

Pool Models

An Introduction

Markus Müller, Holger Metzler, Carlos Sierra

August 13, 2019

Max Planck Institute
for Biogeochemistry



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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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- Introduction
- Linear autonomous
- Generalization to nonlinear nonautonomous systems
- Example application

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4 Generalization to non Well Mixed Systems

- Population Dynamics
- Hydrology

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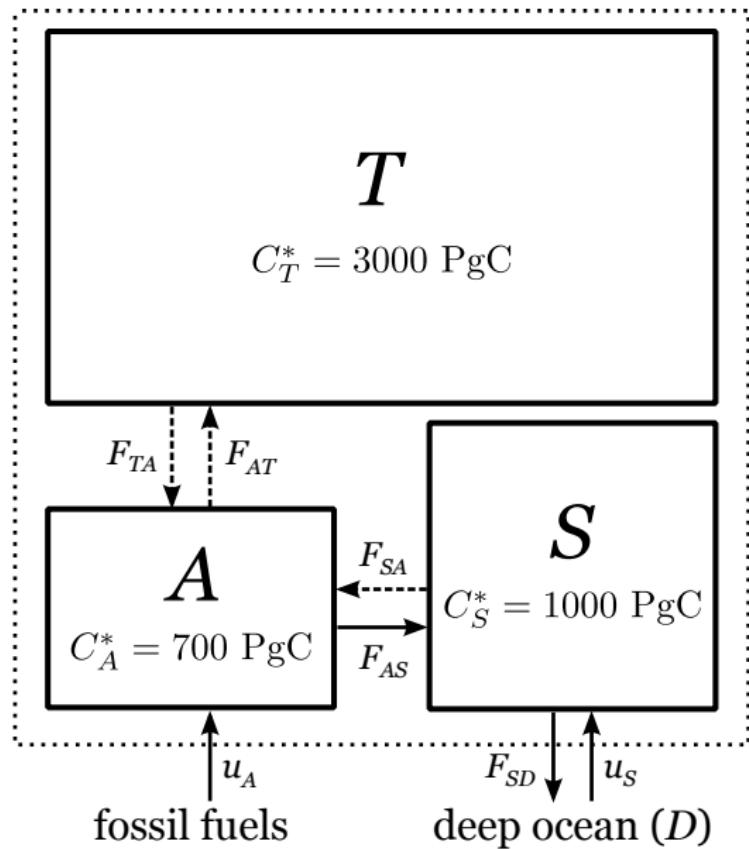
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- Example application

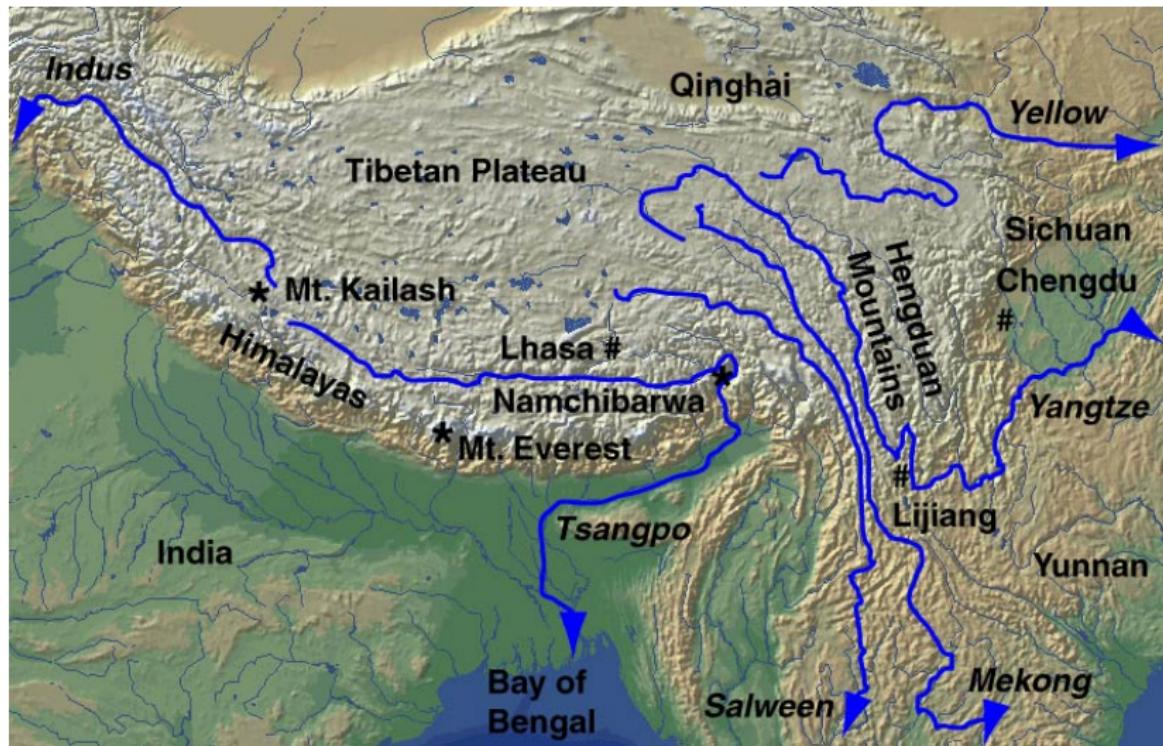
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- Population Dynamics
- Hydrology

Element cycling, e.g. C

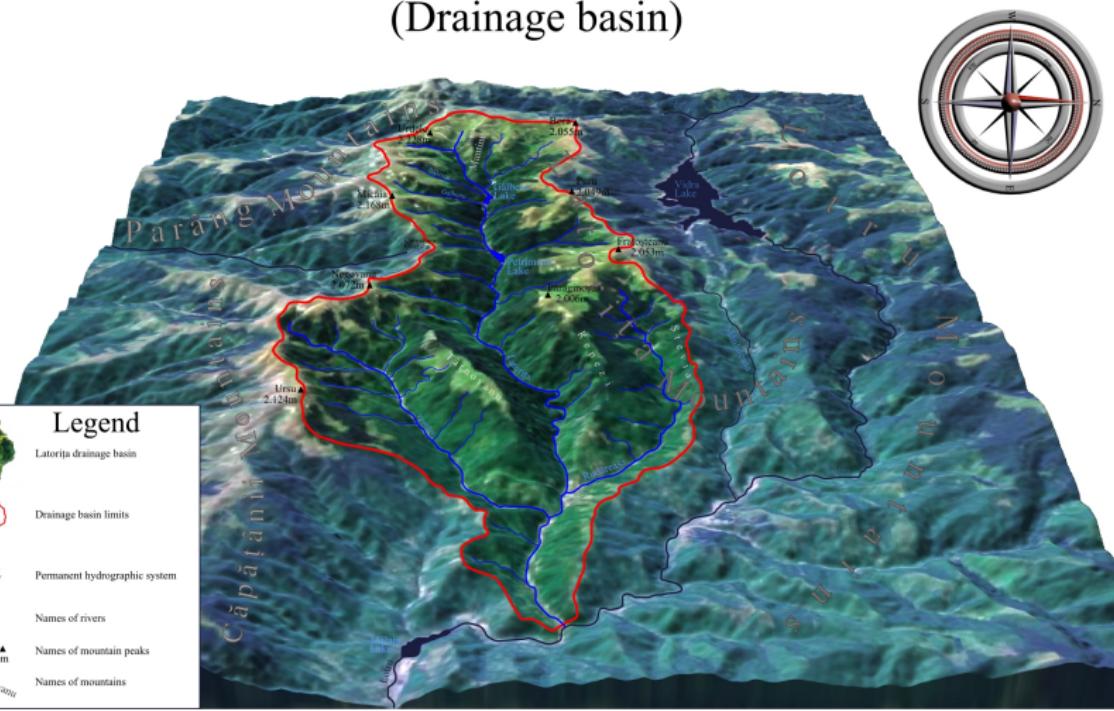


Hydrology, catchments

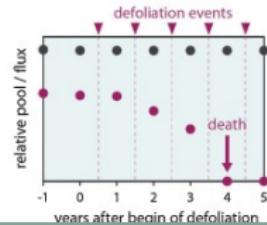
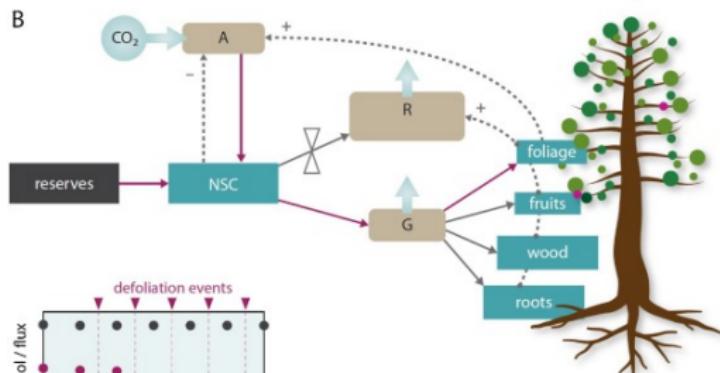
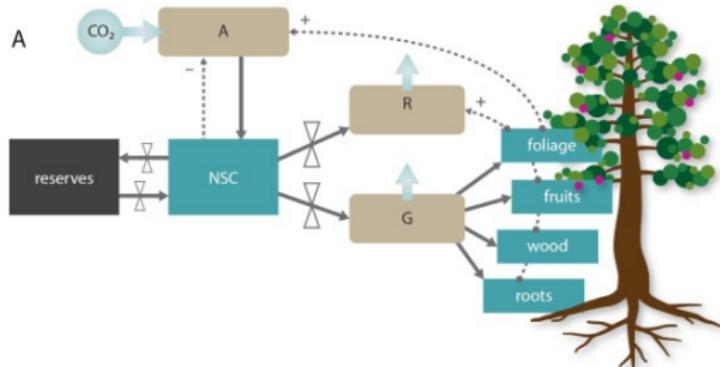


Hydrology, catchments

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

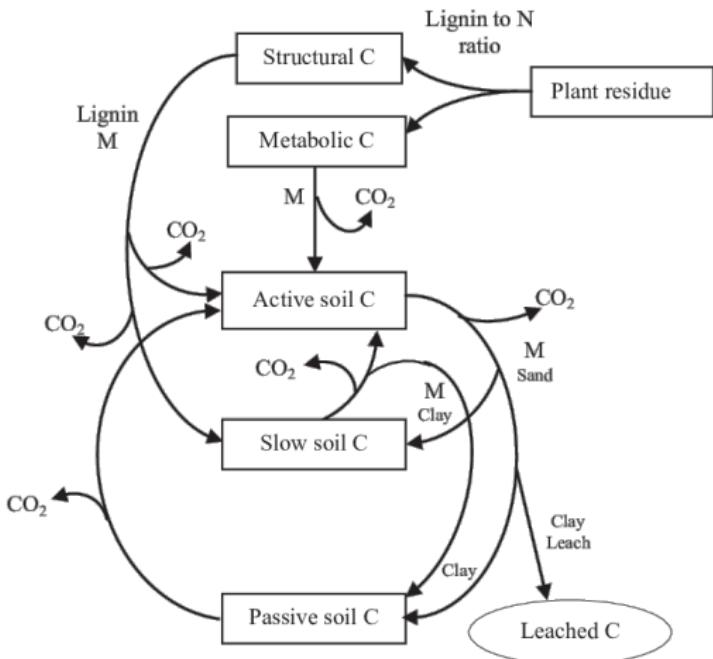
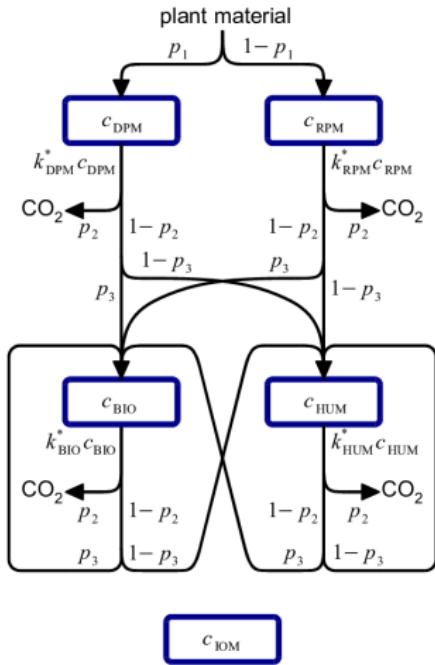


