Reconstruction of tropospheric emissions: A brief tour of DA parameter estimation with (not too) complex models

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Outline

Successful assimilation: It's all about errors

- Context of this talk: Data assimilation and inverse modeling applied to large 3D models, using real data.

- Our observations are wrong
- Our models are wrong
- Even when they are so not wrong, they do not tell the same story!
- So successful data assimilation and especially inverse modeling is all about errors!

- Exception: Global meteorological forecast models are quite good and very well tuned.
- But severe hardships (modeling: complex microphysics, mathematics: integration of complex microphysics, non-Gaussian statistics) are soon as one has to deal with atmospheric constituents (humidity, gas, aerosols, hydrometeors, ashes), oceanic constituent (ice, salt, algae, plankton, fish, nutriments), or model coupling, models feedback, etc.

Focus of this talk

- Focus of this talk: inverse modeling in atmospheric transport and chemistry, and especially estimation of emissions, and other parameters of atmospheric constituents using 3D (offline) models and data assimilation/inverse modeling.

- There is a 15-year history of inverse modeling applied to the estimation of atmospheric constituents (greenhouse gases, regulated pollutants, heavy metals, pollens, radionuclides, etc.).
- This literature is often ignored by DA experts growing an interest in this field.
- The inverse modeling techniques were not mathematically speaking state-of-the-art because the biggest concerns were the 3D models...

- I believe this era has ended

- As a reward, (knowledge of) proper state-of-the art mathematical techniques will
  - tell us if a problem is solvable in finite time
  - tell us about the model, observational and representativeness errors, with often unexpected and dramatic results!
  - help us cut computational load in numerical integrations

Outline

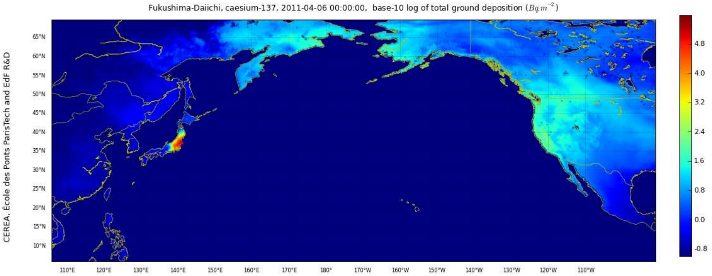
The Fukushima Daiichi source term

- Inverse modeling of the Fukushima Daiichi accident source term (^{137}Cs and ^{131}I) from March 11 to March 27.

- Chronology: March 12: R 1 explosion; March 13-14: R 3 venting + explosion; March 15: R 2 venting + explosion; March 20-22: R 2 R 3 spraying - smokes.

$\longrightarrow$ Source term of major interest for risk/health agencies, NPP operators

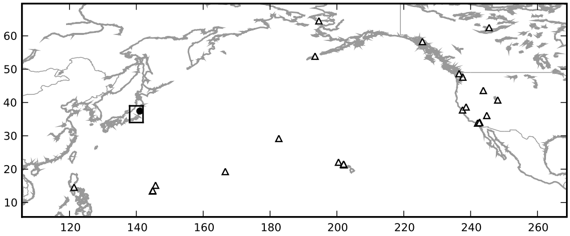
Observations of the Fukushima atmospheric dispersion

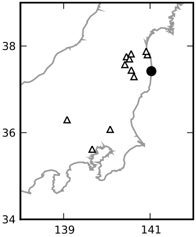


- Very few observations of activity concentrations in the air:
  1. A few hundreds of observations over Japan publicly released.
  2. Several thousands of observations from the CTBO IMS network, only partly publicly available, far away from the release site (except for Tokyo station).
  3. Activity deposition: a few hundreds, but more difficult to exploit (mainly ^{137}Cs).
  4. Hundreds of thousands of gamma dose measurements available on the web: very difficult to exploit.

Fukushima activity concentration observations

- At least two observational scales.





Dispersion model and physics

$$\frac{\partial c}{\partial t} + \underbrace{\mathrm{div}\,(\mathbf{u}c)}_{\text{wind advection}} = \underbrace{\mathrm{div}\,(\mathbf{K}\nabla c)}_{\text{turbulent diffusion}} - \underbrace{\boldsymbol{\Lambda} c}_{\substack{\text{wet scavenging}\\ \text{radioactive decay}}} + \underbrace{\sigma}_{\text{source}}$$

- Simplest reasonable numerical scheme (for demanding DA algorithms)
  - Wet scavenging: relative humidity $\Lambda^s = 3.5\,10^{-5}(RH - RH_t)/(RH_s - RH_t)$ [Pudykiewicz 1989; Brandt 1998; Baklanov 1999]
  - Dry deposition: constant deposition velocity, $v_\mathrm{d} = 0.5$ cm.s^{-1} for $^{131}\mathrm{I}$, $v_\mathrm{d} = 0.2$ cm.s^{-1} for $^{137}\mathrm{Cs}$ and $^{134}\mathrm{Cs}$ over land, much smaller values over the ocean.
  - Vertical turbulent diffusion (K_z): Louis scheme [Louis 1979].
  - Radioactive decay.
- Resolution: $0.25^\circ \times 0.25^\circ$; $N_x = 652$, $N_y = 256$, $N_z = 15$.

Methodology

- Posing the inverse problem (estimate σ knowing μ) with the Jacobian $\mathbf{H}$:

$$\mu = \mathbf{H}\sigma + \varepsilon\,. \tag{1}$$

$\mathbf{H}$ computed with the forward or adjoint model + observation operator.

- Traditional methodology inspired from geophysical data assimilation:

$$\mathscr{J} = \frac{1}{2}(\mu - \mathbf{H}\sigma)^{\mathrm{T}}\mathbf{R}^{-1}(\mu - \mathbf{H}\sigma) + \frac{1}{2}(\sigma - \sigma_b)^{\mathrm{T}}\mathbf{B}^{-1}(\sigma - \sigma_b)\,, \tag{2}$$

- A prior (background) is absolutely necessary if the dataset is not overwhelming!

- In the case of accidental release inverse modeling, such a prior does not exist, or is difficult to establish. Moreover its uncertainty is even more difficult to assess.

- Choices for the first guess: $\sigma_b = \mathbf{0}$, or σ_b estimated from nuclear physics model.

