IMPLEMENTATION OF 4D-VAR WITH RATIO METHOD FOR METHANE AND CARBON DIOXIDE FLUXES

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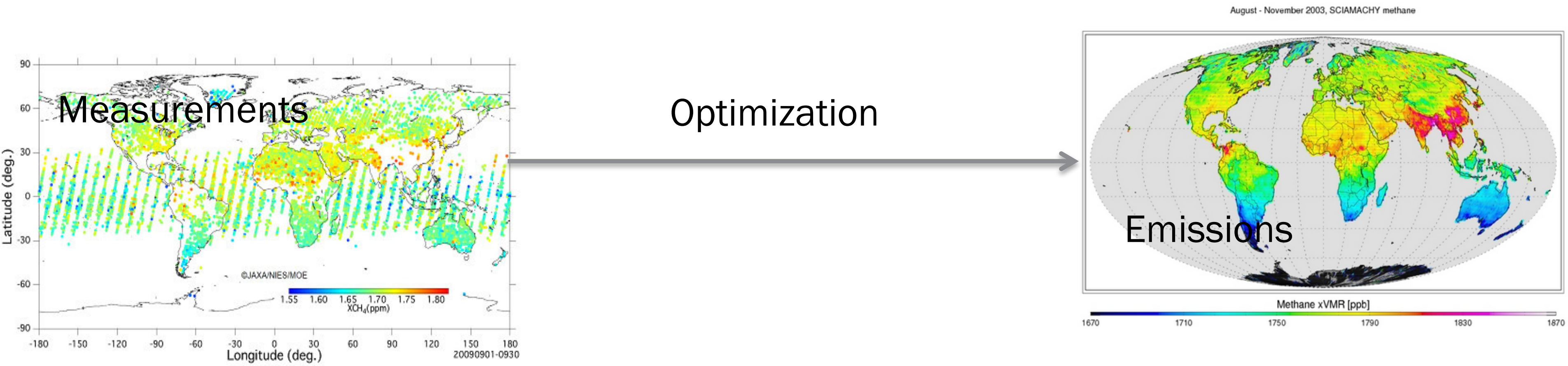
Measurements
Latitude (deg.)
Longitude (deg.)
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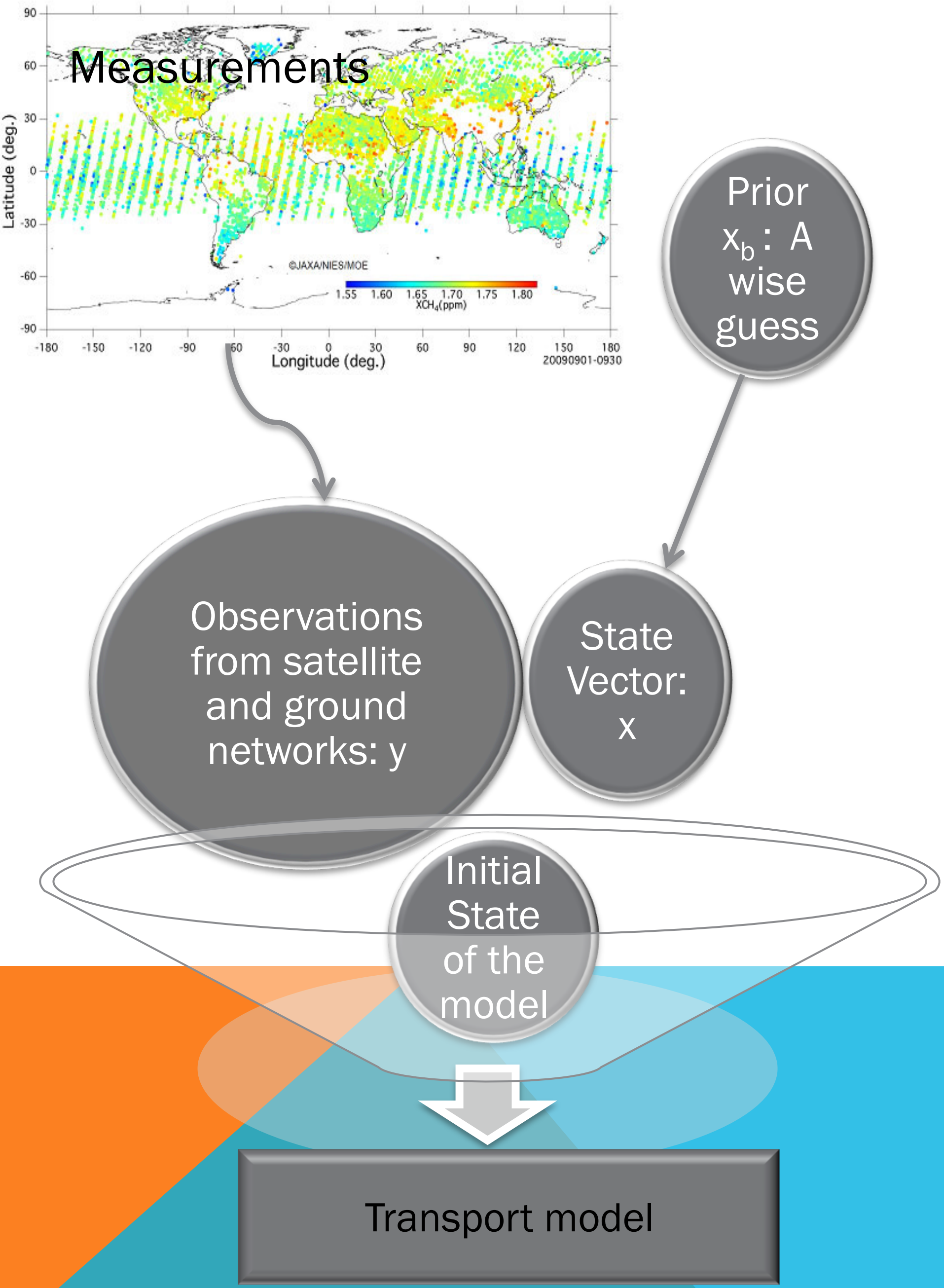
XCH4(ppm)
20090901-0930
Optimization
August - November 2003, SCIAMACHY methane
Emissions
Methane xVMR [ppb]



