

1 Example Applications of Pool Models

2 Reducing Model Complexity

- The Carbon Cycle example
- Asking Simpler Questions
- Answer Questions more simply

3 Compartmental Systems

Pool Models

An Introduction

Markus Müller, Holger Metzler, Carlos Sierra

August 8, 2019

Max Planck Institute
for Biogeochemistry



- What are pool models?
- Why do we need them?
- What can they be used for?
 - ▶ What is needed?
 - ▶ What can we learn from them?

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Outline

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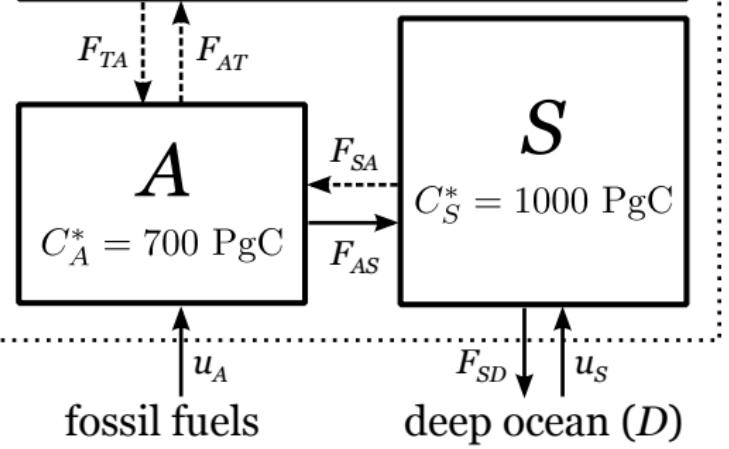
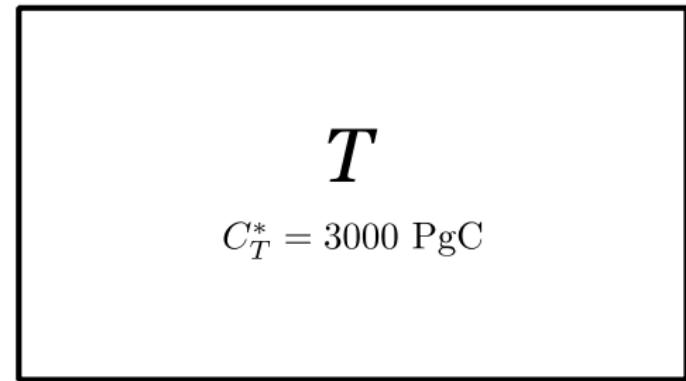
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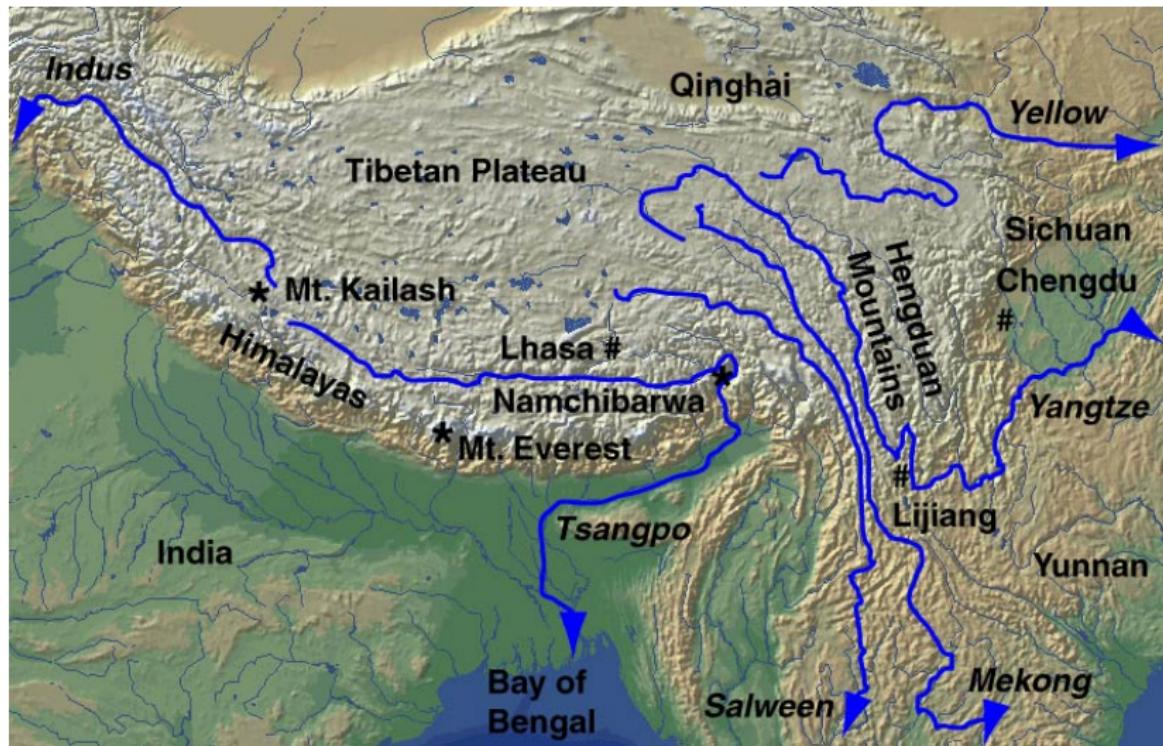
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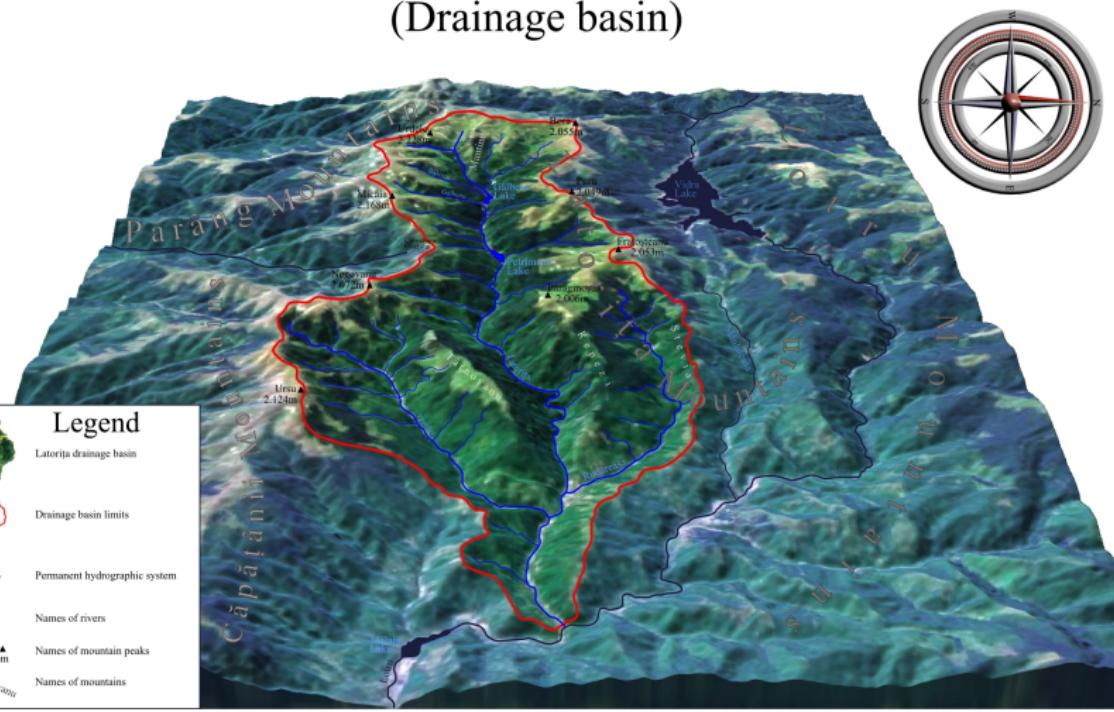


Hydrology Watersheds

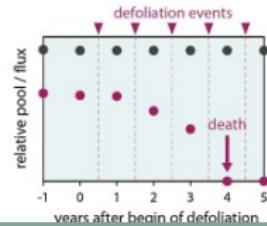
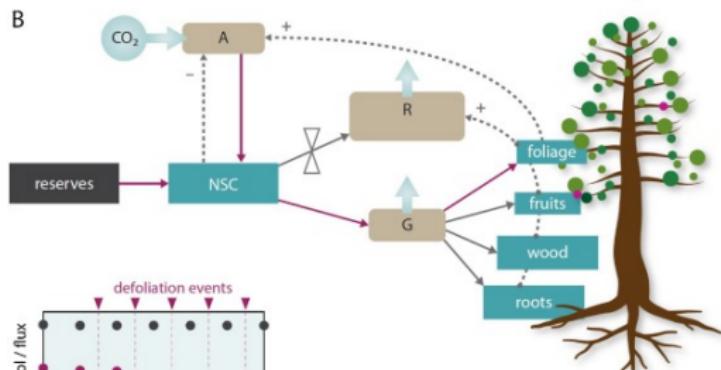
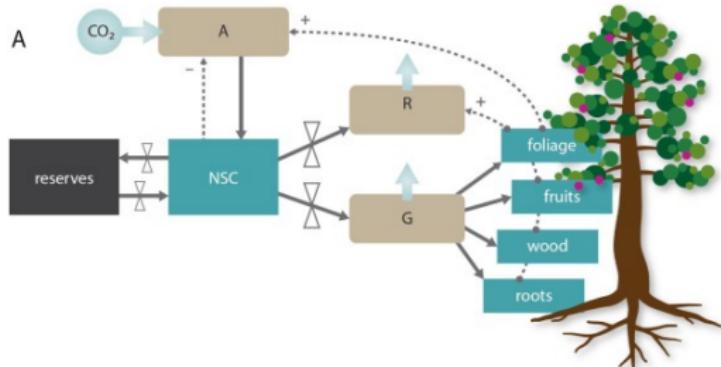


Hydrology Catchments

Latorița River, tributary of the Lotru River (Drainage basin)

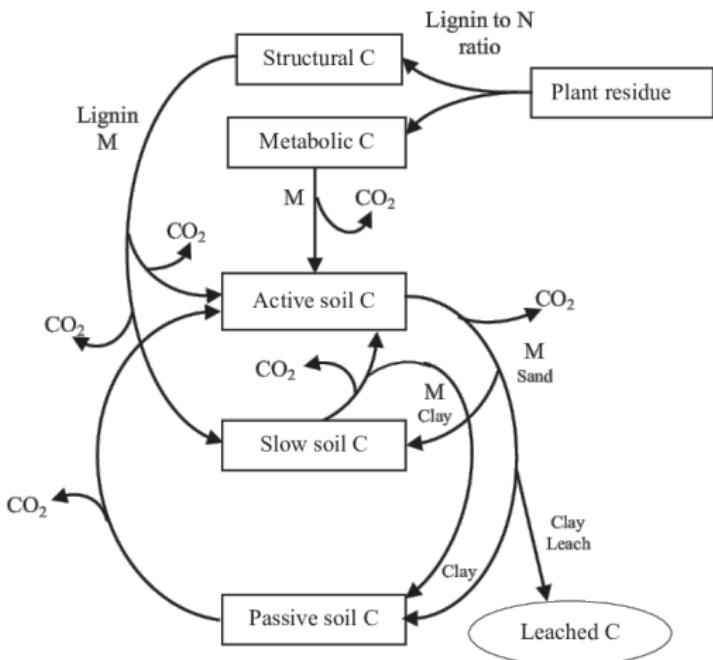
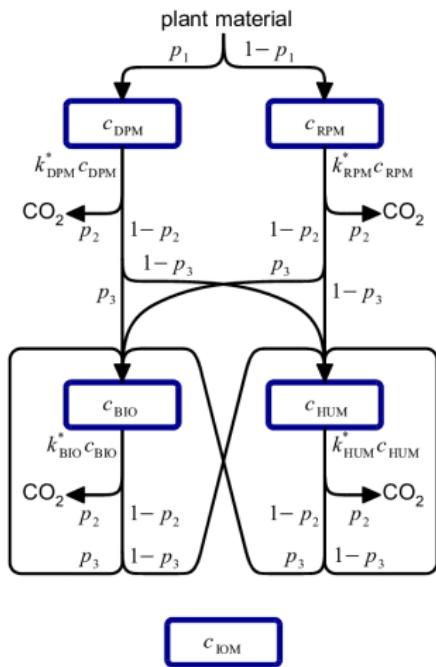