Reconstruction of the Fukushima Daiichi source term

- Retrieval of the cesium-137 source term $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_{384})$ ($\Delta t = 1\text{h}$) using

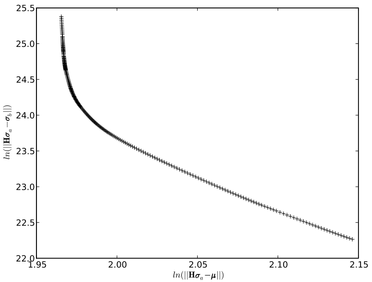
$$\mathscr{J} = \frac{1}{2}(\mu - \mathbf{H}\sigma)^{\mathrm{T}} \mathbf{R}^{-1} (\mu - \mathbf{H}\sigma) + \frac{1}{2}\sigma^{\mathrm{T}}\mathbf{B}^{-1}\sigma \,, \tag{3}$$

where $\mathbf{R} = r^2\mathbf{I}_d$, $\mathbf{B} = m^2\mathbf{I}_N$. Gaussian assumptions on the background (no positivity constraint).

- Three methods will be used to estimate r and m:
  - An L-curve method, coupled with a χ^2 diagnosis.
  - The value screening of the likelihood, to find the parameters that maximize the likelihood.
  - Desroziers' scheme to numerically localize the maximum likelihood parameters.

L-curve and χ^2

- For a given r, one computes $\sigma_a(m)$. The L-curve is given by the plot of $\ln(||\sigma_a - \sigma_b||)$ against $\ln(||\mathbf{H}\sigma_a - \mu||)$.
- The L-curve represents the balance between over-fitting to the data and over-smoothing by regularization.
- The turning point is indicated by the corner of the L-curve.



- For the second degree of freedom, we tune the general level of errors in the system. The quantity $(\mu - \mathbf{H}\sigma_a)^{\mathrm{T}}\mathbf{R}^{-1}(\mu - \mathbf{H}\sigma_a) + (\sigma_a - \sigma_b)^{\mathrm{T}}\mathbf{B}^{-1}(\sigma_a - \sigma_b)$ should have the statistics of a χ^2 if the prior errors are Gaussian, and it should equal the number of observations when the prior statistics matches the genuine ones [Ménard, 2000].

Maximum likelihood principle (1/2)

- The likelihood of the observation set

$$p(\mu) = \int d\sigma\, p(\mu|\sigma) p(\sigma) \tag{4}$$

is actually a function of $(r,\ m)$.

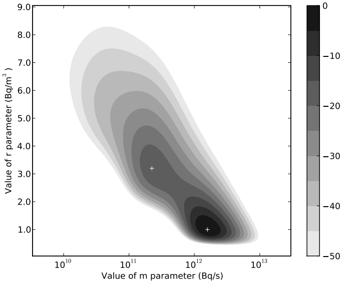
- In the Gaussian context,

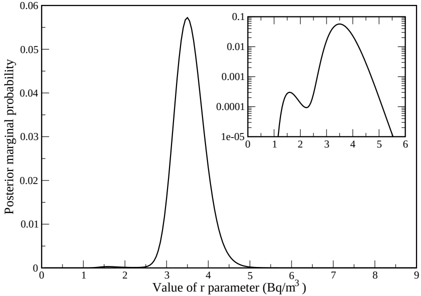
$$p(\mu|r,m) = \frac{e^{-\frac{1}{2}\mu^{\mathrm{T}}\left(\mathbf{HBH}^{\mathrm{T}}+\mathbf{R}\right)^{-1}\mu}}{\sqrt{(2\pi)^d|\mathbf{HBH}^{\mathrm{T}}+\mathbf{R}|}} \tag{5}$$

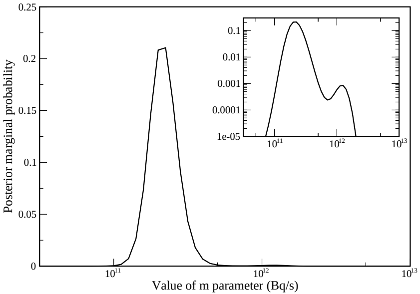
- Two strategies :
  - A numerical scheme [Desroziers, 2001], which converges to a fixed point.
  - The exhaustive value screening of the likelihood.

Maximum likelihood principle (2/2)

- Values screening of likelihood as a function of (r, m).
- Marginals of the hyper-parameters (r and m)







Positivity assumption on the source term

▶ Retrieval of the cesium-137 source term, under semi-Gaussian constraints.

$$\mathscr{J} = \frac{1}{2}(\mu - \mathbf{H}\sigma)^{\mathrm{T}}\mathbf{R}^{-1}(\mu - \mathbf{H}\sigma) + \frac{1}{2}\sigma^{\mathrm{T}}\mathbf{B}^{-1}\sigma\,, \tag{6}$$

under the assumption $\sigma \geq 0$, where $\mathbf{R} = r^2\mathbf{I}_d$, $\mathbf{B} = m^2\mathbf{I}_N$.

▶ Estimation of the hyper-parameters m and r mathematically challenging (sampling of a high-dimensional truncated Gaussian distribution).

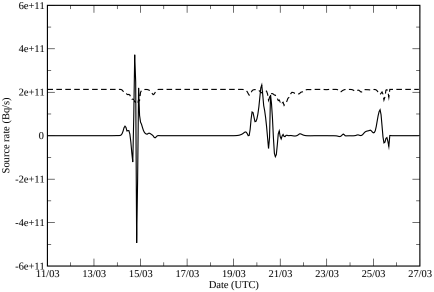
$$p(\mu|r,m) = \frac{e^{-\frac{1}{2}\mu^{\mathrm{T}}\left(\mathbf{HBH}^{\mathrm{T}}+\mathbf{R}\right)^{-1}\mu}}{\sqrt{(2\pi)^d|\mathbf{HBH}^{\mathrm{T}}+\mathbf{R}|}} \times \int_{\sigma\geq 0} \frac{e^{-\frac{1}{2}(\sigma-\sigma^*)^{\mathrm{T}}\mathbf{P}_a^{-1}(\sigma-\sigma^*)}}{\sqrt{(\pi/2)^N|\mathbf{P}_a|}}\mathrm{d}\sigma\,, \tag{7}$$

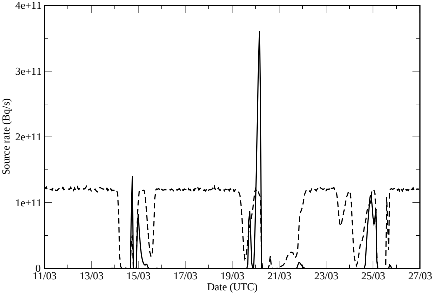
with

$$\begin{aligned} \sigma^* &= \mathbf{BH}^{\mathrm{T}}\left(\mathbf{HBH}^{\mathrm{T}}+\mathbf{R}\right)^{-1}\mu\,, \\ \mathbf{P}_a &= \mathbf{B} - \mathbf{BH}^{\mathrm{T}}\left(\mathbf{HBH}^{\mathrm{T}}+\mathbf{R}\right)^{-1}\mathbf{HB} \end{aligned} \tag{8}$$

