

Supporting the improvement of the carbon observing system by quantitative network design

M. Voßbeck (<http://FastOpt.com>)

T. Kaminski, P. Rayner, M. Scholze, E. Koffi, and R. Giering

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Motivation

What is the question?

Can construct a machinery that,
for a given network and a given target quantity,
can approximate the uncertainty
with which the value of the target quantity is
constrained by the observations

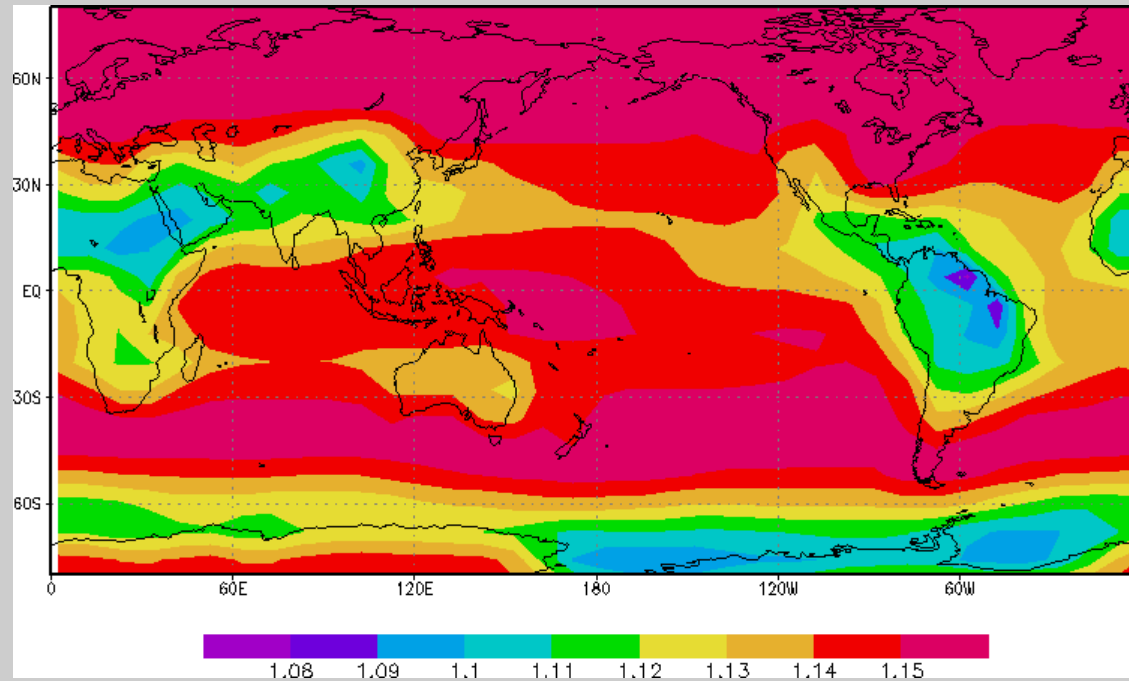
Outline

- Motivation
- Example
- Method
- Demo
- Summary
- Links to further information

Example Linear Model

Target quantity:

Standard deviation of Global Ocean Uptake (GtC/yr)