Plant physiology, carbon allocation

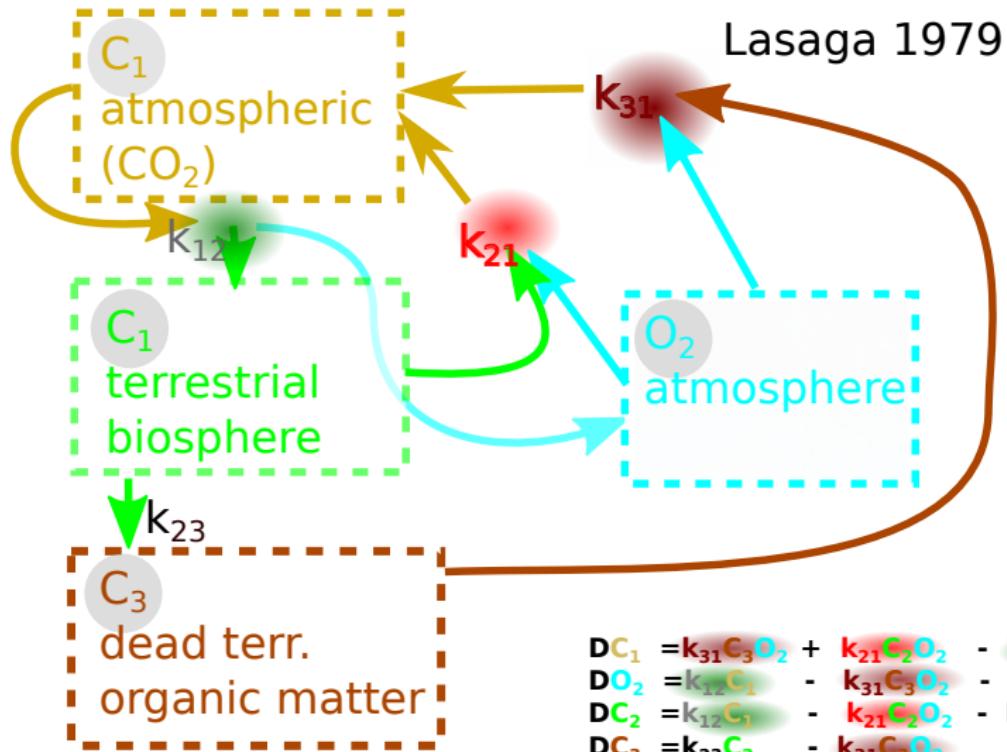


Pool Models

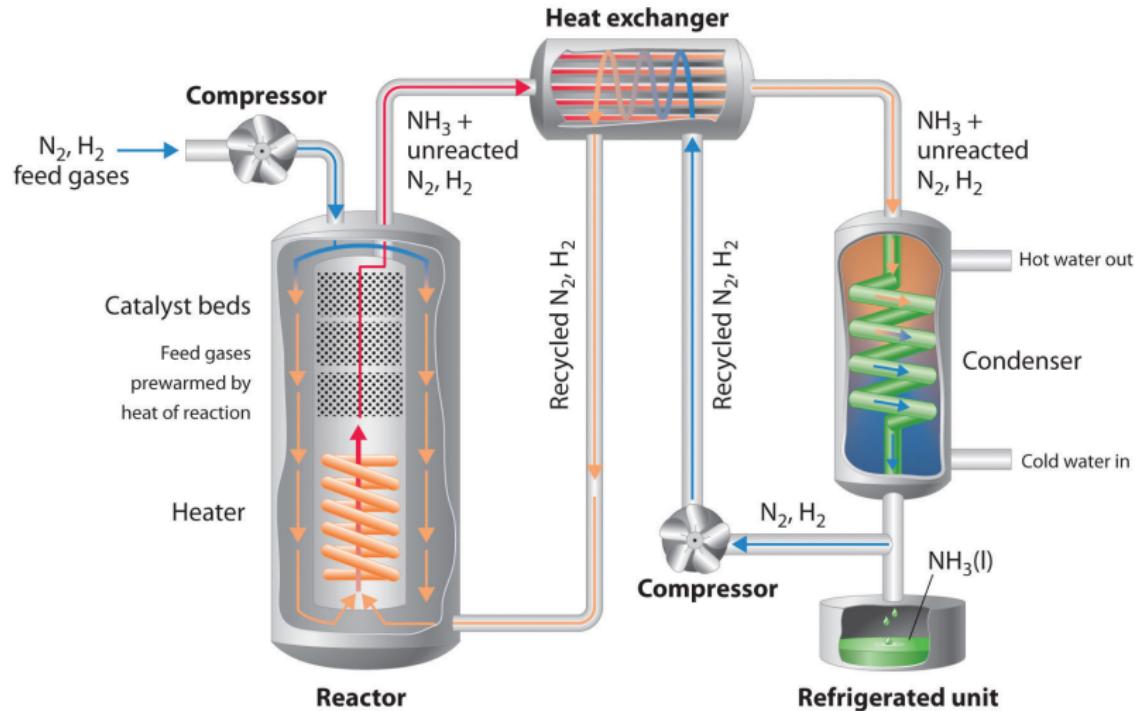
Organic matter decomposition , soil models



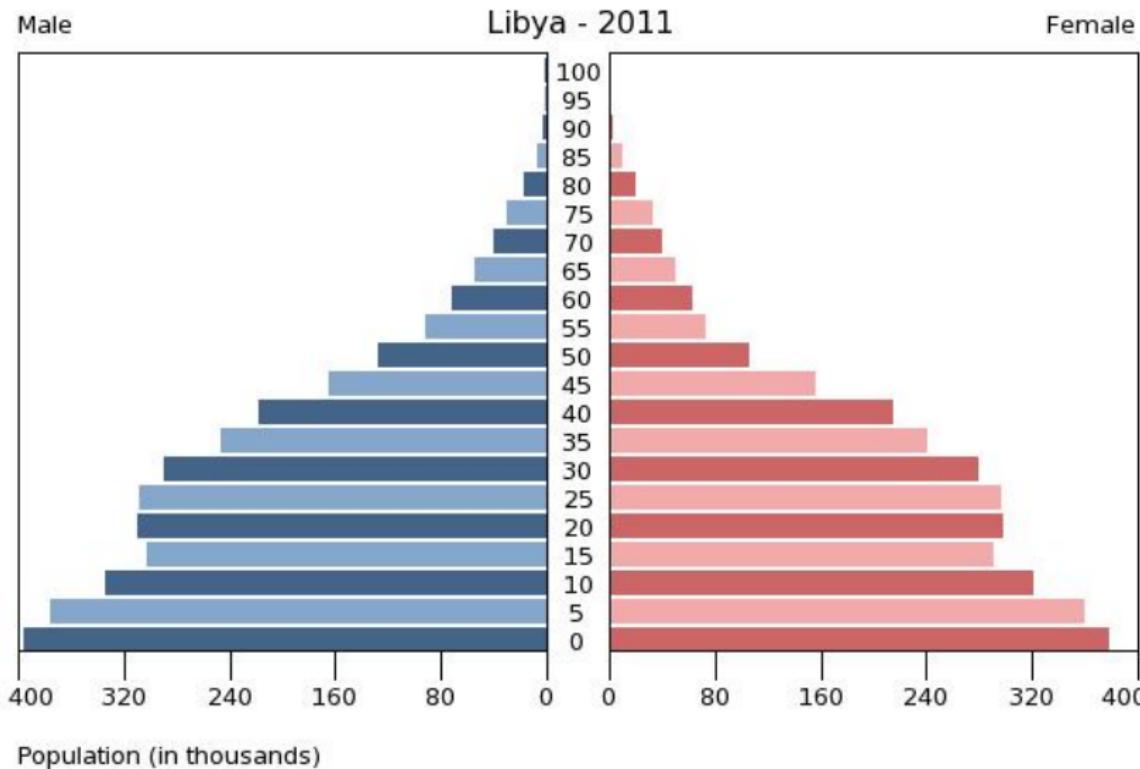
Ecosystem models



Chemical reactors



Population dynamics



1 Example applications of pool models

2 Reducing model complexity

- The carbon cycle example
- Asking simpler questions
- Answer questions more simply

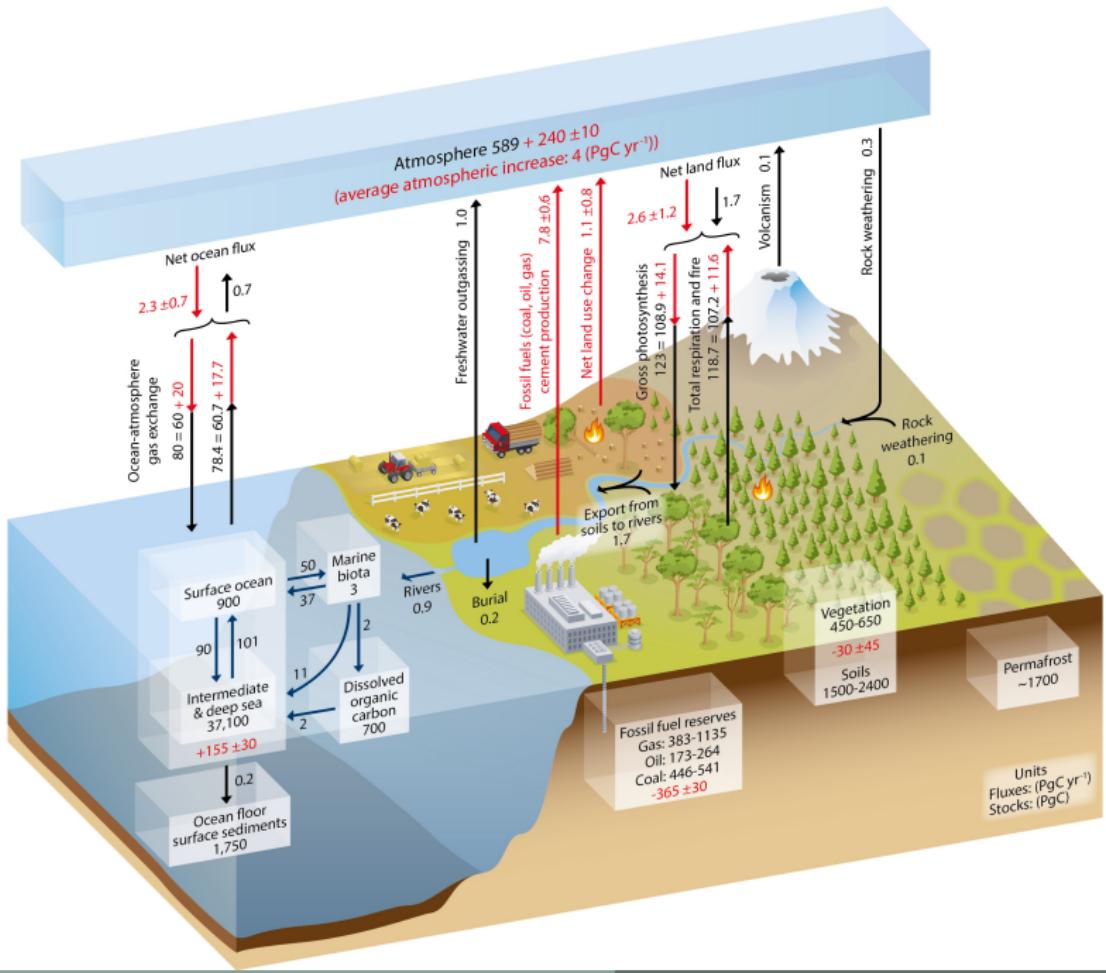
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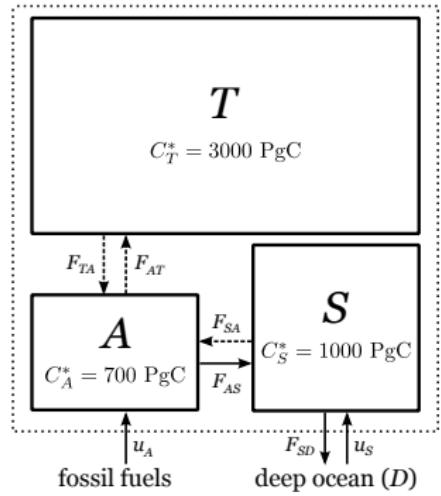
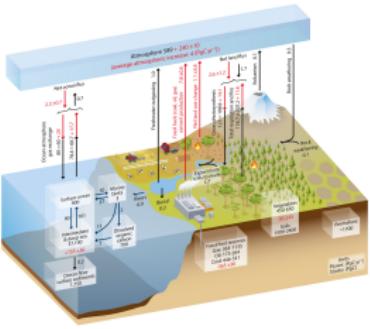
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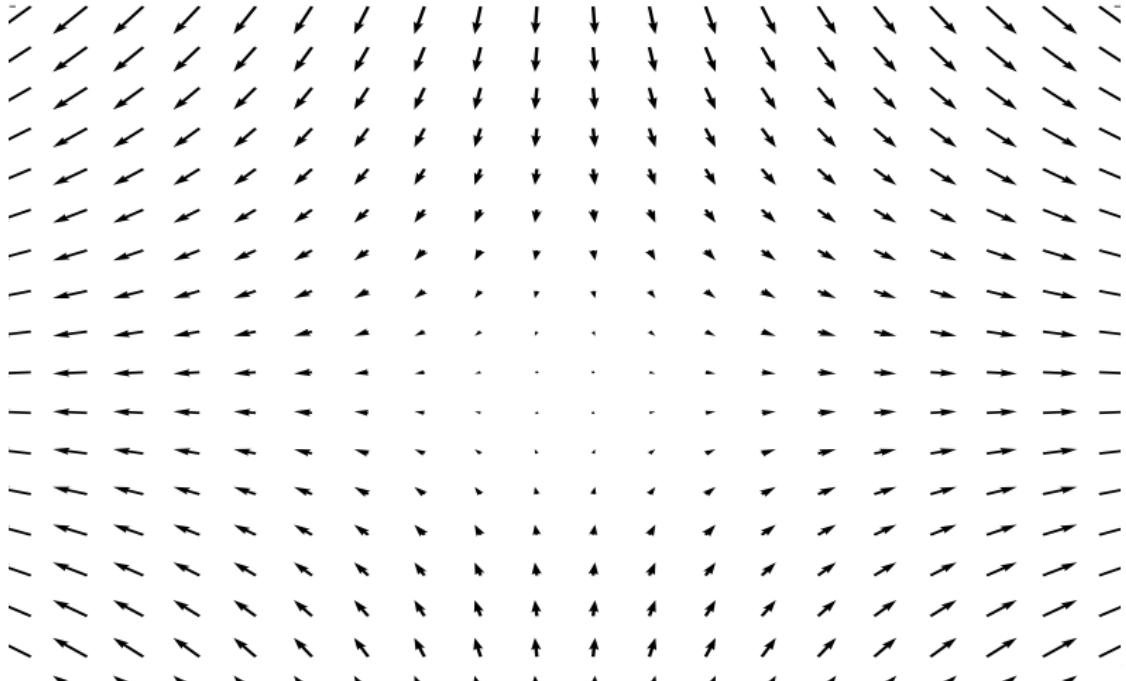
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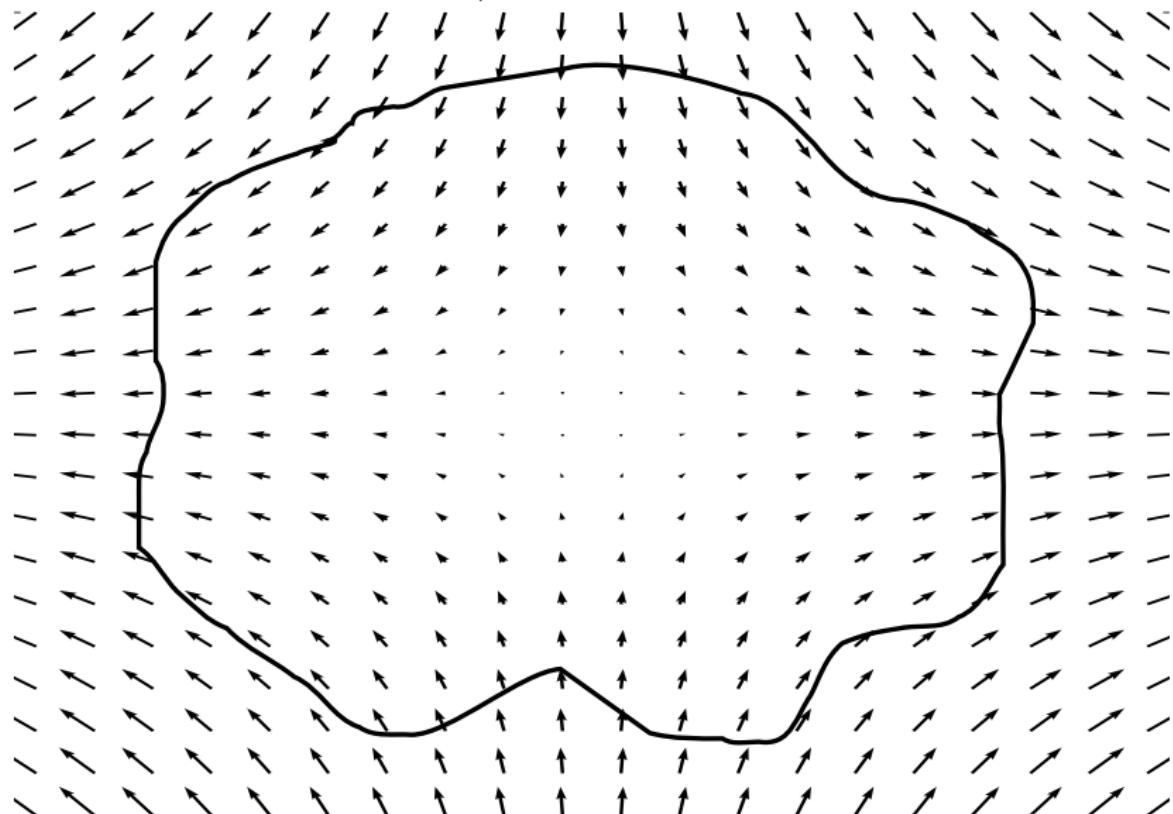
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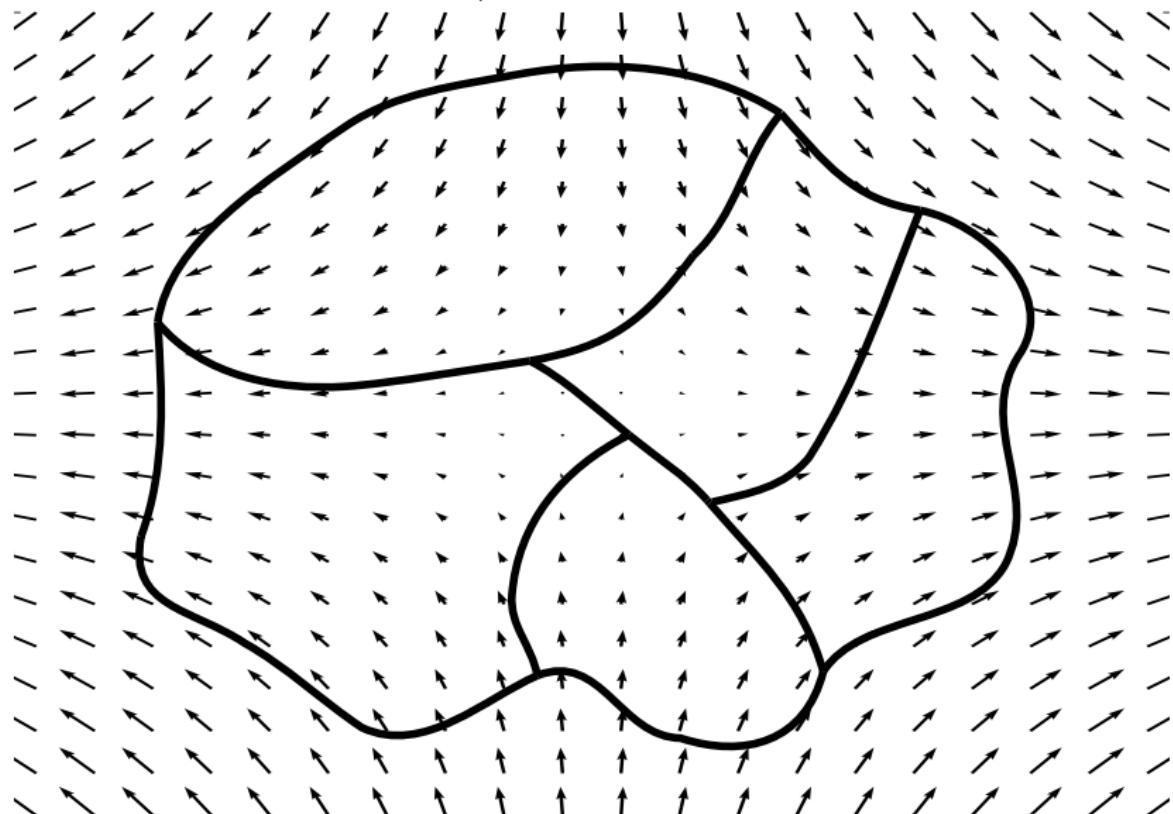