Results (1/3)

- The posterior uncertainty on the retrieved source term is computed through a second-order Monte-Carlo analysis.
- Retrieved profile, Gaussian and non-Gaussian case + uncertainty





Results (2/3)

- Quantitative results and uncertainty on the retrieved activities (cesium-137).

parameter	method	with observations in Japan (104)	with all observations (267)
r (Bq m^{-3})	χ^2 + L-curve	4.55	2.88
	Desroziers's scheme	5.41	2.96
	Maximum likelihood	3.25	1.7
m (Bq s^{-1})	χ^2 + L-curve	3.2×10^{11}	2.0×10^{11}
	Desroziers's scheme	5.3×10^{10}	1.3×10^{11}
	Maximum likelihood	2.0×10^{11}	3.5×10^{11}
Released activity (Bq)	χ^2 + L-curve	1.2×10^{16}	1.3×10^{16}
	Desroziers's scheme	3.3×10^{15}	1.0×10^{16}
	Maximum likelihood	1.2×10^{16}	1.9×10^{16}

Results (3/3)

- Uncertainty (Monte-Carlo).

Species	Released activity (Bq) all observations	Released activity (Bq) observations over Japan (robust results)	std. deviation with pert. observations	std. deviation with pert. obs. and background
cesium-137	1.0×10^{16} - 1.9×10^{16}	$\mathbf{1.2 \times 10^{16}}$	15% - 20%	$60\% - 100\%$
iodine-131	1.9×10^{17} - 7.0×10^{17}	$\mathbf{1.9 \times 10^{17}}$ - $\mathbf{3.8 \times 10^{17}}$	5% - 10%	$40\% - 45\%$

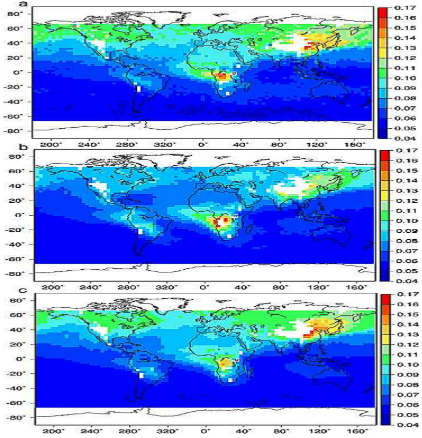
- Order of magnitude of the first Japanese estimation.

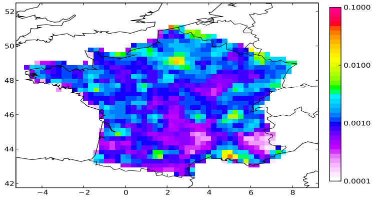
- Emissions (cesium-137 et iodine-131) in the atmosphere 5 to 10 times less important than for Chernobyl (lower bound).

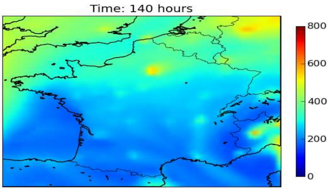
Outline

Emission and modeling of carbon monoxide

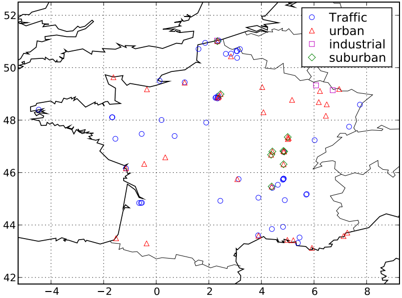
- Usually retrieved from satellite radiance measurements: MOPITT EOS Terra, IASI METOP-A [Fortems-Cheyney et al., 2009-2011; Emmons et al., 2010; Kopacz et al., 2010; Pétron et al., 2004]
- Air quality networks measure CO, but with a different goal, spatial and time scales [Muholland and Seinfeld, 1995; Yuminotoa et al., 2006; Saide et al. 2011].







Inverse modeling of carbon monoxide fluxes at regional scale



- Using the French 600-stations BDQA network: hourly measurements of CO concentrations at about 80 stations.
- Observations highly impacted by representativeness errors (traffic, urban stations).

- Great number of observations (about 10^5 assimilated here, 5×10^5 used for validation).
- Control space: fluxes and volume sources parameterized with about 70×10^3 variables at $0.25^\circ \times 0.25^\circ$ resolution.

$\longrightarrow$ Even in this linear physics context, 4D-Var is a method of choice.

4D-Var

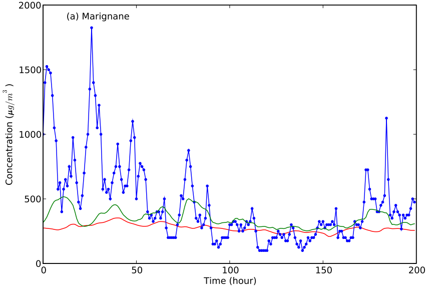
- Gradient obtained from adjoint approximated by the discretization of the continuous adjoint model [Davoine & Bocquet, 2007; Bocquet, 2012].
- Background: EMEP inventory over Europe with an uncertainty of about 100%.
- Cost function:

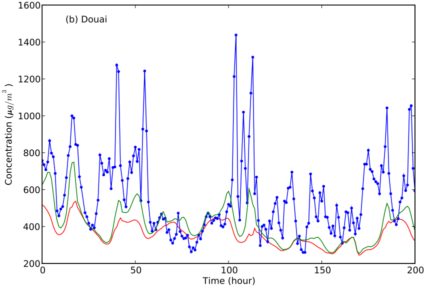
$$
\begin{aligned}
\mathscr{J}(\alpha) \quad = \quad & \frac{1}{2} \sum_{h=0}^{N_\alpha - 1} (\alpha_h - \mathbf{1})^{\mathrm{T}} \mathbf{B}_{\alpha_h}^{-1} (\alpha_h - \mathbf{1}) \\
& + \frac{1}{2} \sum_{k=0}^{N} (\mathbf{y}_k - \mathbf{H}_k \mathbf{c}_k)^{\mathrm{T}} \mathbf{R}_k^{-1} (\mathbf{y}_k - \mathbf{H}_k \mathbf{c}_k) \\
& + \sum_{k=1}^{N} \phi_k^{\mathrm{T}} (\mathbf{c}_k - \mathbf{M}_k \mathbf{c}_{k-1} - \Delta t \mathbf{e}_k)
\end{aligned}
\tag{9}
$$

- α: control vector of scaling parameters that multiply the first guess.
- Observation (representativeness) errors iteratively estimated by χ^2 diagnosis.

