Pool Models

An Introduction

Markus Müller, Holger Metzler, Carlos Sierra

August 13, 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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An Introduction

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Outline

1. Example Applications of Pool Models

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2. Reducing Model Complexity
   - The Carbon Cycle example
   - Asking Simpler Questions
   - Answer Questions more simply

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3. Compartmental Systems

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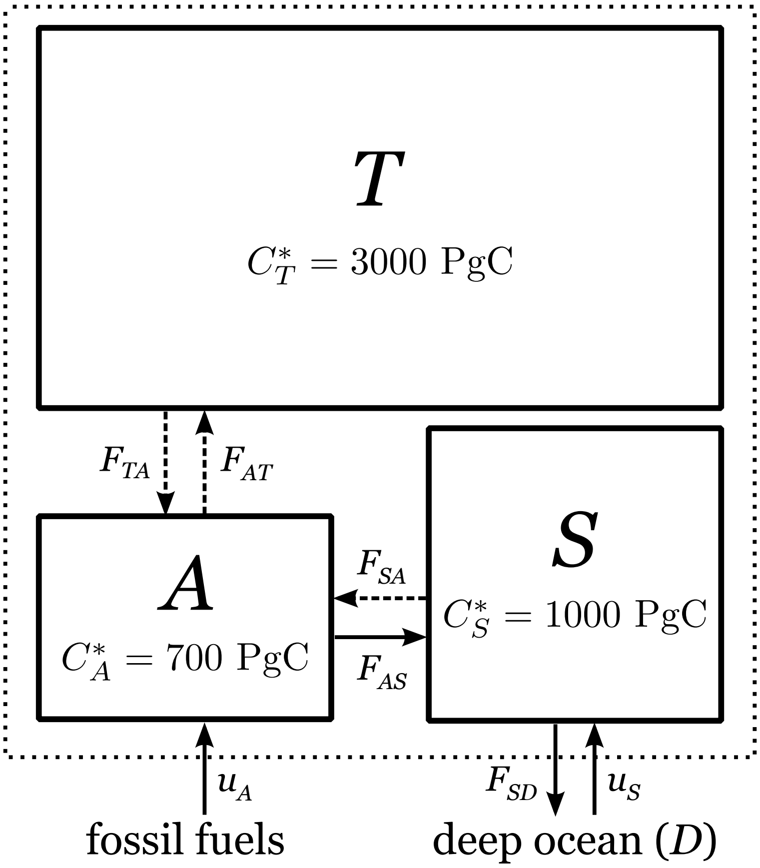
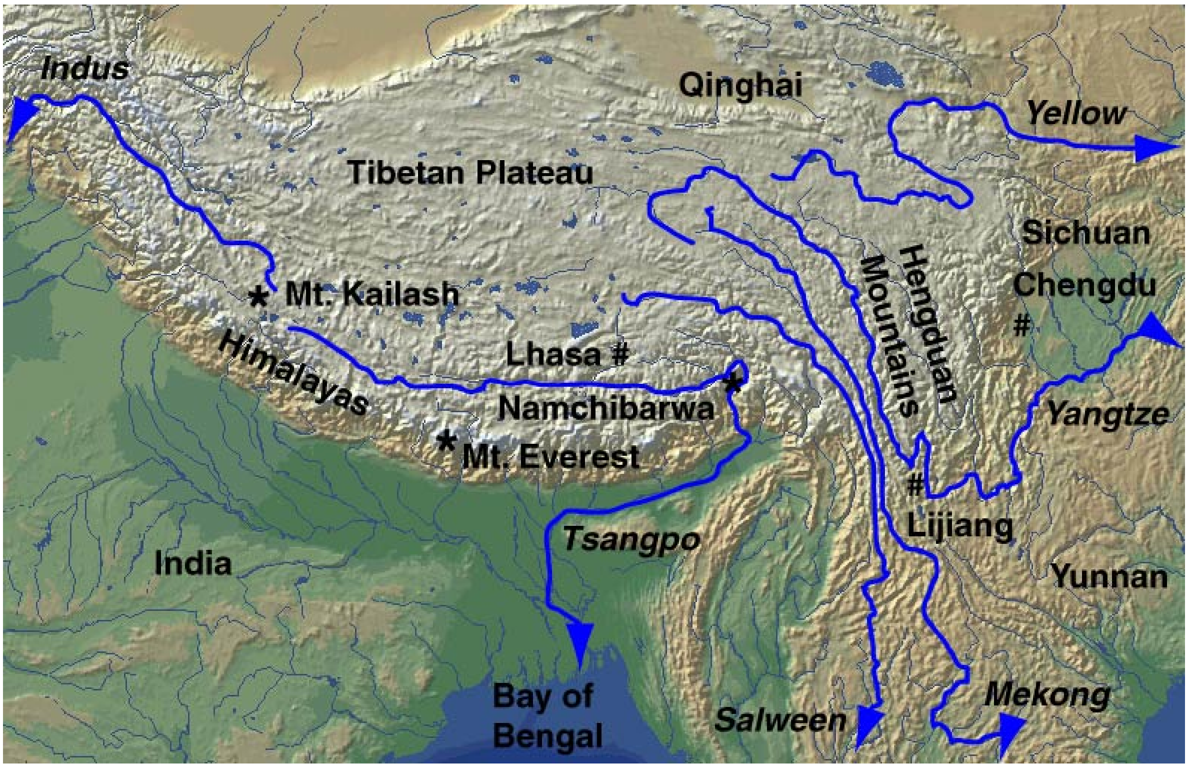
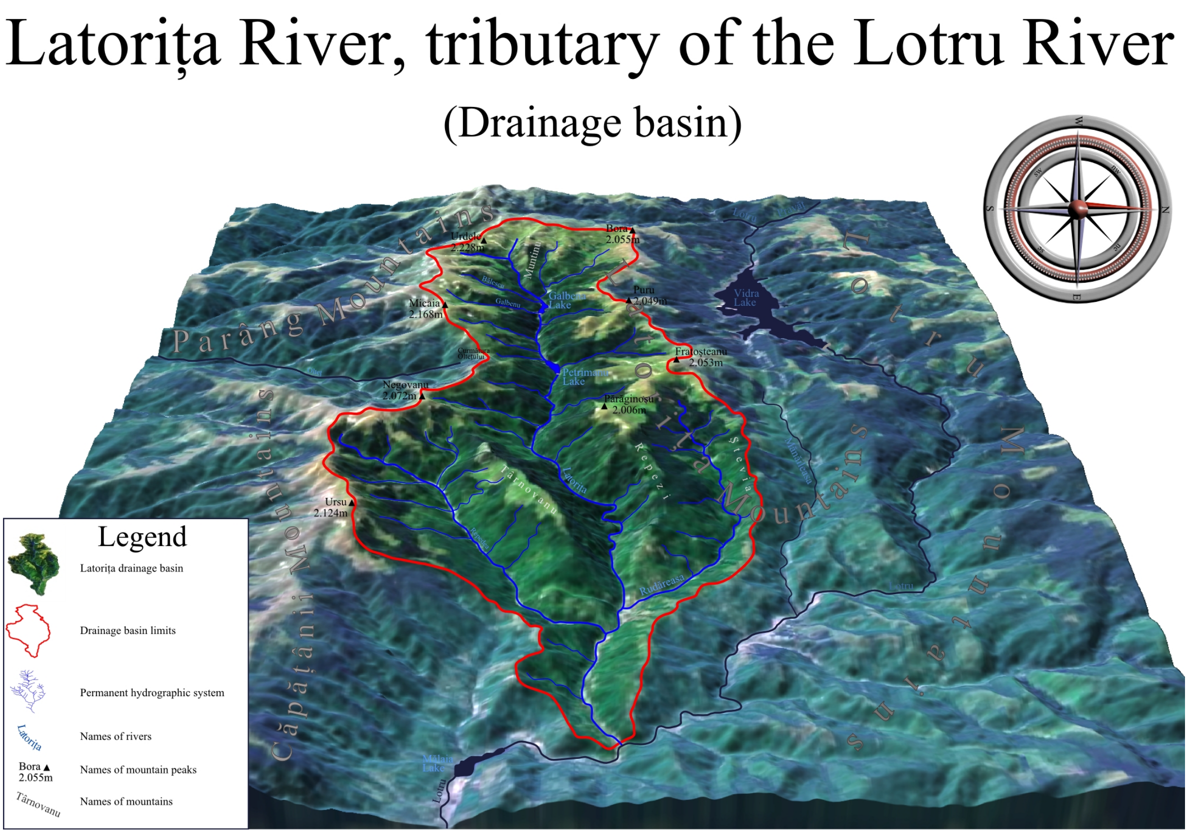
1. Example Applications of Pool Models
2. Reducing Model Complexity
   - The Carbon Cycle example
   - Asking Simpler Questions
   - Answer Questions more simply
3. Compartmental Systems
4. Generalization to non Well Mixed Systems
   - Population Dynamics



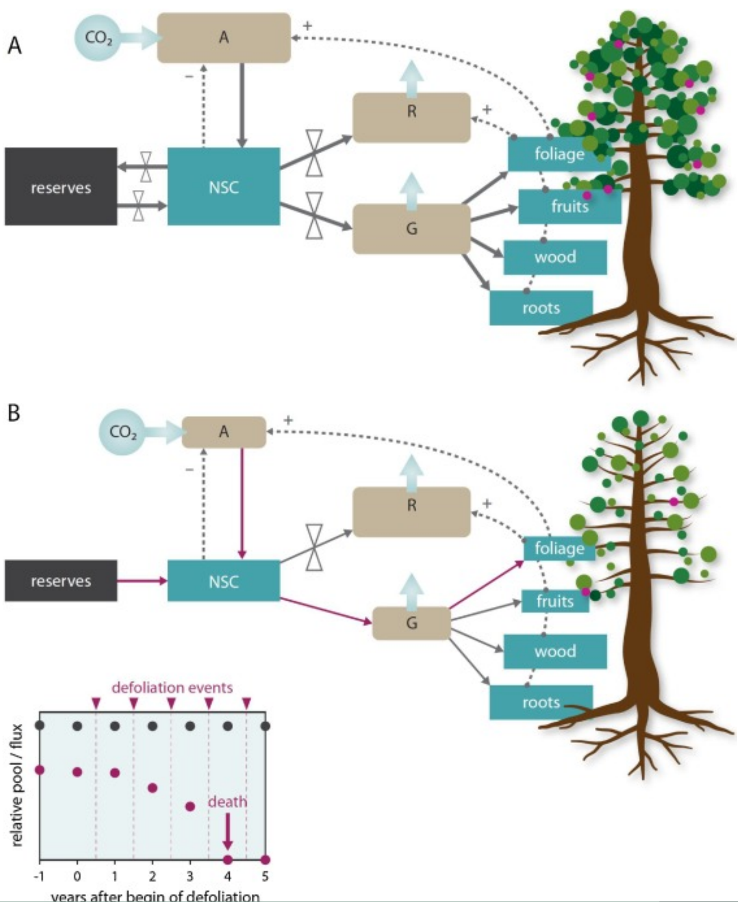
Hydrology Watersheds



Hydrology Catchments



Plant Physiology/ Carbon allocation



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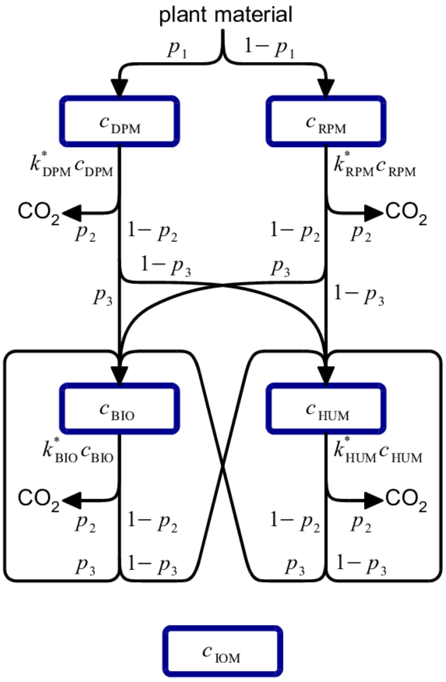
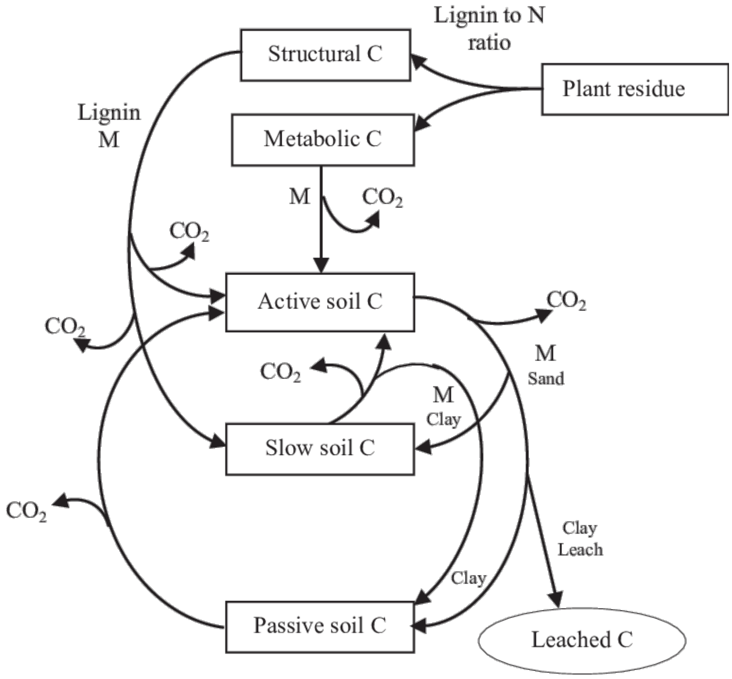
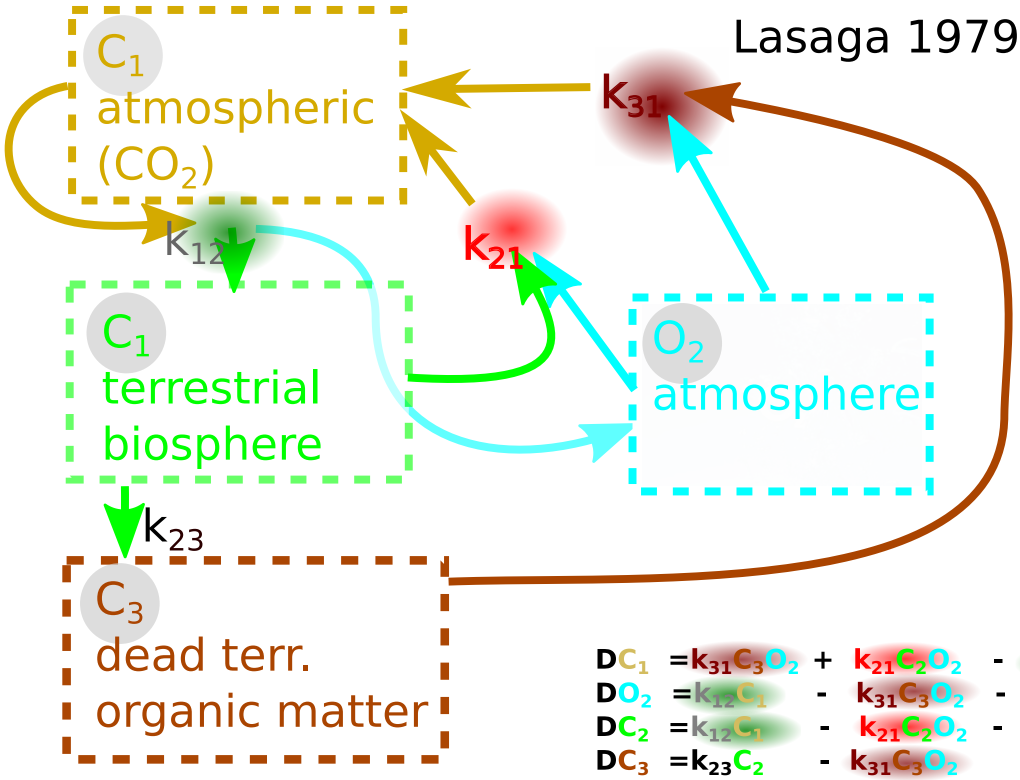
Organic Matter Decomposition / Soil Models





