partial \mathbf{x}_2} = \frac{\mathbf{x}_2 - \mathbf{y}_2}{\sigma_2^2}$$

- At time  $t_1$ :

$$\frac{\partial \mathcal{J}_2}{\partial \mathbf{x}_1} = \mathbf{M}_2^T \left( \frac{\partial \mathcal{J}_2}{\partial \mathbf{x}_2} \right) = \mathbf{M}_2^T \left( \frac{\mathbf{x}_2 - \mathbf{y}_2}{\sigma_2^2} \right)$$

$$\frac{\partial \mathcal{J}_1}{\partial \mathbf{x}_1} = \frac{\mathbf{x}_1 - \mathbf{y}_1}{\sigma_1^2}$$

- At time  $t_0$ :

$$\frac{\partial \mathcal{J}_2}{\partial \mathbf{x}_0} = \mathbf{M}_1^T \left( \frac{\partial \mathcal{J}_2}{\partial \mathbf{x}_1} \right) = \mathbf{M}_1^T \left[ \mathbf{M}_2^T \left( \frac{\mathbf{x}_2 - \mathbf{y}_2}{\sigma_2^2} \right) \right]$$

$$\frac{\partial \mathcal{J}_1}{\partial \mathbf{x}_0} = \mathbf{M}_1^T \left( \frac{\partial \mathcal{J}_1}{\partial \mathbf{x}_1} \right) = \mathbf{M}_1^T \left( \frac{\mathbf{x}_1 - \mathbf{y}_1}{\sigma_1^2} \right)$$

- Finally:

$$\frac{\partial \mathcal{J}}{\partial \mathbf{x}_0} = \frac{\partial \mathcal{J}_1}{\partial \mathbf{x}_0} + \frac{\partial \mathcal{J}_2}{\partial \mathbf{x}_0} = \mathbf{M}_1^T \left( \frac{\mathbf{x}_1 - \mathbf{y}_1}{\sigma_1^2} \right) + \mathbf{M}_1^T \left[ \mathbf{M}_2^T \left( \frac{\mathbf{x}_2 - \mathbf{y}_2}{\sigma_2^2} \right) \right]$$