Efficient uncertainty estimation of atmospheric chemical forecast due to model parameters

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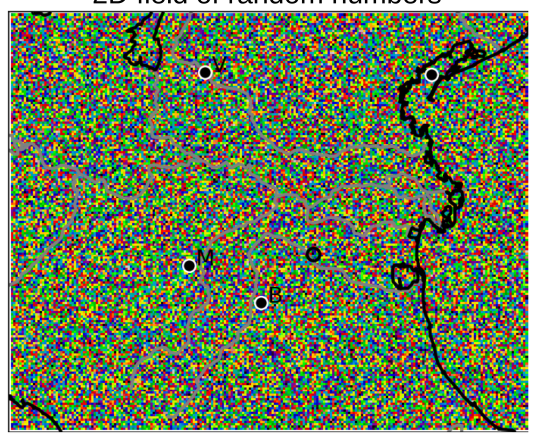
Introduction:

Forecasts of atmospheric chemical composition rely highly on various poorly-known model parameters, e.g. representing emission or deposition processes. However, a feasible estimation of resulting uncertainties by a limited ensemble of forecasts has to deal with the high-dimensionality of the system.

A new algorithm is presented to efficiently estimate forecast uncertainties caused by leading uncertainties in model parameters.

The algorithm is based on the idea, that the dynamical system induces multi-variational coupling of model states and uncertainties. For the application to biogenic emissions, case-dependent uncertainties are considered in form of sensitivities to local atmospheric and terrestrial conditions.

2D field of random numbers



ALGORITHM

Requirements:

1) Efficient calculation of sensitivities
 - consideration of multiple uncertainties, low computational effort for calculation of sensitivities

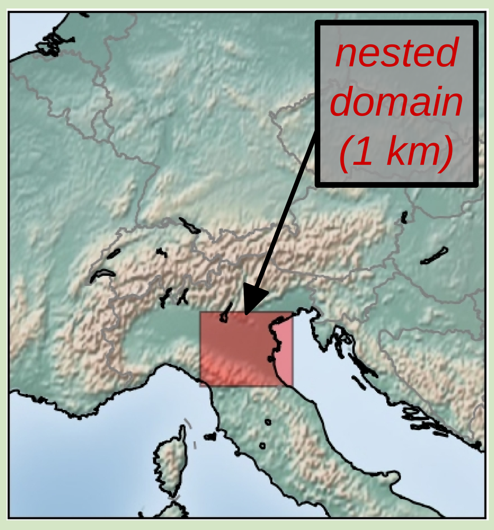
2) Efficient estimation of largest uncertainties
 - representation of largest uncertainties, suitable for high-dimensional systems $O(10^5 - 10^7)$ $\rightarrow O(10^8)$

3) Efficient physical-based ensemble generation $O(10-10^2)$
 - sampling in reduced space, physical-based uncertainty estimation

RESULTS

Modeling setup:

- ***WRF-ARW***[4] v.3.8.1 meteorological driver
- ***EURAD-IM***[1] Eulerian chemistry transport model
- ***MEGAN 2.1***[5] estimate biogenic emissions as function of vegetation distribution, leaf area index, soil moisture, solar radiation, air temperature



- Po valley
- initialization: 11.07.2012 00 UTC
- time of interest: 12.07.2012 00 – 10 UTC
- 5 biogenic gases → here: isoprene

1) Sensitivity estimation:

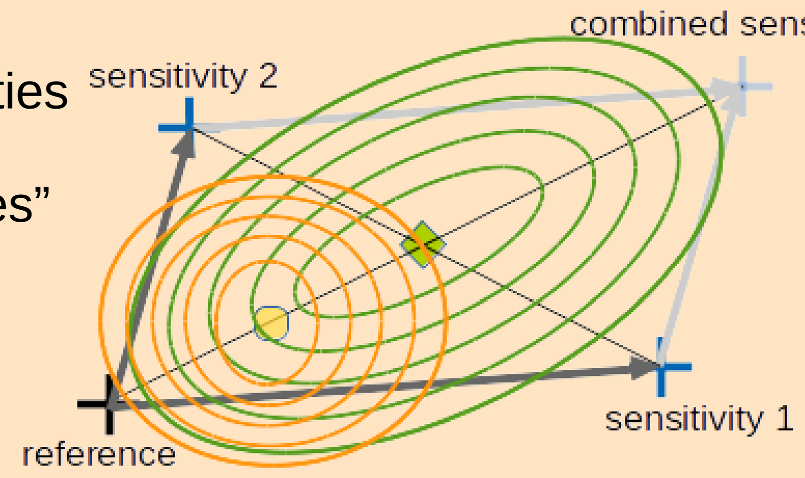
- estimate uncertainties of parameters induced by different input options
- translation to averaged ***factors***[1] w.r.t. reference values:

$$f_{sens}(j,s) := \frac{1}{T}\sum_{t=t_0}^{t_1}\frac{q(j,s,t)}{q(j_{ref},s,t)}$$

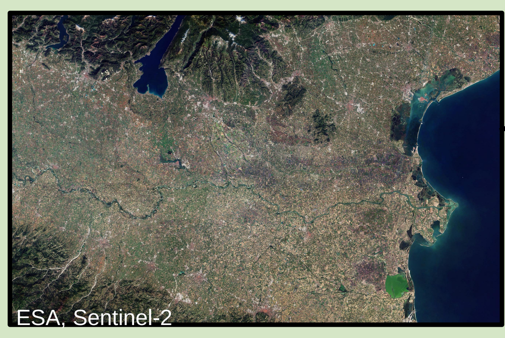
"***independent sensitivities***":
- assume tangent linearity of sensitivities
- approximate combined sensitivities by single "independent sensitivities"

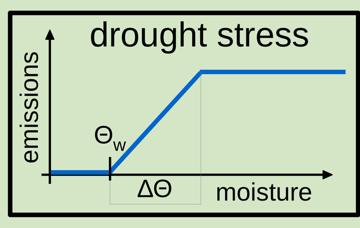
→ calculate only single sensitivities

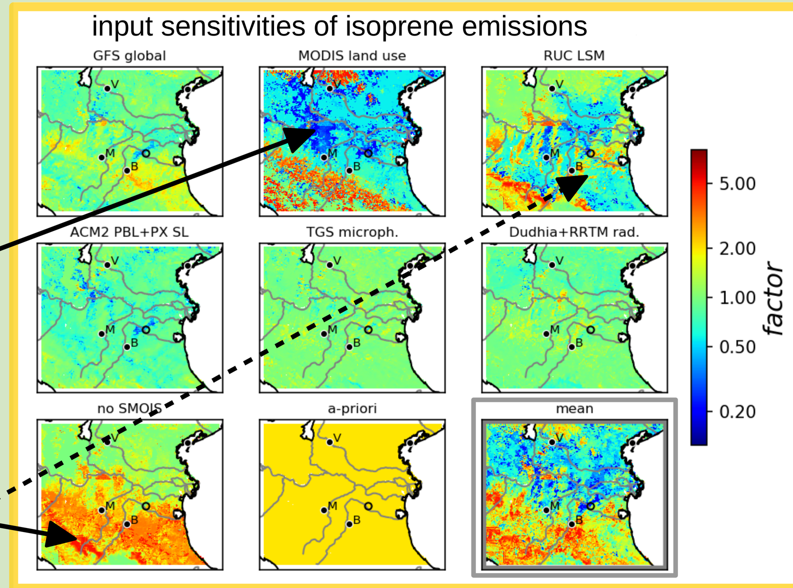
→ include additional uncertainties (with / without direction)



- independent sensitivities to global meteorology, land use information, land surface model, boundary layer-, microphysics- and radiation parameterizations
- additional uncertainties from formulation of drought stress, emission module







→ high sensitivity to vegetation and soil dryness

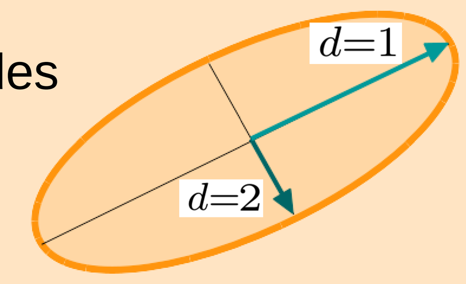
2) Eigenmode decomposition:

- describe uncertainties as covariance matrix
- extract dominating uncertainties as leading eigenmodes

Leading eigenvectors indicate dominant directions of uncertainties

$$\int_S C(s,s')\varphi_d(s')\,ds' = \lambda_d\varphi_d(s)$$

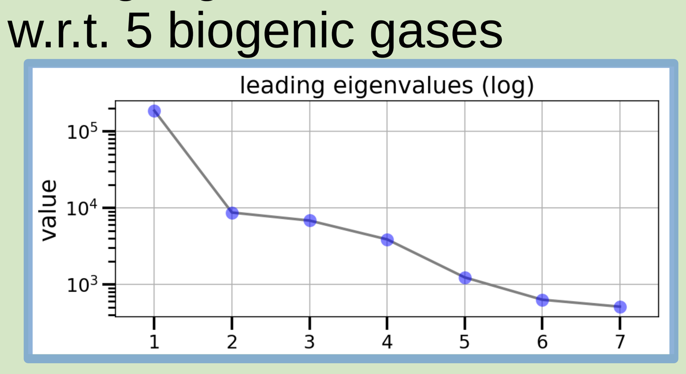
(eigenvalues = length, eigenvectors = direction)

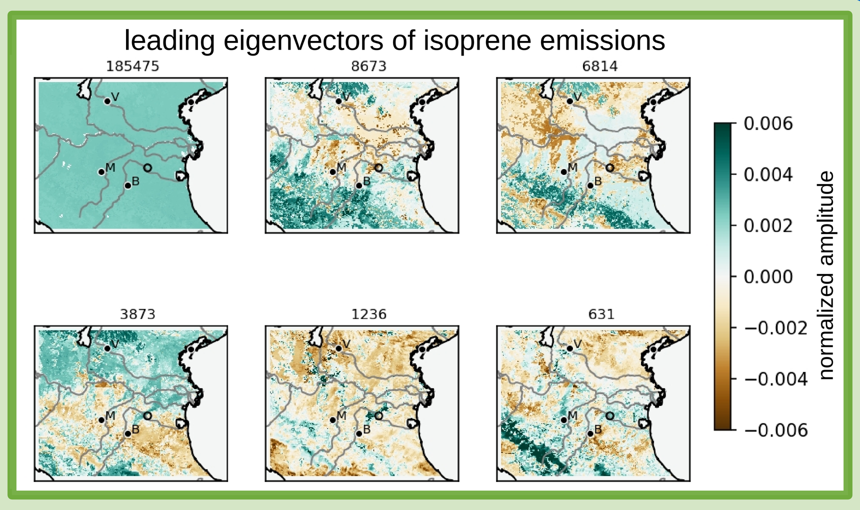


→ numerical solution with PARPACK[2] (sufficient for $C \in \mathbb{R}^{10.000 \cdot 10.000}$)

→ low number of perpendicular uncertainties for high correlations

- leading eigenmodes w.r.t. 5 biogenic gases





→ high correlations in regional domain

3) Generation of perturbations:

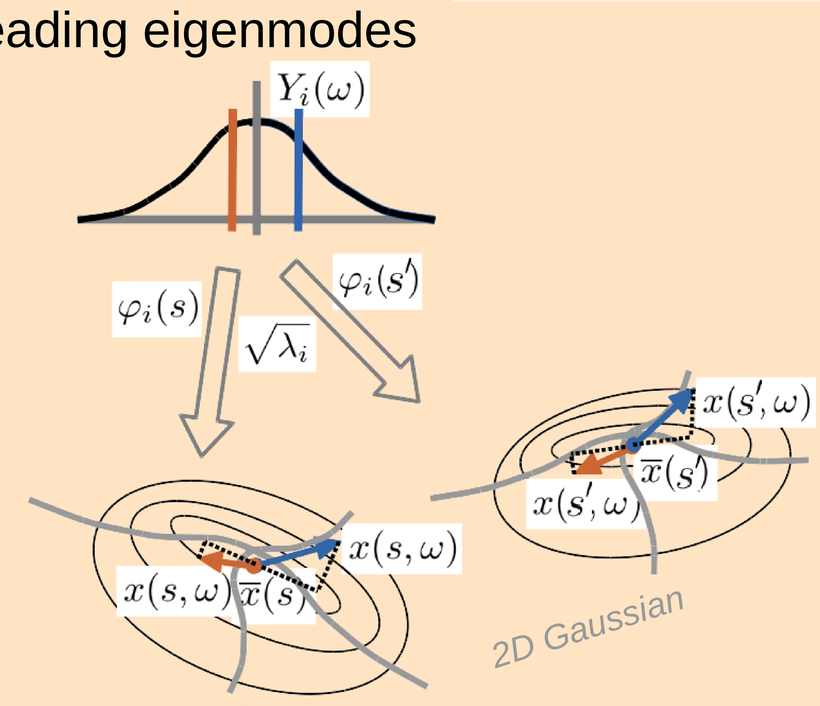
- generate perturbations according to leading eigenmodes
- ***Karhunen-Loève expansion***[3]