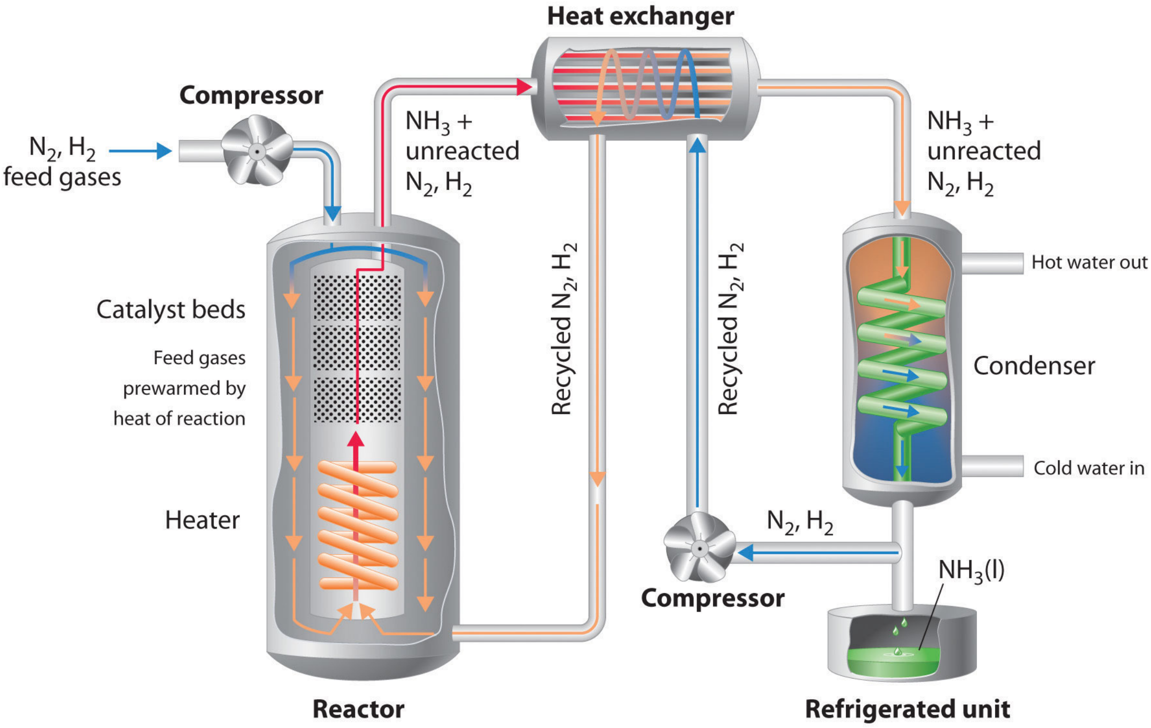
Ecosystem Models

Lasaga 1979

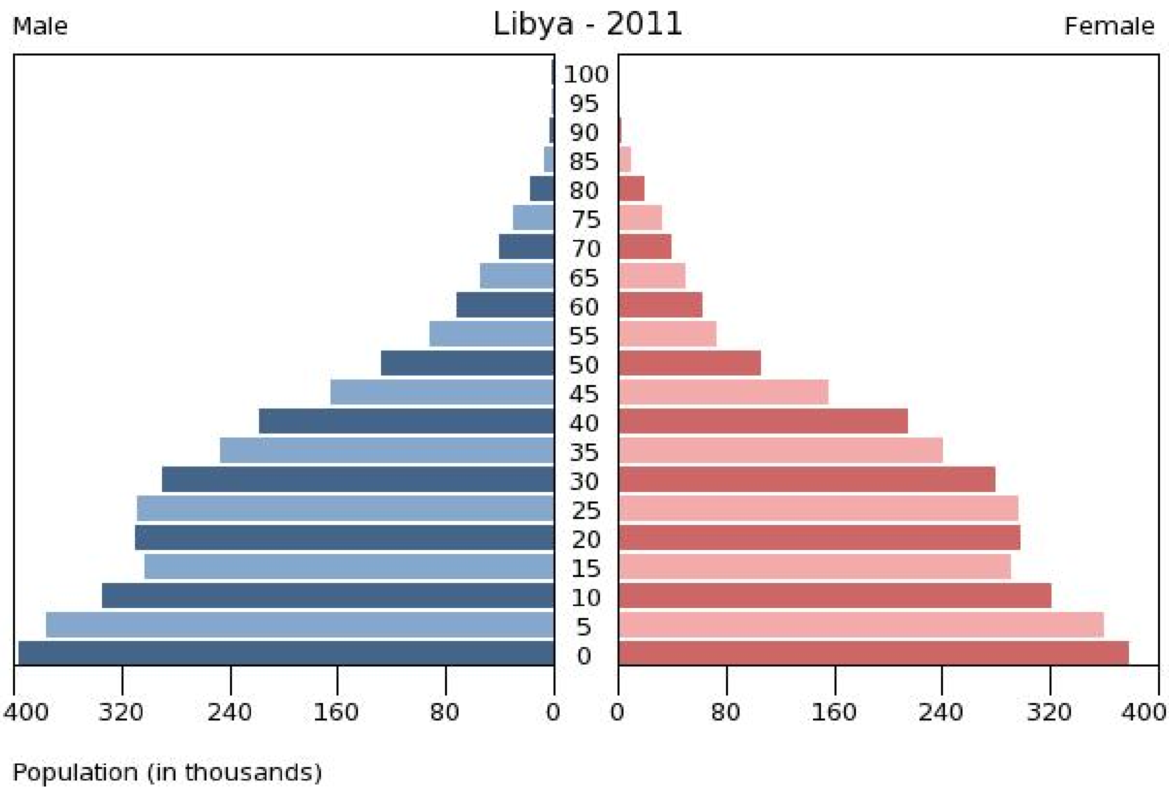


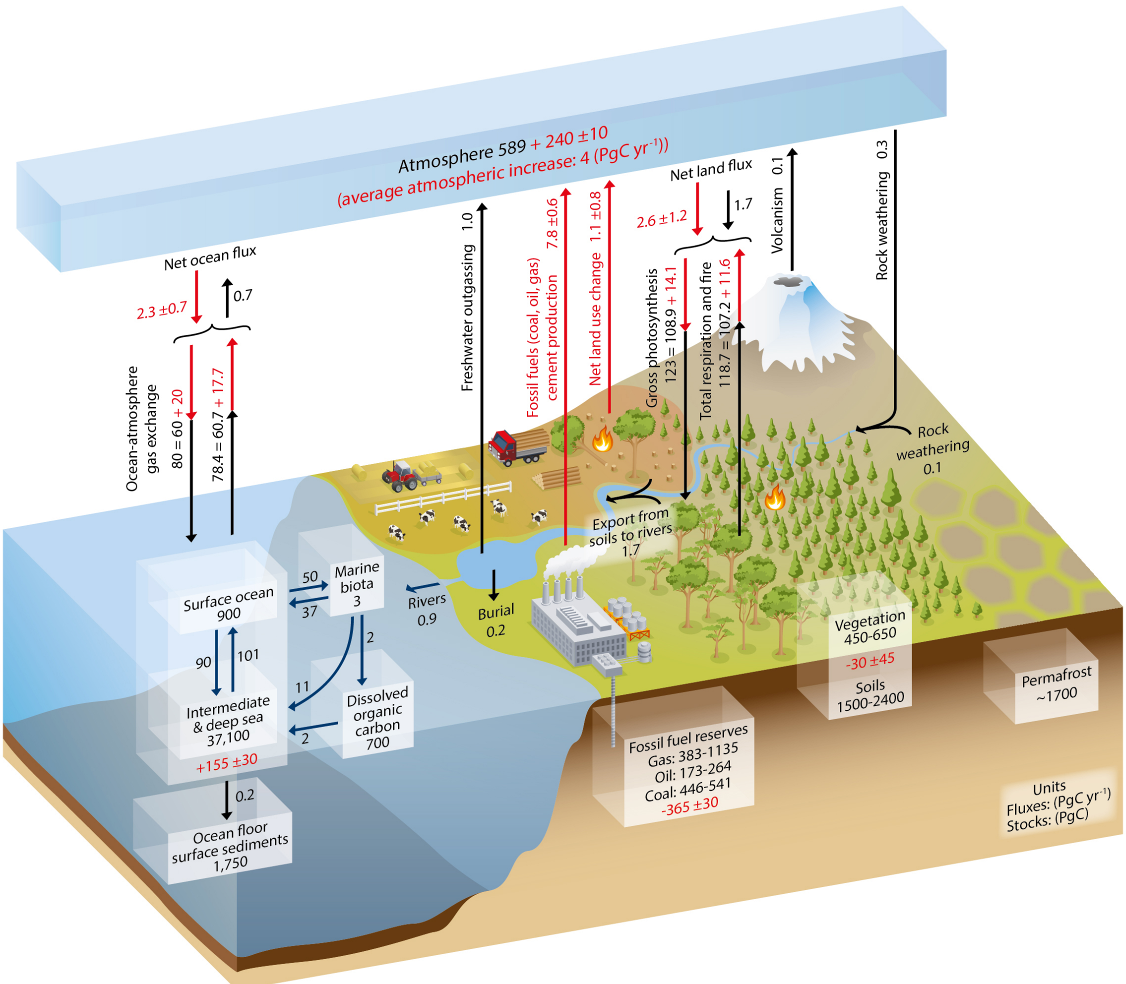
$$DC_1 = k_{31}C_3O_2 + k_{21}C_2O_2 - k_{12}C_1$$
$$DO_2 = k_{12}C_1 - k_{31}C_3O_2 - k_{21}C_2O_2$$
$$DC_2 = k_{12}C_1 - k_{21}C_2O_2 - k_{23}C_2$$
$$DC_3 = k_{23}C_2 - k_{31}C_3O_2$$

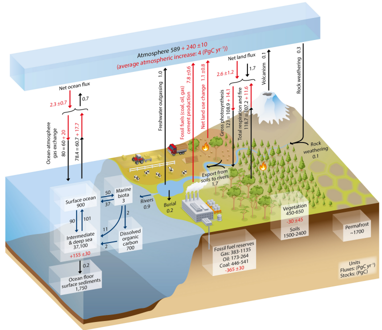
Chemical Reactors

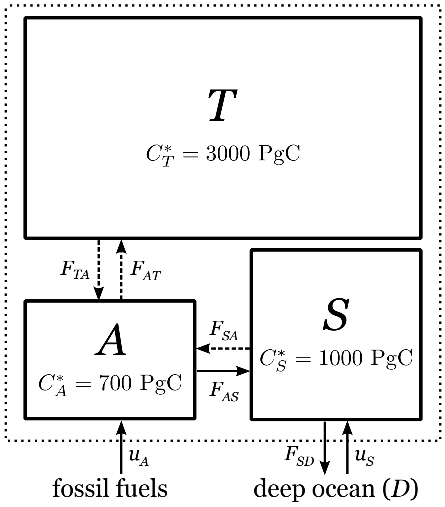


Population Dynamics

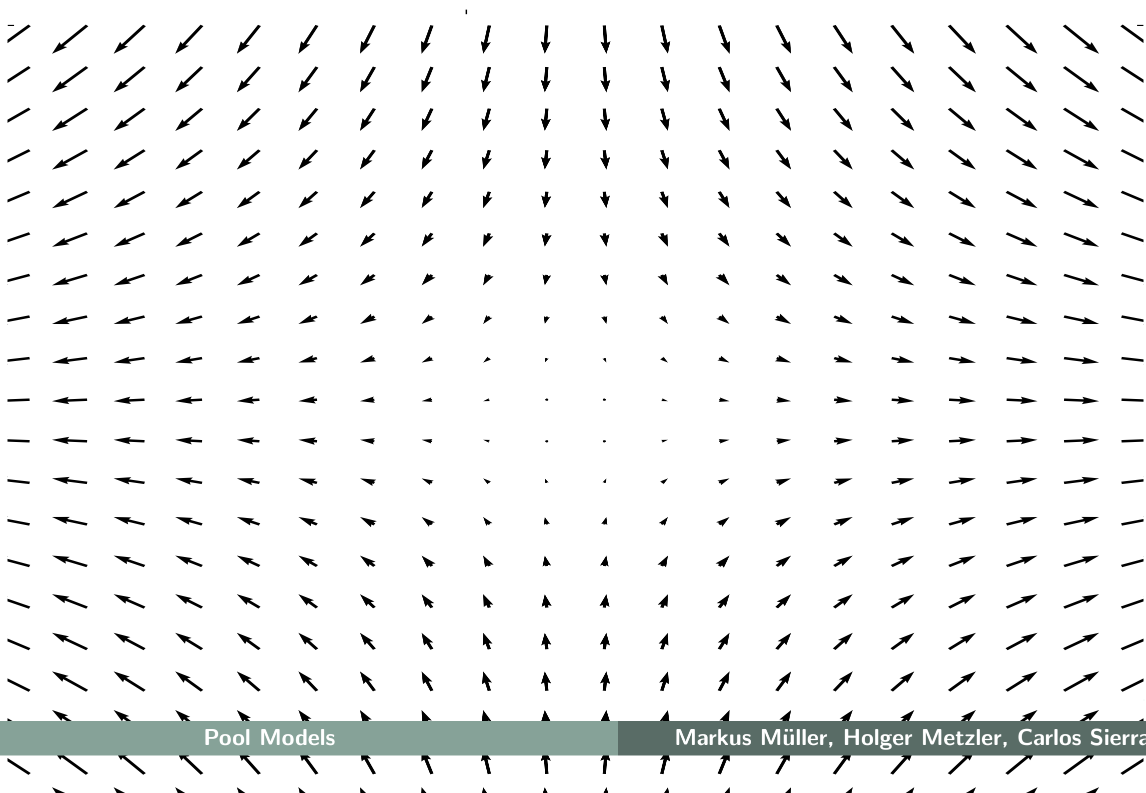


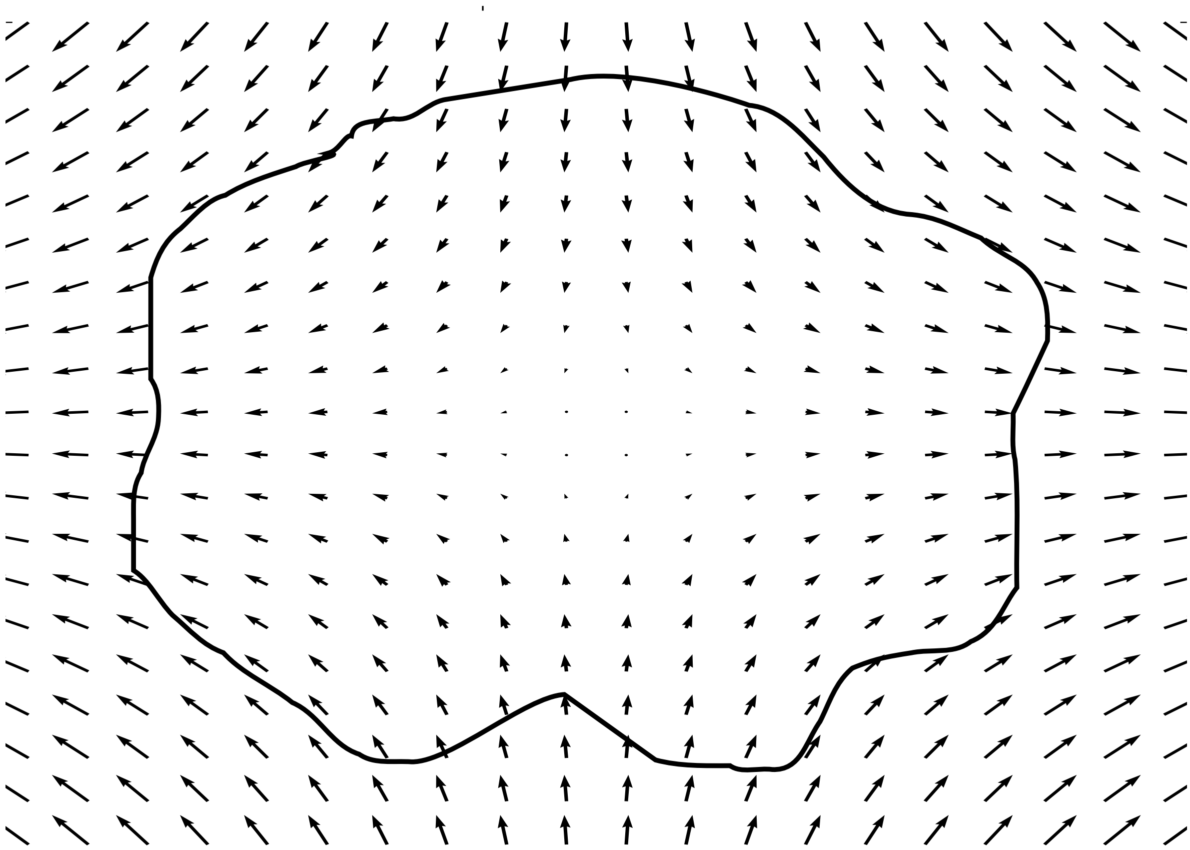

Atmosphere 589 + 240 ±10
(average atmospheric increase: 4 (PgC yr⁻¹))
Net ocean flux
2.3 ±0.7
0.7
Ocean-atmosphere gas exchange
80 = 60 + 20
78.4 = 60.7 + 17.7
Freshwater outgassing 1.0
Fossil fuels (coal, oil, gas) cement production 7.8 ±0.6
Net land use change 1.1 ±0.8
Net land flux
2.6 ±1.2
1.7
Gross photosynthesis 123 = 108.9 + 14.1
Total respiration and fire 118.7 = 107.2 + 11.6
Volcanism 0.1
Rock weathering 0.3
Rock weathering 0.1
Export from soils to rivers 1.7
Surface ocean 900
50
37
Marine biota 3
Rivers 0.9
Burial 0.2
90
101
2
11
Intermediate & deep sea 37,100
+155 ±30
2
Dissolved organic carbon 700
0.2
Ocean floor surface sediments 1,750
Vegetation 450-650
-30 ±45
Soils 1500-2400
Permafrost ~1700
Fossil fuel reserves
Gas: 383-1135
Oil: 173-264
Coal: 446-541
-365 ±30
Units
Fluxes: (PgC yr⁻¹)
Stocks: (PgC)

