

# Atmospheric Science Data Analysis Tools

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GRENE-Arctic

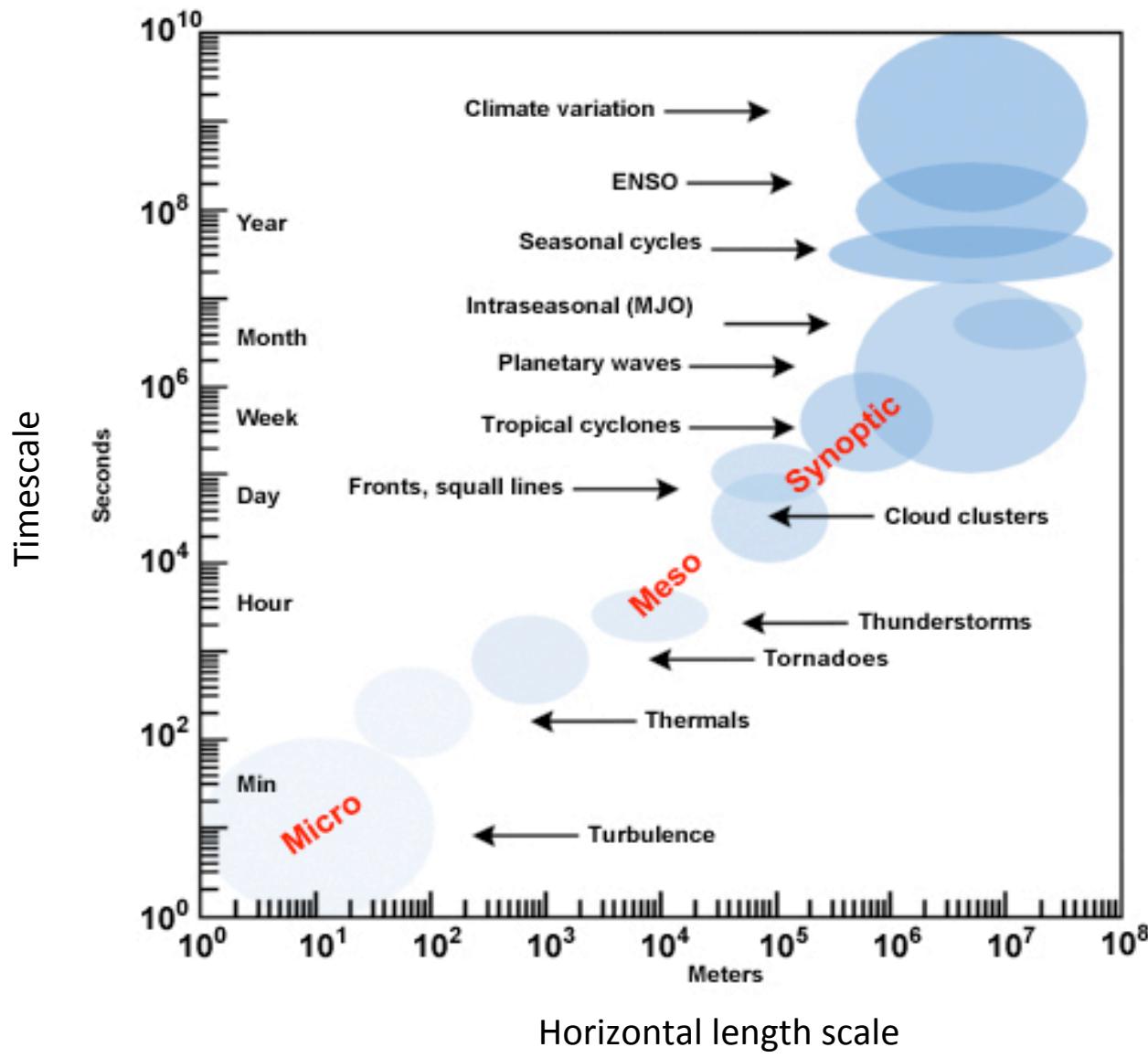


D E G C R

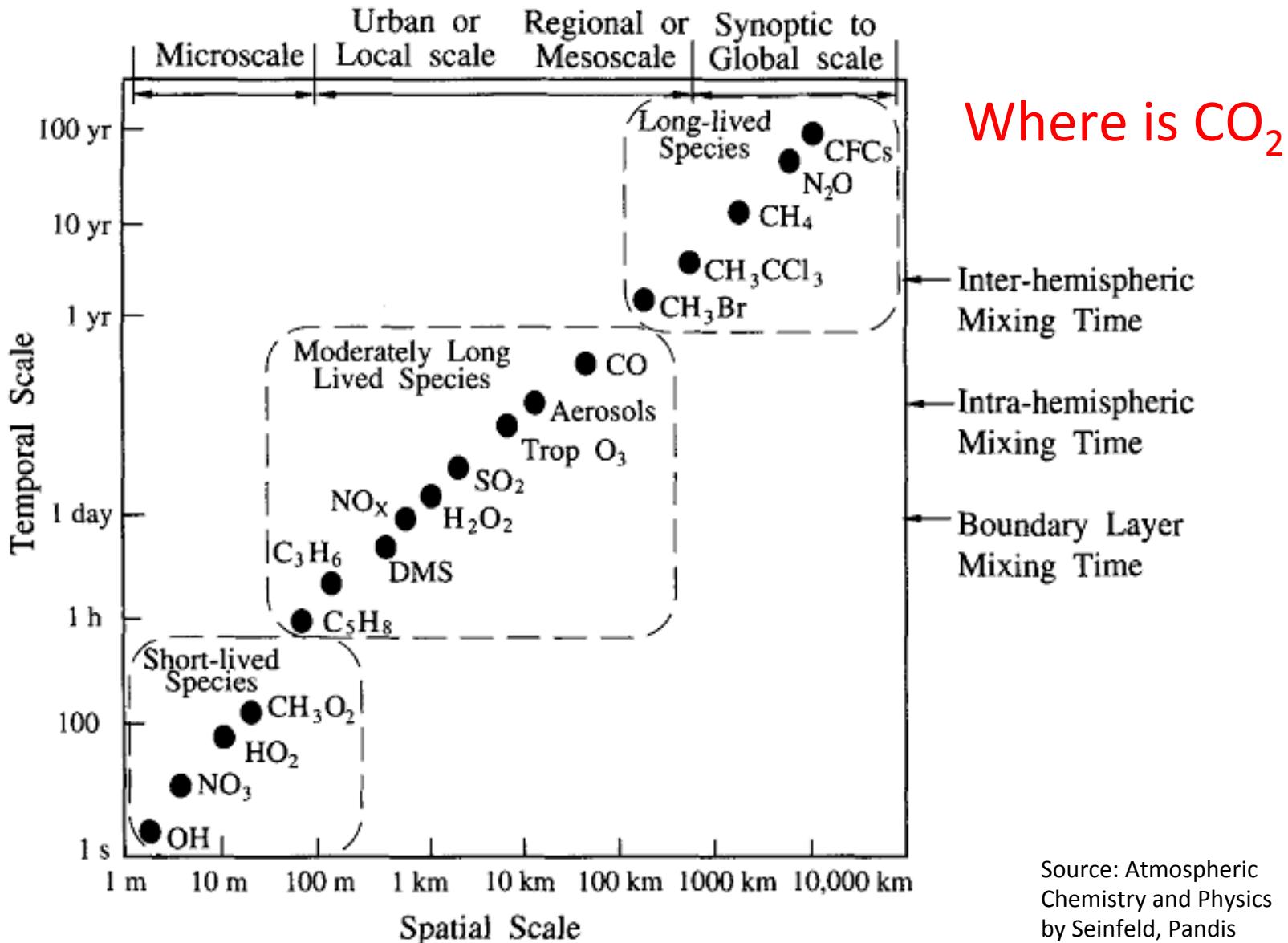
# Is there any universal tool for data analysis?

Year	Event	Research and tools adopted	
1992	Joined Ph. D.	Learned instrumentation, field campaigns, little data analysis, simple software (Fortran, SM graphics, LaTeX)	CNRS  CFCs, CH <sub>4</sub> , N <sub>2</sub> O 
1998	Joined IBM	No data, but model development and analysis (lots of Fortran, 5-dimensional data analysis, data compression technique-PCA, advanced visualisation, GrADS)	 Fortran: originally developed by IBM in the 1950s for scientific and engineering applications
2001	Joined JAMSTEC	Apply optimization tools (Simulated annealing), Bayesian inversion, data assimilation of GHGs; Microsoft Office	MM5, RAMS NCEP FNL
2005	Become older	Apply AGCM to GHG modelling – worked for people, with people. Learned a lot in terms of science	$C_S = (G^T C_D^{-1} G + C_{S_0}^{-1})^{-1}$ $S = S_0 + (G^T C_D^{-1} G + C_{S_0}^{-1})^{-1} G^T C_D^{-1} (D - D_{ACTM})$
2015	Today	Not so much research; hard to learn new tools!	That's probably is one of the reasons I am asked to teach!

# Scales of atmospheric dynamics

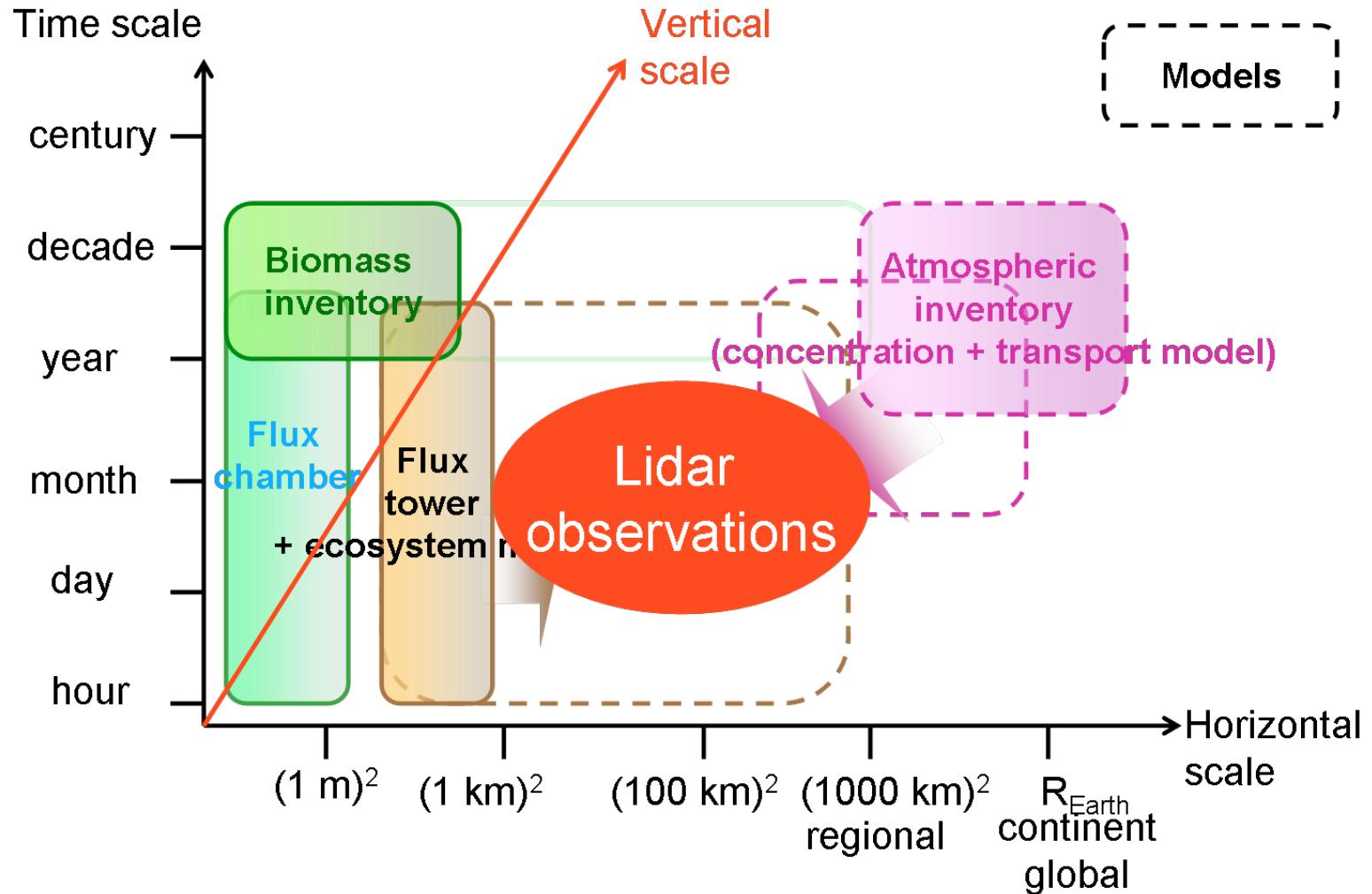


# Scales of atmospheric constituents



Source: Atmospheric  
Chemistry and Physics  
by Seinfeld, Pandis

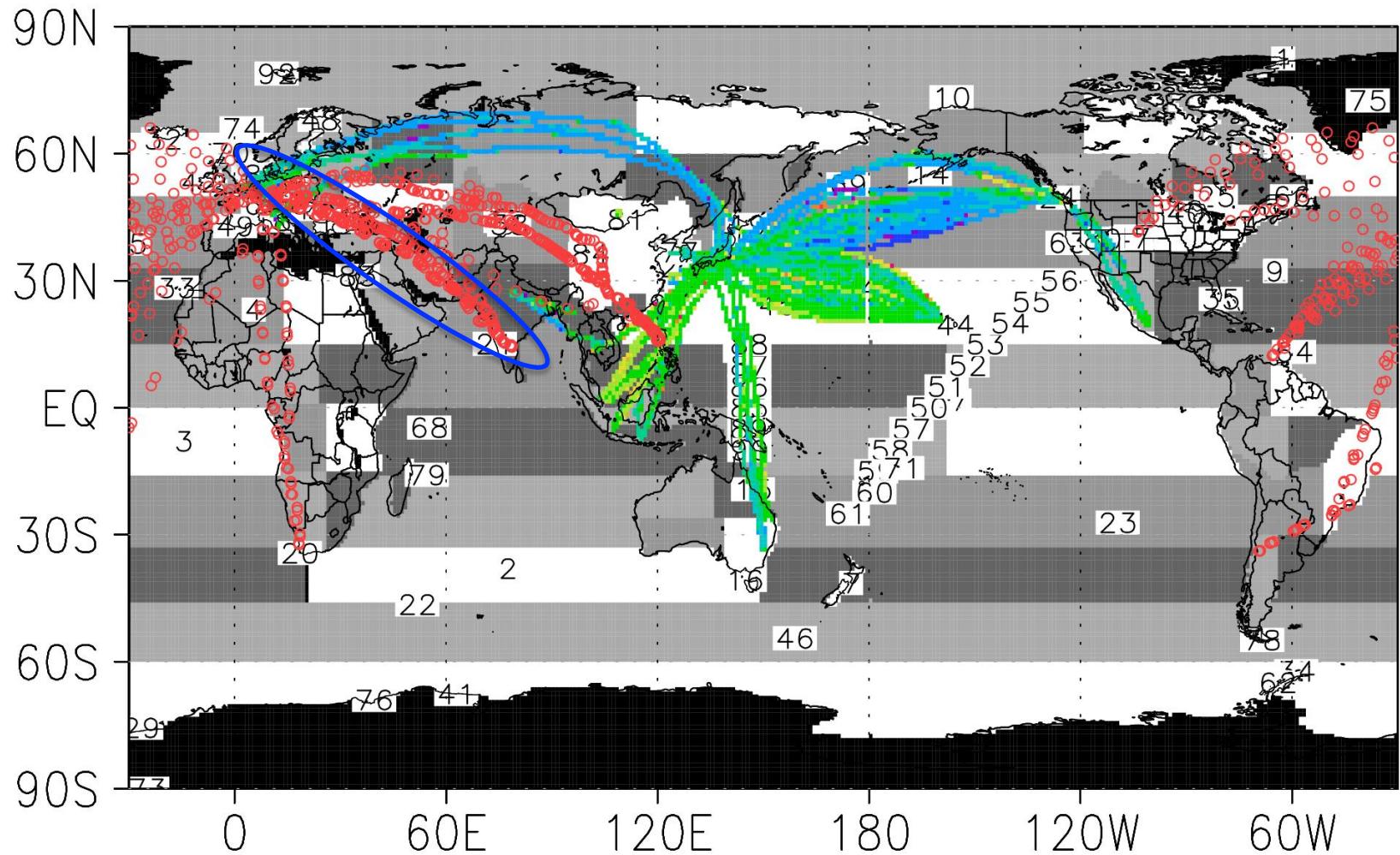
# Scale gaps between CO<sub>2</sub> Surface flux measurements/inventory and atmospheric measurements/models