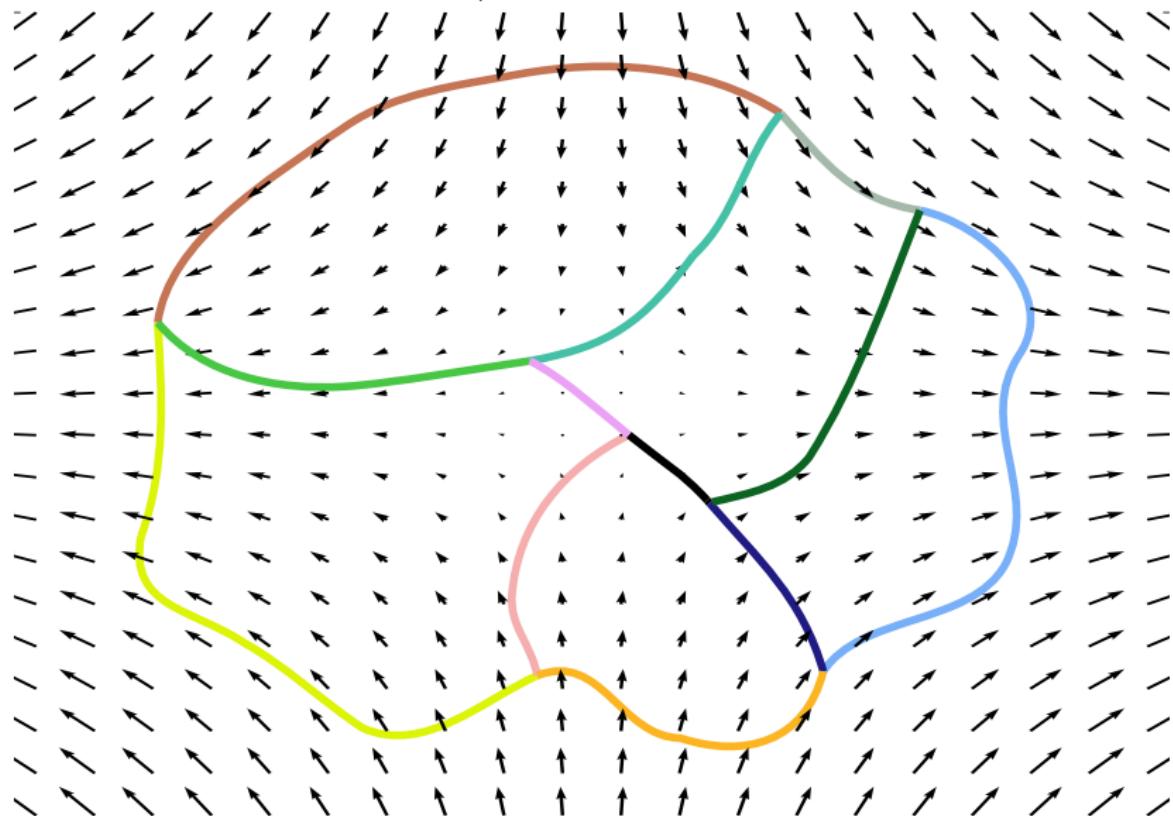


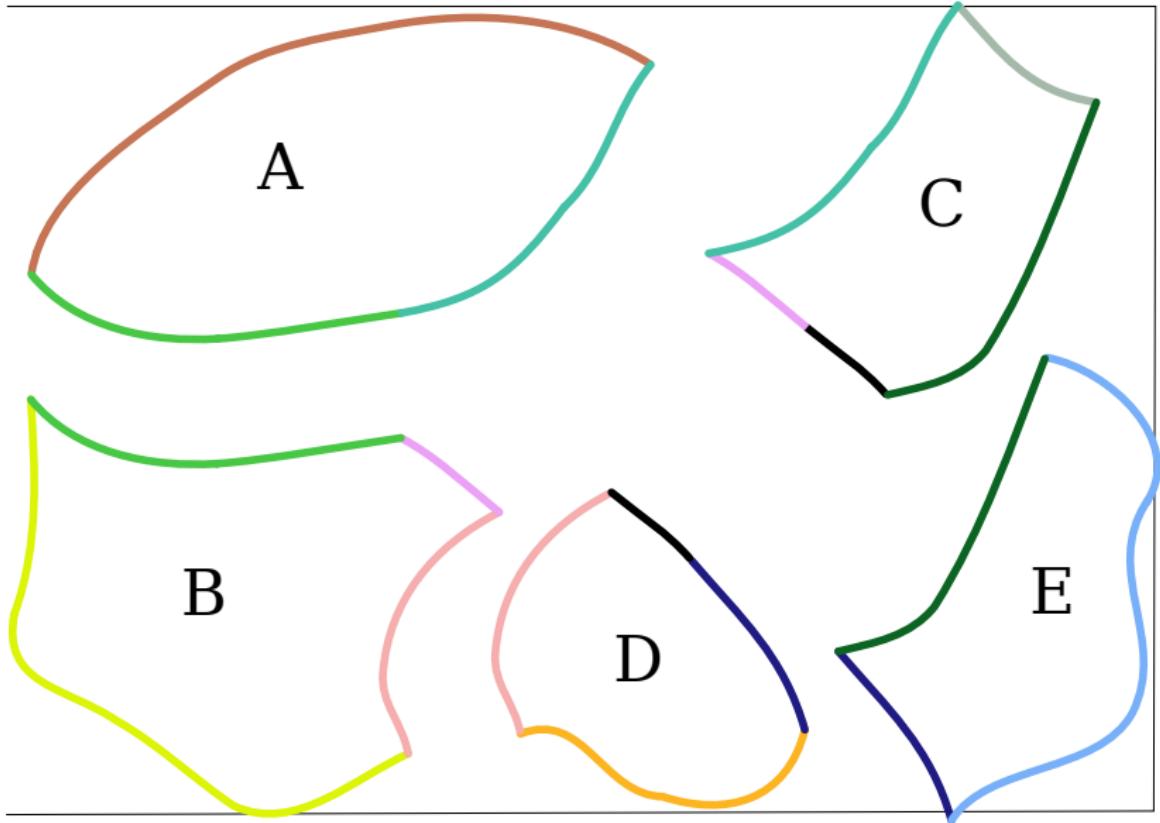


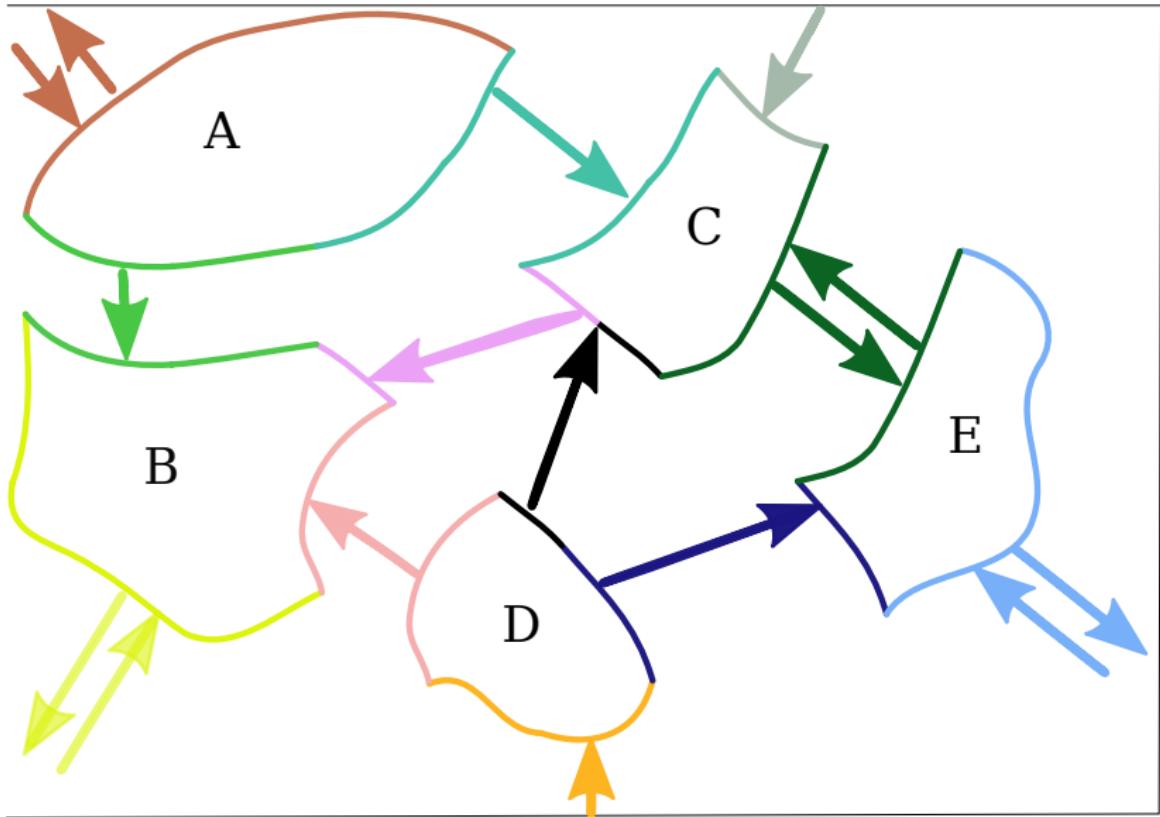


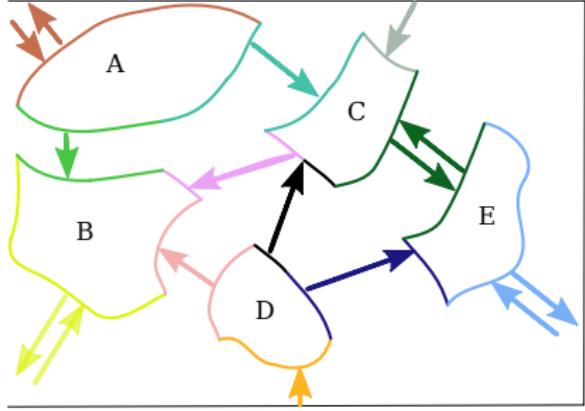
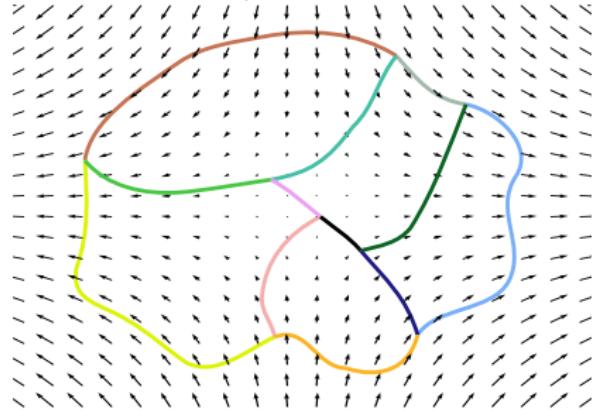