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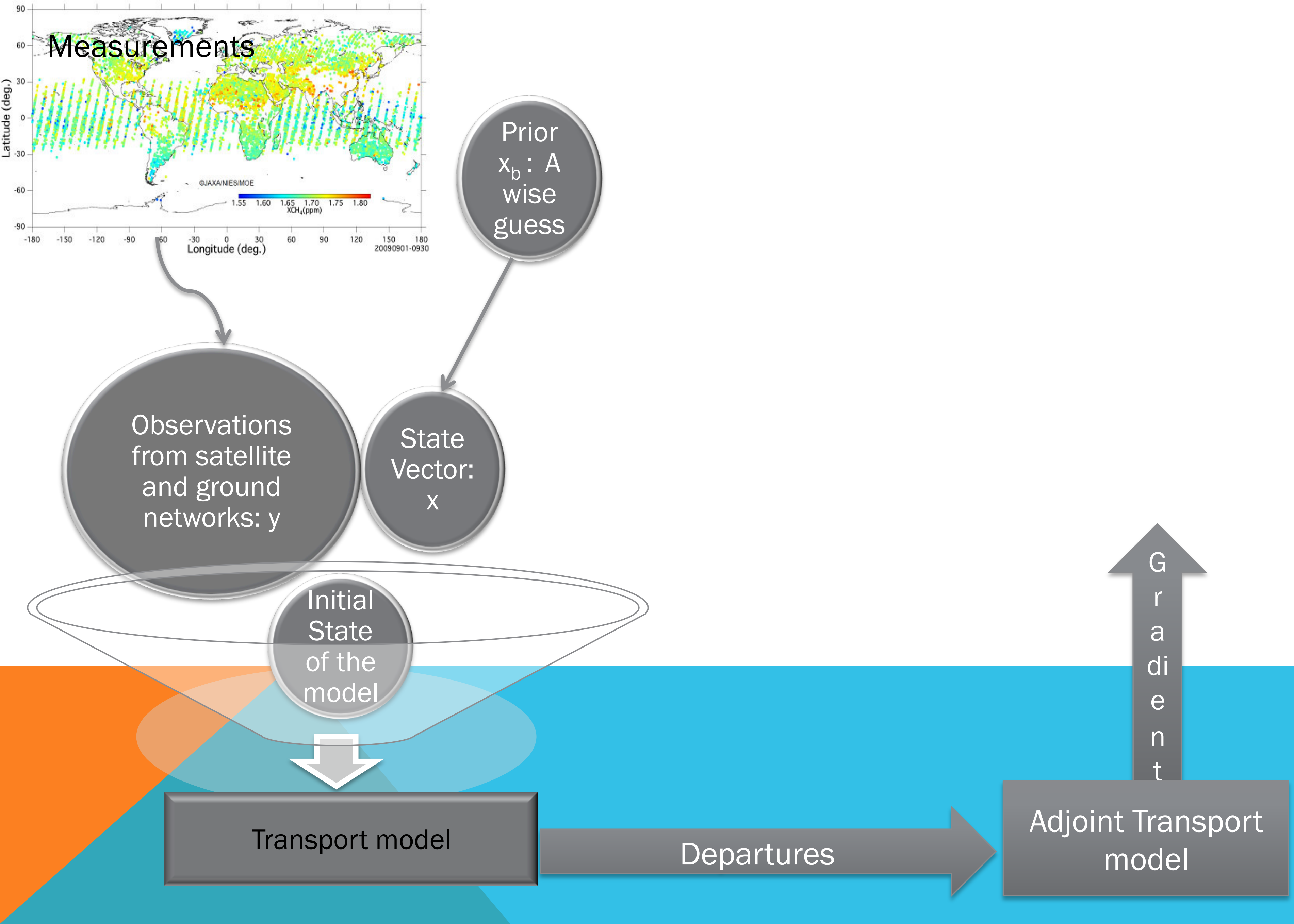
XCH4(ppm)
20090901-0930
Prior x_b : A wise guess
Observations from satellite and ground networks: y
State Vector: x
Initial State of the model
Transport model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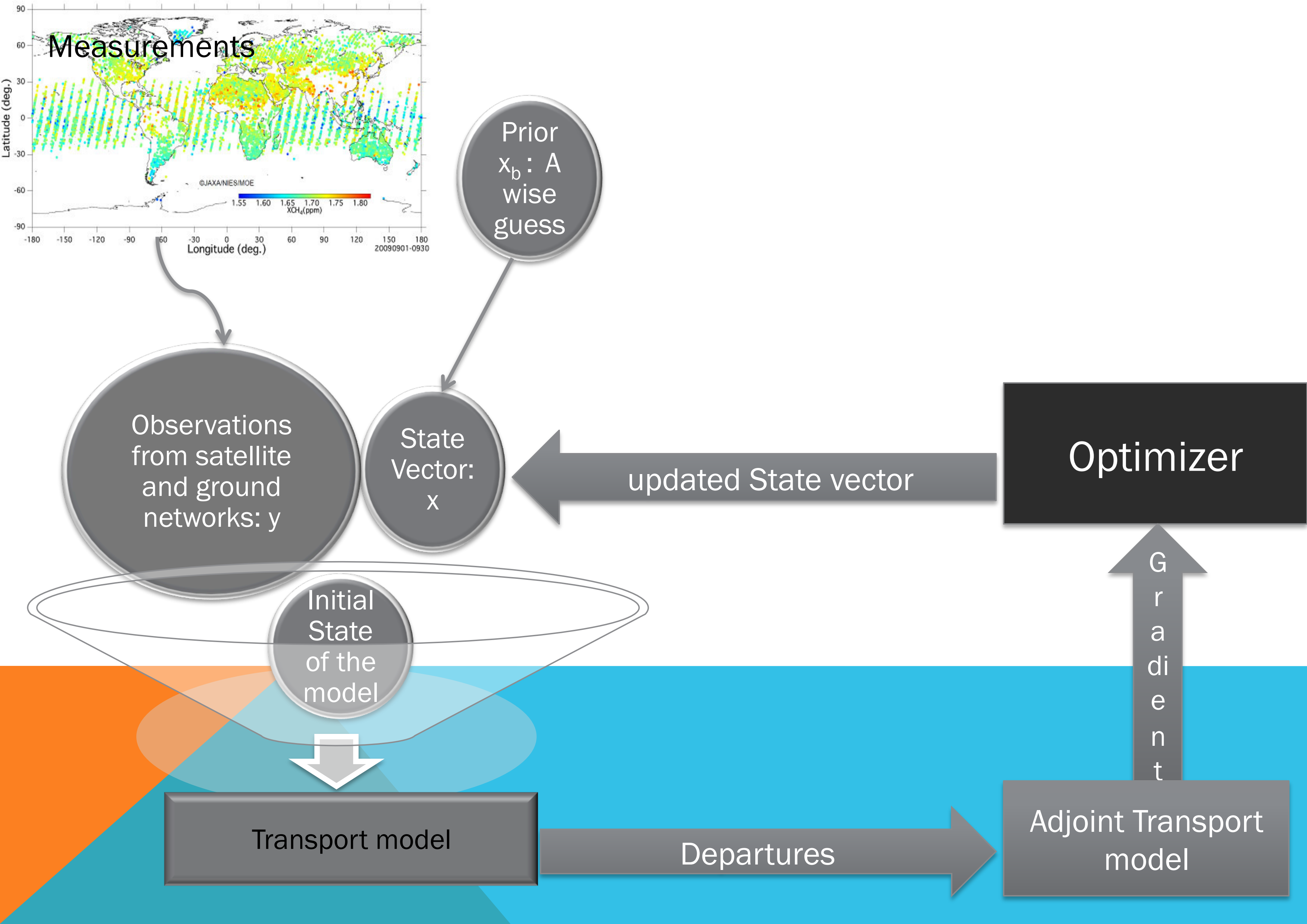
Initial State of the model
Transport model
Departures
Adjoint Transport model
Gradient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Prior
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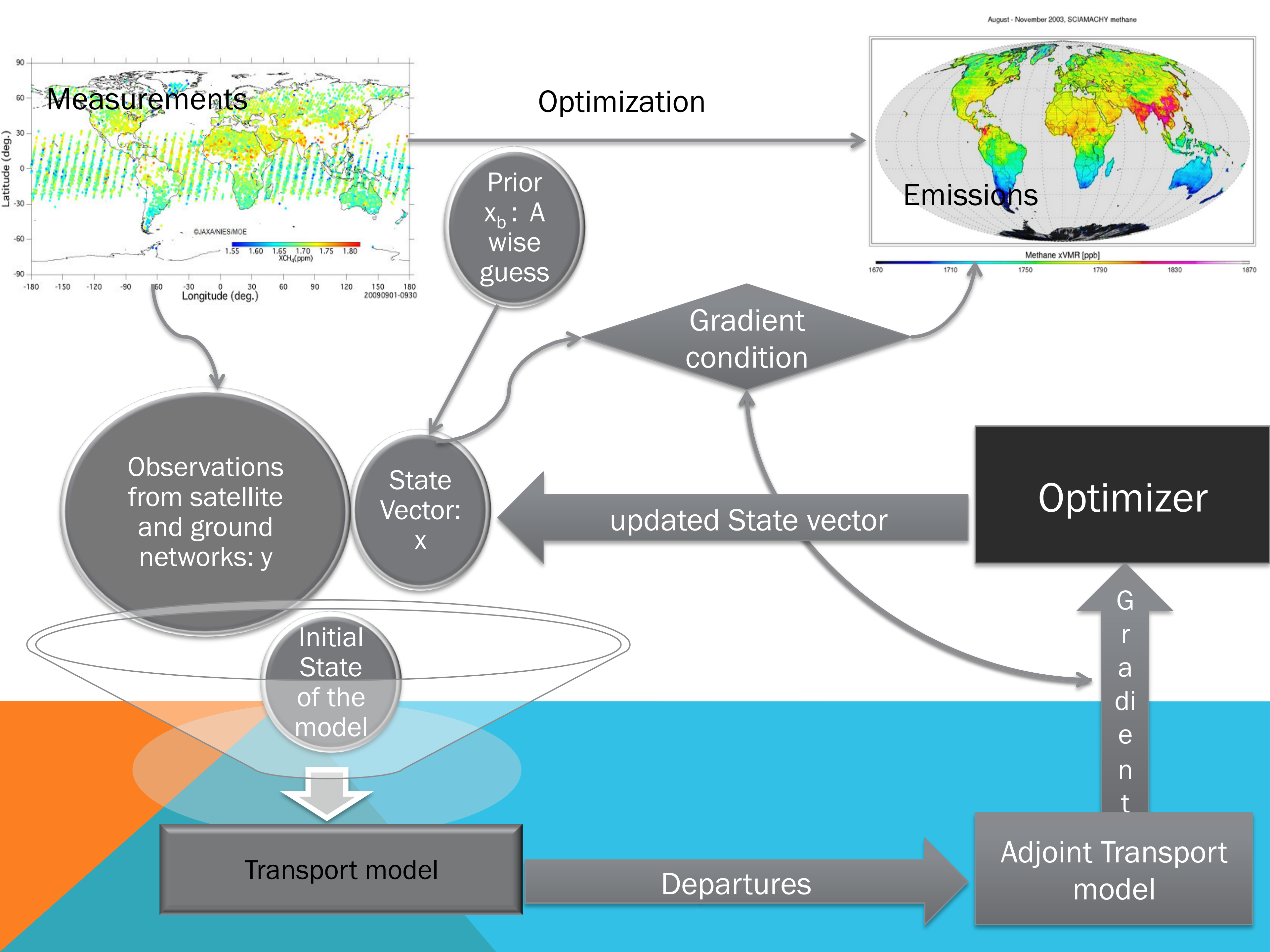
Observations from satellite and ground networks: y
State Vector: x
updated State vector
Optimizer
Gradient
Initial State of the model
Transport model
Departures
Adjoint Transport model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Methane xVMR [ppb]
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Gradient condition
Observations from satellite and ground networks: y
State Vector: x
updated State vector
Optimizer
Gradient
Initial State of the model
Transport model
Departures
Adjoint Transport model