Plant Physiology/ Carbon allocation

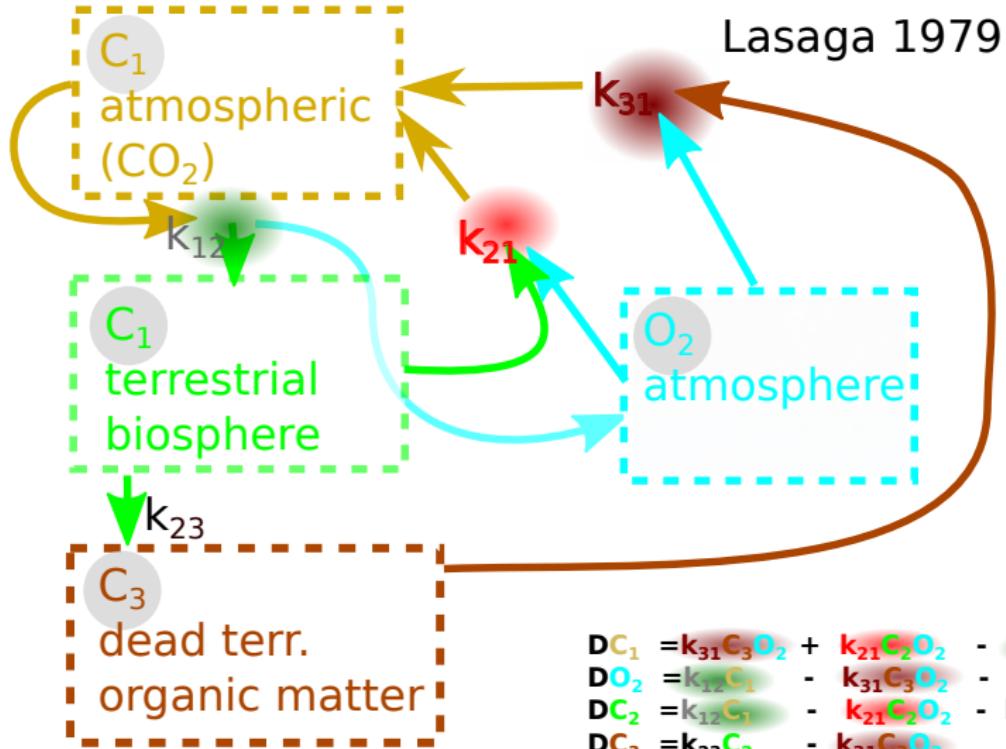


Pool Models

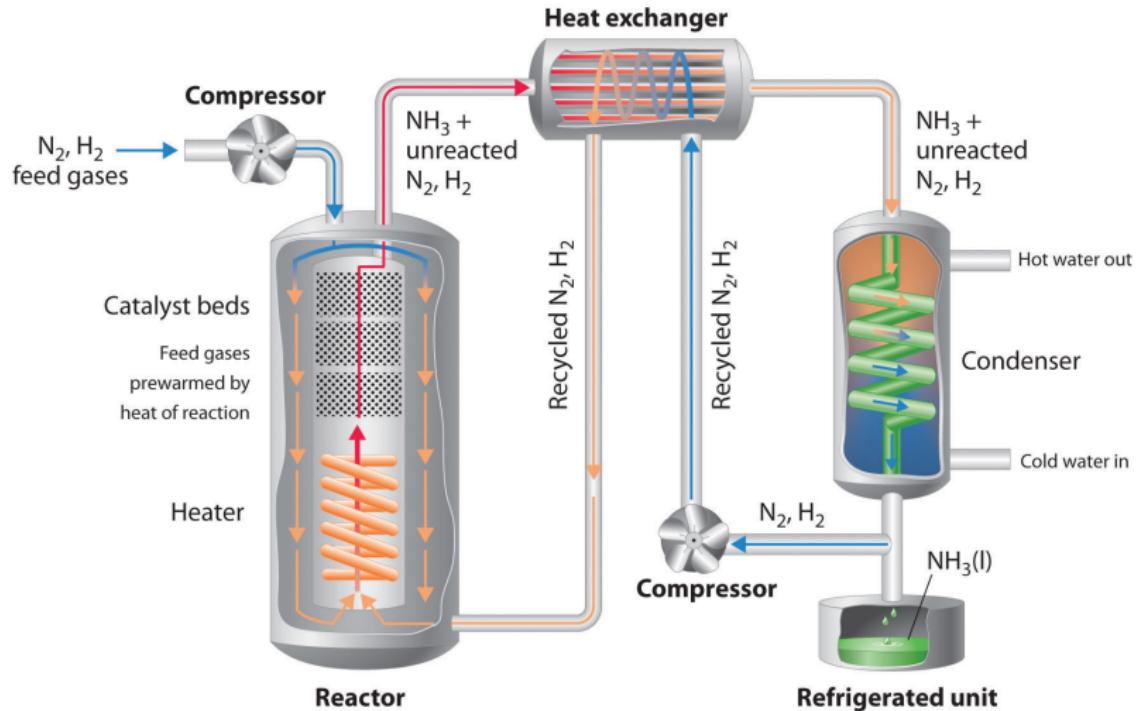
Organic Matter Decomposition / Soil Models



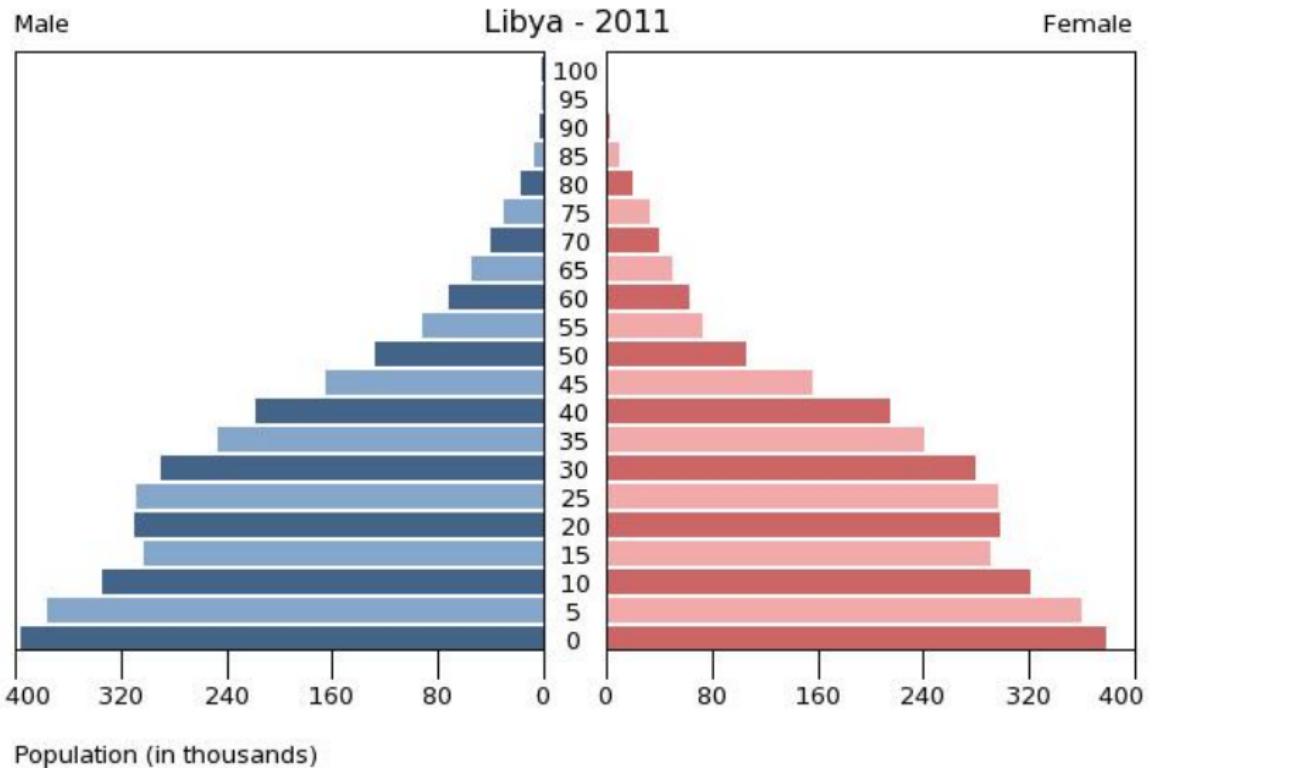
Ecosystem Models



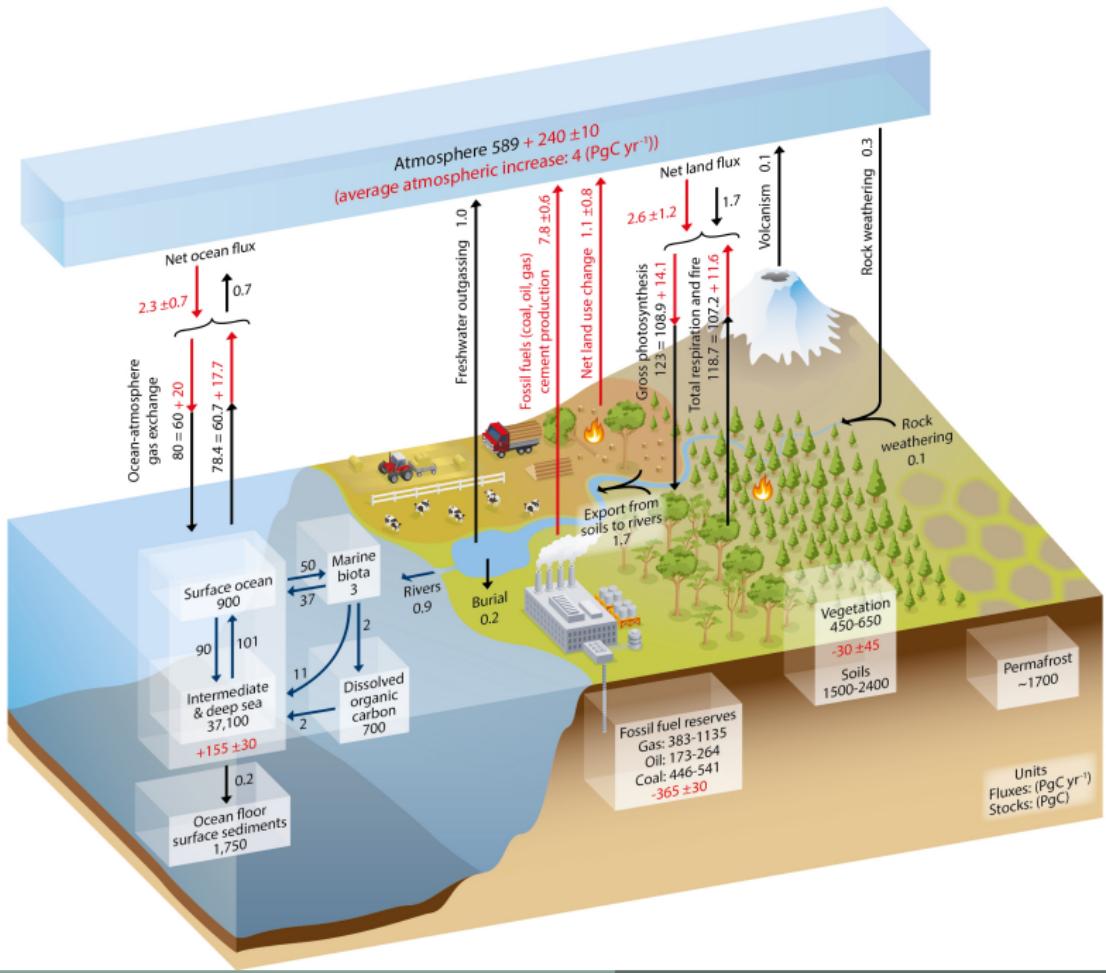
Chemical Reactors

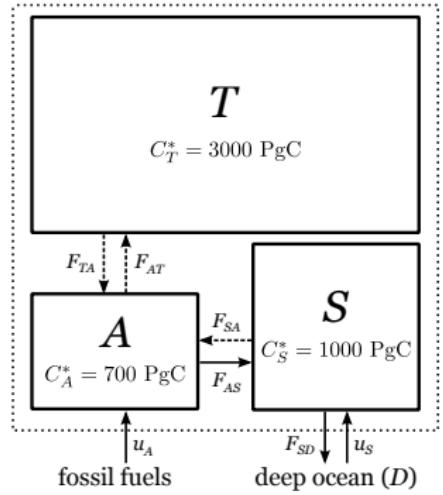
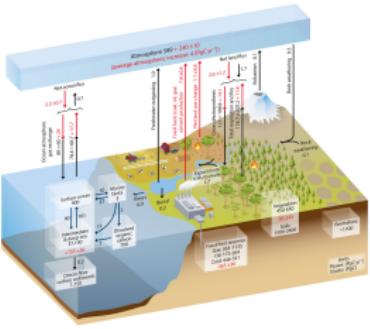


