Using mathematical inverse theory to estimate respiratory and photosynthetic fluxes in a heterogeneous conifer canopy

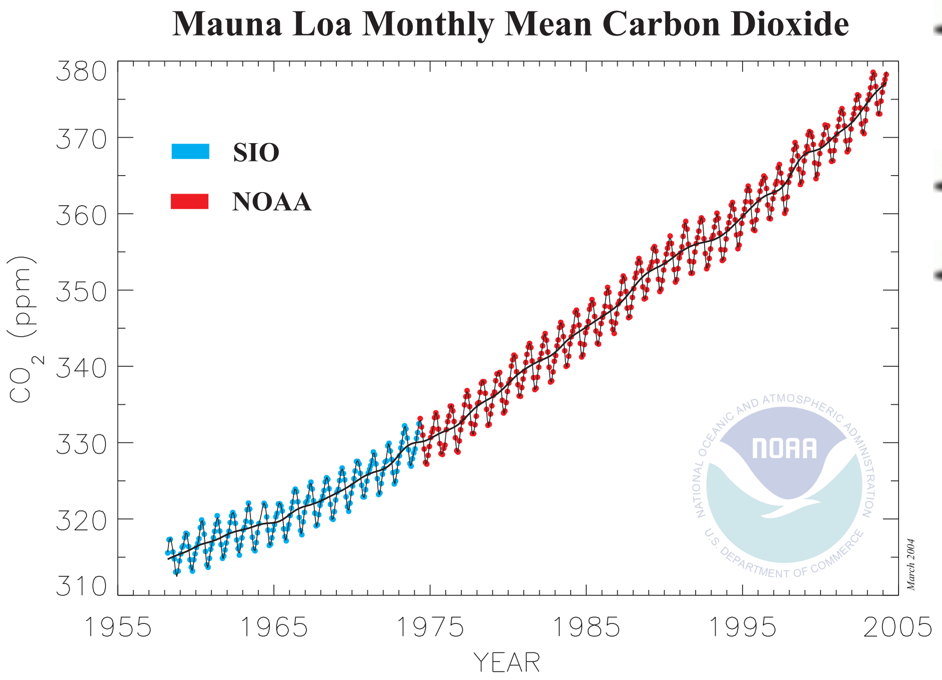
John M. Zobitz
with
David R. Bowling, Frederick R. Adler, James P. Keener, Jerome Ogée

UT-AZ IGERT Summit

Outline

- The Global Carbon Cycle
  - Historical CO_2 trends
  - 1990s Carbon Cycle
  - The influence of multiple scales
- Measuring ecosystem-scale fluxes of CO_2
  - Net Ecosystem Exchange (NEE)
  - Niwot Ridge AmeriFlux tower
  - Components of NEE
- Stable carbon isotopes
- Mathematical inverse theory
  - Traditional approaches to estimate photosynthesis and respiration
  - Probabilistic inverse theory
  - Uncertainty reduction

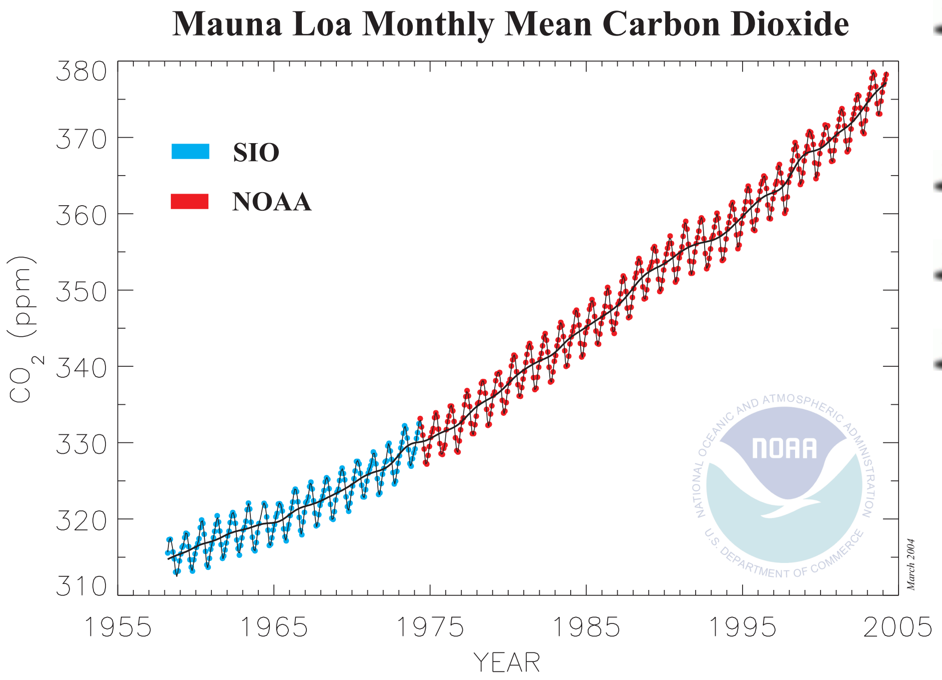
Historical CO_2 trends



Atmospheric carbon dioxide monthly mean mixing ratios. Data prior to May 1974 are from the Scripps Institution of Oceanography (SIO, blue), data since May 1974 are from the National Oceanic and Atmospheric Administration (NOAA, red). A long-term trend curve is fitted to the monthly mean values. Principal investigators: Dr. Pieter Tans, NOAA CMDL Carbon Cycle Greenhouse Gases, Boulder, Colorado, (303) 497-6678, pieter.tans@noaa.gov, and Dr. Charles D. Keeling, SIO, La Jolla, California, (616) 534-6001, cdkeeling@ucsd.edu.