OPTIMIZATION

$$\mathbf{J}(\mathbf{x_o}) = \mathbf{J^b}(\mathbf{x_o}) + \mathbf{J^o}(\mathbf{x_o})$$

$$\mathbf{J^b}(\mathbf{x_o}) = (\mathbf{x_o} - \mathbf{x_o^b})^\mathbf{T}\mathbf{B}^{-1}(\mathbf{x_o} - \mathbf{x_o^b})$$

$$\mathbf{J^o}(\mathbf{x_o}) = \sum_{\mathbf{i=0}}^{\mathbf{n}}(\mathbf{y_i^o} - \mathbf{H_i}(\mathbf{x_i}))^\mathbf{T}\mathbf{R_i}^{-1}(\mathbf{y_i^o} - \mathbf{H_i}(\mathbf{x_i}))$$

where, H is an atmospheric transport model sampled according to the measurements y and forced by the sources and sinks x.

$$\mathbf{x} = \begin{bmatrix}\delta(CO_2)_1 & \delta(CO_2)_2 & \dots & \delta(CH_4)_1 & \delta(CH_4)_2 & \dots\end{bmatrix}$$

The state vector **x** is comprised of the fluxes (represented by *δ* in the equation) and measurements **y** comprises of the ratio of measurements of mixing ratio of CO_2 and CH_4.

$$\mathbf{y} = \begin{bmatrix}\frac{[CO_2]_1}{[CH_4]_1} & \frac{[CO_2]_2}{[CH_4]_2} & \dots\end{bmatrix}$$

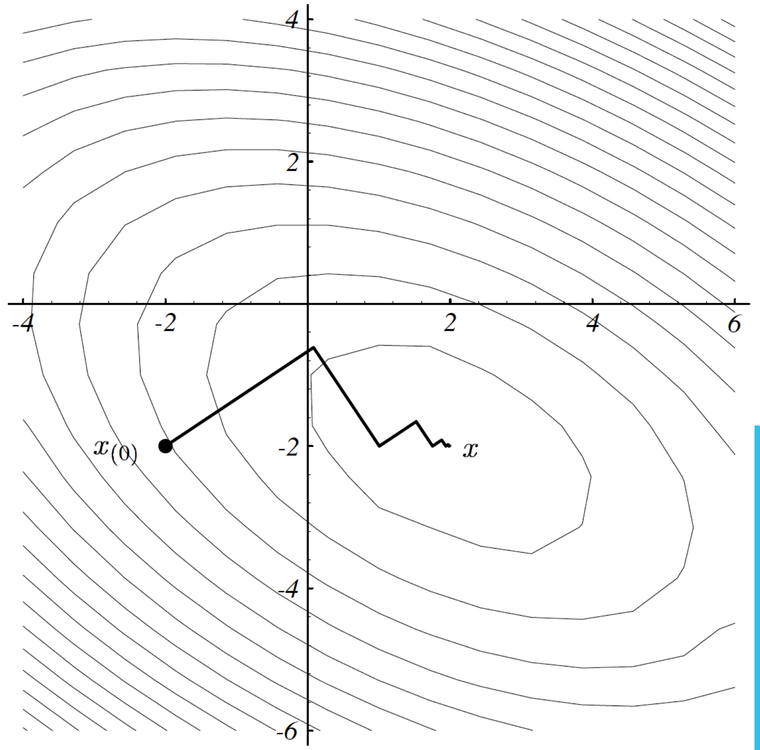
OPTIMIZATION

The minimization of the cost function involves iteratively calculating the **gradient** of the cost function to decide the direction of decent of state vector.