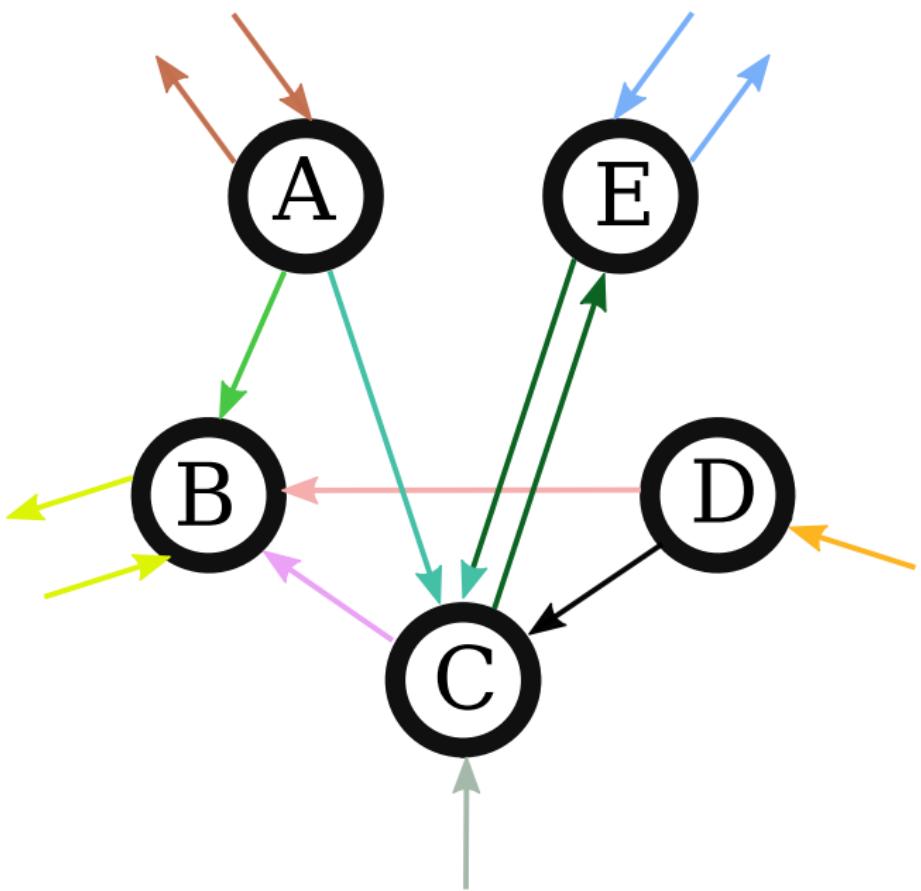


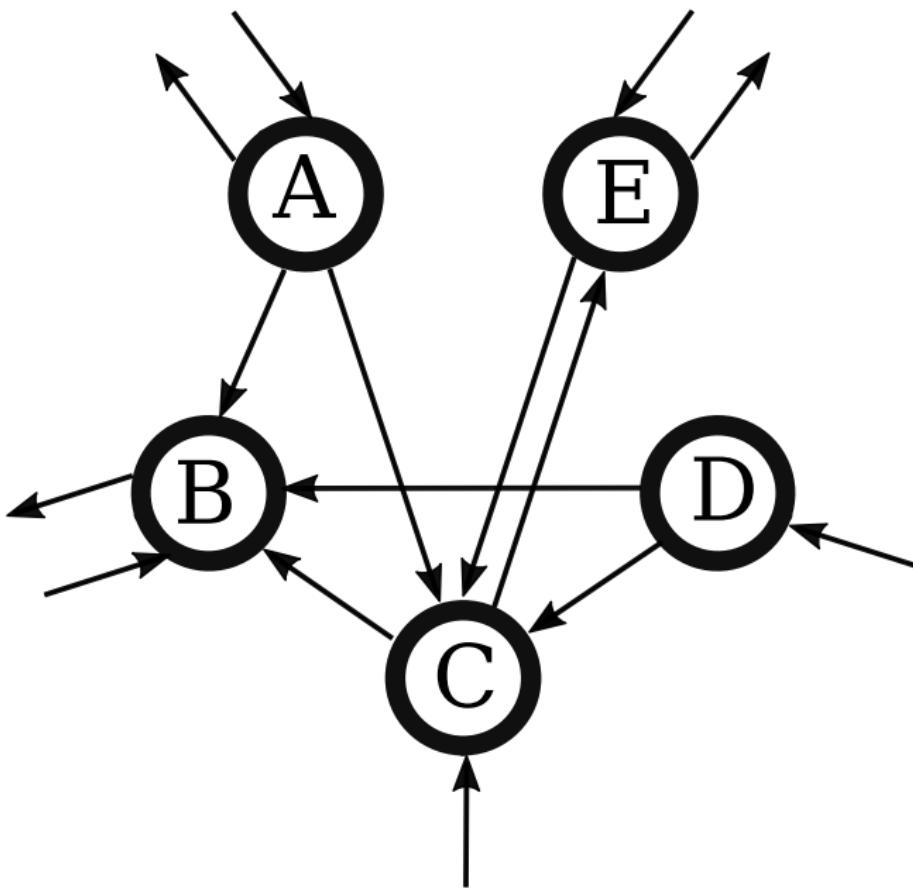










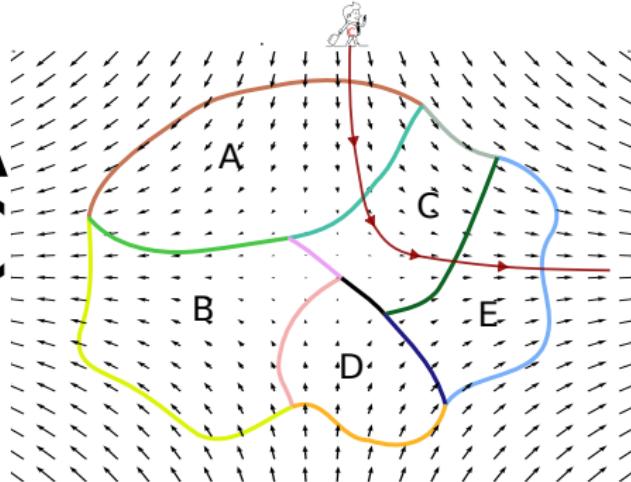




t,x,y,z



A
C
E



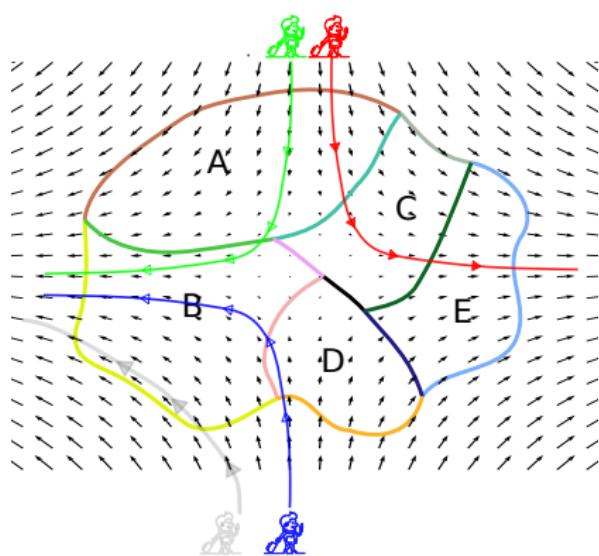
Pools arrival

- | | | |
|---|-----|--------------|
| 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

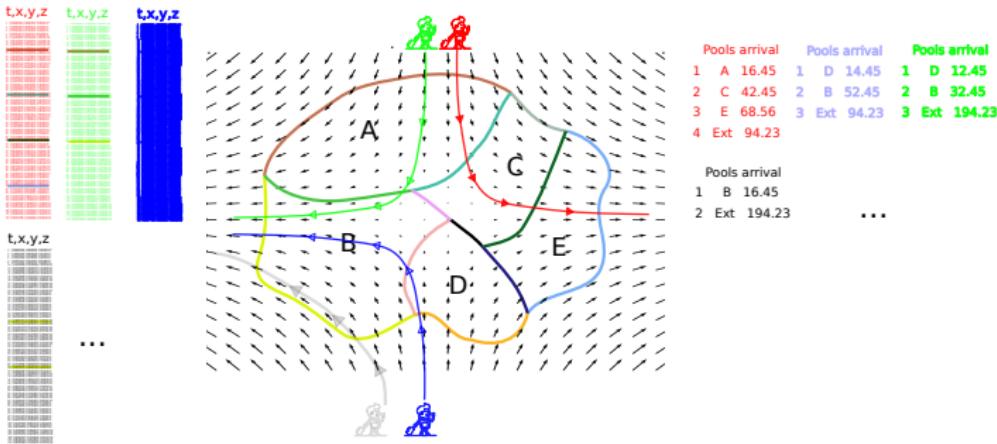
1 D 12.45
2 B 32.45
3 Ext 194.23

Pools arrival

1 B 16.45
2 Ext 194.23

...

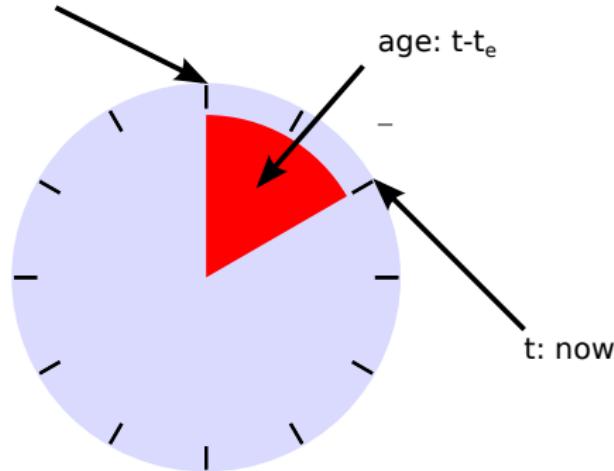
Possible descriptive statistics



- 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.

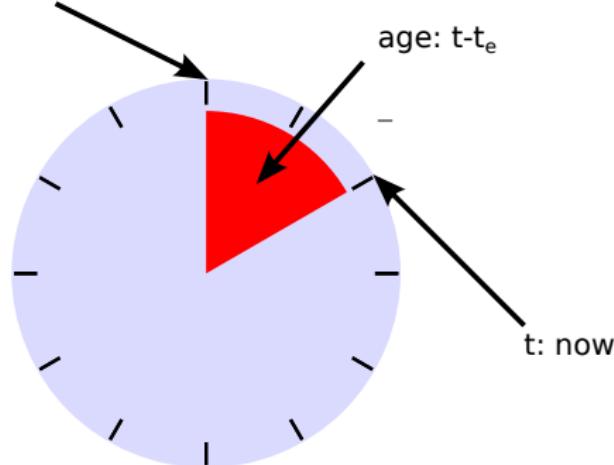
Age of a Particle

t_e : particle enters reservoir



Age of a Particle

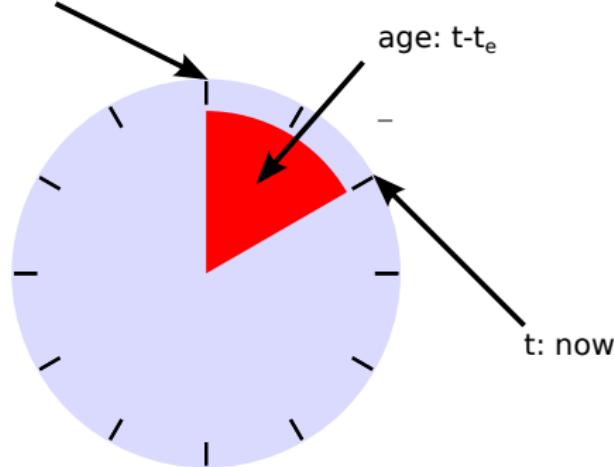
t_e : particle enters reservoir



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

Age of a Particle

t_e : particle enters reservoir



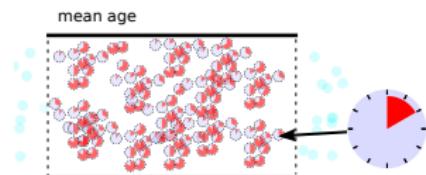
- The “age” can not be negative!

Mean age

- Which set of particles to use for the average?

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

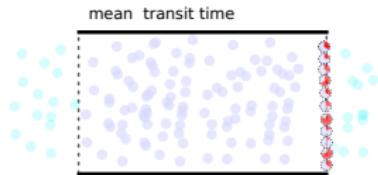
→ usually depends on input rates as well as the dynamics of the system.



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

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

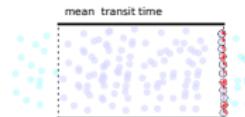
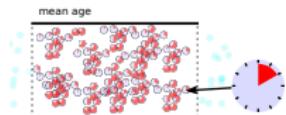
Mean transit time

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

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

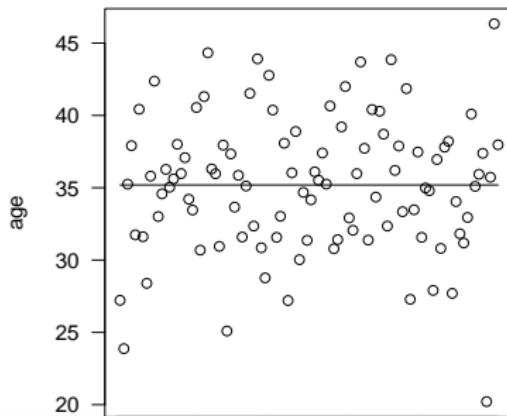
- ① To compute the mean transit time we have to identify the particles just leaving.
- ② Ask every leaving particle when it entered and compute its age.
- ③ Iterate over all particles and compute the average of their ages.

