

Inverse Modelling of Atmospheric Carbon Dioxide

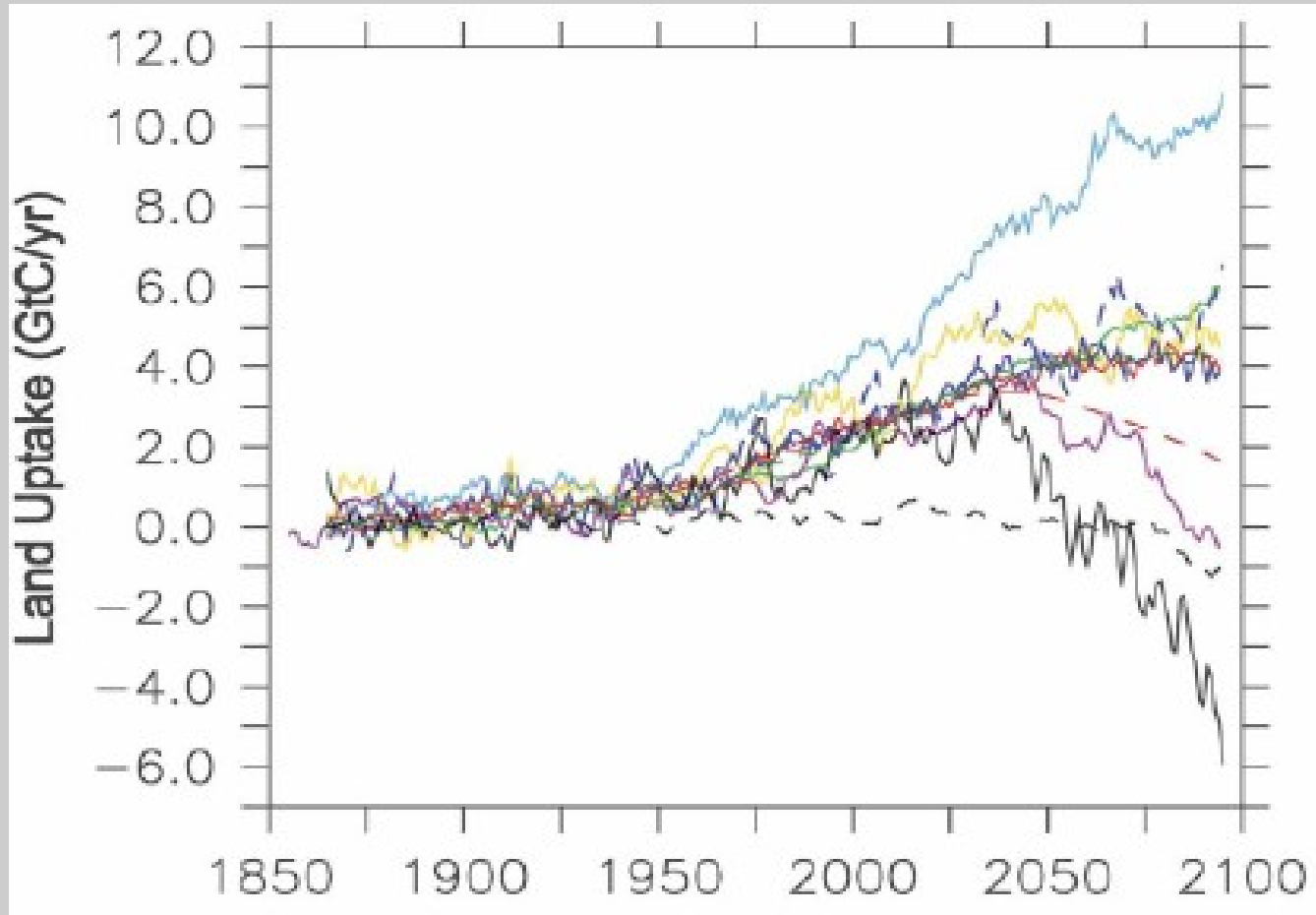
Thomas Kaminski (<http://FastOpt.com>)

2nd Advanced Training Course on Atmospheric Remote Sensing, Juelich, October 2014

Outline

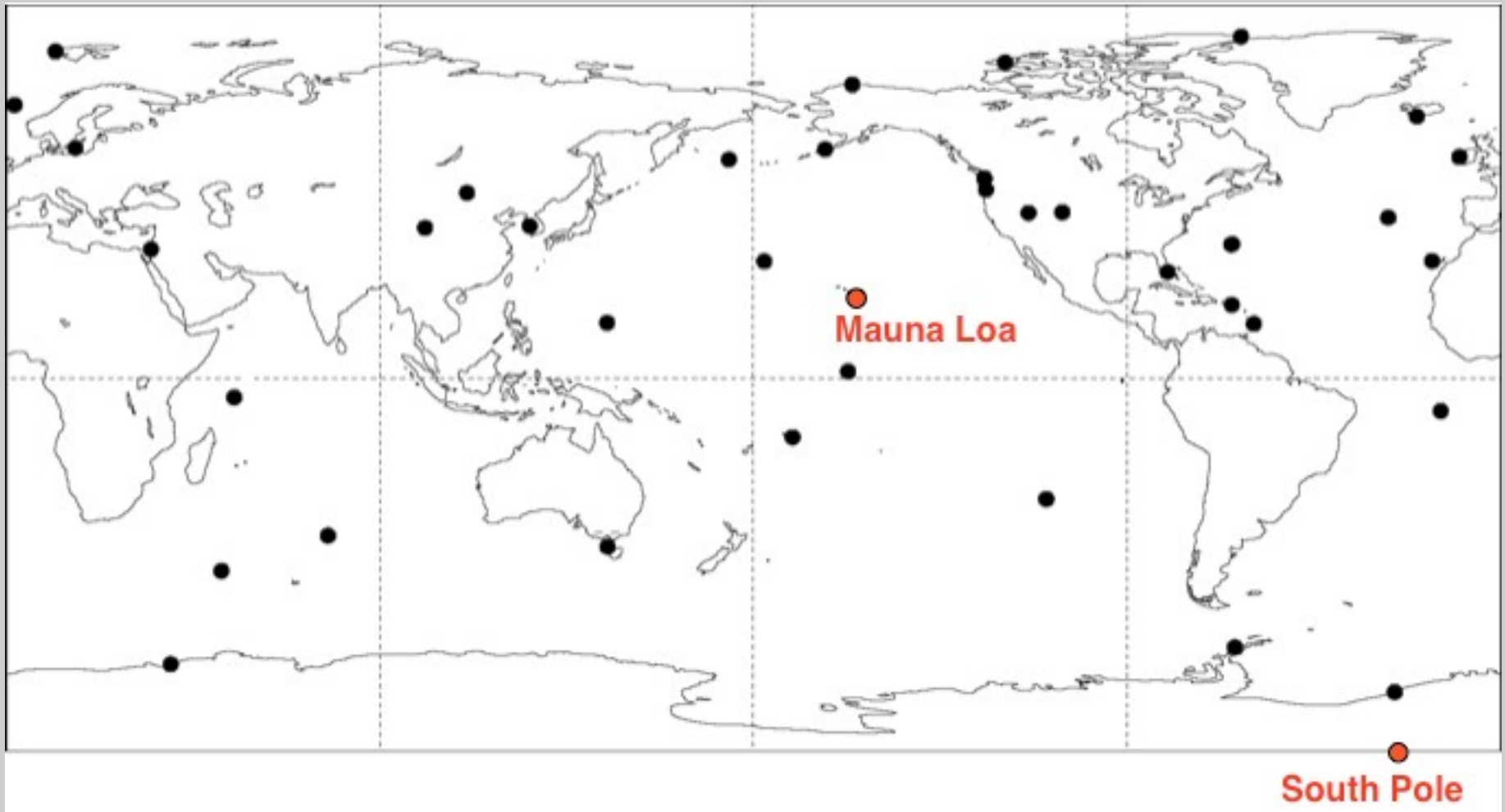
- Motivation
- Transport Inversion
- Underdetermined Inverse Problem, Pitfalls
- Role of Remote Sensing
- Carbon Cycle Data Assimilation System (CCDAS)