$$\nabla \mathbf{J}(\mathbf{x_0}) = \mathbf{2B^{-1}}(\mathbf{x_o} - \mathbf{x_o^b}) - \mathbf{2}\sum \mathbf{H_i^T}\left[\mathbf{y_i^0} - \mathbf{H_i}(\mathbf{x_0})\right]$$

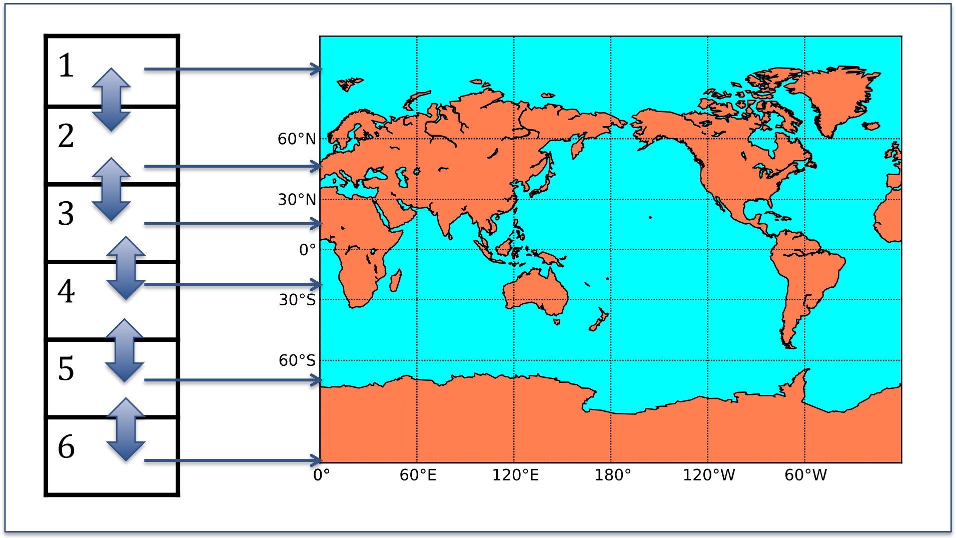
The aim is to minimize the gradient to a desired value, depending upon efficiency of optimization subroutine and the complexity of the problem. When working with satellite data generally the **state vector is in order of 10000.**

We look for gradient minimization of **1000**, typically achieved in **50- 100 iterations.**



TOY MODEL SETUP

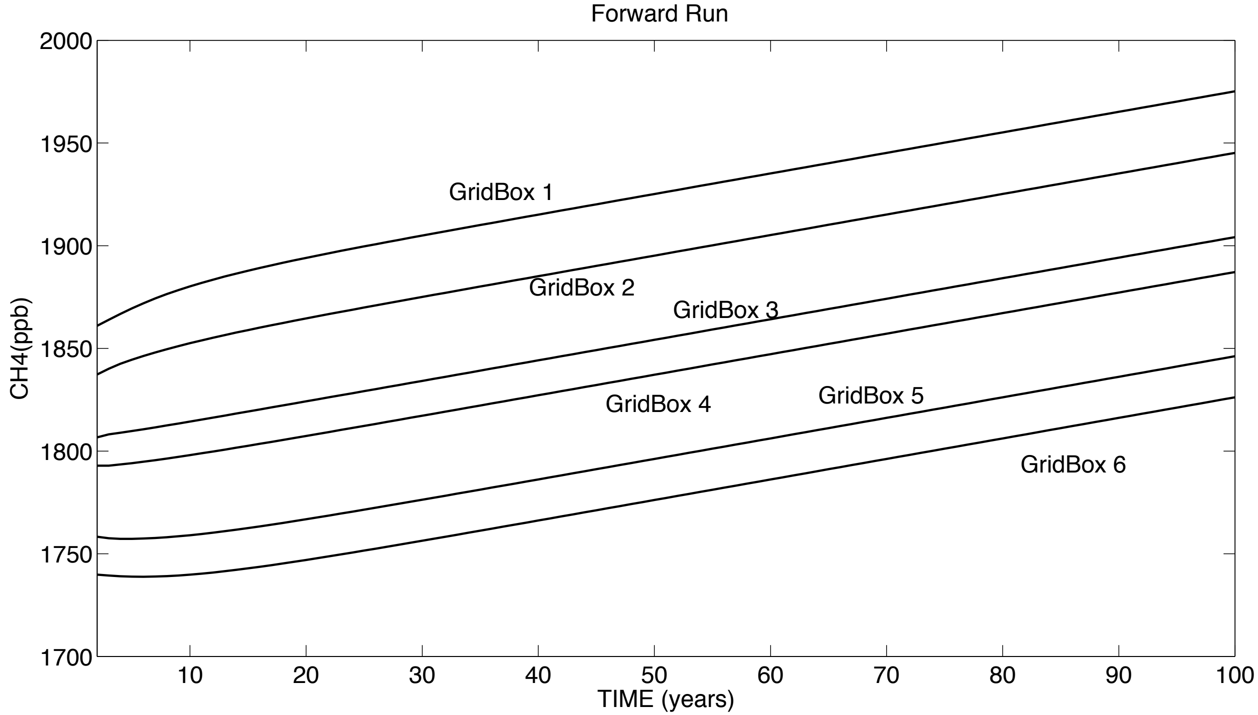
- Toy Model : Simplifies one dimensional transport model.
- 6 grid boxes, one for each climatic zone.
- Prior: The emissions and sink from each zone was taken by integrating the flux values of a resolution of 1° x 1° over each zone.
- Two tracers CO_2 and CH_4 are optimized simultaneously
- Time step: 1 year



FORWARD TRANSPORT MODEL

The transport model gives the mixing ratio of tracers after i timesteps.

$$\mathbf{C_f^k} = \mathbf{C_i^k} + \mathbf{S^K} + \sum_{\mathbf{adjacentzones}} \alpha(\mathbf{\Delta C})_{\mathbf{n}}^{\mathbf{k}}$$



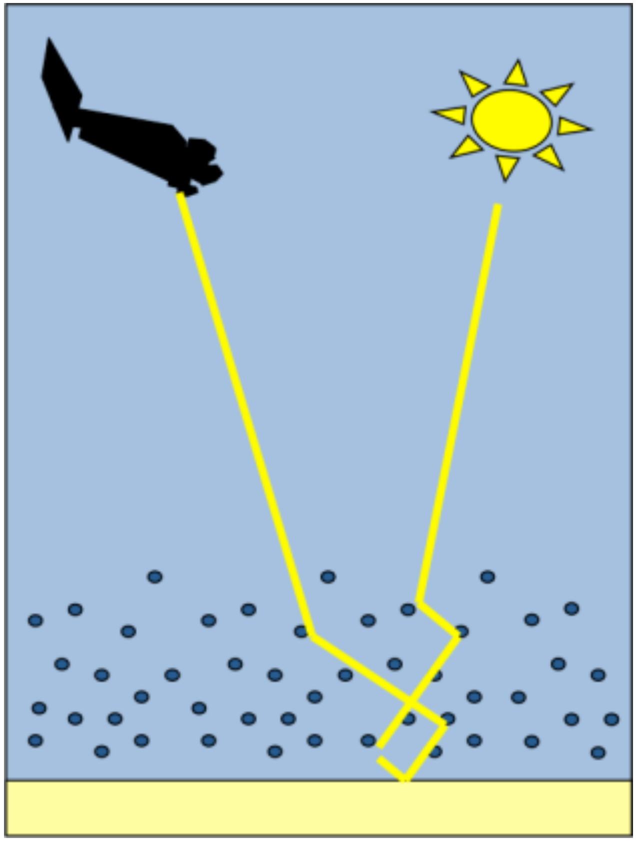
OBSERVATION OPERATOR

- Input : state vector containing concentration of $[CO_2]$ and $[CH_4]$

- Output: the ratio of the $\frac{[CH_4]}{[CO_2]}$

Optimization WRT to this Ratio:

Cancels out the error due **scattering affect** in the atmosphere, hopefully



ADJOINT CODING

- Observation operator is non-linear
- Matrix form not possible, we write a subroutine:
- Adjoint of this subroutine *H*, given by

The Forward Model (H)

```
do i=1,n
   x_ratio(i)= xch4(i)/xco2(i)
 end do
```

The Adjoint Model (H^*)

```
do i = n, 1, -1
      adj_xch4(i)=adj_xch4(i)+ adj_x_ratio(i)//xco2(i)
      adj_xco2(i)= adj_xco2(i) - adj_x_ratio(i)* xch4(i)/(xco2(i))**2
      adj_x_ratio(i)= adj_x_ratio(i)
 end do
```

Adjoint test

$$< H dx, dy >=< dx, H^t dy >$$

RECENTLY IMPLEMENTED FOR TM5

Gradient test

$$\lim_{h \to 0} \left(\frac{H(x+h) - H(x)}{\mathbf{H} h} \right) = 1$$

OPTIMIZATION SUBROUTINES

CONGRAD : Conjugate gradient method

- Pros : most efficient in term of no of iterations needed. Hessian is also calculated which gives posterior error covariance
- Cons: Not good for non linear case.

M1QN3: Quasi Newton method

- Pros : can be used for Non-linear case.
- Con: hessian is not calculated and computationally more demanding.

Good for our case !!!!!!!!!!!

COMPARISON SETUP

Direct Optimization

$$[CH_4]_{obser} = \frac{[CH_4]_{init}}{[CO_2]_{init}} \times [CO_2]_{obser}$$

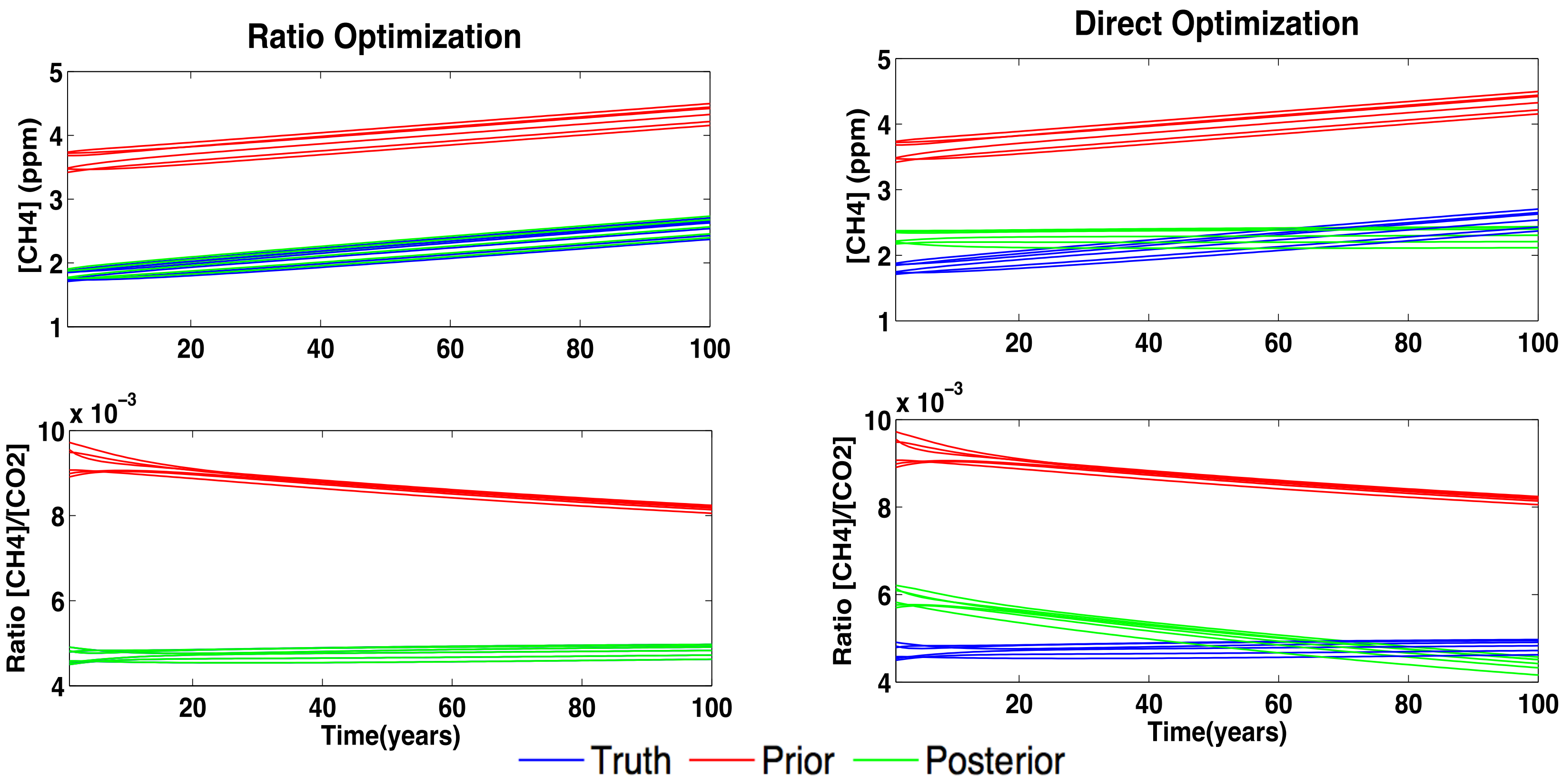
- Linear observation operator
- Congrad subroutine is used as the optimization subroutine

Ratio Optimization

$$\frac{[CH_4]_{init}}{[CO_2]_{init}}$$

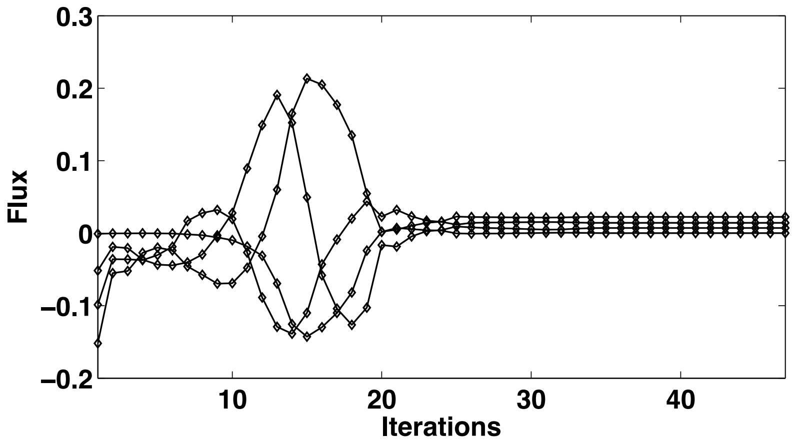
- Nonlinear observation operator
- We use m1qn3 (Gilbert et al., 2009) as our optimization subroutine instead.