Results of (traditional) 4D-Var

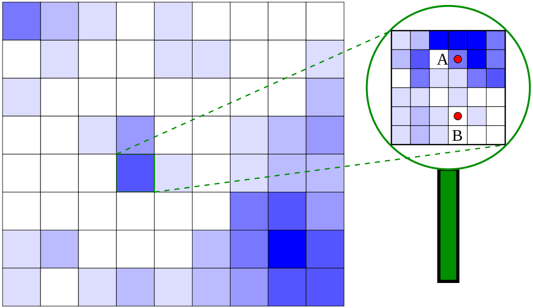
	$\overline{C}$	$\overline{O}$	RMSE	C.Pear.	FA2	FA5
Simulation (01/01–02/26 2005)	303	662	701	0.16	0.52	0.90
Forecast (02/26–03/26 2005)	267	642	648	0.13	0.47	0.88
Optimization of α	396	662	633	0.36	0.59	0.92
Forecast with optimal α	343	642	589	0.33	0.53	0.90





- Tremendous impact of representativeness errors!

Coupling 4D-Var with a simple statistical subgrid model



▶ We would like to take into account the impact of nearby sources that generate peaks on the CO concentration recordings:

$$\varepsilon_{\mathrm{rep}} \simeq \xi \cdot \mathbf{\Pi e} \quad \longrightarrow \quad \mathbf{y} = \mathbf{Hc} + \xi \cdot \mathbf{\Pi e} + \widehat{\varepsilon}. \tag{10}$$

ξ: set of statistical coefficients (influence factors).

Coupling 4D-Var with a simple statistical subgrid model

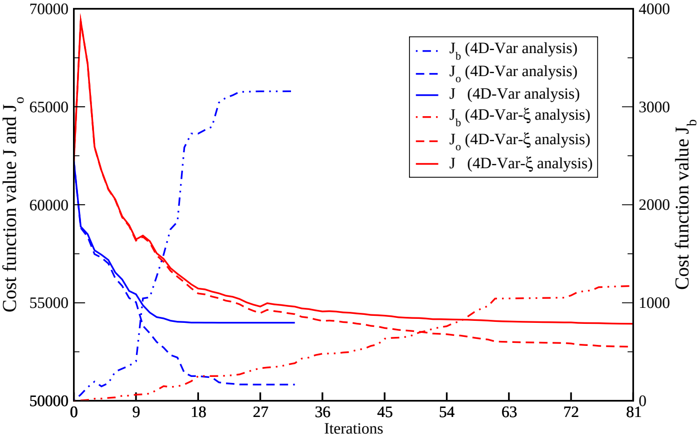
- Cost function of 4D-Var-ξ:

$$\begin{aligned} \mathscr{J}(\alpha,\xi) &= \frac{1}{2}\sum_{h=0}^{N_\alpha-1}(\alpha_h-\mathbf{1})^{\mathrm{T}}\mathbf{B}_{\alpha_h}^{-1}(\alpha_h-\mathbf{1}) \\ &+\frac{1}{2}\sum_{k=0}^{N}(\mathbf{y}_k-\mathbf{H}_k\mathbf{c}_k-\xi\cdot\mathbf{\Pi}\mathbf{e}_k)^{\mathrm{T}}\widehat{\mathbf{R}}_k^{-1}(\mathbf{y}_k-\mathbf{H}_k\mathbf{c}_k-\xi\cdot\mathbf{\Pi}\mathbf{e}_k) \\ &+\sum_{k=1}^{N}\phi_k^{\mathrm{T}}(\mathbf{c}_k-\mathbf{M}_k\mathbf{c}_{k-1}-\Delta t\mathbf{e}_k)\,. \end{aligned} \tag{11}$$

- $\widehat{\mathbf{R}}$ is residual error covariance matrix (smaller than $\mathbf{R}$).

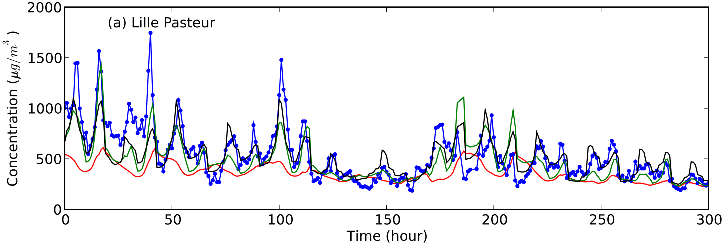
$$\mathbf{R}=\mathrm{E}\left[\varepsilon\varepsilon^{\mathrm{T}}\right]=\xi\cdot\mathbf{\Pi}\mathrm{E}\left[\mathbf{e}\mathbf{e}^{\mathrm{T}}\right]\mathbf{\Pi}^{\mathrm{T}}\cdot\xi^{\mathrm{T}}+\widehat{\mathbf{R}}. \tag{12}$$

Minimization of the cost functions

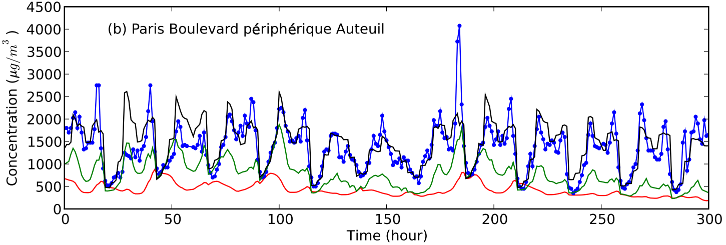


The magnitude of the residual $\widehat{\mathbf{R}}$ is iteratively estimated using a χ^2 diagnostic. The fixed-point equation is actually equivalent to Desroziers'.

Results of 4D-Var-ξ: Profiles (1/7)

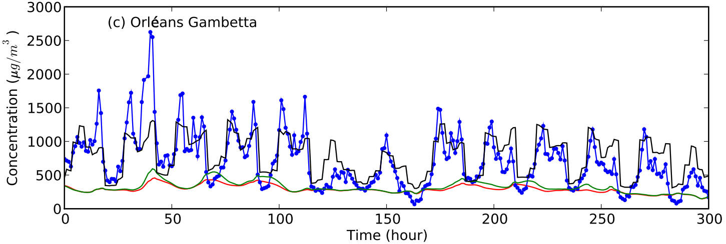


$\xi_i = 0.6$ h.