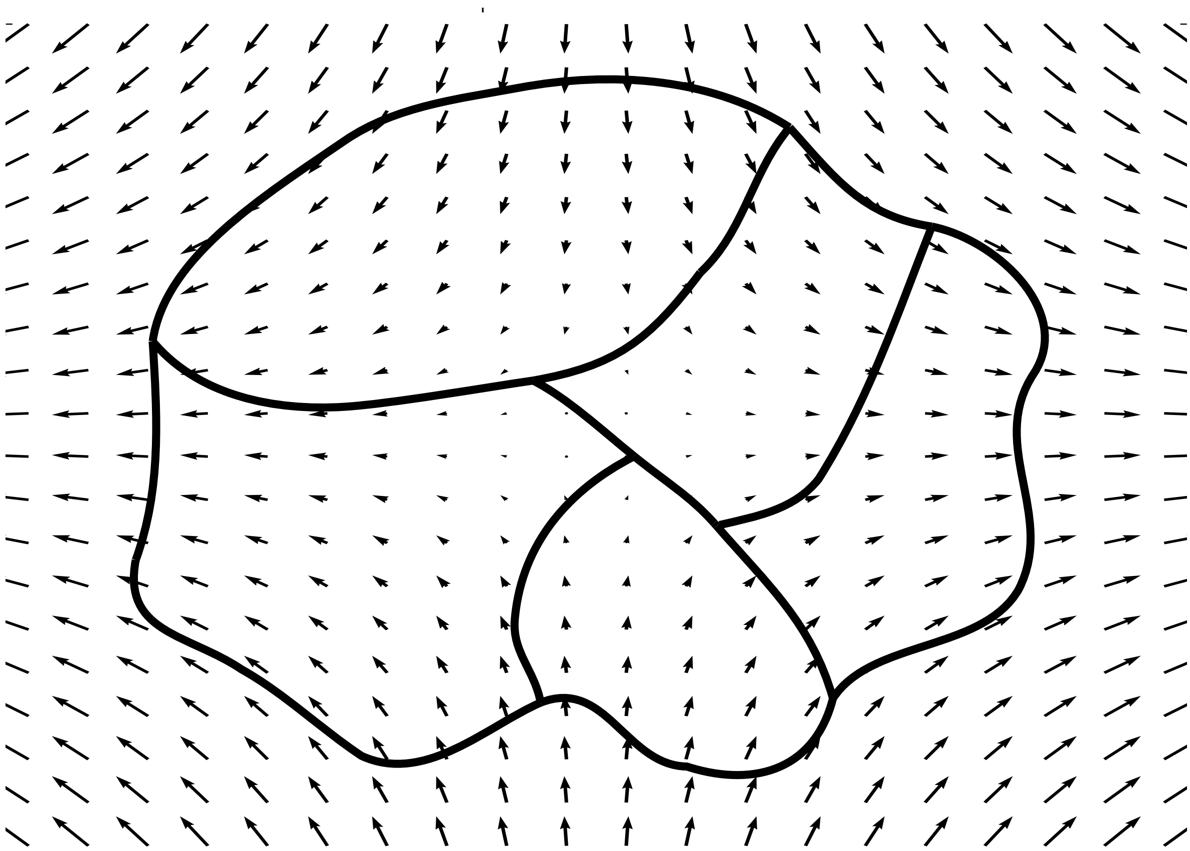


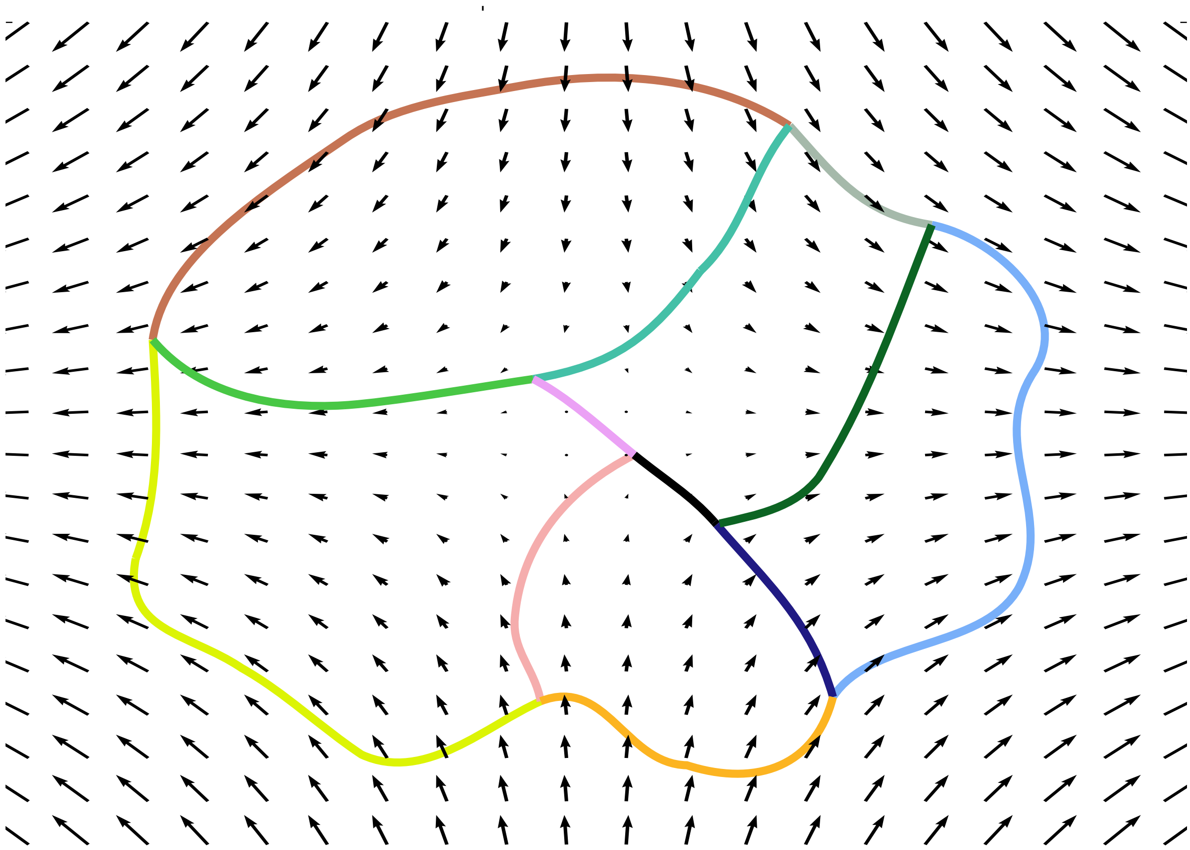


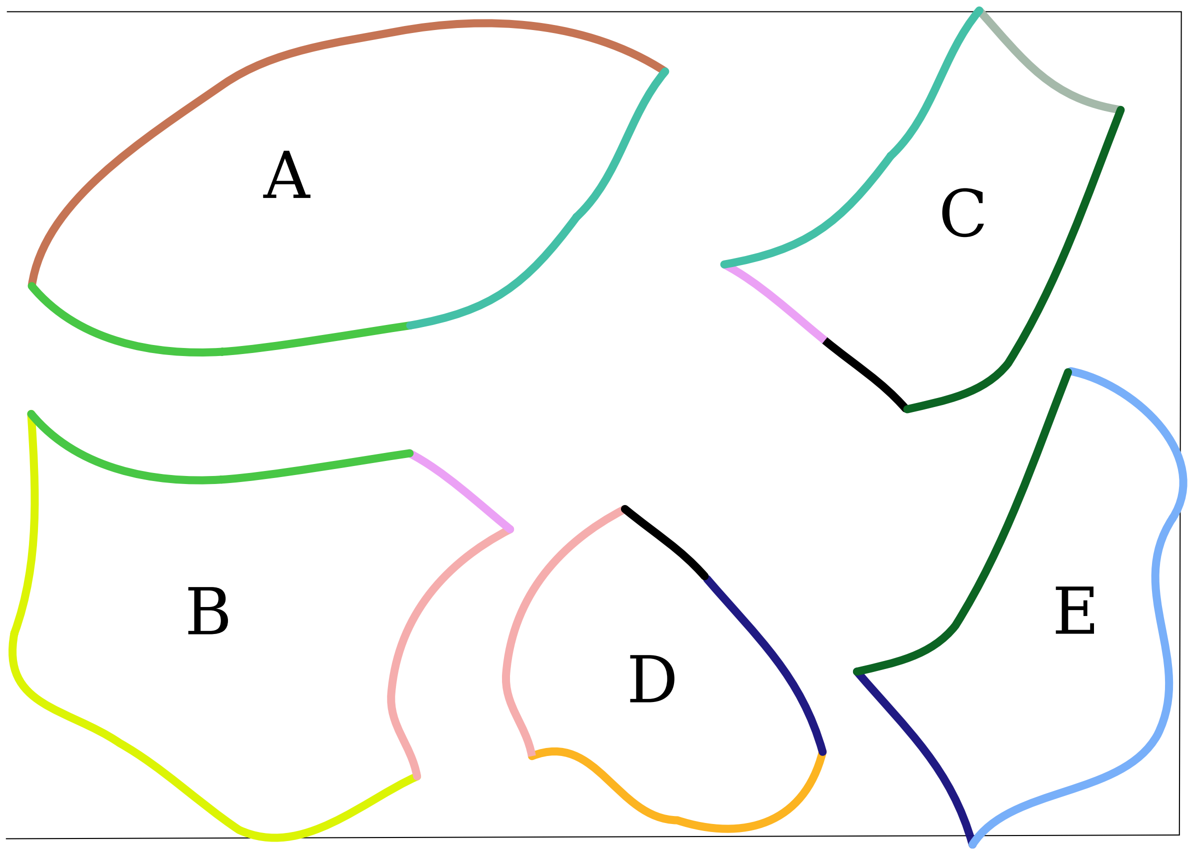
T
$C_T^* = 3000$ PgC
F_{TA}
F_{AT}
A
$C_A^* = 700$ PgC
S
$C_S^* = 1000$ PgC
F_{SA}
F_{AS}
u_A
fossil fuels
F_{SD}
u_S
deep ocean (D)

