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Atmospheric Models with Data

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Contents

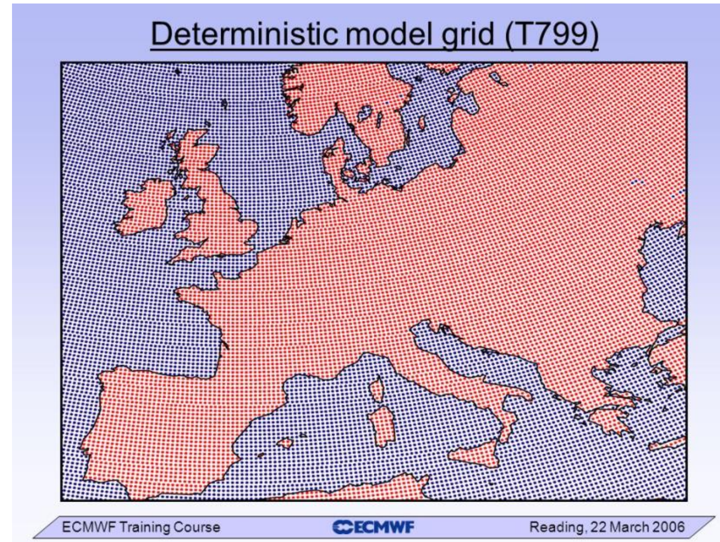
European Centre for Medium-range Weather Forecast numerical model: the dynamic core

$$\frac{\partial U}{\partial t} + \frac{1}{a\cos^2\theta}\left\{U\frac{\partial U}{\partial\lambda} + v\cos\theta\frac{\partial U}{\partial\theta}\right\} + \dot{\eta}\frac{\partial U}{\partial\eta}$$

$$(-fv) + \frac{1}{a}\left\{\frac{\partial\phi}{\partial\lambda} + R_{\mathrm{dry}}T_v\frac{\partial}{\partial\lambda}(\ln p)\right\} = P_U + K_U$$

$$\frac{\partial V}{\partial t} + \frac{1}{a\cos^2\theta}\left\{U\frac{\partial V}{\partial\lambda} + V\cos\theta\frac{\partial V}{\partial\theta} + \sin\theta(U^2+V^2)\right\} + \dot{\eta}\frac{\partial V}{\partial\eta}$$

$$+fU + \frac{\cos\theta}{a}\left\{\frac{\partial\phi}{\partial\theta} + R_{\mathrm{dry}}T_v\frac{\partial}{\partial\theta}(\ln p)\right\} = P_V + K_V$$

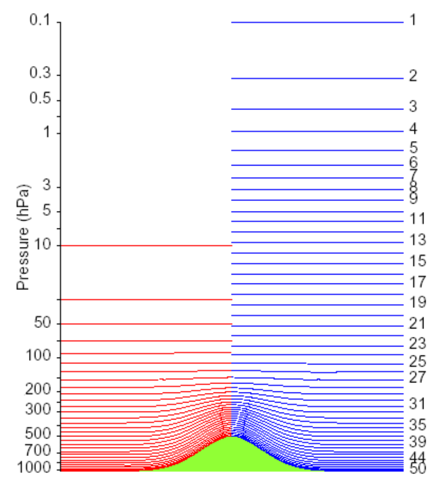


$$\frac{\partial T}{\partial t} + \frac{1}{a\cos^2\theta}\left\{U\frac{\partial T}{\partial\theta} + V\cos\theta\frac{\partial T}{\partial\theta}\right\} + \dot{\eta}\frac{\partial T}{\partial\eta} - \frac{\kappa T_v\omega}{(1+(\delta-1)q)p} = P_T + K_T$$

$$\frac{\partial q}{\partial t} = \frac{1}{a\cos^2\theta}\left\{U\frac{\partial q}{\partial\lambda} + V\cos\theta\frac{\partial q}{\partial\theta}\right\} = \eta\frac{\partial q}{\partial\eta} = P_q + K_q$$

$$\frac{\partial p_{\mathrm{surf}}}{\partial t} = -\int_0^1 \nabla\cdot\left(\mathbf{v}_H\frac{\partial p}{\partial\eta}\right)d\eta \qquad \dot{\eta}\frac{\partial p}{\partial\eta} = -\frac{\partial p}{\partial\eta} - \int_0^\eta \nabla\cdot\left(\mathbf{v}_H\frac{\partial p}{\partial\eta}\right)d\eta$$

$$\eta(0, p_{\mathrm{surf}}) = 0$$



meanwhile T1279L91 (~15 km)

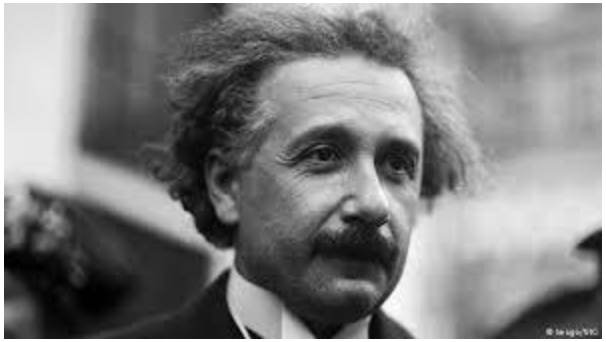
➔

dim **O(10^8)**

Einstein on weather predictability

"When the number of factors coming into play in a phenomenological complex is too large, scientific method in most cases fails**. One need only think of the weather, in which case the prediction even for a few days ahead is impossible**."

— Albert Einstein



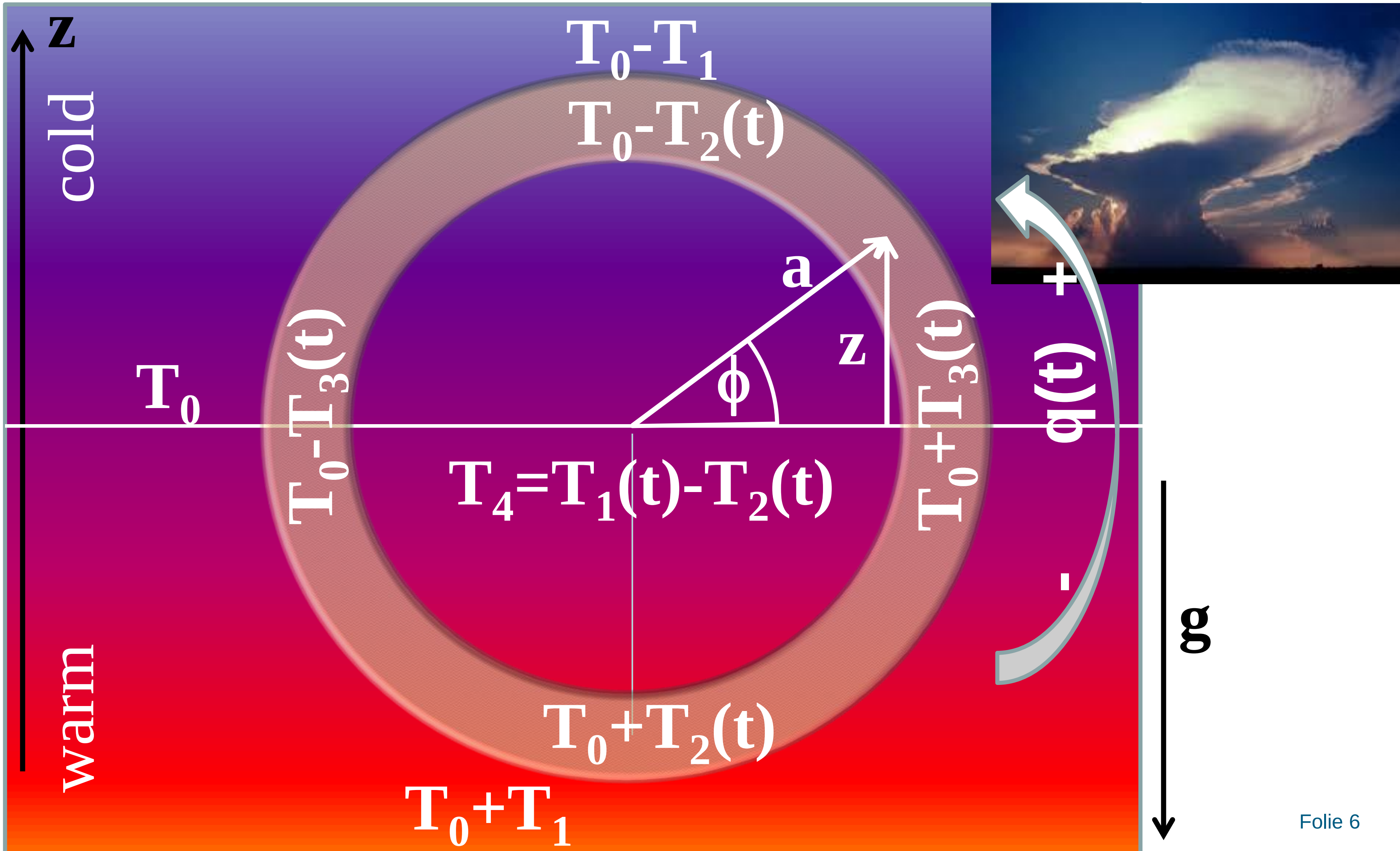
The minimalistic nucleus of (weather) chaos:

Lorenz, E. N. Deterministic non-periodical flow. J. Atmos. Sci. 20, 130–141, (1963).

One of the most influential papers establishing the fundamentals of chaos theory applied to numerical weather prediction.

Lorenz (1963) system:

A technical realisation: Convection in a torus



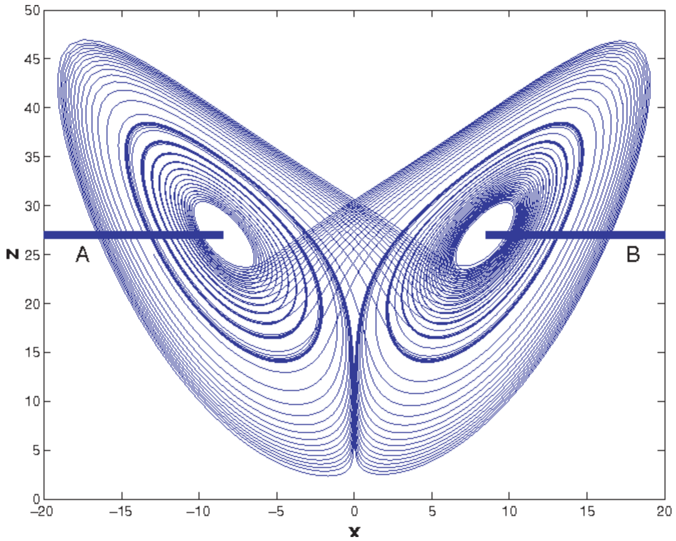
Lorentz (1963) equations

A transition to non-dimensional variables X, Y, Z is achieved by defining

$$X := \frac{q}{aK}, \qquad Y := \frac{g\alpha T_3}{2a\Gamma K}, \qquad Z := \frac{g\alpha T_4}{2a\Gamma K}, \qquad t' := tK,$$

to arrive at

$$\begin{aligned} \frac{dX}{dt} &= -PX + PY \\ \frac{dY}{dt} &= -Y + rX - XZ \\ \frac{dZ}{dt} &= -bZ + XY, \end{aligned}$$



where

$$P := \frac{\Gamma}{K}, Prandtl\, number, \qquad r := \frac{g\alpha T_1}{2a\Gamma K}, Rayleigh\, number \qquad b = 8/3\, heat\, transfer$$

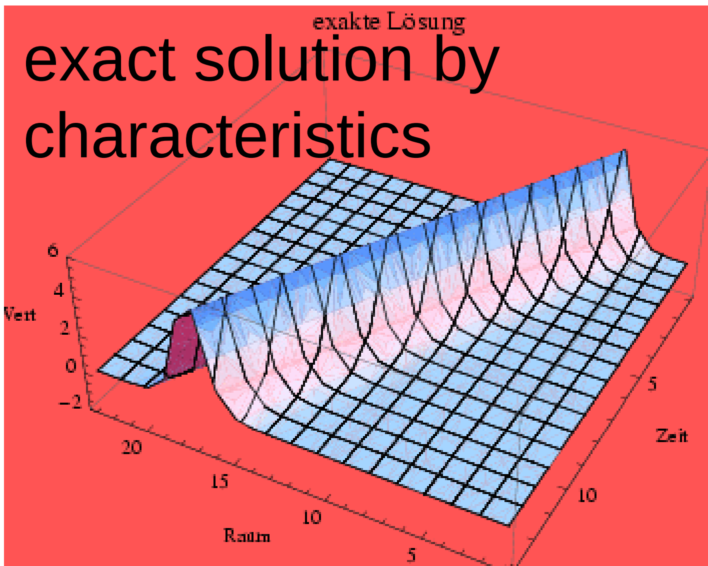
Why poor predictability in practice?