Land Uptake of CO₂

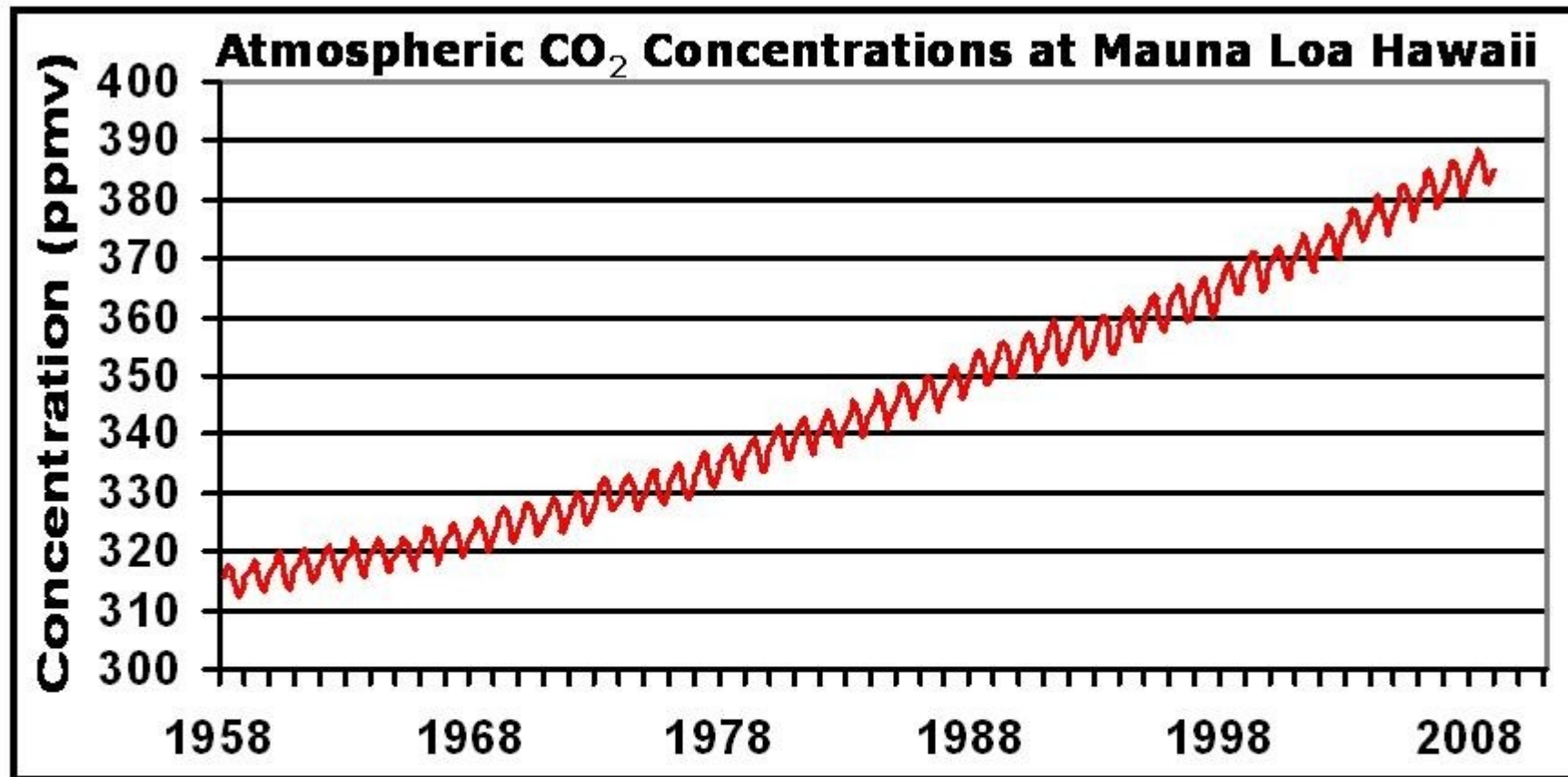


C4MIP results (Friedlingstein et al. 2006)

The atmospheric CO₂ flask sampling network



MLO



Pioneers of Transport Inversion

- Ian Enting's group in Melbourne -> Peter Rayner
- Transport Inversion with formal computation of posterior uncertainty
- History and flavours of transport inversion:



Posterior Uncertainty, linear case

$$J(\tilde{\mathbf{x}}) = \frac{1}{2} [(\mathbf{M}\tilde{\mathbf{x}} - \mathbf{d})^T \mathbf{C}(d)^{-1} (\mathbf{M}\tilde{\mathbf{x}} - \mathbf{d}) + (\tilde{\mathbf{x}} - \mathbf{x}_0)^T \mathbf{C}(x_0)^{-1} (\tilde{\mathbf{x}} - \mathbf{x}_0)]$$