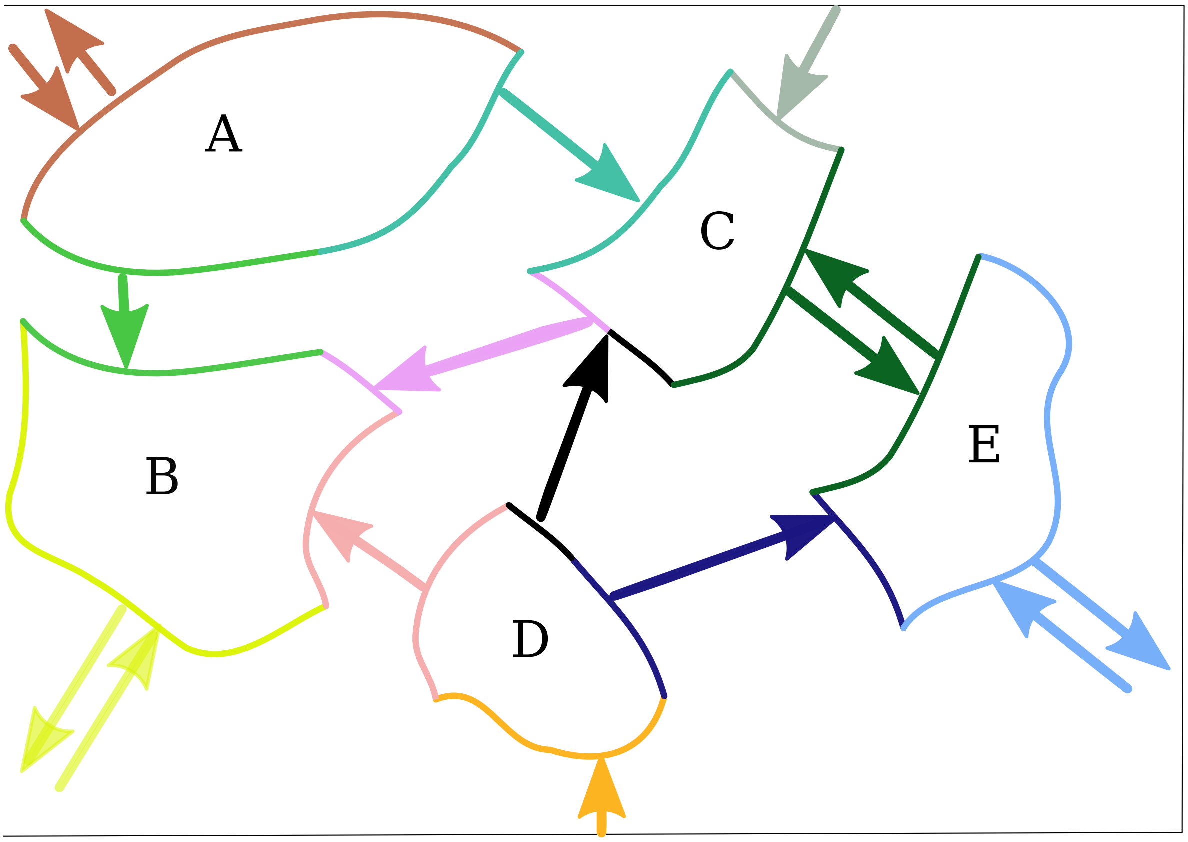









A
B
C
D
E


A
B
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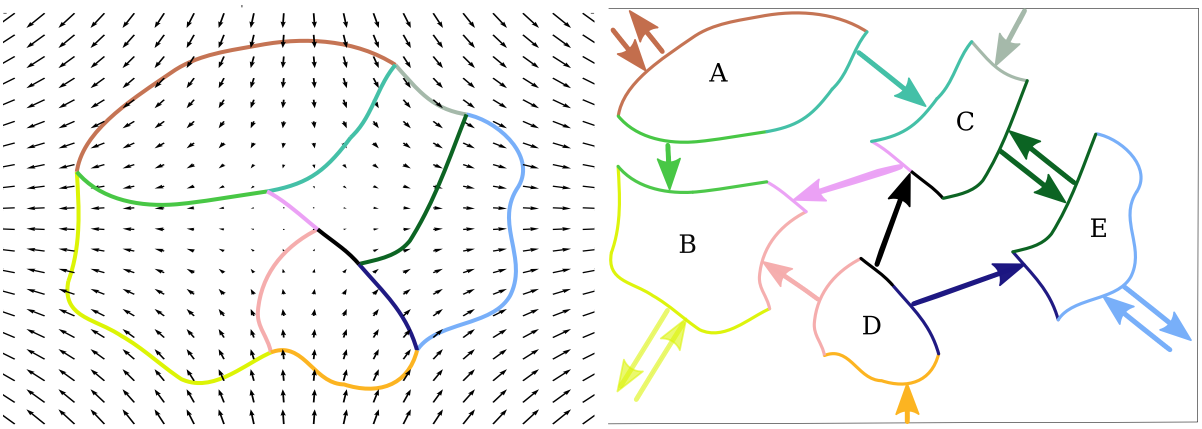
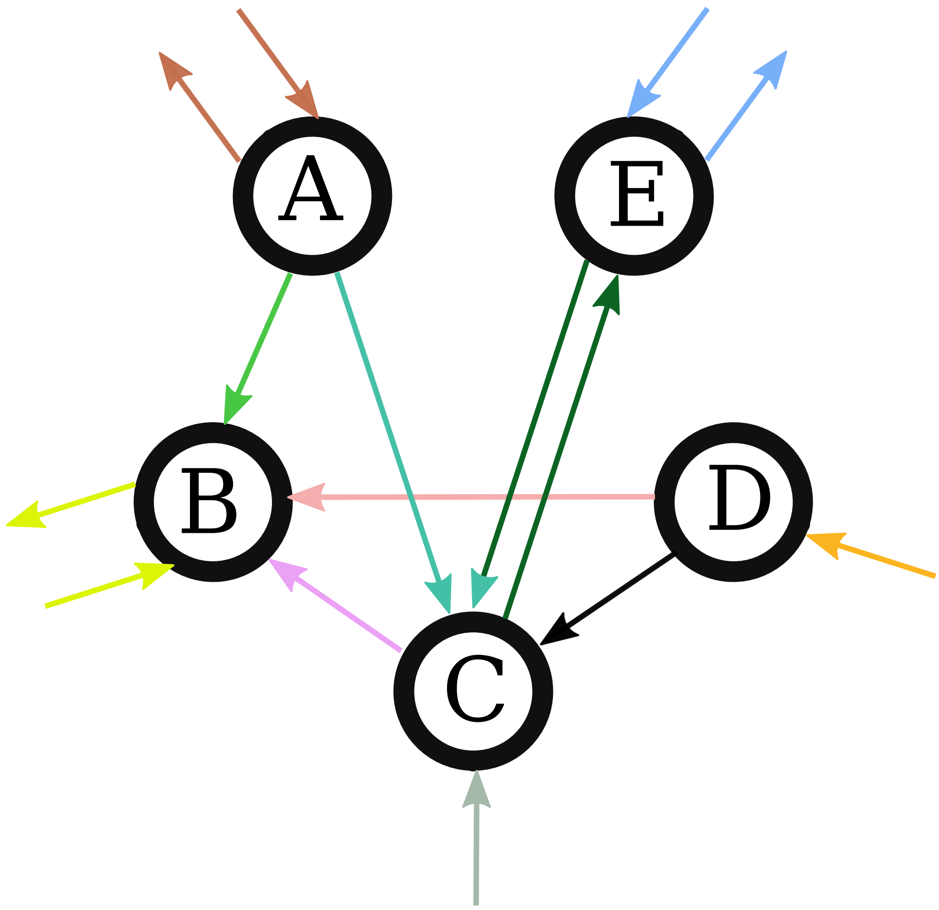
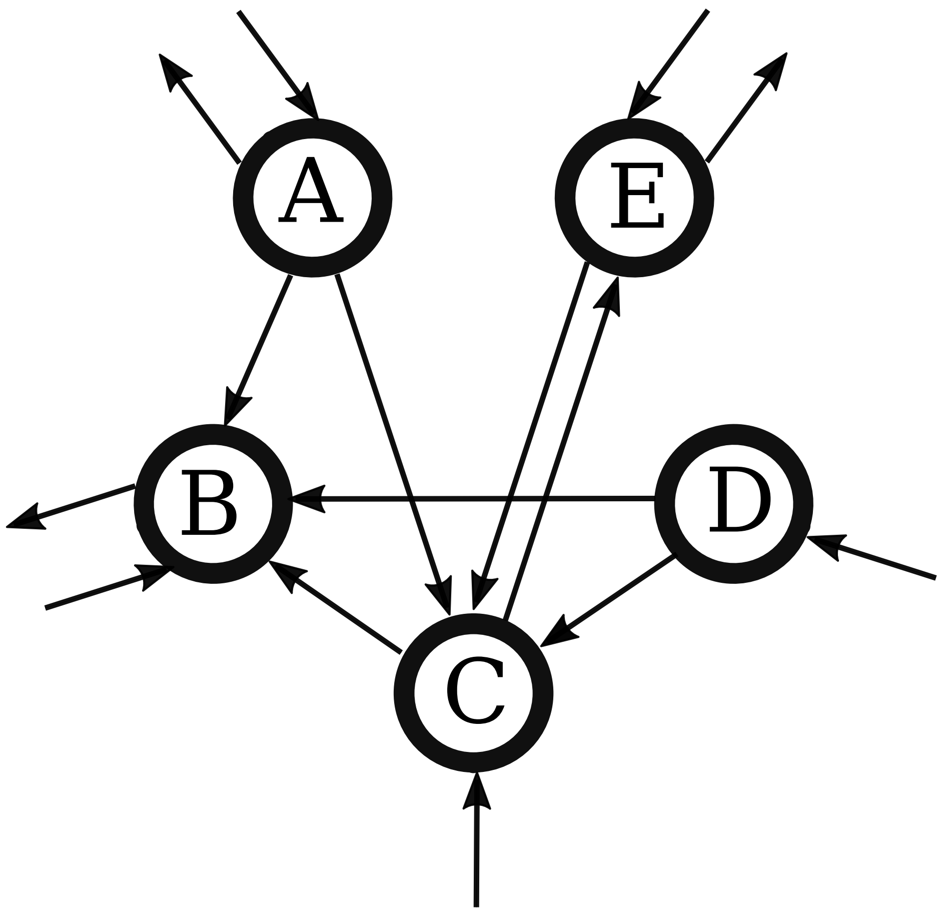
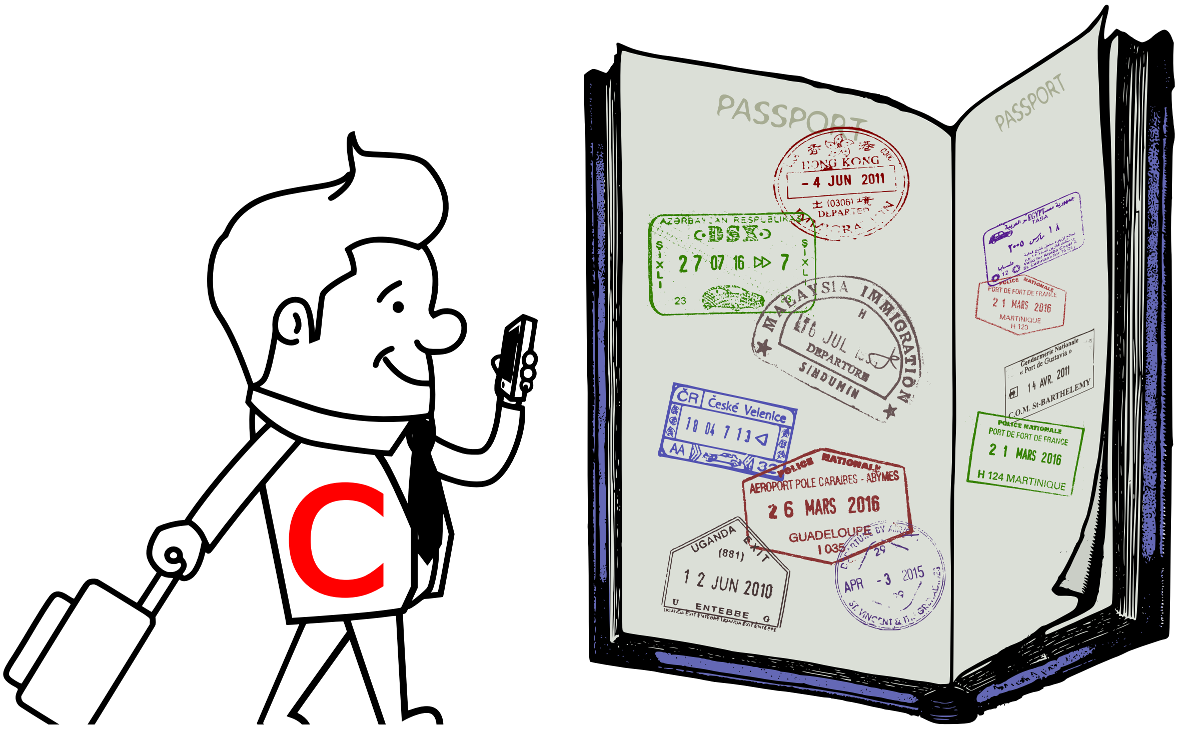
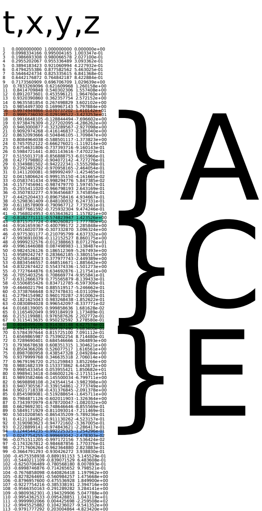
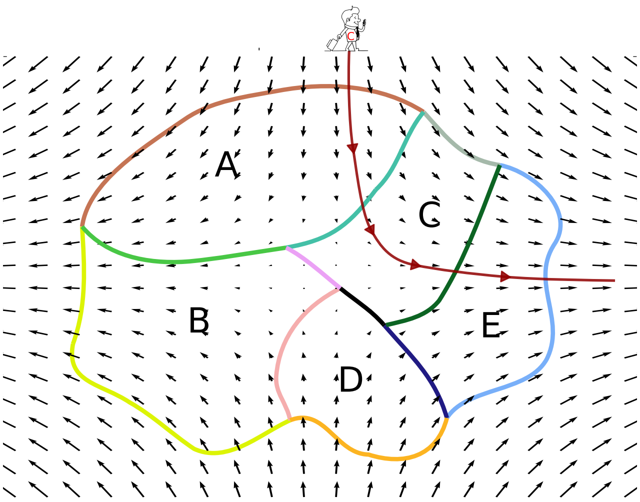

A
B
C
D
E


A
E
B
D
C


A
E
B
D
C

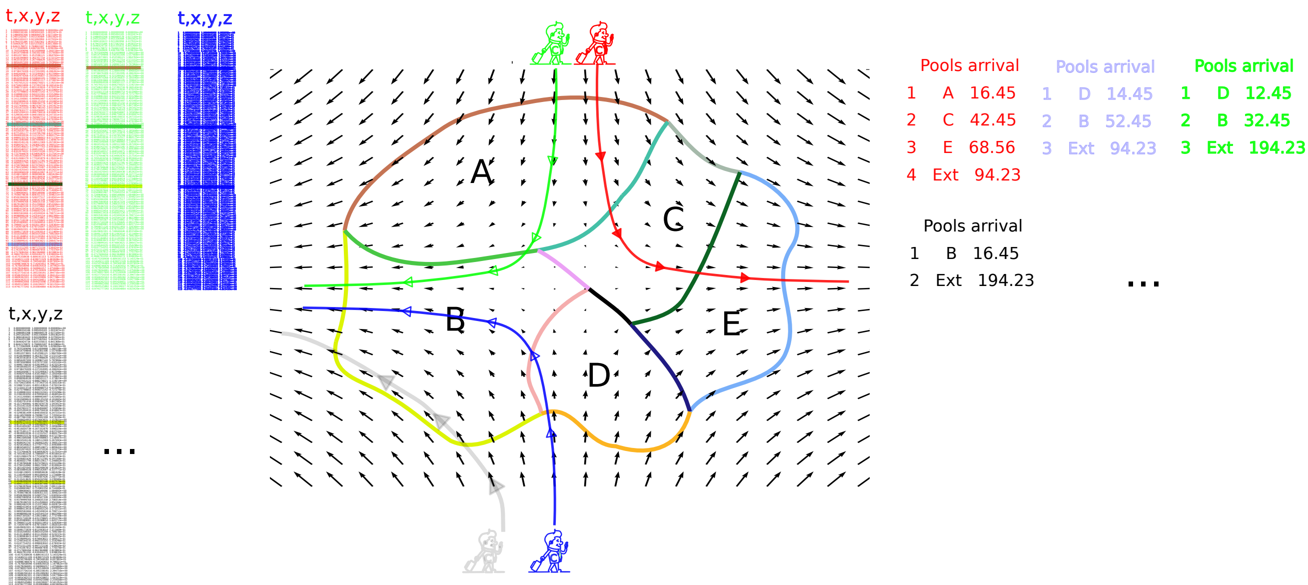




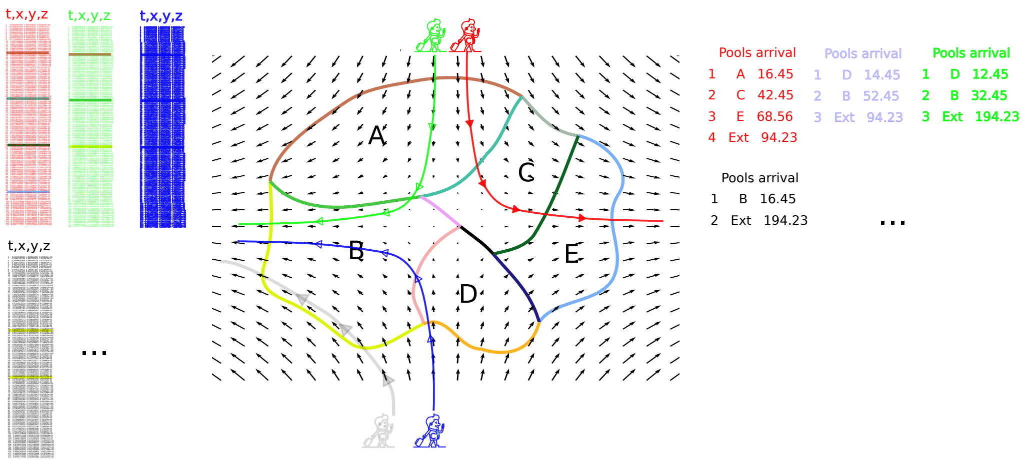


Pools arrival

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

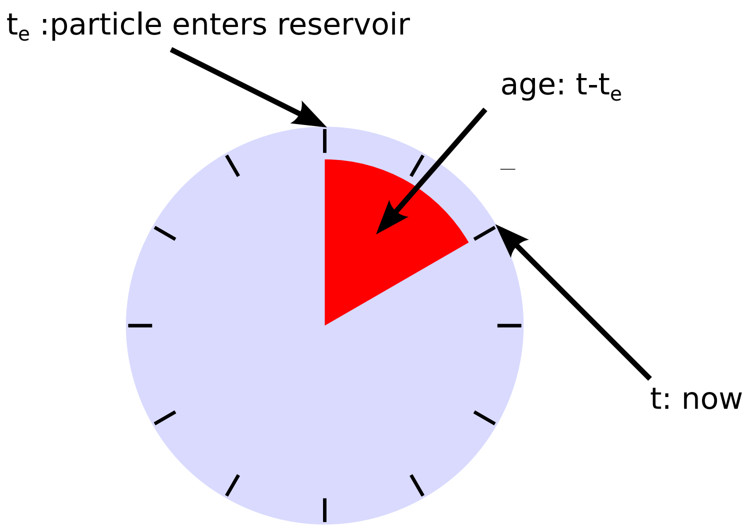


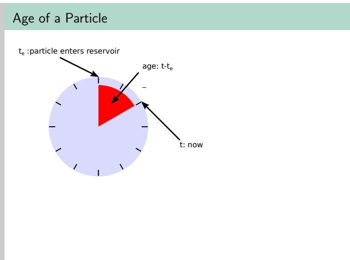
Possible Descriptive Statistics



- 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.

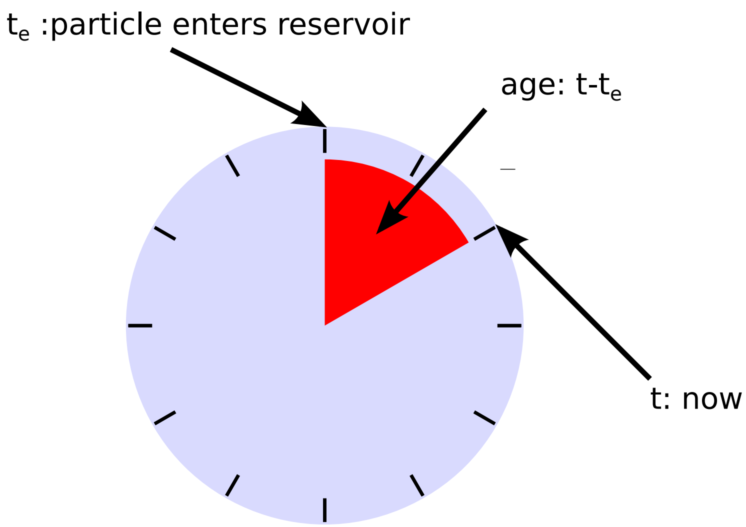
Age of a Particle





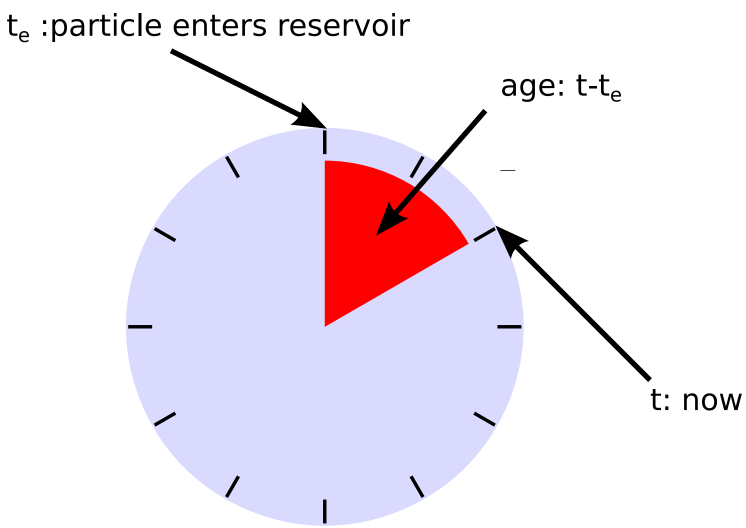
We can define the age of a particle with respect to the reservoir as the time it has spent in it. In the case of the human population this refers to the age in common sense. But in general the age refers not to the time of creation but to the time the reservoir was entered. If the reservoir in question is e.g. the soil and the particle a ^{14}C atom that entered the soil 5 minutes ago it is at least possible that the atom is as old as the universe while its age with respect to the soil is only 5 minutes

Age of a Particle



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

Age of a Particle



- The “age ” can not be negative!

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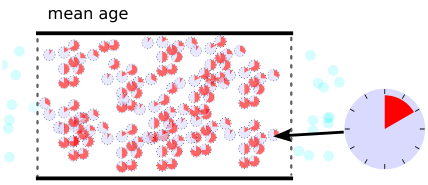
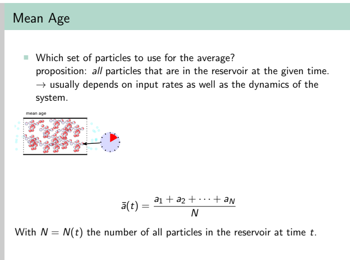
Mean Age

- Which set of particles to use for the average?
  proposition: *all* particles that are in the reservoir at the given time.
  $\rightarrow$ usually depends on input rates as well as the dynamics of the system.



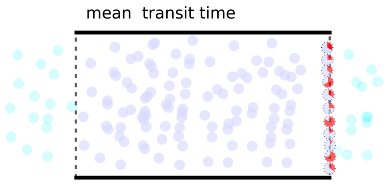
$$\bar{a}(t) = \frac{a_1 + a_2 + \cdots + a_N}{N}$$

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



To compute the average age of the population of the world at a given time we would have to ask everybody how old he is and then compute the mean value. If we treat this room as a reservoir everybody would have started a stopwatch entering the room, press the stop button now and we would have to add all the times and divide them by the number of people.