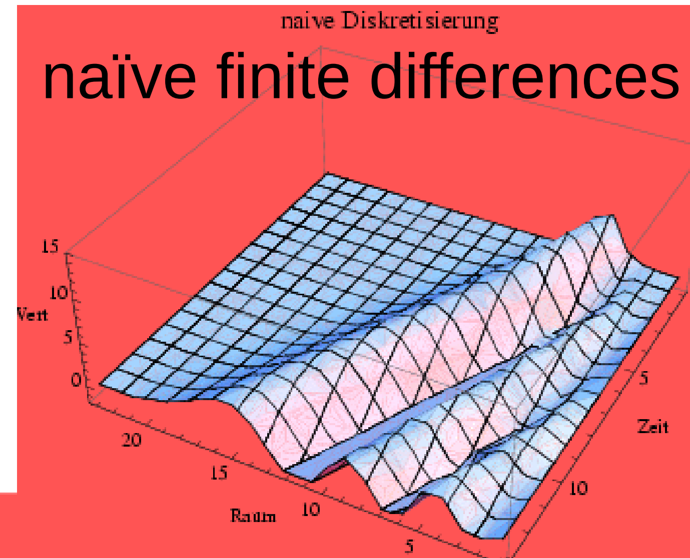
Instabilities:

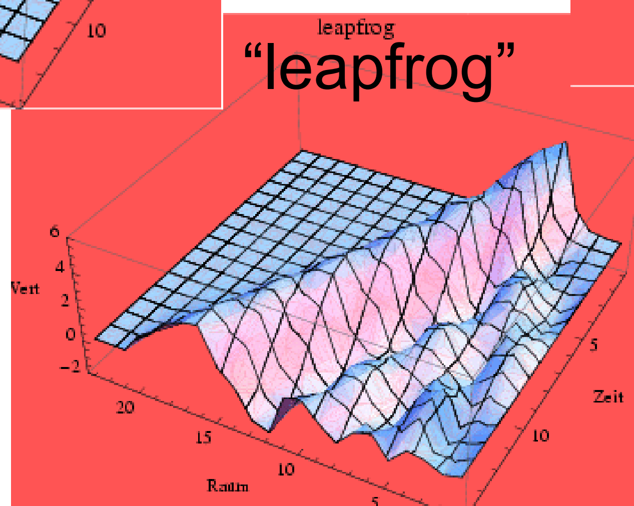
- convective scale clouds and convection
- barotropic instabilities (rotational modes)
- baroclinic instabilities (low pressure systems)
- phase transitions of: water (Earth) , methane (Titan)
-

Another realm of advances: Numerics
a naïve starting point with the advection equation (fails after a few time steps)

$$\frac{\partial \chi(t,\mathbf{r})}{\partial t} + \mathbf{v}(t,\mathbf{r}) \cdot \nabla \chi(t,\mathbf{r}) = g(t,\mathbf{r})$$







for progress see presentation by Tamari Janelidze

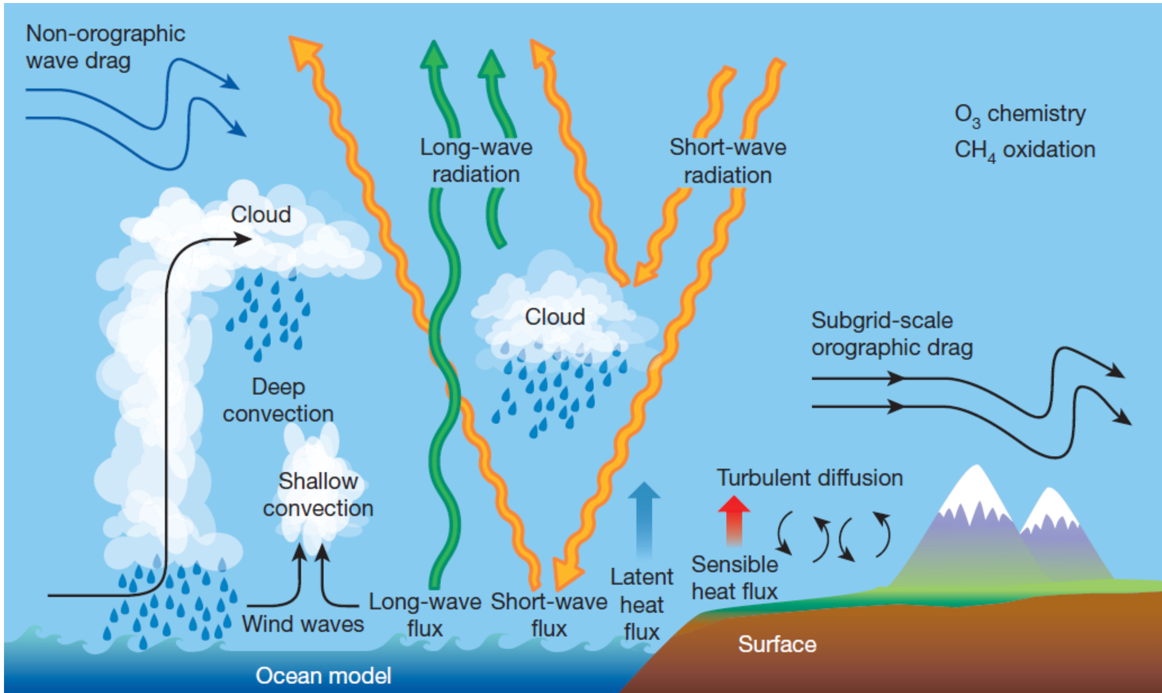
There is more progress: e.g. Nature article 2015
Bauer, Thorpe, Brunet

REVIEW

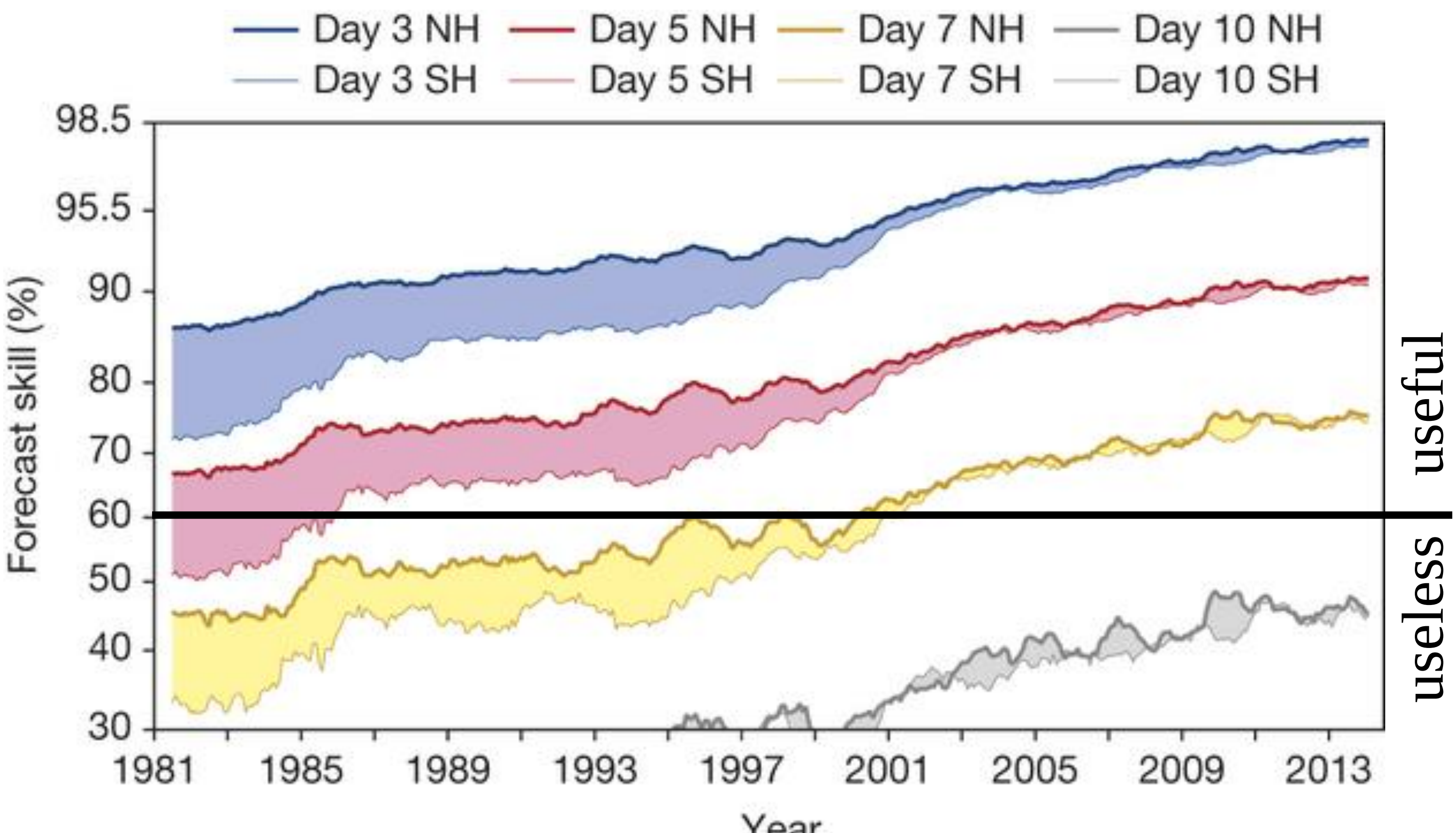
doi:10.1038/nature14956

The quiet revolution of numerical weather prediction

Peter Bauer[1], Alan Thorpe[1] & Gilbert Brunet[2]