$$x_{KL}(\omega,s) = \sum_{d=1}^{D}\sqrt{\lambda_d}\,\varphi_d(s)\,Y_d(\omega)$$

- optimal approximation by finite sum
- generation of different members from global sampling

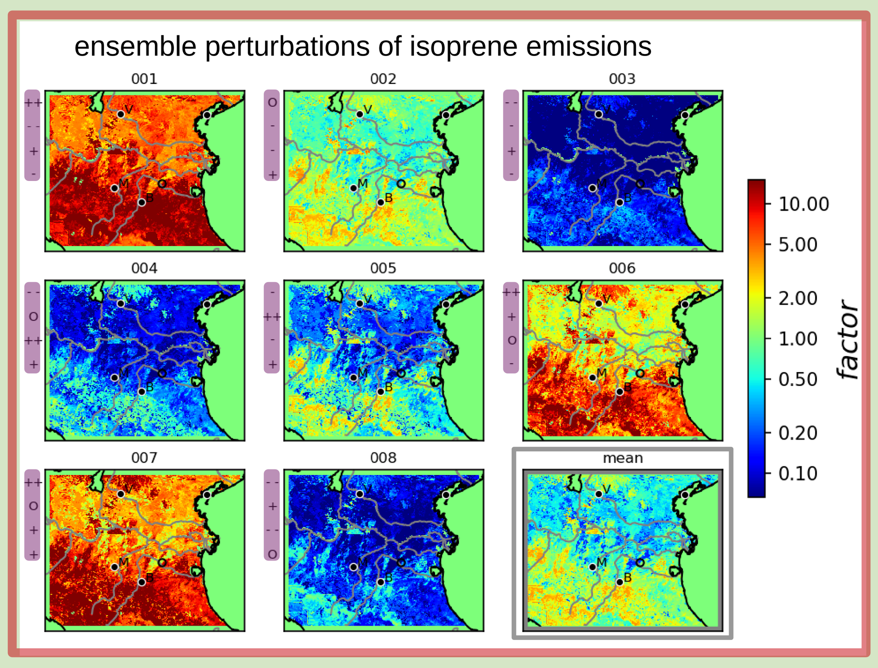
$$q(\omega,s,t) = q(j_{ref},s,t)\cdot f_{KL}(\omega,s)$$

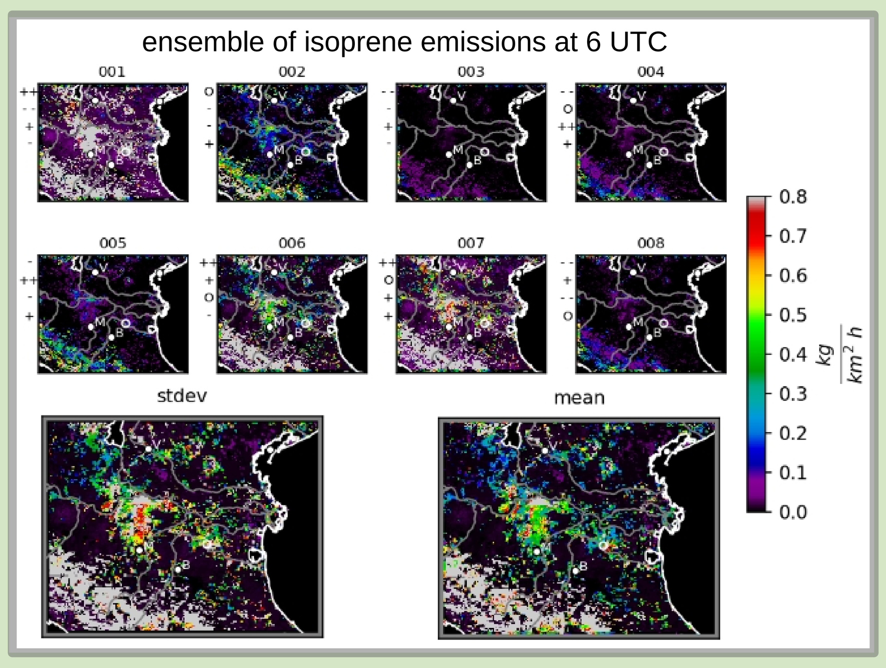
with $f_{KL}(\omega,s) = exp\left[x_{KL}(\omega,s) + \mu(s)\right]$