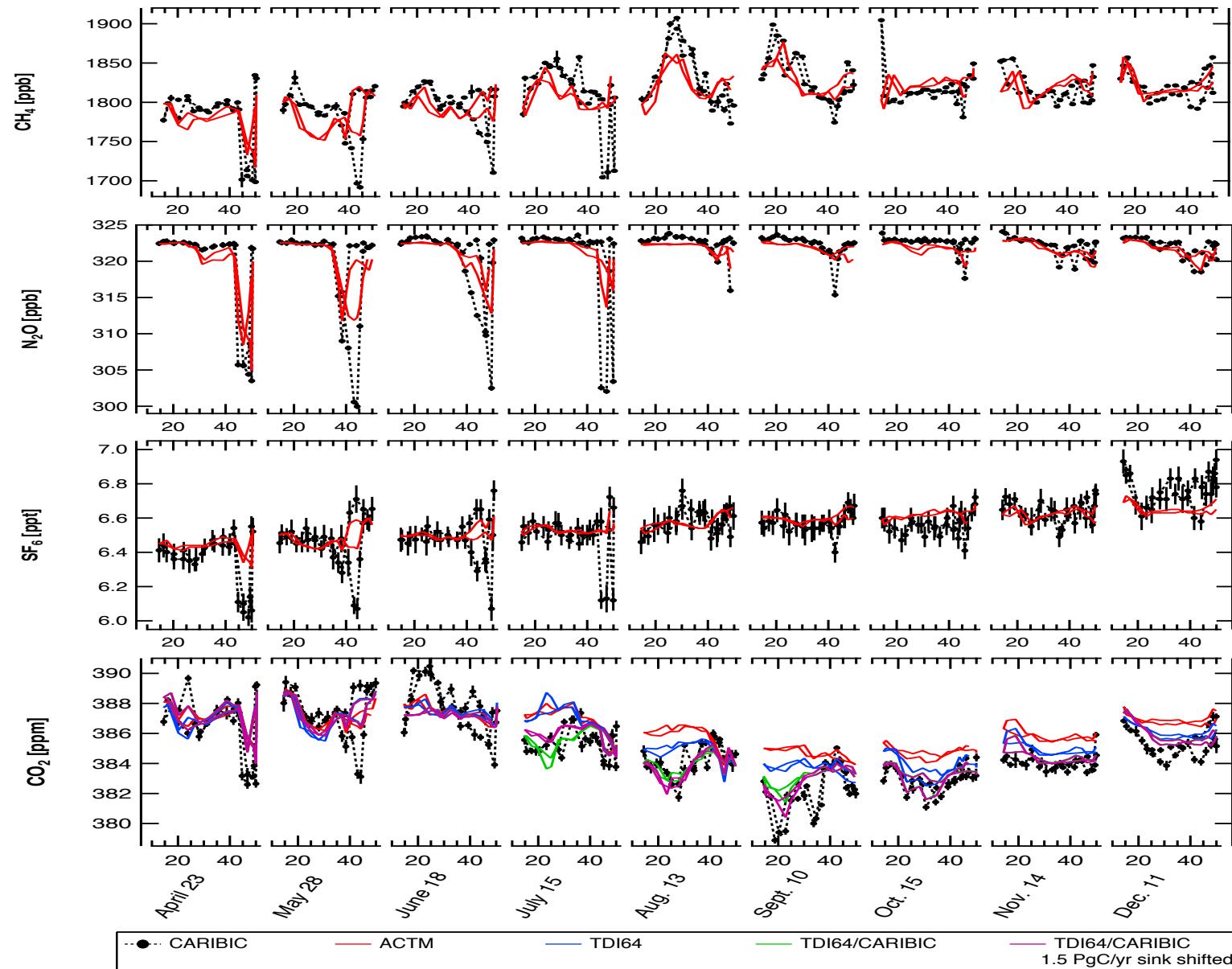
The Research Problem drives the development of tools

## **EXAMPLE ANALYSIS TOOLS**

# In situ (direct) measurement networks: (surface + CONTRAIL + CARIBIC)



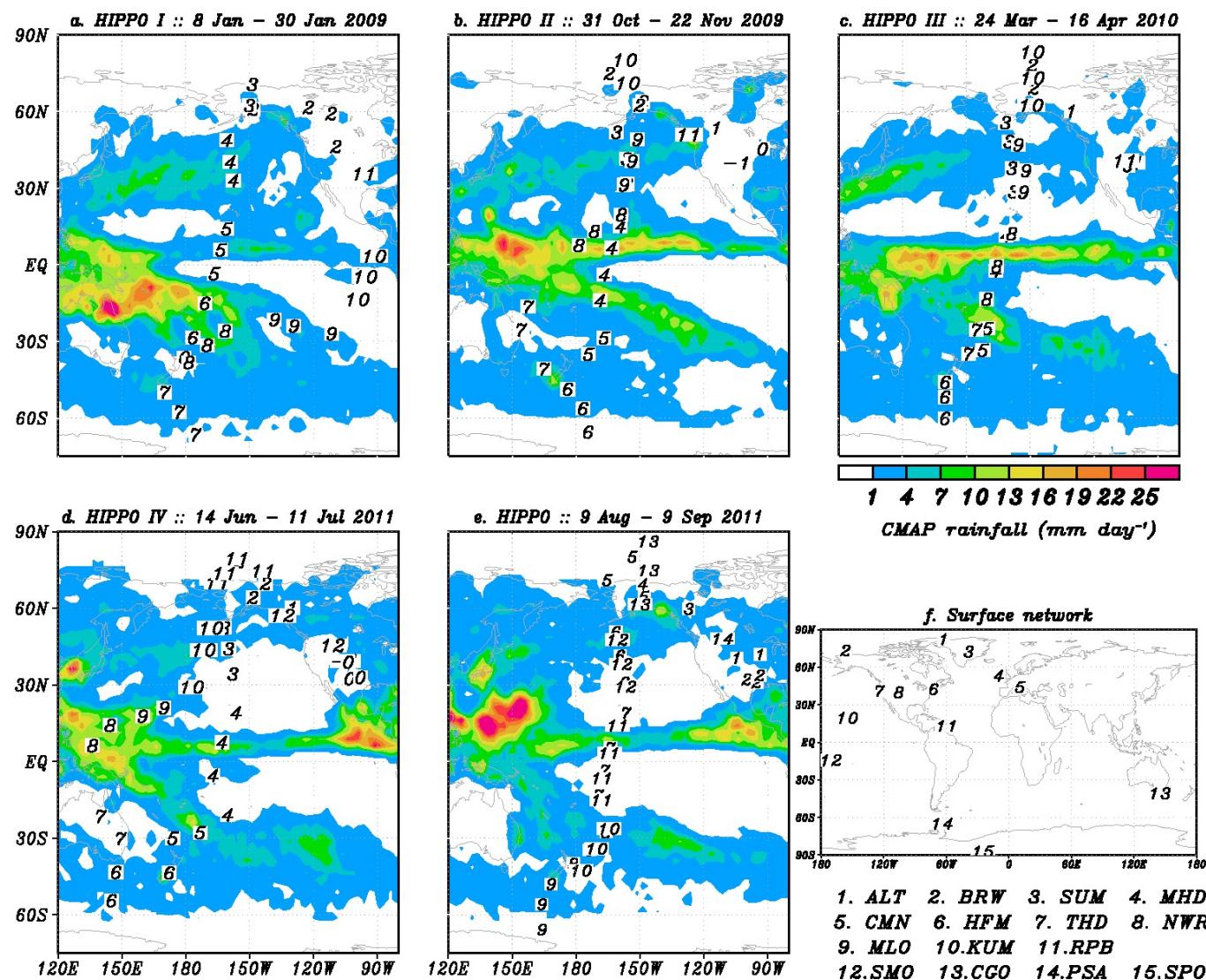
# CARIBIC measurements between Frankfurt and Chennai in comparison with ACTM simulations (an early view of the South Asian GHG fluxes)



Plot for  
Readers

Patra et al., ACP, 2011; plotted by Tanja Schuck using IGOR;  
Baker et al., ACAM, 2015

# Summary of HIPPO flights and CMAP rainfall, and surface network

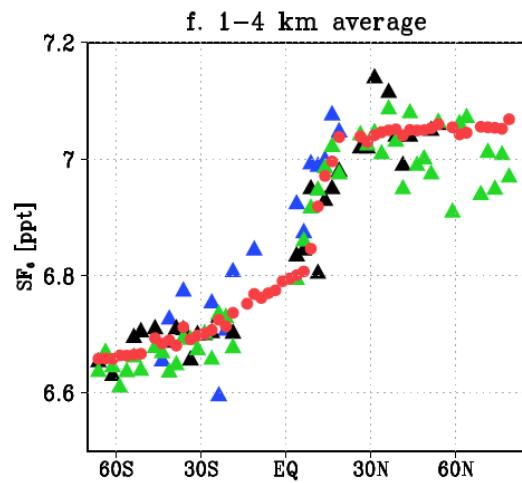
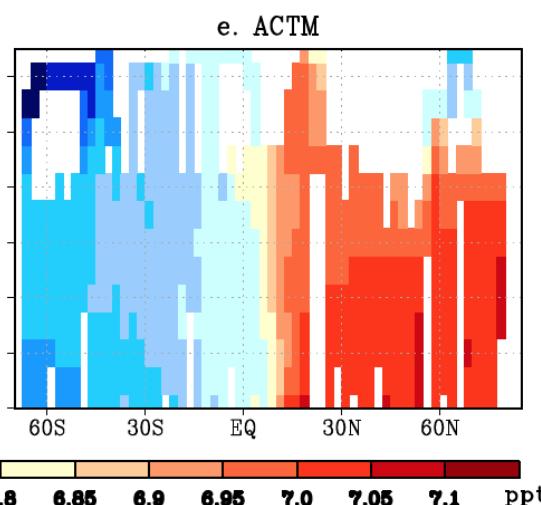
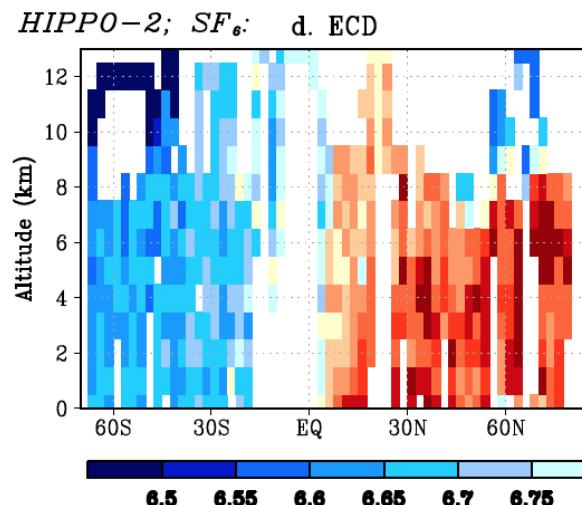
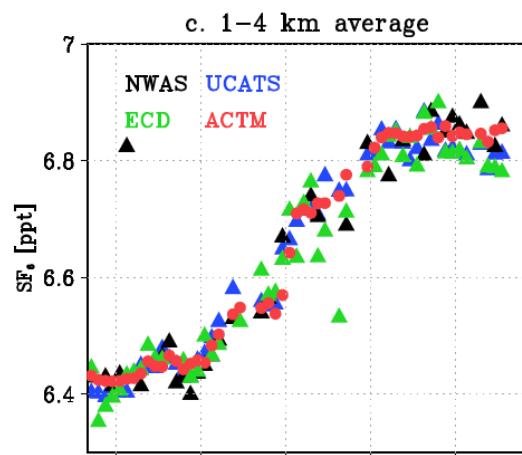
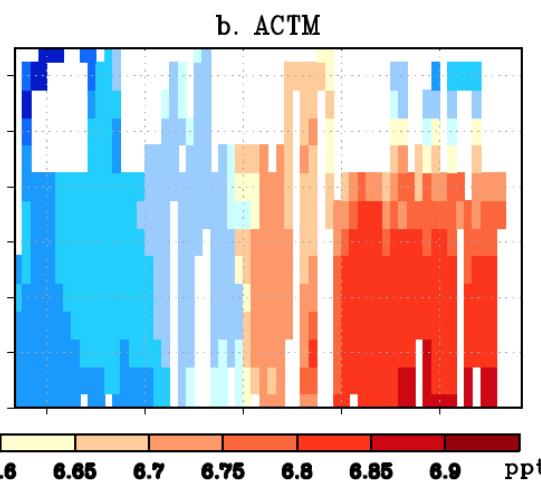
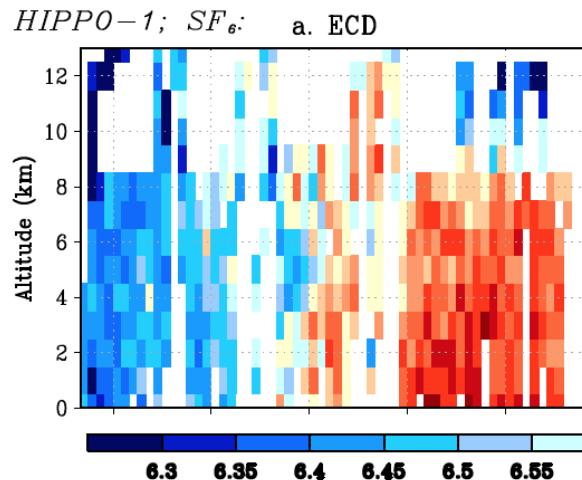


HIPPO data  
from central  
Pacific only

H#	Res. Flt#
1	#2-8
2	#1-7
3	#1-7
4	#1-7
5	#3-9

- 1. ALT    2. BRW    3. SUM    4. MHD
- 5. CMN    6. HFM    7. THD    8. NWR
- 9. MLO    10.KUM    11.RPB
- 12.SMO    13.CGO    14.PSA    15.SPO

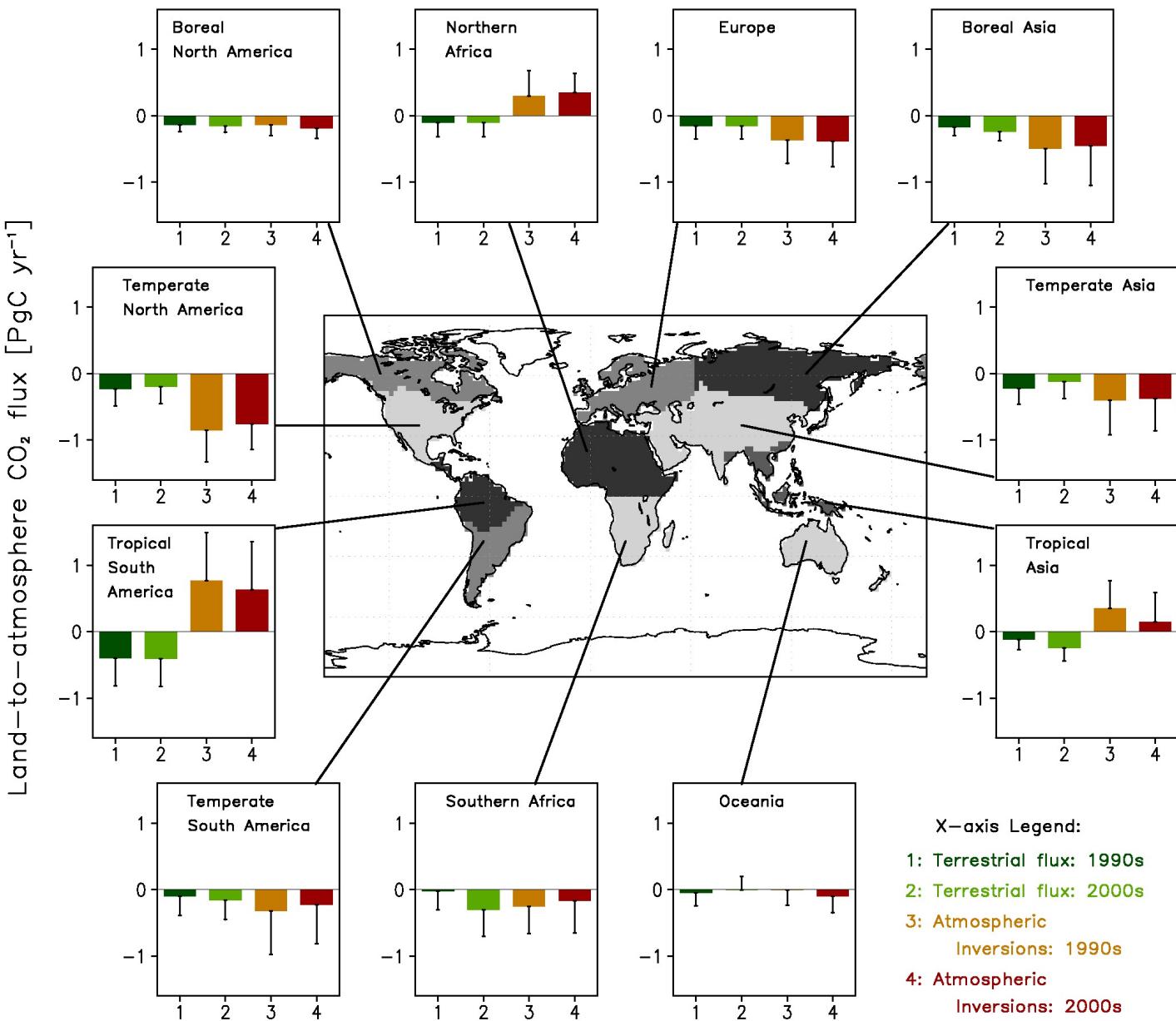
# Latitude-altitude variations of HIPPO & ACTM SF<sub>6</sub> using EDGAR4.2 (validation of NH to SH transport in ACTM)



Obs – Mod (ppt)	H-1	H-2	H-3	H-4	H-5
NH – SH SF <sub>6</sub>	-0.02 (6%)	0.02 (6%)	-0.02 (6%)	0.00 (0%)	-0.01 (3%)

Patra et al.,  
2009, 2011, 2014

# Synthesis of Land fluxes from TDIs and DGVMs



```
'reinit';* 'set display color white';
'set xlopts 1 4 0.44'; 'Set ylopts 1 4
iset mproj off'; 'set font 0'
* Greyscale
iset rgb 50 50 50 50'; 'set rgb 51
iset rgb 52 90 90 90'; 'set rgb 53
iset rgb 54 130 130 130'; 'set rgb 55
iset rgb 56 170 170 170'; 'set rgb 57
iset rgb 58 210 210 210'; 'set rgb 59
iset rgb 60 250 250 250'
iset rgb 61 153 0 2';* warm red
iset rgb 62 196 121 0';* warm orange
iset rgb 63 0 79 0';* warm green
iset rgb 64 0 170 208';* warm blue
iset rgb 65 224 0 0';* bring red
iset rgb 66 239 85 15';* dark orange
iset rgb 67 255 169 0';* warm yellow
iset rgb 68 89 169 0';* bright green
iset rgb 69 0 52 102';* dark blue
iset rgb 70 127 0 110';* dark purple
*
'open ./ctls/flux_summ.ctl'; 'open ./ctls/flux_sum2.ctl'; 'open ./ctls/flux_sum4.ctl'
* Boreal North America
iset vpage 0.5 2.5 4.2 6.2'; 'set gra
iset x 0.5 4.5'; 'set y 1'; 'set z 1'; 'se
iset gxout bar'; 'set bargap 30'; 'se
iset ccolor 63'; 'set baropts filled';
iset ccolor 68'; 'set baropts filled';
iset ccolor 62'; 'set baropts filled';
iset ccolor 61'; 'set baropts filled';
iset ccolor 1'; 'set gxout errbar'; 'se
iset strin
iset strin
iset line
iset vpag
*
Figure 6.15,
IPCC-AR5-WG1,
analysis by P. Patra
```

# Large scale data analysis using Principal Component Analysis

## **Correlations in time series (some preliminaries) :**

Univariate time series :

$$C(\tau) = \langle (x(t) - \bar{x}) (x(t + \tau) - \bar{x}) \rangle$$

Bi-variate time series :

$$C_{x,y}(\tau) = \langle (x(t) - \bar{x}) (y(t) - \bar{y}) \rangle$$

Multivariate time series :  $x_1(t), x_2(t), x_3(t) \dots \dots x_N(t)$

$$t = 1, 2, 3 \dots T$$

Pair wise correlations :  $\frac{N(N + 1)}{2}$

# Principal Component Analysis (PCA/EOFs)

Correlation matrix :  $C = D^T D$

$D$  is  $T \times N$  data matrix, with each column representing a time series.