If the model is linear:

and data + priors have Gaussian PDF, then the posterior PDF is also Gaussian:

$$\rho(x) \sim e^{-J(x)}$$

with mean value:

$$\mathbf{x} = \mathbf{x}_0 + [\mathbf{M}^T \mathbf{C}(d)^{-1} \mathbf{M} + \mathbf{C}(x_0)^{-1}]^{-1} \mathbf{M}^T \mathbf{C}(d)^{-1} (\mathbf{d} - \mathbf{M}\mathbf{x}_0)$$

and uncertainty:

$$\mathbf{C}(x)^{-1} = \mathbf{M}^T \mathbf{C}(d)^{-1} \mathbf{M} + \mathbf{C}(x_0)^{-1}$$

which are related to the Hessian of the cost function:

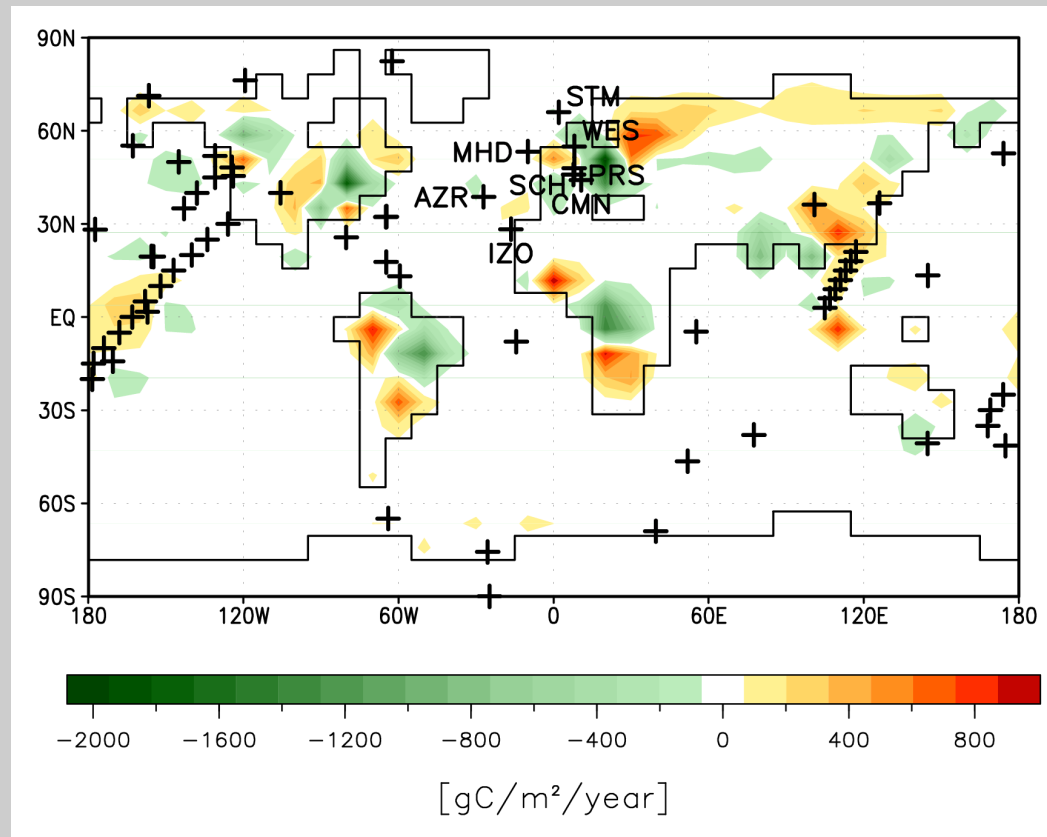
$$\mathbf{C}(x)^{-1} = \mathbf{H}$$

$$\frac{\partial^2 J}{\partial x_i \partial x_j}$$

For a non-linear model, this is an approximation

Transport Inversion

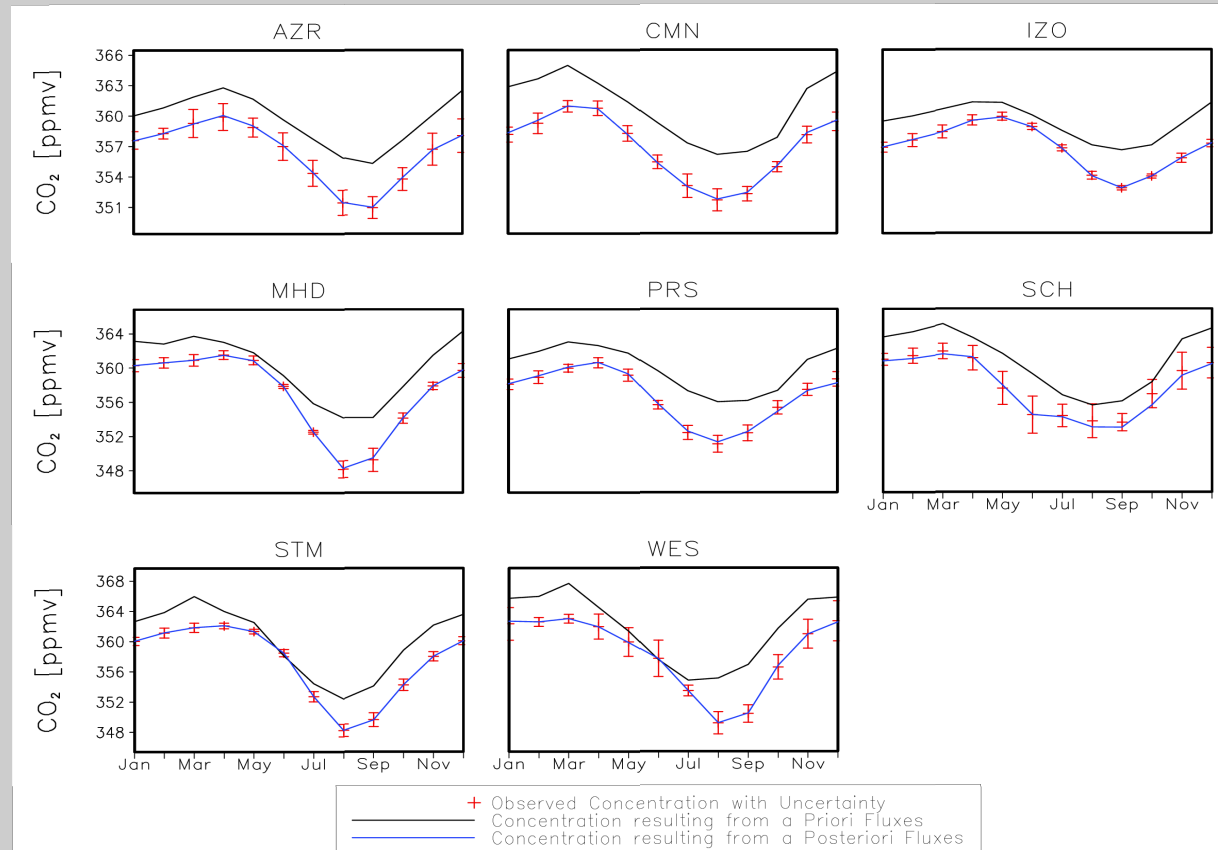
Surface flux field with a 2PgC/year sink over Europe/Hamburg ...