- 1000-1800 CE: ≈ 280 ppm atmospheric [CO_2]
- 1980: ≈ 335 ppm
- 2005: ≈ 375 ppm

Historical CO_2 trends

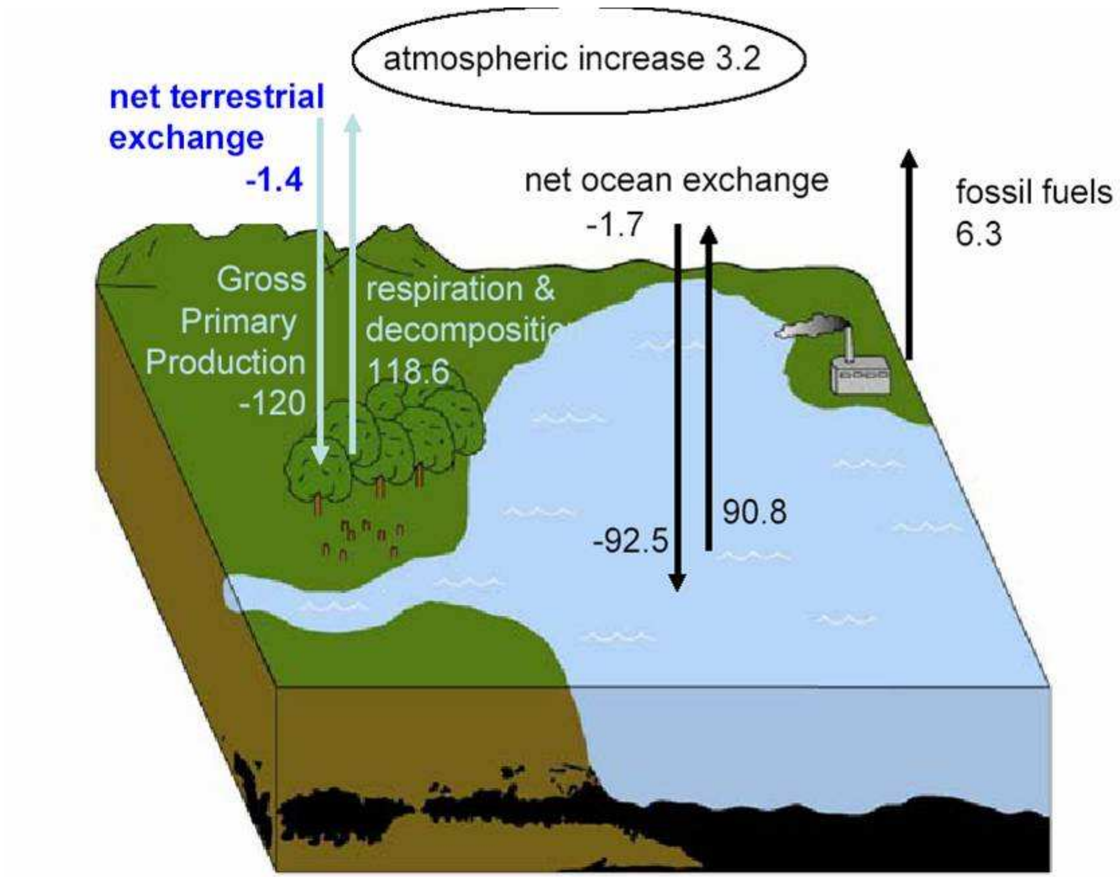


Atmospheric carbon dioxide monthly mean mixing ratios. Data prior to May 1974 are from the Scripps Institution of Oceanography (SIO, blue), data since May 1974 are from the National Oceanic and Atmospheric Administration (NOAA, red). A long-term trend curve is fitted to the monthly mean values. Principal investigators: Dr. Pieter Tans, NOAA CMDL Carbon Cycle Greenhouse Gases, Boulder, Colorado, (303) 497-6678, pieter.tans@noaa.gov, and Dr. Charles D. Keeling, SIO, La Jolla, California, (616) 534-6001, cdkeeling@ucsd.edu.

- 1000-1800 CE: $\approx$ 280 ppm atmospheric [CO_2]
- 1980: $\approx$ 335 ppm
- 2005: $\approx$ 375 ppm
- **42% of the increase has happened during my lifetime!**

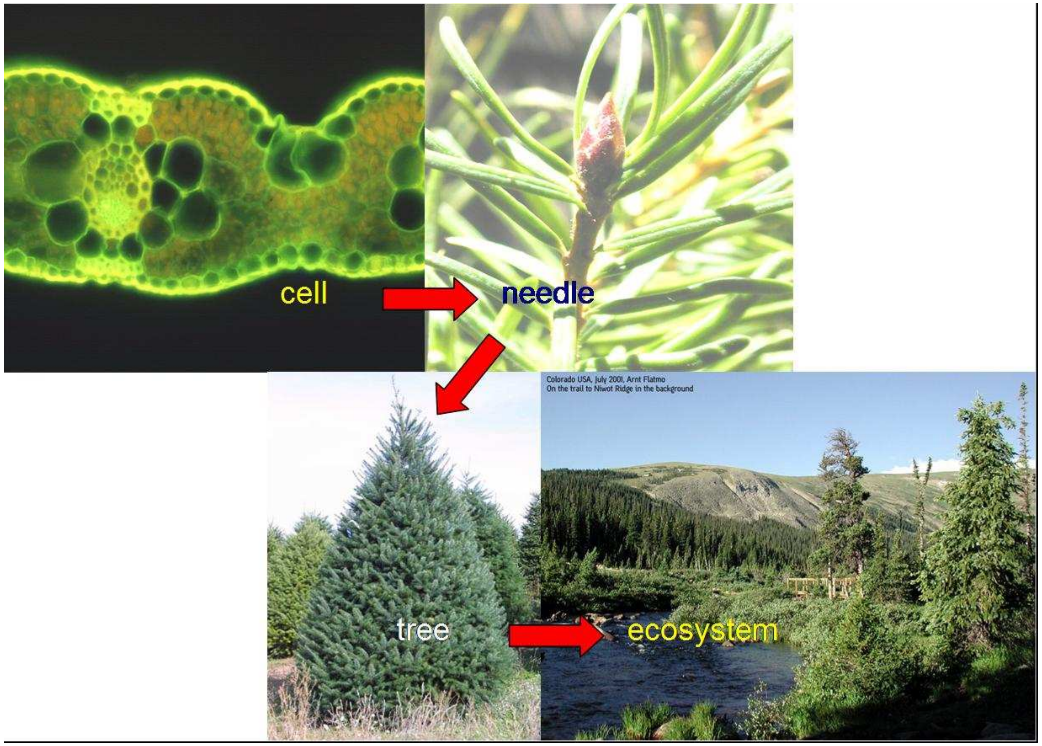
1990s Carbon Cycle

This overall increase in CO_2 is a reflection of perturbations to the global carbon cycle (Schimel and others, 2001) (units Gt C/yr).