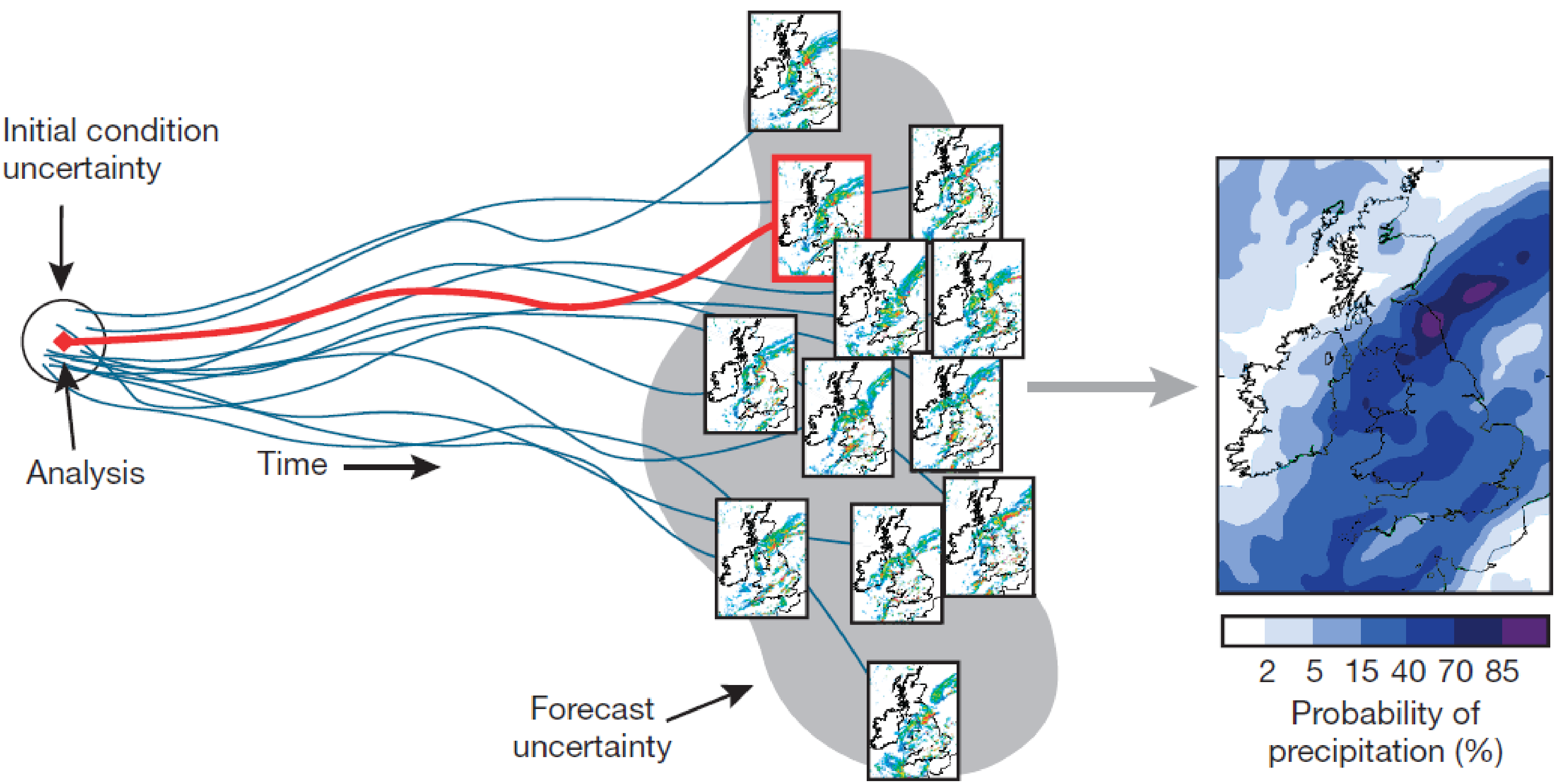
ECMWF forecast skill evolution



Source: ECMWF

Ensemble modelling: predicting uncertainties
O(#50) model integrations

example:
likelihood of precipitation



from Bauer et al, 2015

The main reasons for uncertain forecasts

There are two classes of reasons, why forecasts are uncertain:

- ❑ one is induced by model insufficiencies, and by

- ❑ the uncertainty of initial values.

The latter problem is addressed by data assimilation.

Initial value uncertainty

A quadratic form is reduced, defining a cost function, penalizing discrepancies between observations and a priori knowledge

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

The Hessian of J is the inverted analysis error covariance matrix

$$\nabla^2 J = \mathbf{B}^{-1} + H^T \mathbf{R}^{-1} H =: \mathbf{A}^{-1} \qquad (2)$$

The evolution of the uncertainty as quantified by the analysis error covariance matrix is given by the generalized eigenvector equation

$$M^T M \delta\mathbf{x}(t_0) = -\lambda \mathbf{A}^{-1} \delta\mathbf{x}(t_0) \qquad (1)$$

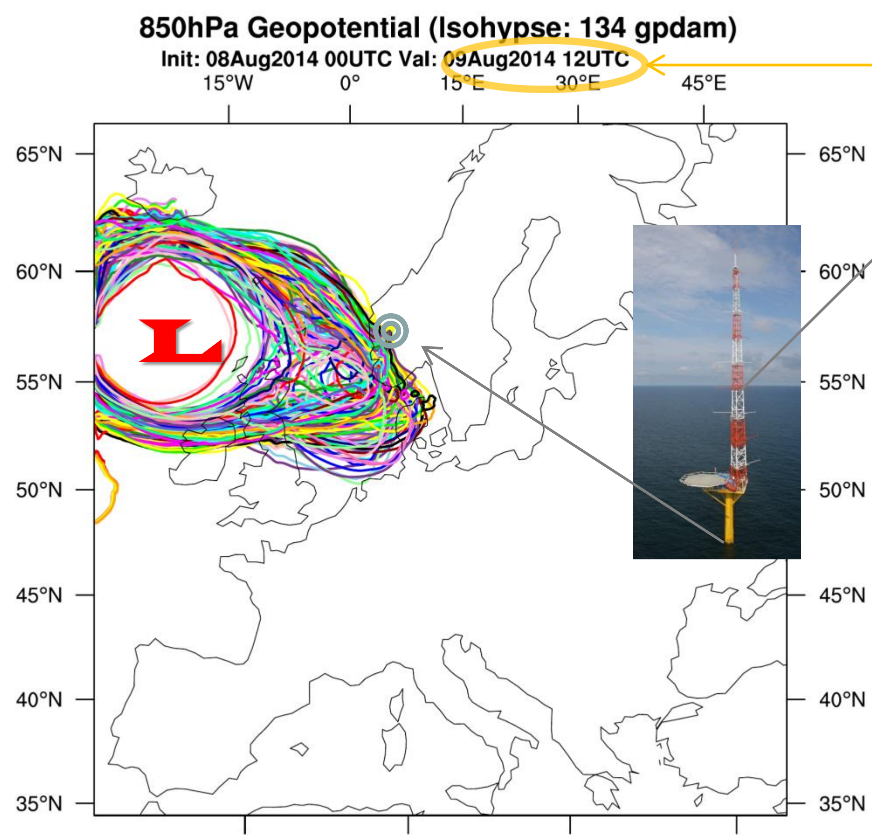
Model uncertainties

Key source of uncertainties result from

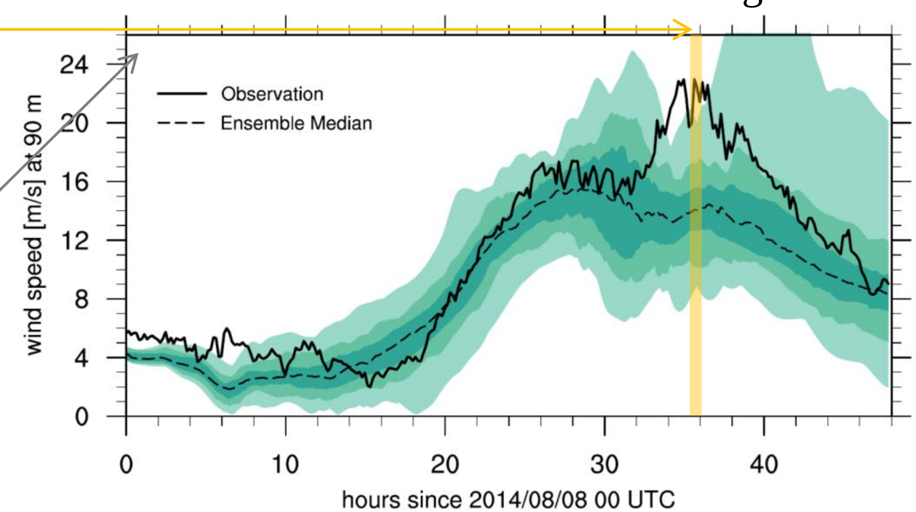
- not sufficiently well known processes and their controlling parameters,
- the finite resolution of calculations due to the model discretization. or errors due to truncation of dynamics and
- unresolved features of "`subgrid processes"'.

Energy meteorology: wind

Can we predict the likelihood of imminent fatal forecast failures?
1000 parallel model runs with WRF



FINO3 measurement tower 101 m height



(Example case
from PhD Jonas Berndt
08.08. - 10.08. 2014)

Ensemble size of (*O*)1000 member to apply a Sequential Importance Resampling Smoother

a **novel, non-linear data assimilation technique in atmospheric science**.

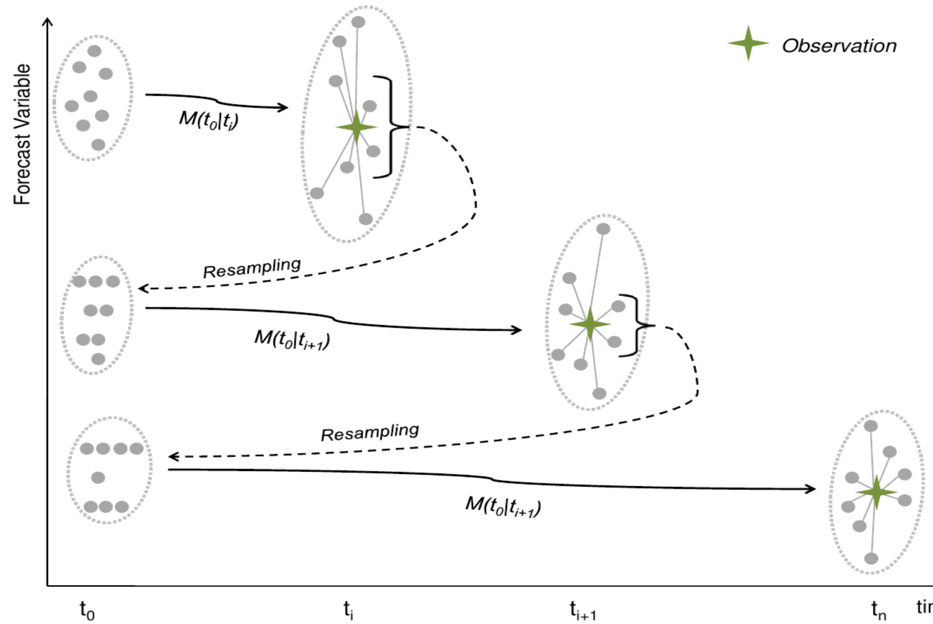
Parcticle filtering consists of representing the initial density of the state by an ensemble of size *N*