Kaminski and Heimann (2001)

Transport Inversion

... fully consistent with atmospheric flask sampling network

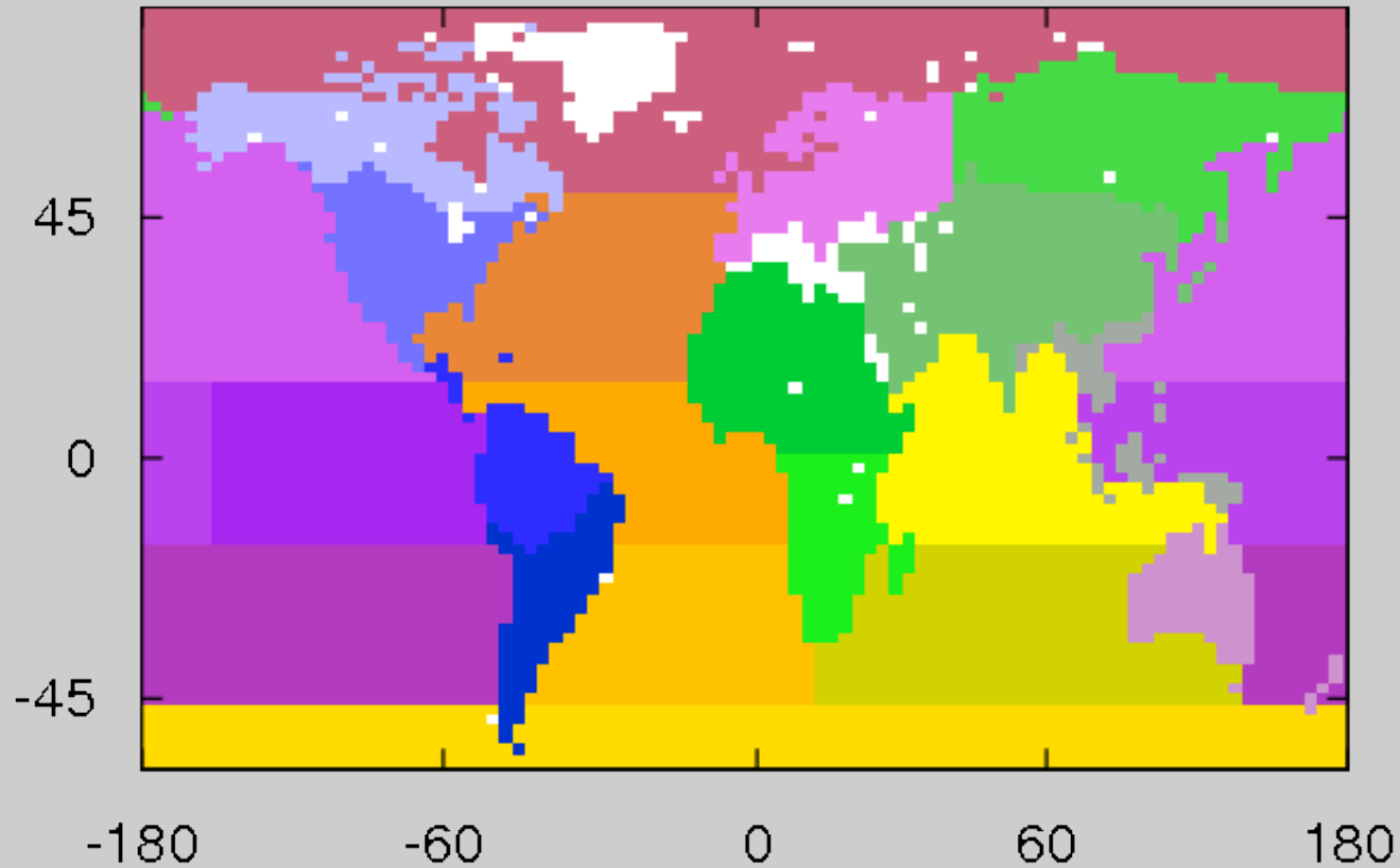


Kaminski and Heimann (2001)