RESULTS


Ratio Optimization
Direct Optimization
[CH4] (ppm)
Ratio [CH4]/[CO2]
x 10^-3
Time(years)
Truth
Prior
Posterior

IS IT WORTH THE TROUBLE?

	Ratio	Direct
Norm Flux diff (ppm)	4.329e-5	1.678e-3
Iterations performed	47	16
Gradient norm reduction	3.8 e-10	0.5299 -13

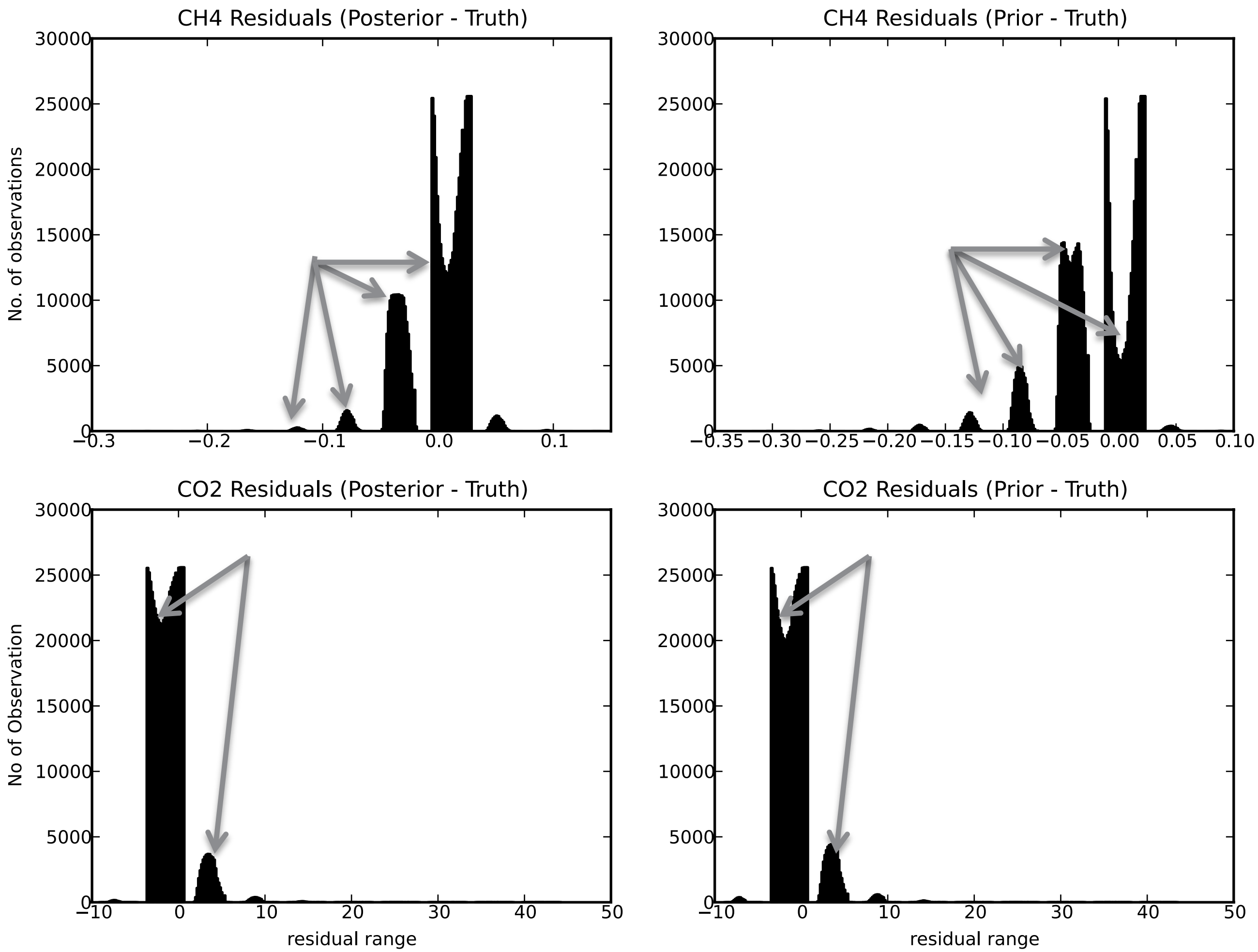


IMPLEMENTATION ON TM5

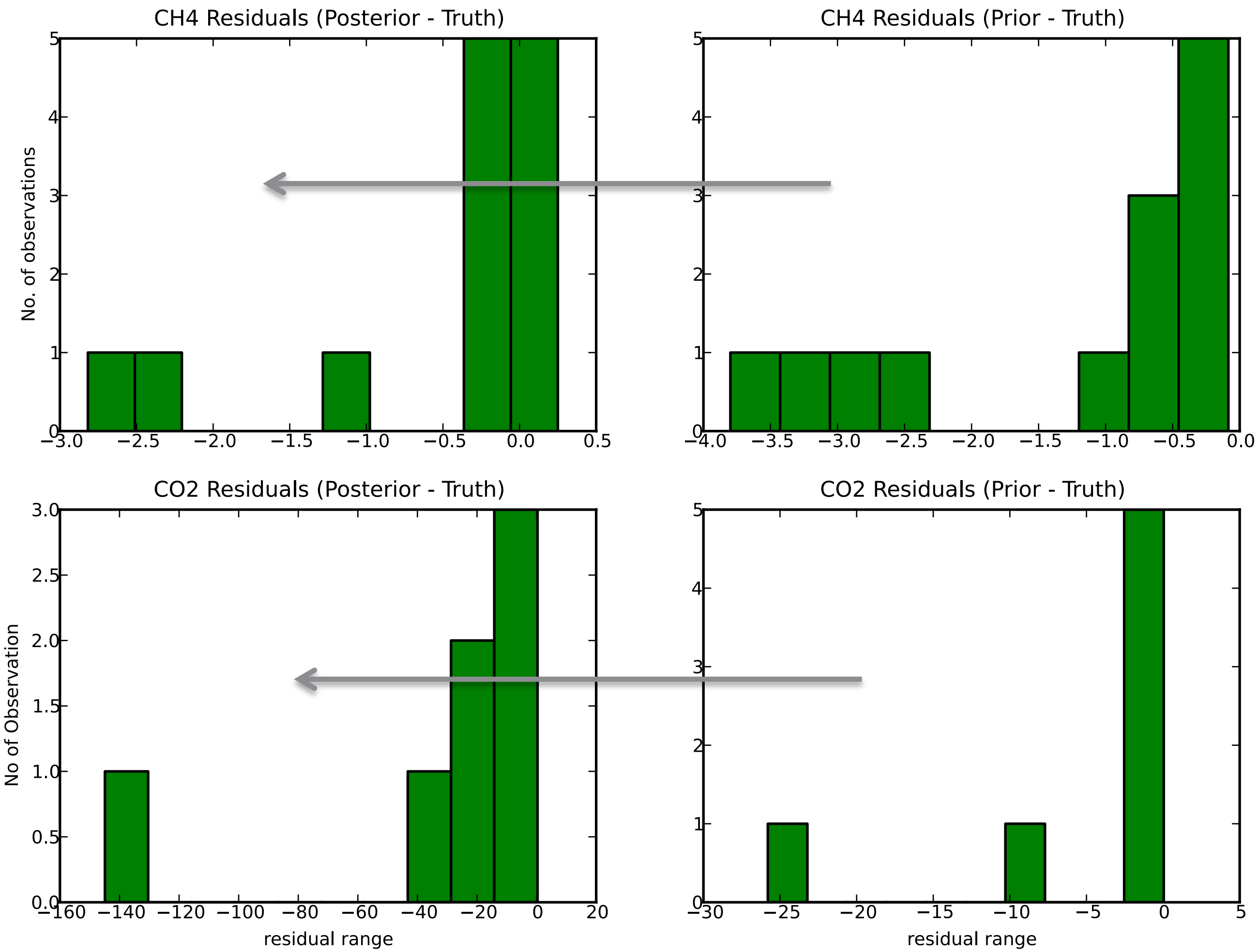
- The TM5 model is a 3D atmospheric chemistry-transport ZOOM model.
- It allows the definition of arbitrary zoom regions, which are 2-way nested into the global model.
- My aim is to make a test setup with can compare the performance of the ratio approach with tradition approach using TM5 as transport .