$$p(\Psi|d) = \sum_{i=1}^{N} w_i \delta(\Psi - \Psi_i)$$

we estimate the posteriori density of the model state, given the observ

$$w_i = \frac{p(d|\Psi_i)}{\sum_{j=1}^{N} p(d|\Psi_j)}.$$

- Each ensemble member gets a certain weight with respect to the observations



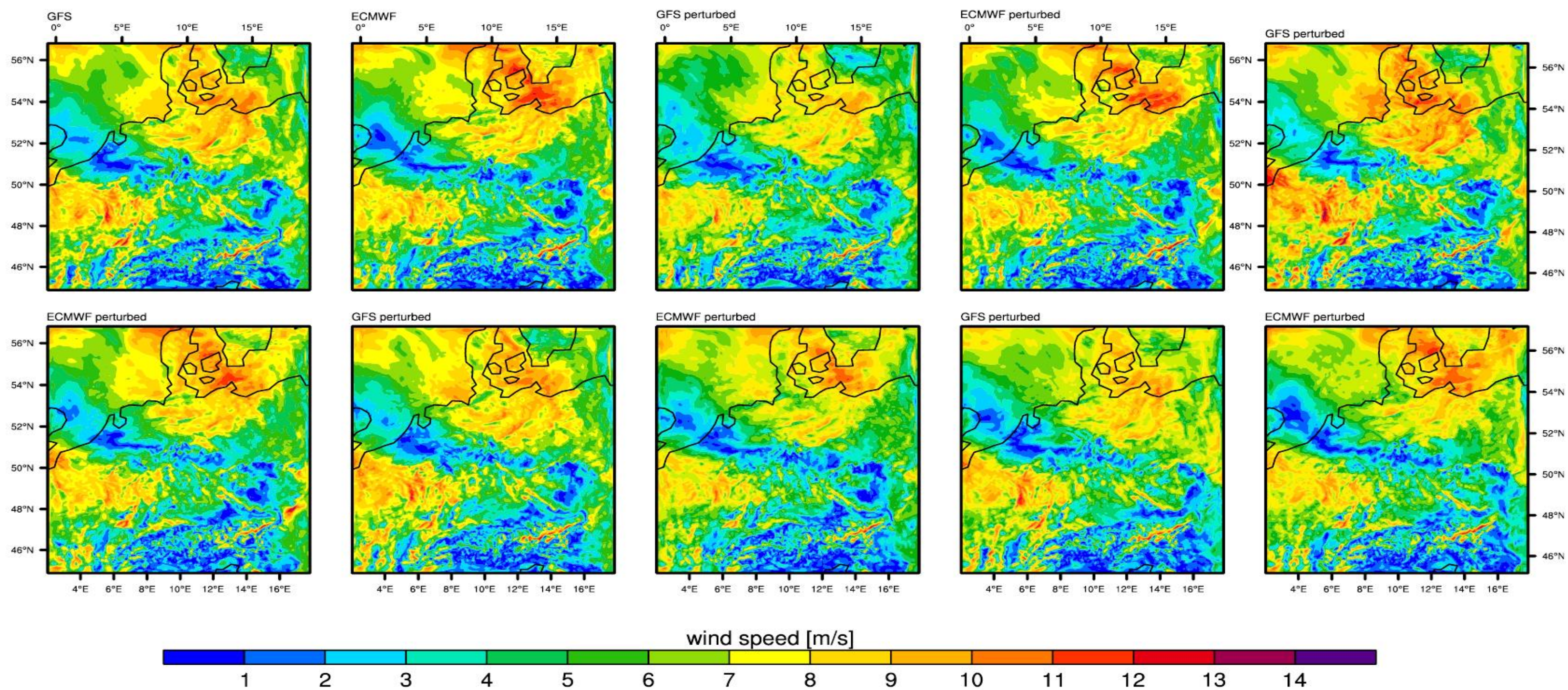
- Minimize ensemble variance by neglecting members with least weights and spawn members with highest weights

ESIAS super ensemble modelling system

(Ensembles for Stochastic Integration of Atmospheric Systems)

Stamp plots of an only 12-member sub-ensensemble selection with either

- GFS or ECMWF boundary and initial conditions and
- SKEBS (Stochastic Kinetic Energy Backscatter Scheme) perturbation.



24 h forecast for 5.09.2014 UTC 00:00

How can data control the prediction?

Observation systems

Observability

Terminology

Inverse Modelling

The inverse modelling problem consists of using the **actual** result of some **measurements** to **infer the values of the parameters** that characterize the system.

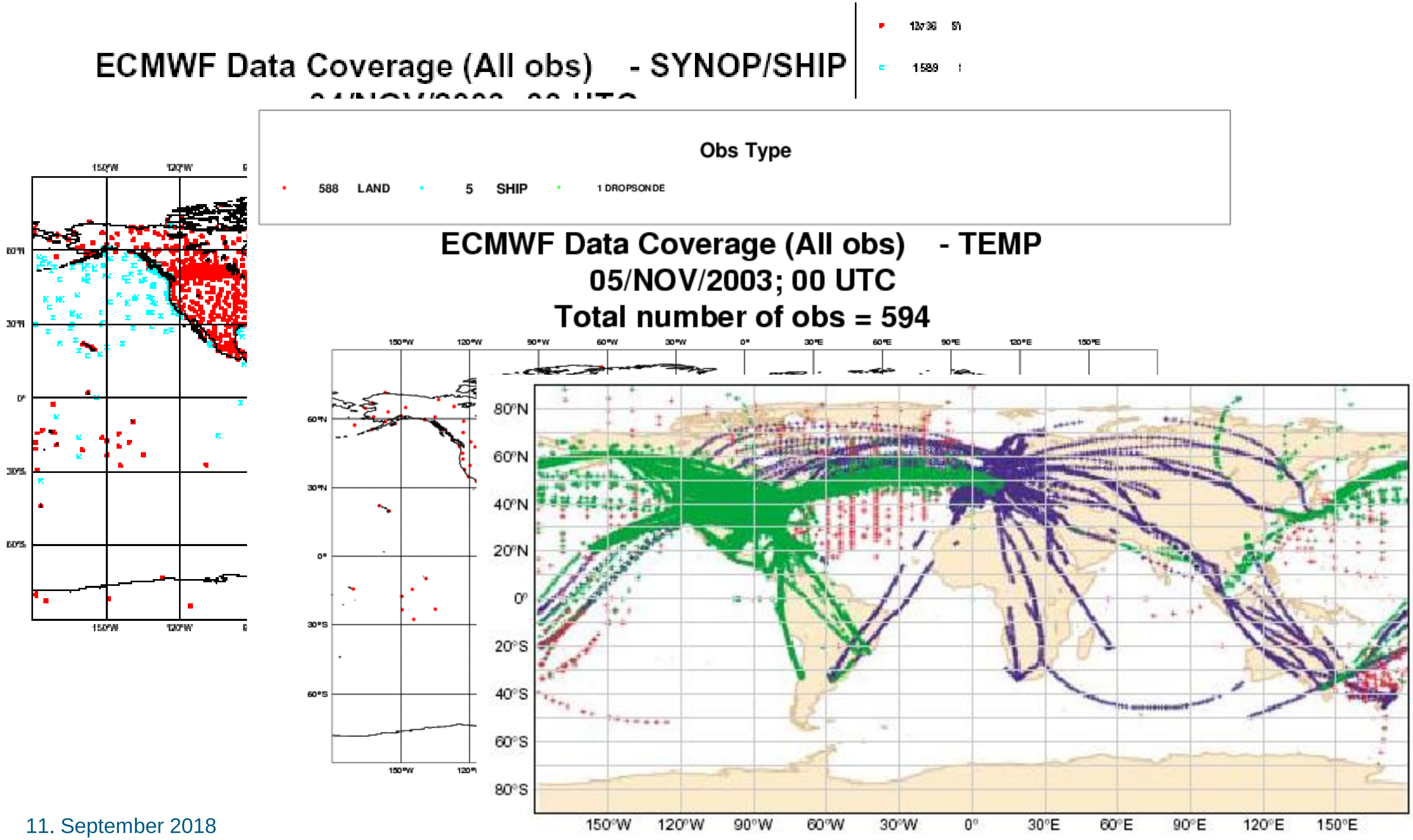
A. Tarantola (2005)

Data Assimilation in general

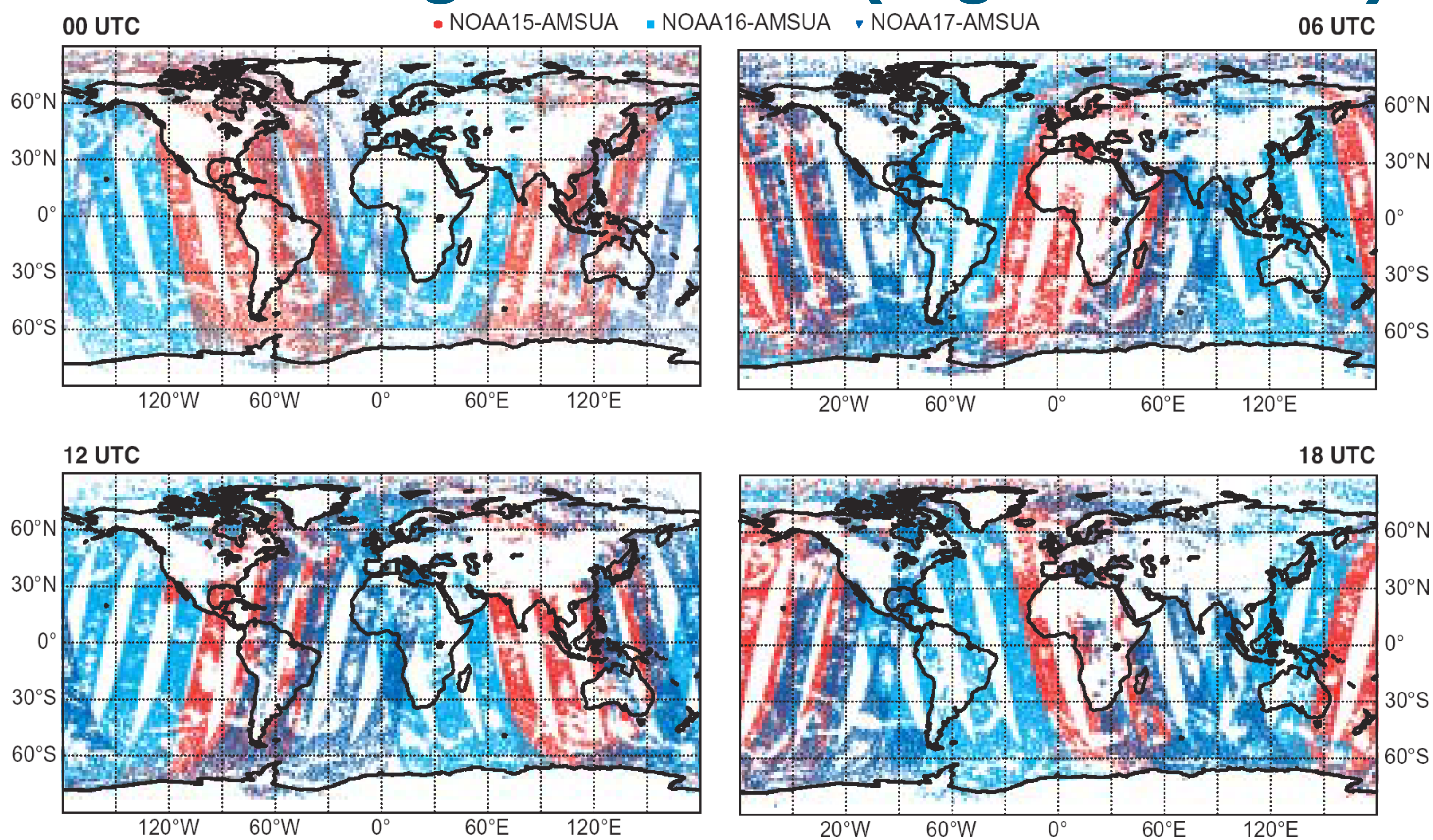
The ambitious and elusive goal of data assimilation is to provide a dynamically consistent motion picture of the atmosphere and oceans, in three space dimensions, with known error bars.