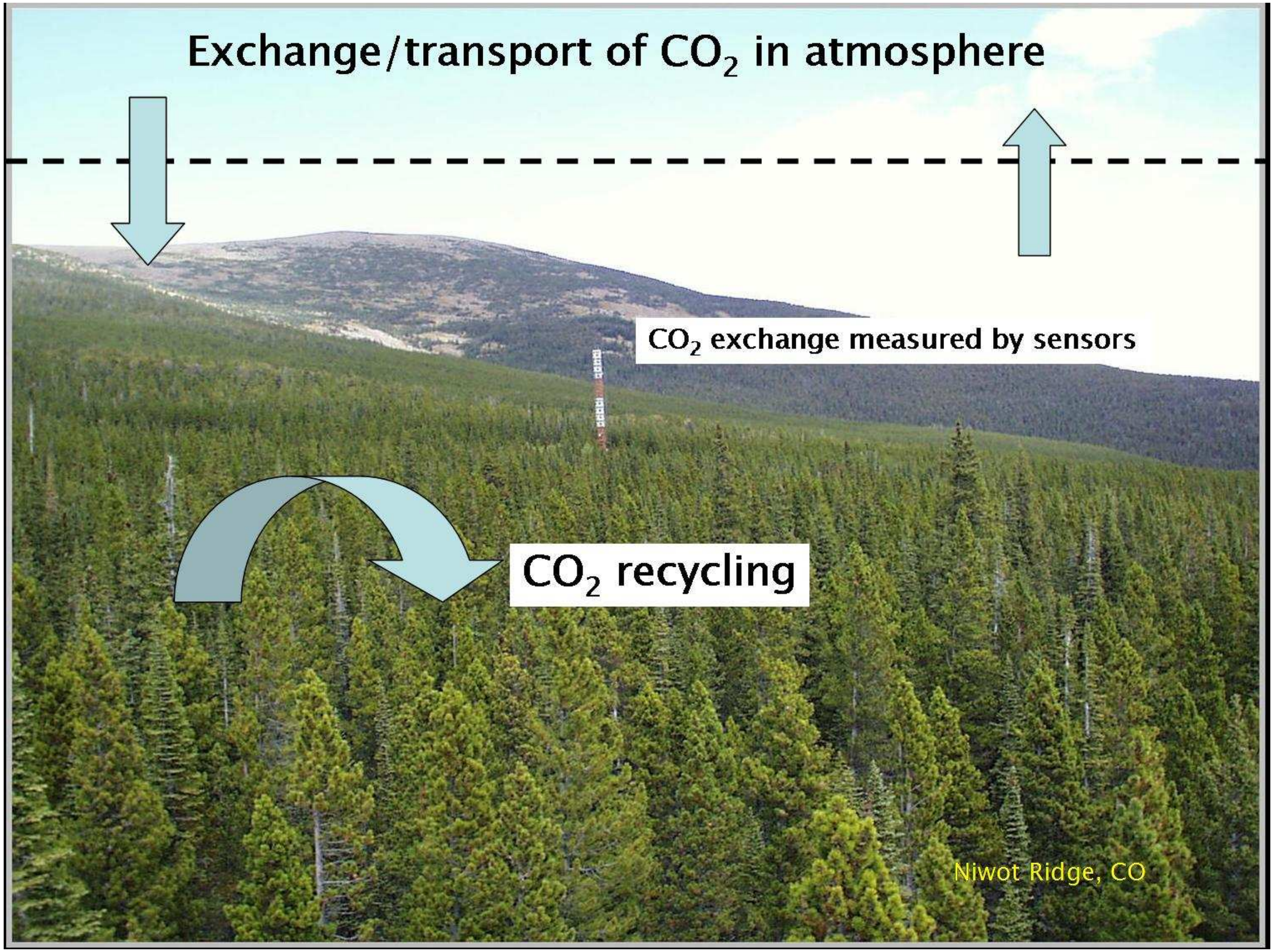


Influence of Multiple Scales

CO_2 is produced on the **cellular** level, but we want a canopy scale measure.

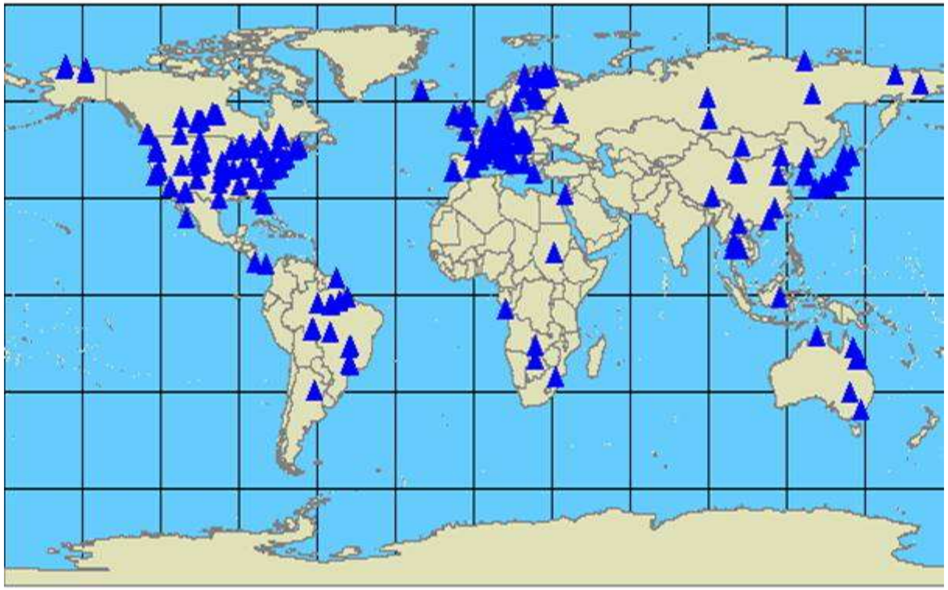


Net Ecosystem Exchange (NEE)



Measuring NEE

NEE is measured at more than 250 sites worldwide This provides a worldwide monitoring network of CO_2 fluxes that allows us to generalize about ecosystem-atmosphere exchange (Baldocchi and others, 2001).