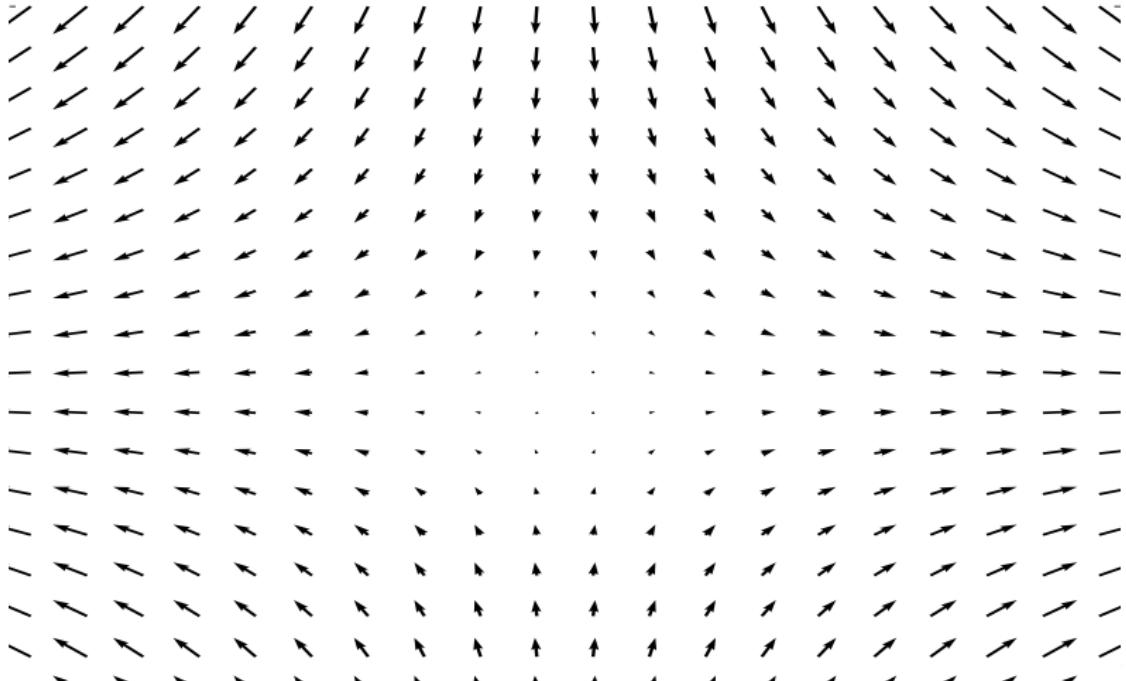
Population Dynamics

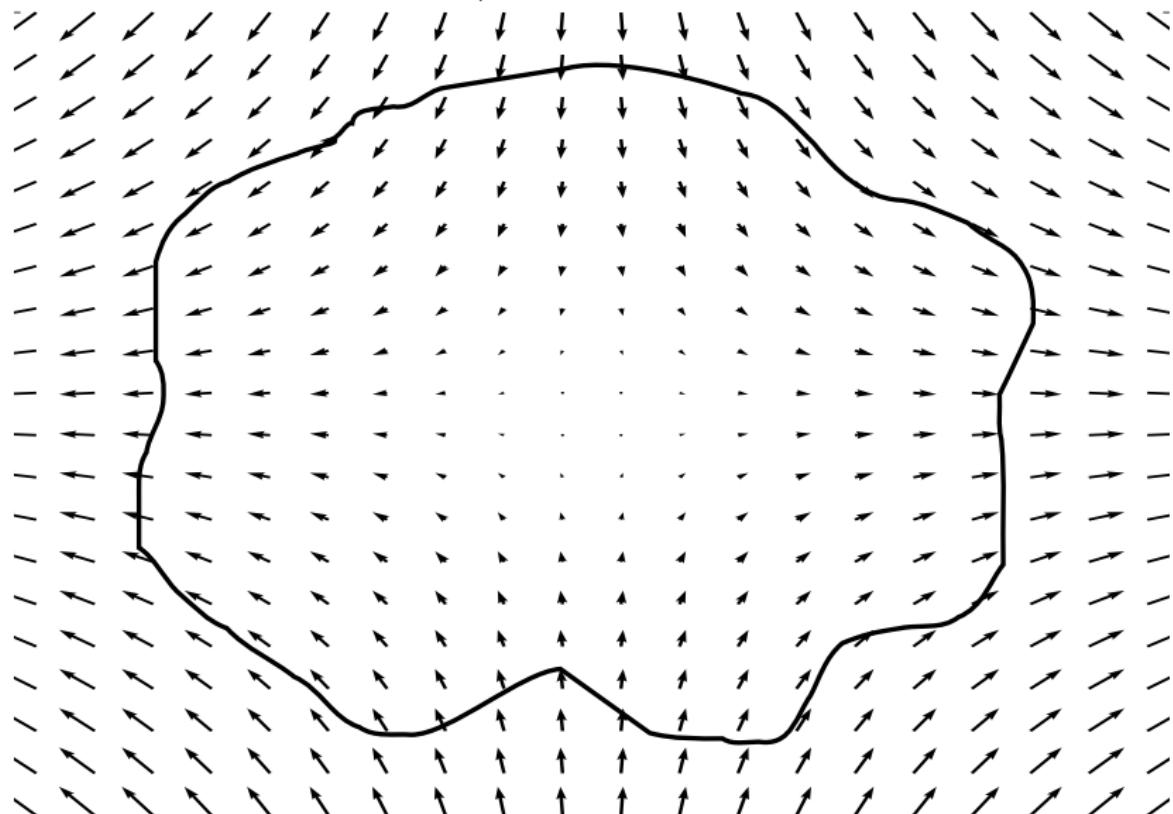


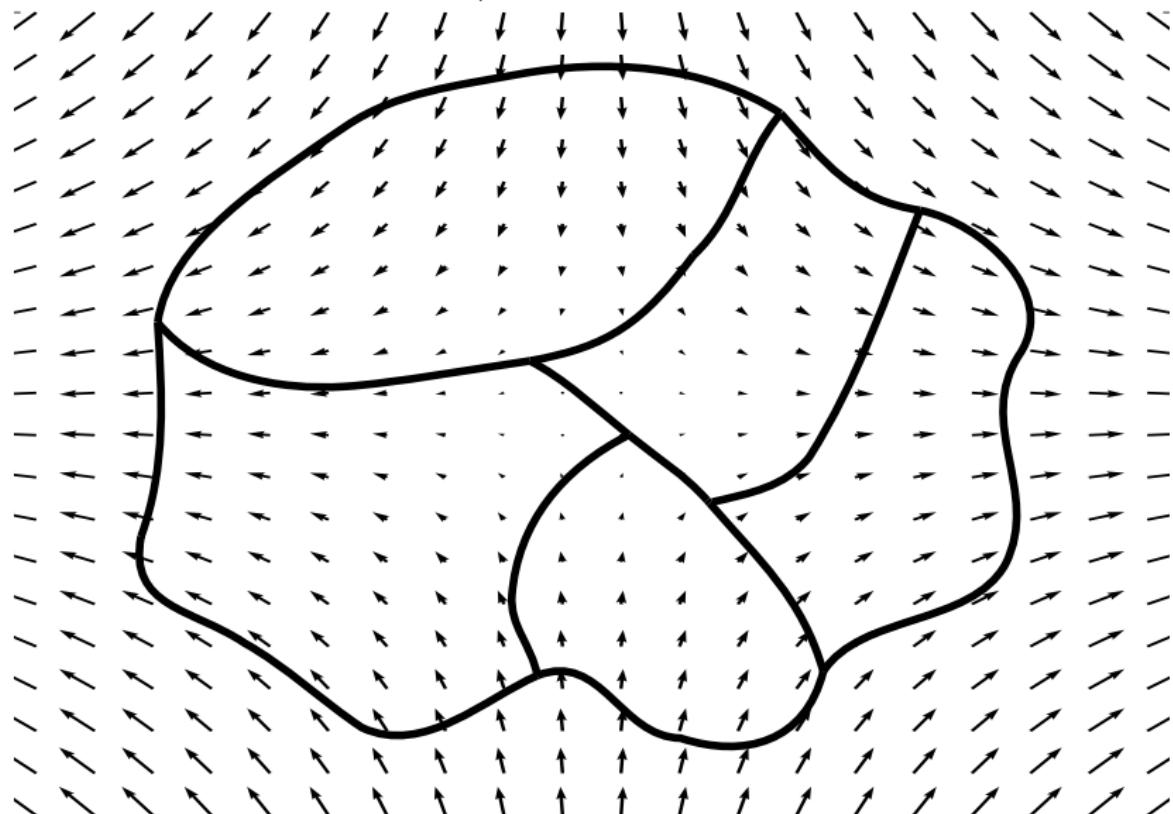


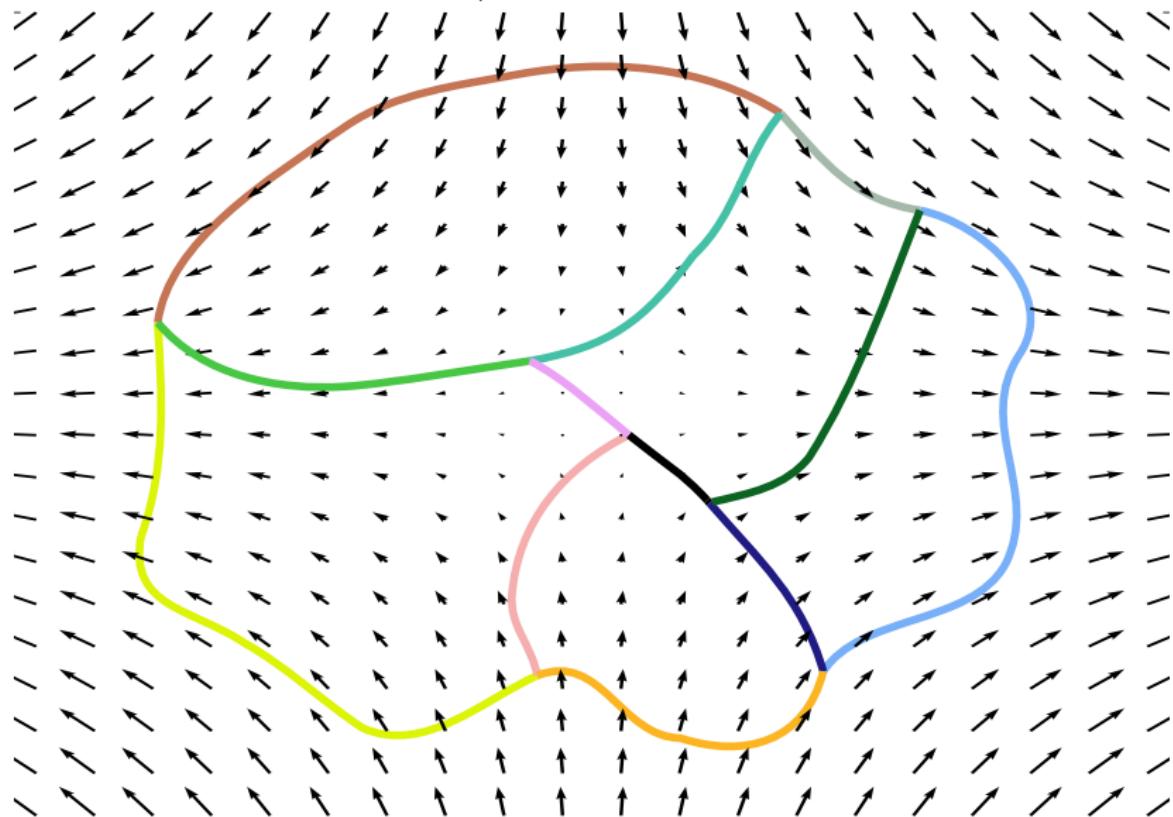


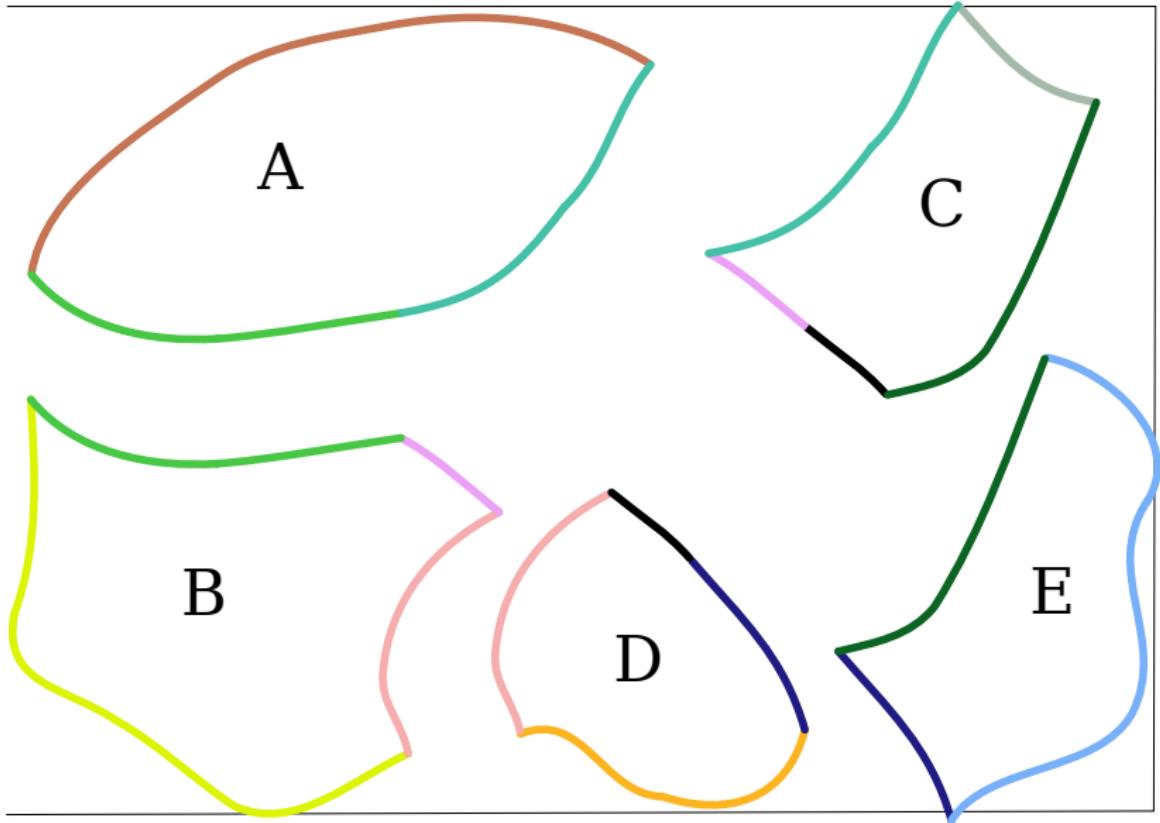


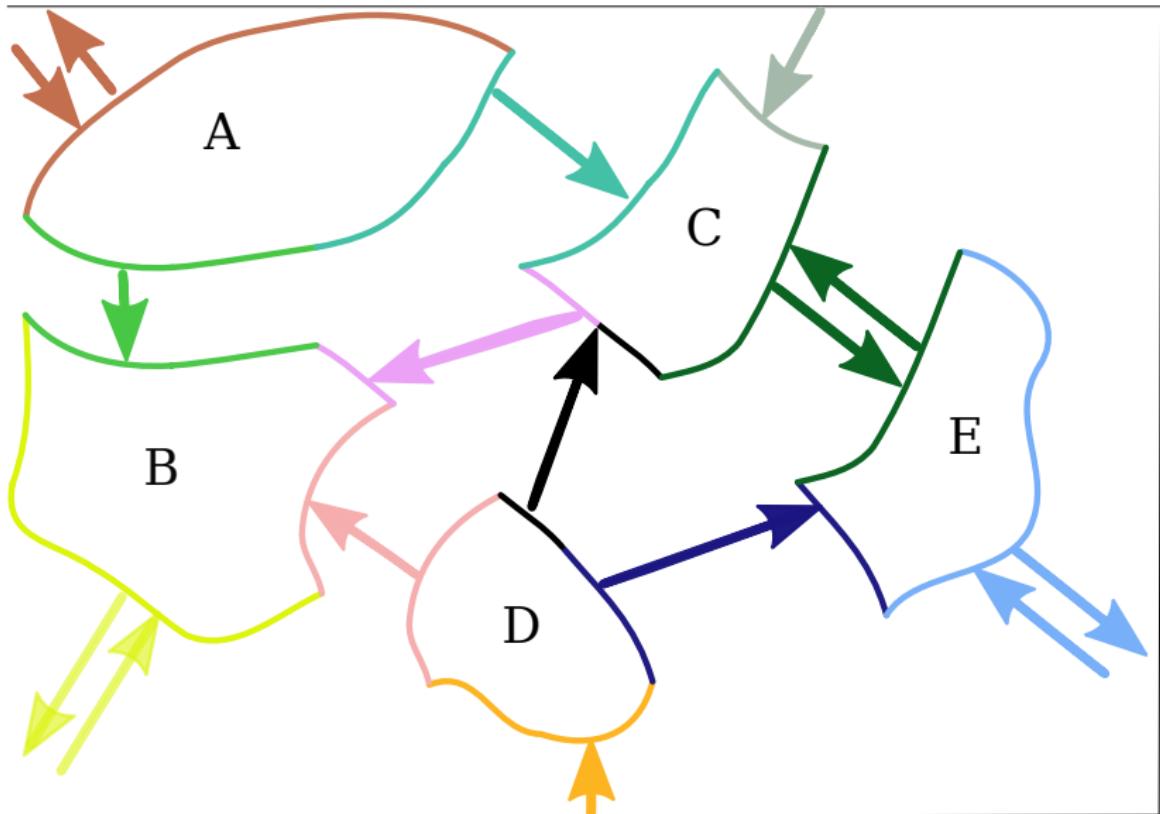


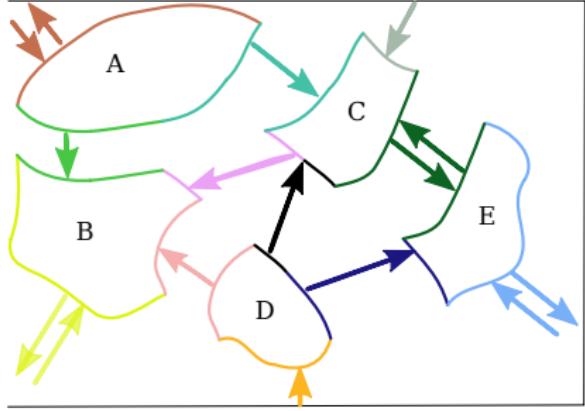
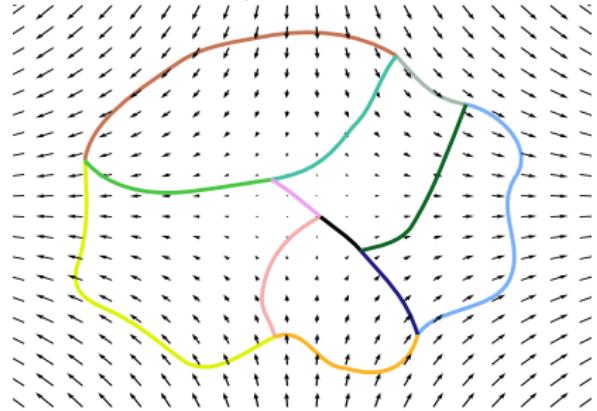