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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

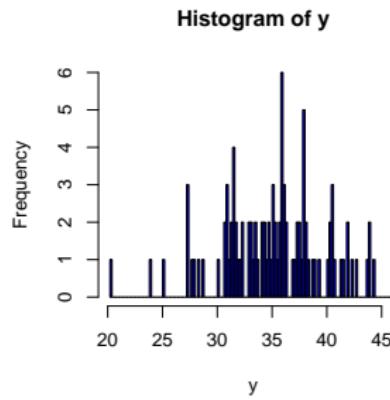
- ① as above
- ② as above + make a histogram of all ages
- ③ iterate over all ages and compute their weighted average

Iteration over all ages

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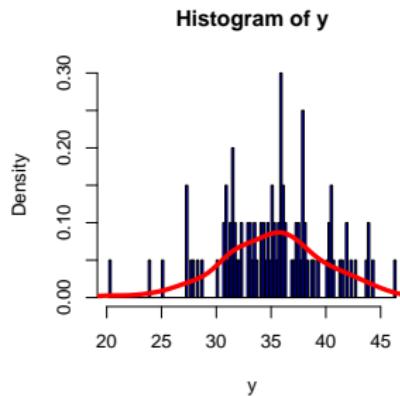
$$\bar{t}_r(t) = \frac{a_1 n_{a_1} + a_2 n_{a_2} + \cdots + a_n n_{a_n}}{n_o}$$

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



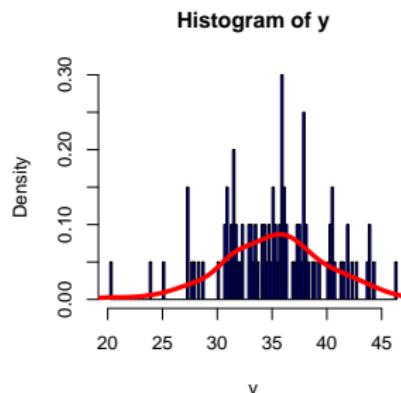
Integration over a density

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

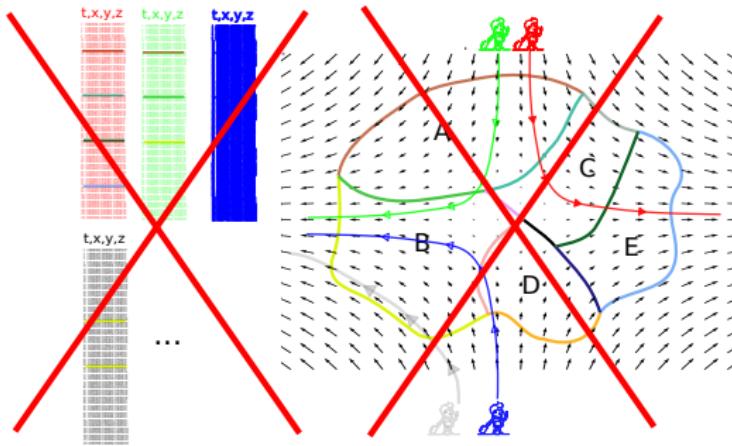


Same procedure for age density

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

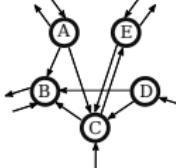


Possible Predictive Statistics ?



	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.

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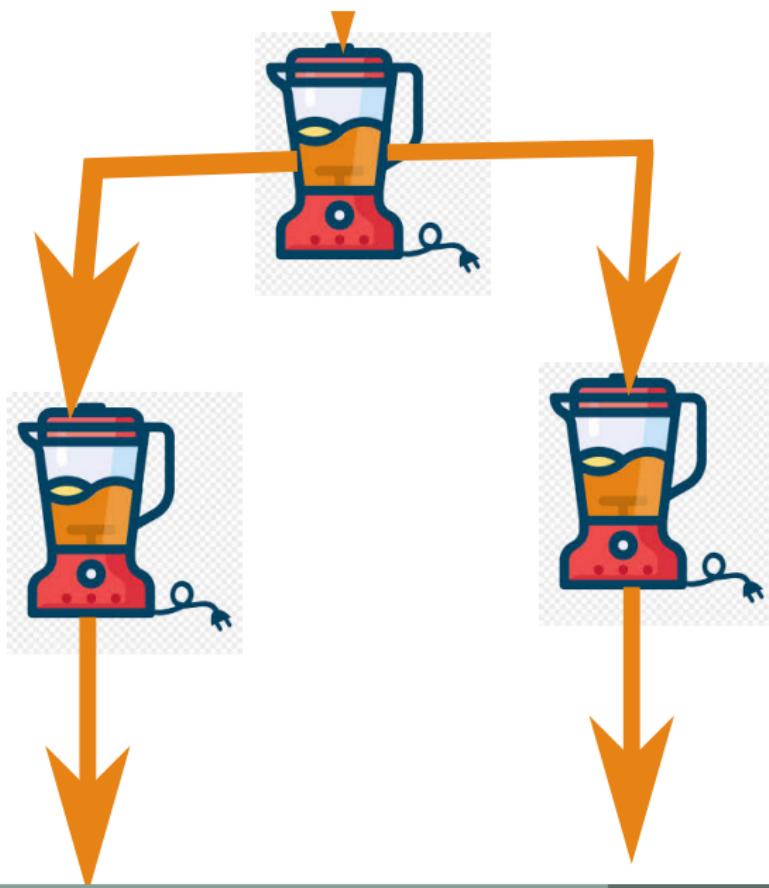
- Population Dynamics
- Hydrology

The simplest pool systems



Pool Models

The simplest pool systems are well mixed



Only the number of particles per Pool counts ...

	Pools	arrival		Pools	arrival		Pools	arrival
1	A	16.45	1	D	14.45	1	D	12.45
2	C	42.45	2	B	52.45	2	B	32.45
3	E	68.56	3	Ext	94.23	3	Ext	194.23
4	Ext	94.23						

	Pools	arrival
1	B	16.45
2	Ext	194.23
		...

Only the number of particles per Pool counts ...

Pools arrival			Pools arrival			Pools arrival		
1	A	16.45	1	D	14.45	1	D	12.45
2	C	42.45	2	B	52.45	2	B	32.45
3	E	68.56	3	Ext	94.23	3	Ext	194.23
4	Ext	94.23						

Pools arrival		
1	B	16.45
2	Ext	194.23
		...

Only the number of particles per Pool counts ...

Pools arrival			Pools arrival			Pools arrival			Pools arrival		
1	A	16.45	1	D	14.45	1	D	12.45	1	D	12.45
2	C	42.45	2	B	52.45	2	B	32.45	2	B	32.45
3	E	68.56	3	Ext	94.23	3	Ext	194.23	3	Ext	44.23
4	Ext	94.23									

leaves too early

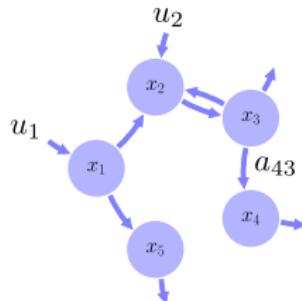
Pools arrival

1 B 66.45 } arrives too late
2 Ext 194.23 ...

How many particles are in pool B at time t = 60?

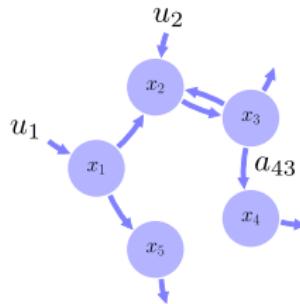
Linear autonomous compartmental models

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



Linear autonomous compartmental models

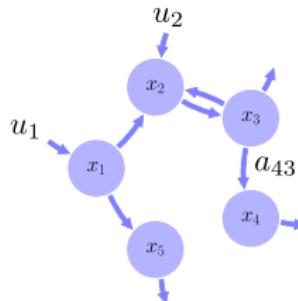
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$\mathbf{x}(t)$ vector of compartment content (e.g. C) at time t

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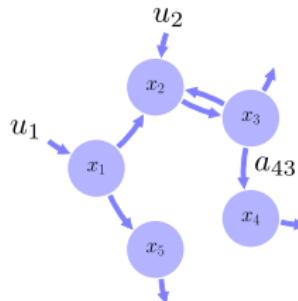


$\mathbf{x}(t)$ vector of compartment content (e.g. C) at time t

\mathbf{u} constant input vector

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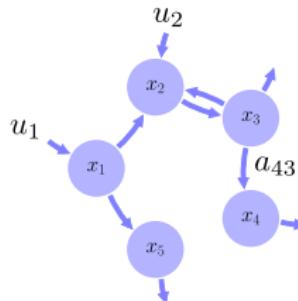
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$A = (a_{ij})$ compartmental matrix

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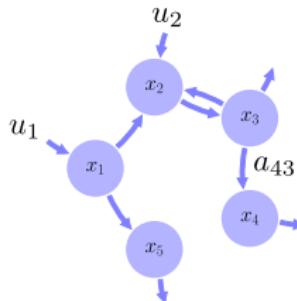
$A = (a_{ij})$ compartmental matrix

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

rate of flow from compartment j to compartment i

Linear autonomous compartmental models

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



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

\mathbf{u} constant input vector

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

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

rate of flow from compartment j to compartment i

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

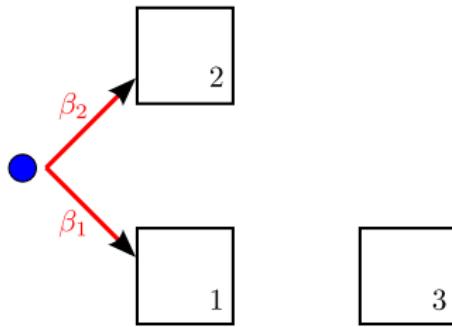
A particle travels

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

$$\begin{array}{c} \boxed{2} \\ u \\ \boxed{1} \quad \boxed{3} \end{array} \quad \begin{array}{ccc} \mathbf{A} & & \mathbf{u} \\ \left(\begin{array}{ccc} -a_{11} & a_{12} & 0 \\ a_{21} & -a_{22} & 0 \\ a_{31} & 0 & -a_{33} \end{array} \right) & & \left(\begin{array}{c} u_1 \\ u_2 \\ 0 \end{array} \right) \\ -\sum & 0 & > 0 & > 0 & \|\mathbf{u}\| \end{array}$$

A particle travels

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



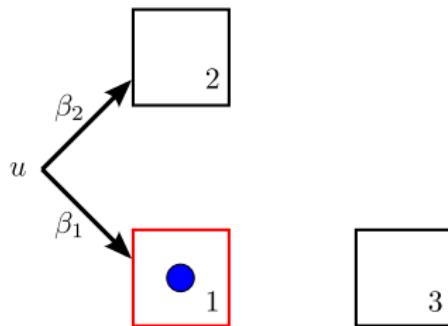
$$\begin{pmatrix} -a_{11} & a_{12} & 0 \\ a_{21} & -a_{22} & 0 \\ a_{31} & 0 & -a_{33} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ 0 \end{pmatrix} - \sum 0 > 0 > 0 \quad \|\mathbf{u}\|$$

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

$$T_0 = 0$$

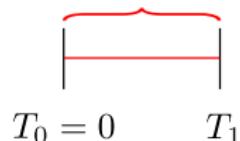
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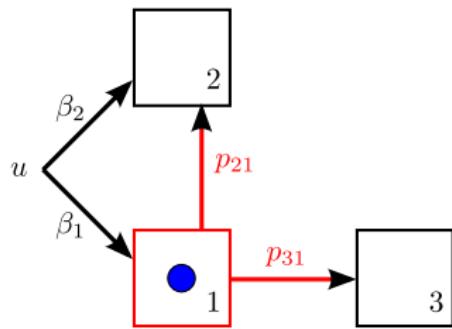
$$\begin{pmatrix} -a_{11} & a_{12} & 0 \\ a_{21} & -a_{22} & 0 \\ a_{31} & 0 & -a_{33} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ 0 \end{pmatrix} - \sum 0 > 0 > 0 \|\mathbf{u}\|$$

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



A particle travels

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



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

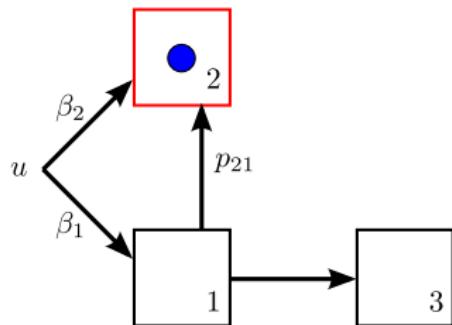
$$p_{21} = \frac{a_{21}}{a_{11}} \quad p_{31} = \frac{a_{31}}{a_{11}}$$

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

The diagram shows a horizontal line segment with a brace above it, indicating its length. Below the line, the value $T_0 = 0$ is written to the left of a vertical tick mark, and the value T_1 is written to the right of the same tick mark.