M. Ghil and P. Malanotte-Rizzoli (1991)

Observation systems (2): In-situ observations

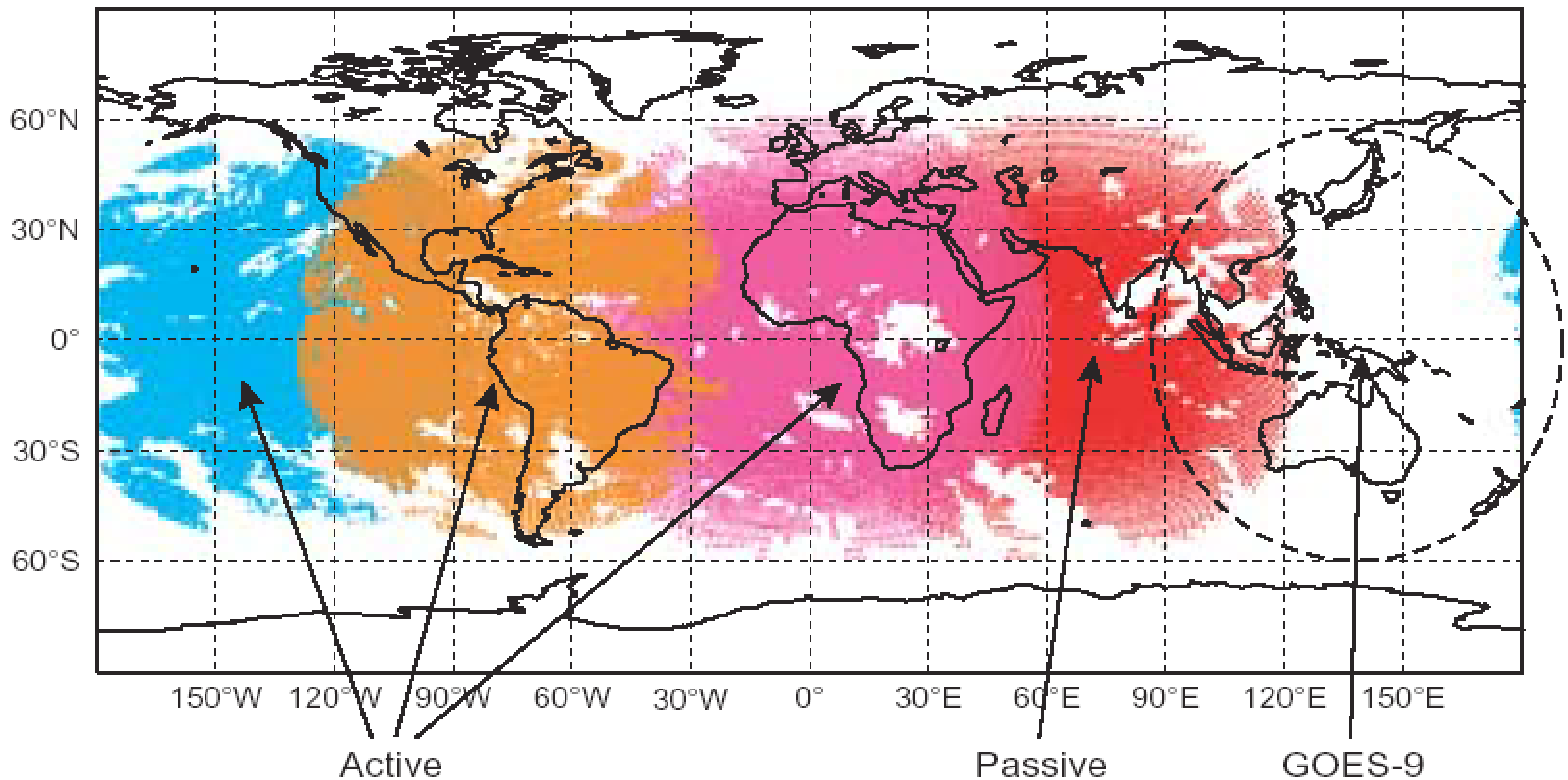


Observation systems (3): polar orbiting satellites (e.g. AMSU-A)



Data coverage for the NOAA-15 (red), NOAA-16 (cyan) and NOAA-17 (blue) AMSU-A instruments, for the four 6-hour periods centred at 00, 06, 12 and 18 UTC 12 November 2002. The plots show the data used for AMSU-A channel 5, which is a temperature-sounding channel in the mid and lower troposphere.

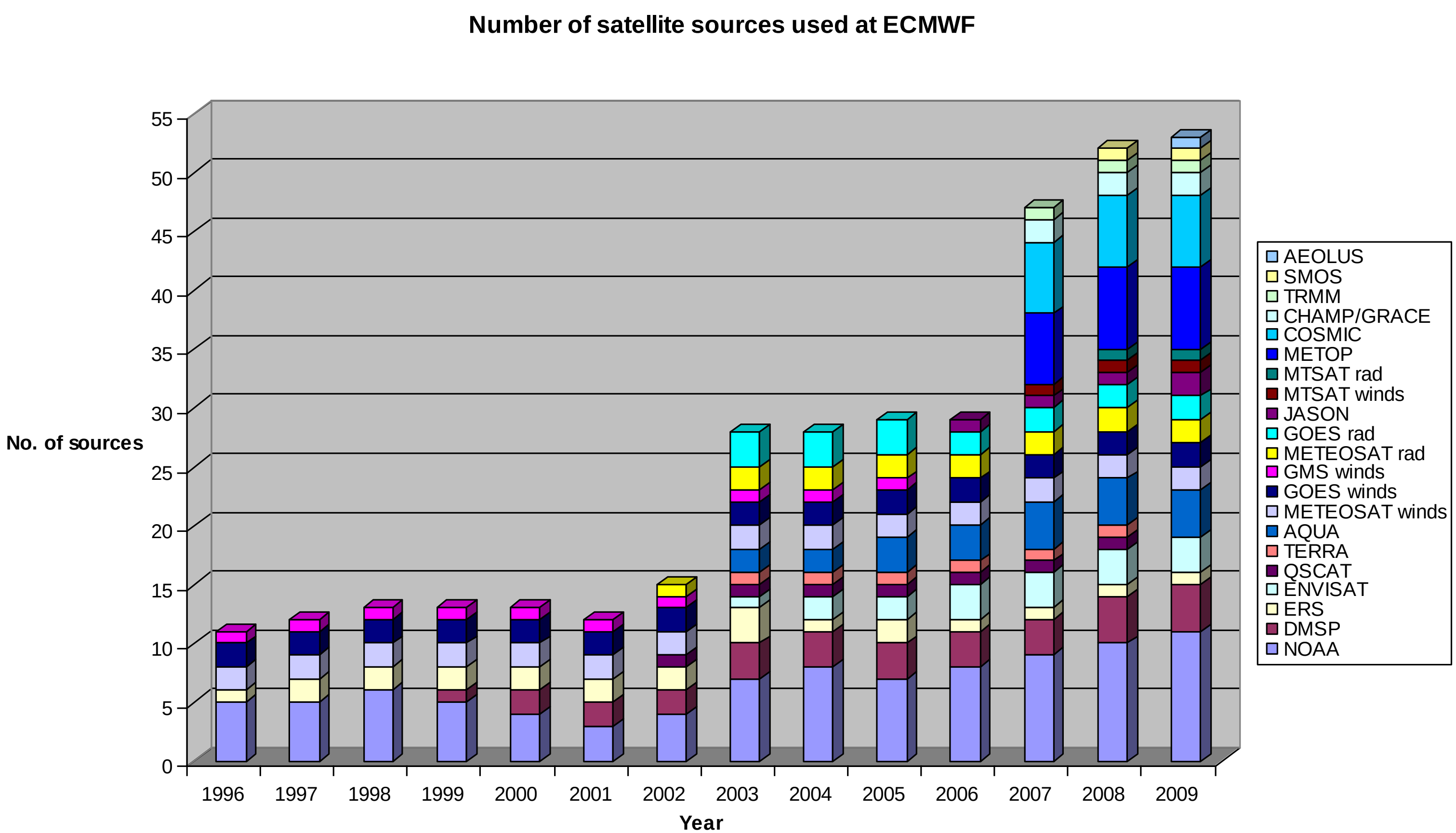
Observation systems (4): geostationary



Data coverage provided by the GOES satellites (cyan and orange) and the METEOSAT satellites (magenta and red) for 00 UTC 10 May 2003. The total number of observations

Source: ECMW

Satellite data sources in 2007+



Source: ECMWF

Improving the quality of analyses by the observation configuration

- optimise the observation network, subject to given **constraints**, [Szunyogh et al. 1999; Langland et al. 1999), Bishop et al. (1999); Berliner et al. (1998), Bellsky et al. 2014),…]

- to evaluate the **value** of individual or types of observations for the analyses, [Cardinali et al. (2004); Cardinali (2009), Liu and Kalnay (2008), Baker and Daley (2000), …]

- to quantify the degree of which the analysis can be influenced by the observations, that is the **sensitivity (Degree of Freedom for Signal)**. [Fisher (2003) Eyre 1990; Rodgers 2000; Rabier et al. 2002; Fourrié et al. 2003; Martynenko et al. 2010), …]

2. How can the observation configuration be optimized?

Given CTM (here RACM and EURAD-IM) acting as tan.-lin. model operator $\mathcal{L}$:

$$\delta\mathbf{c}(t_F) = \mathcal{L}_{t_I,t_F}\,\delta\mathbf{c}(t_I), \quad \mathcal{L}_{t_I,t_F} = \left.\frac{\partial \mathcal{M}_{t_I,t_F}}{\partial \mathbf{c}}\right|_{\mathbf{c}(t_I)}$$

1. Berliner et al., (1998) Statistical design:
"Minimize" the analysis error covariance matrix **A** (say, via trace):

$$\min_{\mathbf{H}} \mathbf{A} = \mathbf{B} - \underbrace{\mathbf{B}\mathbf{H}^T(\mathbf{H}\mathbf{B}\mathbf{H}^T + \mathbf{R})^{-1}\mathbf{H}\mathbf{B}}_{\text{to be maximized by } \mathbf{H}}$$

For this find maximal eigenvectors as observation operators **H,** which configure observations.

$$\mathcal{L}_{t_I,t_F}\mathbf{B}\mathcal{L}^T_{t_I,t_F}\mathbf{H}^T = \lambda\mathbf{H}^T$$

2. Palmer (1995) Singular vector analysis:
Observe maximal SV configuration:

$$\max_{\delta\mathbf{c}(t_I)} \frac{\|\delta\mathbf{c}(t_F)\|^2_{\mathbf{B}}}{\|\delta\mathbf{c}(t_I)\|^2_{\mathbf{B}}} = \max_{\delta\mathbf{c}(t_I)} \frac{\delta\mathbf{c}(t_I)^T\mathcal{L}^T_{t_I,t_F}\mathbf{B}\,\mathcal{L}_{t_I,t_F}\delta\mathbf{c}(t_I)}{\delta\mathbf{c}(t_I)^T\mathbf{B}\,\delta\mathbf{c}(t_I)},$$

Phase space variables per grid point stratospheric chemistry example

167 gas phase reactions +

10 heterogeneous reactions on polar strat. clou

Table 3. Heterogeneous reactions included in the SACADA reaction scheme. The notation "(c)" indicates a species in the condensed (liquid or solid) phase. The term "products" represents constituents which are not considered in the reaction scheme.