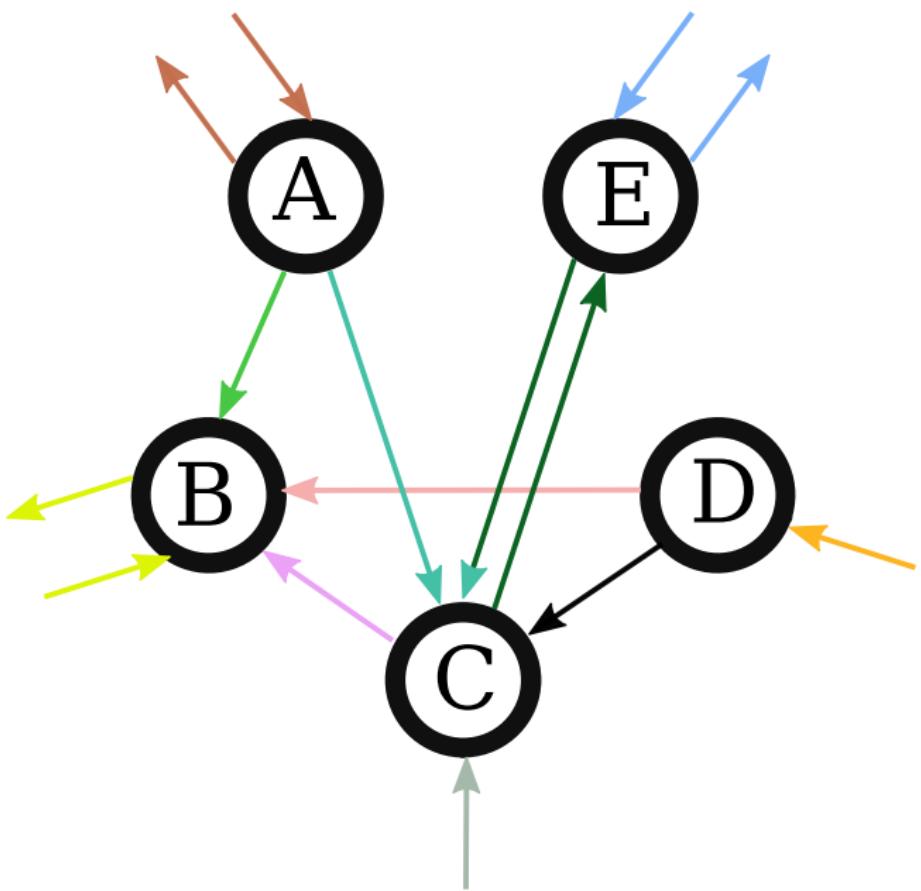


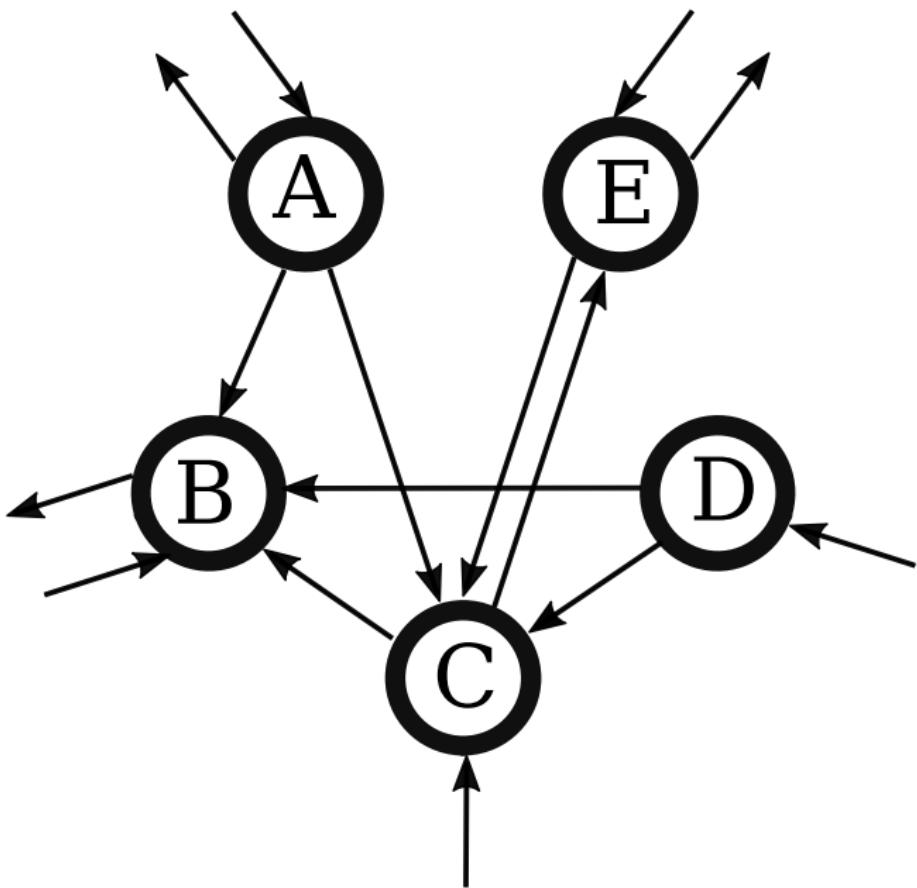






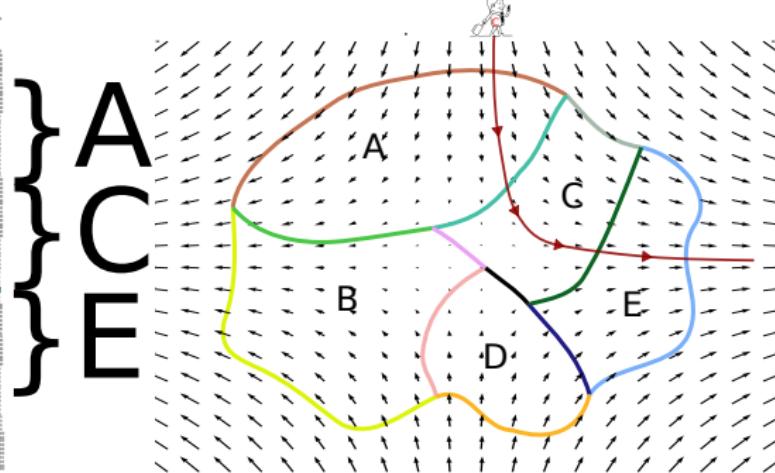








t,x,y,z



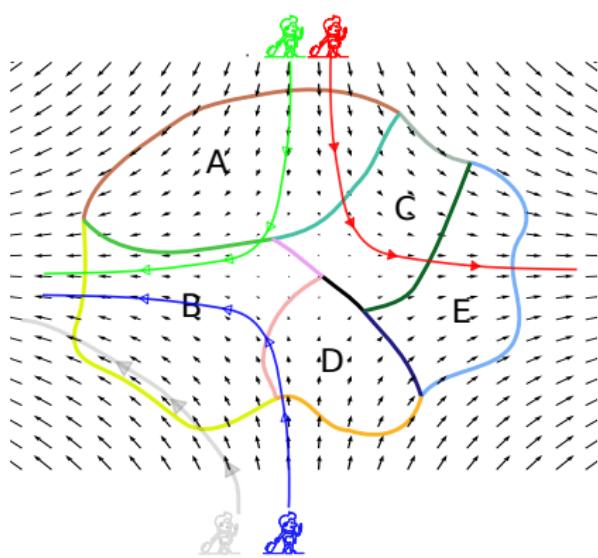
Pools arrival

1	A	16.45
2	C	42.45
3	E	68.56
4	Ext	94.23
...		

t,x,y,z

t,x,y,z
...

t,x,y,z



Pools arrival

1 A 16.45
2 C 42.45
3 E 68.56
4 Ext 94.23

Pools arrival

1 D 14.45
2 B 52.45
3 Ext 94.23

Pools arrival

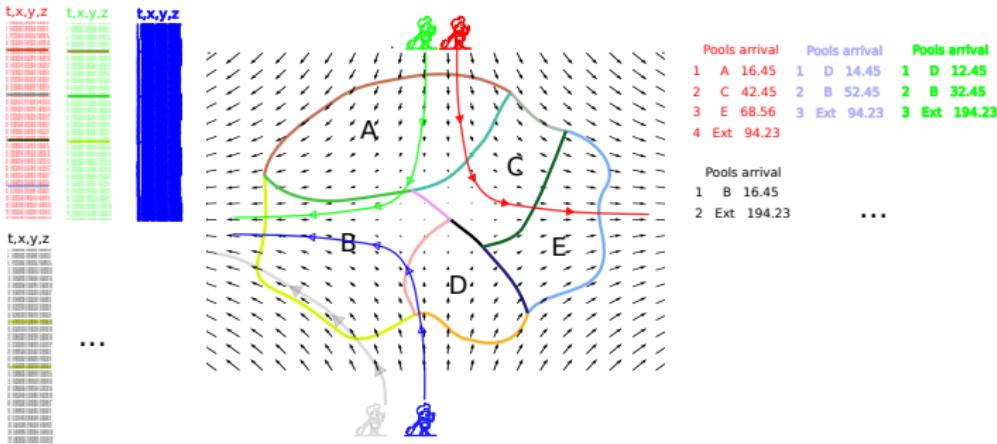
1 D 12.45
2 B 32.45
3 Ext 194.23

Pools arrival

1 B 16.45
2 Ext 194.23

...

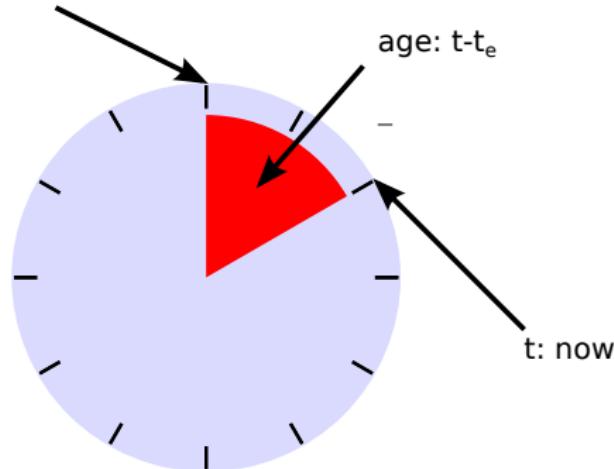
Possible Descriptive Statistics



- number / mass of particles in pool A, B, ...
- average time spent in a pool A ,B...
- average time spent in the whole system
- average time of particles spent between pool C and E under the assumption of having entered by pool D (weird but possible...)
- deathrate of pool A.

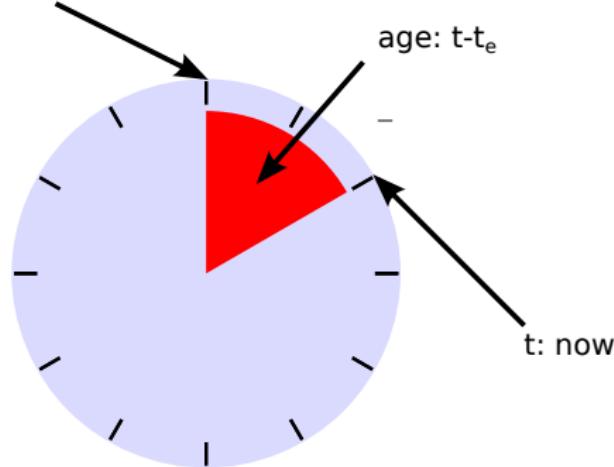
Age of a Particle

t_e : particle enters reservoir



Age of a Particle

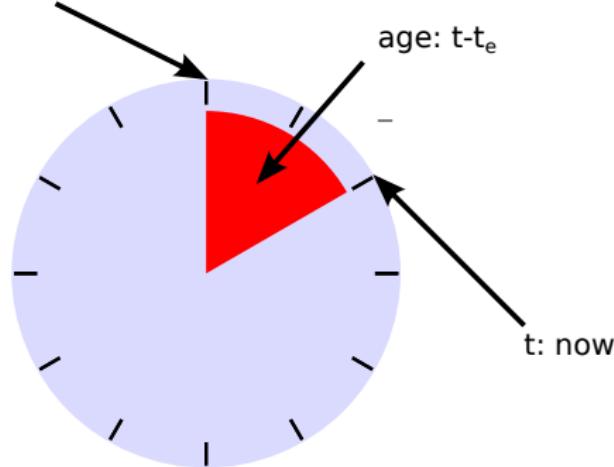
t_e : particle enters reservoir



- The “age” is always defined in *context* of the reservoir

Age of a Particle

t_e : particle enters reservoir



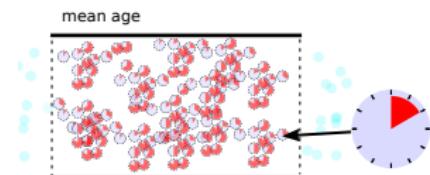
- The “age” can not be negative!

Mean Age

- Which set of particles to use for the average?

proposition: *all* particles that are in the reservoir at the given time.

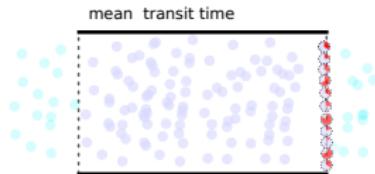
→ usually depends on input rates as well as the dynamics of the system.



$$\bar{a}(t) = \frac{a_1 + a_2 + \cdots + a_N}{N}$$

With $N = N(t)$ the number of all particles in the reservoir at time t .

Mean Transit Time



$$\bar{t}_r(t) = \frac{a_1 + a_2 + \cdots + a_{n_o}}{n_o}$$

With $n_o = n_o(t)$ the number of particles **just leaving** at time t

- Can be time dependent as well

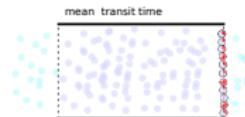
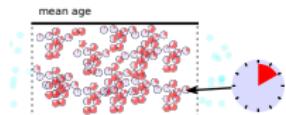
Mean Transit Time

$$\bar{t}_r(t) = \frac{a_1 + a_2 + \cdots + a_{n_o}}{n_o}$$

With $n_o = n_o(t)$ the number of particles **just leaving** at time t

- Can be time dependent as well
- Includes only the subset of particles that are just leaving at the given time. (Can only be computed when there is an output stream)

Differences between mean age and mean transit time



- Includes **all** particles that are in the reservoir at the given time.
- Directly coupled to input rates
- Includes only the subset of particles that are **just leaving** at the given time.
- Indirectly coupled to inputs

Iteration over all particles

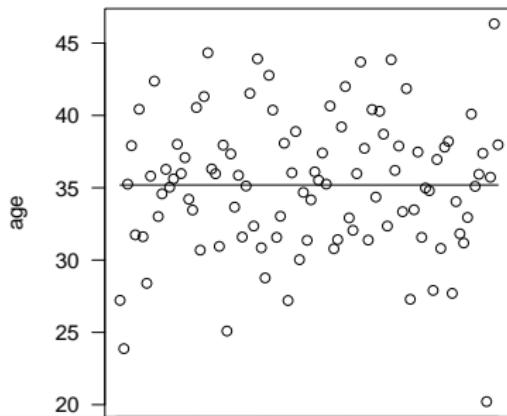
- ① To compute the mean transit time we have to identify the particles just leaving.
- ② Ask every leaving particle when it entered and compute its age.
- ③ Iterate over all particles and compute the average of their ages.