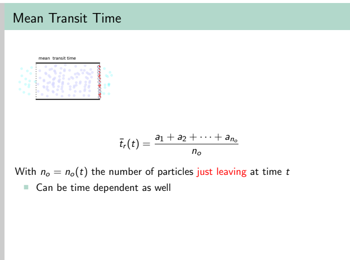
Mean Transit Time



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

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

- Can be time dependent as well



In the example of the world population it would be sufficient to observe the grave yards. We would investigate the birth date of every person who dies and compute the average of the live spans. We ignore all the people still alive and concentrate only on the people just dying. In this room it would be hard to compute the average transit time right now, because nobody is leaving at the moment. (dropping of to sleep does not count as leaving). But we could after the talk. Every person would press the stop bottom at its watch in the moment she passes the door. If two or more people would leave in the same moment we could compute the average of the times. It is also

Mean Transit Time

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- 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)

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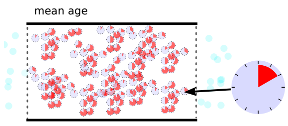
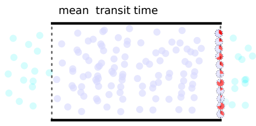
Differences between mean age and mean transit time





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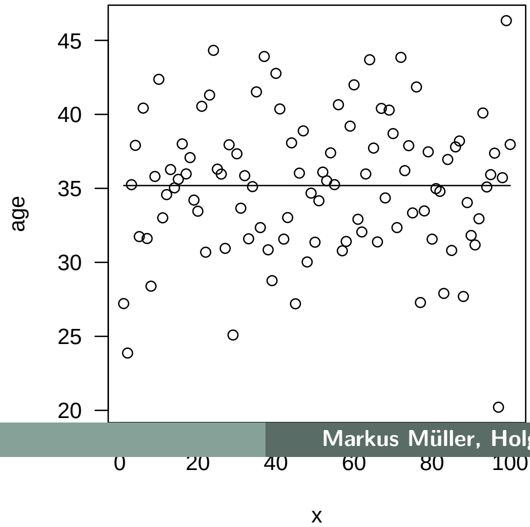
$$\bar{t}_r(t) = \frac{a_1 + a_2 + \cdots + a_{n_o}}{n_o}$$

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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2. as above + make a histogram of all ages
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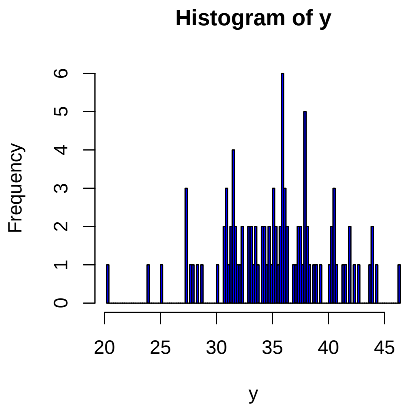
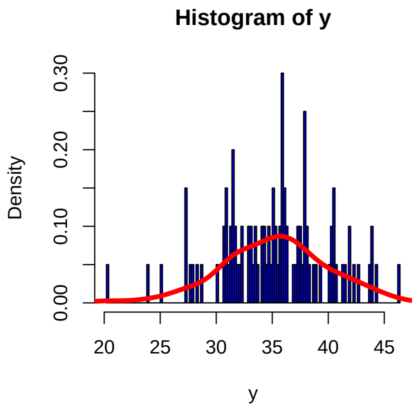
$$\bar{t}_r(t) = \frac{a_1 n_{a_1} + a_2 n_{a_2} + \cdots + a_n n_{a_n}}{n_o}$$

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



Integration over a density

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

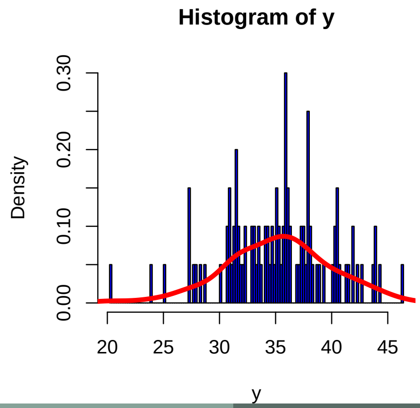


Same procedure for age density

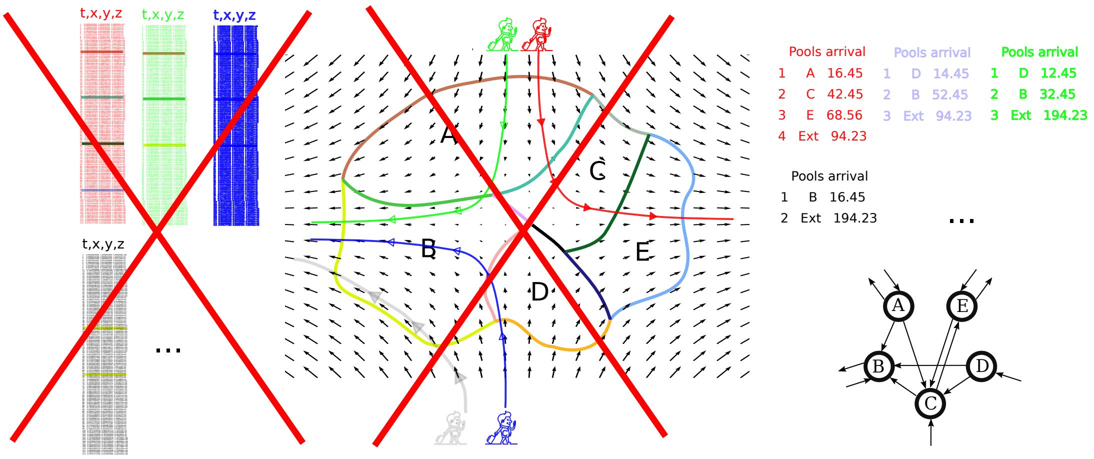
$$\bar{a}(t) = \lim_{n\to\infty} \frac{a_1 n_{a_1} + a_2 n_{a_2} + \cdots + a_n n_{a_n}}{n_p}$$

$$= \lim_{n\to\infty} \sum_{minage}^{maxage} a \frac{n(a)}{n_p} da$$

$$= \int_{minage}^{maxage} a\phi(a)da$$



Possible Predictive Statistics ?



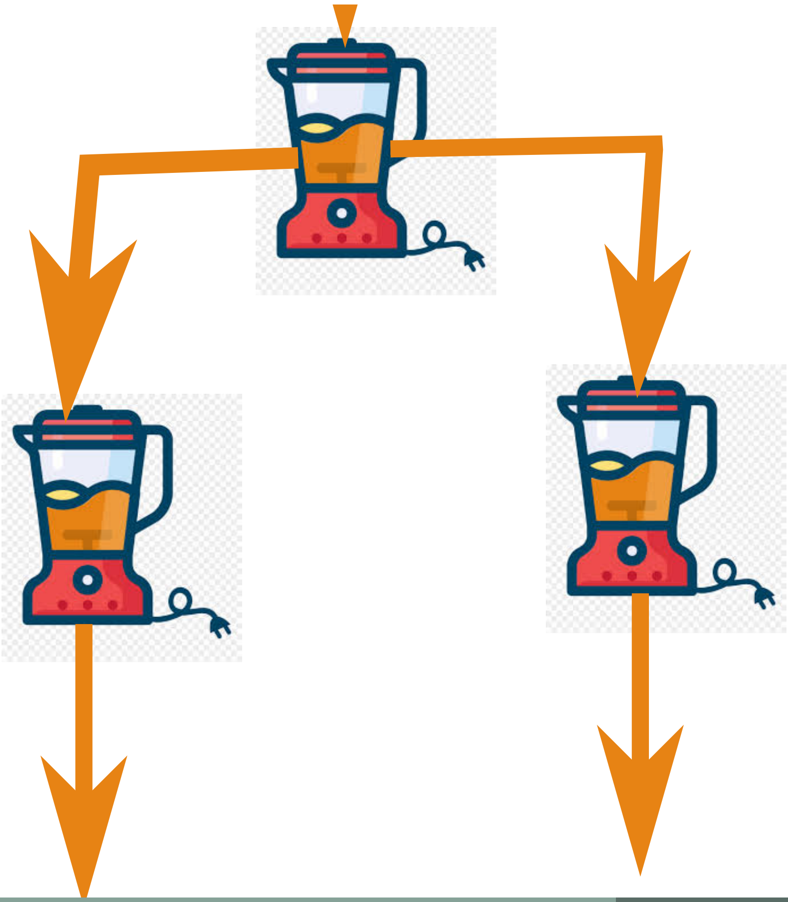
- Could we make a rule to predict the number of particles exiting from Pool E at time using only the particle passports? (Assuming that the exit from E is not recorded.)
- Could we make a rule to predict the age distribution of particles exiting from Pool E at time using only the particle passports?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

Intermediate Summary

1. Pool descriptions condense complex information to a time series of pool changes.(A series of stamps in the passport)
2. 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,
3. Pool Models predict = model some of these exclusively with respect to the information obtainable from (all) passports.
4. The most common even disregard most of the information in the passports.

The simplest pool yystems

The simplest pool systems are well mixed



Only the number of particles per Pool counts ...

	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

...

Only the number of particles per Pool counts ...

	Pools	arrival
1	A	16.45
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	Pools	arrival
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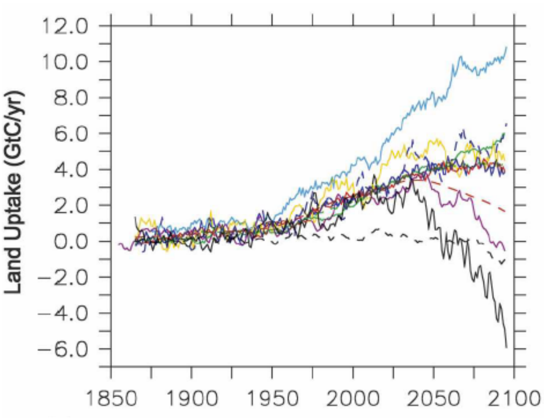
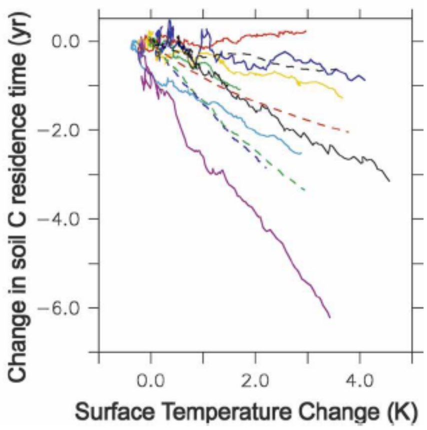
...

Diverse model predictions





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Model comparison

Key quantities

Model comparison

Key quantities

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

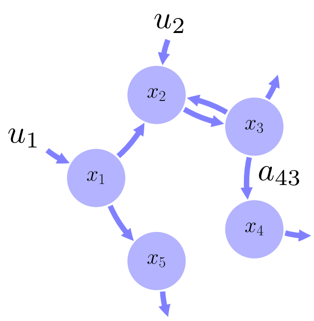
Model comparison

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

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



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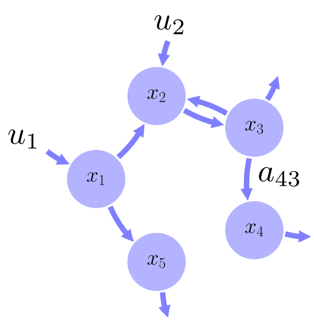

$\mathbf{x}(t)$ vector of compartment content (e.g. C) at time t

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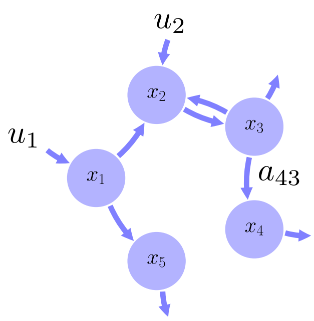

$\mathbf{x}(t)$	vector of compartment content (e.g. C) at time t
$\mathbf{u}$	constant input vector

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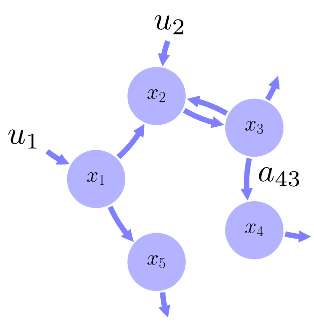

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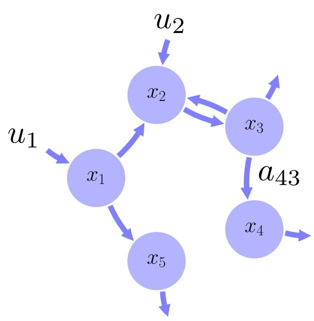

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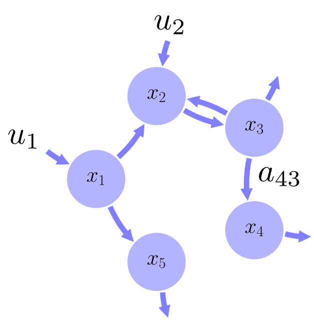

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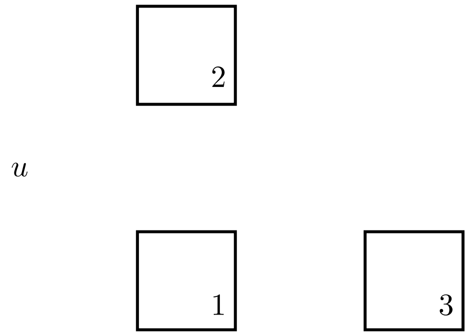
$-a_{ii} > 0$	rate of flow out of compartment i

A particle travels

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



$$\begin{array}{cc} \mathrm{A} & \mathbf{u} \\ \begin{pmatrix} -a_{11} & a_{12} & 0 \\ a_{21} & -a_{22} & 0 \\ a_{31} & 0 & -a_{33} \end{pmatrix} & \begin{pmatrix} u_1 \\ u_2 \\ 0 \end{pmatrix} \end{array}$$

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

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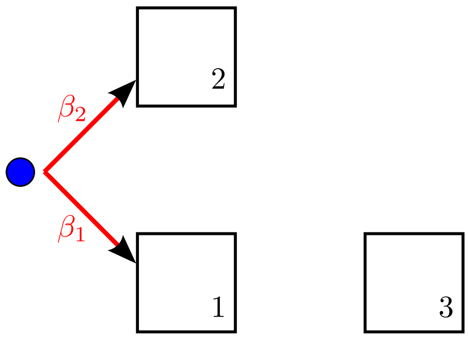

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$$-\sum \quad 0 \quad > 0 \quad > 0 \qquad \|\mathbf{u}\|$$

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

$T_0 = 0$

A particle travels

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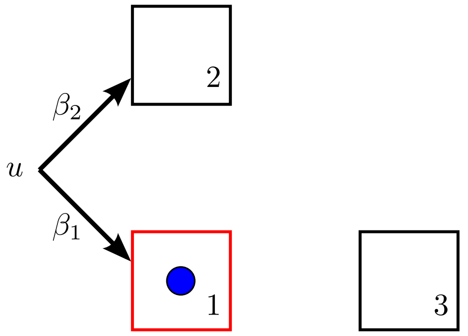
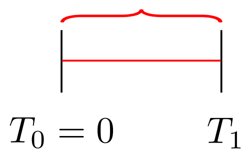


$$\begin{array}{c|ccc|c} & & \mathrm{A} & & \mathbf{u} \\ & \begin{pmatrix} -a_{11} & a_{12} & 0 \\ a_{21} & -a_{22} & 0 \\ a_{31} & 0 & -a_{33} \end{pmatrix} & & & \begin{pmatrix} u_1 \\ u_2 \\ 0 \end{pmatrix} \\ -\sum & 0 & >0 & >0 & \|\mathbf{u}\| \end{array}$$

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



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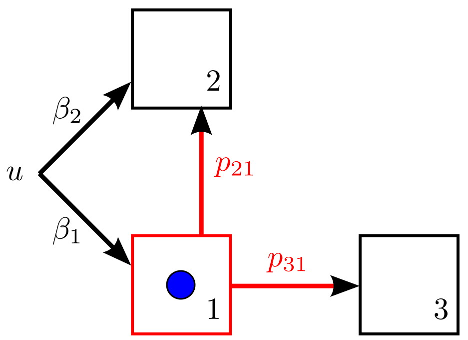

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$$p_{21} = \frac{a_{21}}{a_{11}} \qquad p_{31} = \frac{a_{31}}{a_{11}}$$

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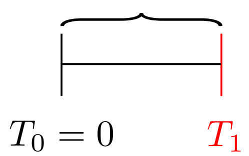
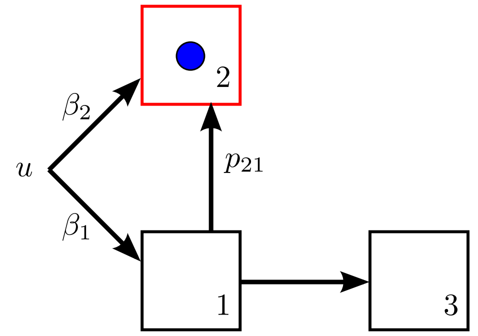


A particle travels $\quad \frac{d}{dt}\mathbf{x}(t) = \mathrm{A}\,\mathbf{x}(t) + \mathbf{u}$



$$
\begin{array}{c|c}
\mathrm{A} & \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} \\
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\end{array}
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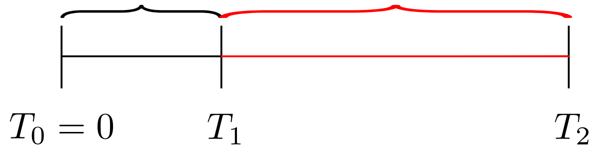
$T_1 \sim \mathrm{Exp}(a_{11})$

$T_2 - T_1 \sim \mathrm{Exp}(a_{22})$



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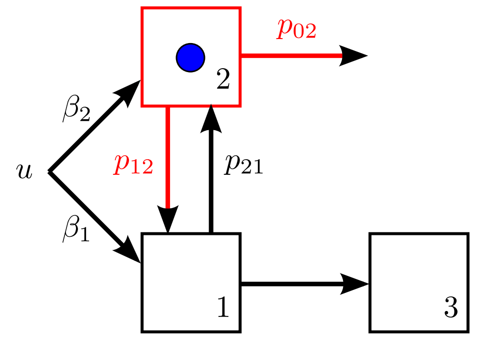

$$
\begin{array}{c|c}
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\begin{pmatrix} -a_{11} & a_{12} & 0 \\ a_{21} & -a_{22} & 0 \\ a_{31} & 0 & -a_{33} \end{pmatrix} & \begin{pmatrix} u_1 \\ u_2 \\ 0 \end{pmatrix} \\
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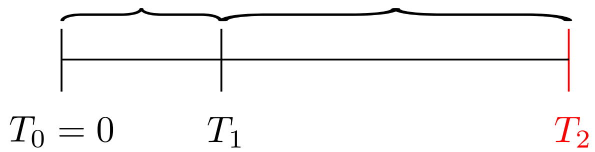
\end{array}
$$

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

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

$T_2 - T_1 \sim \mathrm{Exp}(a_{22})$



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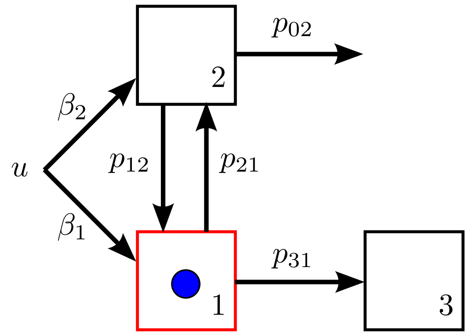

$$
\begin{array}{ccc}
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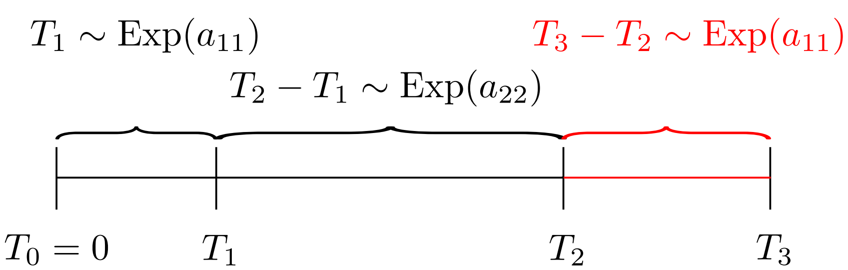