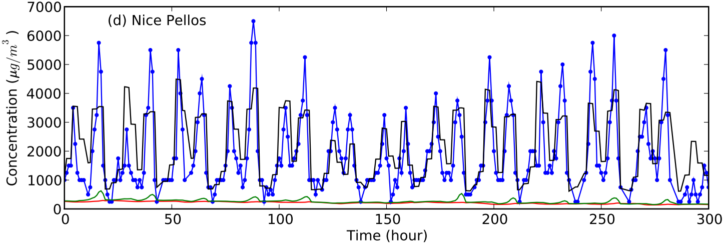


$\xi_i = 2.7$ h.

Results of 4D-Var-ξ: Profiles (2/7)

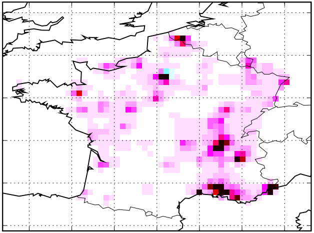


$\xi_i = 11.9$ h.

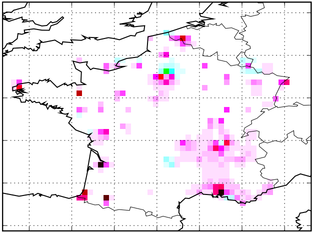


$\xi_i = 45.8$ h.

Results of 4D-Var-ξ: Space analysis (3/7)



(a)



(b)

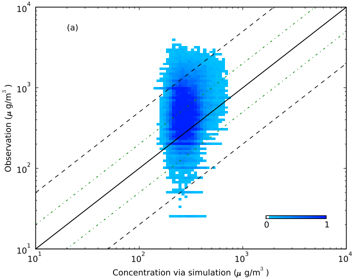
Results of 4D-Var-ξ: Scores (4/7)

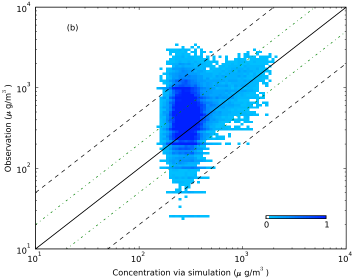
- Skills:

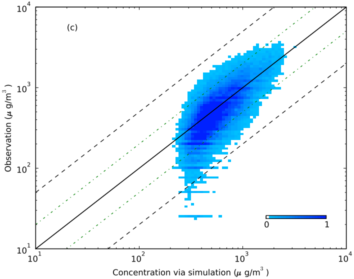
	$\overline{C}$	$\overline{O}$	RMSE	C.Pear.	FA2	FA5
Simulation (01/01–02/26 2005)	303	662	701	0.16	0.52	0.90
Forecast (02/26–03/26 2005)	267	642	648	0.13	0.47	0.88
Optimization of α	396	662	633	0.36	0.59	0.92
Forecast with optimal α	343	642	589	0.33	0.53	0.90
Optimization of ξ	615	662	503	0.57	0.73	0.96
Forecast with optimal ξ	574	642	451	0.56	0.76	0.97
Coupled optimization of ξ, α	671	662	418	0.73	0.79	0.97
Forecast with optimal ξ, α	631	642	340	0.68	0.81	0.98

- We found an increase of 9% in the French CO total emission. Consistent with satellite retrieval for Western Europe.

Results of 4D-Var-ξ: Scatterplot (5/7)



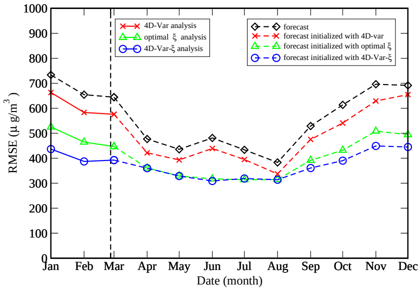


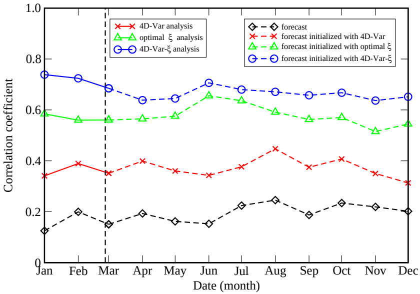


- (a) Simulation
- (b) 4D-Var analysis
- (c) 4D-Var-ξ analysis

Results of 4D-Var-ξ: Forecast (6/7)

- Validation of a 10-month forecast after the 8-week assimilation window (2005)

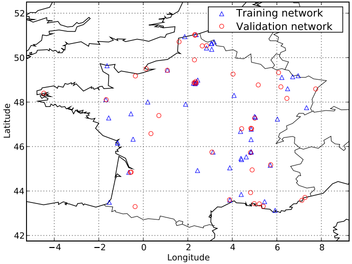


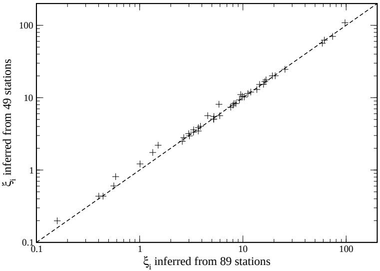


- Skills almost as good in the forecast period as in the assimilation time window!
- Seasonal effects impacting scores.

Results of 4D-Var-ξ: Cross-validation (7/7)

- Training and validation sets:





- Cross-validation experiments:

Used inventory	$\overline{C}$	$\overline{O}$	NB	RMSE	R	FA_2	FA_5	Total mass
Background	296	697	-0.81	771	0.16	0.51	0.88	1.06 (1.06)
4D-Var	357	697	-0.65	726	0.28	0.57	0.89	1.25 (1.44)
4D-Var-ξ	310	697	-0.77	758	0.22	0.52	0.89	1.14 (1.16)
Background + climatological ξ	644	697	-0.08	538	0.60	0.73	0.96	1.06 (1.06)
4D-Var + climatological ξ	968	697	0.33	1216	0.40	0.67	0.94	1.25 (1.44)
4D-Var-ξ + climatological ξ	674	697	-0.03	514	0.64	0.75	0.96	1.14 (1.16)

Outline

Model parameter estimation (besides emissions)

- Data assimilation methods:
  - Kalman filter, extended Kalman filter, extended ensemble Kalman filter and particle filter [Aksoy et al., 2006] [Vossepoel and van Leeuwen, 2007], [Kondrashov et al., 2008], [Wirth and Verron, 2008], [Barbu et al., 2008], [Ruiz et al., 2012] . . . ,
  - Simulated annealing, and other stochastic methods [Jackson et al., 2004], [Liu, 2005], [Bocquet, 2012], . . .
  - Kalman smoothers (emerging),
  - Variational methods [Pulido and Thuburn, 2006], [Bocquet, 2012], ...