Then,  $C$  is a square matrix of order  $N$ .

Spectra of correlation matrix  $C$ .

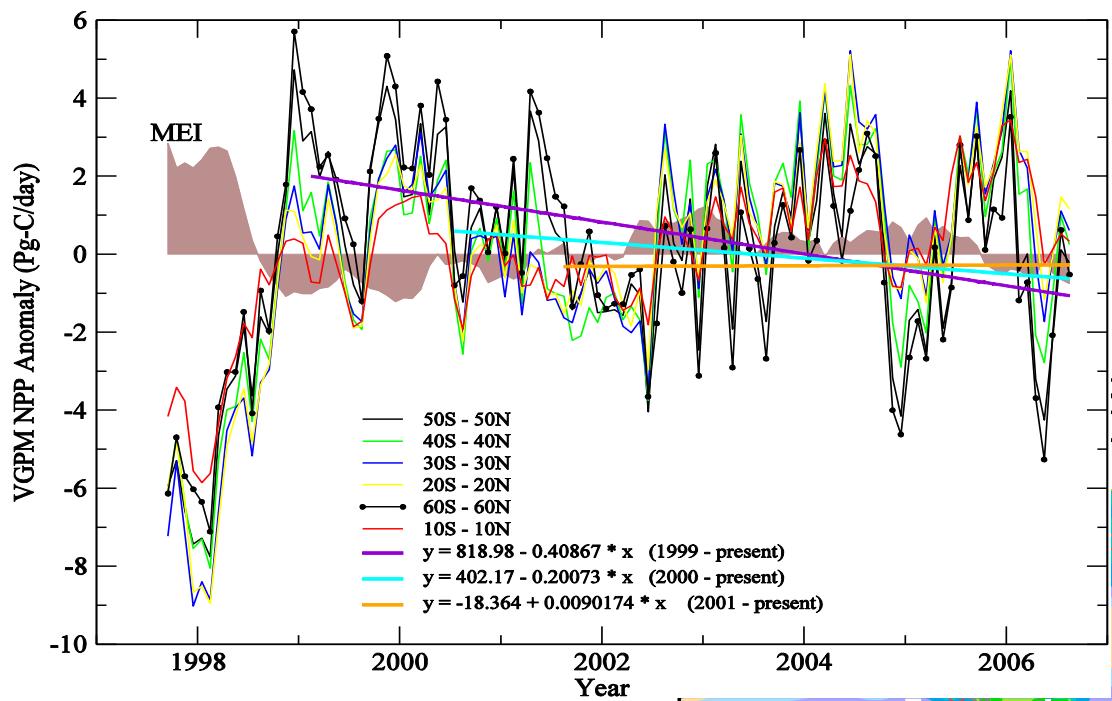
$$C u_i = \lambda_i u_i, \quad i = 1, 2, \dots, N$$

Positive semi-definite eigenvalues :  $\lambda_i \geq 0$

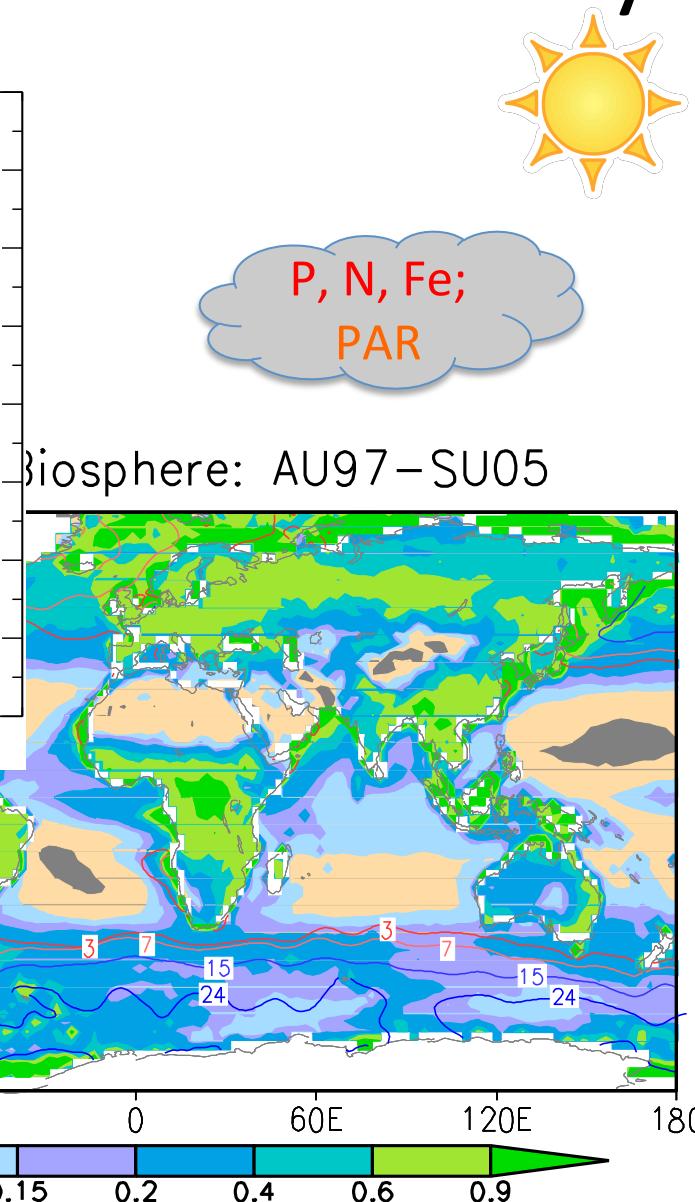
Real, symmetric :

$$C = C^T$$

# Our biosphere: trends and variability



Behrenfeld et al., 2006 (Edited)



# Principal component analysis: Empirical orthogonal function (EOF)

M. S. SANTHANAM AND PRABIR K. PATRA

PHYSICAL REVIEW E 64 016102

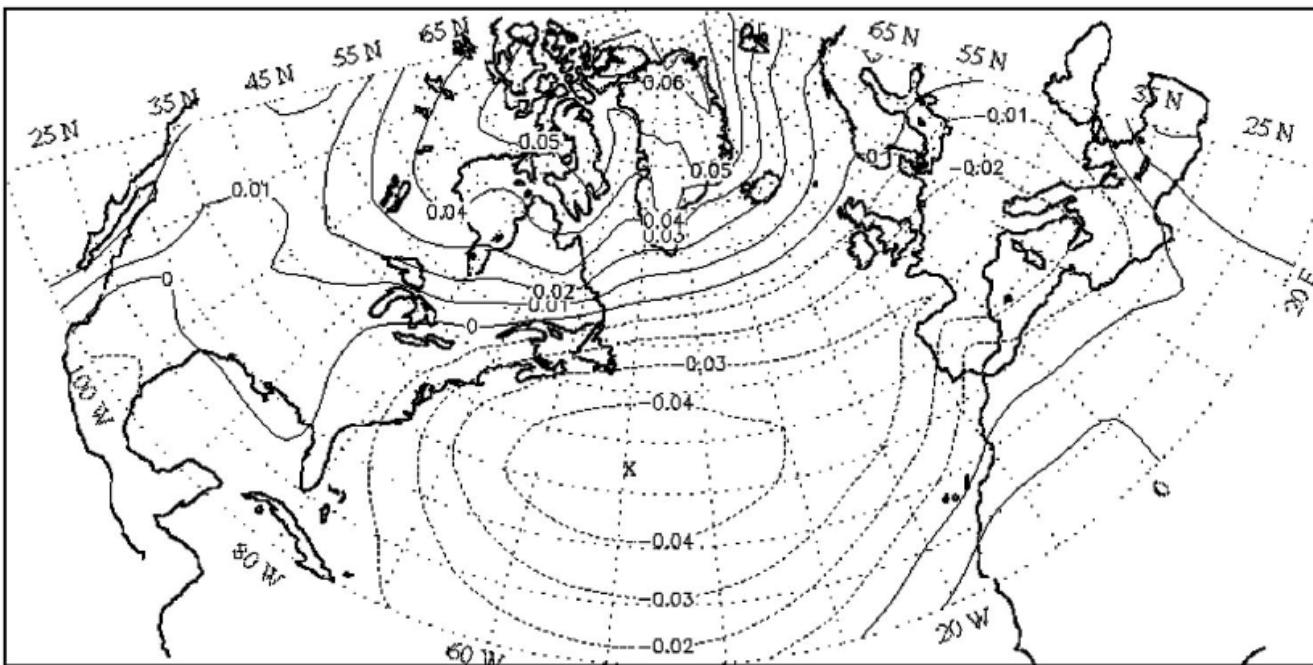


FIG. 1. The NAO pattern from the EOFs of monthly mean SLP correlation matrix with the geographical map of the domain of analysis in the background. The contours are drawn after averaging over the first two dominant EOFs. Note the north-south dipole shown as closed contours, in mid Atlantic (dotted contour) and over Greenland (solid contours).

anomaly  $z'(x,t)$  will be used that will have zero mean [ $\bar{z}'(x)=0$ ] and is rescaled such that its variance  $\langle z'(x)^2 \rangle$  is unity. If the observations were taken  $n$  times at each of the  $p$  spatial locations and the corresponding anomalies  $z'(x,t)$  assembled in the data matrix  $\mathbf{Z}$  of order  $p \times n$ , then the spatial correlation matrix of the anomalies is given by

$$\mathbf{S} = \frac{1}{n} \mathbf{Z} \mathbf{Z}^\dagger. \quad (2.1)$$

location. If the eigenvalue corresponding to the  $m$ th eigenmode is  $\lambda_m$ , then the percentage variance associated with that mode is given by

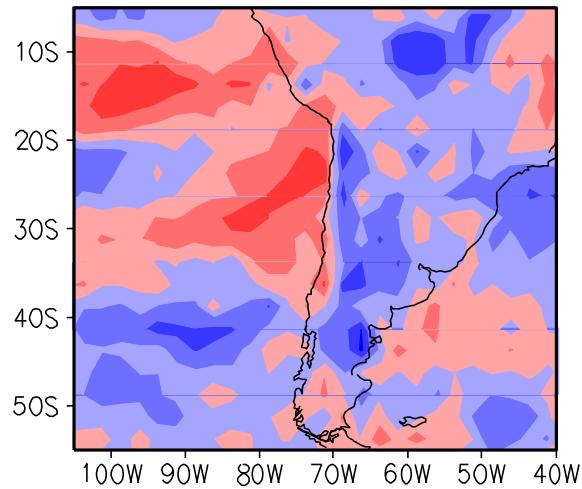
$$\lambda_m / \sum_{i=1}^p \lambda_i \times 100,$$

$p$  denotes the total number of eigenmodes. The PCs for each modes of variability ( $u_m$ ) can be calculated as

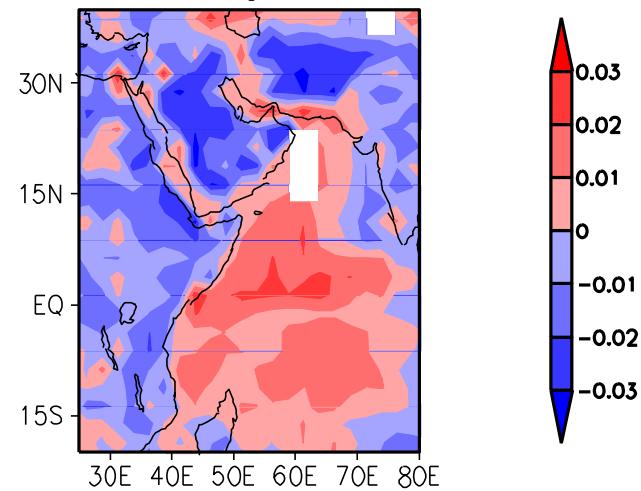
$$u_m = \sum_i e_{im} x_i.$$

# EOF-1 for selected regions

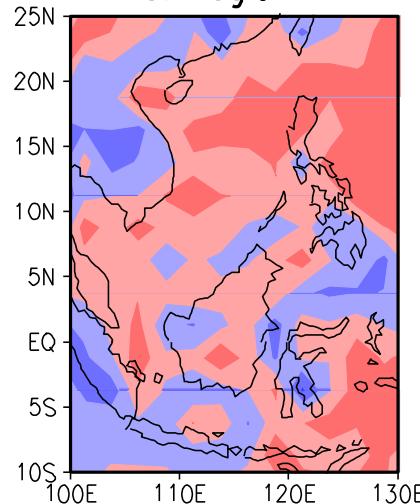
A. Region 1 and 2 (EOF 1)



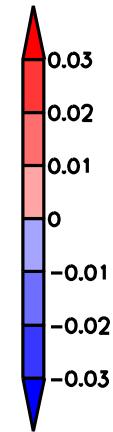
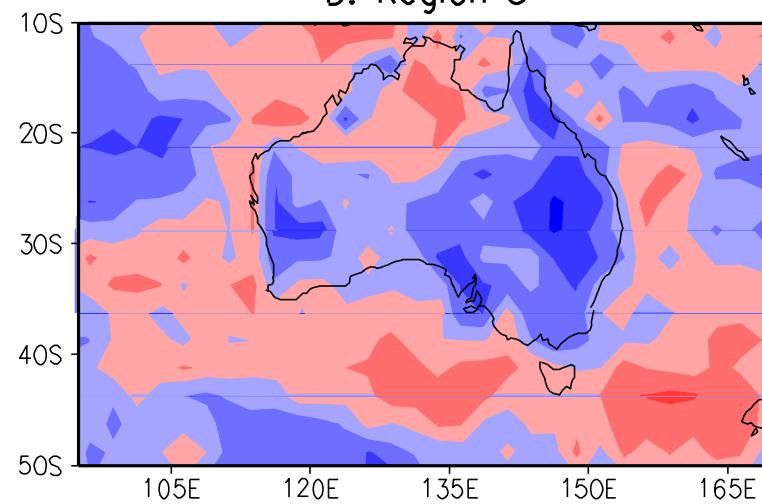
B. Region 3



C. Region 4



D. Region 5

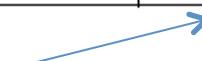


# Possible mechanism of strong land-ocean coupling – correlations of timeseries for 10 years

Lead-lag correlation for identifying the cause-and-effect relationship

	Chl-a/ SST	NDVI/ PCP	Chl-a/ NDVI
Region 1 (105°W-50°W, 35°S-5°S)	-0.54 (-2)	0.44 (-2)	-0.27 ( 0)
Region 2 (75°W-50°W, 55°S-30°S)	-0.39 (-1)	0.17 (-2)	-0.26 (-4)
Region 3 (25°E-80°E, 20°S-40°N)	-0.61 ( 0)	0.46 (-2)	-0.70 ( 1)
Region 4 (100°E-130°E, 10°S-25°N)	-0.70 ( 0)	0.36 ( 0)	-0.42 ( 0)
Region 5 (105°E-170°E, 50°S-25°S)	-0.44 (-1)	0.41 (-2)	-0.34 (-4)