→ reduce degrees of freedom for random sampling to directions of largest uncertainties according to covariances

- perturbation factors and resulting emissions for 8 ensemble members





→ ensemble spread ≥ mean emissions

Conclusions:

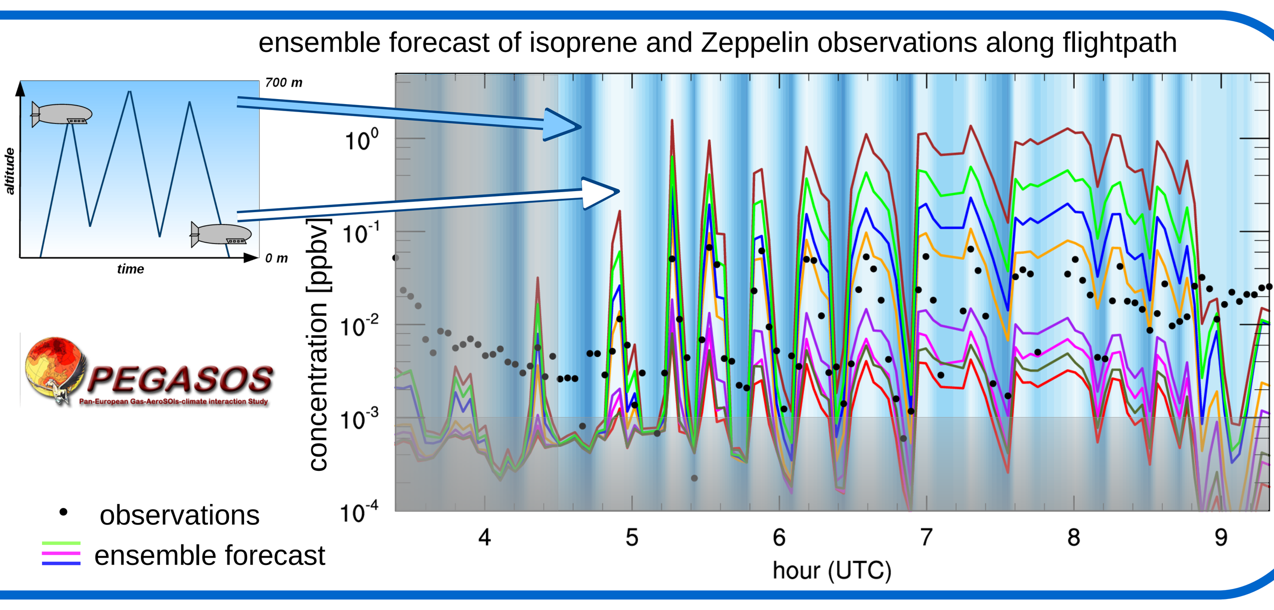
- combination of different kinds of uncertainties
- representation of largest uncertainties with low ensemble size
- high sensitivity to generation of covariances

sufficient estimation of forecast uncertainties

- high sensitivity of vegetation and soil dryness
- high cross-correlations between gases
- ensemble spread ≥ mean emissions
- high uncertainty confirmed by observations

predictability of biogenic gases limited to regions, not forecast time

ensemble forecast of isoprene and Zeppelin observations along flightpath



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for further details see PhD thesis A.Vogel, University of Cologne, 2020

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