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$$\bar{t}_r(t) = \frac{a_1 + a_2 + \cdots + a_{n_o}}{n_o}$$

With $n_o = n_o(t)$ the number of particles just leaving at time t



Iteration over all ages

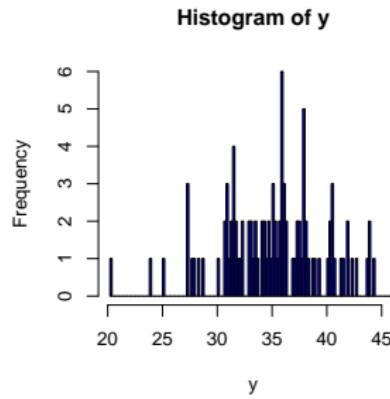
- ① as above
- ② as above + make a histogram of all ages
- ③ iterate over all ages and compute their weighted average

Iteration over all ages

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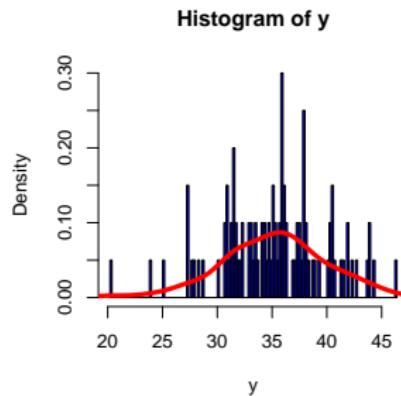
$$\bar{t}_r(t) = \frac{a_1 n_{a_1} + a_2 n_{a_2} + \cdots + a_n n_{a_n}}{n_o}$$

With $n_o = n_o(t) = n_{a_1} + n_{a_2} + \cdots + n_{a_n}$



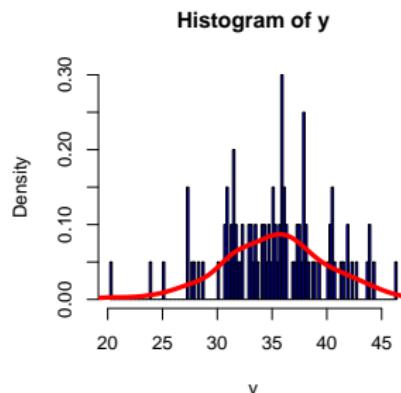
Integration over a density

$$\begin{aligned}\bar{t}_r(t) &= \lim_{n \rightarrow \infty} \frac{a_1 n_{a_1} + a_2 n_{a_2} + \cdots + a_n n_{a_n}}{n_o} \\ &= \lim_{n \rightarrow \infty} \sum_{\substack{\text{maxage} \\ \text{minage}}} a \frac{n(a)}{n_o} da \\ &= \int_{\text{minage}}^{\text{maxage}} a \psi(a) da\end{aligned}$$

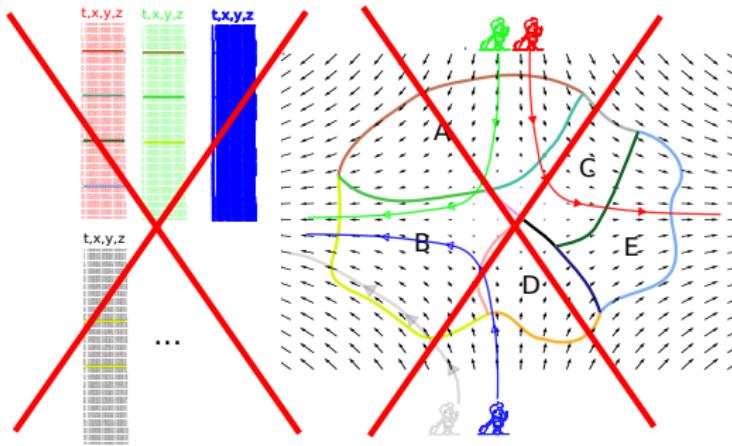


Same procedure for age density

$$\begin{aligned}\bar{a}(t) &= \lim_{n \rightarrow \infty} \frac{a_1 n_{a_1} + a_2 n_{a_2} + \cdots + a_n n_{a_n}}{n_p} \\ &= \lim_{n \rightarrow \infty} \sum_{\substack{\text{minage} \\ \text{maxage}}} a \frac{n(a)}{n_p} da \\ &= \int_{\text{minage}}^{\text{maxage}} a \phi(a) da\end{aligned}$$

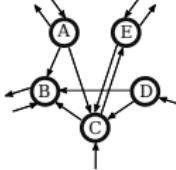


Possible Predictive Statistics ?



	Pools arrival	Pools arrival	Pools arrival
1	A 16.45	1	D 14.45
2	C 42.45	2	B 52.45
3	E 68.56	3	Ext 94.23
4	Ext 94.23		3 Ext 194.23

	Pools arrival
1	B 16.45
2	Ext 194.23



- Could we make a rule to predict the number of particles exiting from Pool E at time using only the particle passports? (Assuming that the exit from E is not recorded.)
- Could we make a rule to predict the age distribution of particles exiting from Pool E at time using only the particle passports? (Assuming again that the exit from E is not recorded.)

Intermediate Summary

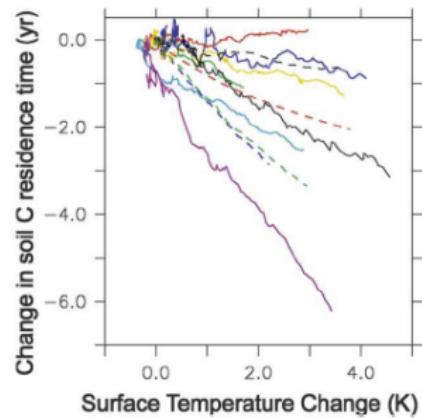
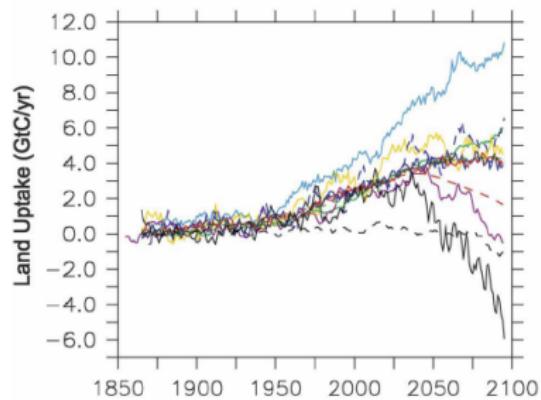
- ➊ Pool descriptions condense complex information to a time series of pool changes.(A series of stamps in the passport)
- ➋ There are many possible statistics on sets of these time series, usually related to numbers of particles and times. (e.g. the number of particles in a pool,
- ➌ Pool **Models** predict = model some of these **exclusively** with respect to the information obtainable from (all) passports.
- ➍ The most common even disregard most of the information in the passports.

The simplest Pool Systems



Pool Models

Diverse model predictions



?

Model comparison

Key quantities

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- **transit time**
 - ▶ the time that particles need to travel through the system
 - ▶ exit time - entry time

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- **transit time**
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- **system age**
 - ▶ for particles in the system
 - ▶ current time - entry time

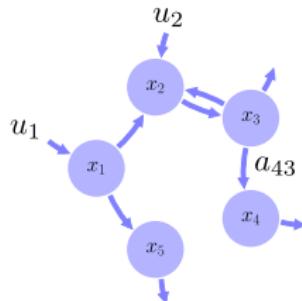
Model comparison

Key quantities

- **transit time**
 - ▶ the time that particles need to travel through the system
 - ▶ exit time - entry time
- **system age**
 - ▶ for particles in the system
 - ▶ current time - entry time
- **compartment age**
 - ▶ system age of particles in a compartment

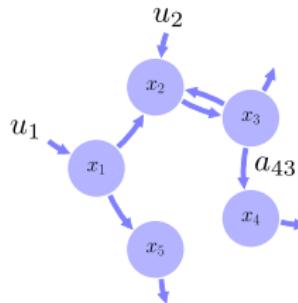
Linear autonomous compartmental models

$$\frac{d}{dt} \mathbf{x}(t) = A \mathbf{x}(t) + \mathbf{u}$$



Linear autonomous compartmental models

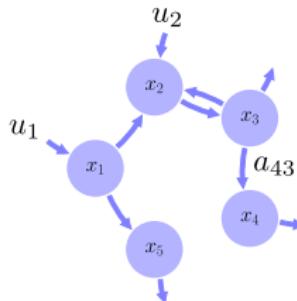
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$\mathbf{x}(t)$ vector of compartment content (e.g. C) at time t

Linear autonomous compartmental models

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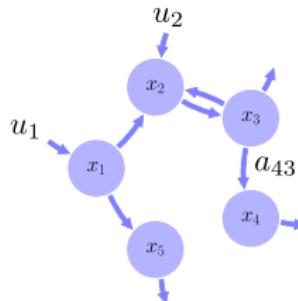


$\mathbf{x}(t)$ vector of compartment content (e.g. C) at time t

\mathbf{u} constant input vector

Linear autonomous compartmental models

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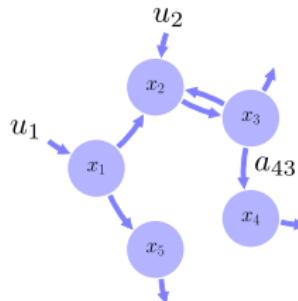
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$A = (a_{ij})$ compartmental matrix

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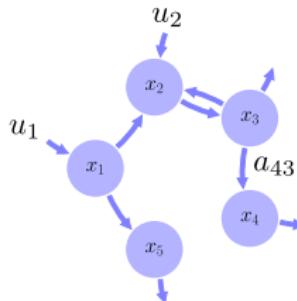
$A = (a_{ij})$ compartmental matrix

$a_{ij} (i \neq j)$ fractional transfer coefficients,

rate of flow from compartment j to compartment i

Linear autonomous compartmental models

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$\mathbf{x}(t)$ vector of compartment content (e.g. C) at time t

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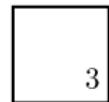
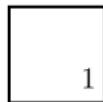
$-a_{ii} > 0$ rate of flow out of compartment i

A particle travels

$$\frac{d}{dt} \mathbf{x}(t) = \mathbf{A} \mathbf{x}(t) + \mathbf{u}$$



u



$$-\sum$$

$$\begin{pmatrix} -a_{11} & a_{12} & 0 \\ a_{21} & -a_{22} & 0 \\ a_{31} & 0 & -a_{33} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ 0 \end{pmatrix}$$

$$0$$

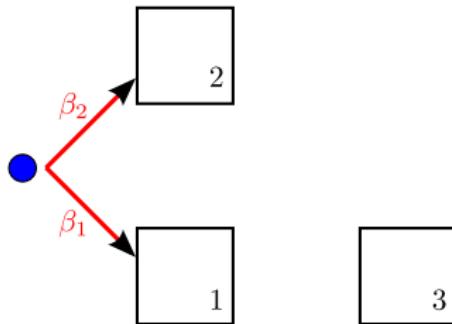
$$> 0$$

$$> 0$$

$$\|\mathbf{u}\|$$

A particle travels

$$\frac{d}{dt} \mathbf{x}(t) = \mathbf{A} \mathbf{x}(t) + \mathbf{u}$$

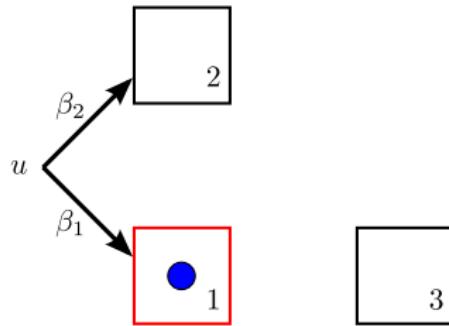


$$\begin{pmatrix} -a_{11} & a_{12} & 0 \\ a_{21} & -a_{22} & 0 \\ a_{31} & 0 & -a_{33} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ 0 \end{pmatrix} - \sum 0 > 0 > 0 \quad \|\mathbf{u}\|$$

$$\beta_1 = \frac{u_1}{u_1+u_2} \quad \beta_2 = \frac{u_2}{u_1+u_2}$$

$$T_0 = 0$$

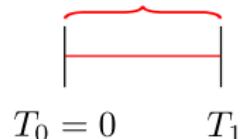
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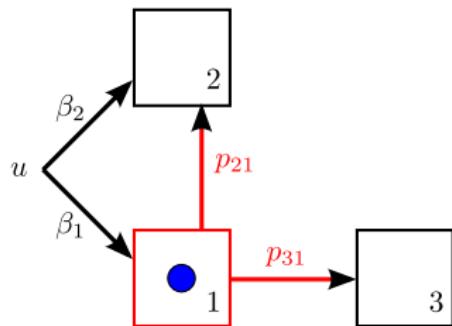
$$\begin{pmatrix} -a_{11} & a_{12} & 0 \\ a_{21} & -a_{22} & 0 \\ a_{31} & 0 & -a_{33} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ 0 \end{pmatrix} - \sum 0 > 0 > 0 \|\mathbf{u}\|$$

$$T_1 \sim \text{Exp}(a_{11})$$



A particle travels

$$\frac{d}{dt} \mathbf{x}(t) = \mathbf{A} \mathbf{x}(t) + \mathbf{u}$$



$$\begin{pmatrix} -a_{11} & a_{12} & 0 \\ a_{21} & -a_{22} & 0 \\ a_{31} & 0 & -a_{33} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ 0 \end{pmatrix}$$

$$- \sum \quad 0 \quad > 0 \quad > 0 \quad \|\mathbf{u}\|$$

$$p_{21} = \frac{a_{21}}{a_{11}} \quad p_{31} = \frac{a_{31}}{a_{11}}$$

$$T_1 \sim \text{Exp}(a_{11})$$

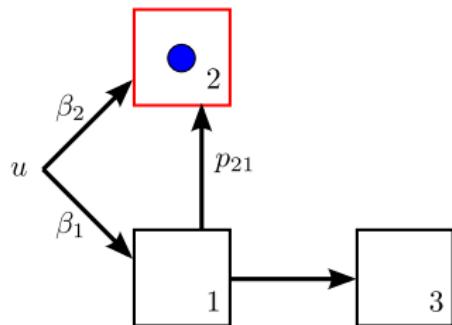


$$T_0 = 0$$

$$T_1$$

A particle travels

$$\frac{d}{dt} \mathbf{x}(t) = \mathbf{A} \mathbf{x}(t) + \mathbf{u}$$



$$\begin{pmatrix} -a_{11} & a_{12} & 0 \\ a_{21} & -a_{22} & 0 \\ a_{31} & 0 & -a_{33} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ 0 \end{pmatrix}$$

$$- \sum$$

$$0$$

$$> 0$$

$$> 0$$

$$\|\mathbf{u}\|$$

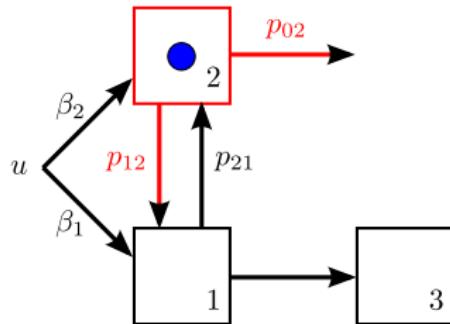
$$T_1 \sim \text{Exp}(a_{11})$$

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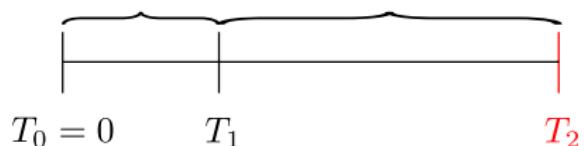
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$$- \sum 0 > 0 > 0 \quad \|\mathbf{u}\|$$

$$p_{12} = \frac{a_{12}}{a_{22}} \quad p_{02} = 1 - \frac{a_{12}}{a_{22}}$$

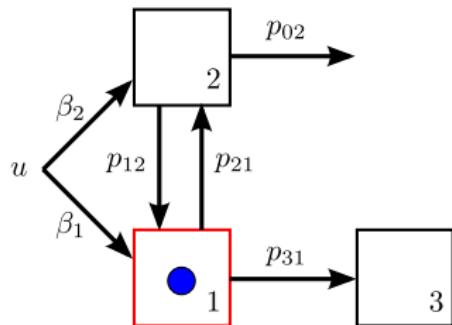
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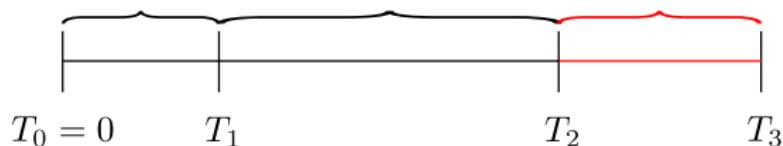


$$\begin{pmatrix} -\mathbf{a}_{11} & \mathbf{a}_{12} & 0 \\ \mathbf{a}_{21} & -\mathbf{a}_{22} & 0 \\ \mathbf{a}_{31} & 0 & -\mathbf{a}_{33} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ 0 \end{pmatrix} - \sum 0 > 0 > 0 \|\mathbf{u}\|$$