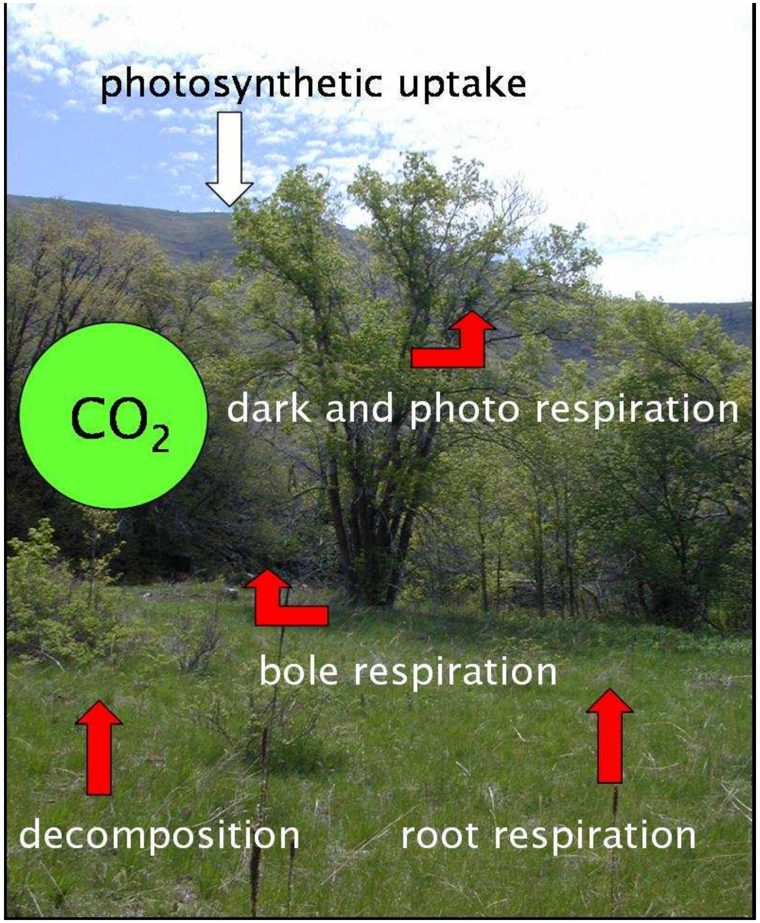
Niwot Ridge AmeriFlux tower, CO

Niwot Ridge photo
taken May 6, 2005 by Sean P. Burns

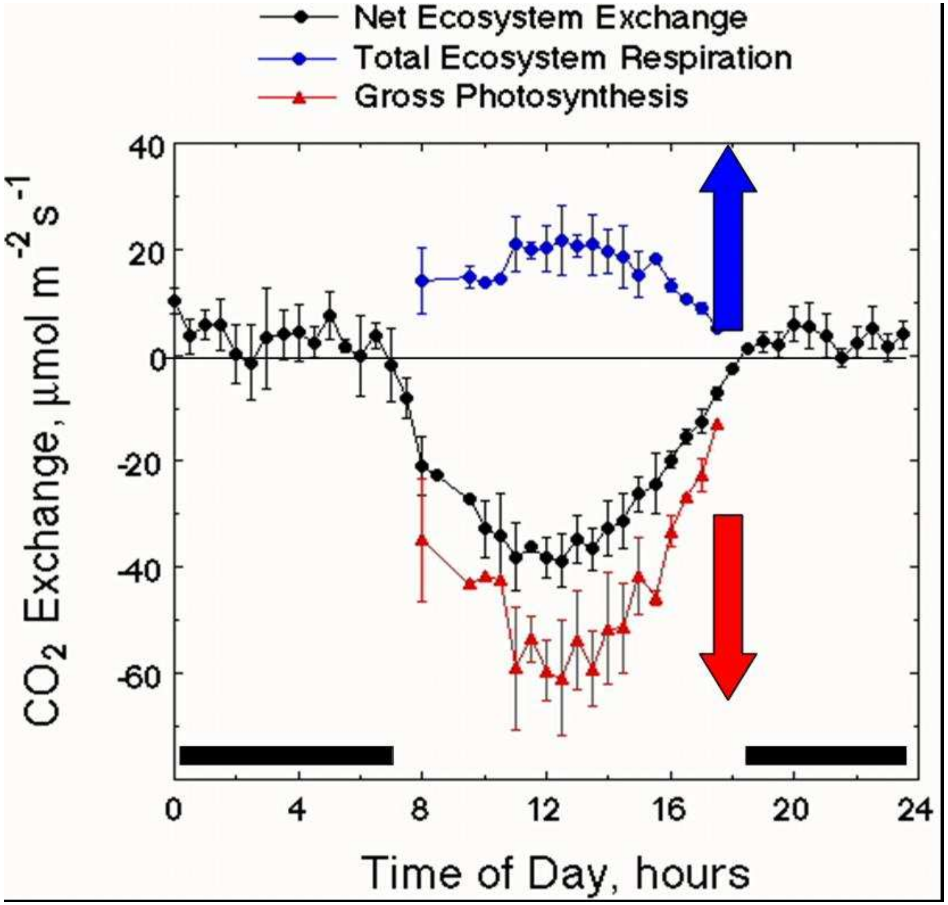
- subalpine forest west of Boulder, CO
- 3 dominant species:
  - lodgepole pine *Pinus contorta*
  - Engelmann spruce *Picea engelmannii*
  - subalpine fir *Abies lasiocarpa*
- 3050 m (10,000 ft) elev

Components of NEE

- NEE is made up of two components:
  - Gross Primary Productivity (F_A) = Flux due to photosynthesis
  - Total Ecosystem Respiration (F_R)= Fluxes due to respiration + decomposition
- The sum of these two determine an ecosystem's terrestrial carbon budget



Diurnal pattern of NEE



Flanagan and Pattey, unpublished

Stable Carbon Isotopes

- In order to estimate F_A and F_R, we need to use stable carbon isotopes.

Average terrestrial abundance		**Average atmospheric content**	
^{12}C	98.89%	$^{12}CO_2$	370 μmol mol^{-1}
^{13}C	1.11%	$^{13}CO_2$	4 μmol mol^{-1}

Dawson et al. (2002)

Stable Carbon Isotopes

- Since the absolute abundance of ^{13}C is so small, measurements are expressed with dimensionless units "permil" (‰) as a ratio compared to ^{12}C:

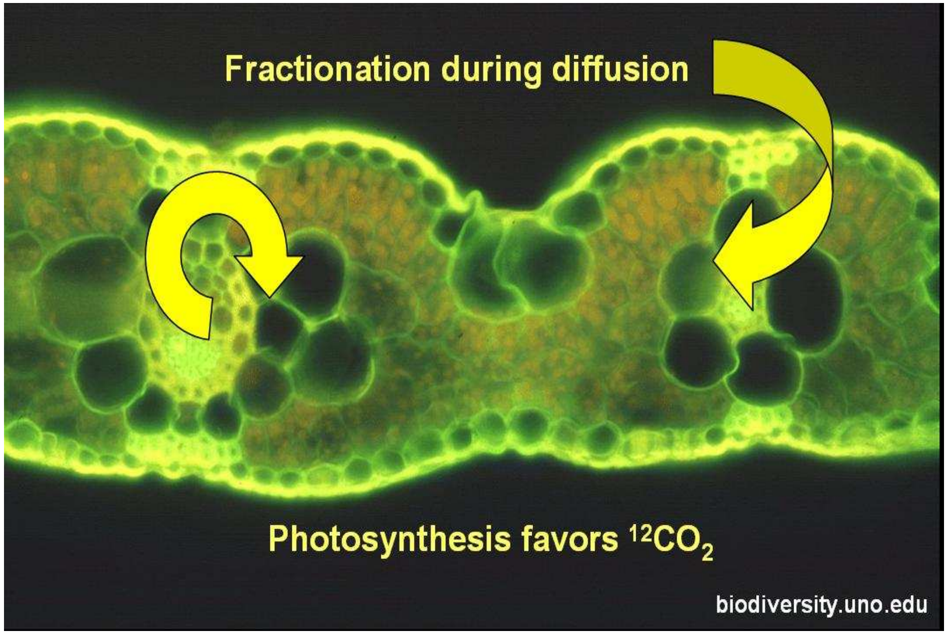
$$\delta^{13}C \ (‰) = \frac{(^{13}C/^{12}C)_{sample} - (^{13}C/^{12}C)_{standard}}{(^{13}C/^{12}C)_{standard}} \times 1000 \qquad (1)$$