Chl-a lags SST

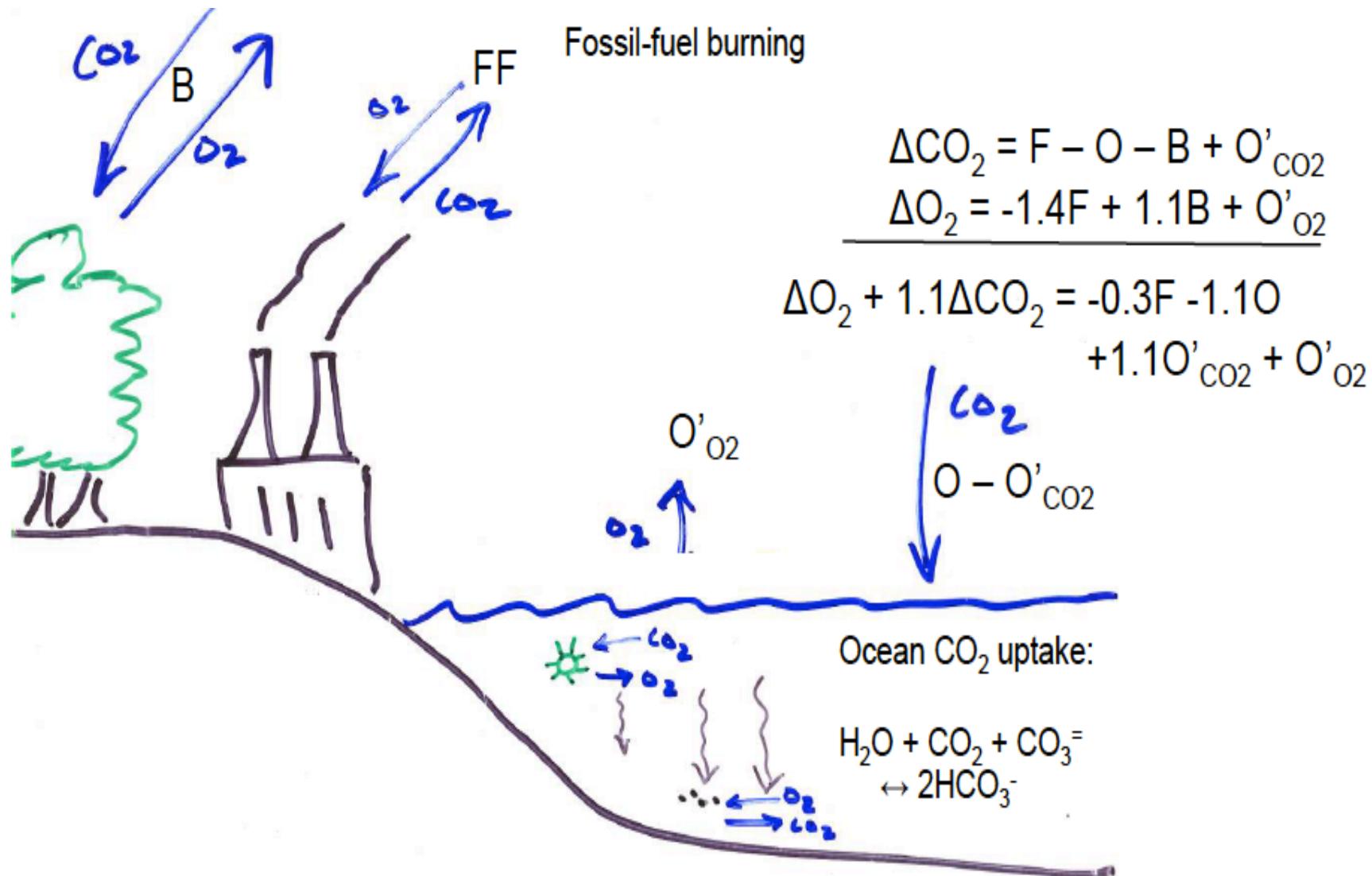


# My little Fortran code – notable is memory allocation

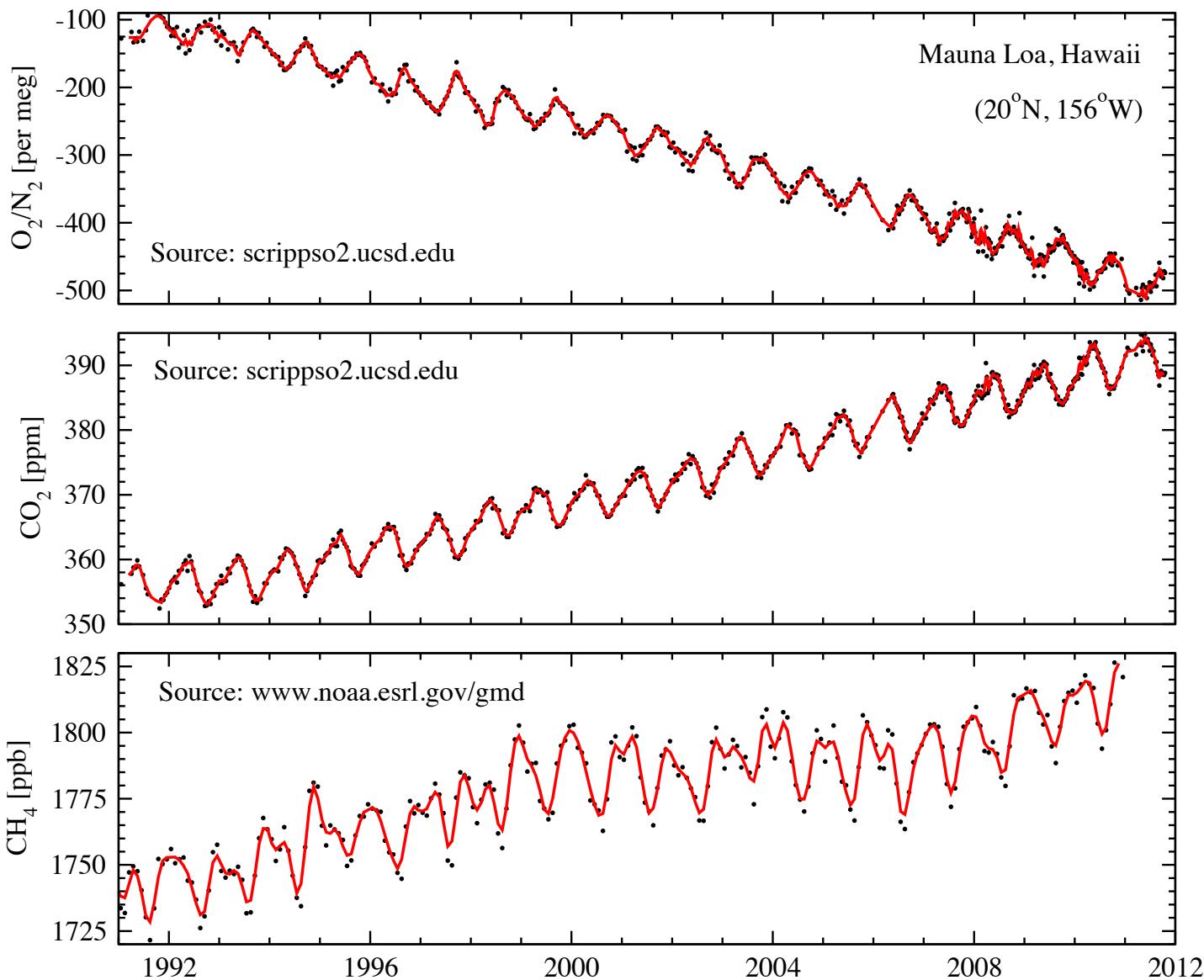
```
! compile with : ifort eofbios2p5.f90 -r8 (-L/usr/local/lib) -llapack -lblas
!
PROGRAM EOFBIO
implicit none
integer :: nyear,nmon,nlat,nlon,nlat1,nlat2,nun,iun,count
parameter (nyear=9, nmon=4, nlat=72, nlon=144,nun=20)
integer :: i,j,k,iy,im,idim,jdim,kdim,idx,idy,irec,num0
real :: c1,sum,lb,ub
real *4 :: LS(nlon,nlat)
real,allocatable :: cov(:,:,:),cor(:,:,:),avg(:,:,:)
real*4,allocatable :: BIO(:,:,(:,:,)),BI0p(:,:,(:,:,)),BI0a(:,:,(:,:,)), chla(:,:,(:,:,)), ndvi(:,:,(:,:,))
real,allocatable :: d(:),e(:),tau(:),work(:),w(:),z(:,:)
real*4,allocatable :: evec(:,:,:),pca(:,:)
integer, allocatable :: IWORK(:),IFAIL(:)
integer :: n,ml,m5,nev,m,info,il,iu,ils,jls,iev,nls,ndim
character*1 JOBZ,RANGE,UPLO
!
OPEN(31,FILE='./data/sw_chlo2.grd',status='old',form='unformatted',access='direct',recl=nlon*nlat)
OPEN(32,FILE='./data/sw_ndvi2.grd',status='old',form='unformatted',access='direct',recl=nlon*nlat)
OPEN(33,FILE='./data/sw_bios2.grd',status='unknown',form='unformatted',access='direct',recl=nlon*nlat)
OPEN(71,FILE='evalbios.dat',status='unknown')
OPEN(62,FILE='pcabios.dat',status='unknown')
!
allocate ( BIO(1:nyear,1:nmon,1:nlat,1:nlon) ); BIO = 66.83439
allocate ( chla(1:nlat,1:nlon) ); chla = 66.83439
allocate ( ndvi(1:nlat,1:nlon) ); ndvi = 66.83439
allocate ( BI0a(1:nmon,1:nlat,1:nlon) ); BI0a = 66.83439
allocate ( BI0p(1:nyear,1:nmon,1:nlat,1:nlon) ); BI0p = 66.83439
!include "time.h"
irec = 0 ! 0 (nyear=8), 4 (nyear=7)
do iy = 1, nyear; do im = 1, nmon; irec = irec + 1 !; print *, 'irec =',irec
  read (31, rec=irec) ((chla(j,i), i=1,nlon), j=1,nlat) ! 1x1 deg Grads
  read (32, rec=irec) ((ndvi(j,i), i=1,nlon), j=1,nlat) ! 1x1 deg Grads
  do i = 1, nlon; do j = 1, nlat
    if ( chla(j,i) .le. 60.0) then
      BIO(iy,im,j,i) = chla(j,i)
    else if ( ndvi(j,i) .le. 60.0) then
      BIO(iy,im,j,i) = ndvi(j,i)
    end if
  end do
end do
!
```

# **EVALUATION OF MODELS – CO<sub>2</sub> EXAMPLE**

# Coupled CO<sub>2</sub> and O<sub>2</sub> system (source: Keeling and Keeling)



# What's the evidence of increased CO<sub>2</sub> loading?



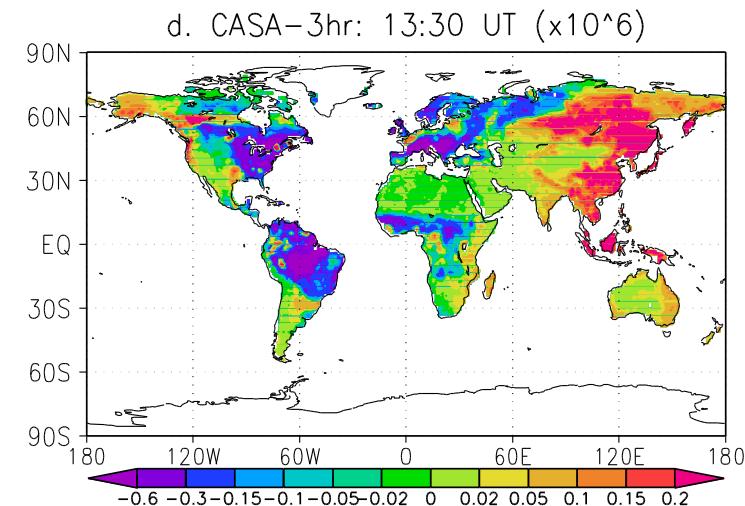
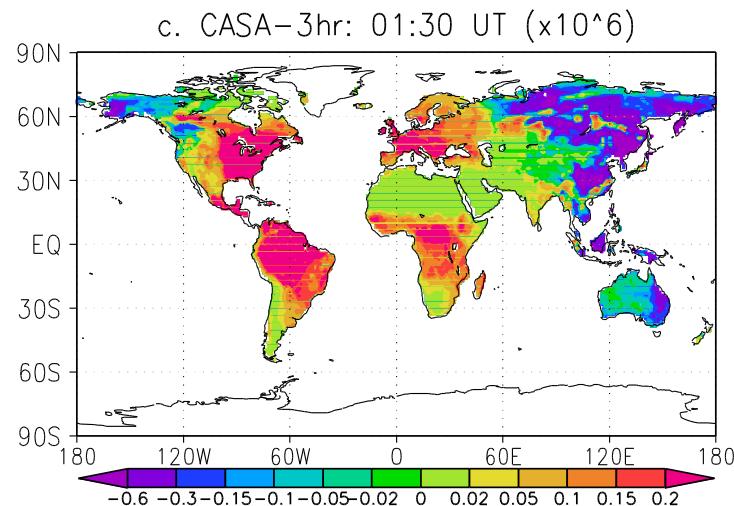
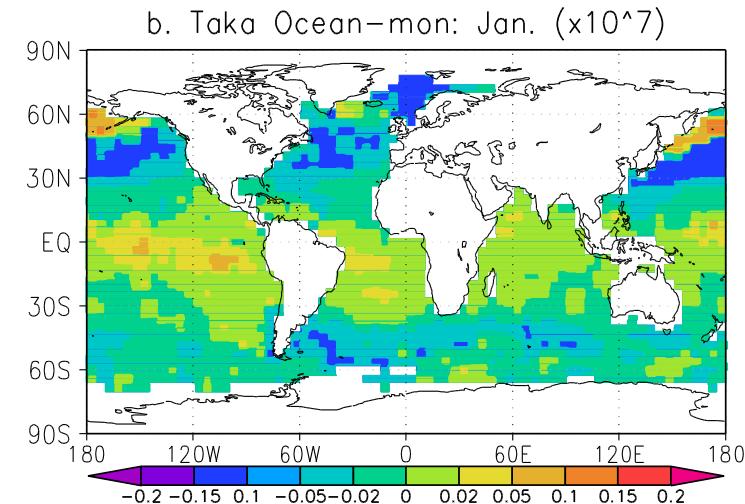
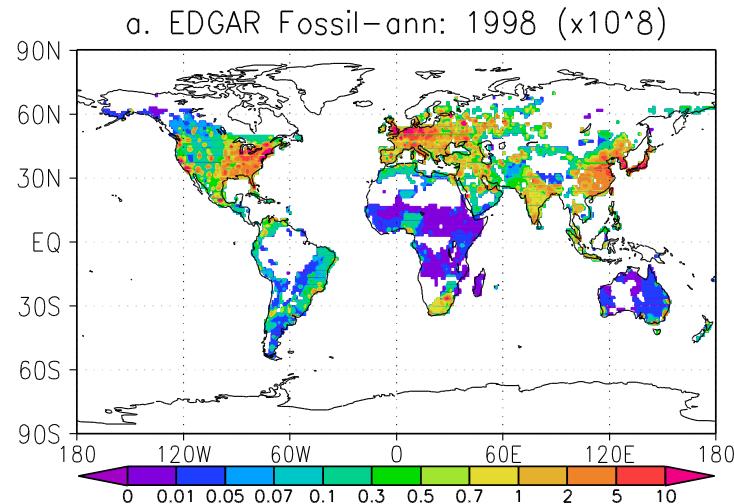
For ACTM  
simulations:

Ishidoya et al.,  
2012

Patra et al.,  
2011a

Patra et al.,  
2011b

# Surface flux distributions – overview



unit: kg-CO<sub>2</sub>/m<sup>2</sup>/s

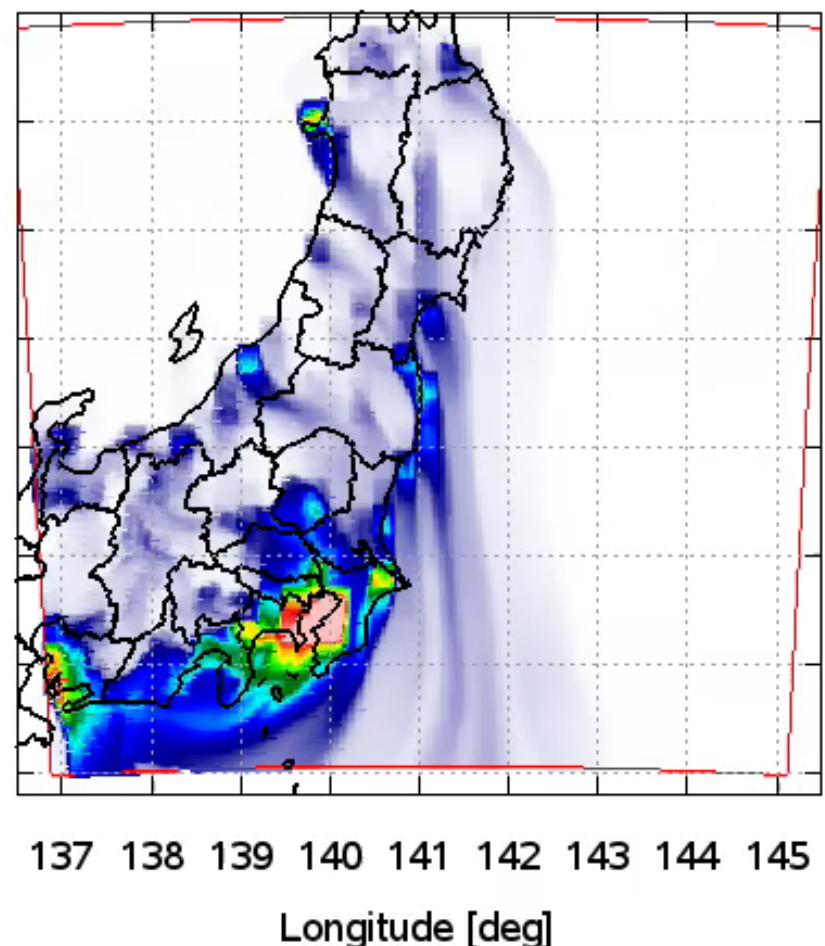
EDGAR: JRC/PBL

CASA: Randerson et al., 1997

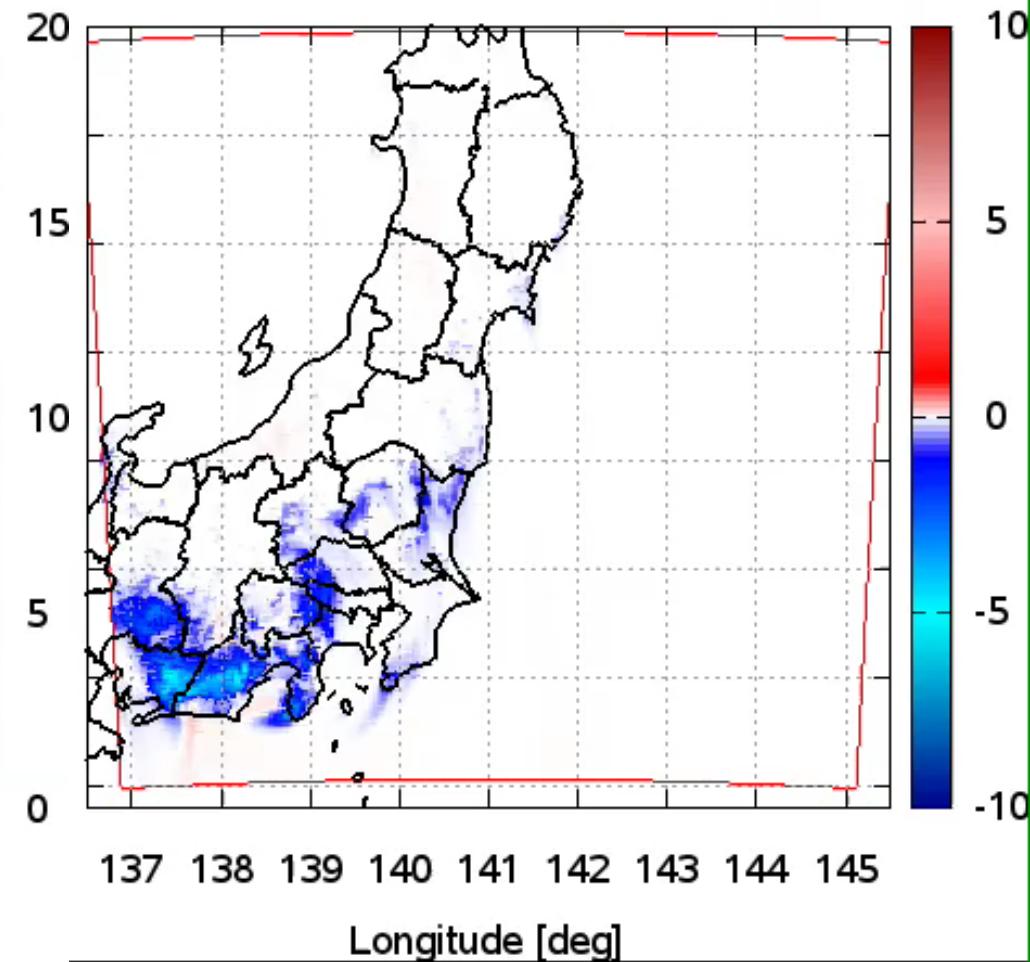
Ocean: Takahashi et al., 2009

# Movies of WRF-CO<sub>2</sub> simulations

Anthro. CO<sub>2</sub> at 00:00 JST 01/03/2011 [ppmv]