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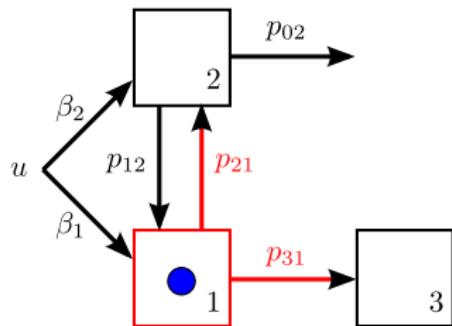
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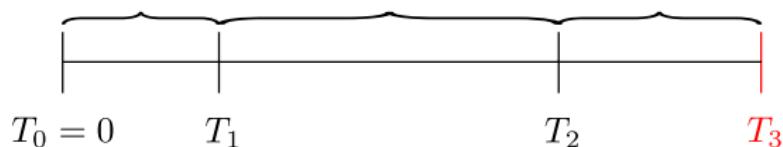
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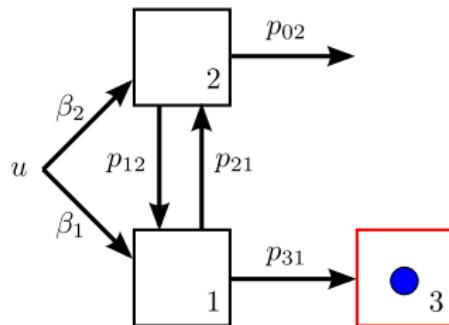
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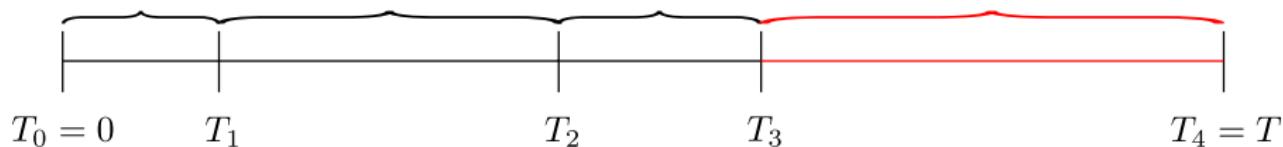
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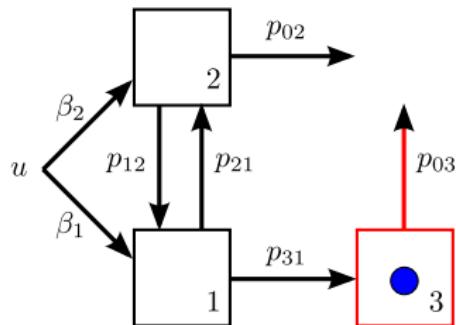
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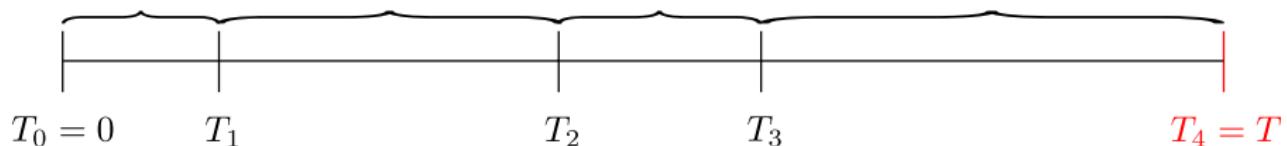
$$p_{03} = 1$$

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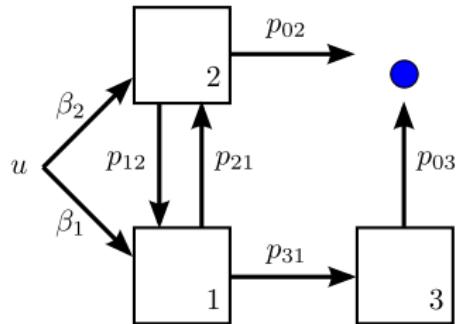
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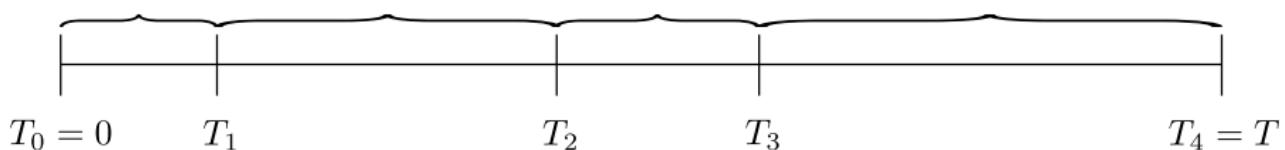
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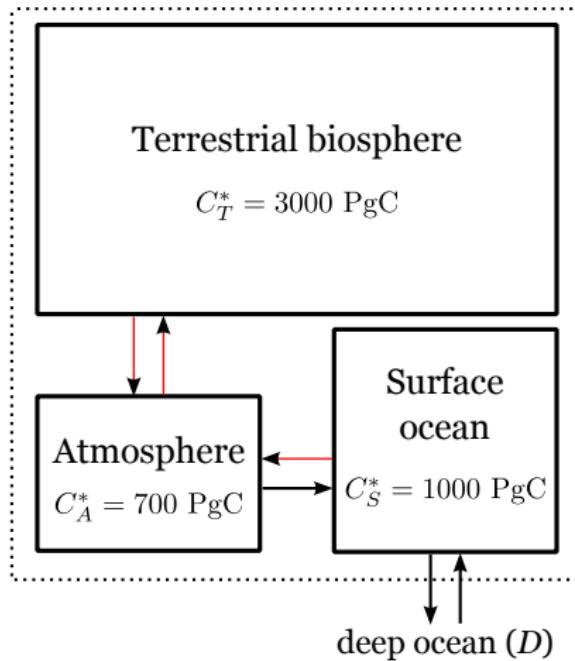
→ $T \sim \text{PH}(\beta, A)$

General, simple, explicit formulas

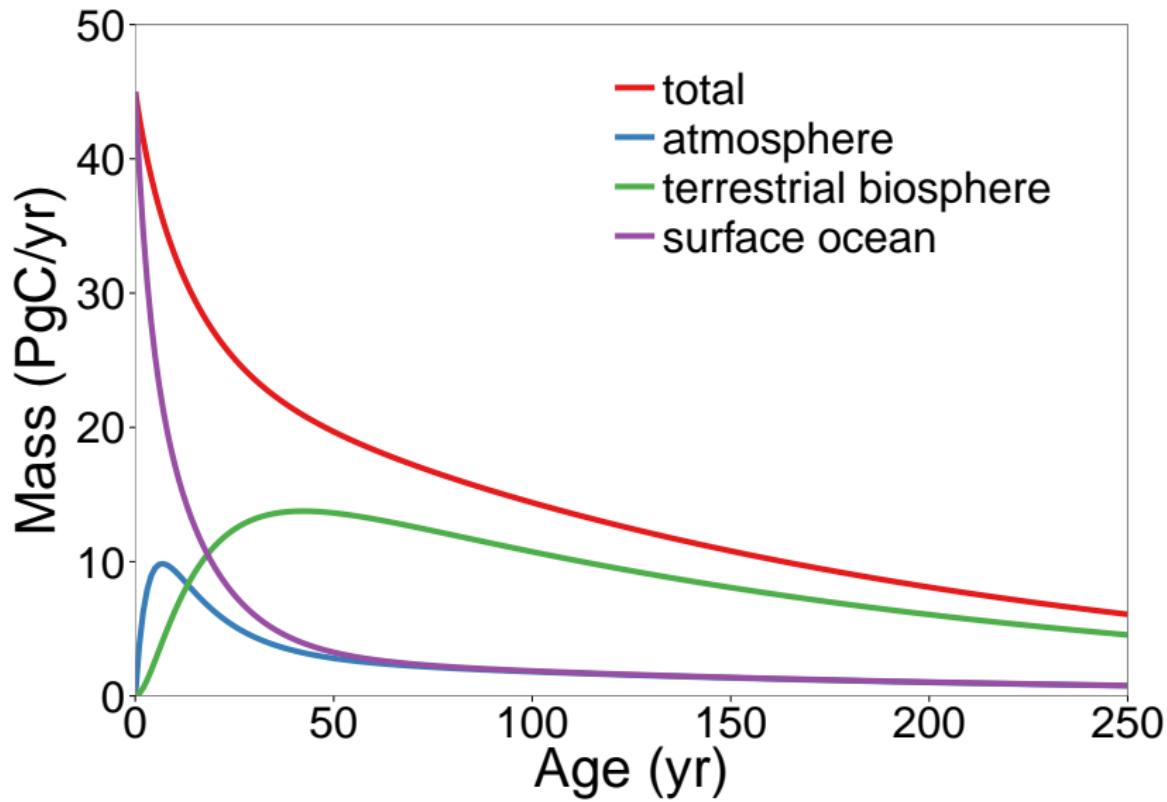
- phase-type distribution is well known:
 - ▶ probability density
 - ▶ cumulative distribution function
 - ▶ quantiles
 - ▶ mean and higher order moments
 - ★ $\mathbb{E}[T] = \|A^{-1}\beta\| = \frac{\|\mathbf{x}^*\|}{\|\mathbf{u}\|}$ (mean transit time)
- system age is also phase-type distributed
 - ▶ parameters $\eta := \frac{\mathbf{x}^*}{\|\mathbf{x}^*\|}, A$
- probability density of compartmental age
 - ▶ $f_a(y) = (X^*)^{-1} e^{yA} \mathbf{u}$

Application to a nonlinear carbon cycle model

Nonlinear model in steady state [?] with three compartments



Equilibrium age densities



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mass with age a at time t

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- solution to the matrix ordinary differential equation

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- \mathbf{p}^0 is a given age distribution of the initial content vector \mathbf{x}^0

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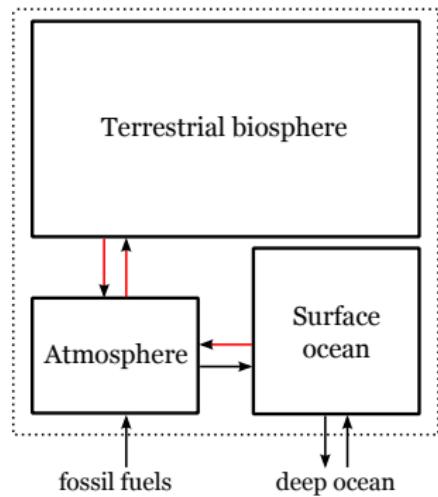
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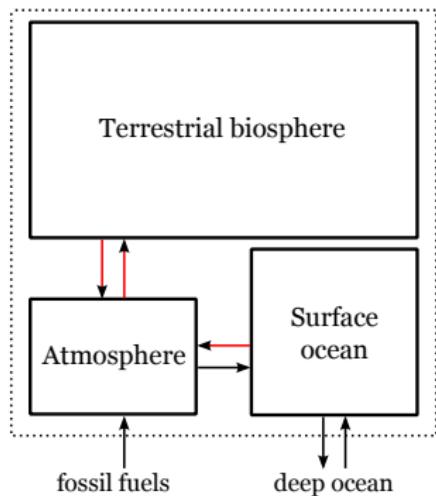
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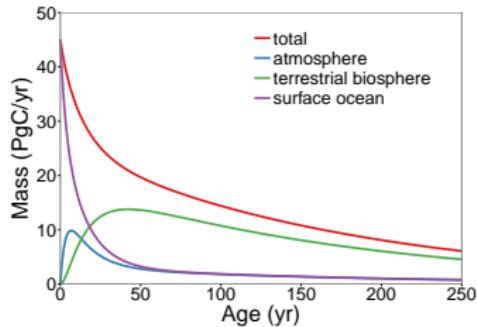
A global carbon cycle model



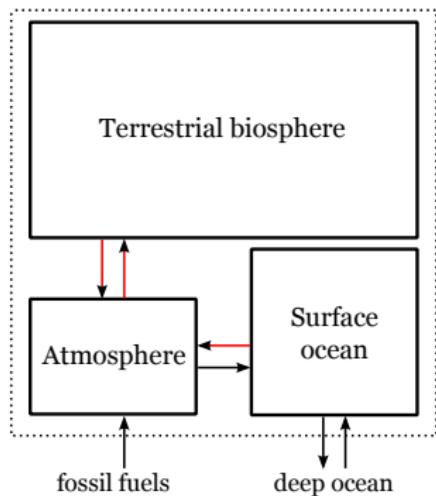
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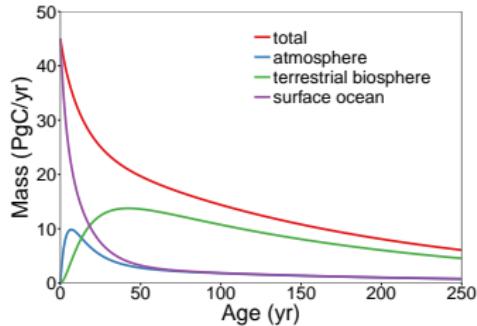
Equilibrium age densities in 1765