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$$- \sum$$

$$0$$

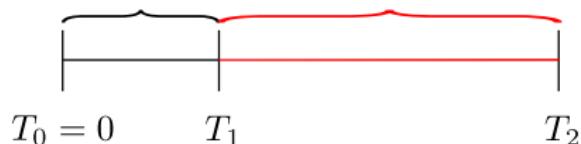
$$> 0$$

$$> 0$$

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

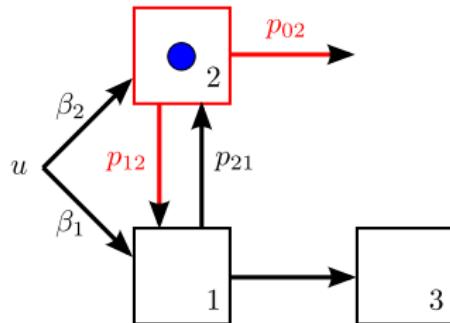
$$T_1 \sim \text{Exp}(a_{11})$$

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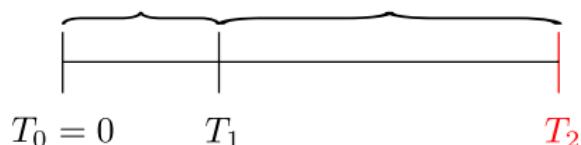


$$\mathbf{A} = \begin{pmatrix} -a_{11} & a_{12} & 0 \\ a_{21} & -a_{22} & 0 \\ a_{31} & 0 & -a_{33} \end{pmatrix}, \quad \mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \\ 0 \end{pmatrix}$$
$$-\sum 0 > 0 > 0 \quad \|\mathbf{u}\|$$

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

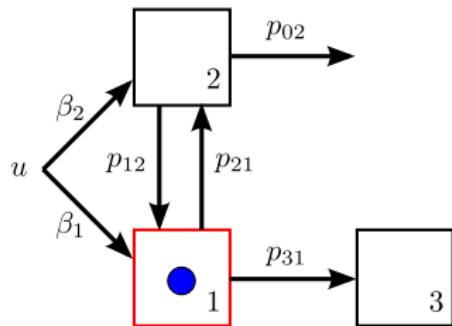
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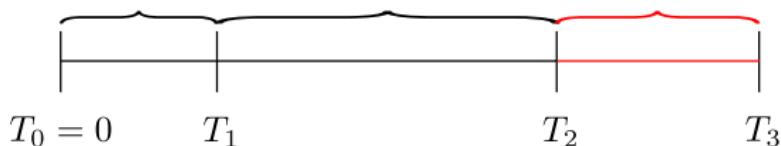


$$\begin{pmatrix} -\mathbf{a}_{11} & \mathbf{a}_{12} & 0 \\ \mathbf{a}_{21} & -\mathbf{a}_{22} & 0 \\ \mathbf{a}_{31} & 0 & -\mathbf{a}_{33} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ 0 \end{pmatrix} - \sum 0 > 0 > 0 \|\mathbf{u}\|$$

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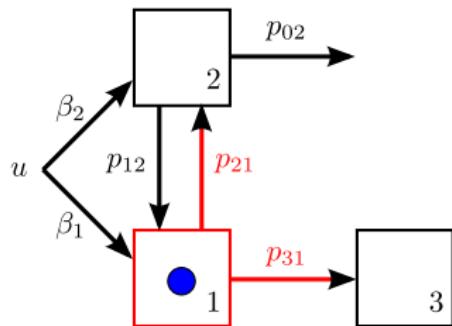
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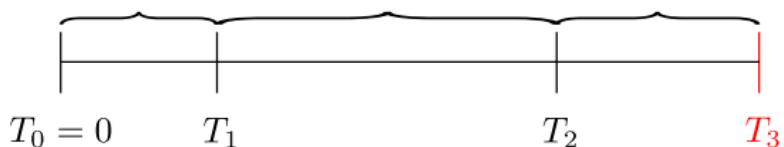
$$- \sum \quad 0 \quad > 0 \quad > 0 \quad \|\mathbf{u}\|$$

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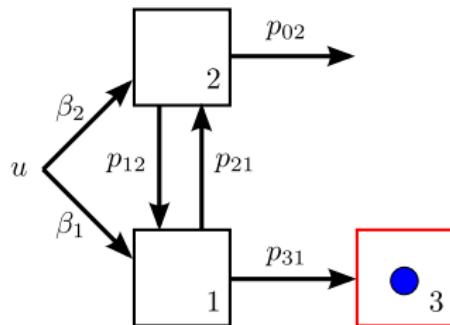
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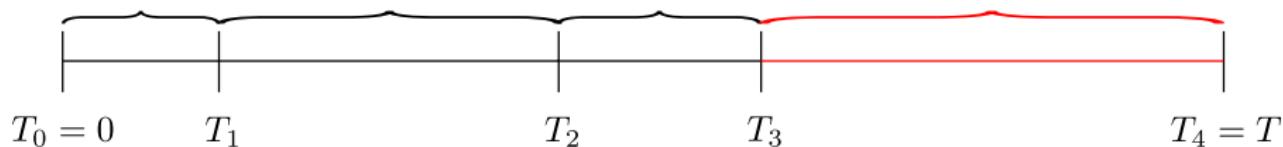
$$\begin{array}{ccc} \mathbf{A} & & \mathbf{u} \\ \left(\begin{array}{ccc} -a_{11} & a_{12} & 0 \\ a_{21} & -a_{22} & 0 \\ a_{31} & 0 & -a_{33} \end{array} \right) & & \left(\begin{array}{c} u_1 \\ u_2 \\ 0 \end{array} \right) \\ -\sum & 0 & > 0 & > 0 \\ & & & \|\mathbf{u}\| \end{array}$$

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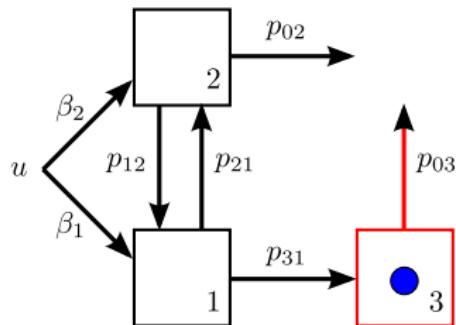
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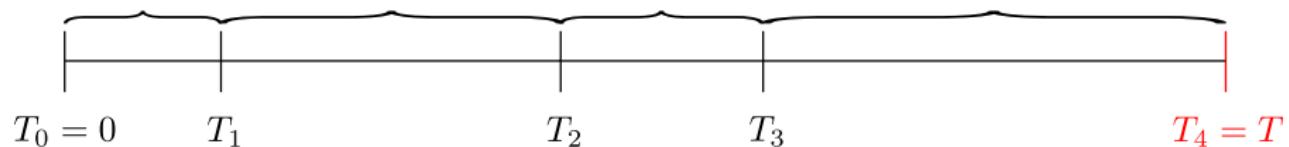
$$p_{03} = 1$$

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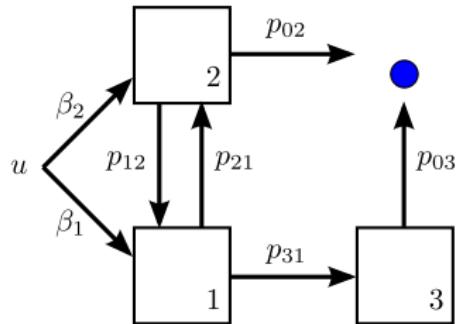
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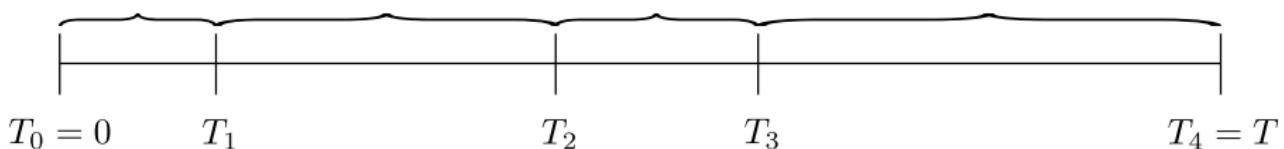
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Transit time distribution

- transit time computation:

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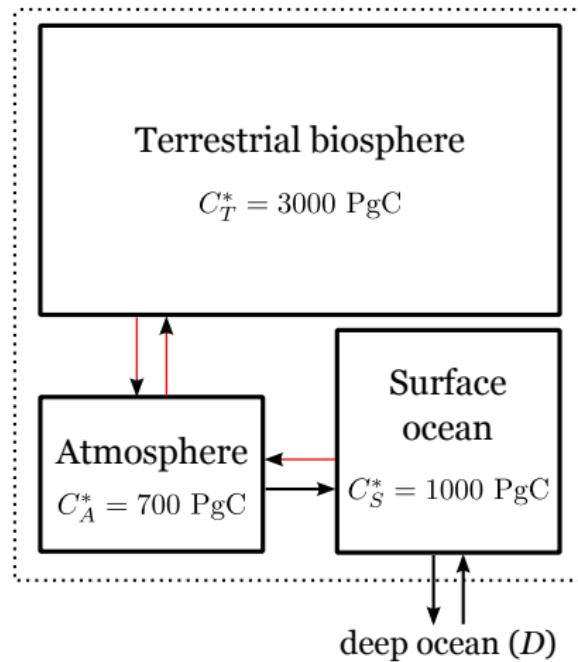
→ $T \sim \text{PH}(\beta, A)$

General, simple, explicit formulas

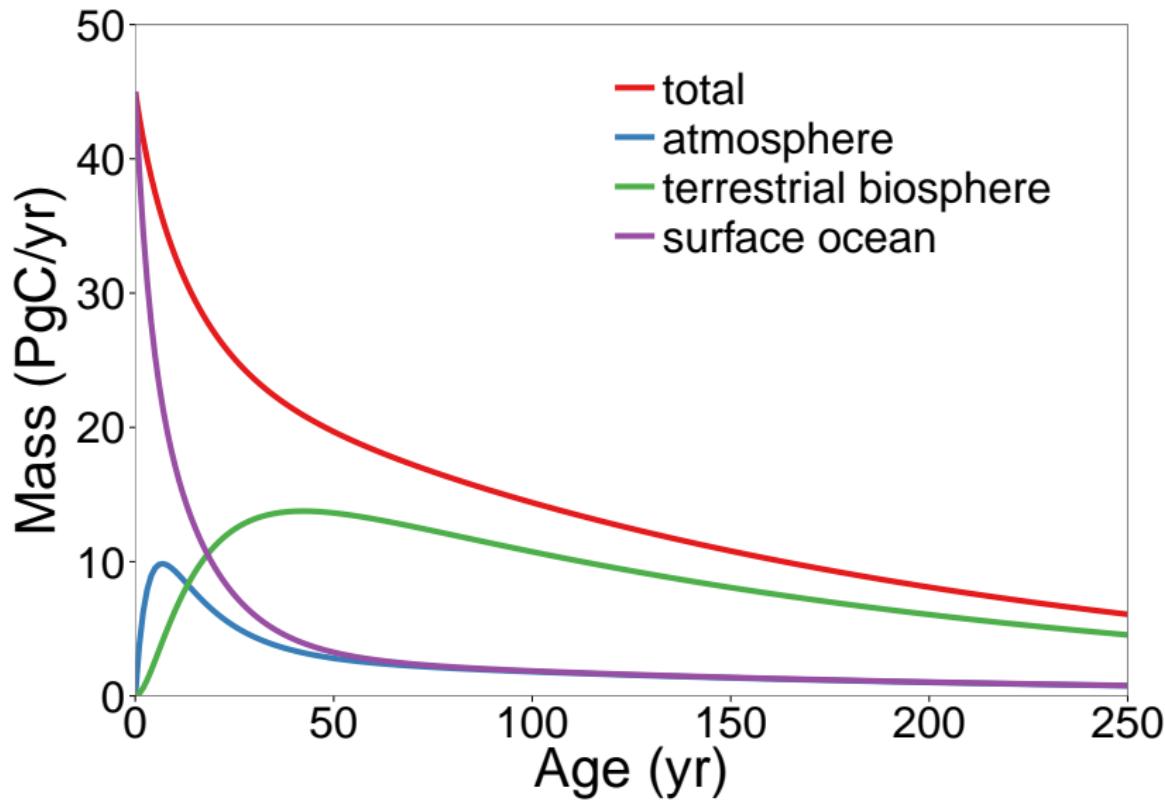
- phase-type distribution is well known:
 - ▶ probability density
 - ▶ cumulative distribution function
 - ▶ quantiles
 - ▶ mean and higher order moments
 - ★ $\mathbb{E}[T] = \|A^{-1}\beta\| = \frac{\|\mathbf{x}^*\|}{\|\mathbf{u}\|}$ (mean transit time)
- system age is also phase-type distributed
 - ▶ 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 [Rodhe and Björkström, 1979] with three compartments



Equilibrium age densities



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mass with age $t-s$ at time t

$$\Rightarrow \underbrace{\Phi(t, t-a) \mathbf{u}(t-a)}$$

mass with age a at time t

The state transition operator Φ

- solution to the matrix ordinary differential equation

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- we can always obtain it (at least numerically)

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

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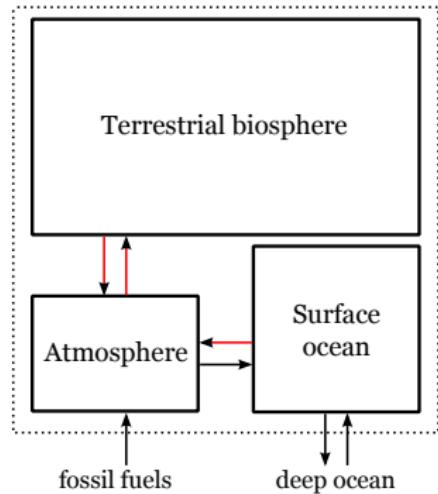
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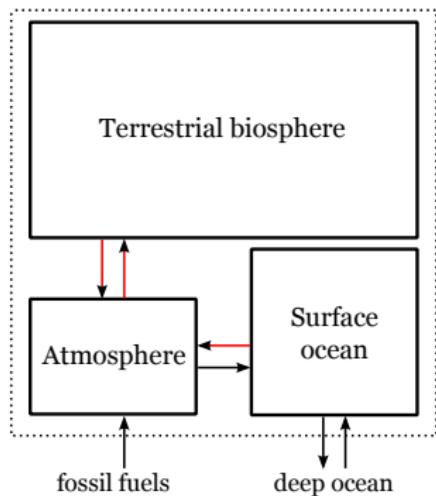
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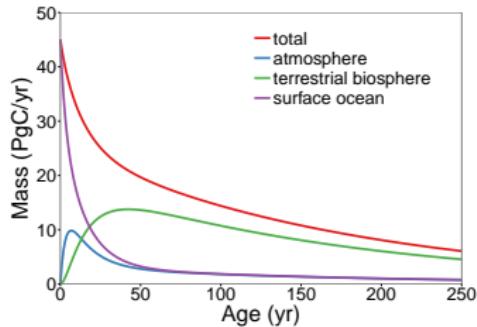
A global carbon cycle model



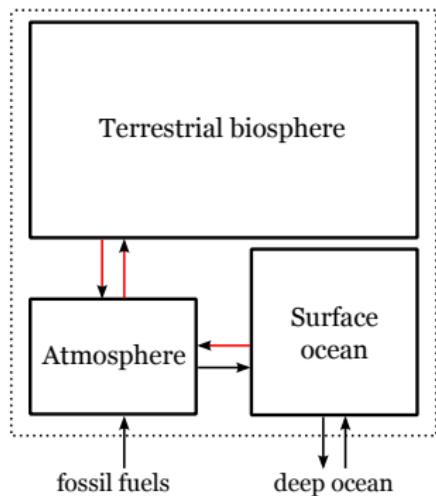
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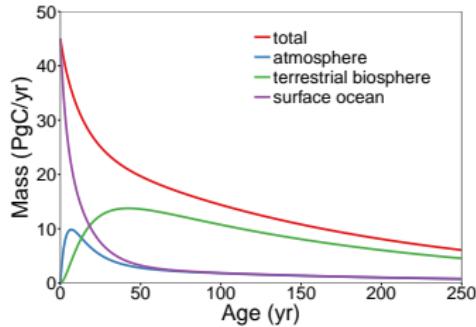
Equilibrium age densities in 1765