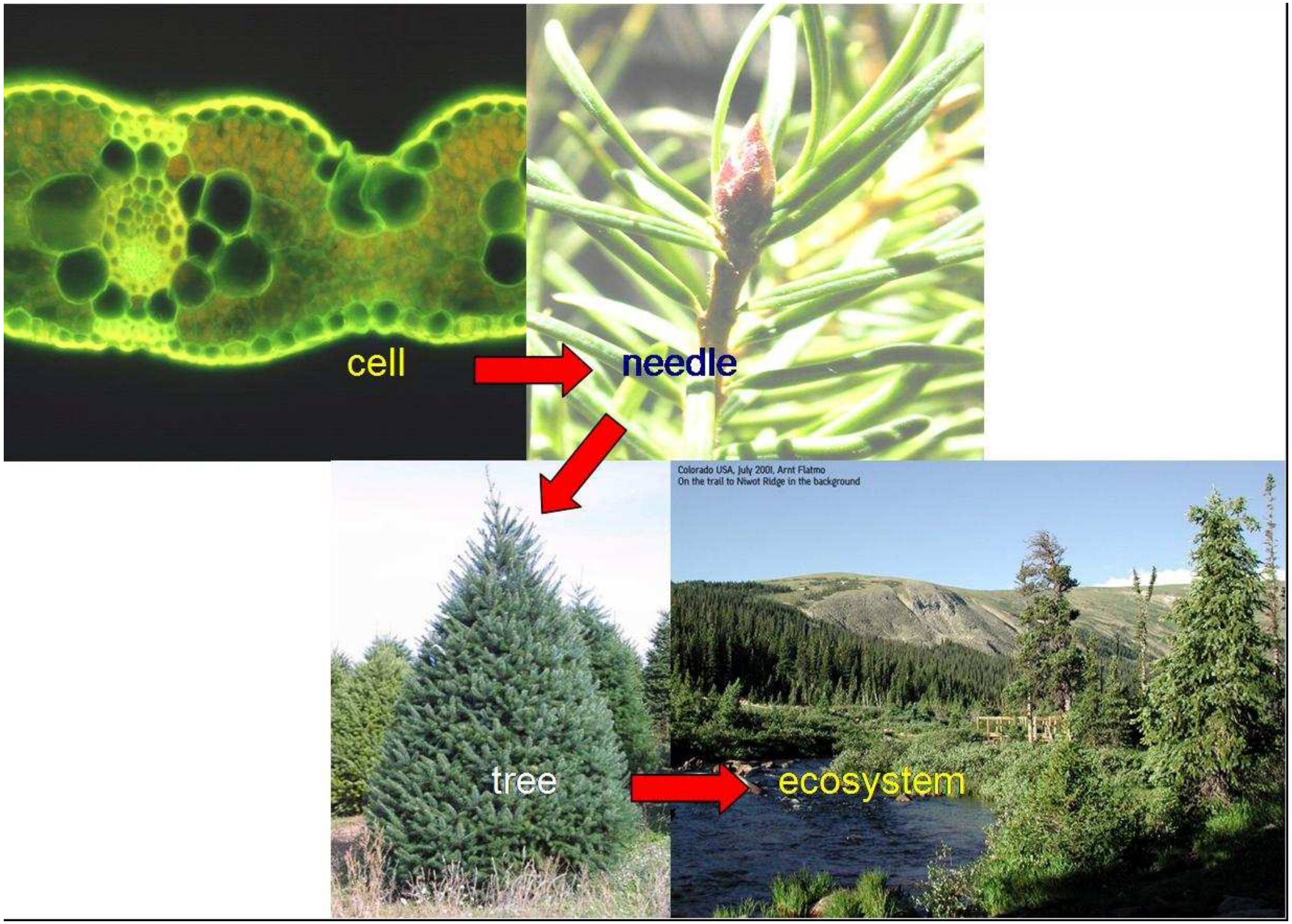
PDB Standard	0‰ by definition
CO_2 in air	-8‰ (-7 to -15‰)
C_3 plant biomass	-24 to -30‰
Respired CO_2	-24 to -30‰

- Negative numbers mean that the sample is depleted of ^{13}C relative to a standard.

Stable Carbon Isotopes

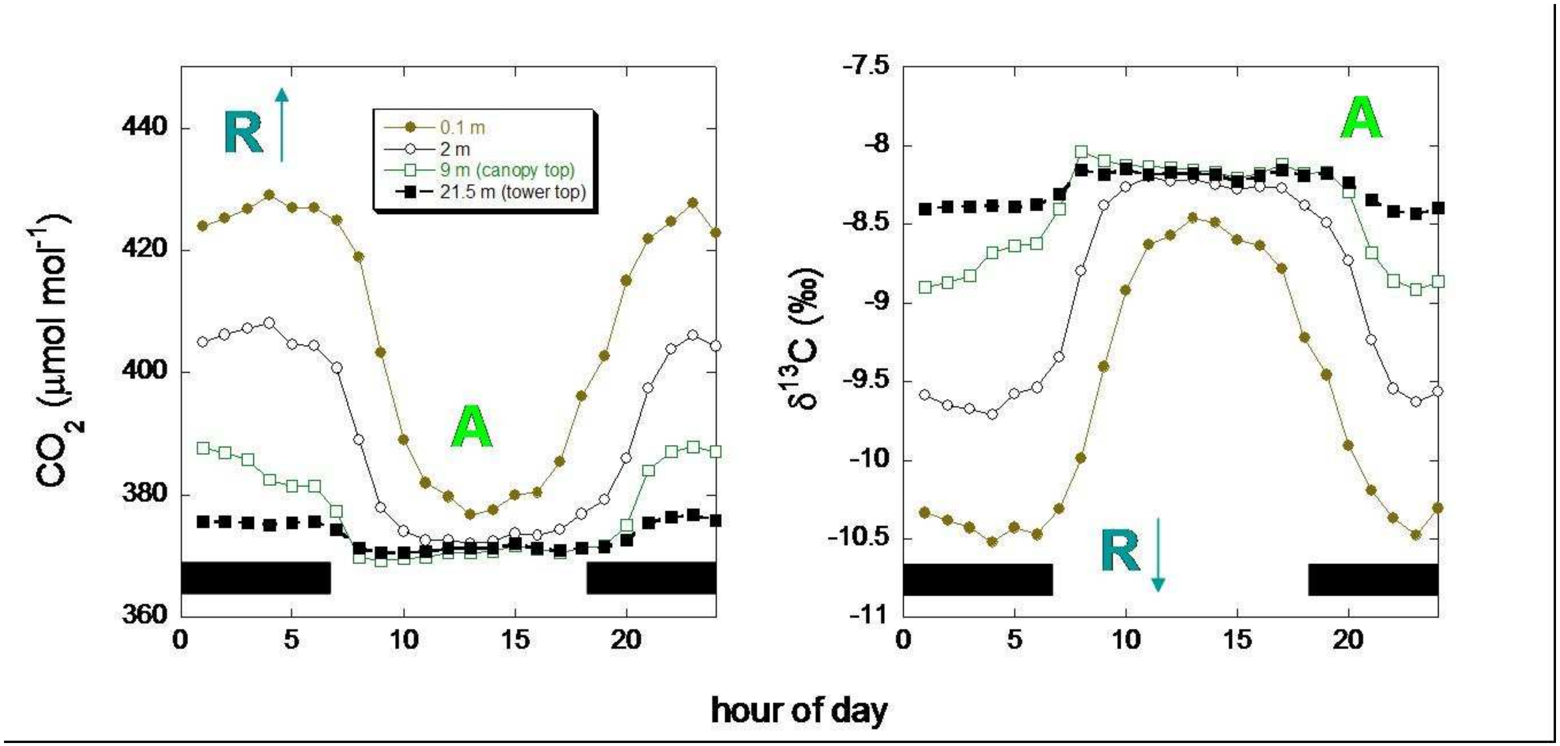
- $^{13}CO_2$ is a heavier molecule than $^{12}CO_2$, so it will diffuse more slowly to the sites of photosynthesis.
- This has an effect of making the atmosphere more *enriched* in $^{13}CO_2$.
- During photosynthesis, $^{12}CO_2$ is biochemically preferred, making photosynthesized carbon *depleted* in $^{13}CO_2$