- Fundamental issue:
  - Do we invert an unobserved parameter or do we just compensate for another source of model error?
  - If we compensate, how useful are the results, how do we interpret them?

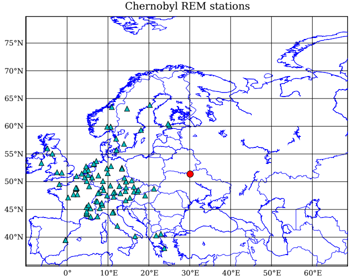
The Chernobyl accident

- On the 25th April 1986, 21:23 local time, reactor-4 of the Chernobyl power plant ran astray. As a result a steam explosion lifted up the reactor core and blasted off the reactor structure. Radionuclides were released into the atmosphere.

- Radionuclides of health impact and available for long-range transport:

	iodine-131	cesium-137	cesium-134
Half-life	8 days	30 years	2 years
Physical form	Gas, particles	Particles	Particles
OECD/NEA/UNSCEAR	1760×10^{15} Bq	85×10^{15} Bq	54×10^{15} Bq

- This study is based on the REM observation data-base of air activity concentrations.



Case study: Optimization of dry deposition and wet scavenging

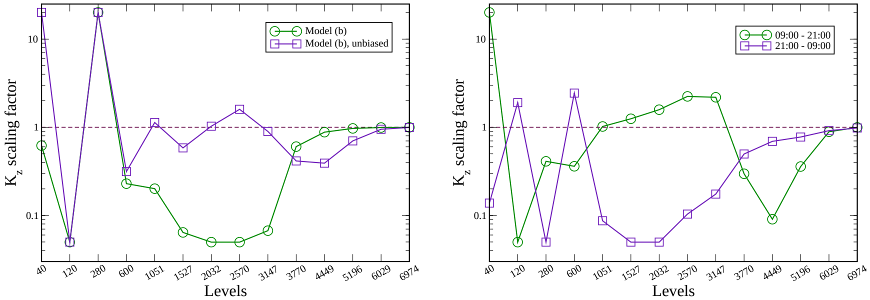
- Cesium-137: optimal value of v^{dep} by 4D-Var or value screening

Model	$\mathrm{v}^{\mathrm{dep}}$ cm s^{-1} (4D-Var)	$\mathrm{v}^{\mathrm{dep}}$ cm s^{-1} (screening)	Cost function
(a)	0.081	0.081 ± 0.005	2984 (3189)
(b)	0.137	0.136 ± 0.010	2792 (2864)
(c)	0.069	0.071 ± 0.005	2905 (3157)

- Iodine-131: optimal value of the scavenging ratio by 4D-Var or value screening

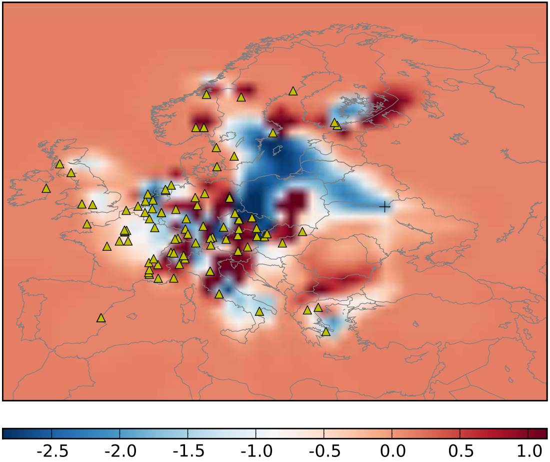
Model	ratio $\times 10^{-4}$ (4D-Var)	ratio $\times 10^{-4}$ (screening)	Cost function $\times 10^{5}$
(a)	0.97	0.96 ± 0.08	1.084 (1.110)
(b)	2.55	2.53 ± 0.20	1.146 (1.227)
(c)	0.88	0.86 ± 0.08	1.072 (1.109)

Case study: Optimal rescaling of the K_z field (cesium-137)



- Without debiasing, no hope to make sense of the retrieved parameters!
- Decreases diffusivity during night, slight increase during day, as expected!

Case study: Optimization of the 2D dry deposition field (1/2)



- Certainly non-physical but maybe useful?

Case study: Optimization of the 2D dry deposition field (2/2)

- Cross-validation from cesium-137 to cesium-134

Optimization	Validation	J (MSE)	Mean	MBE	NMSE	C.Pear.
^{137}Cs	^{137}Cs	1626	0.89	0.09	1.45	0.78
^{137}Cs	^{134}Cs	423	0.61	-0.04	1.23	0.79

- Cross-validation from cesium-134 to cesium-137

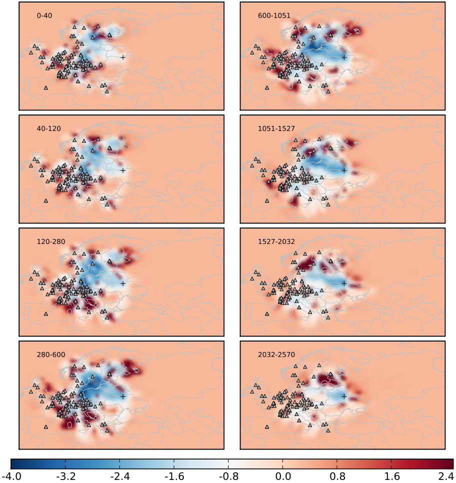
Optimization	Validation	J (MSE)	Mean	MBE	NMSE	C.Pear.
^{134}Cs	^{134}Cs	386	0.86	0.05	1.33	0.81
^{134}Cs	^{137}Cs	1715	0.76	0.23	1.79	0.78

- Very efficient statistical adaptation!

