Pool Models

A classification by required and obtainable information

Markus Müller, Holger Metzler, Carlos Sierra

August 5, 2019

- 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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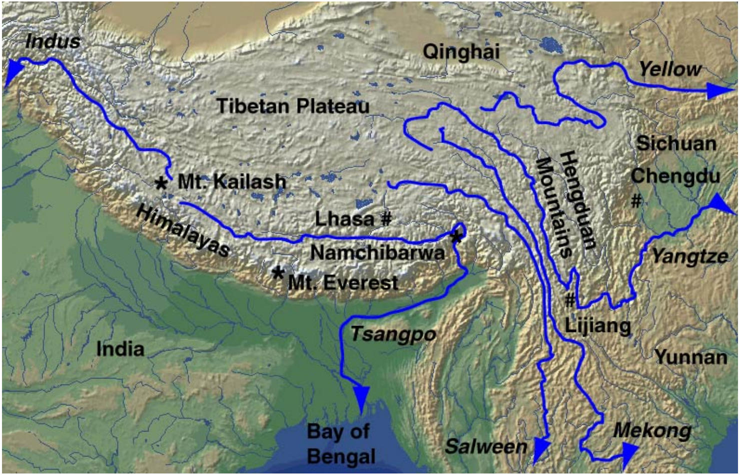
1. Example Applications of Pool Models
2. Reducing Model Complexity
   - The carbon cycle as (de)motivating example
   - Asking Simpler Questions
   - Answer Questions more simply
3. Our proposed solution
   - Definitions
   - Algorithms
   - Comparison to standard theory
4. Example
   - Results

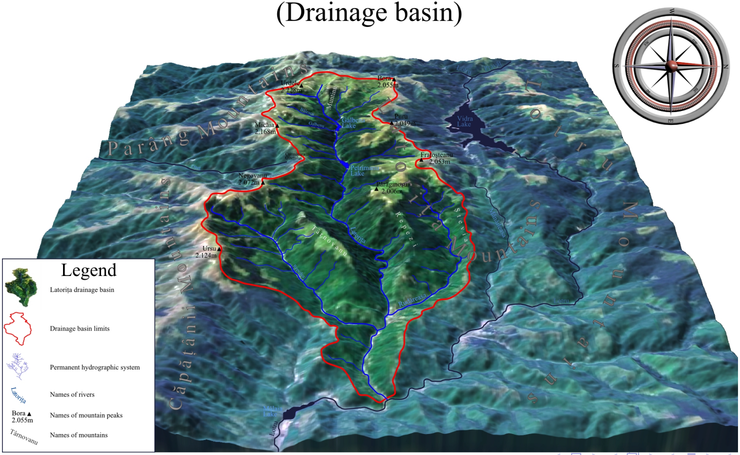
Hydrology Watersheds



Hydrology Catchments

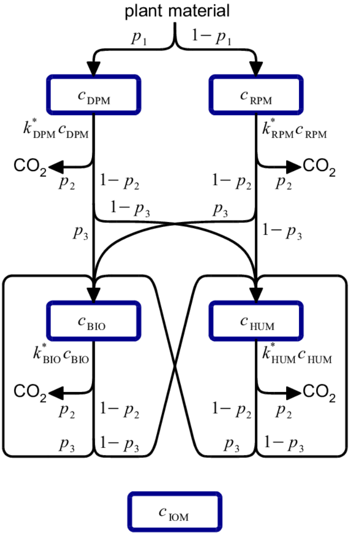
Latorița River, tributary of the Lotru River

(Drainage basin)