Colorado USA, July 2001, Arnt Flatmo
On the trail to Niwot Ridge in the background

Niwot Ridge Diurnal CO_2 and $^{13}CO_2$



3 week averages, summer 2003 Bowling et al. (in review)

Biological Formulation of the Problem

- It is possible to write an equation for conservation of $^{13}CO_2$ (Yakir and Wang, 1996; Bowling et al., 2001).
- Using standard notation, it can be written as a linear combination of F_A and F_R:

$$F_A + F_R = F_{Net} \text{ (conservation of CO}_2\text{)} \quad (2)$$

$$\delta_A F_A + \delta_R F_R = F_\delta \text{ (conservation of }^{13}\text{CO}_2\text{)} \quad (3)$$

- Where:
  - F_{Net} = Net Ecosystem Exchange (NEE)
  - δ_A: Isotopic signature of photosynthesis ($\approx$-18 to -30‰)
  - δ_R: Isotopic signature of respiration ($\approx$-20 to -28‰)
  - F_δ: NEE of $^{13}CO_2$

Flux partitioning as an inverse problem

- We want to estimate F_A and F_R by measuring CO_2 fluxes.
- There is an exact functional relationship between our measured quantities and estimated parameters:

$$F_A + F_R = F_{Net} \tag{4}$$

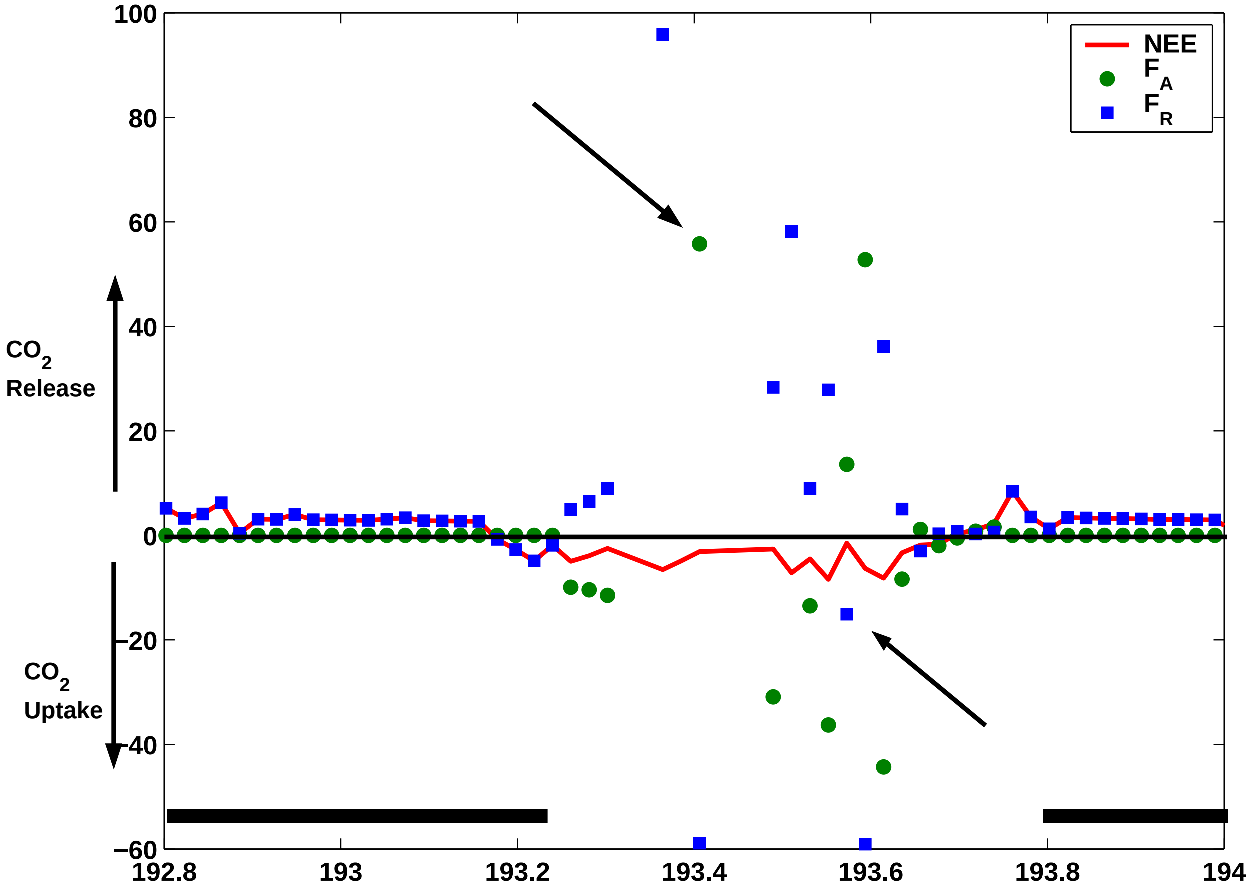
$$\delta_A F_A + \delta_R F_R = F_\delta \tag{5}$$

$$\Downarrow \Downarrow \tag{6}$$

$$g(m) = d_{obs} \tag{7}$$

- We have two equations, two unknowns, so let's solve!
- Determining F_A and F_R is called “flux partitioning.”

Results



vertical axis units: μmol/m^2/sec

What went wrong?

$$F_A + F_R = F_{Net}$$

$$\delta_A F_A + \delta_R F_R = F_\delta$$

$$\Downarrow\Downarrow$$

$$g(m) = d_{obs}$$

- Note that when $\delta_A \approx \delta_R$, we cannot find a unique solution!
- Furthermore there are parameter constraints: $F_A \leq 0$, $F_R \geq 0$.
- We also know that $F_A \approx -10 \pm 5$, $F_R \approx 5 \pm 5$, so why not use this information?

Probabilistic Inverse Theory

- Inverse problems define a relationship between estimated parameters m and measured data d_{obs}:

$$g(m) = d_{obs}$$

- Bayes' Theorem informally states that:

$$P(A|B) = P(B|A)P(A)$$

- Assume that our distributions on m and d_{obs} are Gaussian. When we apply Bayes' Theorem to the joint manifold $X = D \bigcup M$, then the posterior distribution on m will be Gaussian.