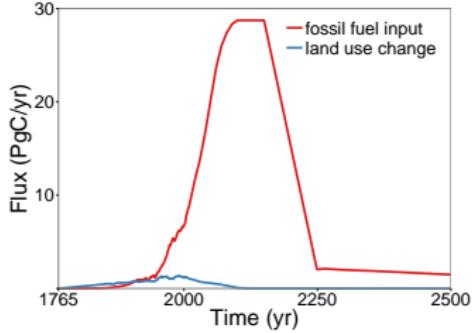
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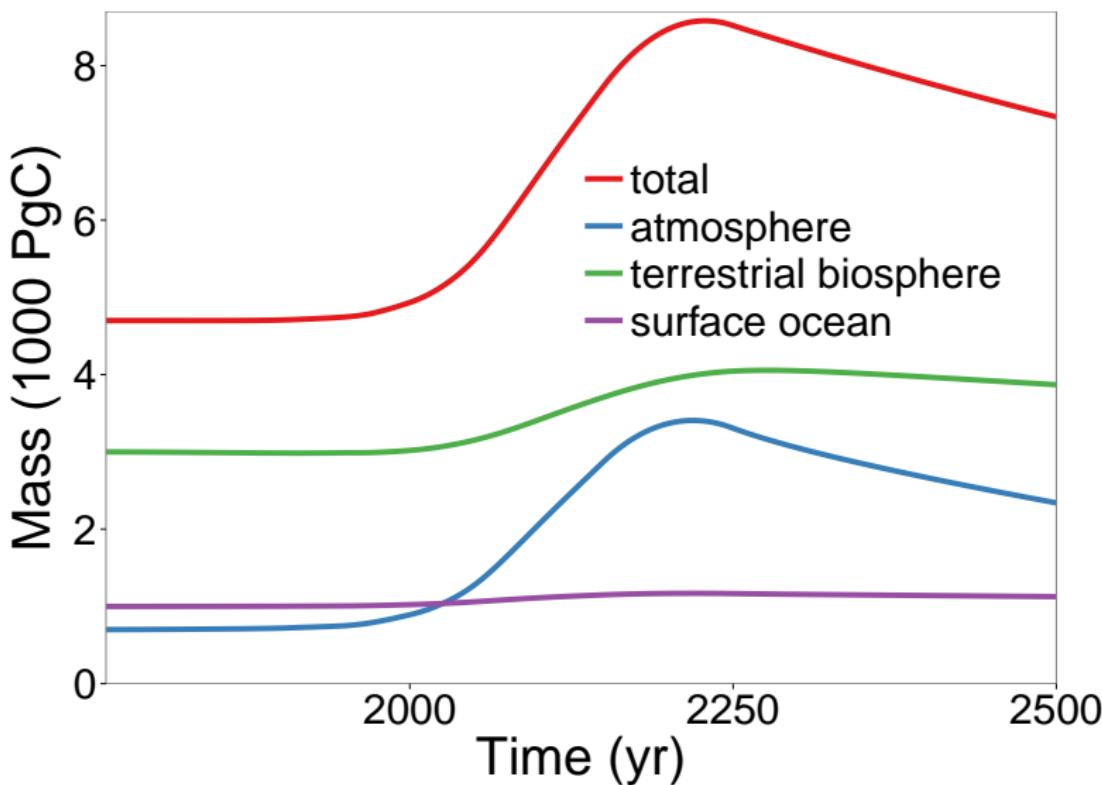
Equilibrium age densities in 1765



RCP8.5 scenario



Time-dependent carbon contents



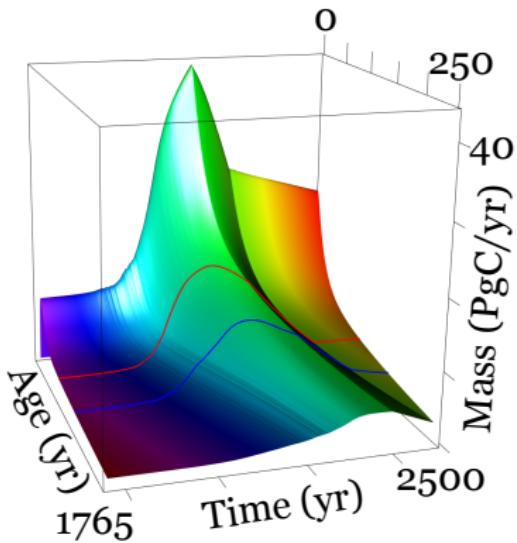
Questions of high scientific and societal interest

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Time evolution of the atmosphere's carbon age density.



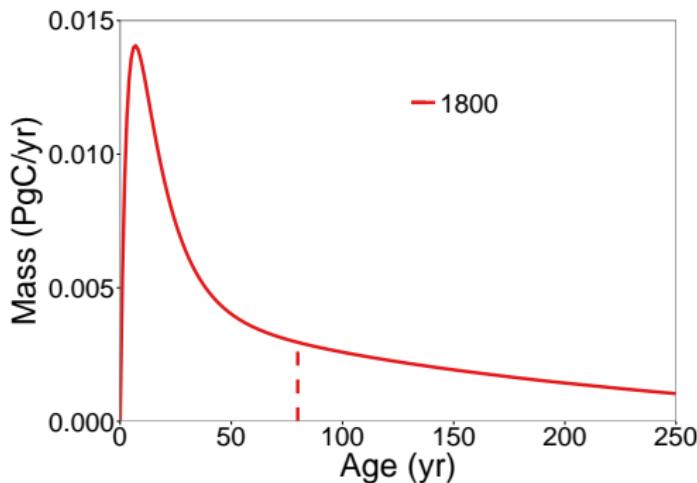
- median age
- mean age
- surface color constant along the time-age diagonal such that the color reflects the moment of entry into the system.
- left edge equilibrium age density of the atmosphere's carbon at (time = 1765 yr)
- lower edge (age = 250 yr) mass is in the system with age equal to 250 yr

Questions of high scientific and societal interest

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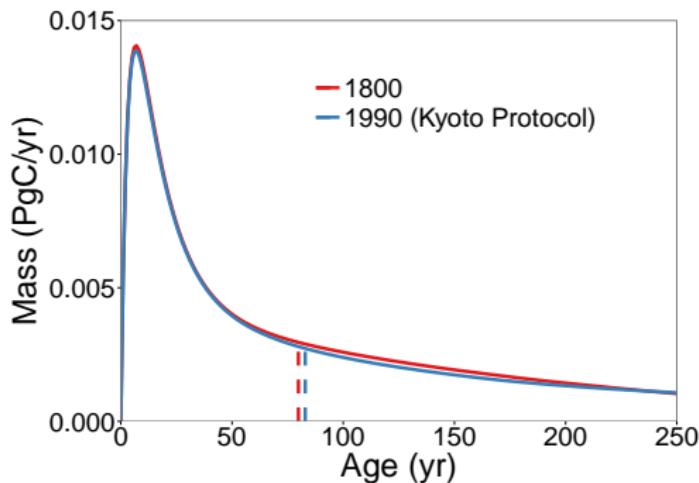
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- medians (dashed vertical lines) increase until the year 2170 and then start decreasing.

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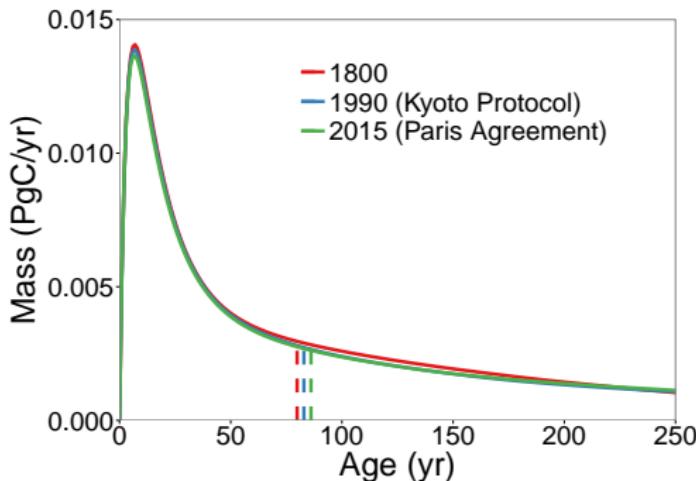
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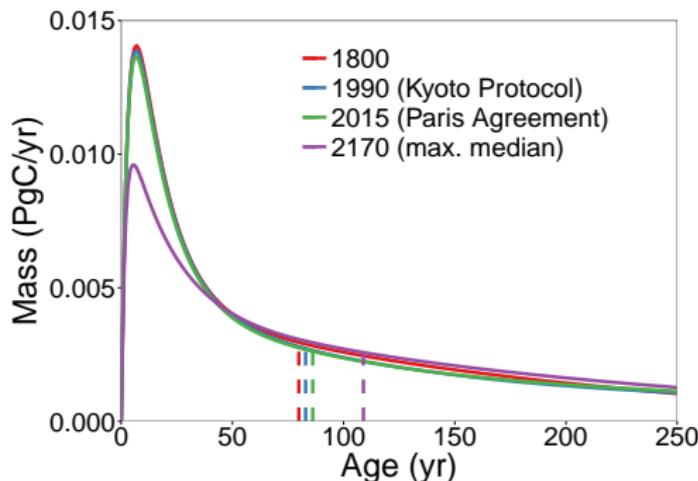
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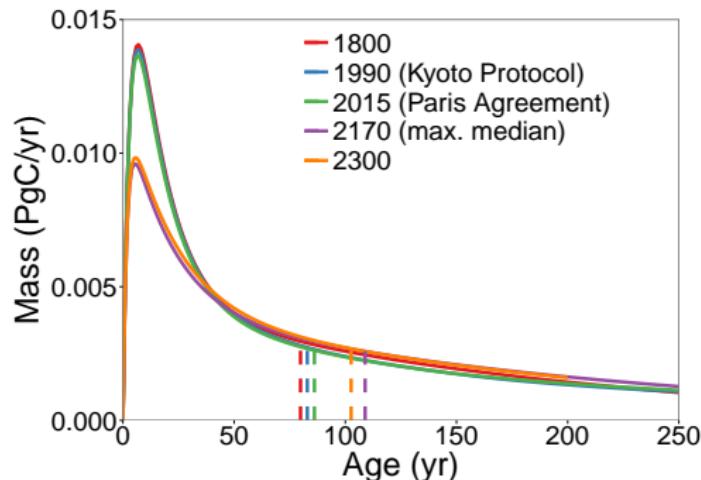
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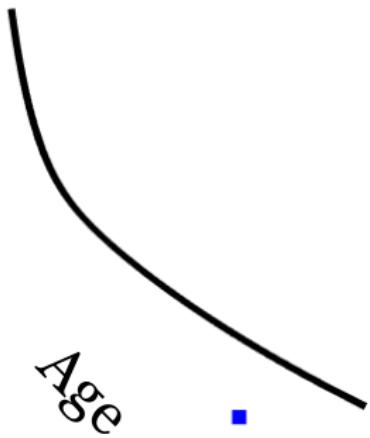
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- **two Python packages**
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 - ★ <http://github.com/goujou/LAPM>
 - ▶ (numerical) computation of age and transit time properties for nonlinear nonautonomous systems