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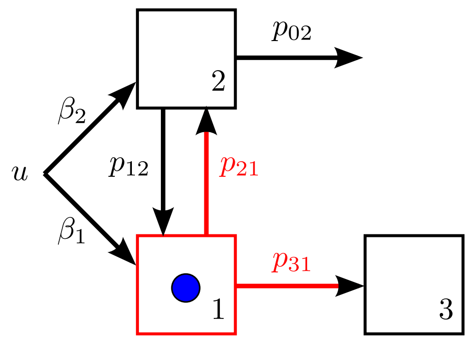

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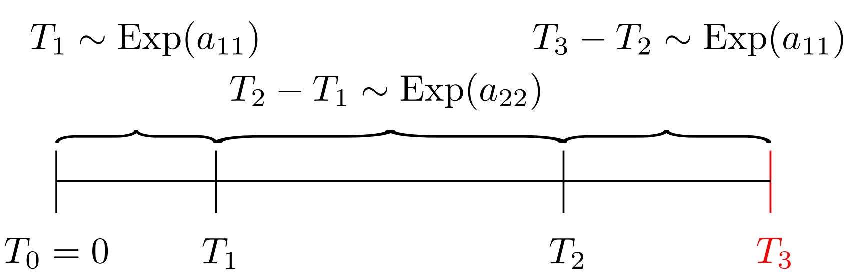

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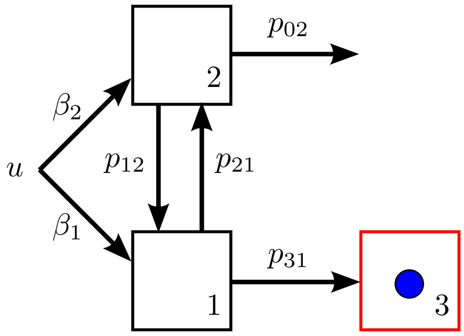

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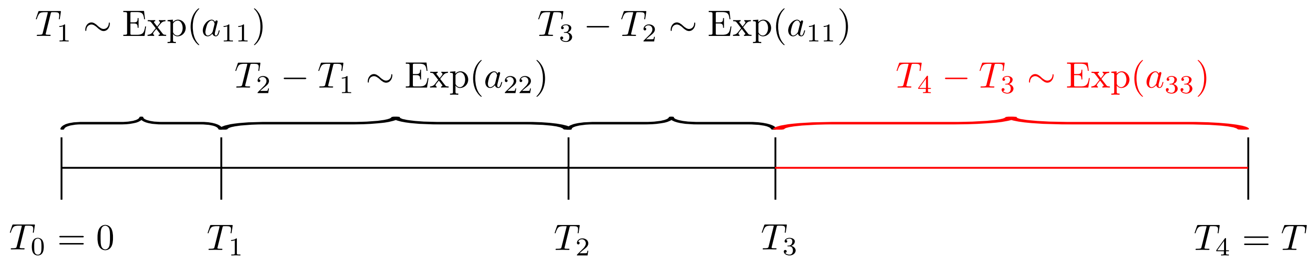

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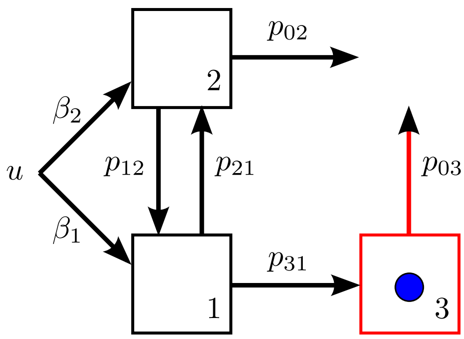

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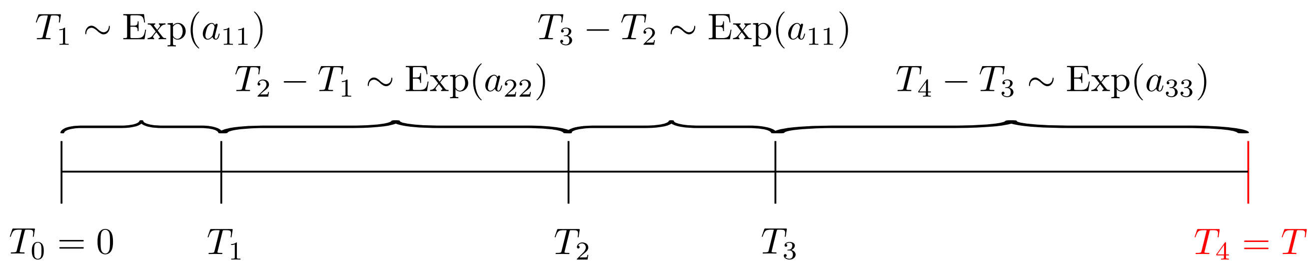
$$p_{03} = 1$$



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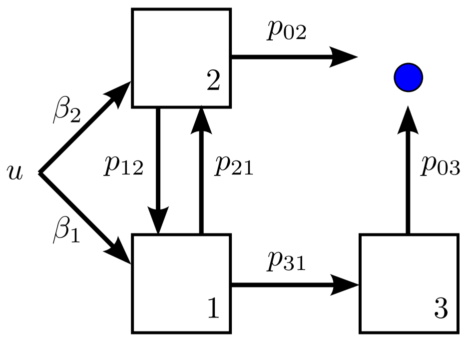

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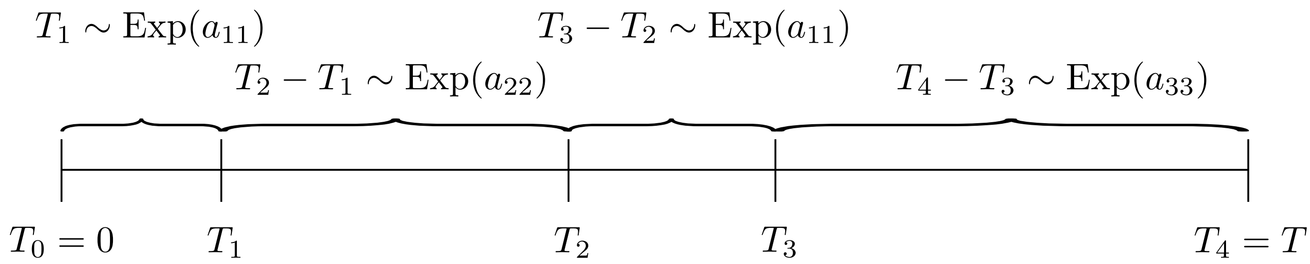

Transit time distribution

- transit time computation:

$$T = \underbrace{(T_1 - T_0)}_{\sim\mathrm{Exp}(a_{11})} + \underbrace{(T_2 - T_1)}_{\sim\mathrm{Exp}(a_{22})} + \underbrace{(T_3 - T_2)}_{\sim\mathrm{Exp}(a_{11})} + \underbrace{(T_4 - T_3)}_{\sim\mathrm{Exp}(a_{33})}$$

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- mixture of exponential distributions

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- length of mixture is stochastic

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→ T follows phase-type distribution with parameters β, A

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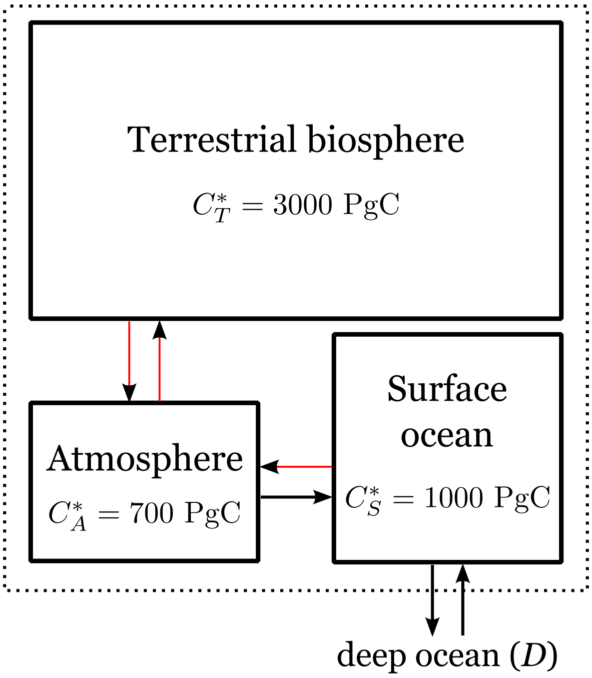
→ $T \sim \mathrm{PH}(\beta, \mathrm{A})$

General, simple, explicit formulas

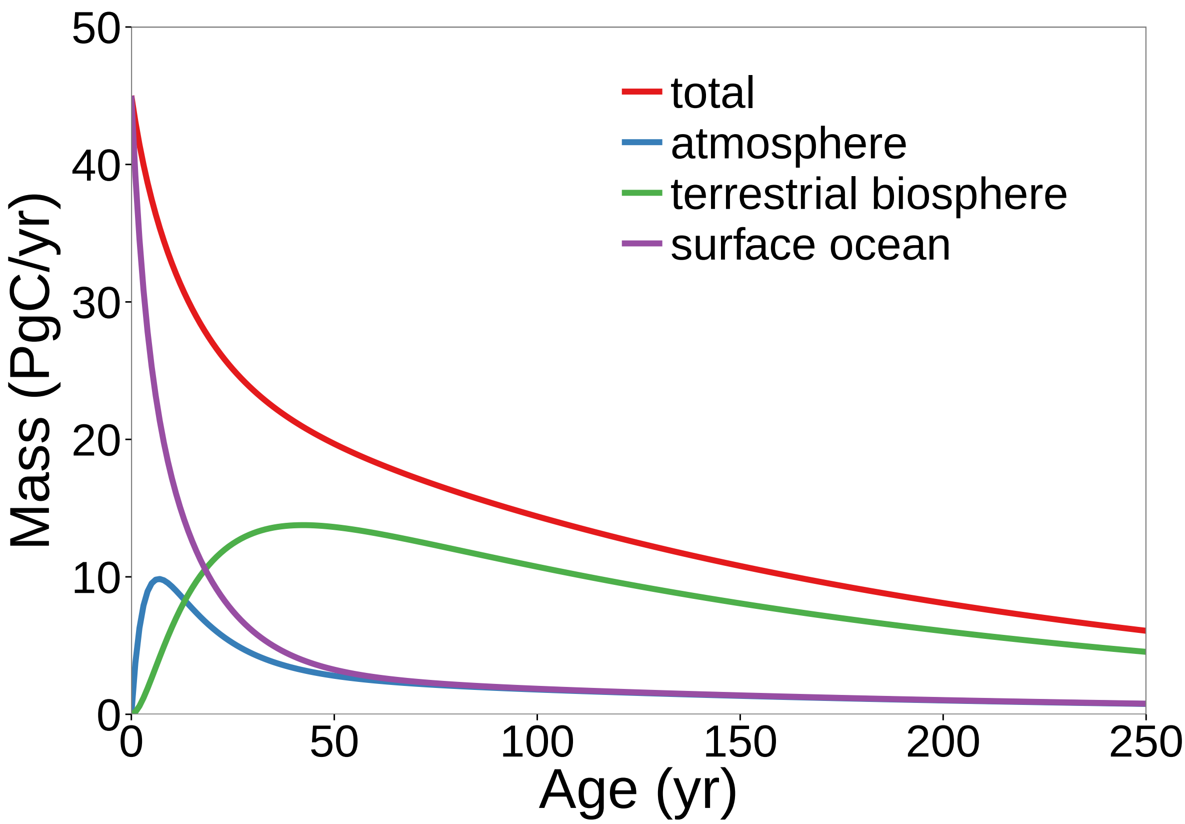
- phase-type distribution is well known:
  - probability density
  - cumulative distribution function
  - quantiles
  - mean and higher order moments
    - $\mathbb{E}[T] = \|\mathrm{A}^{-1}\,\beta\| = \frac{\|\mathbf{x}^*\|}{\|\mathbf{u}\|}$ (mean transit time)
- system age is also phase-type distributed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

Application to a nonlinear carbon cycle model

Nonlinear model in steady state [?] with three compartments



Equilibrium age densities



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- **general solution**

$$\mathbf{x}(t) = \Phi(t,0)\,\mathbf{x}^0 + \int_0^t \Phi(t,s)\,\mathbf{u}(s)\,ds$$

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$$\mathbf{x}(t) = e^{t\,\mathrm{A}}\,\mathbf{x}^0 + \int_0^t e^{(t-s)\,\mathrm{A}}\,\mathbf{u}\,ds$$

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Linear nonautonomous systems

$$\underbrace{\Phi(t,s)\,\mathbf{u}(\mathbf{s})}_{\text{mass with age } t-s \text{ at time } t}$$

Linear nonautonomous systems

$$\underbrace{\Phi(t,s)\,\mathbf{u}(\mathbf{s})}_{\text{mass with age } t-s \text{ at time } t}$$

$$\Rightarrow \underbrace{\Phi(t,t-a)\,\mathbf{u}(t-a)}_{\text{mass with age } a \text{ at time } t}$$

The state transition operator Φ

- solution to the matrix ordinary differential equation

$$\frac{d}{dt}\,\Phi(t,s) = \mathrm{A}(t)\,\Phi(t,s), \quad \text{initial condition } \Phi(\mathrm{s},\mathrm{s}) = \mathrm{I}$$

The state transition operator Φ

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- time-independent system

$$\Phi(t,s) = e^{(t-s)\,\mathrm{A}} \quad \text{(matrix exponential)}$$

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- time-independent system

$$\Phi(t,s) = e^{(t-s)\,\mathrm{A}} \quad \text{(matrix exponential)}$$

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$$\Phi(t,s) = e^{-\lambda\,(t-s)} \quad \text{(exponential function)}$$

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→ we can always obtain it (at least numerically)

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- we split the system into two parts

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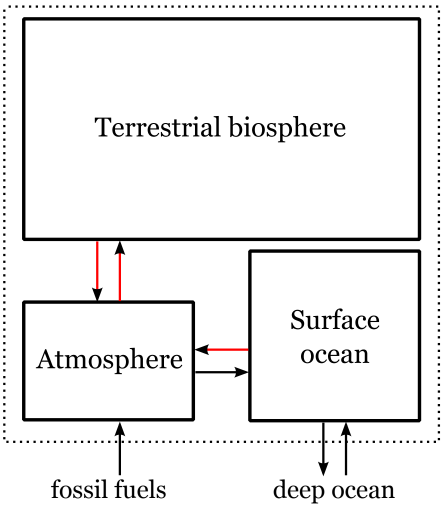
A global carbon cycle model



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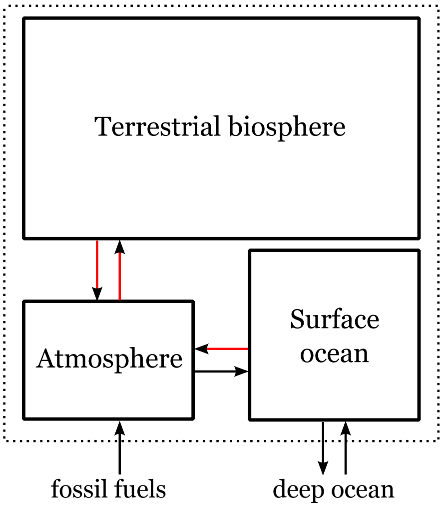
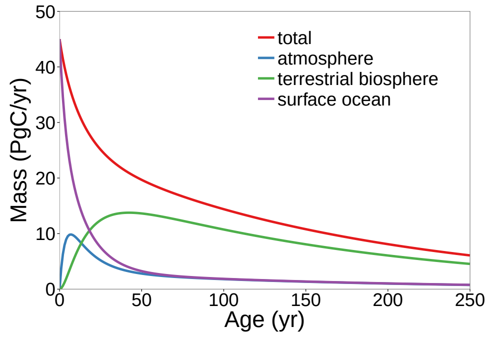


Equilibrium age densities in 1765



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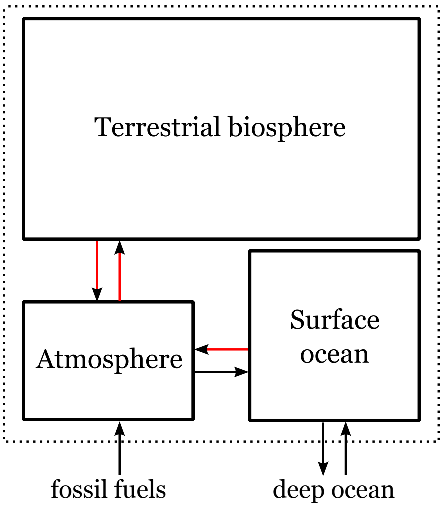