Reaction		Uptake coefficient		
		liquid/STS	NAT	ice
(R168)	$BrONO_2 + H_2O(c) \rightarrow HOBr + HNO_3$	$f(t, p_{H_2O})^a$	-	0.26
(R169)	$N_2O_5 + H_2O(c) \rightarrow HNO_3 + HNO_3$	$f(t, p_{H_2O})^a$	0.0004	0.02
(R170)	$ClONO_2 + H_2O(c) \rightarrow HNO_3 + HOCl$	$f(t, p_{H_2O}, p_{HCl})^b$	0.004	0.3
(R171)	$ClONO_2 + HCl(c) \rightarrow Cl_2 + HNO_3$	$f(t, p_{H_2O}, p_{HCl})^b$	0.2	0.3
(R172)	$HOCl + HCl(c) \rightarrow Cl_2 + H_2O$	$f(t, p_{H_2O}, p_{HCl})^b$	0.1	0.2
(R173)	$N_2O_5 + HCl(c) \rightarrow HNO_3$ + products	-	0.003	0.03
(R174)	$HOBr + HCl(c) \rightarrow BrCl + H_2O$	0.01	-	0.3
(R175)	$ClONO_2 + HBr(c) \rightarrow BrCl + HNO_3$	-	0.3	0.3
(R176)	$HOCl + HBr(c) \rightarrow BrCl + H_2O$	-	-	0.05
(R177)	$BrONO_2 + HCl(c) \rightarrow BrCl + HNO_3$	0.3	-	0.3

a: as recommended by *Sander et al.* [2006]

b: *Shi et al.* [2001], as recommended by *Sander et al.* [2006]

Transport-diffusion-reaction equation and its adjoint

Tendency Equations

direct chemistry transport equation

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (\mathbf{v} c_i) - \nabla \cdot (\rho \mathbf{K} \nabla \frac{c_i}{\rho}) - \Sigma_{r=1}^{R} \left(k(r) \left(s_i(r_+) - s_i(r_-) \right) \Pi_{j=1}^{U} c_j^{s_j(r_-)} \right) = E_i + D_i$$

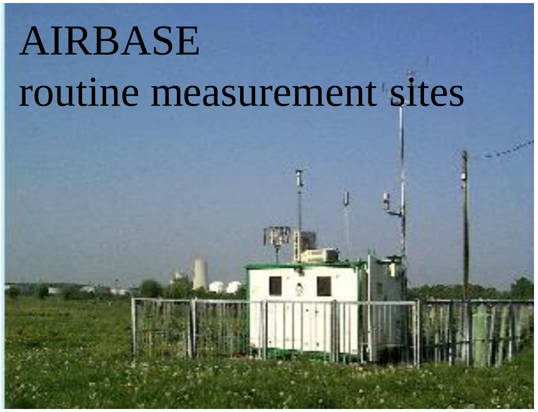
c_i	concentration of species i	c_i^*	adjoint of concentration of species i
$\mathbf{v}$	wind velocity	s	stoichiometric coefficient
$k(r)$	reaction rate of reaction r	$\mathbf{K}$	diffusion coefficient
U	number of species in the mechanism	R	number of reactions in the mechanism
E_i	emission rate of species i (source)	D_i	deposition rate of species i (sink)

adjoint chemistry transport equation

$$-\frac{\partial \delta c_i^*}{\partial t} - \mathbf{v} \nabla \delta c_i^* - \frac{1}{\rho} \nabla \cdot (\rho \mathbf{K} \nabla \delta c_i^*) + \Sigma_{r=1}^{R} \left(k(r) \frac{s_i(r_-)}{c_i} \Pi_{j=1}^{U} \bar{c}_j^{\,s_j(r_-)} \Sigma_{n=1}^{U} \left(s_n(r_+) - s_n(r_-) \right) \delta c_n^* \right) = 0$$

Use of In Situ and Remote Sensing Data

In Situ



Remote Sensing

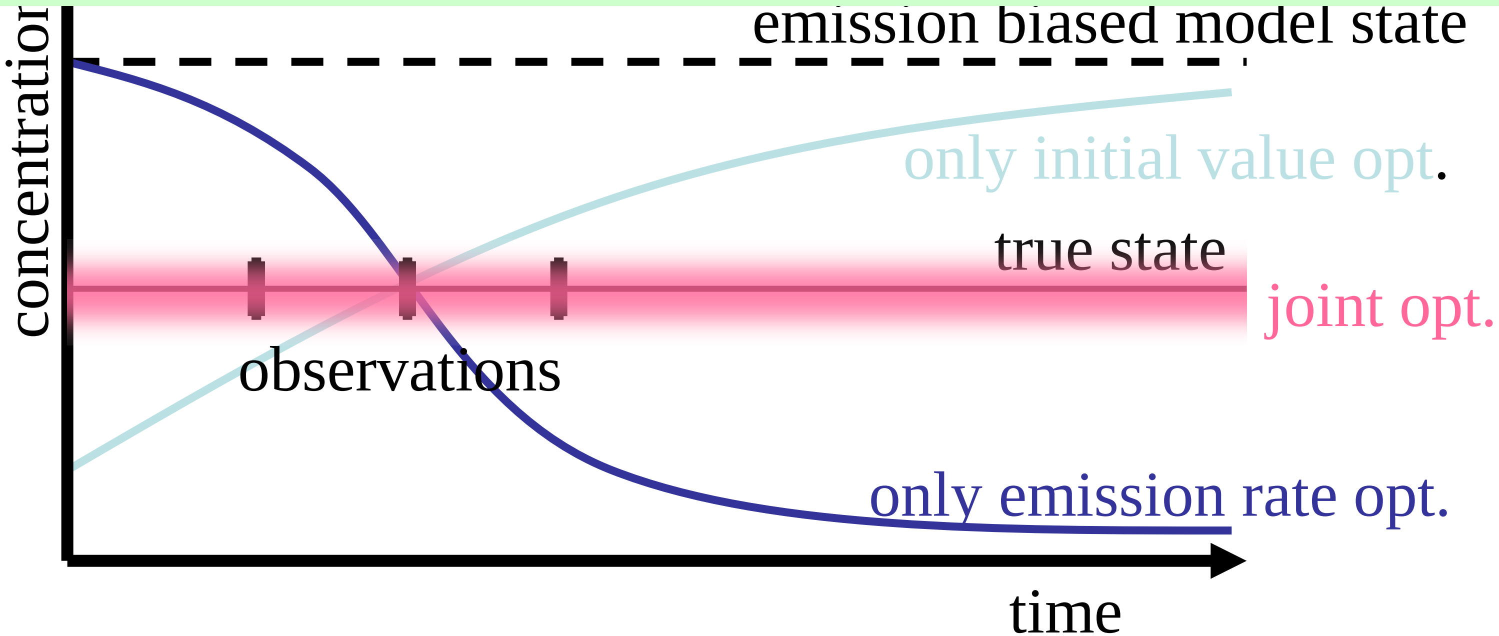
For an optimal observation network design two central questions :

1. Is the observation system sensitive to both initial value and emission rate optimisation?

2. Which chemical constituents should be observed with preference? And

Key question: Which parameter is to be optimised by inverse modelling?

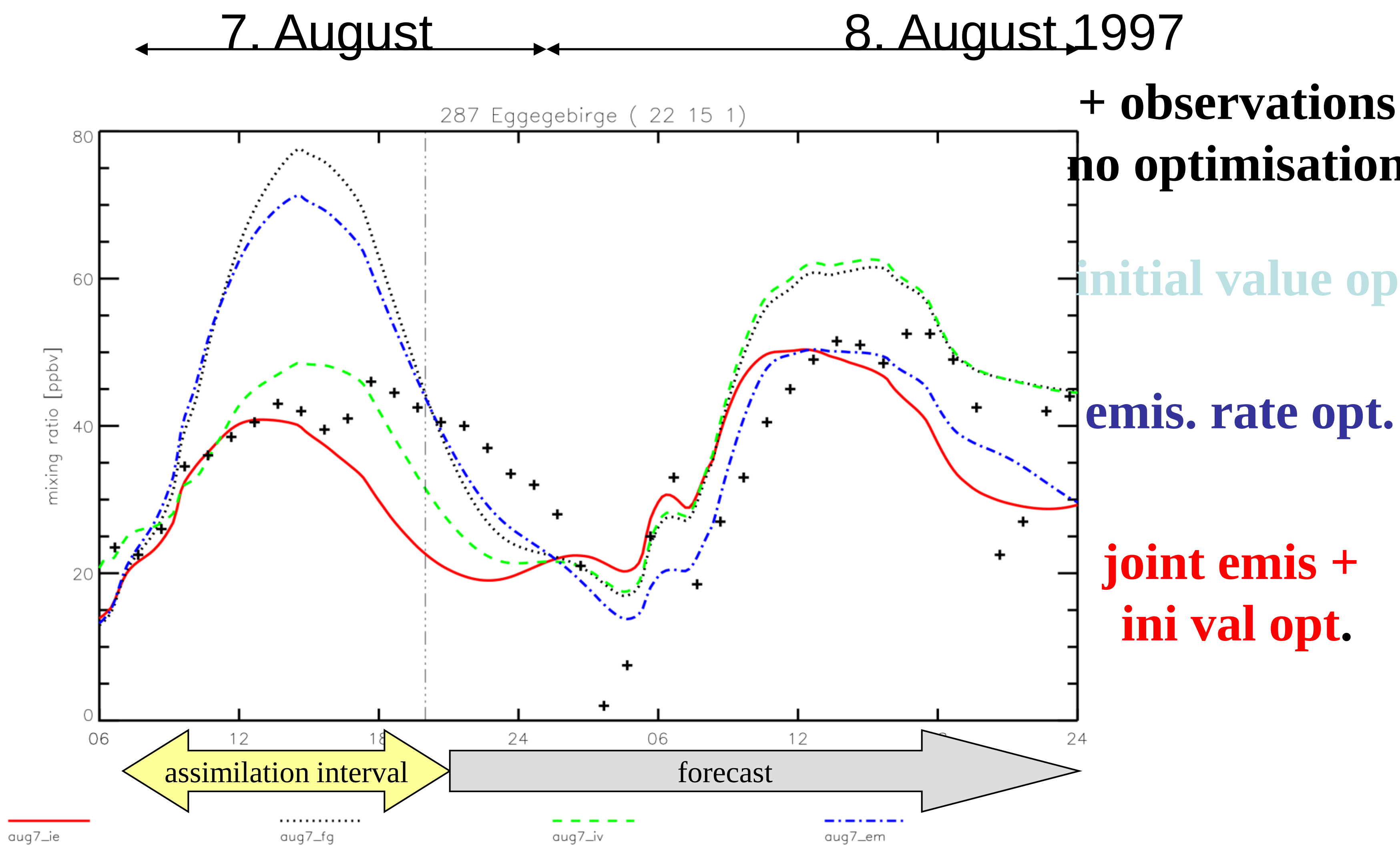
In the troposphere, for emission rates, the product (*paucity of knowledge) x (importance for forecast)* is high



Additional "emission observations" would be desirable for balancing (e.g. via Damköhler number).

An example from air quality inversion

Semi-rural measurement site Eggegebirge



1. Observation location impact assessment on parameter optimisation by Ensemble Kalman Smoother

We seek to infer **normalised sensitivity maps**, which exhibit the control capacity of observations on parameters to be optimised: here ***emission rates*** and ***initial values***

separate vector sections
initial values,
emission rates

Extended model with emission rates

$$\begin{pmatrix} \delta c(t) \\ \delta e(t) \end{pmatrix} = \begin{pmatrix} M(t,t_0) & \int_{t_0}^{t} M(t,s)M_e(s,t_0)ds \\ 0 & M_e(t,t_0) \end{pmatrix} \begin{pmatrix} \delta c(t_0) \\ \delta e(t_0) \end{pmatrix}.$$

Typically, there is no direct observation for emissions.

$$\delta y(t) = [H(t), 0_{n\times n}] \begin{pmatrix} \delta c(t) \\ \delta e(t) \end{pmatrix} + \nu(t),$$

where $0_{n\times n}$ is a $n \times n$ matrix with zero elements.

from Wu, Elbern, Jacob , SIAM, 2016, and GMDD, 2017

Is the information needed available?