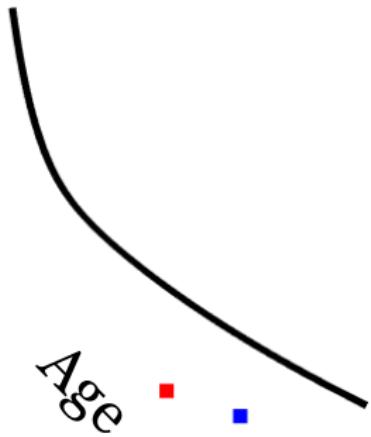
System age



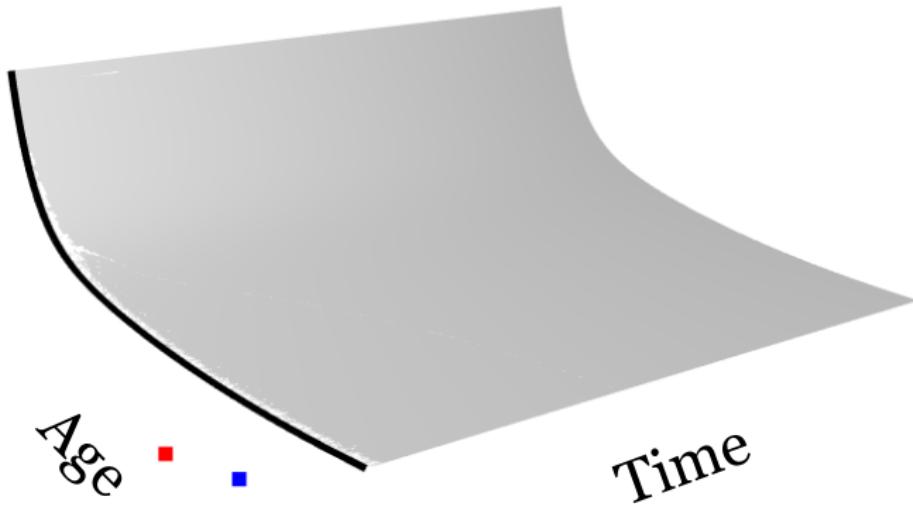
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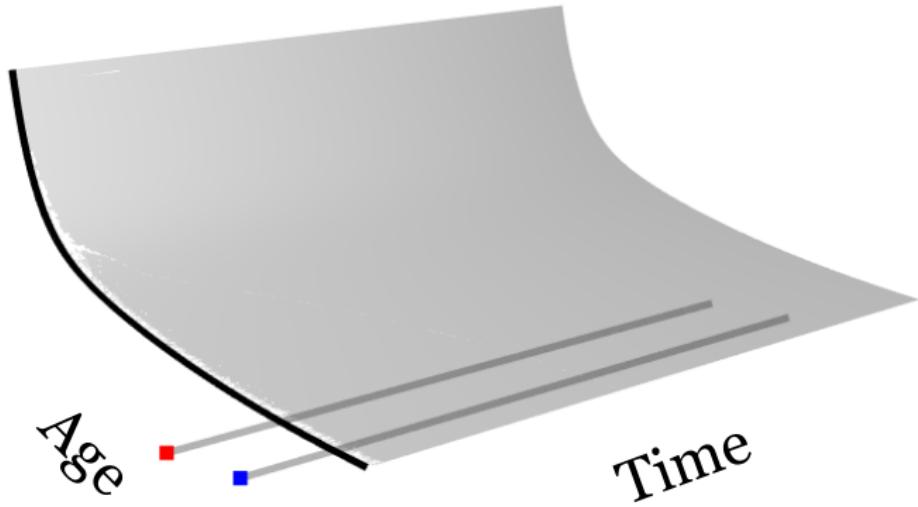
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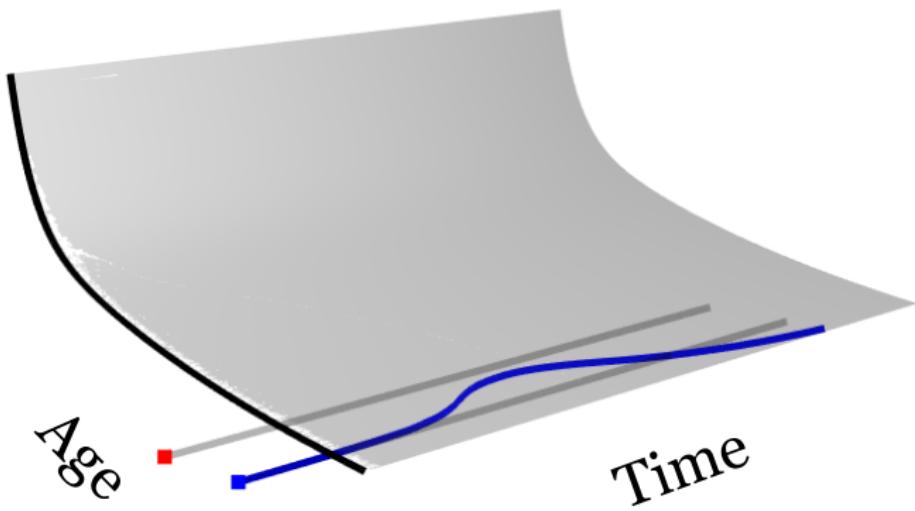
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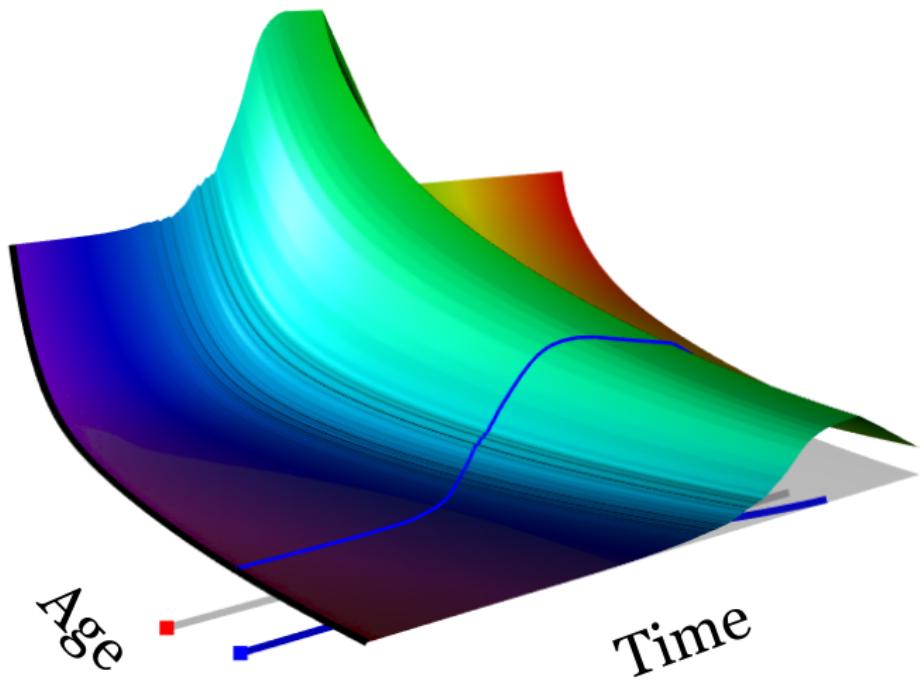
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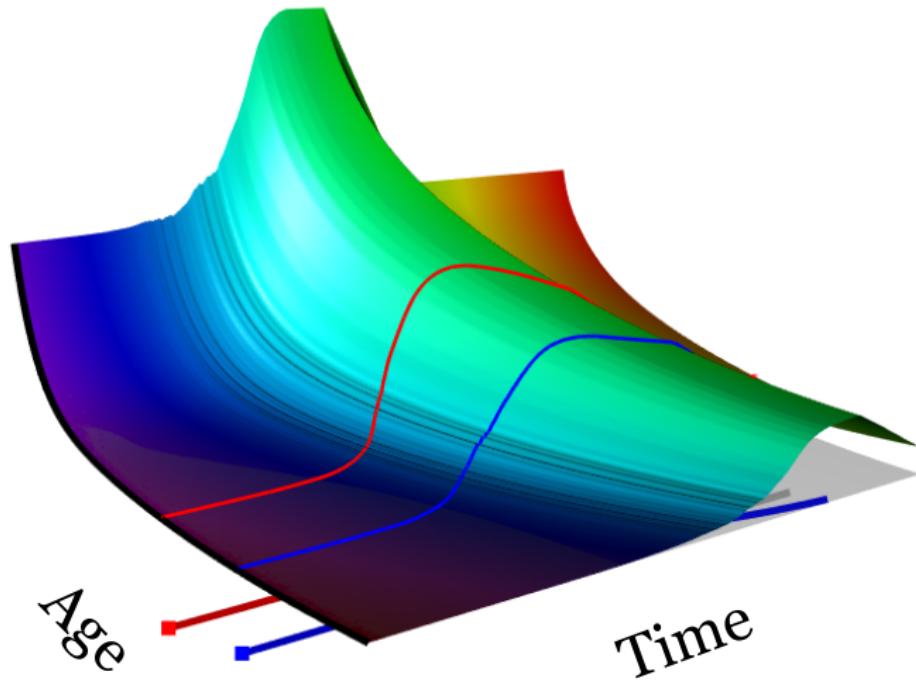
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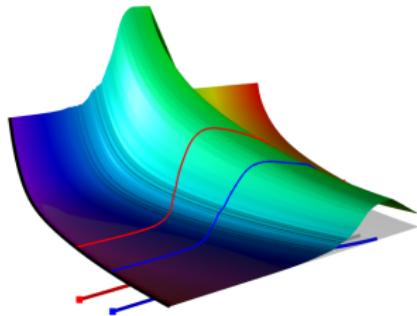
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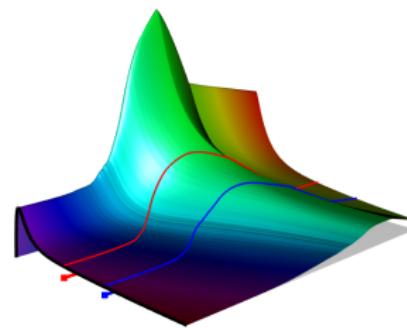
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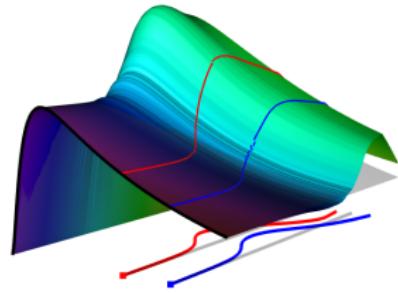
System



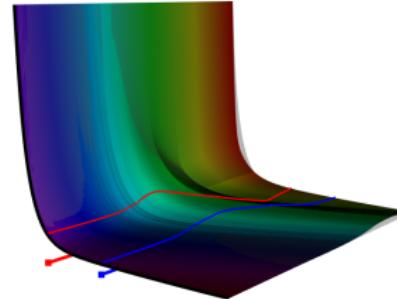
Atmosphere



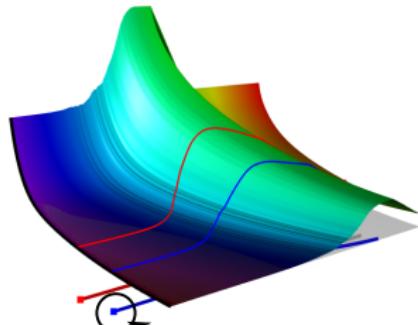
Terrestrial biosphere



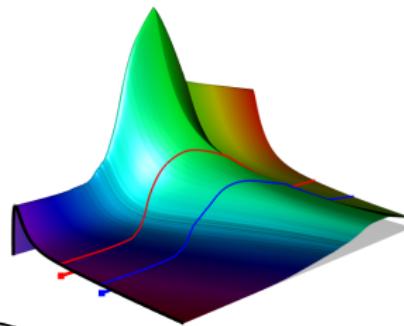
Surface ocean



System

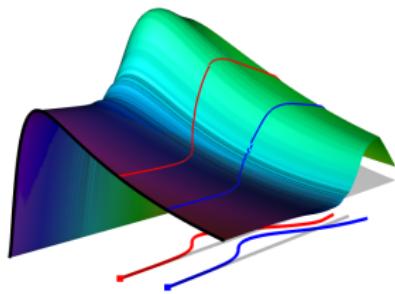


Atmosphere

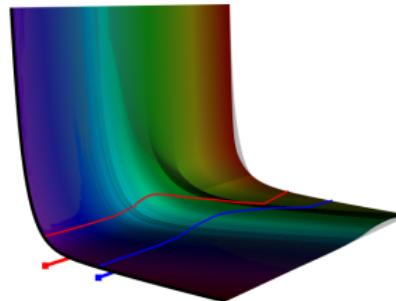


early 2016

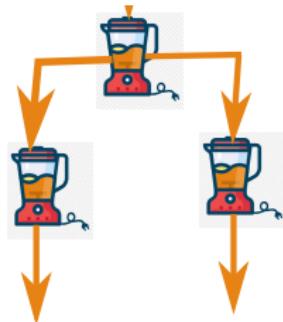
Terrestrial biosphere



Surface ocean



Examples for “Well-mixed Systems”



- Century



- Reactors



- RothC



- Carbon



- Allocation



- Element Cycling Models

- ...

1 Example applications of pool models

2 Reducing model complexity

- The carbon cycle example
- Asking simpler questions
- Answer questions more simply

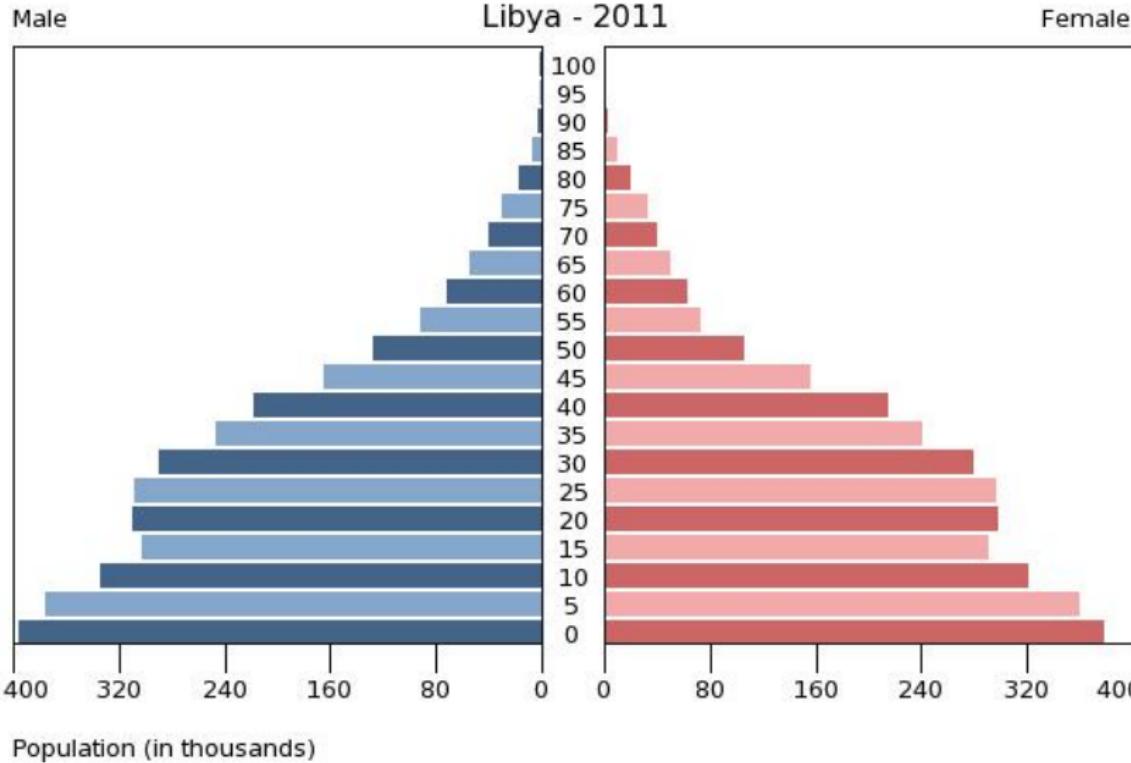
3 Compartmental systems

- Introduction
- Linear autonomous
- Generalization to nonlinear nonautonomous systems
- Example application

4 Generalization to non Well Mixed Systems

- Population Dynamics
- Hydrology

Population Dynamics $\phi(a)$



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

McKendrick–von Foerster Equation

- original:

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

The “deathrate” $m(a)$ depends on the age a .

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

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- in compartmental systems

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

$m(\textcolor{red}{t})$ depends only on time $\textcolor{red}{t}$.

Age and transit-time distributions for catchments

- Single catchment
 - ▶ identical equations as for population dynamics
 - ▶ “deathrate” → “age selection function”.
- multiple connected catchments
 - ▶ Possible: Prediction of age selection function for systems of well mixed pools. (from transit time and age distributions)
 - ▶ Challenge: Prediction of age selection function for systems of **non** well mixed pools. (global age selection functions from pool wise age selection functions)

Summary

- Pool models greatly simplify:
 - ▶ The questions (that can be) asked
 - ▶ The way questions are answered by exploiting symmetries
- Natural descriptive statistics are time related distributions (age and transit time , per pool per system ...)
- The simplest and most prominent pool models with the most theory are “well mixed ” or “compartmental systems” modeled by ordinary differential equations.
- Much more general pool models are possible including non constant deathrates (age selection functions) or delays, that have to be solved with different mathematical tools. (partial differential equations, integral equations, delay equations, Monte Carlo simulations ...) still much simpler than the underlying complete models.

Thanks

Funding



bibliography

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Environmental and Experimental Botany, 152:7 – 18, 2018. doi: <https://doi.org/10.1016/j.envexpbot.2018.03.011>. URL <http://www.sciencedirect.com/science/article/pii/S0098847218303915>.

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