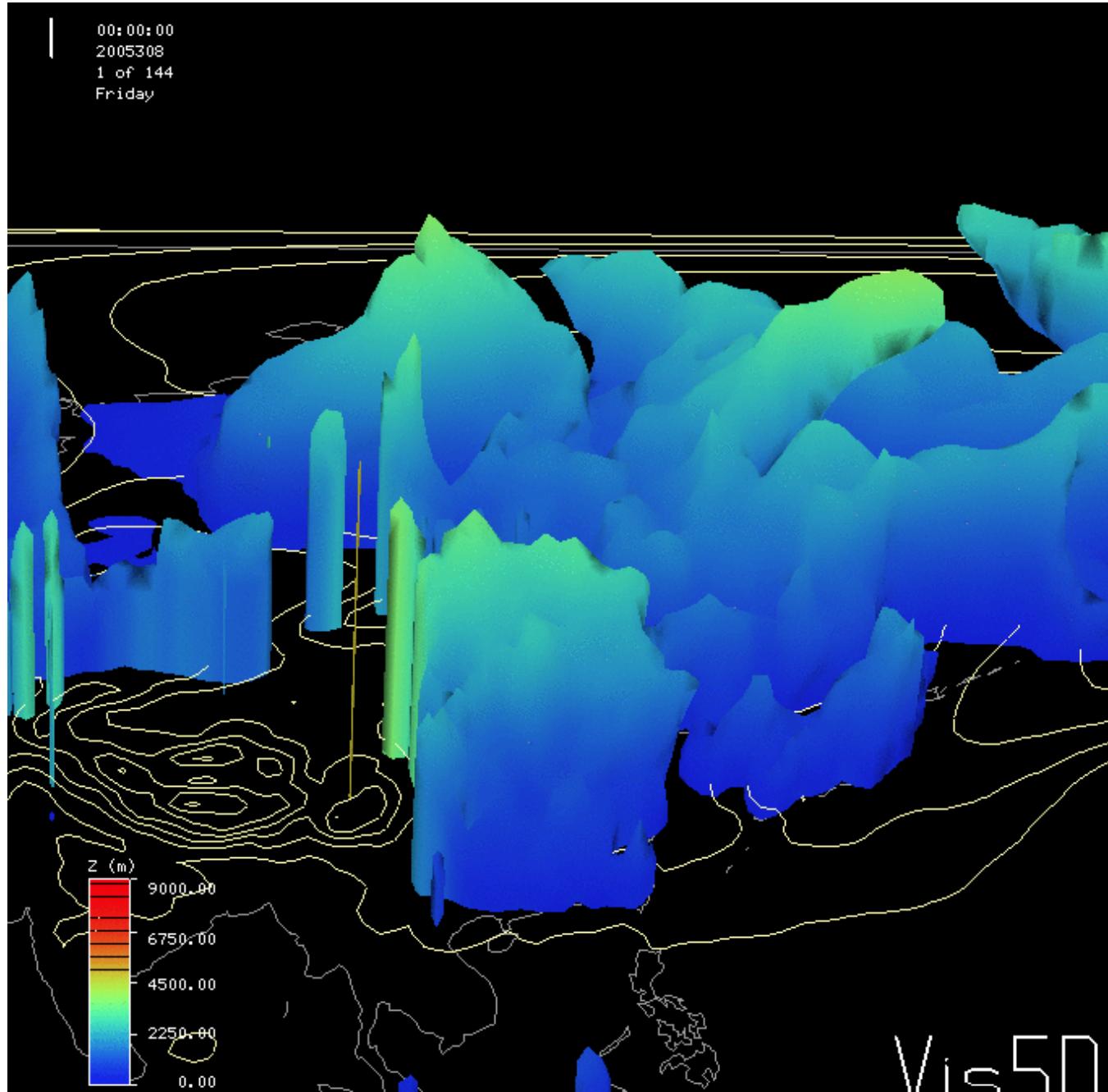
Biogenic CO<sub>2</sub> at 00:00 JST 01/03/2011 [ppmv]



# Spatial scales of atmospheric-CO<sub>2</sub> hourly variations

00:00:00  
2005308  
1 of 144  
Friday

DoY 308-313;  
4-9 Nov 2005



With help from M. Takigawa

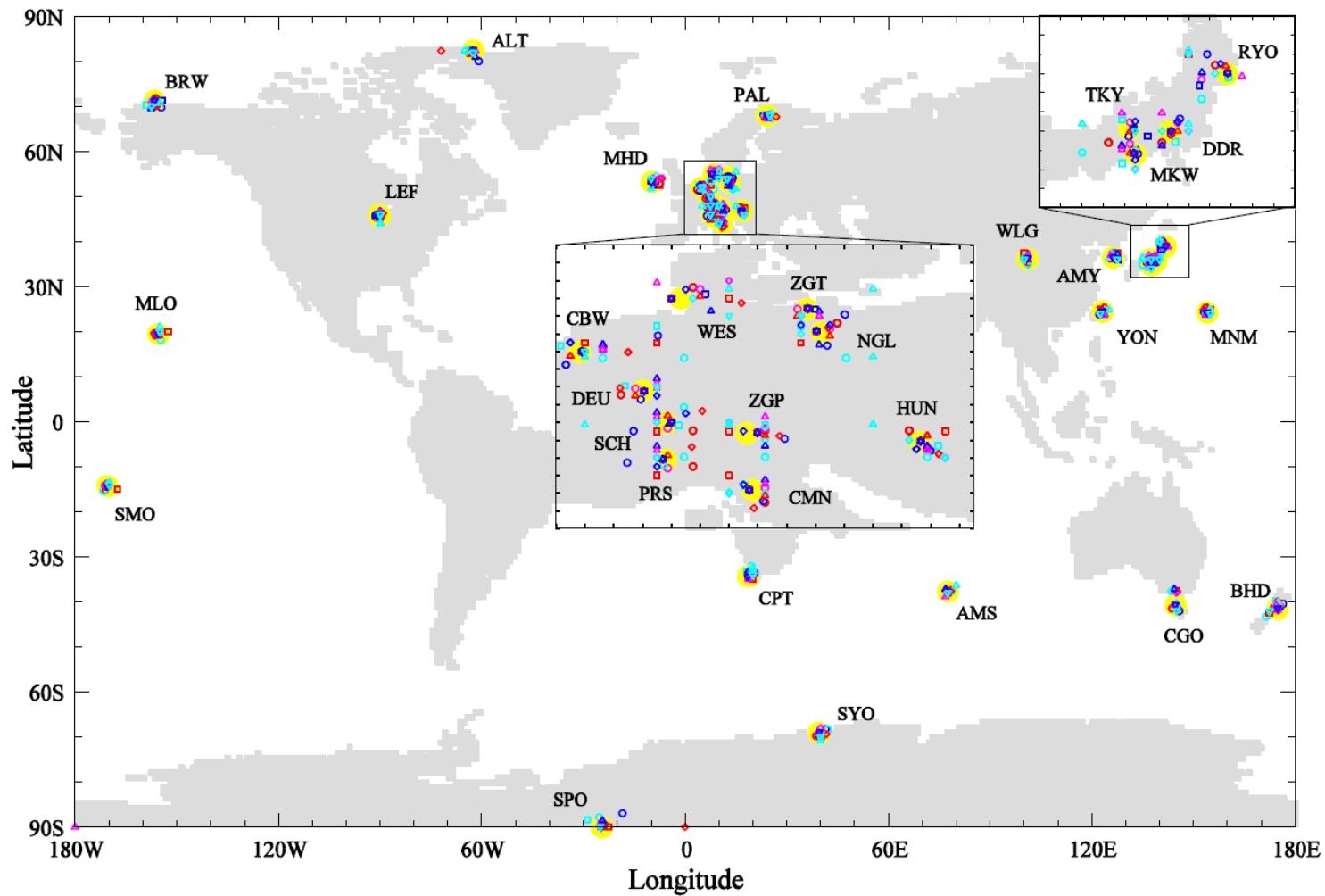
Isosurface of  
380 ppm CO<sub>2</sub>  
concentrations  
coloured by  
Height  
(blue: ground  
red: ~9km  
height)

White contour:  
Sea-level Pressure

Monthly average  
CO<sub>2</sub> shows mainly  
inter-hemispheric  
difference

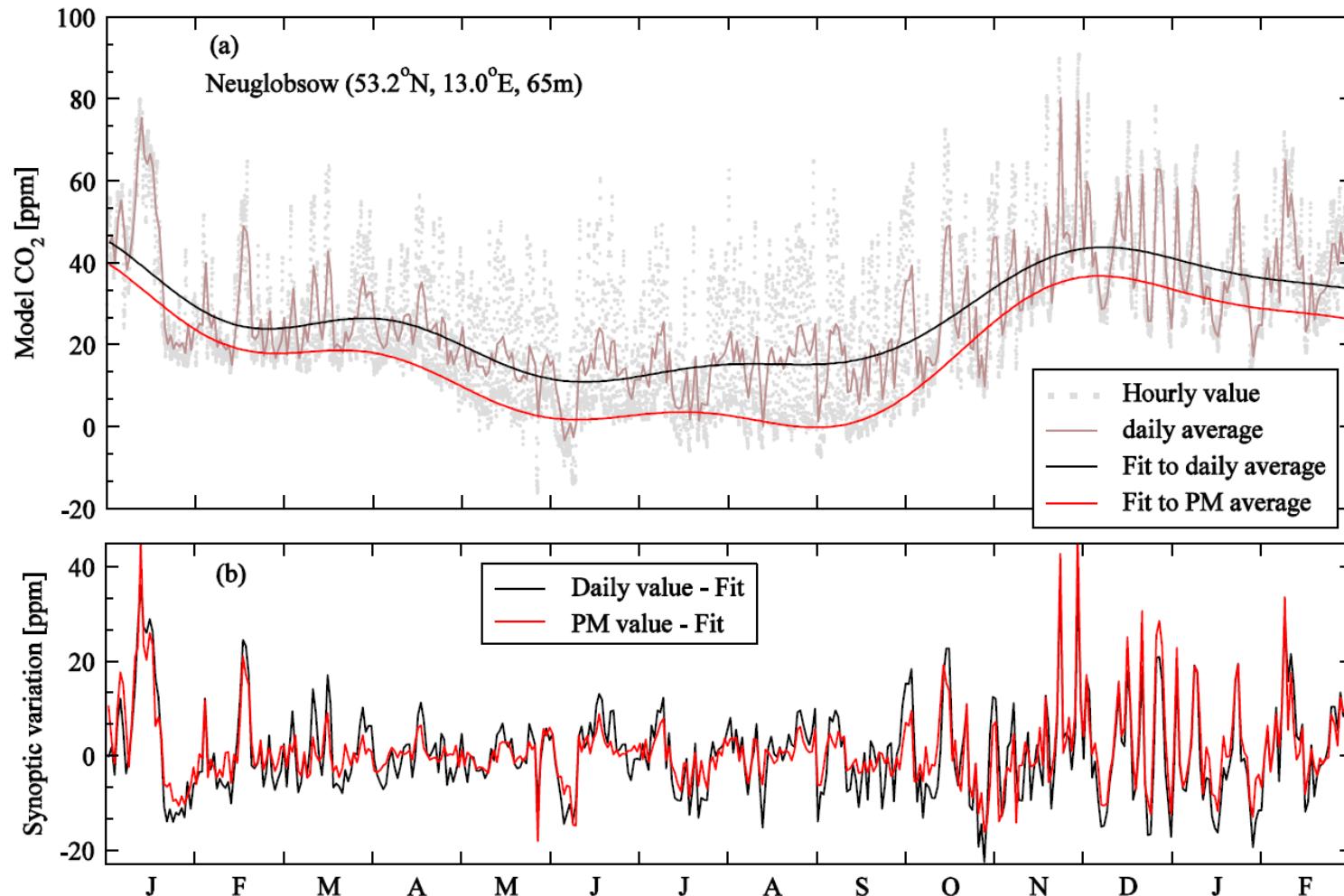
Vis5D

# Measurement locations of Hourly CO<sub>2</sub>

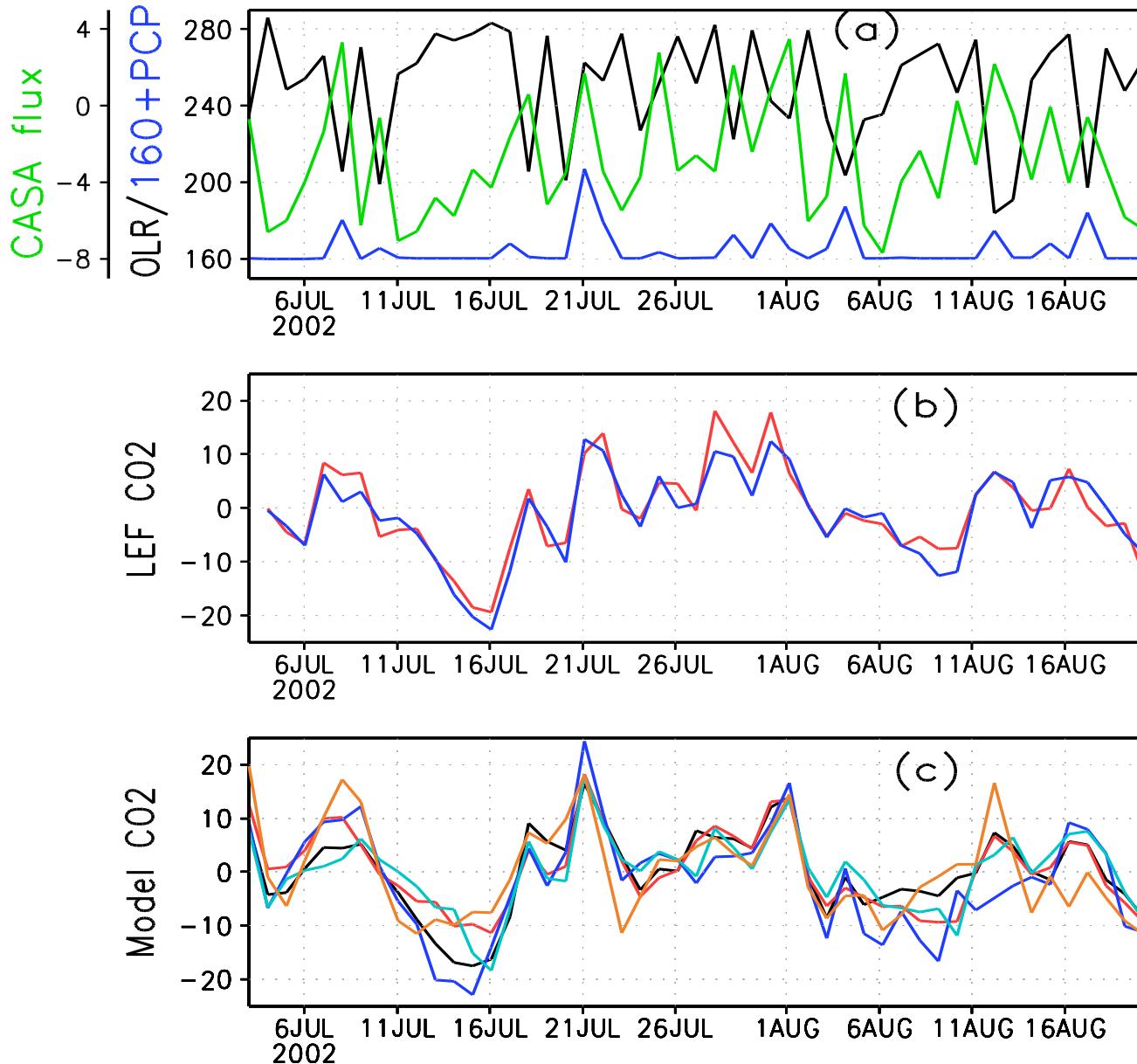


TransCom (Transport model inter-comparison project) – CO<sub>2</sub> continuous experiment  
Law et al., GBC, 2008; Patra et al., GBC, 2008