ONE MONTH RUN (TM5)

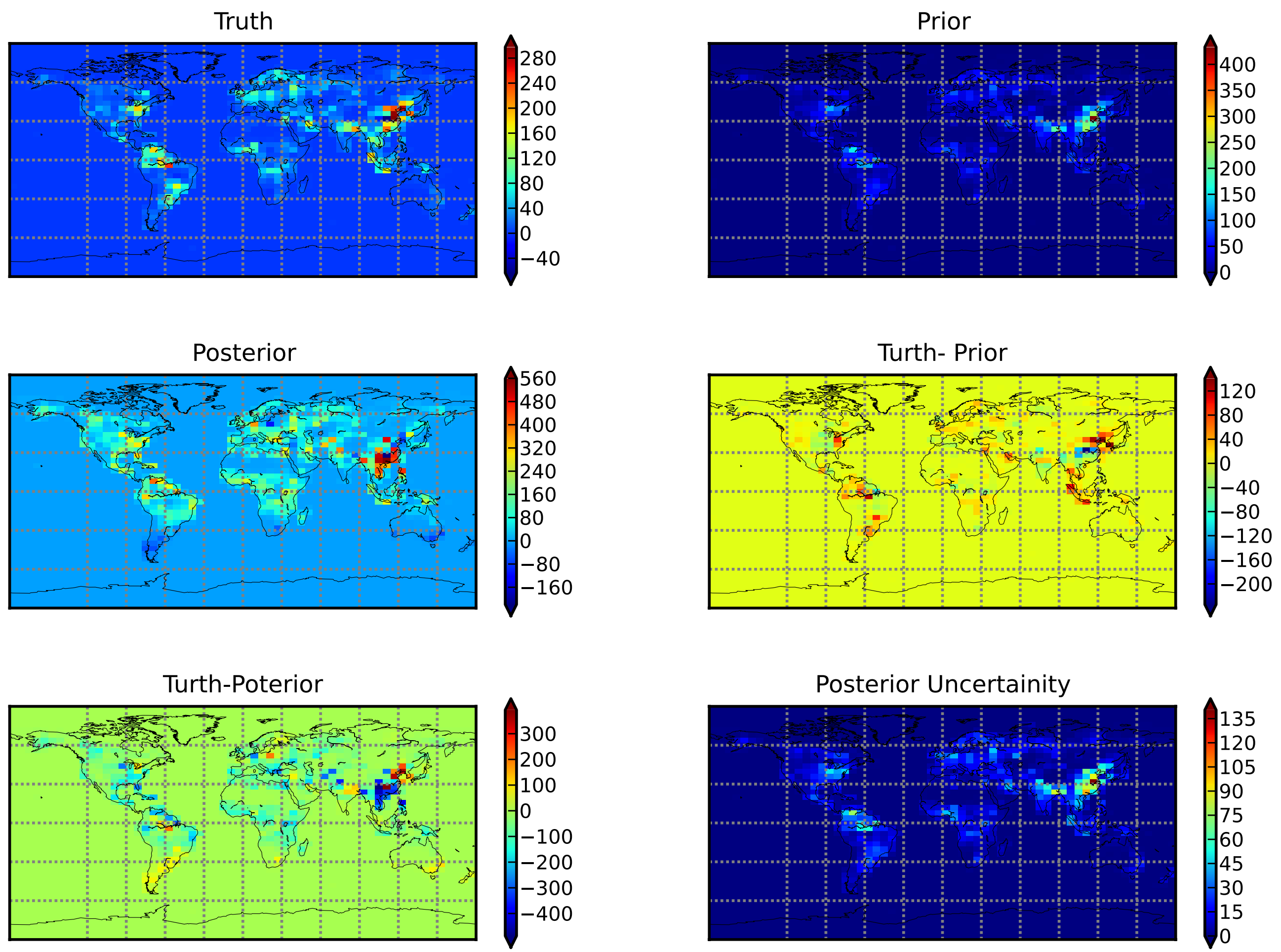
The simultaneous optimization for CO_2 and CH_4 is implemented.