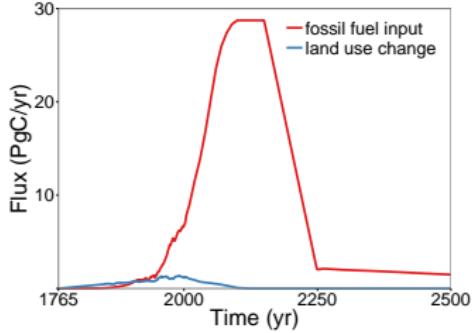
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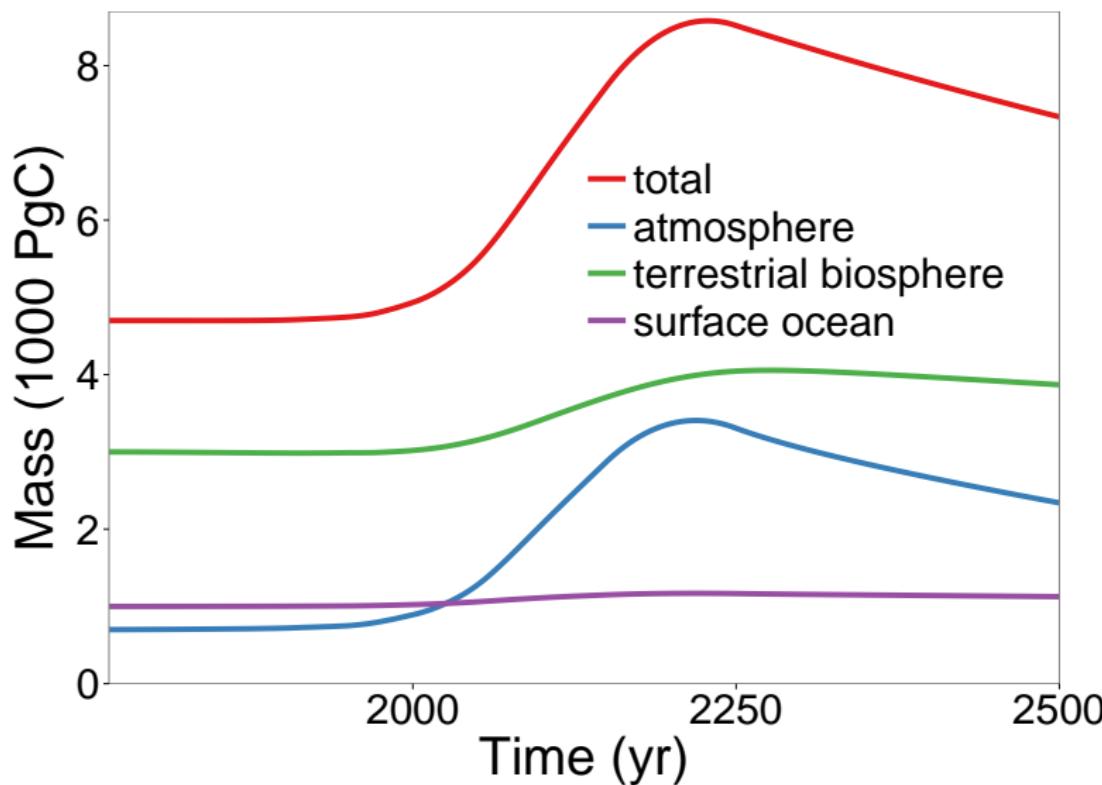
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RCP8.5 scenario



Time-dependent carbon contents

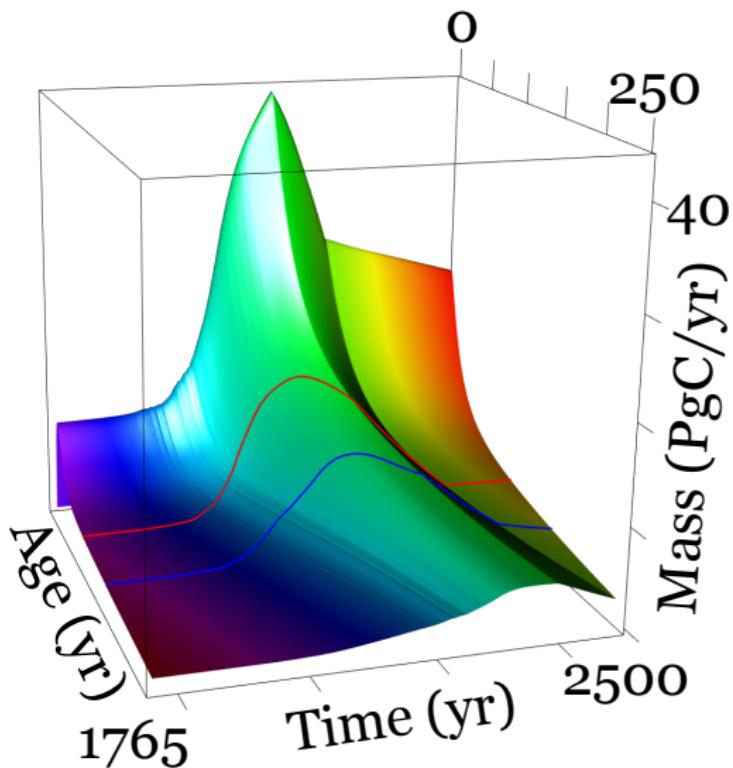


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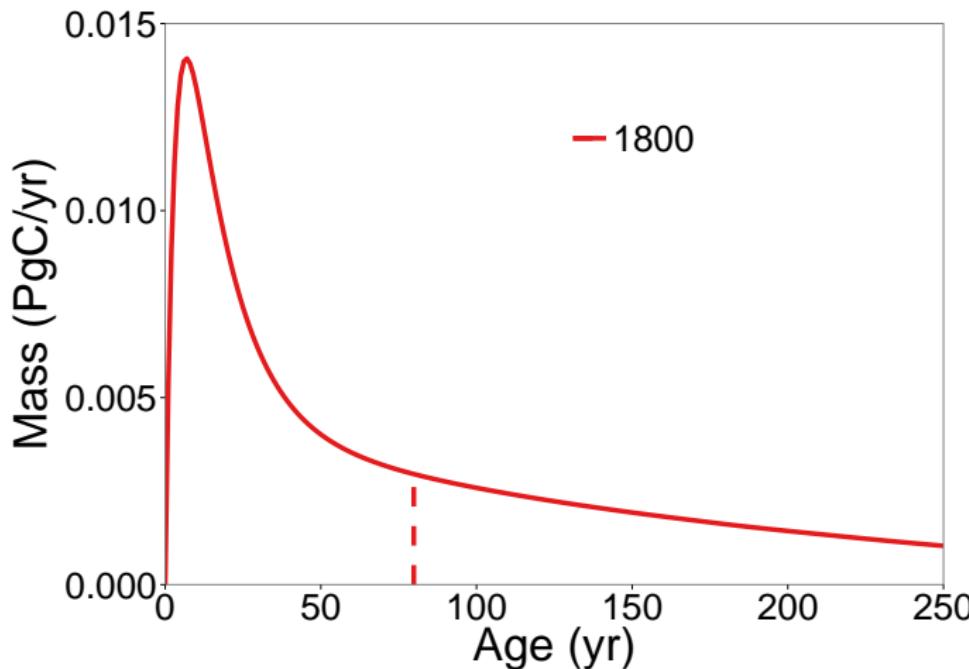


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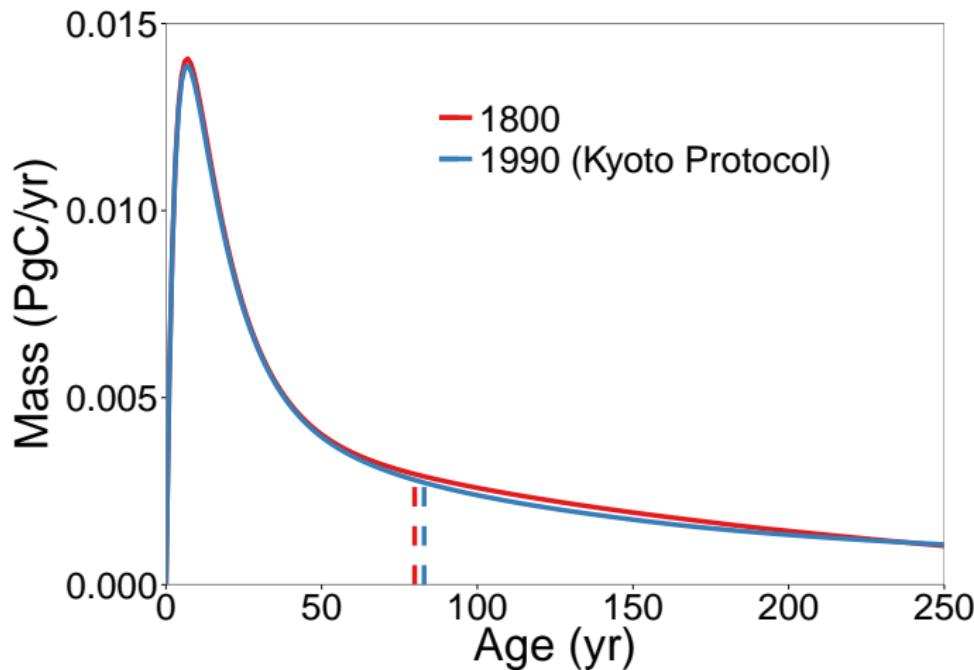
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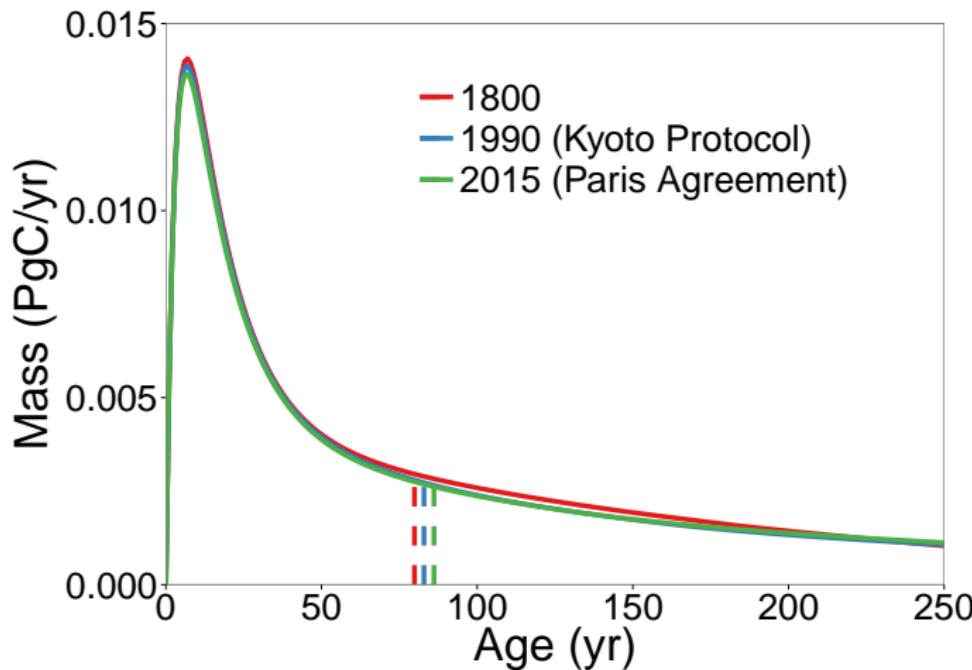
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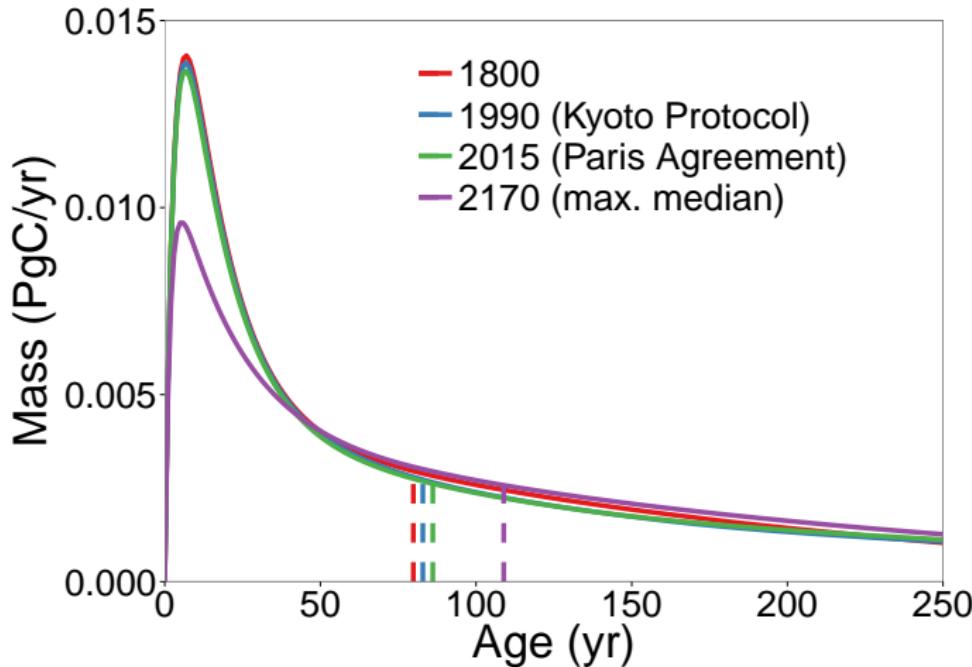
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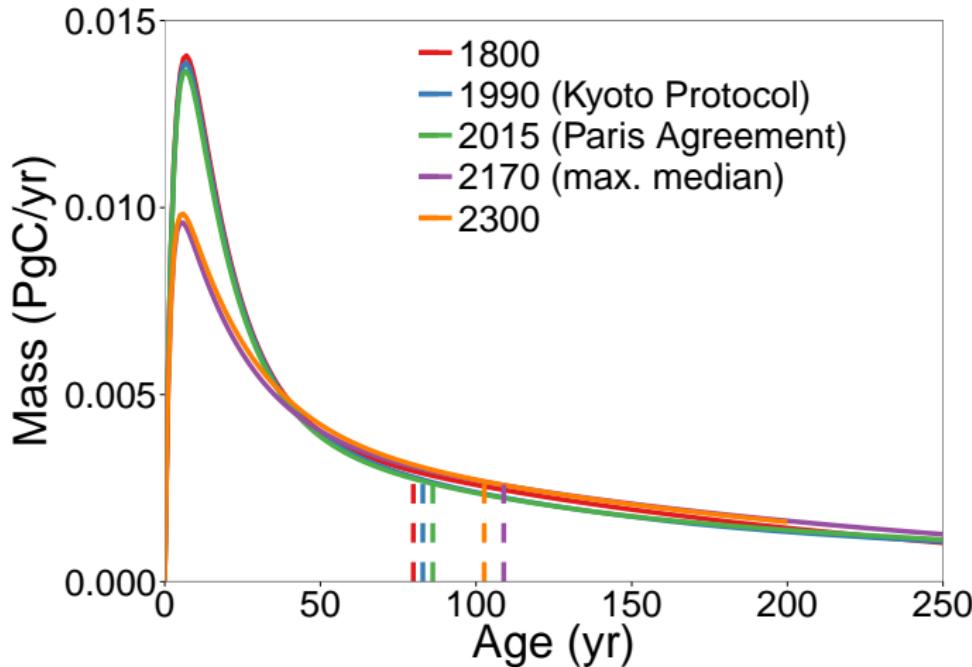
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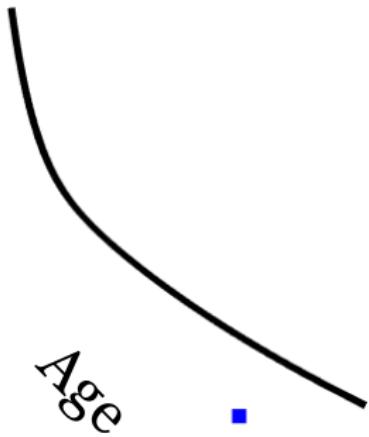
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- **two Python packages**
 - ▶ (symbolic) computation of age and transit time properties for autonomous systems in steady state
 - ★ <http://github.com/goujou/LAPM>
 - ▶ (numerical) computation of age and transit time properties for nonlinear nonautonomous systems