Transport Inversion

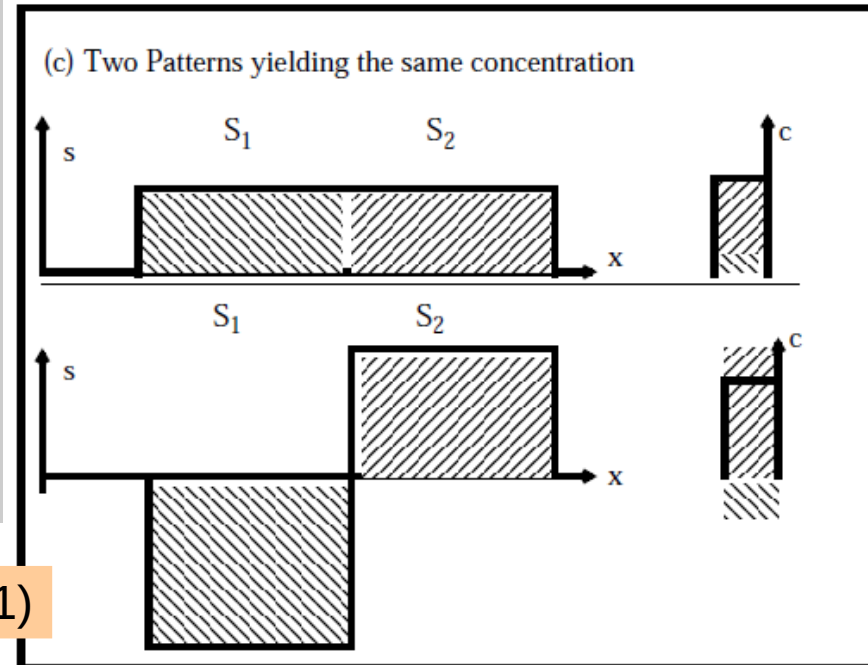
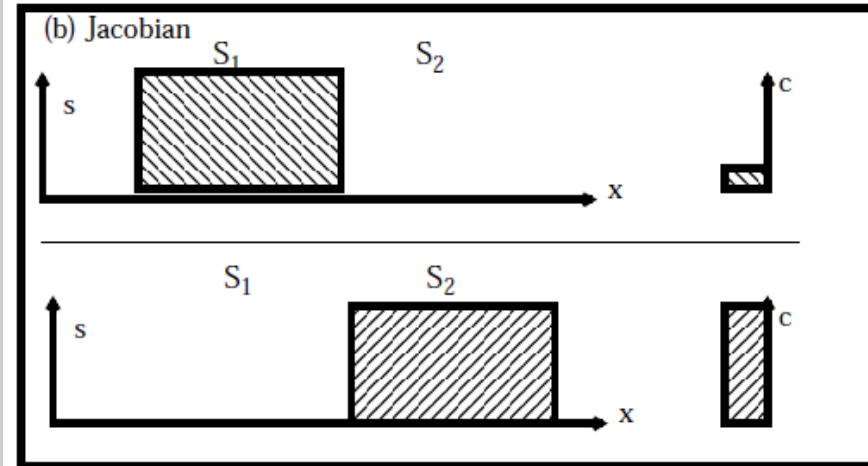
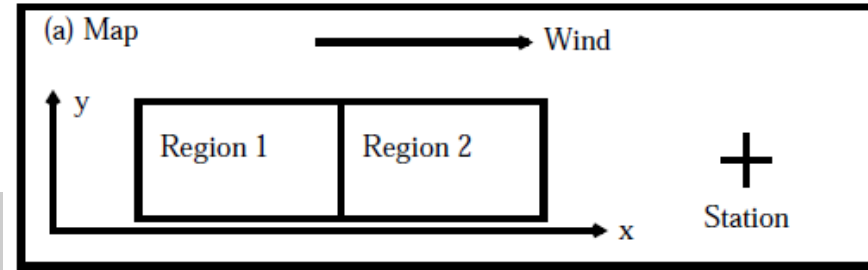
- Cannot infer 2 d flux field from point observations
- Can “hide” arbitrary sink in null space of transport inversion
- Underdetermined inverse problem needs to be stabilised by extra information, which determines solution to large extent

Extra Information through prescribed flux patterns, or spatial correlations



Aggregation Error

- Flux error can have same magnitude as flux
- Should solve for flux on full model grid
- Computationally challenging



Kaminski et al. (2001)

More Data

GEOPHYSICAL RESEARCH LETTERS, VOL. 28, NO. 1, PAGES 175-178, JANUARY 1, 2001

The utility of remotely sensed CO₂ concentration data in surface source inversions

P. J. Rayner

Cooperative Research Centre for Southern Hemisphere Meteorology and CSIRO Atmospheric Research, Aspendale, Victoria, Australia

D. M. O'Brien

CSIRO Atmospheric Research, Aspendale, Victoria, Australia

Abstract. This paper aims to establish the required precision for column-integrated CO₂ concentration data to be useful in constraining surface sources. We use the method of synthesis inversion and compare the uncertainties in regional sources calculated from a moderate-sized surface network and either global or oceanic coverage of column-integrated pseudodata. With a simple measure of total uncertainty, we require precision of monthly averaged column data better than 2.5 ppmv on a 8° × 10° footprint for comparable performance with the existing surface network. If coverage is only oceanic we require 1.5 ppmv precision. We recommend more detailed studies on the feasibility of obtaining such observations from current and future satellite instruments.

In this paper we aim to establish the required precision for column-integrated CO₂ concentration data to be useful in constraining surface sources. The motivation is the suggestion that although imprecisely, at least from existing satellite missions [e.g.

There are several potential sources of uncertainty in the formation on atmospheric CO₂ concentration. For example we can measure the concentration of CO₂ in different bands of CO₂. Similar techniques have been used for CH₄ and O₃ [see for example Rayner *et al.* 1995]. The techniques for measuring temperature profile and humidity (H₂O) are known. Coverage

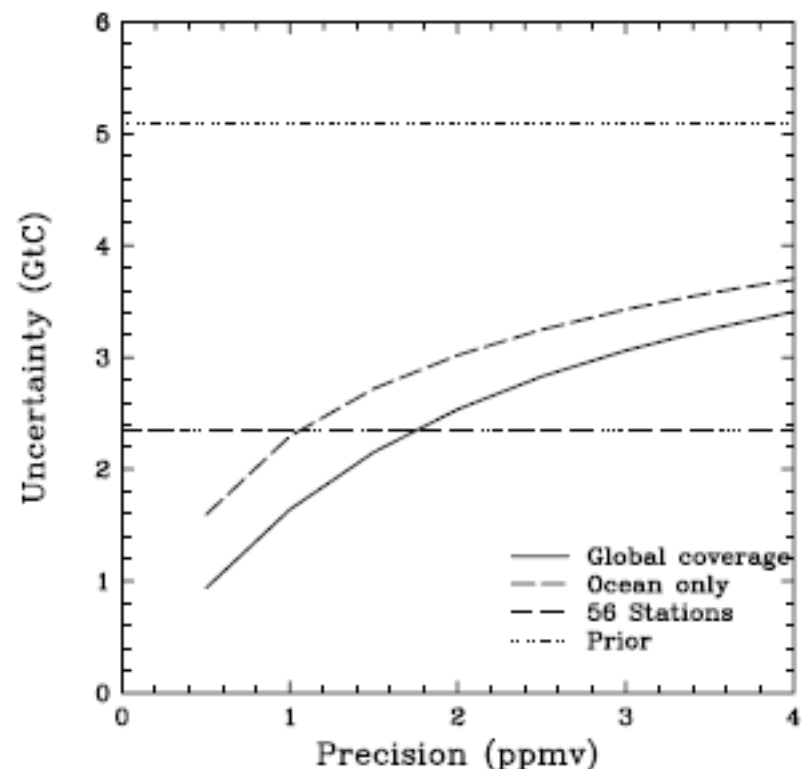


Figure 3. Plot of “total uncertainty” (see Eq. 1) in GtC yr⁻¹ against the precision (ppmv) of column-integrated data. The dotted horizontal line shows the prior uncertainty while the dash-dot horizontal line shows the case for the surface network of Fig. 1.