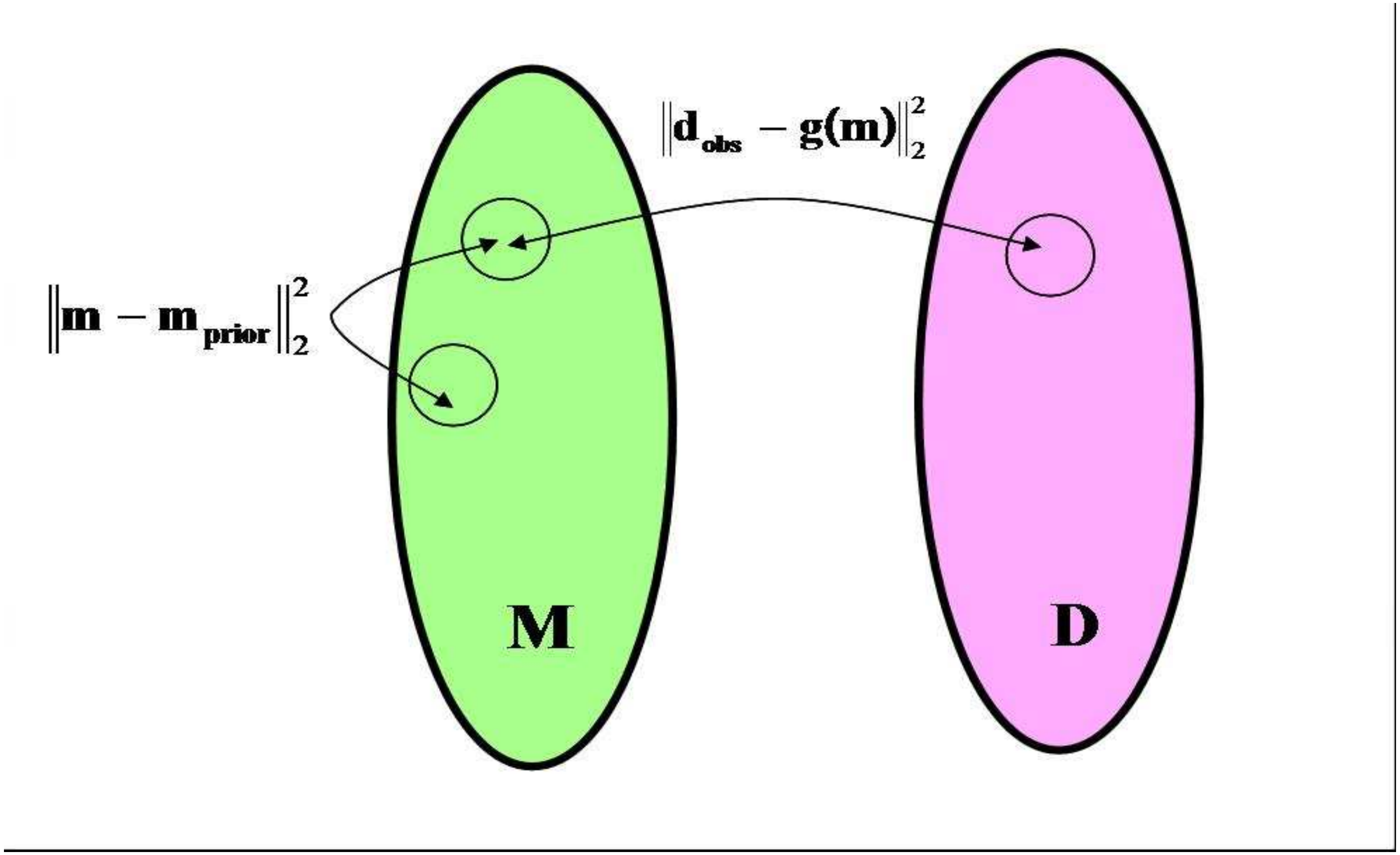
Equivalence to a least-squares condition

- Define a linear space $M \in \mathbb{R}^m$, $D \in \mathbb{R}^n$, where $g : \mathbb{R}^m \rightarrow \mathbb{R}^n$.
- Under the assumptions of Gaussian distributions, it is possible to find the best parameters m that produce d_{obs} by minimizing the following functional: (Tarantola, 2005)

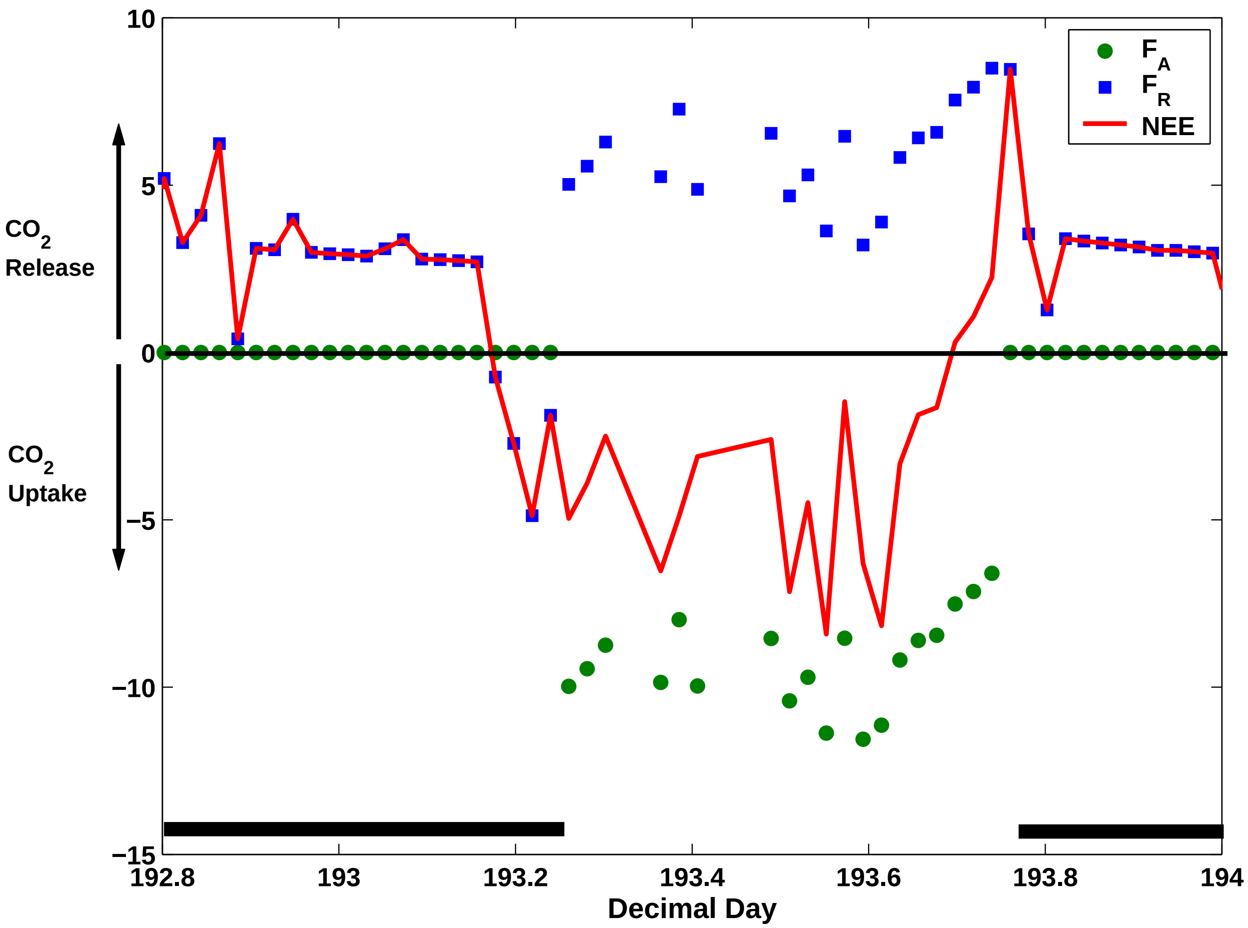
$$S(m) = \|d_{obs} - g(m)\|^2 + \|m - m_{prior}\|^2,$$

- where:
  - m_{prior}: Prior estimates on parameters m.