# What is synoptic variability in CO<sub>2</sub>?



# Model-data comparison



**LEF Tower, 76m  
Wisconsin**

a. Weather conditions  
and flux

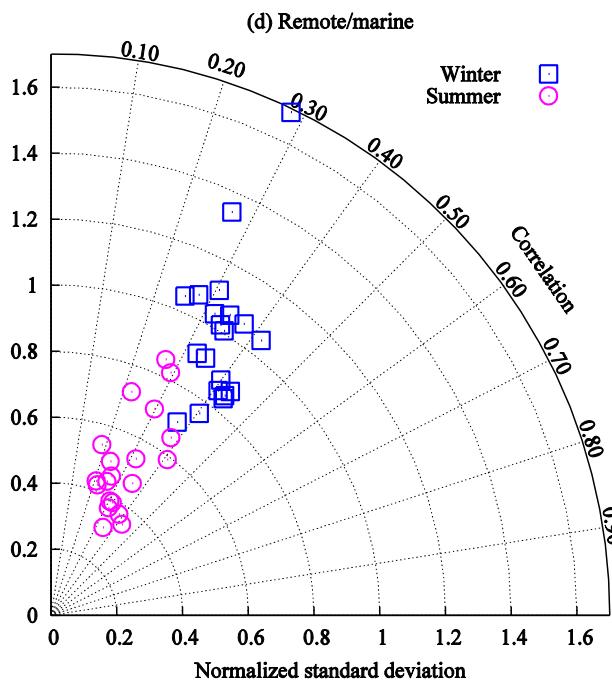
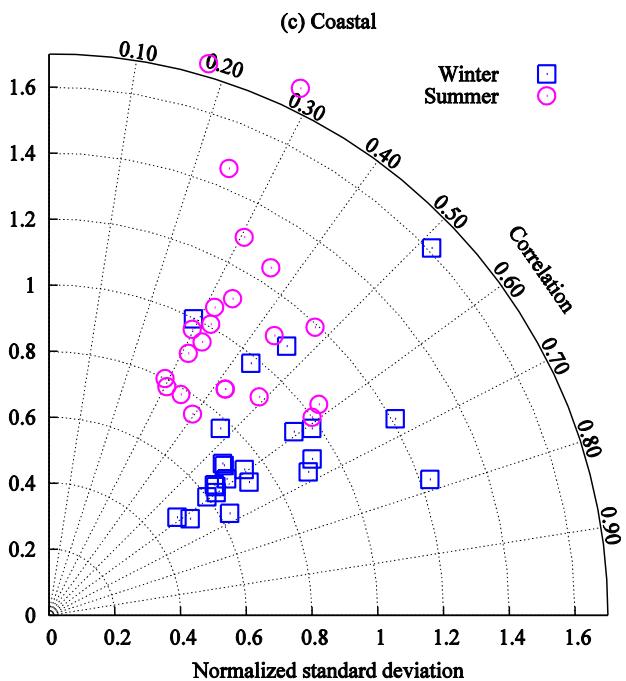
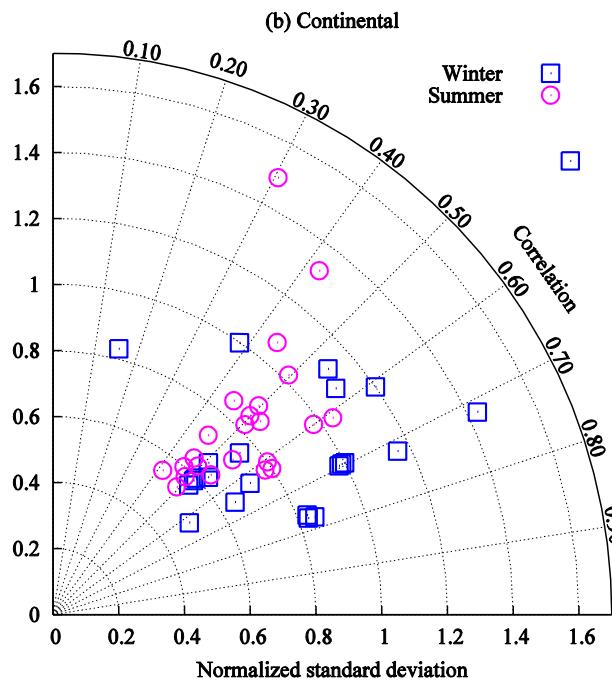
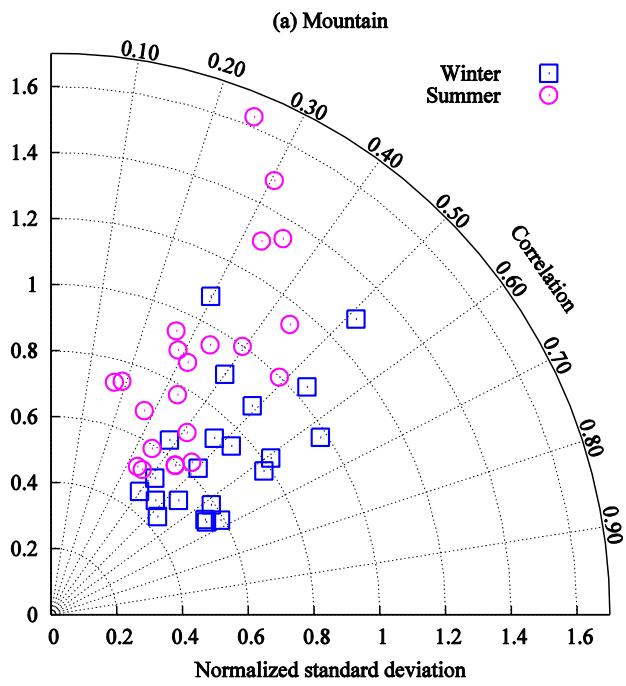
b. Observed CO<sub>2</sub>  
synoptic variability

c. Modelled variability

**Correlation (R):**  
phase of model-data  
comparison

**NSD ( $Sd_{mod}/SD_{obs}$ ) :**  
amplitude of  
variability (1 ideally)

# Taylor Diagrams



Salient features:

Simulations accuracy during winter is better than summer

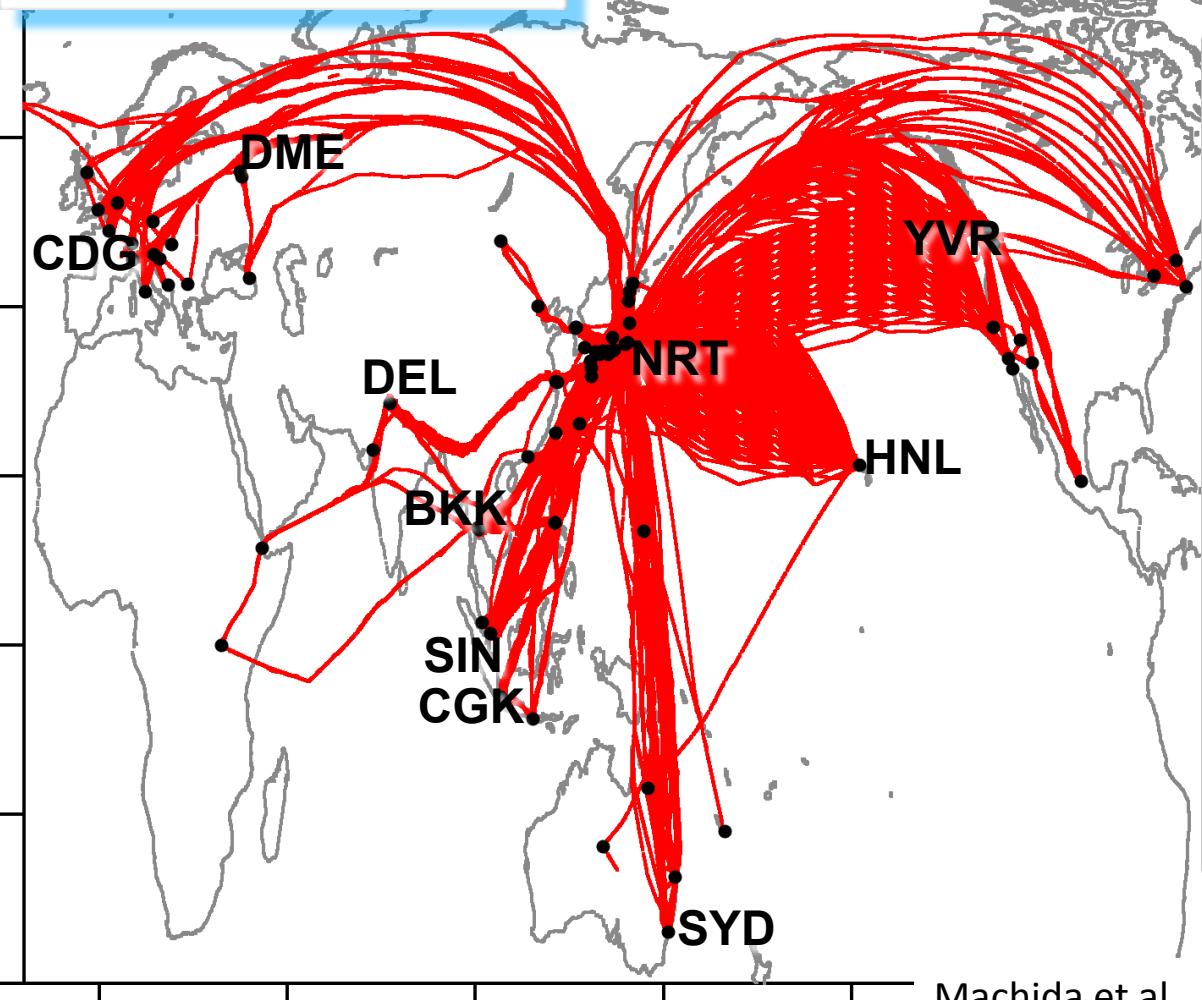
a. Sampling at mountain sites is tricky

b. Continental sites are best simulated. Note diurnally varying flux

d. Oceanic flux variability is weaker

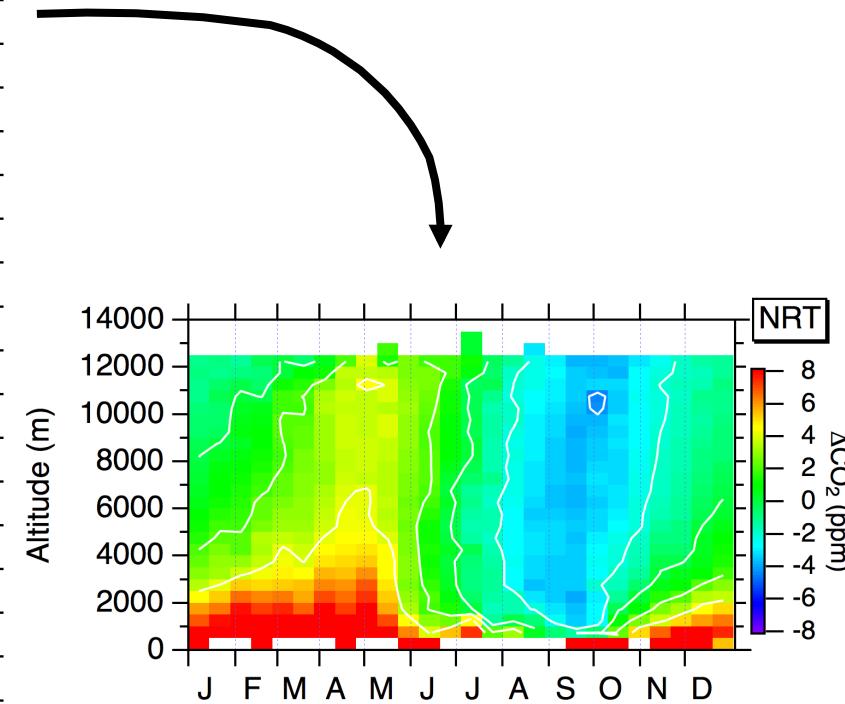
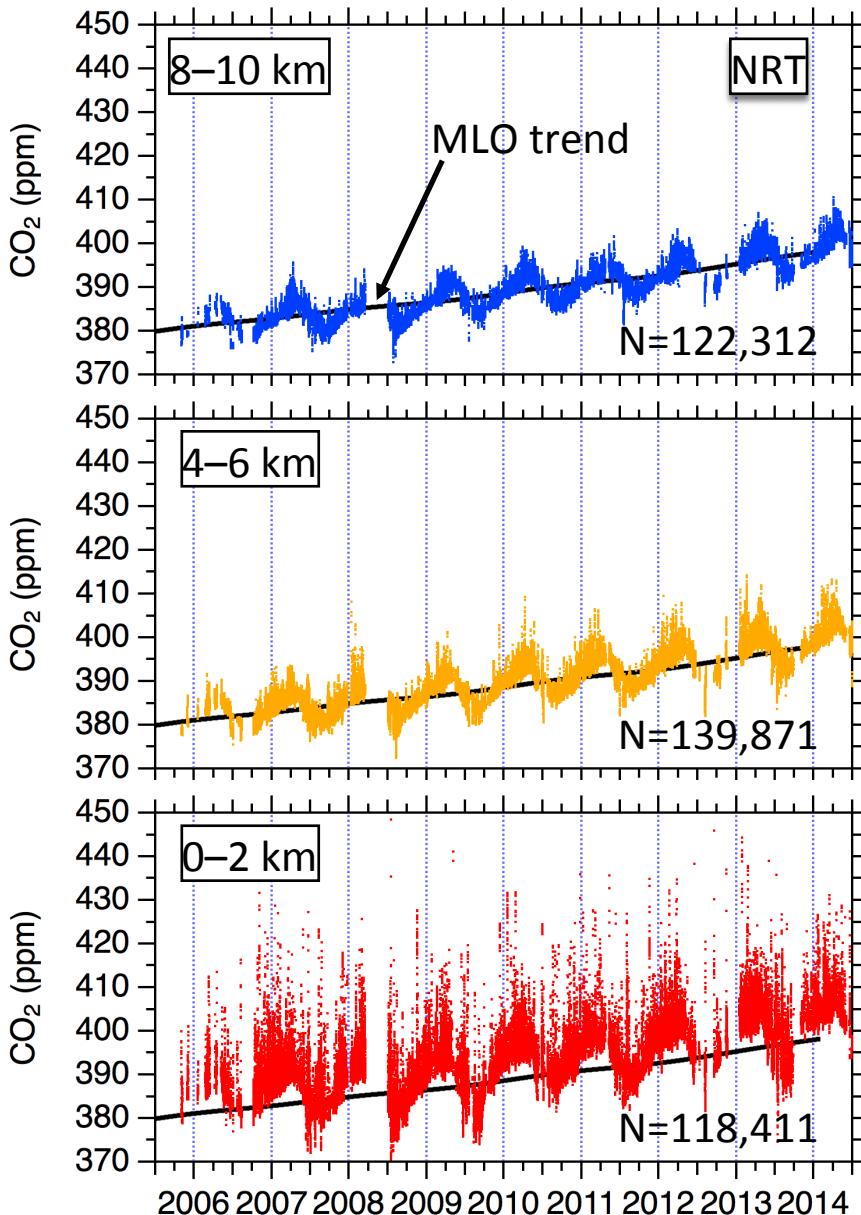
# Flight statistics CME (Nov. 2005–Dec. 2014)

~12,000 flights  
~23,000 vertical profiles  
~7.0 million data



1. **NRT, Japan** 7270
2. **HND, Japan** 2937
3. **SYD, Australia** 1581
4. **HNL, Hawaii** 1455
5. **BKK, Thailand** 1273
6. **NGO, Japan** 855
7. **DEL, India** 787
8. **SIN, Singapore** 686
9. **CDG, France** 683
10. **KIX, Japan** 635
11. **YVR, Canada** 440
12. **CGK, Indonesia** 422
13. **DME, Russia** 409
14. **SFO, California** 366
15. **AMS, the Netherlands** 238
16. **ICN, South Korea** 199
17. **LHR, UK** 196
18. **FUK, Japan** 189

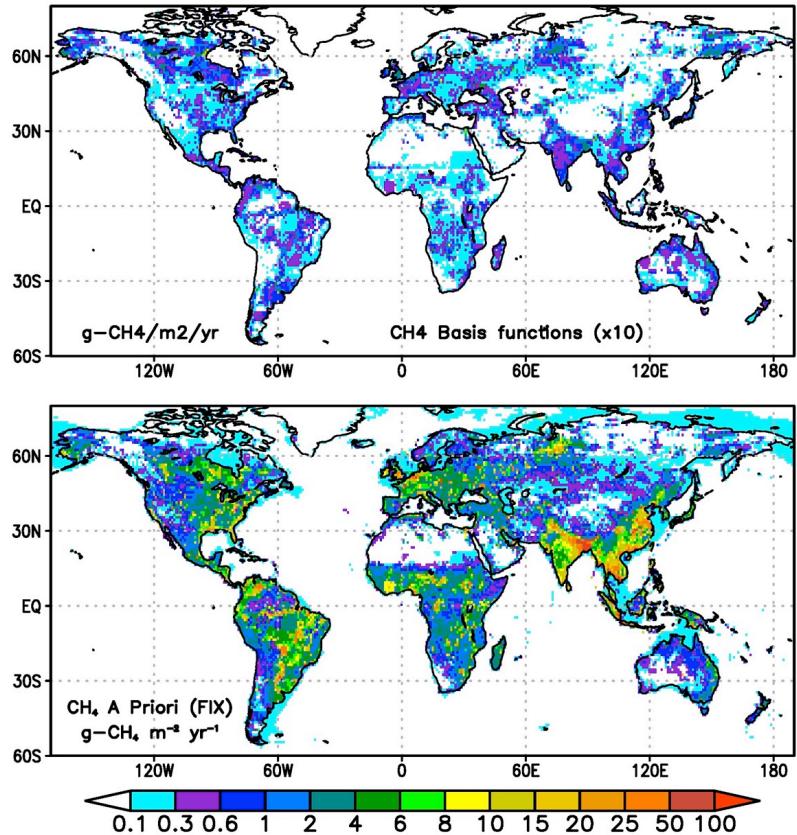
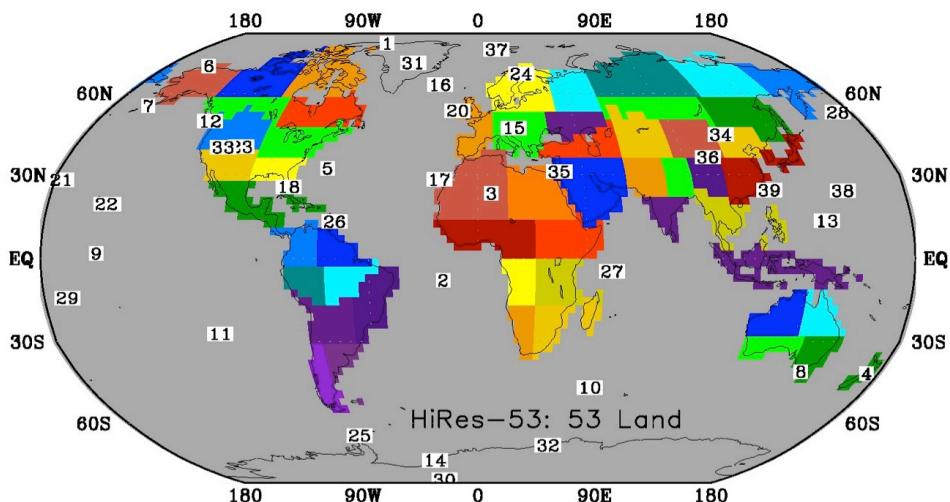
# CO<sub>2</sub> over Tokyo, Japan (NRT)