-> more in MB's lecture

Posterior Uncertainty, linear case

$$J(\tilde{\mathbf{x}}) = \frac{1}{2} [(\mathbf{M}\tilde{\mathbf{x}} - \mathbf{d})^T \mathbf{C}(d)^{-1} (\mathbf{M}\tilde{\mathbf{x}} - \mathbf{d}) + (\tilde{\mathbf{x}} - \mathbf{x}_0)^T \mathbf{C}(x_0)^{-1} (\tilde{\mathbf{x}} - \mathbf{x}_0)]$$

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with mean value:

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and uncertainty:

$$\mathbf{C}(x)^{-1} = \mathbf{M}^T \mathbf{C}(d)^{-1} \mathbf{M} + \mathbf{C}(x_0)^{-1}$$

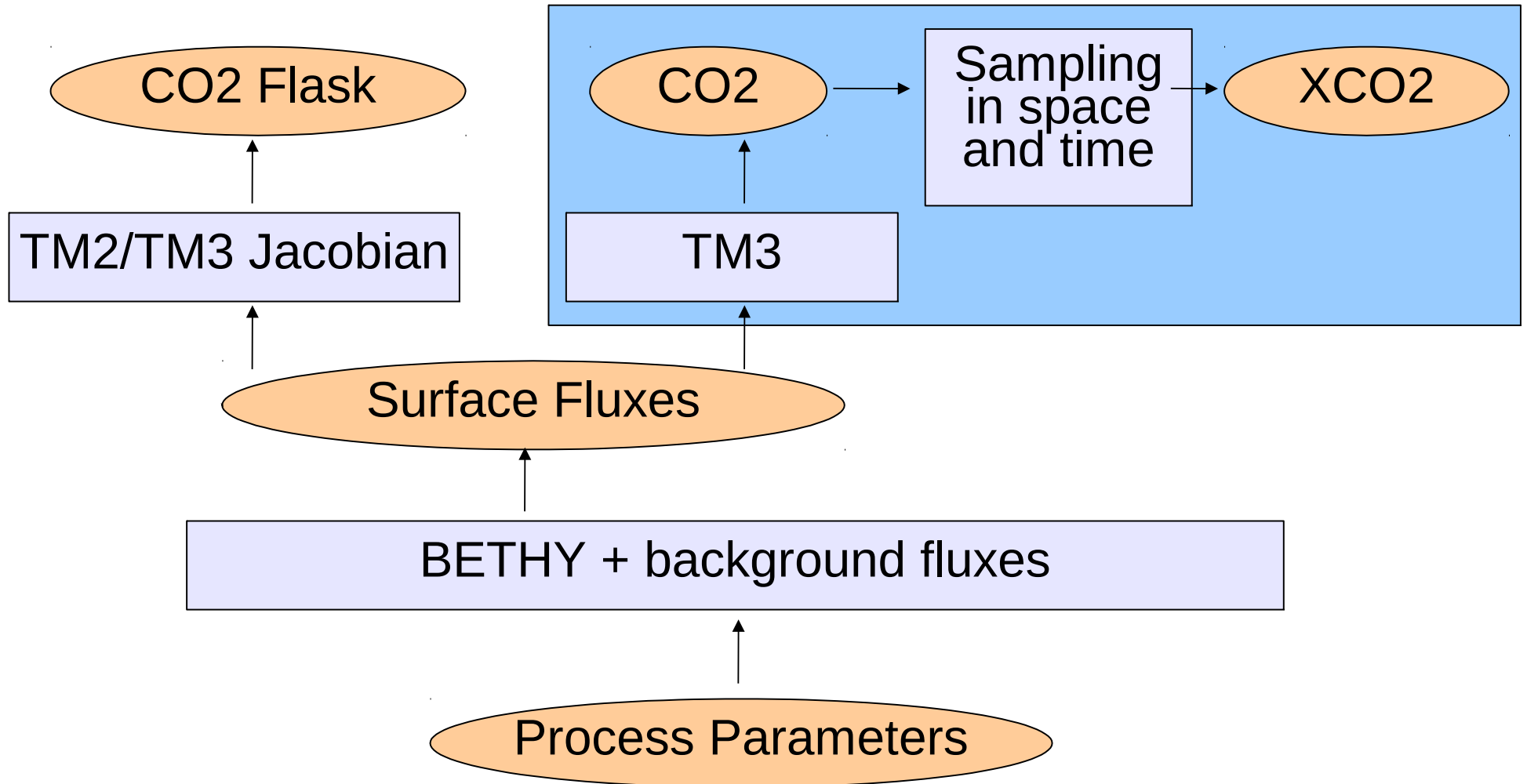
which are related to the Hessian of the cost function:

$$\mathbf{C}(x)^{-1} = \mathbf{H}$$

$$\frac{\partial^2 J}{\partial x_i \partial x_j}$$

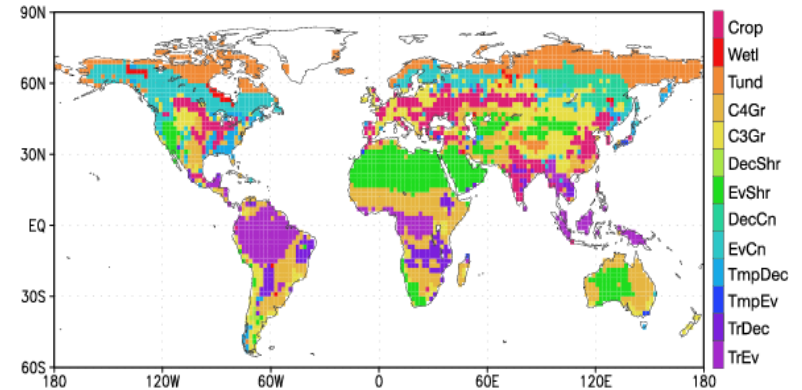
For a non-linear model, this is an approximation