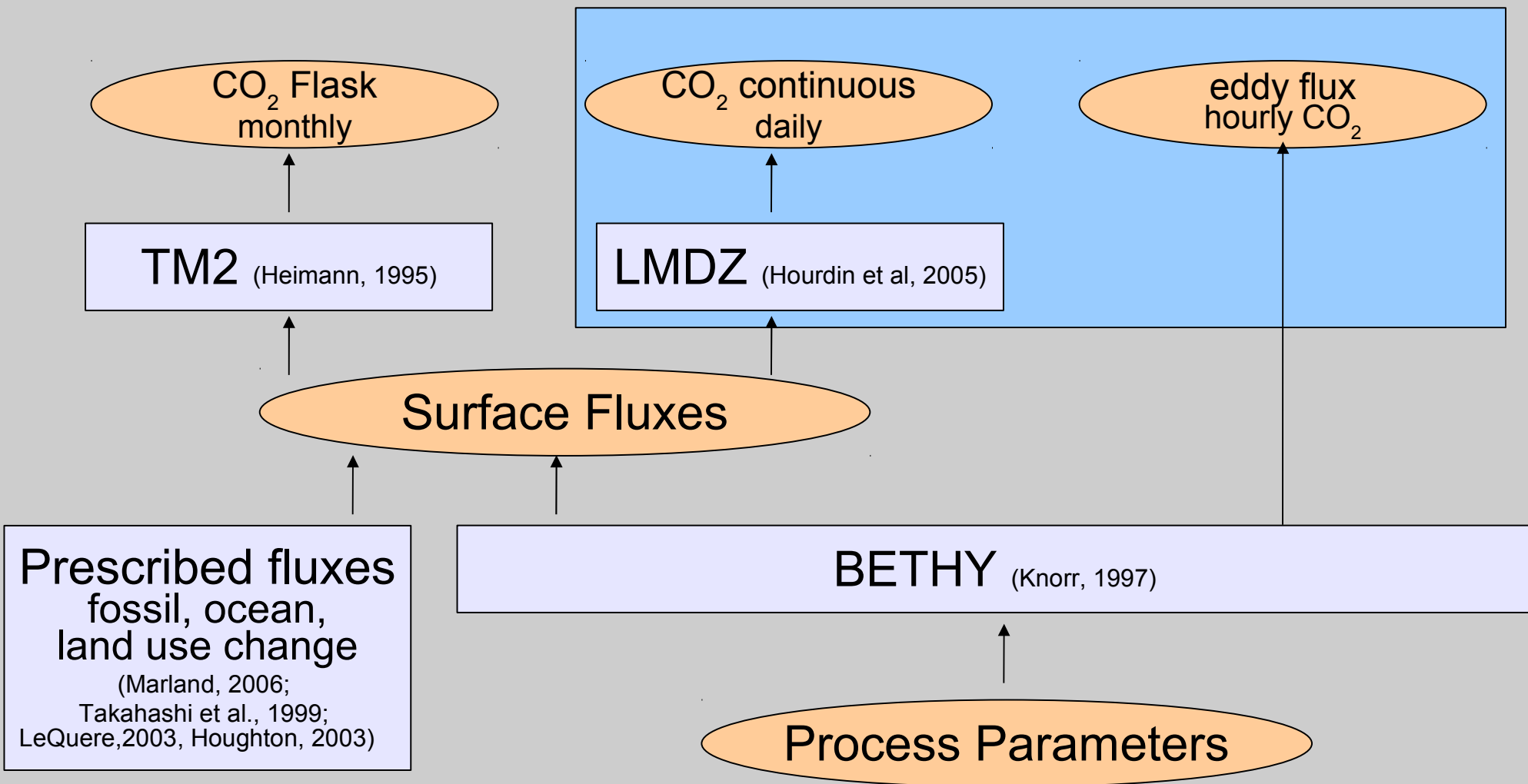
Rayner et al.
(Tellus, 1996)

Inverse model based
on atmospheric tracer
model

Existing network yields
1.16 GtC/yr

- Global constraints with narrow uncertainty on “ocean uptake + terrestrial uptake” couples information from disparate regions:
Improvement in knowledge of Amazonian fluxes improves knowledge of both total land and ocean fluxes!

Carbon Cycle Data Assimilation System (CCDAS) Forward Modelling Chain



Model and Observational Uncertainties

- No observation/no model is perfect.
- It is convenient to quantify observations and their model counterpart by probability density functions (PDFs).
- The simplest assumption is that they are Gaussian.

$$\sigma_d^2 = \sigma_{obs}^2 + \sigma_{mod}^2$$

total uncertainty

uncertainty from model error

uncertainty from observational error

- If the observation refers to a point in space and time, there is a representation error because the counterpart simulated by the model refers to a box in space and time:
the corresponding uncertainty must be accounted for either by the observational or by the model contribution to total uncertainty.