Exhibiting the control capacity of observations on parameters to be optimised

Infer **normalised sensitivity maps**, for here **emission rates** and **initial values**

Costly:
calculate the **observability Gramian** matrix (control theory) by forward and adjoint model M, observation operators H, and observation error covariance matrix.

$$\mathcal{G} = \begin{pmatrix} H(t_0)M(t_0,t_0) \\ H(t_1)M(t_1,t_0) \\ \vdots \\ H(t_N)M(t_N,t_0) \end{pmatrix}, \rightarrow \quad \mathcal{G}^T\mathcal{R}\mathcal{G}$$

from Wu et al. , GMDD, 2017

Recall Kalman Filter equations

Extended Kalman filter equations

Forecast step:

$$\boldsymbol{x}^{\mathrm{b}}(t_i) = M_{i-1}\left[x^{\mathrm{a}}(t_{i-1})\right]$$

$$\mathbf{P}(t_0|t_{-1}) = \mathbf{L}_{i-1}\mathbf{P}(t_0|t_N)(t_{i-1})\mathbf{L}_{i-1}^T + \mathbf{Q}(t_{i-1})$$

Analysis step:

$$\boldsymbol{x}^{\mathrm{a}}(t_i) = \boldsymbol{x}^{\mathrm{b}}(t_i) + \mathbf{K}(t_i)\left(\boldsymbol{y} - H\left[\boldsymbol{x}^{\mathrm{b}}(t_i)\right]\right)$$

$$\mathbf{P}(t_0|t_N) = (\mathbf{I} - \mathbf{K}(t_i)\mathbf{H})\,\mathbf{P}(t_0|t_{-1})$$

where

$M_i :=$ Model operator

$\mathbf{L}_i :=$ Tangent linear model operator

$$\mathbf{K}(t_i) := \mathbf{P}(t_0|t_{-1})\mathbf{H}^T\left[\mathbf{R} + \mathbf{HP}(t_0|t_{-1})\mathbf{H}^T\right]^{-1}$$

$\mathbf{Q}(t_i) :=$ Model error covariance matrix

$\mathbf{P}(t_0|t_{-1}) :=$ Background error covariance matrix

$\mathbf{P}(t_0|t_N) :=$ Analysis error covariance matrix

$\mathbf{R}(t_i) :=$ Observation error covariance matrix

Singular vectors for initial state and emission sensitivity

Define the ***relative improvement covariance matrix***

(scaled forecast – analysis error covariance matrix from KS)

$$\begin{aligned}\tilde{P} &= P^{-\frac{1}{2}}(t_0|t_{-1})(P(t_0|t_{-1}) - P(t_0|t_N))P(t_0|t_{-1}) \\ &= I - (I + P^{\frac{1}{2}}(t_0|t_{-1})\mathcal{G}^\top \mathcal{R}^{-1}\mathcal{G}P^{\frac{1}{2}}(t_0|t_{-1}))^{-1} \\ &= I - (I + VSS^\top V^\top)^{-1} = \ldots = \\ &= V(I - (I + SS^\top)^{-1})V^\top \\ &= \sum_{i=1}^{r} \frac{s_i^2}{1+s_i^2} v_i v_i^\top,\end{aligned}$$

singular value decomposition

separate singular vector sections initial values,

emission rates

$$\tilde{P} = \begin{pmatrix} \tilde{P}^c & \tilde{P}^{ce} \\ \tilde{P}^{ec} & \tilde{P}^e \end{pmatrix} = \sum_{i=1}^{2n} \frac{s_i^2}{1+s_i^2} \begin{pmatrix} v_i^c \\ v_i^e \end{pmatrix} ({v_i^c}^\top, {v_i^e}^\top) \in R^{2n \times 2n},$$

$$\|\tilde{P}^c\|_1 = \sum_{i=1}^{2n} \frac{s_i^2}{1+s_i^2} \mathrm{tr}(v_i^c {v_i^c}^\top), \qquad \|\tilde{P}^e\|_1 = \sum_{i=1}^{2n} \frac{s_i^2}{1+s_i^2} \mathrm{tr}(v_i^e {v_i^e}^\top).$$

from Wu et al. , GMDD, 2017

Sensitivity by partial singular vectors

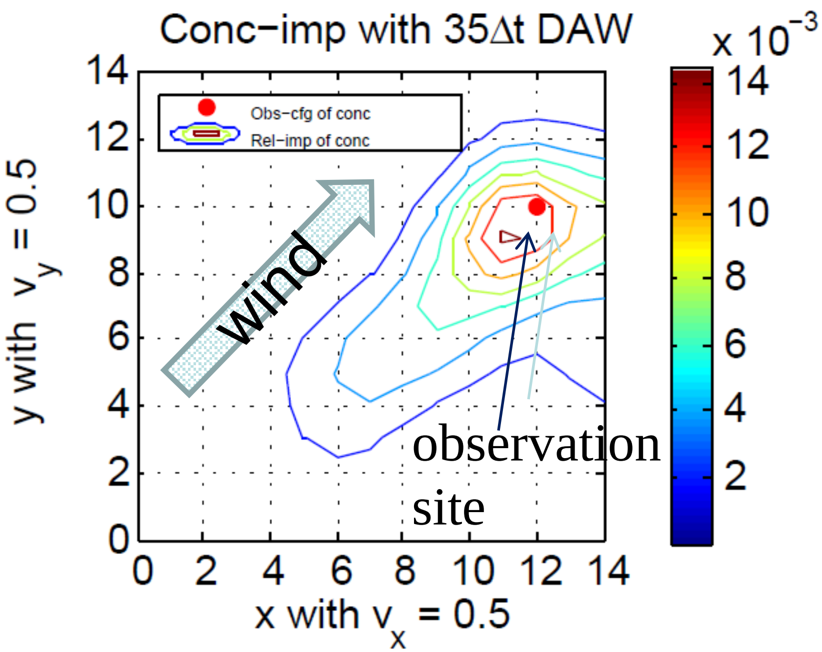
Given:

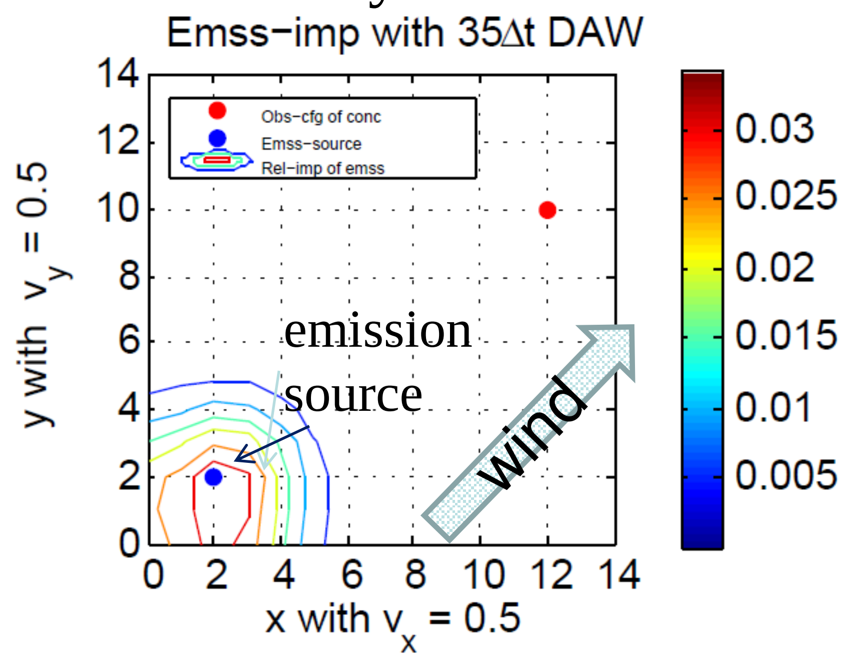
1 observation site 1 windward emission source location

assimilation window: advection time source → observation (35 units)

Question:

can **both** initial values and emission rates be analysed?





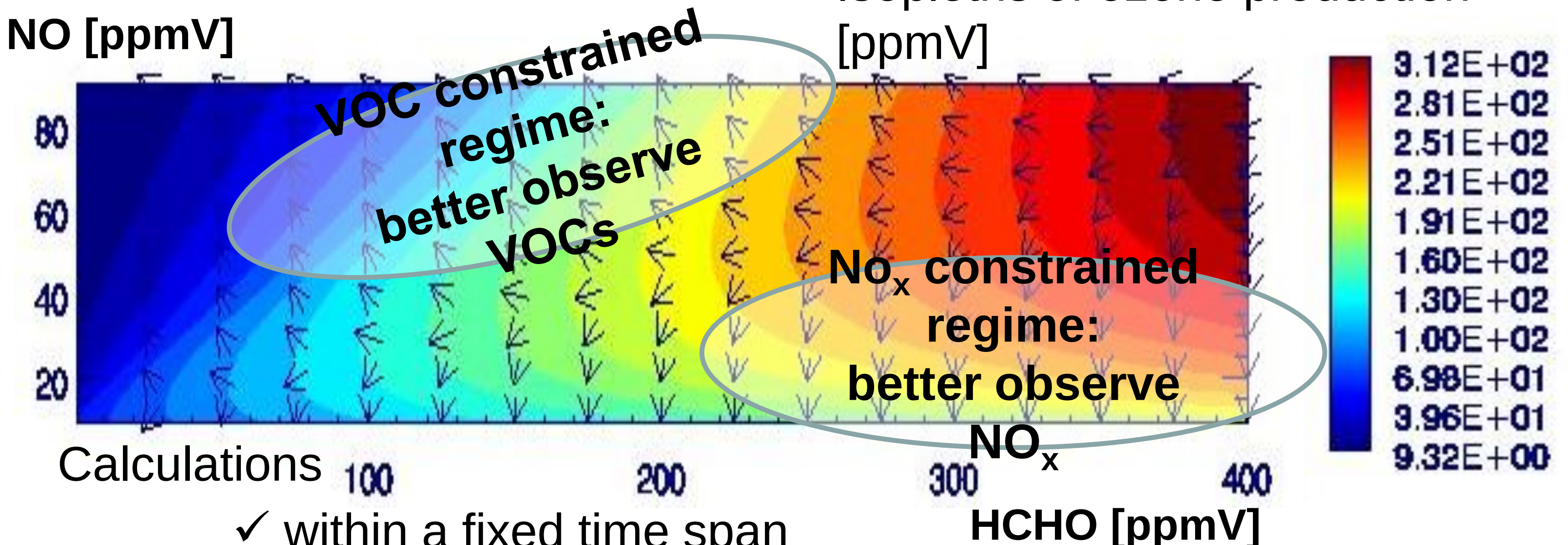
maximal sensitivities: ini. val. $P^c = 0.45$ emi rate $P^e = 0.55$

Answer: **Yes, both sensitivities are of same order**

from Wu et al., GMDD, 2017

What should be observed?

Is NO_x always <u>the</u> controlling key to ozone production? And consequently, its observation the key to better forecast?



Calculations

- ✓ within a fixed time span
- ✓ initial conventrations of NO / HCHO were varied
- ✓ change of final concentration is given by colour
- ✓gradients (SVs) of maximyl ozone production given by arrows

from Goris and Elbern , ACP, 2013

Singular value analysis

to identify the direction of maximal error/perturbation growth

model operator ($t_i \rightarrow t_f$) $\mathbf{c}(t_F) = \mathcal{M}_{t_I,t_F}\,\mathbf{c}(t_I)$

with initial perturbation $\delta\mathbf{c}(t_I)$

error evolution with : tangent-linear model $\delta\mathbf{c}(t_F) = \mathbf{L}_{t_I,t_F}\,\delta\mathbf{c}(t_I)$

maximise

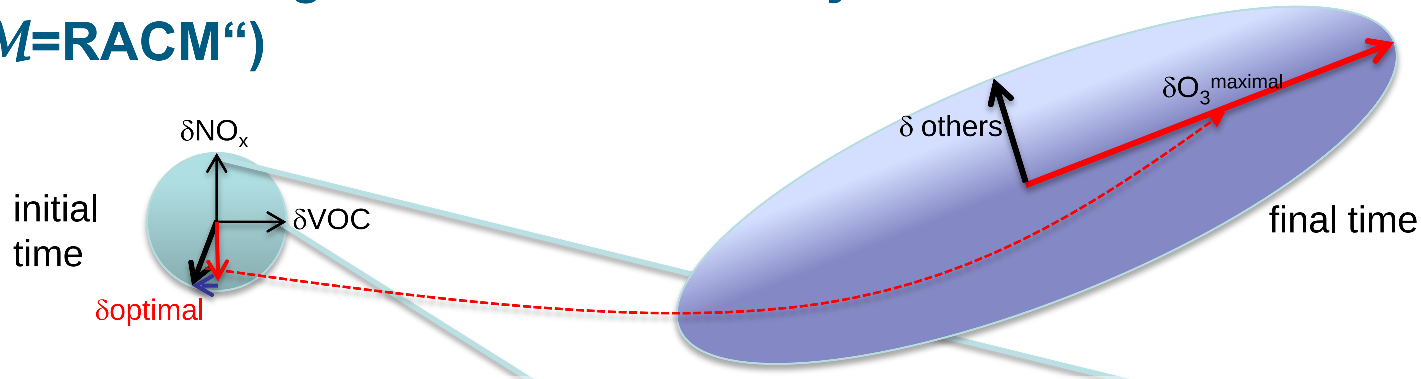
$$\frac{\|\,\delta\mathbf{c}(t_F)\,\|_2}{\|\,\delta\mathbf{c}(t_I)\,\|_2} = \frac{\sqrt{\delta\mathbf{c}(t_I)^T\,\mathbf{L}_{t_I,t_F}^T\,\mathbf{L}_{t_I,t_F}\,\delta\mathbf{c}(t_I)}}{\sqrt{\delta\mathbf{c}(t_I)^T\delta\mathbf{c}(t_I)}}$$