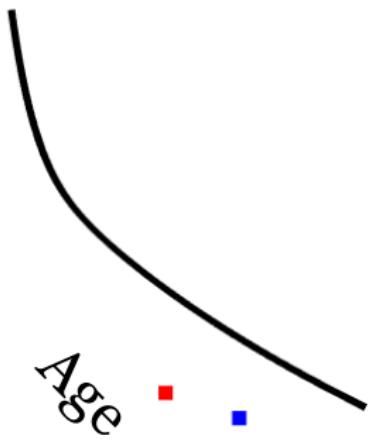
System age



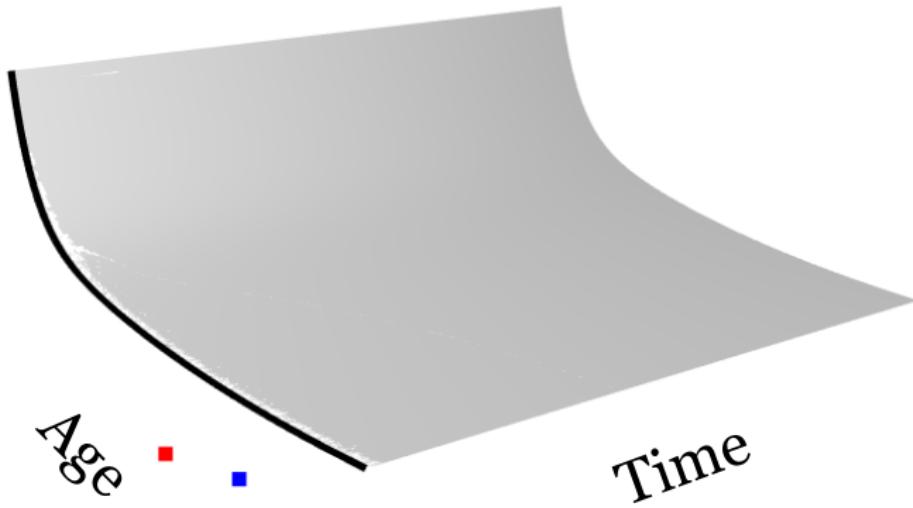
System age



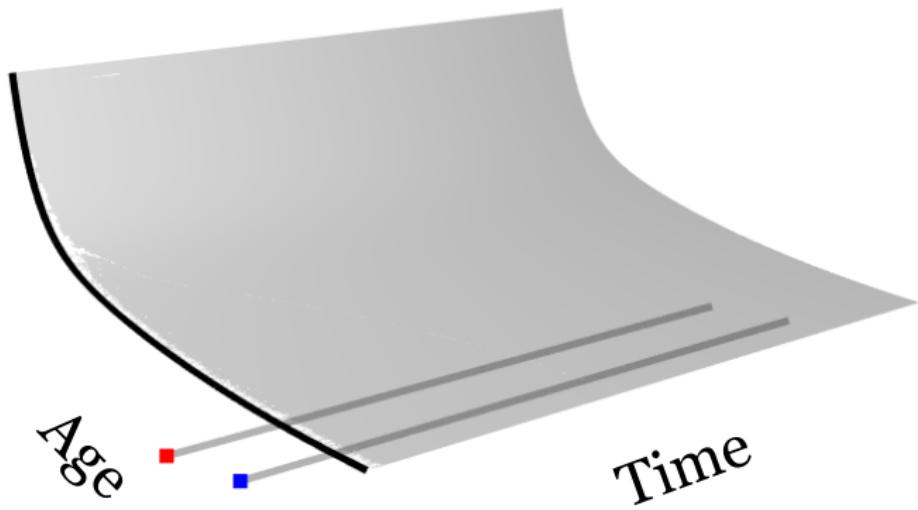
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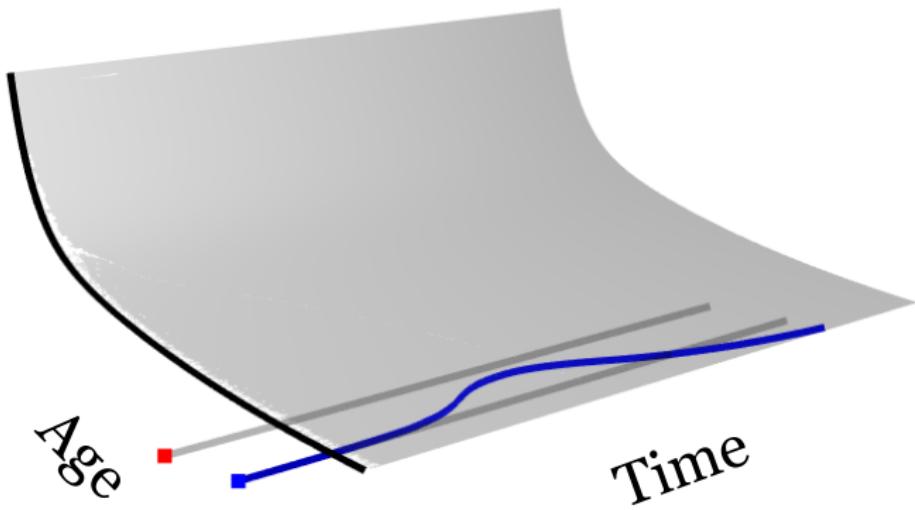
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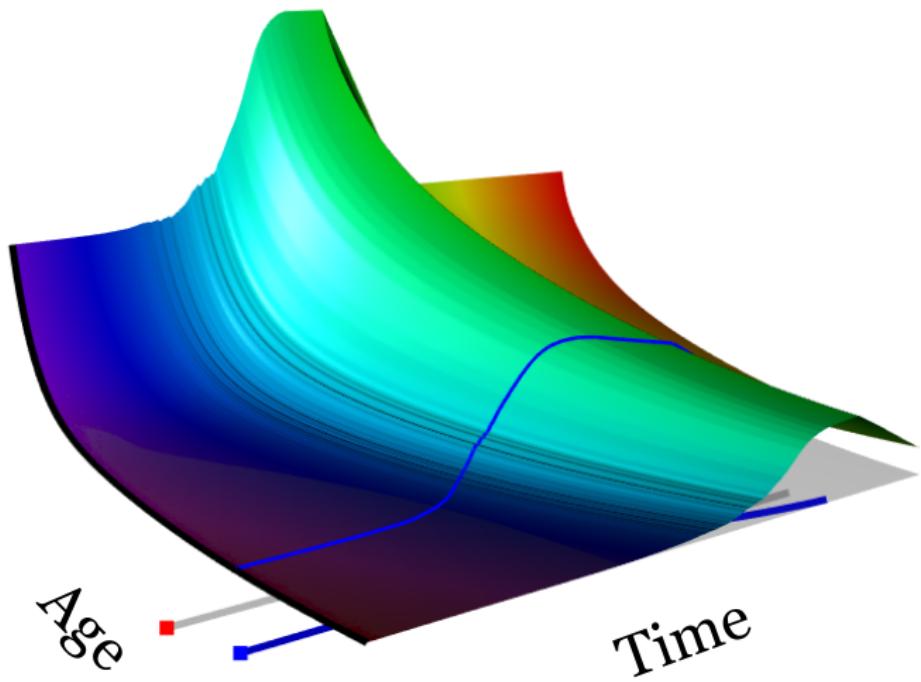
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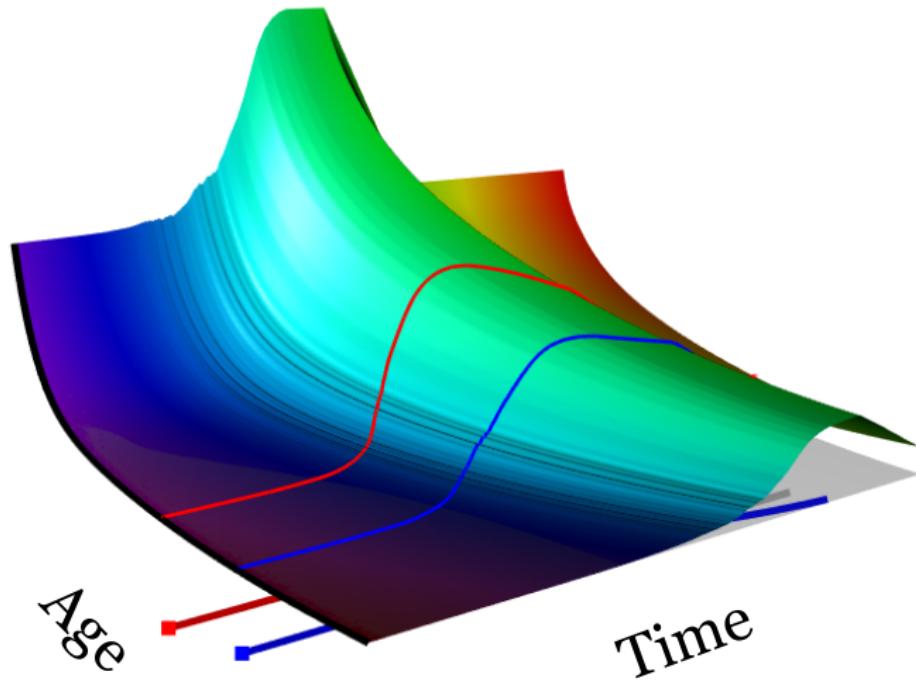
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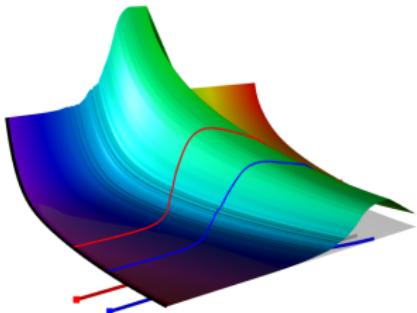
System age



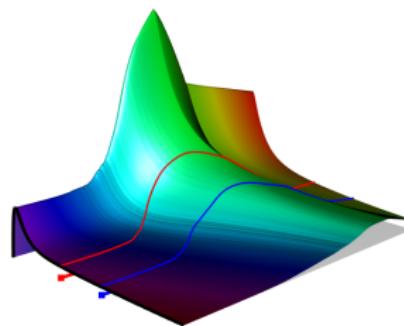
System age



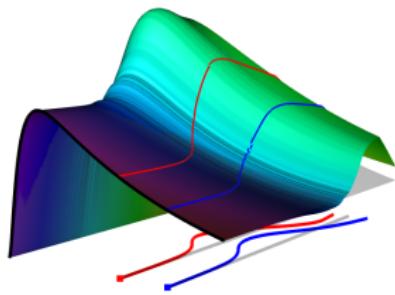
System



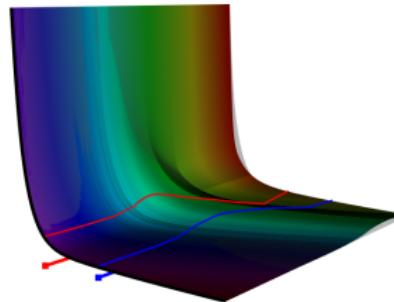
Atmosphere



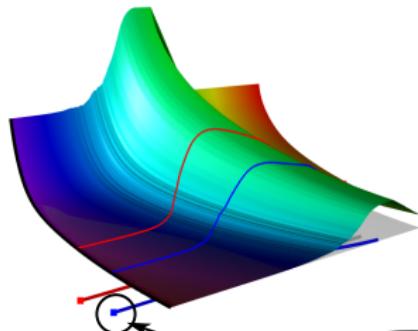
Terrestrial biosphere



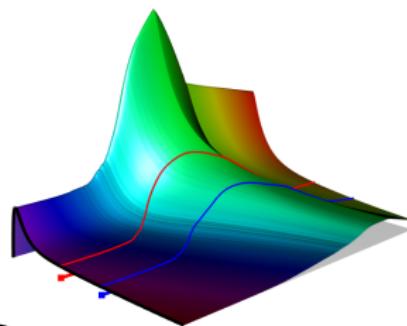
Surface ocean



System

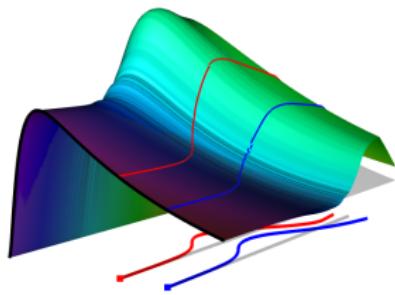


Atmosphere

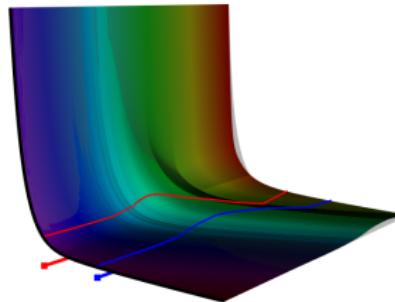


early 2016

Terrestrial biosphere



Surface ocean



Thanks

Funding



Thank you for your attention

$$\begin{aligned} I &= \int \sqrt{1+(1+u^2)^2} \frac{u du}{1+u^2}, \quad z = 1+u^2, \quad dz \\ &\int \frac{1+z^2}{z\sqrt{1+z^2}} dz = \frac{1}{2} \sqrt{1+z^2} + \frac{1}{2} \ln |z|, \quad I_1 = \int \frac{1}{z\sqrt{1+z^2}} dz, \quad z = 1/t, \quad dz = -\frac{dt}{t^2} \\ I_1 &= \int \frac{-\frac{dt}{t^2}}{\frac{1}{t}\sqrt{1+\frac{1}{t^2}}} = -\ln \left(t + \sqrt{1+t^2} \right) + C_1 \\ &= \ln z - \ln \left(1 + \sqrt{1+z^2} \right) + C_1 = \ln \left(\frac{1}{z} - \sqrt{1+\frac{1}{z^2}} \right) + C_1 \\ &= \ln \left(1 + \tan^2 x \right) - \ln \left(1 + \sqrt{1 + \left(\frac{1}{\cos^2 x} \right)} \right) + C_1 \\ &= \ln \left(\cos^2 x + \sqrt{\cos^4 x + 1} \right) + 2 \ln |\cos x| + C_1 \end{aligned}$$

bibliography

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