Computing posterior parameter uncertainty

- $M: x \rightarrow d$ maps the process parameters onto the observations
(CO₂ concentrations, flask and continuous, CO₂ hourly fluxes)

- Introduce cost function:

$$J(x) = \frac{1}{2} [(Mx-d)^T C_d^{-1} (Mx-d) + (x - x_{pr})^T C_{pr}^{-1} (x - x_{pr})]$$

- x_{pr} : priori information on the process parameter
 C_d, C_{pr} : covariance matrices of uncertainties in observations and prior parameters respectively.

- If model M is **linear**, and if data d and priors x_{pr} have Gaussian PDF, then posterior PDF is also Gaussian (Tarantola 87):

$$\rho(x) = K * \exp(-\frac{1}{2}(x - x_{po})^T C_{po}^{-1} (x - x_{po}))$$

with mean value:

$$x_{po} = x_{pr} + [M^T C_d^{-1} M + C_{pr}^{-1}]^{-1} M^T C_d^{-1} (d - Mx_{pr})$$

- x_{po} minimises $J(x)$
- Uncertainty given by:

$$C_{po}^{-1} = M^T C_d^{-1} M + C_{pr}^{-1} = d^2 J(x_{po}) / dx^2$$

Computing posterior parameter uncertainty

- For **non-linear, differentiable** model M posterior distribution of parameters is still approximately Gaussian (Tarantola 87)

$$\rho(x) \approx K * \exp(-1/2(x - x_{po})^T C_{po}^{-1}(x - x_{po}))$$

- Equation for posterior uncertainties holds as approximation:

$$C_{po} \approx (d^2J(x_{po}) / dx^2)^{-1}$$

- x_{po} now determined by minimising cost function J
- Use gradient based optimisation to solve, x_{po} fullfills:

$$dJ(x_{po}) / dx = 0$$

- Efficient first and second order derivatives required, use adjoint code for first order derivatives
- All derivative code generated from model code by automatic differentiation tool **TAF** (Giering and Kaminski, 1998)

Network Design Tool: Simplifications of implementation

- For a number of $i = 1, \dots, n_d$ of **uncorrelated** observations (C_d diagonal matrix) with (user provided) standard deviations σ_{d_i} the cost function can be written:

$$J(x) = \frac{1}{2} (x - x_{pr}) C_{pr}^{-1} (x - x_{pr}) + \frac{1}{2} \sum_{i=1}^{n_d} ((M_i(x) - d_i) / \sigma_{d_i})^2$$

with:

$$C_{po}^{-1} = d^2 J(x_{po}) / dx^2 = C_{pr}^{-1} + \sum_{i=1}^{n_d} (1 / \sigma_{d_i}^2) d^2 / dx^2 (M_i(x) - d_i)^2$$