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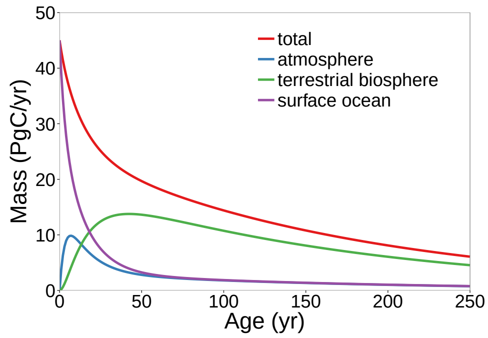
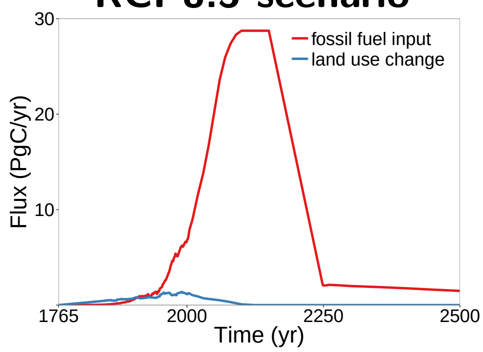
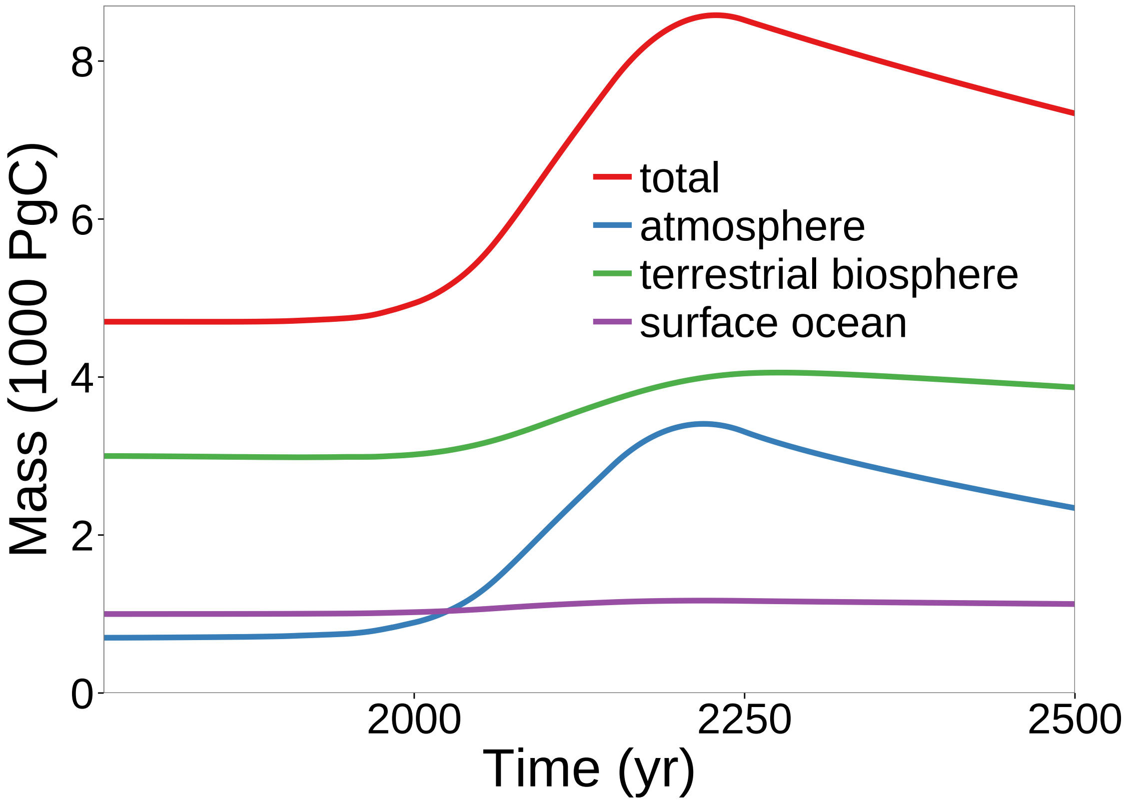


RCP8.5 scenario



Time-dependent carbon contents



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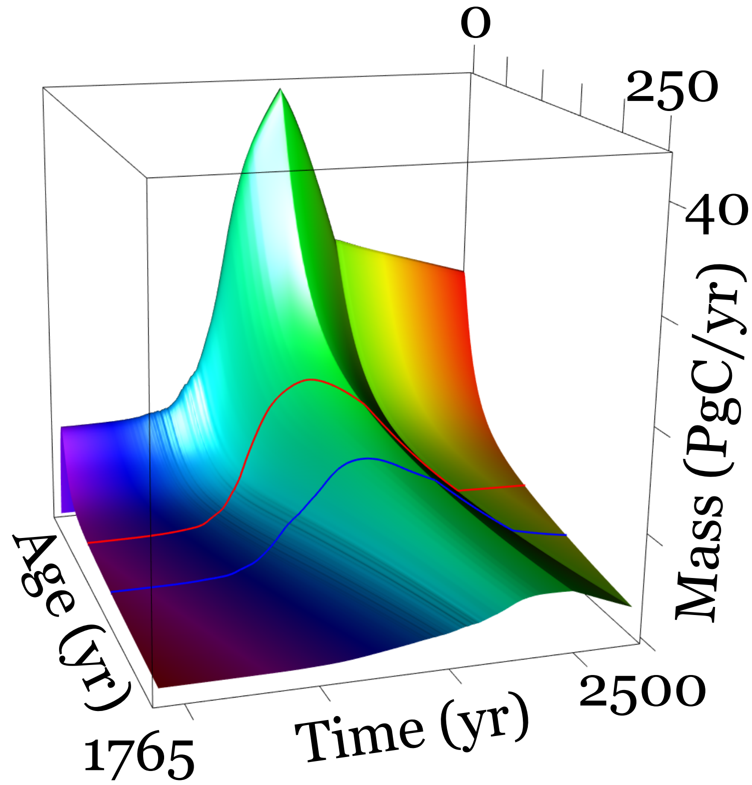

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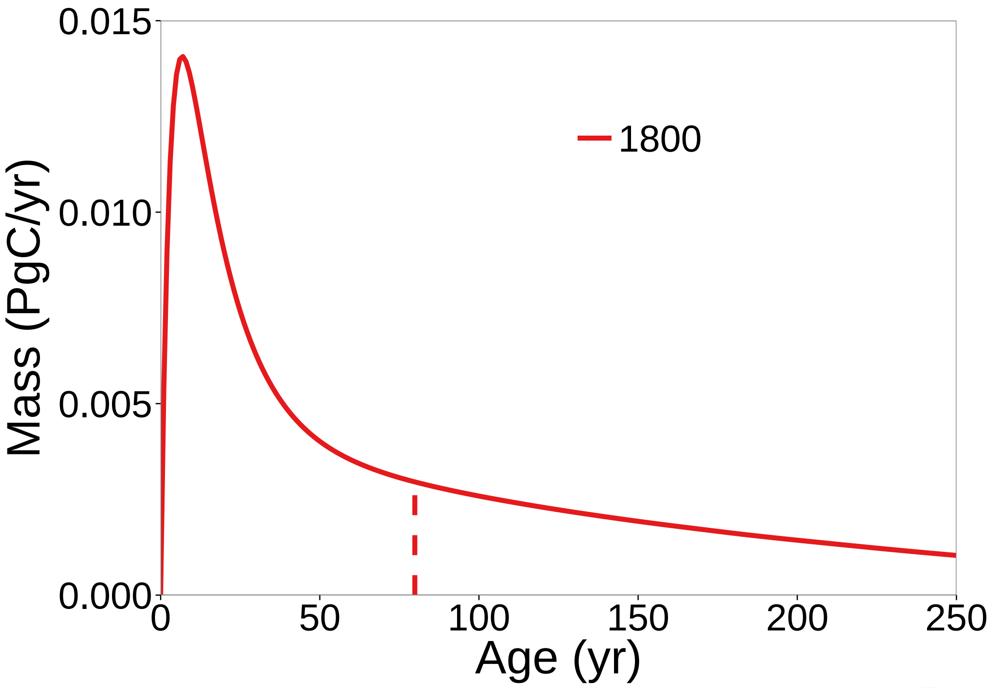

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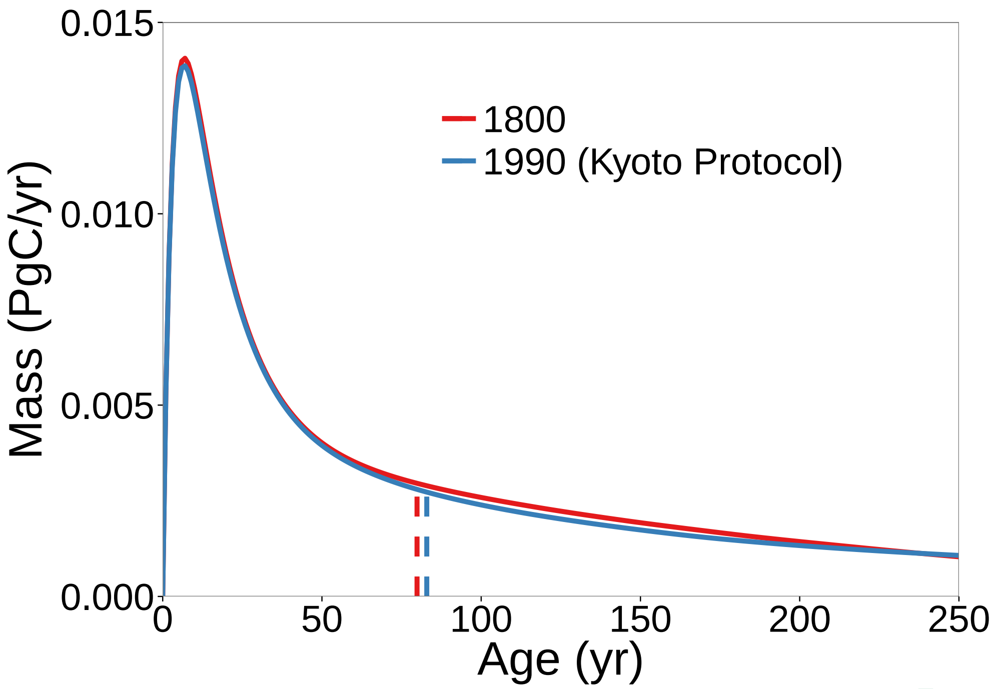

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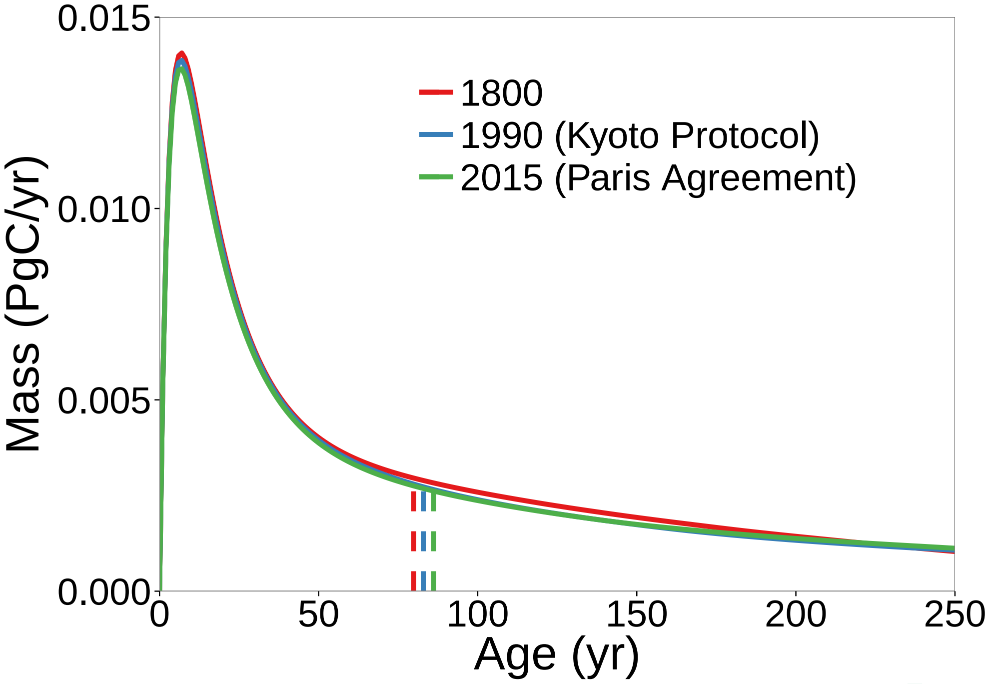

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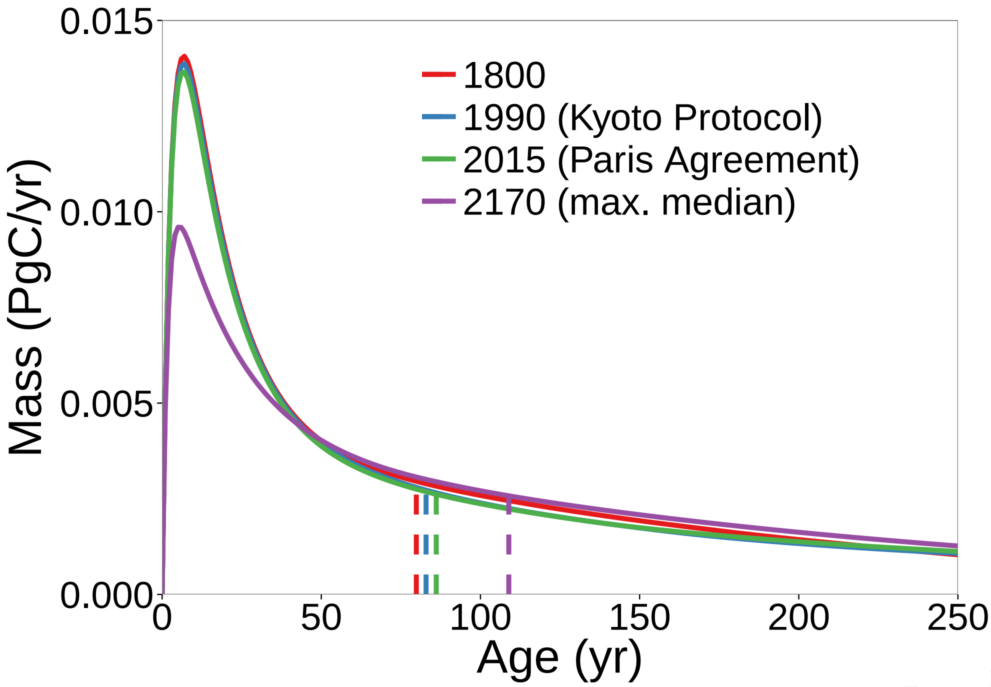

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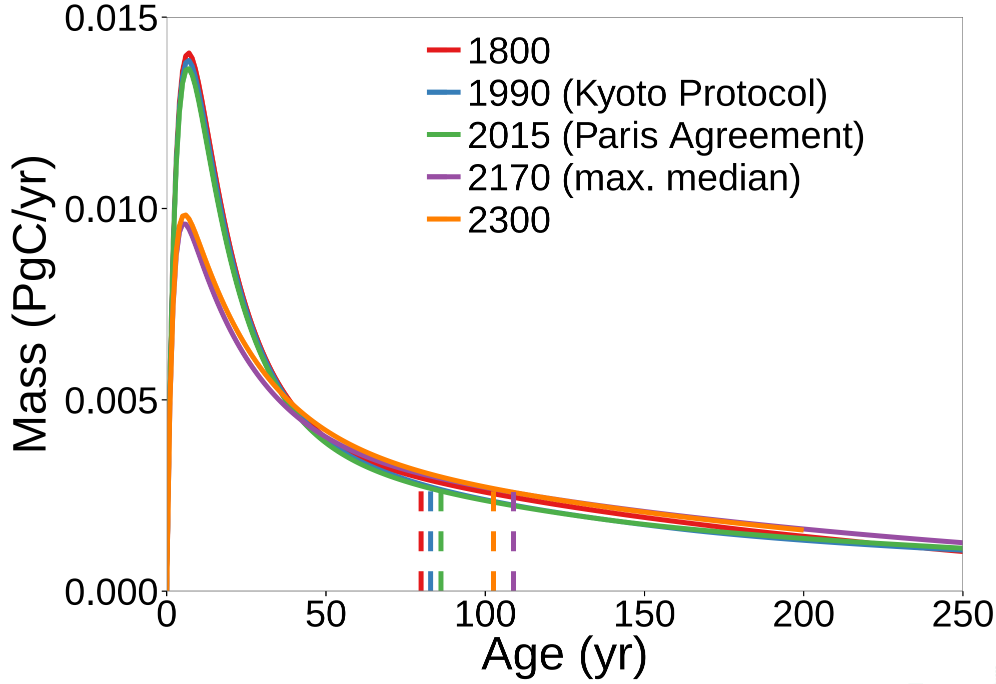

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- **two Python packages**
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    - http://github.com/goujou/LAPM
  - (numerical) computation of age and transit time properties for nonlinear nonautonomous systems

System age

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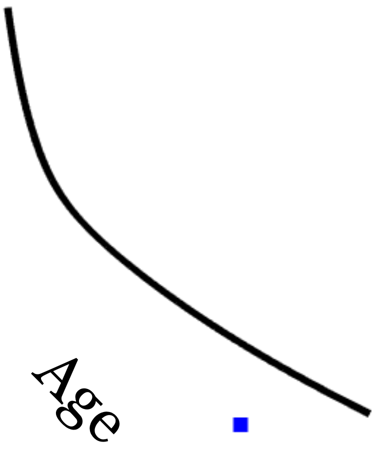

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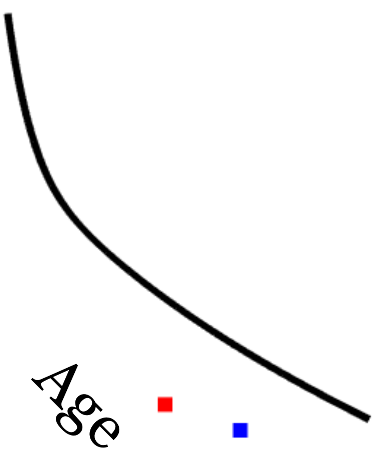