Plant Physiology/ Carbon allocation

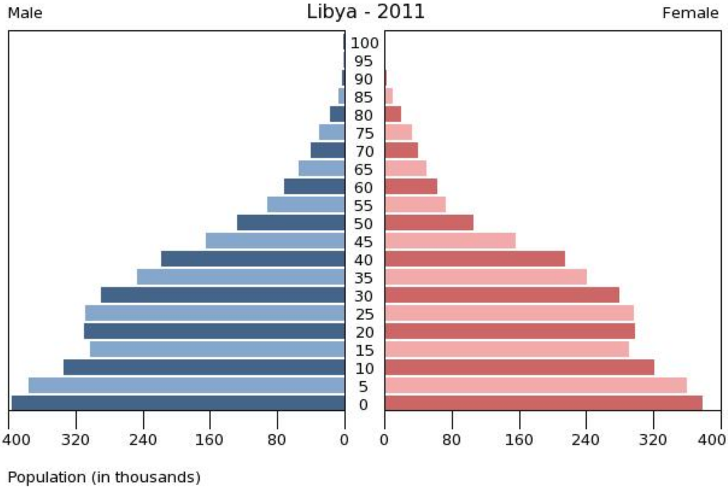
Organic Matter Decomposition / Soil Models

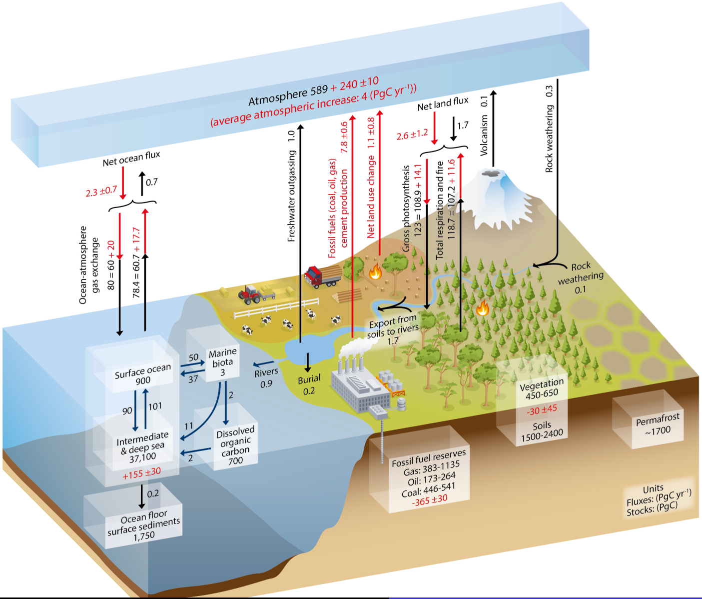


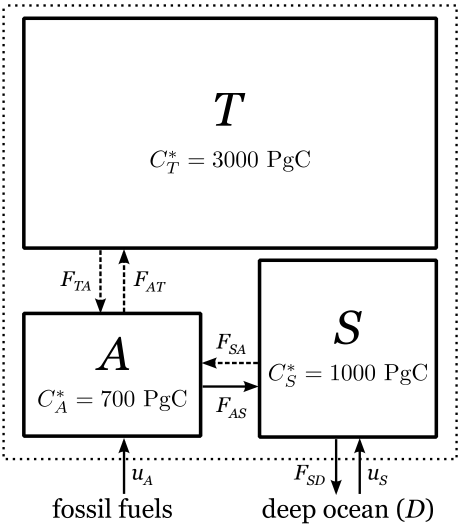
Ecosystem Models

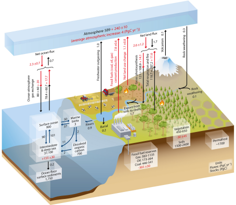
Chemical Reactors

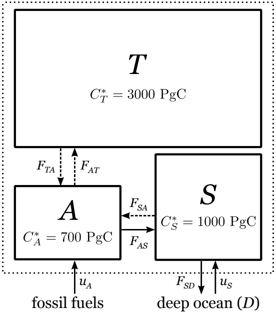
Population Dynamics




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
Rivers 0.9
Burial 0.2
Surface ocean 900
50
37
Marine biota 3
90
101
2
11
Intermediate & deep sea 37,100
+155 ±30
Dissolved organic carbon 700
2
0.2
Ocean floor surface sediments 1,750
Fossil fuel reserves
Gas: 383-1135
Oil: 173-264
Coal: 446-541
-365 ±30
Vegetation 450-650
-30 ±45
Soils 1500-2400
Permafrost ~1700
Units
Fluxes: (PgC yr⁻¹)
Stocks: (PgC)