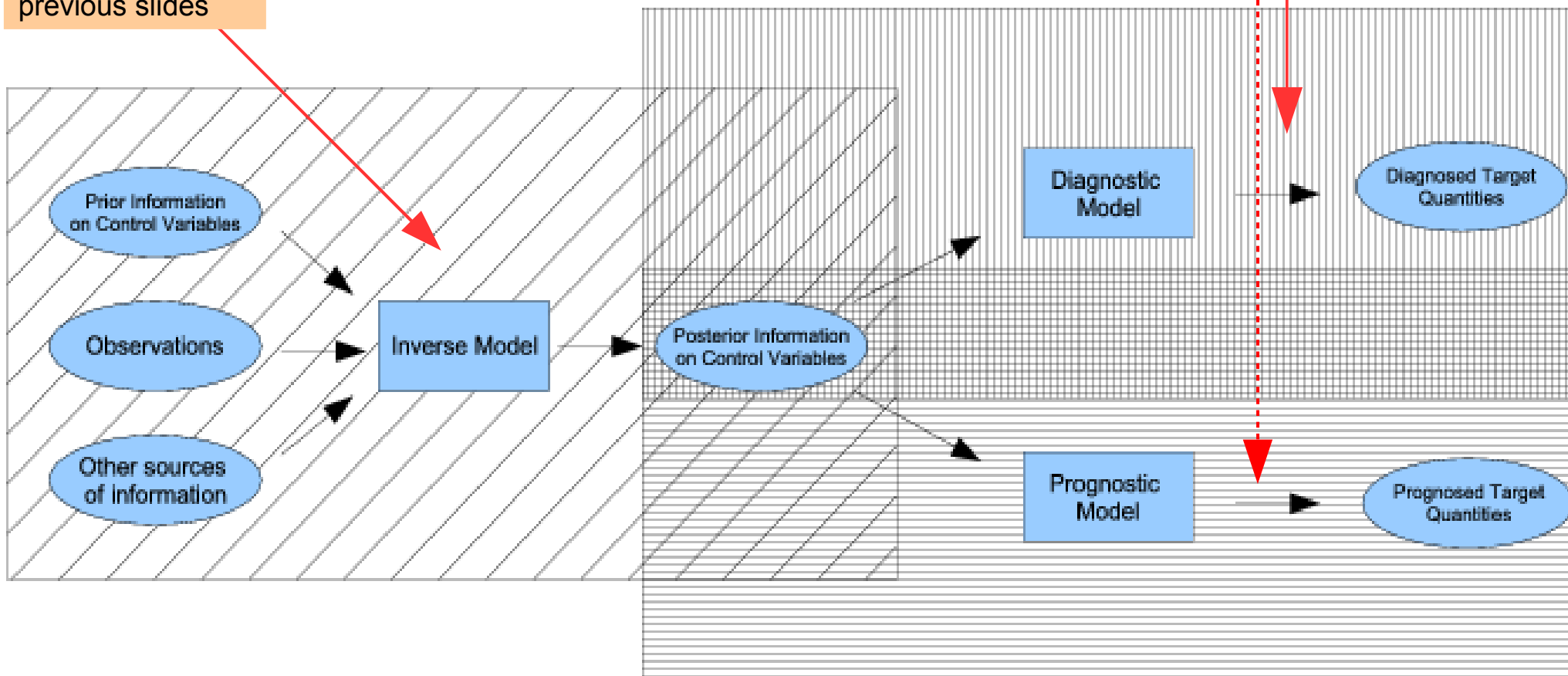
- Using synthetic data $d = M(x)$, model contribution in formula for C_{po} can be precomputed (do not depend on user input!)

uncertainties in observations **AND** model

CCDAS scheme

Inversion step:
described on
previous slides

Propagation step: shown next



Propagation step

- $N: x \rightarrow y$ maps process parameters onto the target quantity (diagnostic or prognostic)
- Diagnostic run means that it is based on same domain (spatial and temporal) as used in the inversion step, whereas prognostic run is (at least in parts) outside this domain