We need more and more data mining tools – data volume beyond human searching of signals

Annual mean, seasonal cycle and  
anomalies for climate analysis

# 53-Regions (land only) Inverse Model for CH<sub>4</sub>



$$C_S = (G^T C_D^{-1} G + C_{S_0}^{-1})^{-1}$$

$$S = S_0 + (G^T C_D^{-1} G + C_{S_0}^{-1})^{-1} G^T C_D^{-1} (D - D_{ACTM})$$

$S_0$  = regional prior sources

$C_{S_0}$  = Prior source covariance = 50% of region-total emission for each month

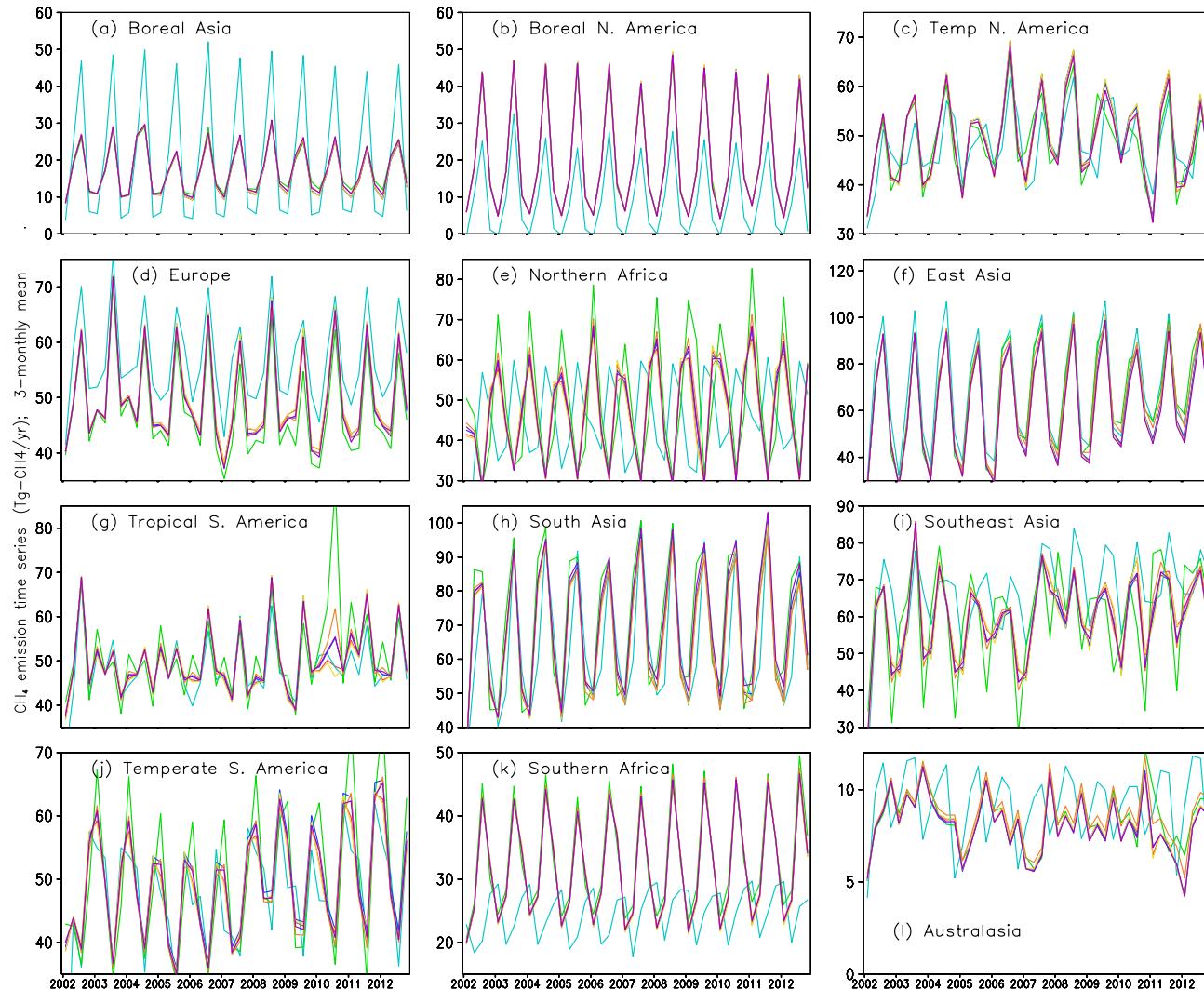
$D$  = atmospheric concentration data

Data covariance  $C_D$  = 10 ppb; 5 ppb for measurements + 5 ppb for model uncertainty

$D_{ACTM}$  = ACTM simulation using  $S_0$

$G$  = Green's functions for regional source-receptor relationships

# CH<sub>4</sub> fluxes: 3-monthly time series for 2002-2012



A Priori(s) (Grey lines)

A Posteriori (Coloured):

(Inv08: 39 sites,  $C_b=5+SD/2$ ,  $C_{so}=E*.7$ )

CH<sub>4</sub>AGS

CH<sub>4</sub>E42

CH<sub>4</sub>ONG

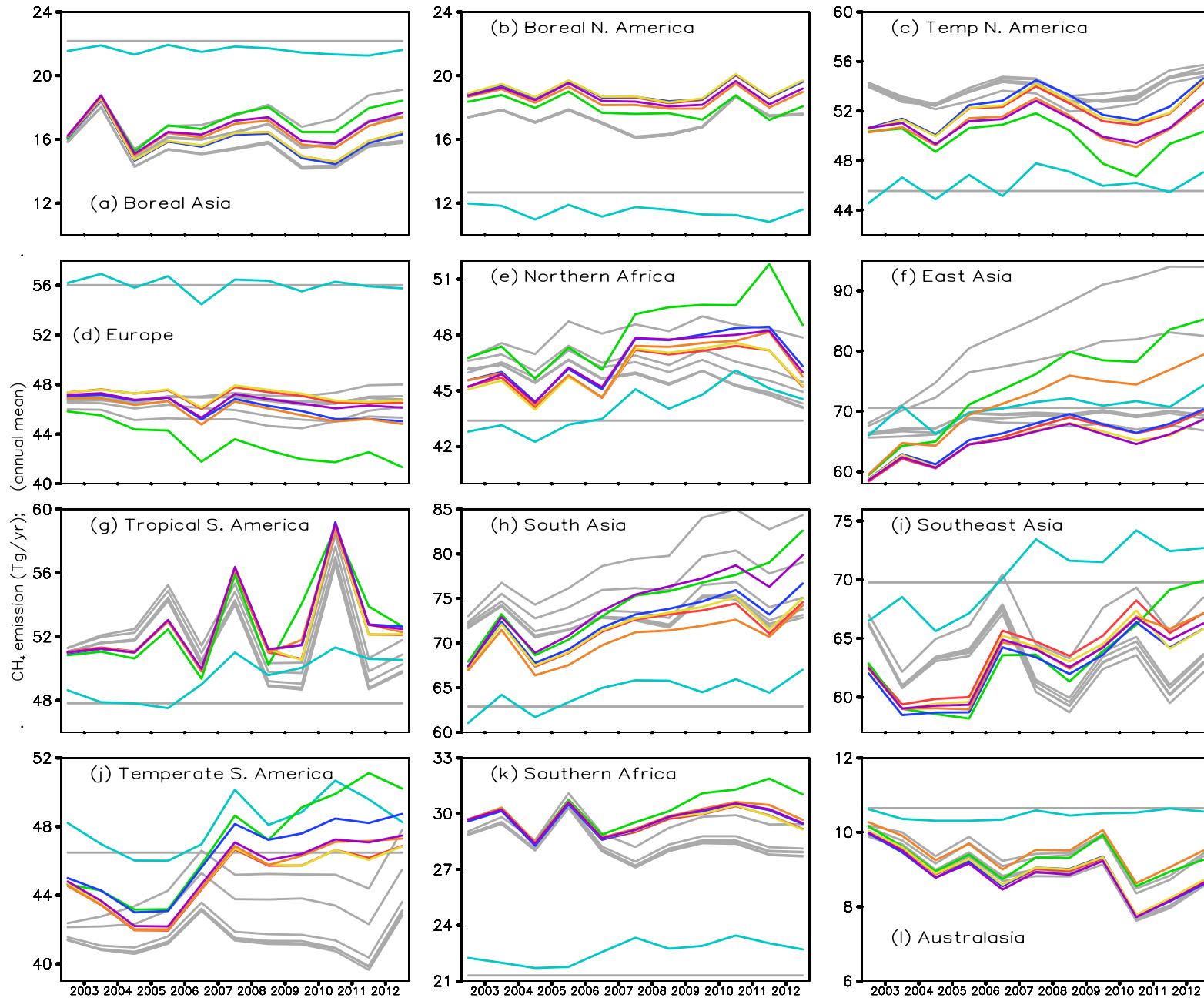
CH<sub>4</sub>ENF

CH<sub>4</sub>FIX

CH<sub>4</sub>CTL

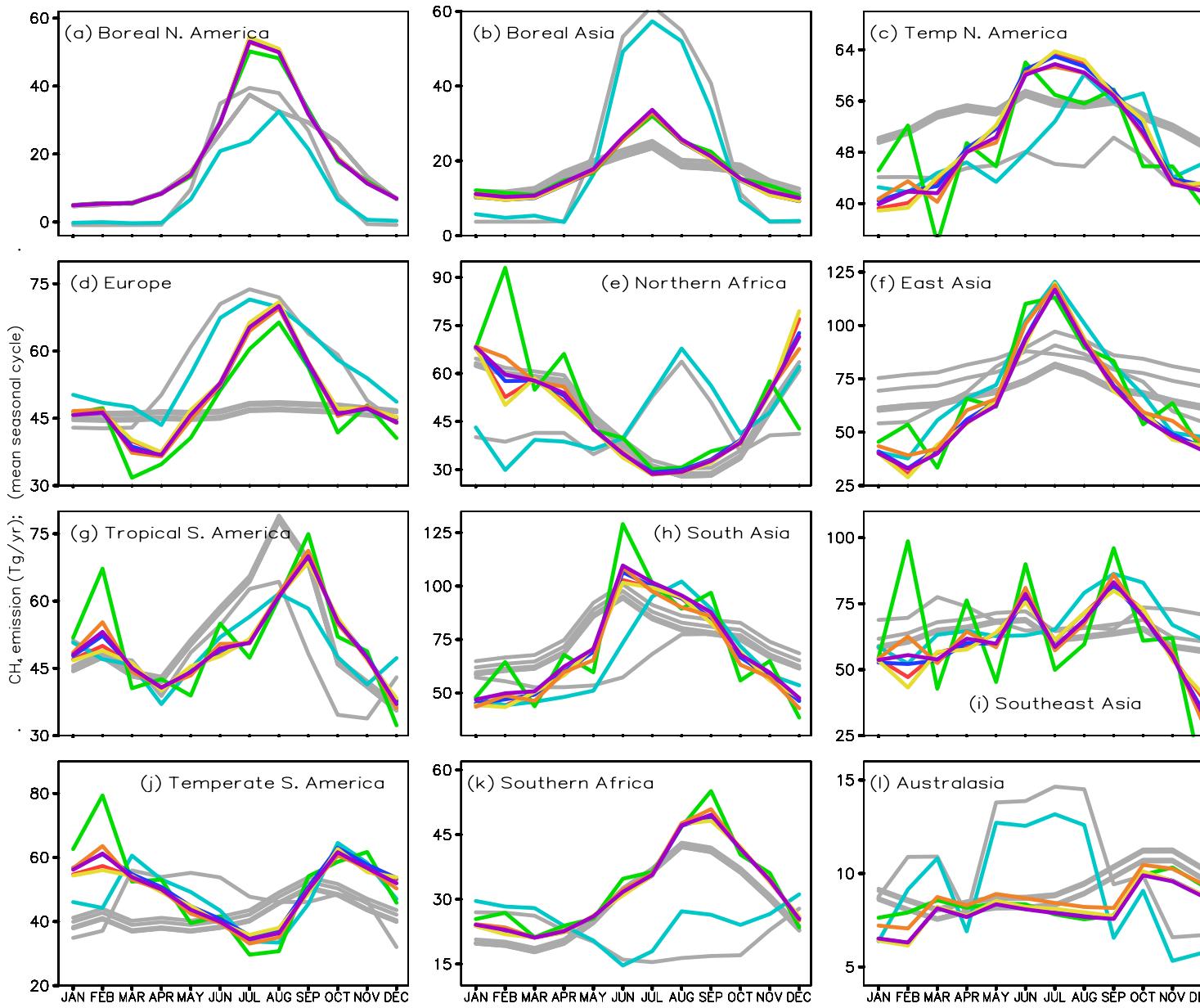
CH<sub>4</sub>FUG

# $\text{CH}_4$ fluxes : annual means for the period 2002-2012



A priori  
A Poste:  
 AGS E42  
 ENF FIX  
 FUG ONG  
 CTL

# $\text{CH}_4$ fluxes: Mean (2002-2012) Seasonal Cycle

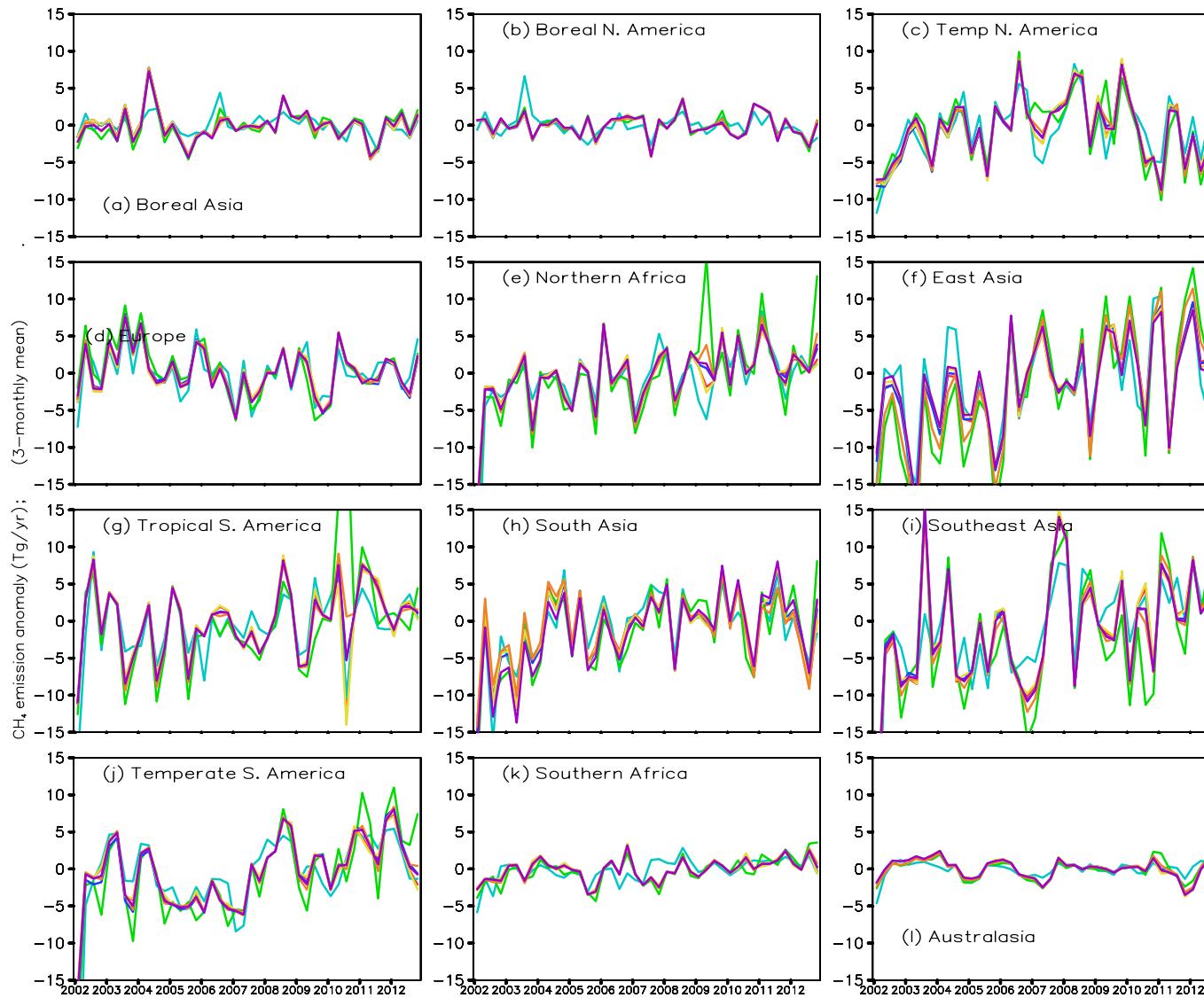


Results do  
not match!

Is it a good  
or bad  
thing?