RIU

JÜLICH FORSCHUNGSZENTRUM

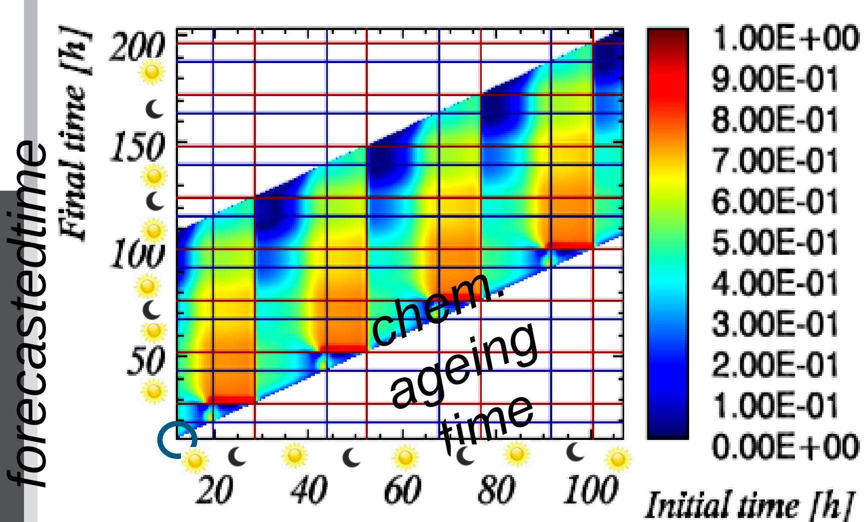
What should be observed?

Basic 0-D Regional Atm. Chemistry Mechanism („$\mathcal{M}$=RACM“)

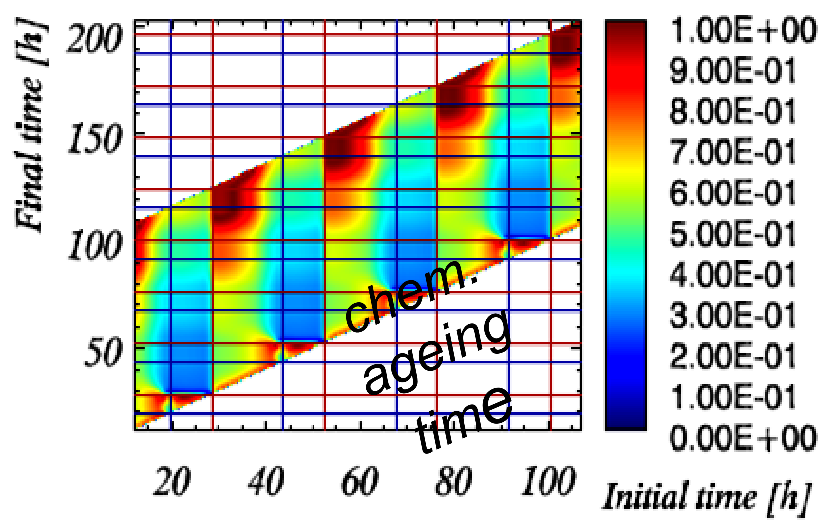


- **Optimal perturbations (Singular Vectors) for** scenario MARINE

1st Grouped Singular Vectors (δVOC)



1st Grouped Singular Vectors (δNO_x)

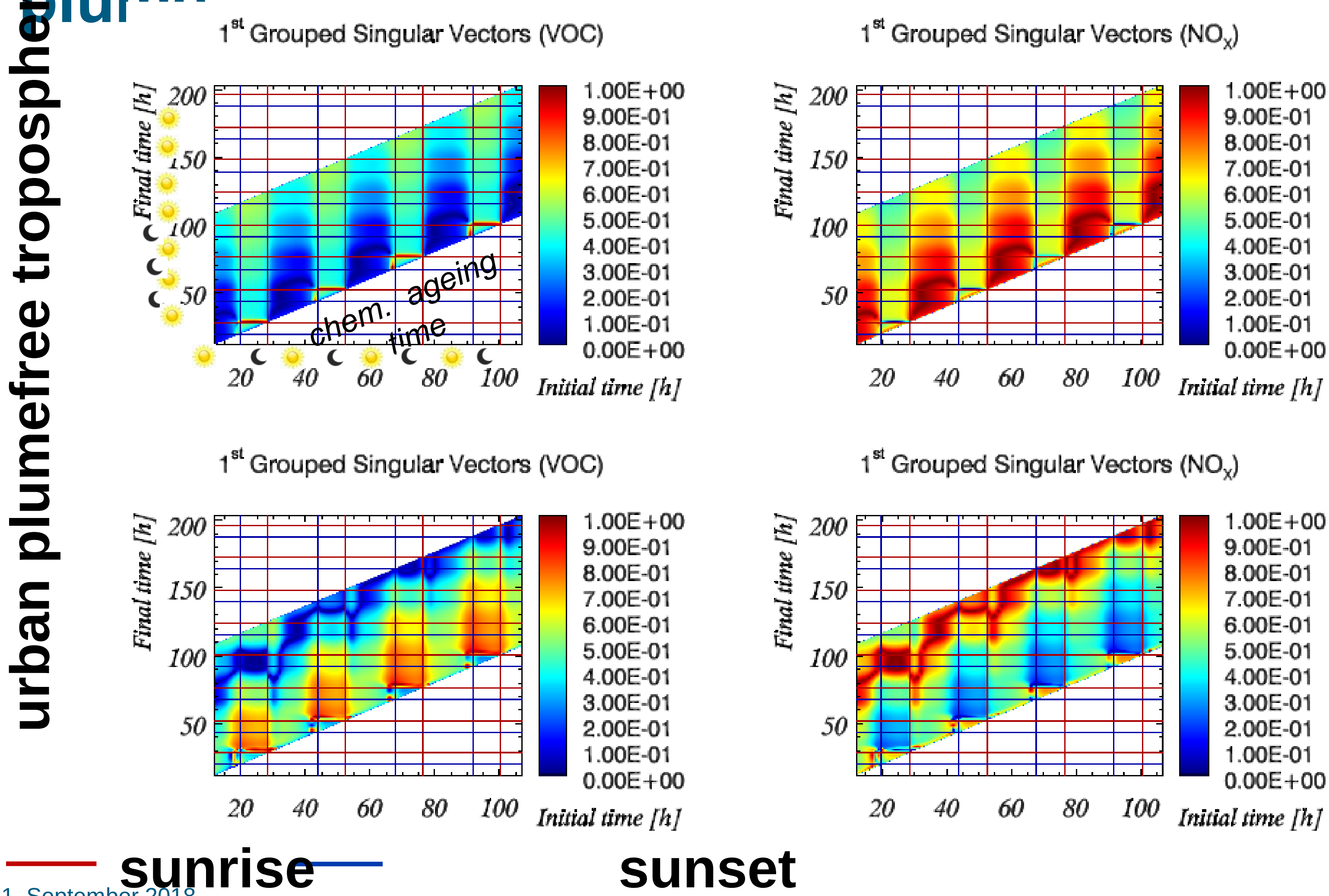


not | very important to observe

sunrise   sunset

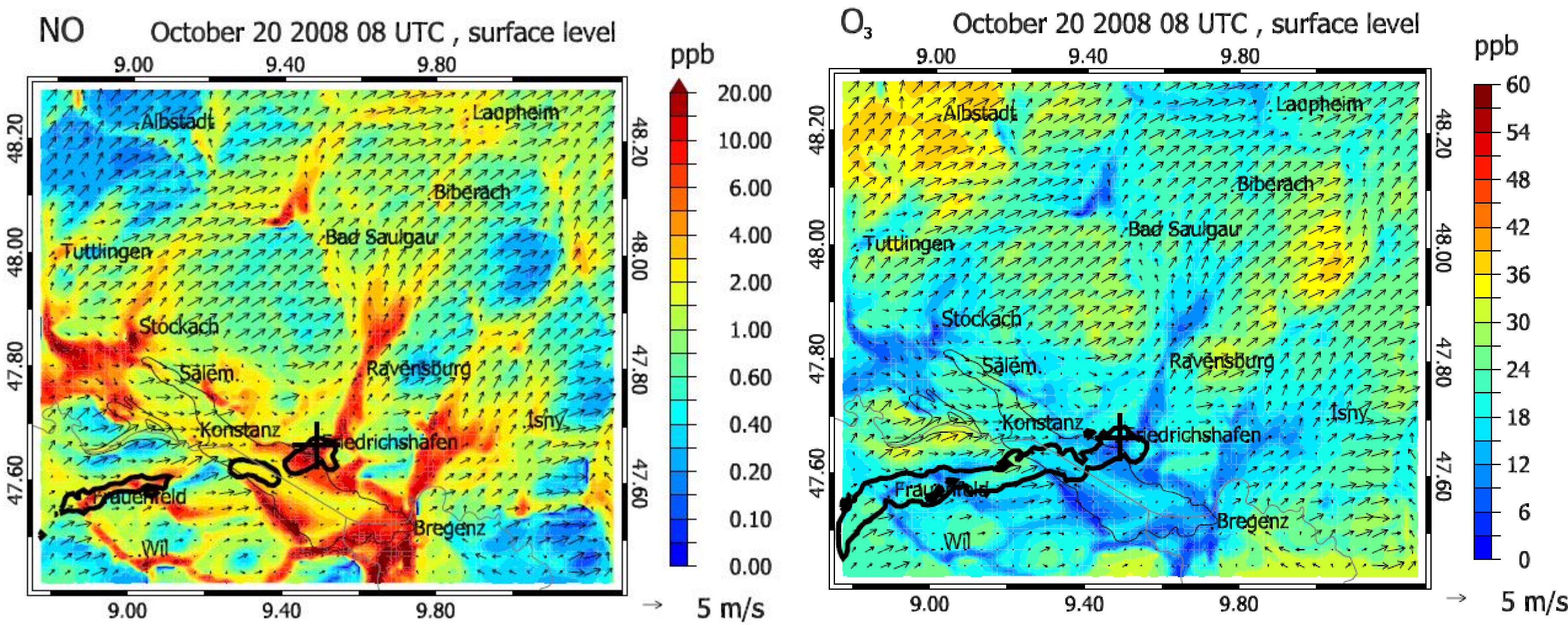
Goris and Elbern, ACP, 2013

SV components VOC (left) and NO_x (right) for scenarios "free troposphere" and "urban plume"



from Goris and Elbern , ACP, 2013

Example observation targeting:
SV optimal placement of observation sites



Initial concentrations and optimal horizontal placement of NO (left) and O3 (right) at surface level . Isopleths of the optimal horizontal placement are indicated with black lines.

from Goris and Elbern , GMD, 2015

Conclusions and outlook

There is still progress possible in improving predictive skills of atmospheric models

- ❑ quantify uncertainties on predictive time scales, “tiny causes, large impacts”

→**improved ensembles, “slow manifold identification”**

- ❑ adaptive observations and remote sensing: can we observe “tiny causes” early enough?

→**improved data selection, weighting, and deployment**

- ❑ Process plethora of ensemble and observation data by big data analytics