Case study: Optimization of the 3D K_h field

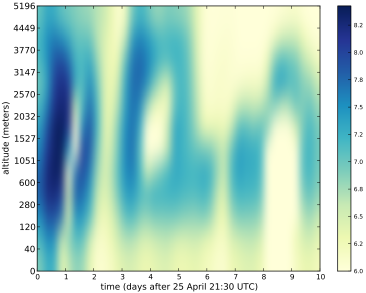
- Similar optimization with the 3D field K_h

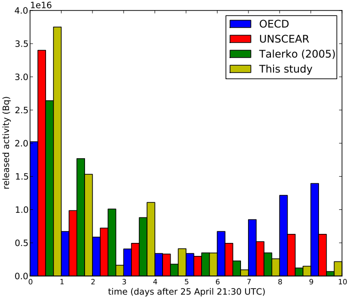
$\longrightarrow$ very similar result: unphysical but very efficient statistical adaptation.



Final word on the cesium 137 source term

▶ A solution of the inverse problem using source positivity constraints, reduction of model error biases, and hyper-parameter estimation.





Model	J(MSE)	Mean	MBE	NMSE	C.Pear.	J(MSE) via SA	Ret.Act.
Optimization of the daily factors							
(b)	2526	0.80	0.19	2.52	0.62	2524	$8.50\,10^{16}$
Optimization of the daily factors using the unbiased $v^{\rm dep}$, λ and source term							
(b)	2187	0.93	0.05	1.86	0.66	2178	$8.70\,10^{16}$
Optimization of the diurnal and nocturnal factors using the unbiased $v^{\rm dep}$, λ and source term							
(b)	2165	0.89	0.09	1.93	0.68	2158	$8.70\,10^{16}$

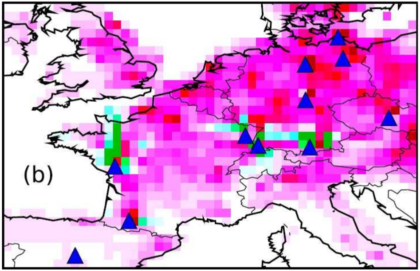
Outline

Conclusions

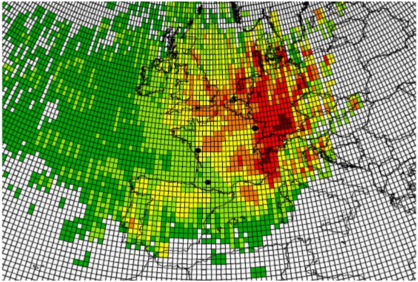
- Methods that are used for parameter estimation: 4D-Var, stochastic optimization, EnKF, PF, matrix BLUE (Jacobian) + adequate (non-Gaussian random) variable representations.
- Prior information on the parameters are difficult to obtain/model (different from forecasting).
  $\longrightarrow$ hyperparameter estimation often needed.
- Correction of parameters may compensate for model errors these parameters are not meant to represent.
  $\longrightarrow$ Global understanding needed of all errors in a problem.
- Proper or improper tuning of parameters may lead to dramatic improvement in model forecast/nowcasting performance!
- Prior distributions of the parameters often non-Gaussian.
  $\longrightarrow$ mathematical hardships.

Realizing I am a DADA too!

- Ongoing comparison (CARBOSOR project) bewteen the DA inverse modelling solution of VOC emissions over Europe (Koohkan et al., 2012) and D&A reconstruction of VOC emissions over Europe (Sauvage et al., 2008).



DA Inversion of acetylene fluxes



D&A Spatialized contribution of traffic VOC using PMF

References I

- Aksoy, A., Zhang, F., Nielsen-Gammon, J., 2006. Ensemble-based simultaneous state and parameter estimation in a two-dimensional sea-breeze model. Mon. Wea. Rev. 134, 2951–2969.
- Aster, R. C., Borchers, B., Thuber, C. H., 2006. Parameter Estimation and Inverse Problems. Elsevier Academic Press.
- Backus, G. E., Gilbert, J. F., 1968. The resolving power of gross earth data. Geophysical Journal of the Royal Astronomical Society 16, 169–205.
- Baklanov, A., 1999. Parameterisation of the deposition processes and radioactive decay: a review and some preliminary results with the DERMA model. Tech. Rep. 99-4, DMI, Copenhagen, Denmark.
- Barbu, A. L., Segers, A. J., Schaap, M., Heemink, A. W., Builtjes, P. J. H., 2009. A multi-component data assimilation experiment directed to sulphur dioxide and sulphate over Europe. Atmos. Env. 43, 1622–1631.
- Bennett, A. F., 1992. Inverse Methods in Physical Oceanography. Cambridge University Press, New York, NY.
- Bennett, A. F., 2002. Inverse Modeling of the Ocean and Atmosphere. Cambridge University Press.
- Bocquet, M., 2005a. Grid resolution dependence in the reconstruction of an atmospheric tracer source. Nonlin. Processes Geophys. 12, 219–233.
- Bocquet, M., 2005b. Reconstruction of an atmospheric tracer source using the principle of maximum entropy. I: Theory. Q. J. Roy. Meteor. Soc. 131, 2191–2208.
- Bocquet, M., 2005c. Reconstruction of an atmospheric tracer source using the principle of maximum entropy. II: Applications. Q. J. Roy. Meteor. Soc. 131, 2209–2223.

References II

- Bocquet, M., 2008. Inverse modelling of atmospheric tracers: Non-Gaussian methods and second-order sensitivity analysis. Nonlin. Processes Geophys. 15, 127–143.
- Bocquet, M., 2012a. An introduction to inverse modelling and parameter estimation for atmospheric and oceanic sciences. In: Blayo, E., Bocquet, M., Cosme, E. (Eds.), Advanced data assimilation for geosciences. Oxford University Press, Les Houches school of physics.
- Bocquet, M., 2012b. Parameter field estimation for atmospheric dispersion: Application to the Chernobyl accident using 4D-Var. Q. J. Roy. Meteor. Soc. 138, 664–681.
- Brandt, J., Christensen, J. H., Frohn, M., 2002. Modelling transport and deposition of caesium and iodine from chernobyl accident using the dream model. Atmos. Chem. Phys. 2, 397–417.
- Chapnik, B., Desroziers, G., Rabier, F., Talagrand, O., 2004. Properties and first application of an error-statistics tuning method in variational assimilation. Q. J. Roy. Meteor. Soc. 130, 2253–2275.
- Davoine, X., Bocquet, M., 2007. Inverse modelling-based reconstruction of the Chernobyl source term available for long-range transport. Atmos. Chem. Phys. 7, 1549–1564.
- Dee, D. P., 1995. On-line estimation of error covariance parameters for atmospheric data assimilation. Mon. Wea. Rev. 123, 1128–1145.
- Desroziers, G., Berre, L., Chapnik, B., Poli, P., 2005. Diagnosis of observation, background and analysis-error statistics in observation space. Q. J. Roy. Meteor. Soc. 131, 3385–3396.
- Desroziers, G., Ivanov, S., 2001. Diagnosis and adaptive tuning of observation-error parameters in a variational assimilation. Q. J. Roy. Meteor. Soc. 127, 1433–1452.