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

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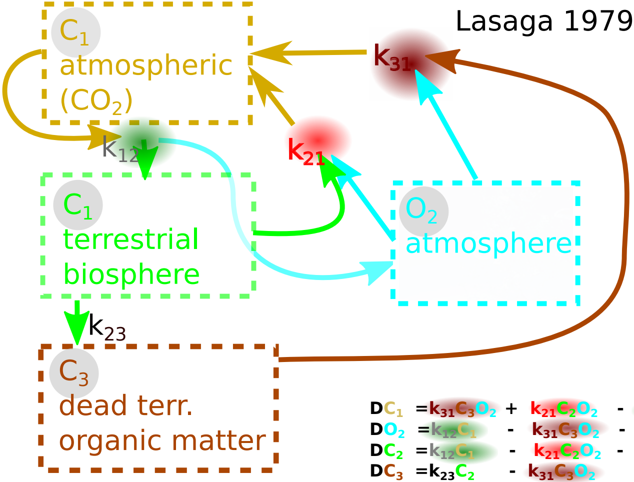
C
PASSPORT
PASSPORT
HONG KONG
- 4 JUN 2011
MALAYSIA IMMIGRATION
DEPARTURE
České Velenice
AEROPORT POLE CARAIBES - ABYMES
2 6 MARS 2016
GUADELOUPE
UGANDA
1 2 JUN 2010
ENTEBBE
2 1 MARS 2016
H 124 MARTINIQUE
14 AVR. 2011

Example Model

Lasaga 1979



$$
\begin{aligned}
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 \\
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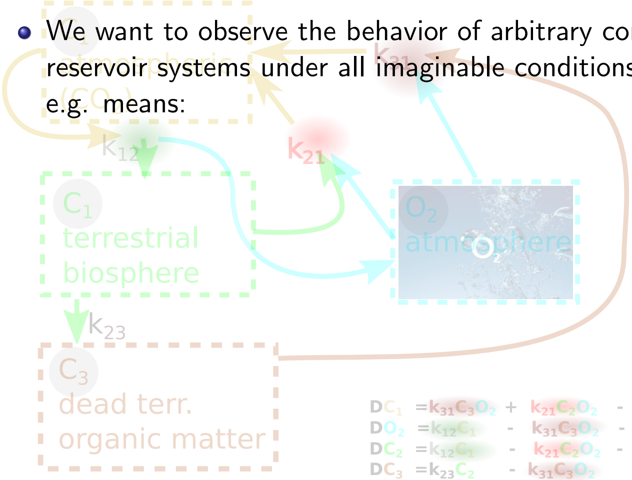
Example Model

- We want to observe the behavior of arbitrary complex reservoir systems under all imaginable conditions,which e.g. means:



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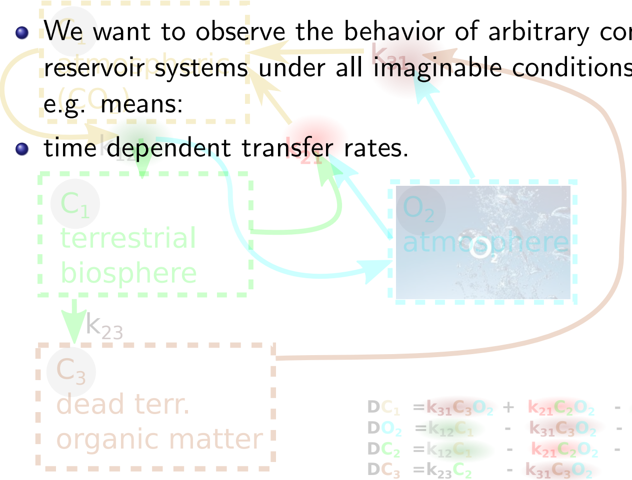