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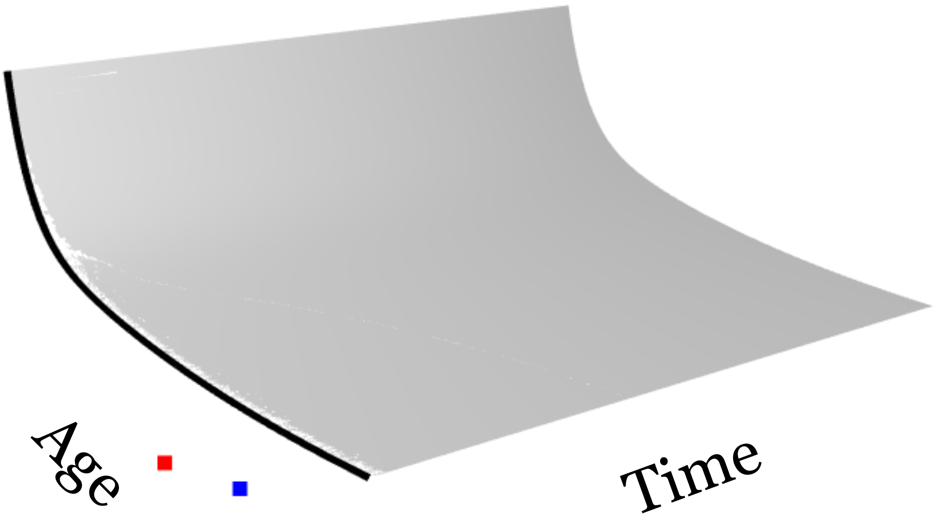

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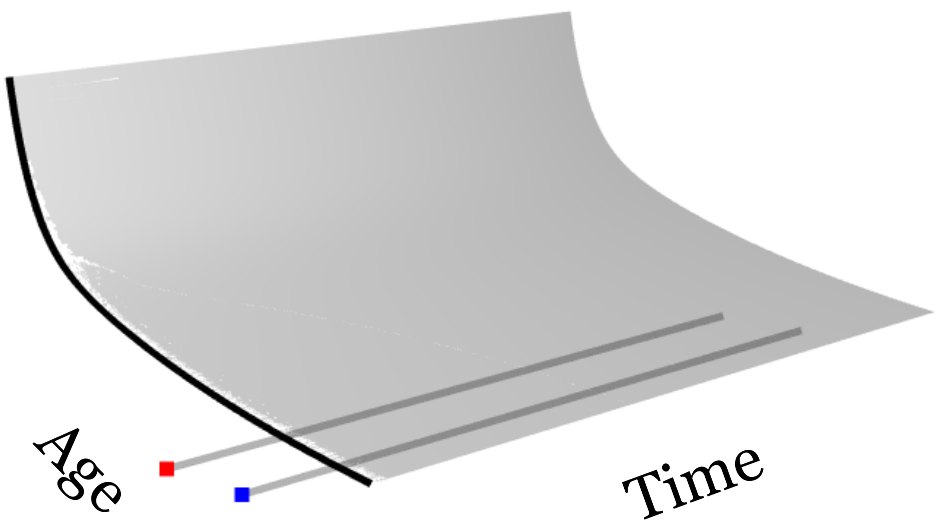

Pool Models Markus Müller, Holger Metzler, Carlos Sierra 61 / 64

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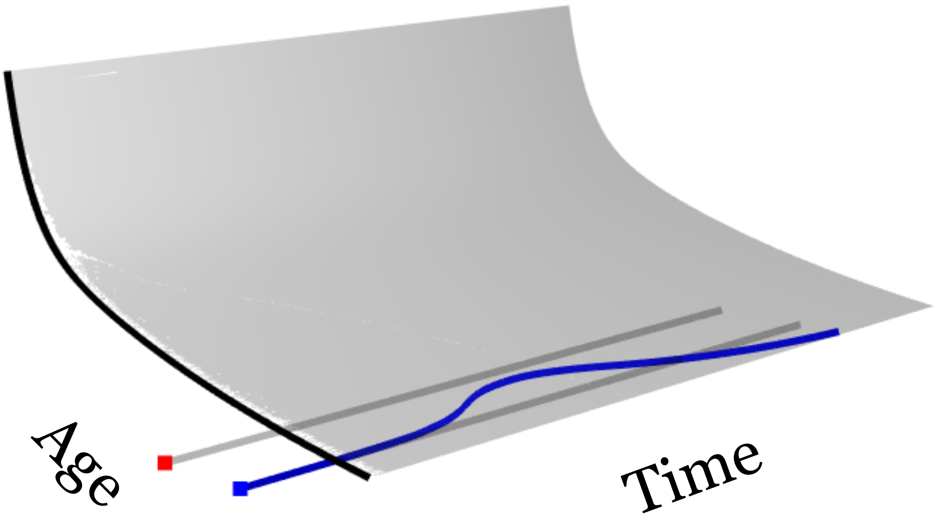

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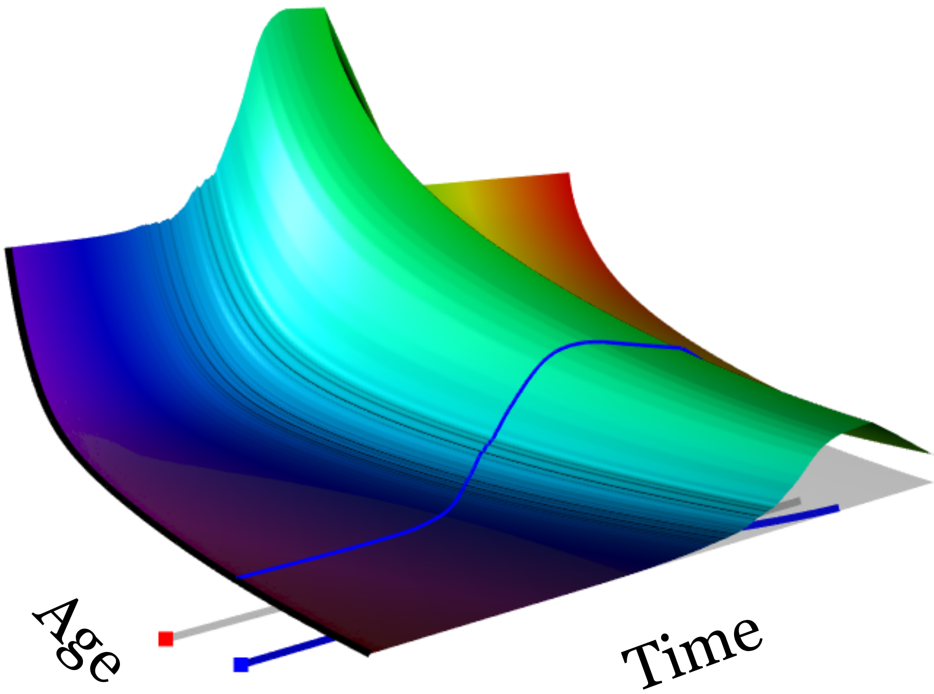

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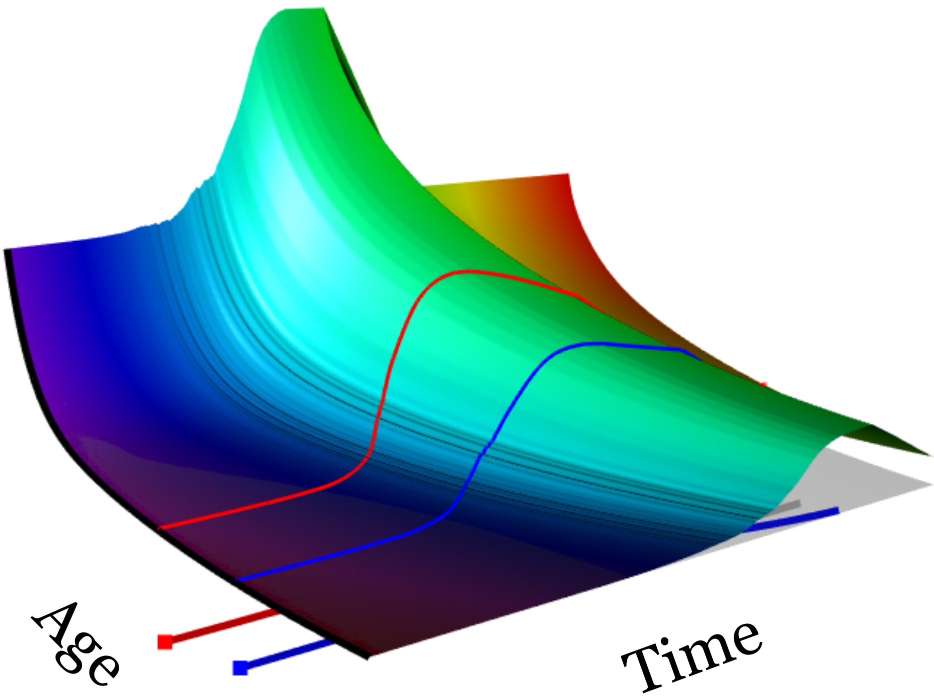
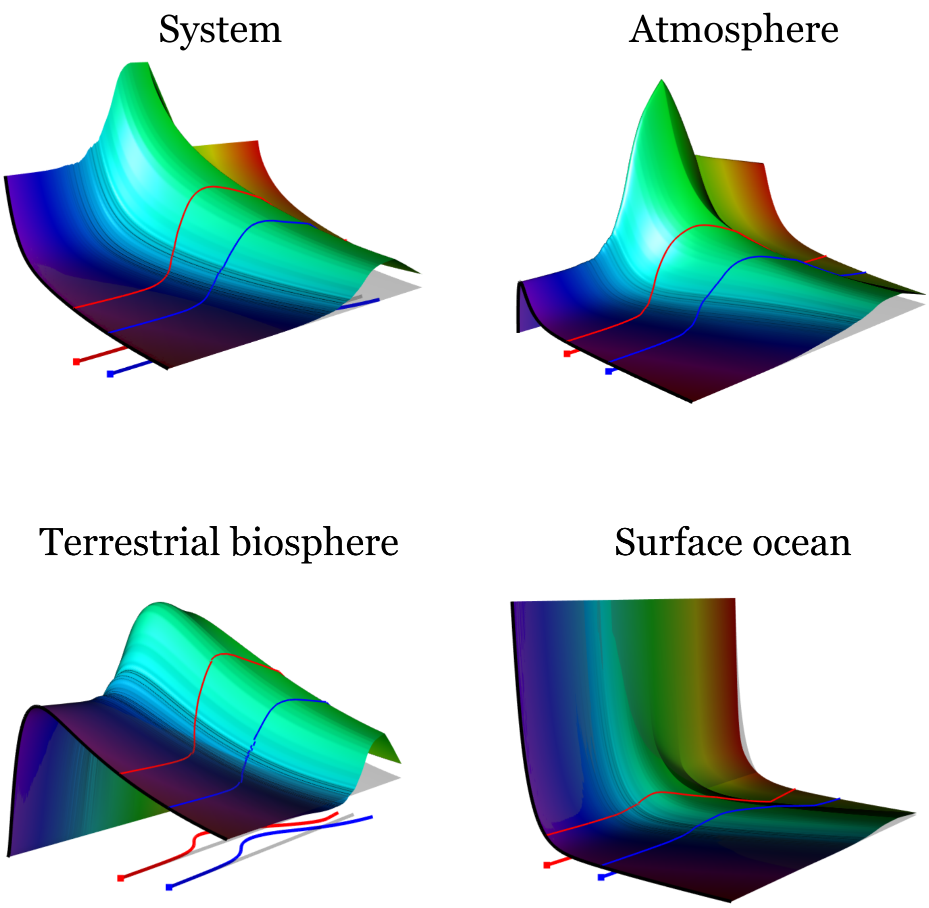
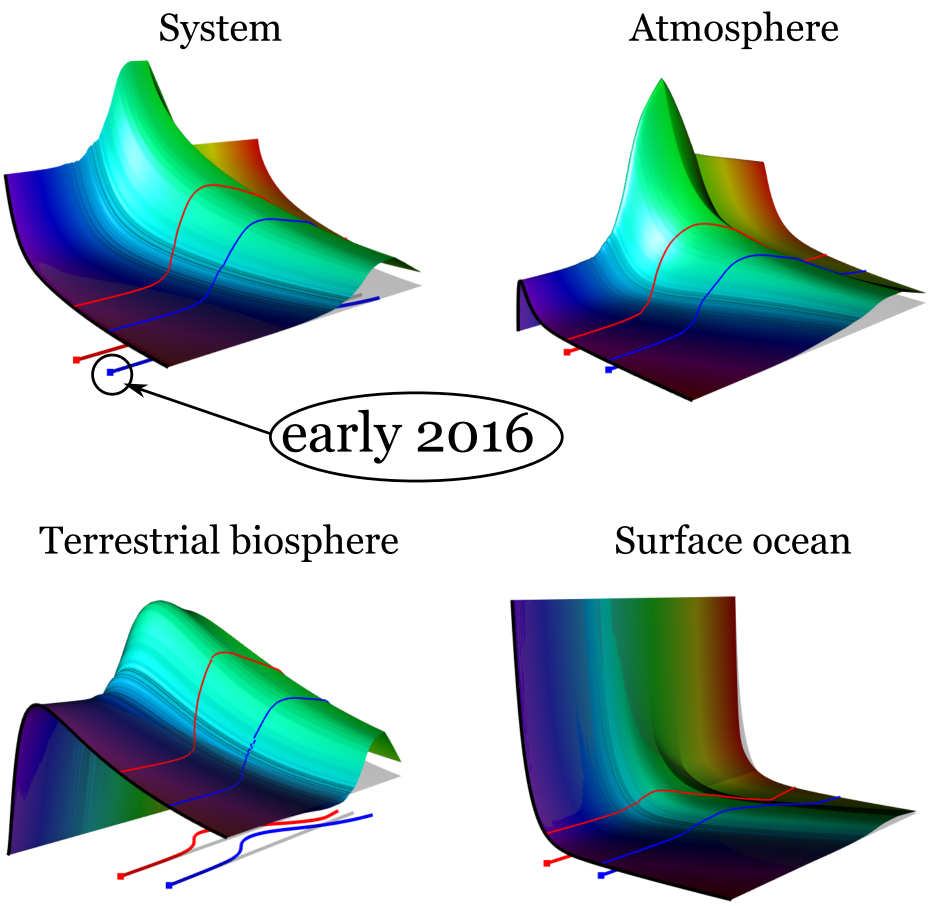
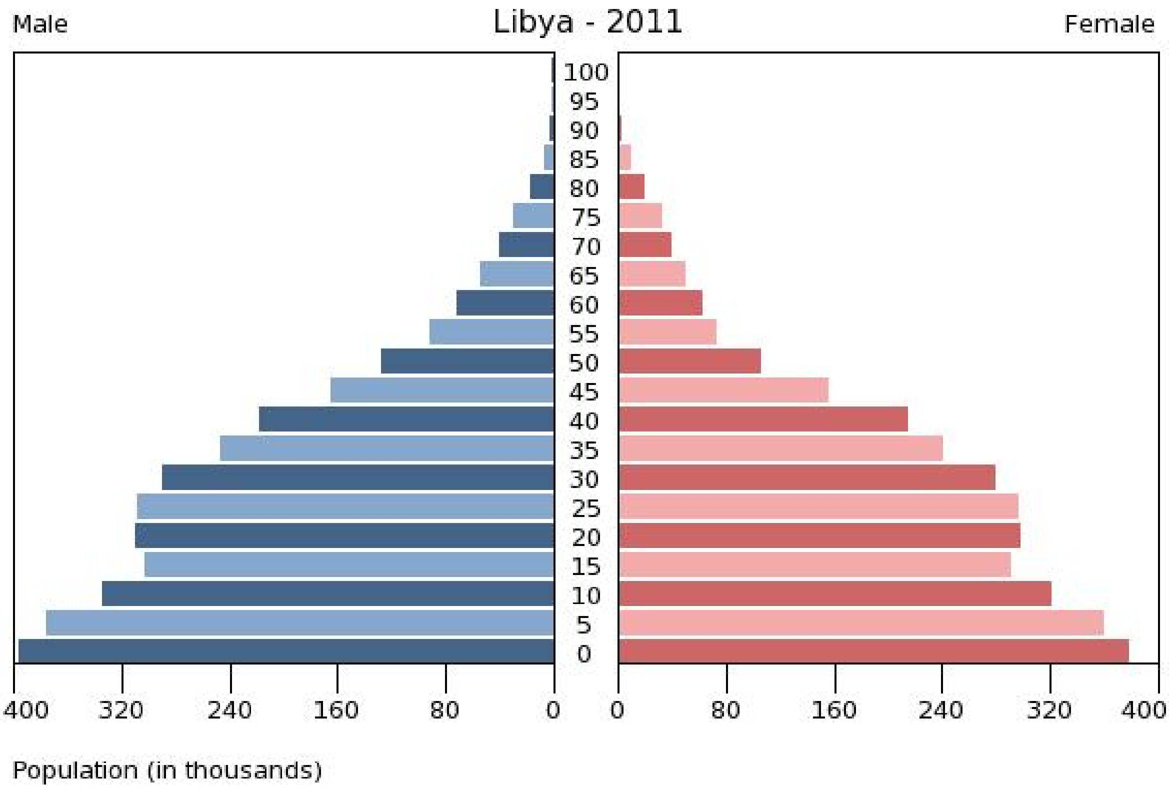

Age
Time


System
Atmosphere
Terrestrial biosphere
Surface ocean



Population Dynamics $\phi(a)$



Age distribution varies with time. $\phi(a) = \phi(a, t)$

McKendrick–von Foerster Equation

- original:

$$\frac{\partial \phi}{\partial a} + \frac{\partial \phi}{\partial t} = m(a)\phi$$

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- in compartmental systems

$$\frac{\partial \phi}{\partial a} + \frac{\partial \phi}{\partial t} = m(t)\phi$$

  $m(t)$ depends only on time t.

Thanks

Funding

bibliography