Mathematical Formulation



Results



vertical axis units: μmol/m^2/sec

Discrete-time Smoothing

- Alternatively, we can consider correlations of our parameters between timesteps:

$$g(m^{(t)}) = d_{obs}^{(t)}$$
$$m^{(t+1)} = f(m^{(t)})$$

Discrete-time Smoothing

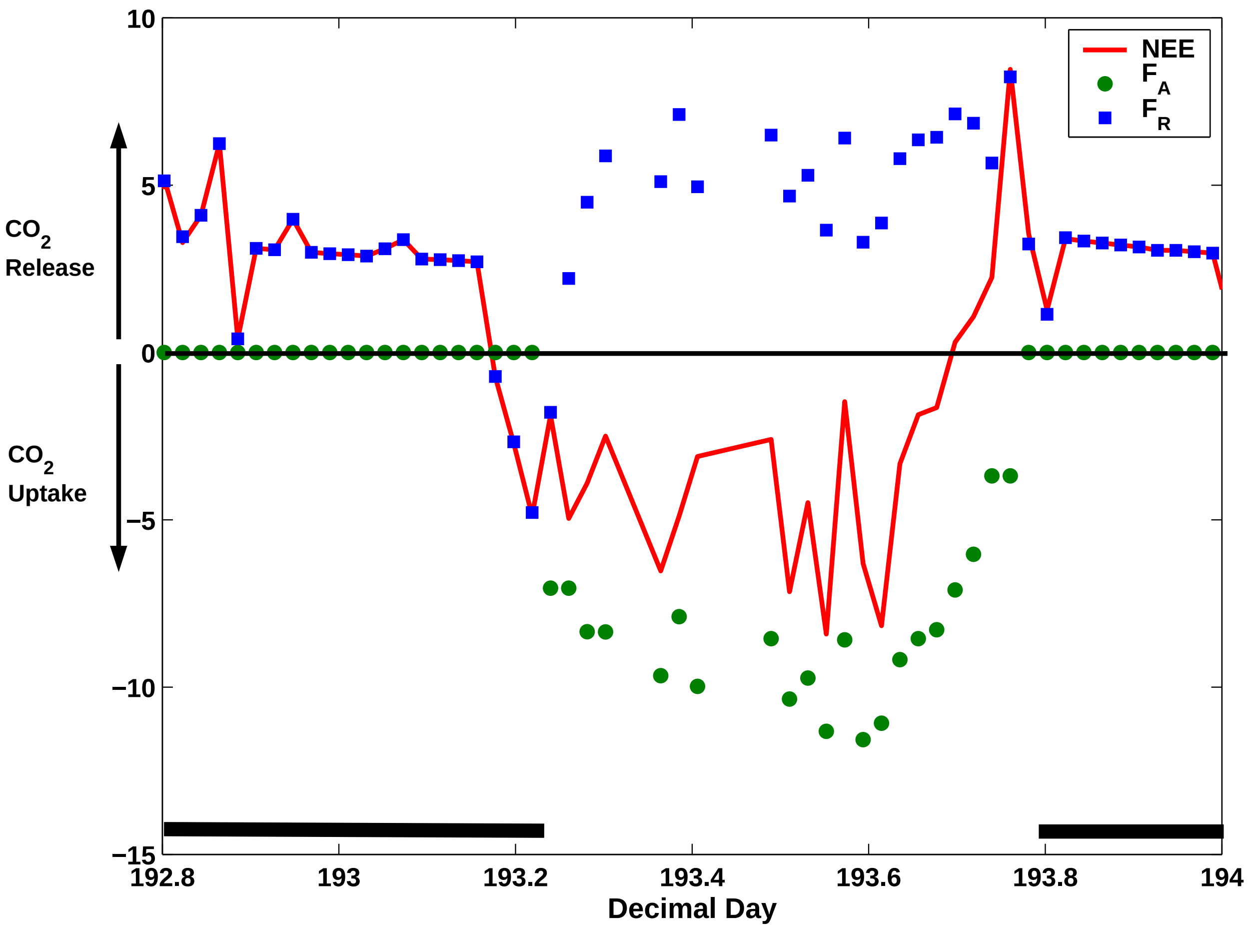
- Alternatively, we can consider correlations of our parameters between timesteps:

$$g(m^{(t)}) = d_{obs}^{(t)}$$
$$m^{(t+1)} = f(m^{(t)})$$

- We can still apply Bayes' Theorem.
- The case we consider is $m^{(t+1)} - m^{(t)} \sim N(0, \sigma_m)$.
- When this is done, we can define the following functional:

$$S(m) = \|d_{obs} - g(m)\|^2 + \|m - m_{prior}\|^2 + \|Dm\|^2,$$

Results



vertical axis units: μmol/m^2/sec

Uncertainty Reduction

	Maximum Uncertainty in F_A (μmol/m^2/sec)	**Maximum Uncertainty in F_R (μmol/m^2/sec)**
Prior values	5	5
Traditional Partitioning	581.75	580.45
Unsmoothed Partitioning	3.64	3.62
Smoothed Partitioning	2.89	2.89

Work in Progress

- Application of other methods (Backus-Gilbert, etc)
- More careful characterization of $g(m) = d_{obs}$
- Understanding the influence of prior values

References

Baldocchi, D. D., et al., 2001. FLUXNET: A New Tool to Study the Temporal and Spatial Variability of Ecosystem-Scale Carbon Dioxide, Water Vapor, and Energy Flux Densities. Bulletin of the American Meterological Society 82 (11), 2415–2434.

Bowling, D. R., Burns, S. P., Conway, T. J., Monson, R. K., White, J. W. C., in review. Extensive observations of CO_2 carbon isotope content in and above a high-elevation subalpine forest. Global Biogeochemical Cycles.

Bowling, D. R., Tans, P. P., Monson, R. K., 2001. Partitioning net ecosystem carbon exchange with isotopic fluxes of CO_2. Global Change Biology 7, 127–145.

Dawson, T. E., Mambelli, S., Plamboeck, A. H., et al., 2002. Stable Isotopes in Plant Ecology. Annual Review of Ecological Systems 33, 507–59.

Schimel, D. S., et al., 2001. Recent patterns and mechanisms of carbon exchange by terrestrial ecosystems. Nature 414, 169–172.

Tarantola, A., 2005. Inverse Problem Theory and Model Parameter Estimation. SIAM Books, Philadelphia, PA.

Yakir, D., Wang, X.-F., 1996. Fluxes of CO_2 and water between terrestrial vegetation and the atmosphere estimated from isotope measurements. Nature 380, 515–517.