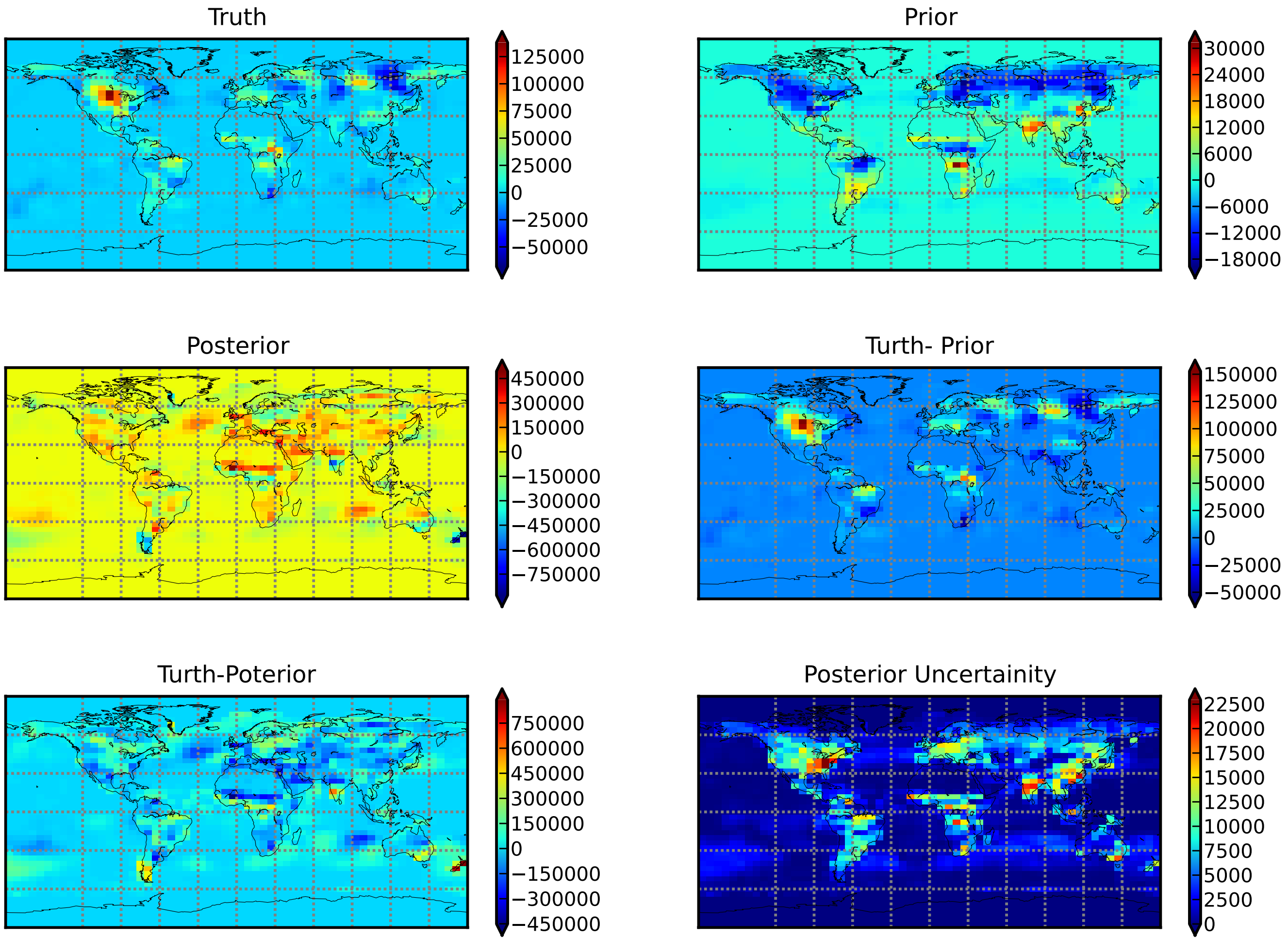
POINT OBSERVATIONS



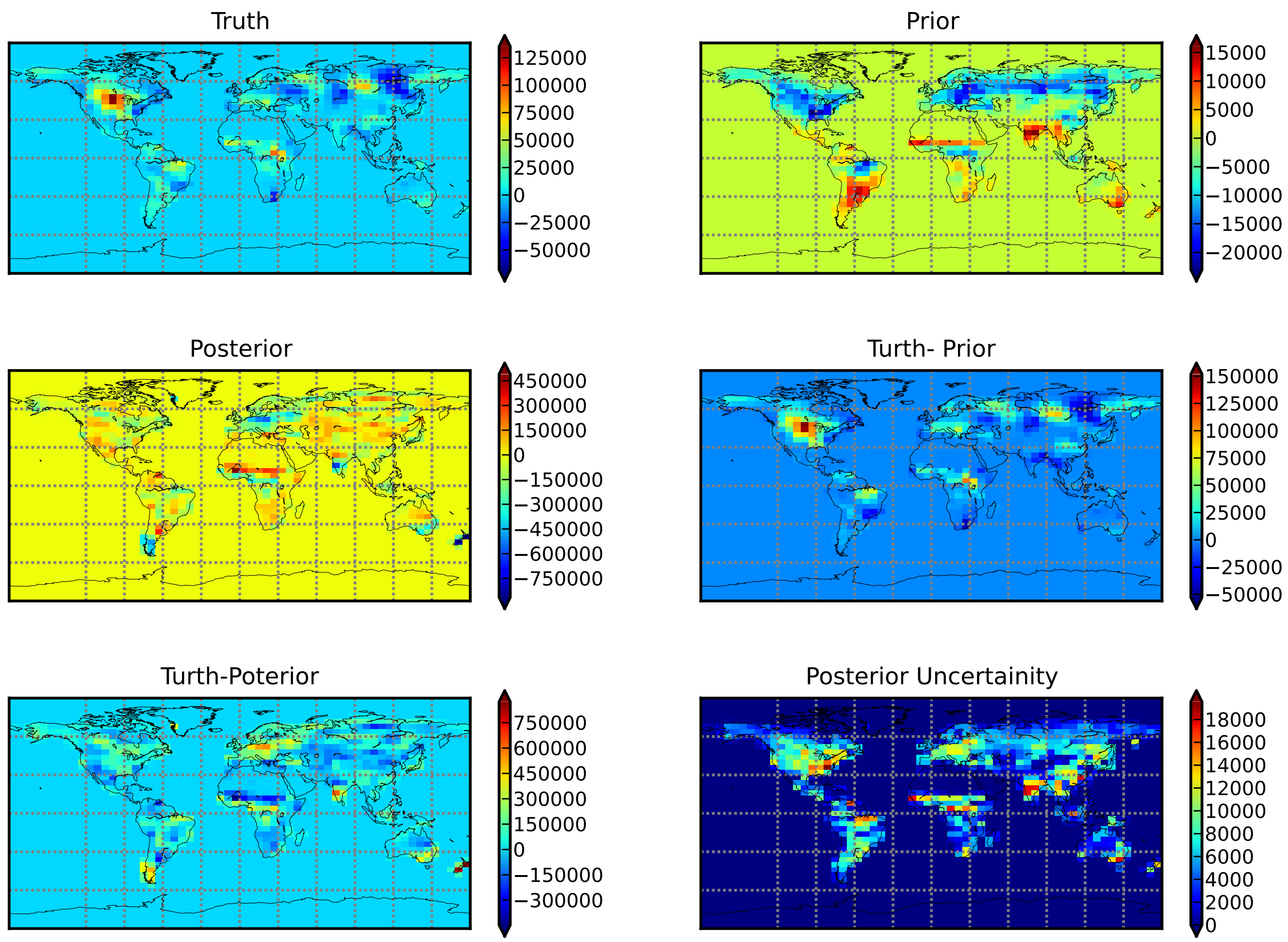
CH4


Truth
280
240
200
160
120
80
40
0
−40
Prior
400
350
300
250
200
150
100
50
0
Posterior
560
480
400
320
240
160
80
0
−80
−160
Turth- Prior
120
80
40
0
−40
−80
−120
−160
−200
Turth-Poterior
300
200
100
0
−100
−200
−300
−400
Posterior Uncertainity
135
120
105
90
75
60
45
30
15
0

CO2


Truth
125000
100000
75000
50000
25000
0
−25000
−50000
Prior
30000
24000
18000
12000
6000
0
−6000
−12000
−18000
Posterior
450000
300000
150000
0
−150000
−300000
−450000
−600000
−750000
Turth- Prior
150000
125000
100000
75000
50000
25000
0
−25000
−50000
Turth-Poterior
750000
600000
450000
300000
150000
0
−150000
−300000
−450000
Posterior Uncertainity
22500
20000
17500
15000
12500
10000
7500
5000
2500
0

CO2 (BIOSPHERE FLUX)



CONCLUSION

- M1qn3 can solve the non-linear optimization problem for ratio measurements of CO_2 and CH_4
- Good solutions can be found in less than 15 iterations
- Compared to direct method, Ratio method is able to optimize the fluxes and concentrations more efficiently in Toy model Setup.

DANK U WEL……