Opportunity  
vs  
obviousness

# $\text{CH}_4$ fluxes: 3-monthly anomalies (2002-2012)



Can we now conclude that we understand / estimate the  $\text{CH}_4$  flux anomalies better than their annual means at regional scale

# Outlook

- Be open minded – as Gabi said the credit for discovery of “ozone hole” probably went to wrong person/group
-

# Survey

- Research interests (2-3 key words, e.g., aerosol, gases, dynamics)
- Method of research (model, satellite or in situ measurements)
- Research tools (Fortran, C, IDL, python, R, matlab)
- Years in research field
- Social media participation (Facebook, WhatsApp)
- Academic goal (optional)

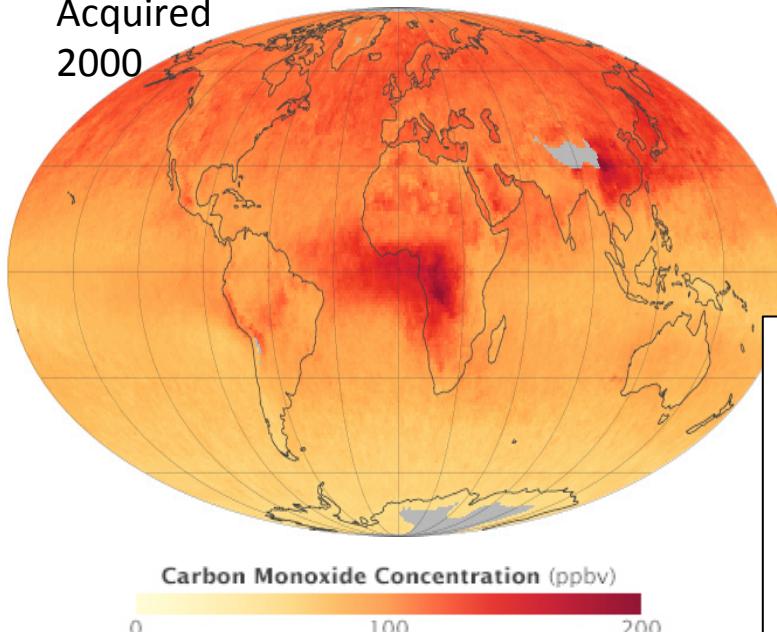
# CO<sub>2</sub>, CH<sub>4</sub>, CO growth rates

Make plots like CH<sub>4</sub> by Saeki-san

# CO from MOPITT

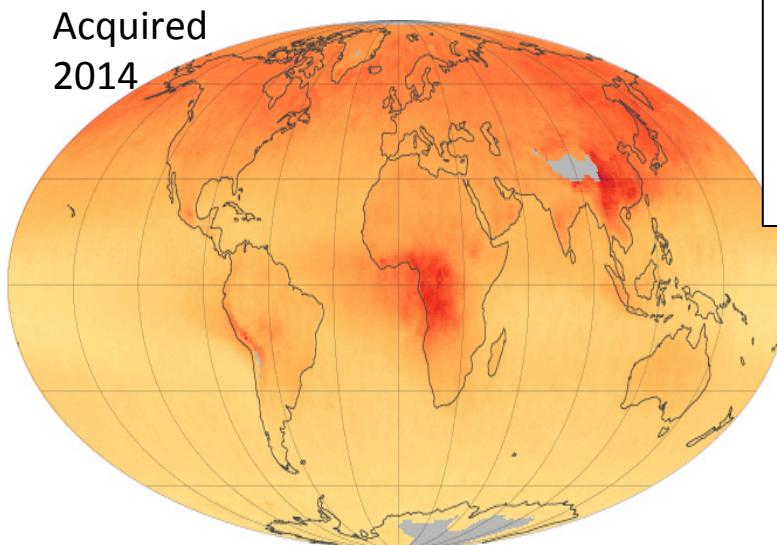
Acquired

2000



Acquired

2014



<http://earthobservatory.nasa.gov/IOTD/view.php?id=85967&src=eoia-iotd>

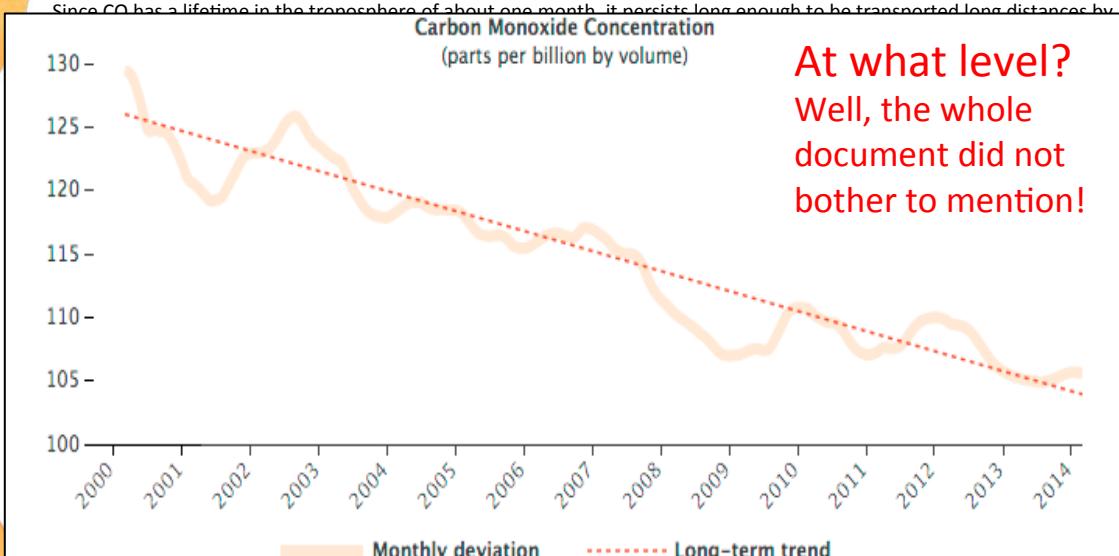
Carbon monoxide is perhaps best known for the lethal effects it can have in homes with faulty appliances and poor ventilation. In the United States, the colorless, odorless gas kills about 430 people each year.

However, the importance of carbon monoxide (CO) extends well beyond the indoor environment. Indoors or outdoors, the gas can disrupt the transport of oxygen by the blood, leading to heart and health problems. CO also contributes to the formation of tropospheric ozone, another air pollutant with unhealthy effects. And though carbon monoxide does not cause climate change directly, its presence affects the abundance of greenhouse gases such as methane and carbon dioxide.

Carbon monoxide forms whenever carbon-based fuels—including coal, oil, natural gas, and wood—are burned. As a result, many human activities and inventions emit carbon monoxide, including: the combustion engines in cars, trucks, planes, ships, and other vehicles; the fires lit by farmers to clear forests or fields; and industrial processes that involve the combustion of fossil fuels. In addition, wildfires and volcanoes are natural sources of the gas.

Little was known about the global distribution of carbon monoxide until the launch of the Terra satellite in 1999. Terra carries a sensor—Measurements of Pollution in the Troposphere (MOPITT)—that can measure carbon monoxide in a consistent fashion on a global scale. With a swath width of 640 kilometers (400 miles), MOPITT scans the entire atmosphere of Earth every three days.

Since CO has a lifetime in the troposphere of about one month, it persists long enough to be transported long distances by wind.

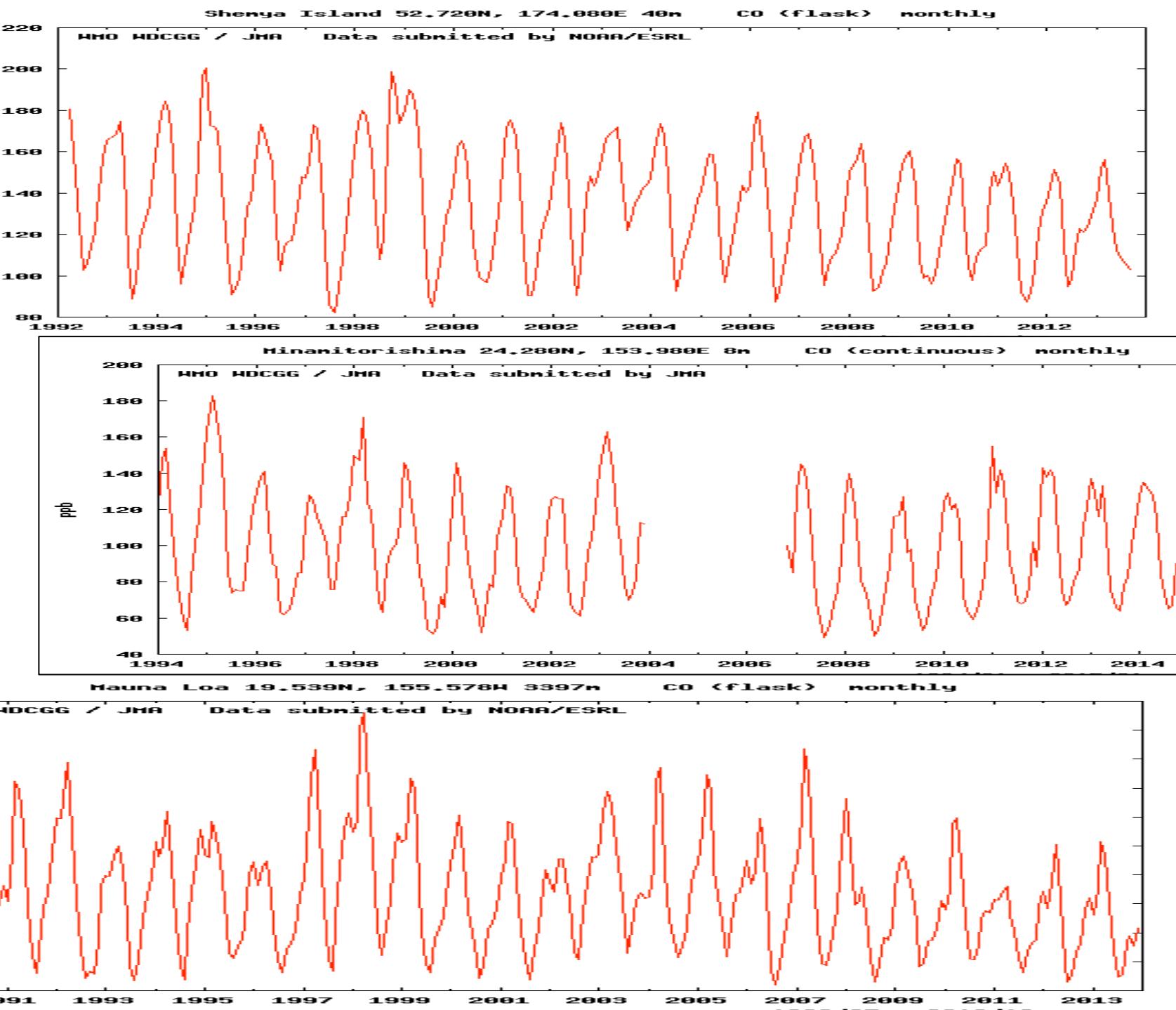


carbon monoxide over China and India, satellites and emissions inventories have shown that other pollutants like sulfur dioxide and nitrogen dioxide have risen during the same period.

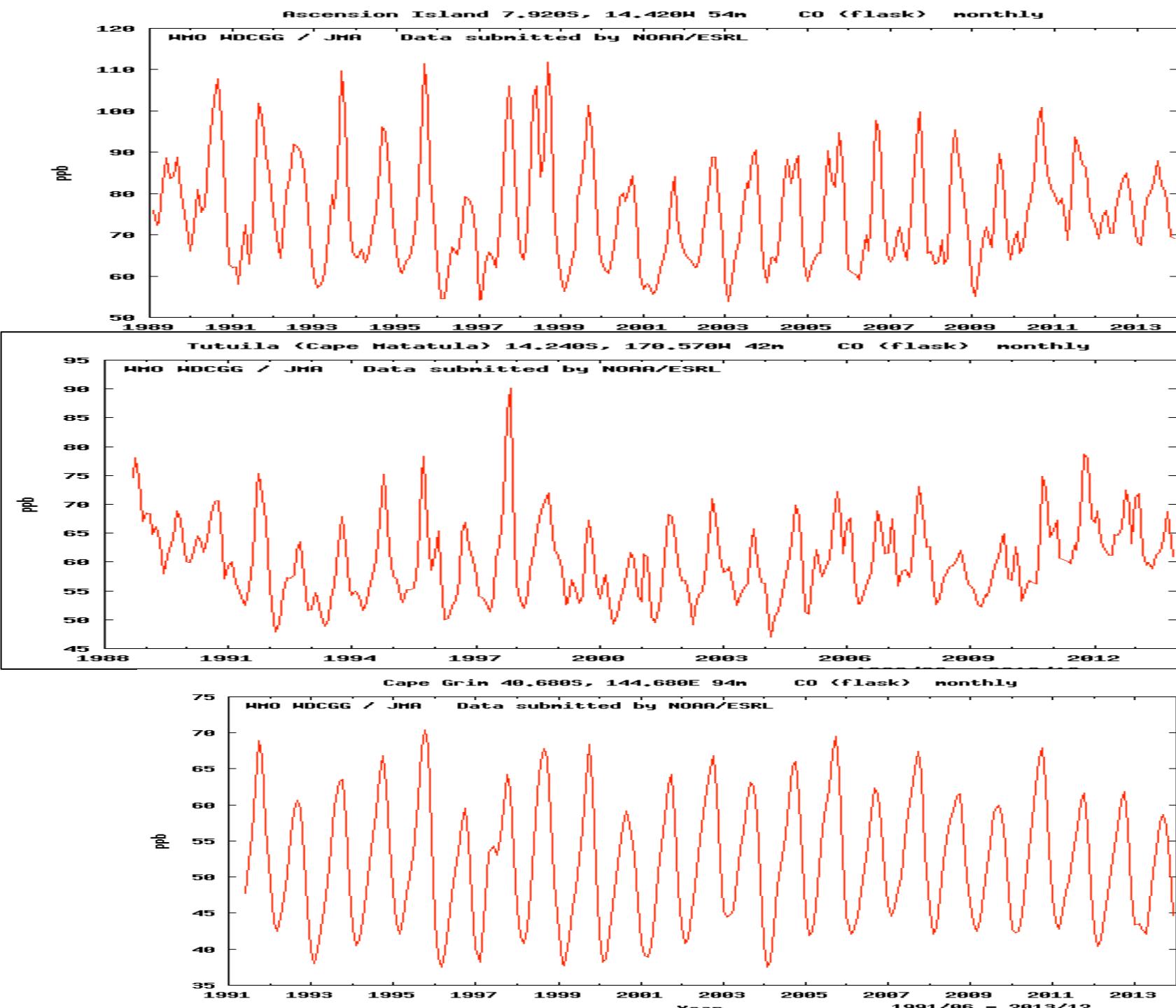
"For China, nitrogen dioxide emissions are mostly from the power and transportation sectors and have grown significantly since 2000 with the increase in demand for electricity," explained Helen Worden, an atmospheric scientist from the National Center for Atmospheric Research. "Carbon monoxide emissions, however, have a relatively small contribution (less than 2 percent) from the power sector, so vehicle emissions standards and improved combustion efficiency for newer cars have lowered carbon monoxide in the atmosphere despite the fact that there are more vehicles on the road burning more fossil fuel."

As illustrated by the maps, the news is also generally positive for the Southern Hemisphere, where deforestation and agricultural fires are the primary source of carbon monoxide. In South America, MOPITT observed a slight decrease in carbon monoxide; other satellites have observed decreases in the number of small fires and areas burned, suggesting a decrease in deforestation fires since 2005. Likewise, MOPITT has observed decreases in the amount of carbon monoxide

# CO from Surface sites (Northern Hemisphere)



# CO from Surface sites (Southern Hemisphere)



# Decadal trends in global CO emissions as seen by MOPITT

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**Abstract.** Negative trends of carbon monoxide (CO) concentrations are observed in the recent decade by both surface measurements and satellite retrievals over many regions, but they are not well explained by current emission inventories. Here, we attribute the observed CO concentration decline with an atmospheric inversion that simultaneously optimizes the two main CO sources (surface emissions and atmospheric hydrocarbon oxidations) and the main CO sink (atmospheric hydroxyl radical OH oxidation) by assimilating observations of CO and other chemically related tracers. Satellite CO column retrievals from Measurements of Pollution in the Troposphere (MOPITT), version 6, and surface in-situ measurements of methane and methyl-chloroform mole fractions are assimilated jointly for the period of 2002–2011. Compared to the prior simulation, the optimized CO concentrations show better agreement with independent surface in-situ measurements in terms of both distributions and trends. At the global scale, the atmospheric inversion primarily interprets the CO concentration decline as a decrease in the CO emissions, and finds noticeable trends neither in the chemical oxidation sources of CO, nor in the OH concentrations that regulate CO sinks. The latitudinal comparison of the model state with independent formaldehyde ( $\text{CH}_2\text{O}$ ) columns retrieved from the Ozone Measurement Instrument (OMI) confirms the absence of large-scale trends in the atmospheric source of CO. The global CO emission decreased by 17% during the decade, more than twice the negative trend estimated by emission inventories. The spatial distribution of the inferred decrease of CO emissions indicates contributions from both a decrease in fossil- and bio-fuel emissions over Europe, the USA and Asia, and from a decrease in biomass burning emissions in South America, Indonesia, Australia and Boreal regions. An emission decrease of  $2\% \text{ yr}^{-1}$  is inferred in China, one of the main emitting regions, in contradiction with the bottom-up inventories that report an increase of  $2\% \text{ yr}^{-1}$  during the study period. A large decrease in CO emission factors due to technology improvements would outweigh the increase of carbon fuel combustions and may explain the observed decrease. In Africa, instead of the negative trend ( $1\% \text{ yr}^{-1}$ ) reported by CO emission inventories mainly contributed by biomass burning, a positive trend ( $1.5\% \text{ yr}^{-1}$ ) is found by the atmospheric inversion, suggesting different trends between satellite-detected burned areas and CO emissions.

**Citation:** Yin, Y., Chevallier, F., Ciais, P., Broquet, G., Fortems-Cheiney, A., Pison, I., and Saunois, M., Global CO emissions as seen by MOPITT, *Atmos. Chem. Phys. Discuss.*, 15, 14505–14547, doi:10.5194/acpd-15-14505-2015, 2015.

**Review Status**  
This discussion paper is under review for the journal *Atmospheric Chemistry and Physics (ACP)*.