References III

- Doicu, A., Trautmann, T., Schreier, F., 2010. Numerical Regularization for Atmospheric Inverse Problems. Springer and Praxis publishing.
- Elbern, H., Strunk, A., Schmidt, H., Talagrand, O., 2007. Emission rate and chemical state estimation by 4-dimensional variational inversion. Atmos. Chem. Phys. 7, 3749–3769.
- Ellis, R. S., 1985. Entropy, Large Deviations, and Statistical Mechanics. Springer.
- Engl, H. W., Hanke, M., Neubauer, A., 2000. Regularization of Inverse Problems. Mathematics and Its Applications. Kluwer Academic Publishers.
- Enting, I. G., 2002. Inverse Problems in Atmospheric Constituent Transport. Cambridge, Atmospheric and Space Science Series.
- Groestsch, C. W., 1993. Inverse Problems in the Mathematical Sciences. Vieweg and Verlag.
- Hansen, P. C., 1992. Analysis of discrete ill-posed problems by means of the L-curve. SIAM Review 34, 561–580.
- Hansen, P. C., 2010. Discrete Inverse Problems: Insight and Algorithms. Applied Mathematical Sciences. SIAM, Philadelphia.
- Hestenes, M. R., Stiefel, E., 1952. Methods of conjugate graidents for solvinf linear systems. J. Res. Nat. Bur. Standards 49, 409–436.
- Jackson, C., Sen, M. K., Stoffa, P. L., 2004. An efficient stochastic Bayesian approach to optimal parameter and uncertainty estimation for climate model predictsions. Journal of Climate 17, 2828–2841.
- Kaipio, J., Somersalo, E., 2005. Statistical and Computational Inverse Problems. Springer.

References IV

- Kondrashov, D., Sun, C., Ghil, M., 2008. Data assimilation for a coupled ocean atmosphere model. Part ii: Parameter estimation. Mon. Wea. Rev. 5, 5062–5076.
- Krysta, M., Bocquet, M., 2007. Source reconstruction of an accidental radionuclide release at European scale. Q. J. Roy. Meteor. Soc. 133, 529–544.
- Lauvernet, C., Brankart, J.-M., Castruccio, F., Broquet, G., Brasseur, P., Verron, J., 2009. A truncated Gaussian filter for data assimilation with inequality constraints: Application to the hydrostatic stability condition in ocean models. Ocean Model. 27, 1–17.
- Le Besnerais, G., Bercher, J.-F., Demoment, G., 1999. A new look at entropy for solving linear inverse problems. Information Theory, IEEE Transactions on 45, 1565–1578.
- Liu, Y., Gupta, H. V., Sorooshian, S., Bastidas, L. A., Shuttlewort, W. J., 2005. Constraining land surface and atmospheric parameters of a locally coupled model using observational data. Journal of Hydrometeorology 6, 156–172.
- Morozov, V. A., 1966. On the solution of functional equations by the method of regularization. Soviet Mathematics Doklady 7, 414–417.
- Nocedal, J., Wright, S. J., 2006. Numerical Optimization. Springer Series in Operations Research. Springer.
- Pudykiewicz, J. A., 1998. Application of adjoint transport tracer equations for evaluating source parameters. Atmos. Env. 32, 3039–3050.
- Pulido, M., Thuburn, J., 2006. Gravity wave drag estimation from global analyses using variational data assimilation principles. Part ii: A case study. Q. J. Roy. Meteor. Soc. 132, 1527–1543.

References V

- Rodgers, C. D., 2000. Inverse methods for atmospheric sounding. Vol. 2. World Scientific, Series on Atmospheric, Oceanic and Planetary Physics.
- Ruiz, J. J., Pulido, M., Miyoshi, T., 2012. Estimating model parameters with ensemble-based data assimilation. Mon. Wea. Rev. 0, 0–0.
- Shore, J. E., 1984. Inversion as logical inference - theory and applications of maximum entropy and minimum cross-entropy. Vol. 14. SIAMS-AMS Proceedings.
- Talerko, N., 2005a. Mesoscale modelling of radioactive contamination formation in ukraine caused by the chernobyl accident. J. Environ. Radioactivity 78, 311–329.
- Talerko, N., 2005b. Reconstruction of ^{131}I radioactive contamination in Ukraine caused by the Chernobyl accident using atmospheric transport modelling. J. Environ. Radioactivity 84, 343–362.
- Tarantola, A., 1987. Inverse Problem Theory. Elsevier.
- Tarantola, A., 2005. Inverse Problem Theory and Methods for Model Parameter Estimation. SIAM.
- Tarantola, A., Valette, B., 1982. Inverse problems = quest for information. Journal of Geophysics 50, 159–170.
- Tikhonov, A. N., Arsenin, V., Y., 1977. Solutions of Ill-Posed Problems. Winston, Washington DC.
- Vogel, C. R., 2002. Computational Methods for Inverse Problems. SIAM, Frontiers in Applied Mathematics.
- Vossepoel, F. C., van Leeuwen, P. J., 2007. Parameter estimation using a particle method: Inferring mixing coefficients from sea level observations. Mon. Wea. Rev. 135, 1006–1020.

References VI

- Wahba, G., 1990. Spline Models for Observational Data. CBMS-NSF Regional Conference Series in Applied Mathematics 59. SIAM, Philadelphia.
- Wahba, G., Johnson, D. R., Gao, F., Gong, J., 1995. Adaptive tuning of numerical weather prediction models: Randomized gcv in three- and four-dimensional data assimilation. Mon. Wea. Rev. 123, 3358–3369.
- Winiarek, V., Bocquet, M., Saunier, O., Mathieu, A., 2012. Estimation of errors in the inverse modeling of accidental release of atmospheric pollutant: Application to the reconstruction of the cesium-137 and iodine-131 source terms from the Fukushima Daiichi power plant. J. Geophys. Res. 117, D05122.
- Wirth, A., Verron, J., 2008. Estimation of friction parameters and laws in 1.5D shallow-water gravity currents on the f-plane, by data assimilation. Ocean Dynamics 58, 247–257.
- Wunsch, C., 2006. Discrete Inverse and State Estimation Problems with Geophysical Fluid Applications. Cambridge University Press.