- PDF of y can again be approximated by a Gaussian with mean

$$y_{po} = N(x_{po})$$

and covariance

$$C(y_{po}) = D(N) C_{po} D(N)^T + C(y_{mod})$$

- $D(N) = dN(x_{po})/dx$ is the linearisation of N around x_{po} (Jacobian),

$C(y_{mod})$ accounts for the uncertainty of the target quantity for errors in N

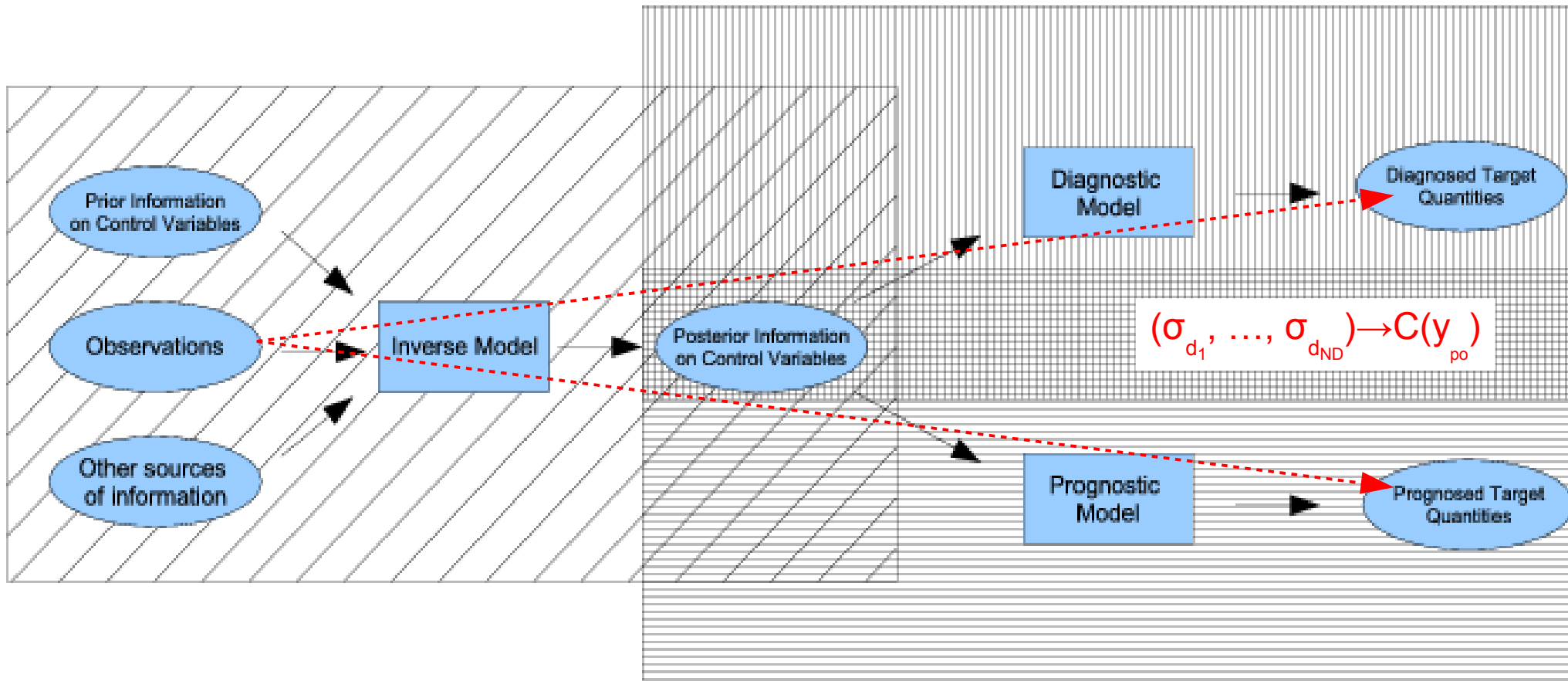
- Recall $C_{po}^{-1} = C_{pr}^{-1} + \sum_{i=1}^{nd} (1/\sigma_{d_i}^2) d^2/dx^2 (M_i(x) - d_i)^2$

- Answers the initial question and eventually yields mapping from uncertainties of (potential) observations to uncertainty of the target quantity:

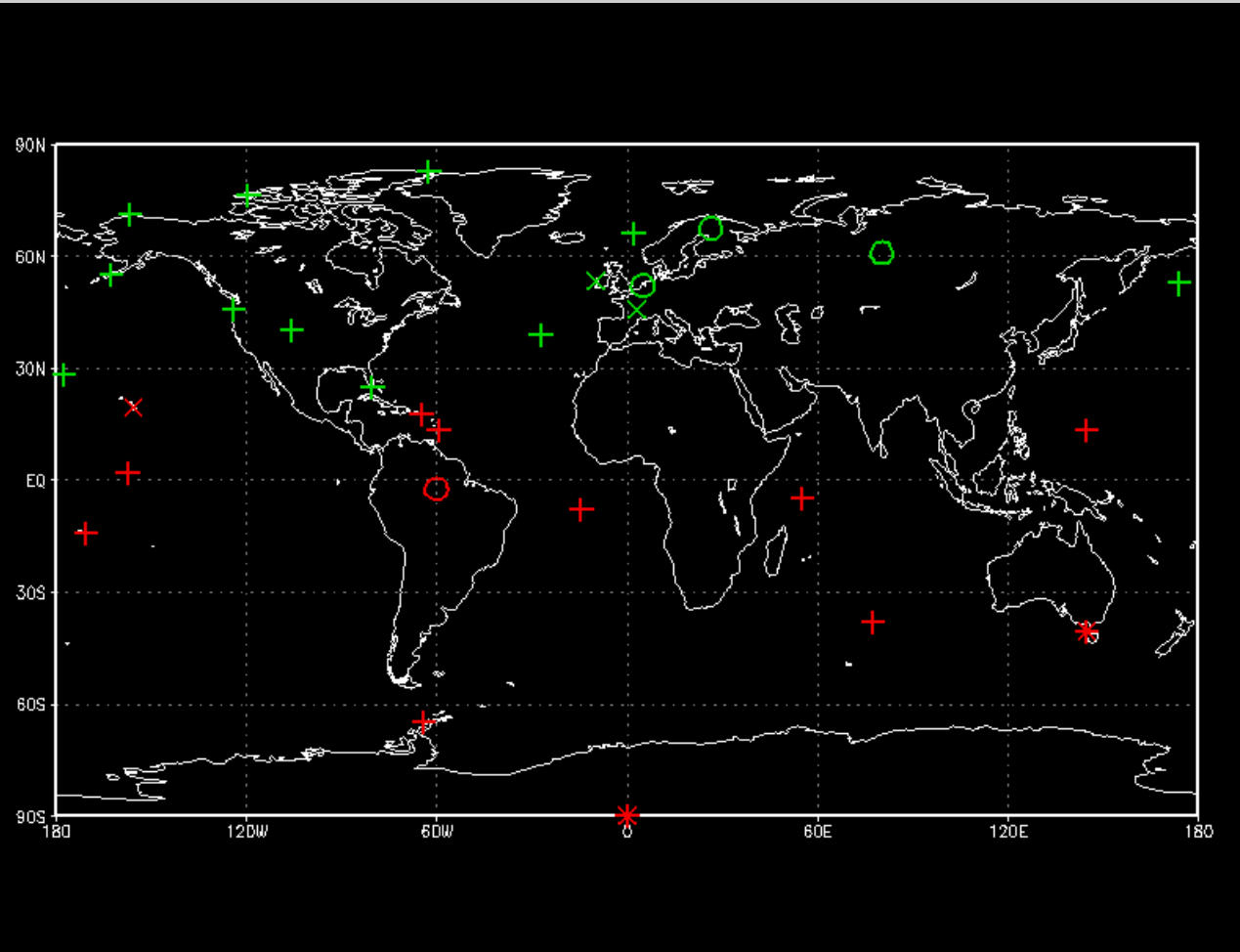
$$C(y_{po}) = C(y_{po}; \sigma_{d_1}, \dots, \sigma_{d_{ND}})$$

Propagation step also requires derivatives!

Uncertainties of Target Quantities



Sketch of Network DesignTool



Observations [sigma]

- + Flask [enter]
- x Continuous [enter]
- o Eddy Flux [enter]

Compute

Targets [sigma]

- European Uptake []
- Global Uptake []

Demo: Network Design Tool

Summary: Assumptions and Ingredients

Assumptions:

- Gaussian uncertainties on priors, observations, and from model error (or function of Gaussian, e.g. lognormal)
- Model not too non linear

Ingredients:

- Assimilation system that can (efficiently) propagate uncertainties; helpful: Adjoint, Hessian, and Jacobian codes
- Ability to estimate uncertainties for priors, observations and due to model error; requires expertise of observationalists and modellers
- Need to take logistic constraints into account

Further Information

Terrestrial assimilation system applications and papers:
<http://CCDAS.org>

The corresponding network design project:
<http://IMECC.CCDAS.org>

with links to papers on network design

More assimilation systems, applications and papers:
<http://FastOpt.com>