CCDAS-Processing Chain

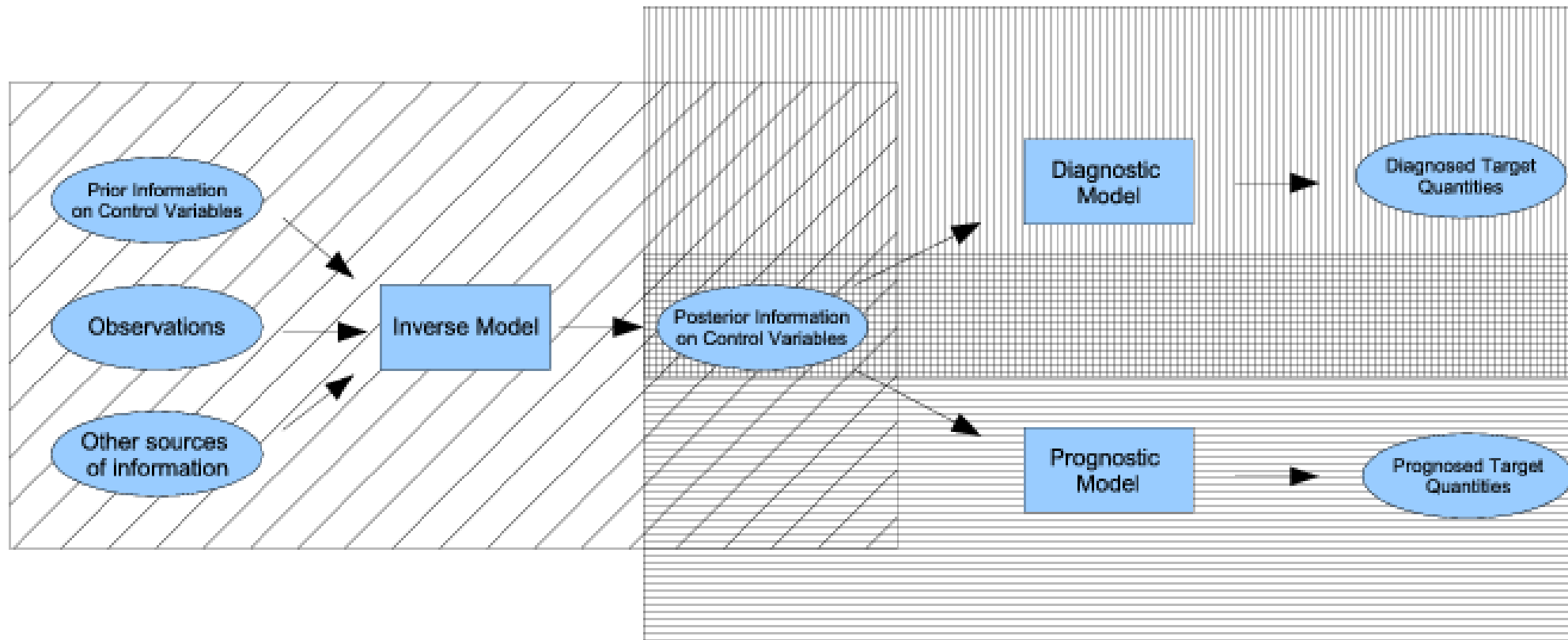


BETHY setup

- 2 by 2 degrees, global
- 13 Plant Functional Types
- 57 Process Parameters (Initial Conditions)
 - † 3 PFT specific
 - † 17 not PFT specific
 - † 1 atmospheric
- Parameter values taken from Scholze et al. (2007)
- Prior parameter uncertainties taken from Scholze et al. (2007), in the order of 25%



CCDAS scheme



Scholze et al. (2007)

Uncertainty calculation in 2 steps

Inverse step:

$$J(x) = \frac{1}{2} (x - x_{pr})^T C_{pr}^{-1} (x - x_{pr}) + \frac{1}{2} \sum_{i=1,nd} \left(\frac{M_i(x) - d_i}{\sigma_{d_i}} \right)^2$$

$$\frac{d^2 J(x)}{dx^2} = C_{pr}^{-1} + \sum_{i=1,nd} \frac{1}{\sigma_{d_i}^2} \frac{d^2}{dx^2} (M_i(x) - d_i)^2$$

- Hessian independent of x for linear model
- For synthetic data use $d = M(x)$.
- Decomposes nicely, can precompute model contribution

**uncertainty
in observations
AND model**

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

Propagation step:

$$\sigma_y^2 \approx \frac{dy(x_{po})}{dx} C_{po} \frac{dy(x_{po})}{dx}^T \approx \frac{dy(x_{po})}{dx} \frac{d^2 J(x_{po})}{dx^2}^{-1} \frac{dy(x_{po})}{dx}^T$$

**All derivative code
generated from model code
by automatic differentiation
tool TAF**

x : Parameters

x_{pr} : Priors

C_{pr} : Uncertainties

$M(x)$: Model

d : Observations

C_d : Their uncertainties

σ_{d_i} : Uncorrelated!

$J(x)$: Cost function

$\frac{d^2 J(x)}{dx^2}$: Hessian

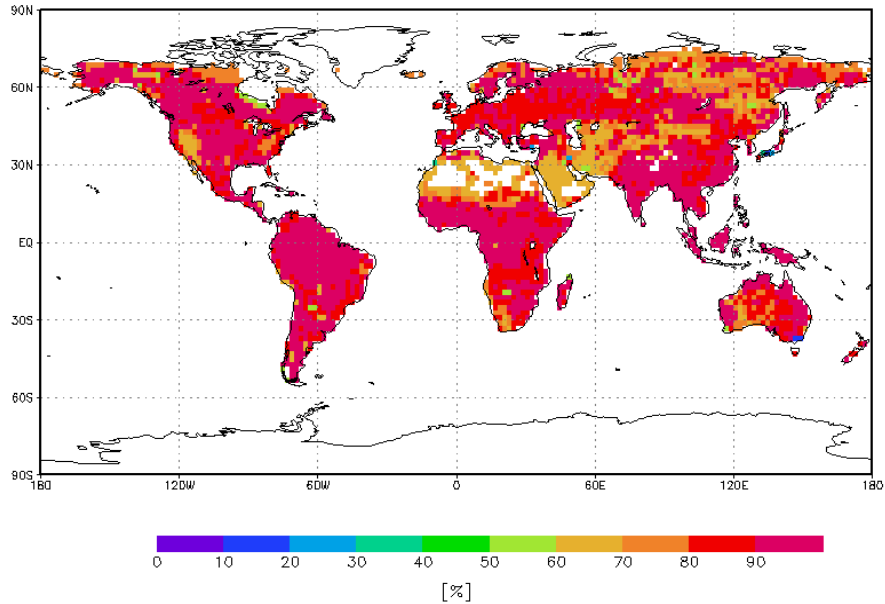
x_{po} : Posterior parameters

C_{po} : Posterior uncertainties

$y(x)$: Target quantity

σ_y : Its uncertainty

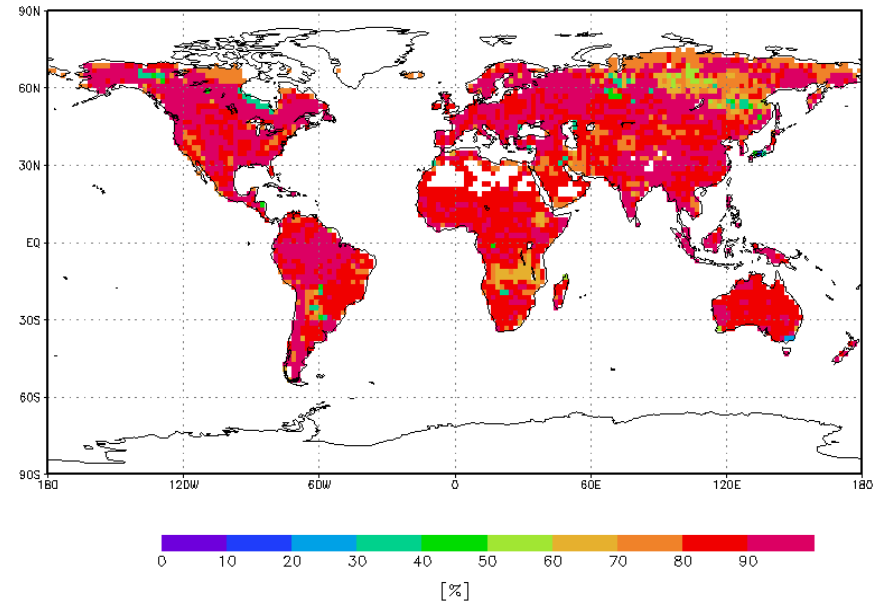
BESD biased vs flask samples



GrADS: COLA/IGES

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**BESD (Reuter et al., 2001)
one year**

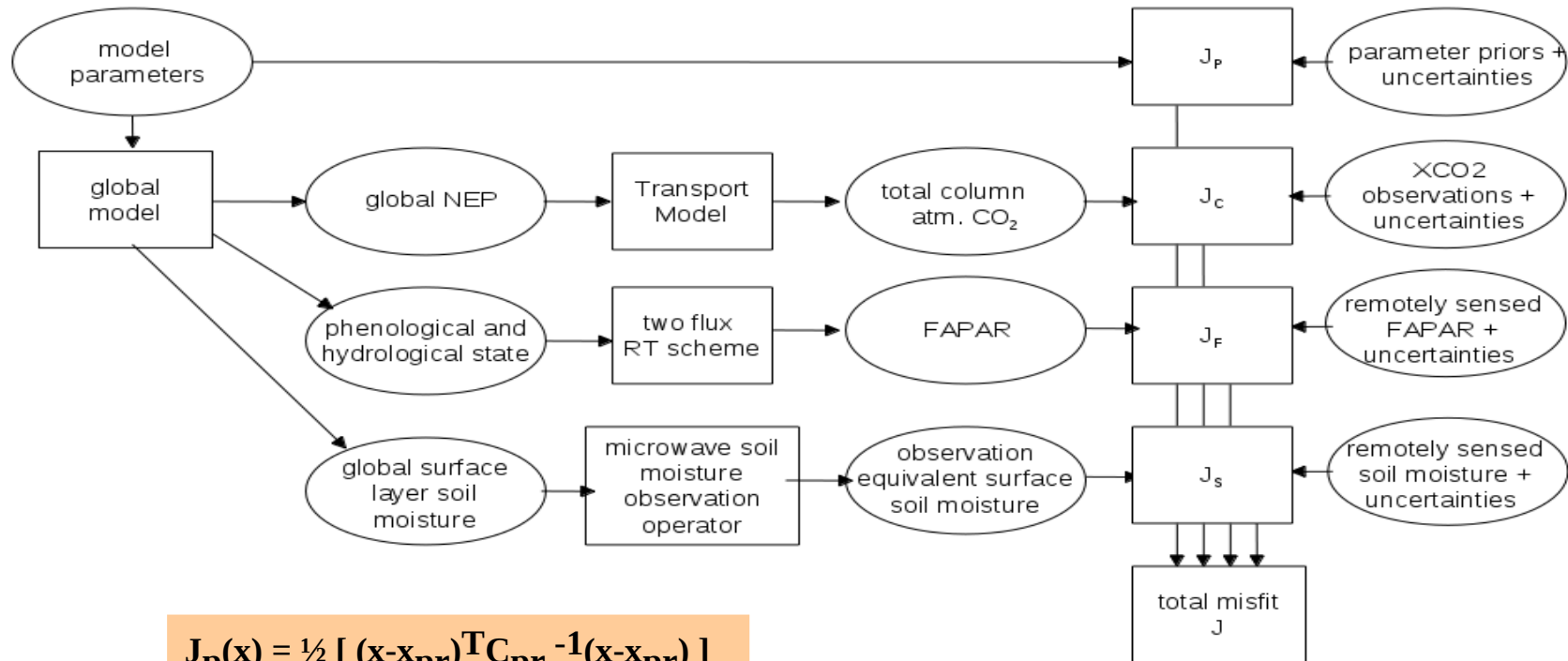


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**flask samples
20 years**

CCDAS can integrate multiple data streams



$$J_p(x) = \frac{1}{2} [(x-x_{pr})^T C_{pr}^{-1} (x-x_{pr})]$$

$$J_d(x) = \frac{1}{2} [(M(x)-d)^T C_d^{-1} (M(x)-d)]$$

Consistent Assimilation :

- all data streams jointly
- in a single long assimilation window