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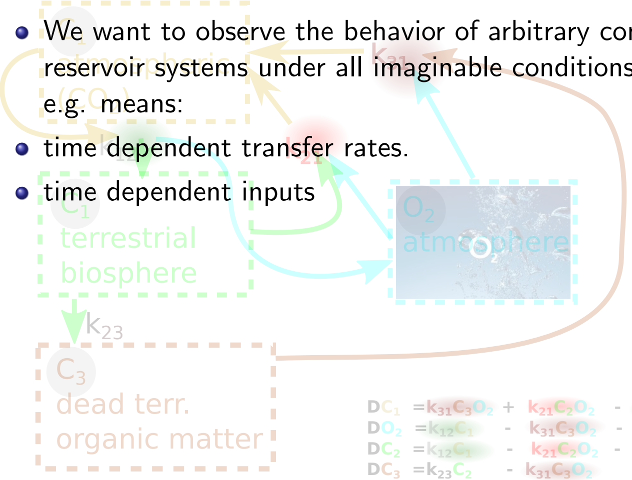

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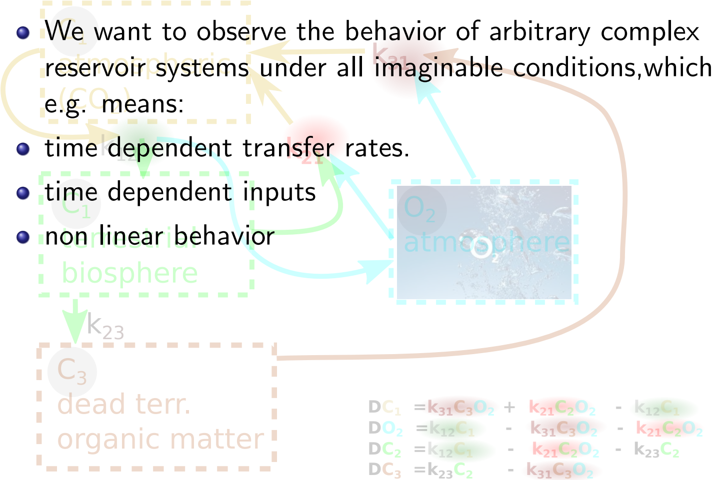

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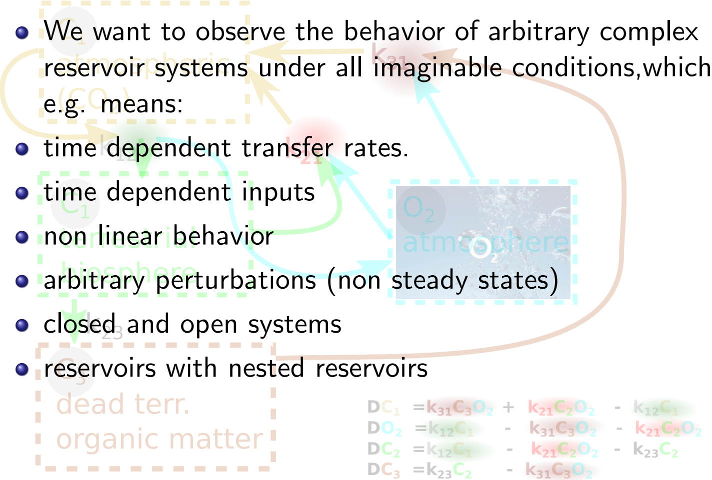
- arbitrary perturbations (non steady states)
- closed and open systems
- reservoirs with nested reservoirs



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  $\rightarrow$ misleading into wrong generalizations
  $\rightarrow$ motivation for a numerical counterpart where all the assumptions (if any) should be intuitive and obvious.

Requirements for definitions

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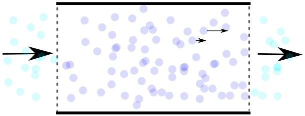
   2. definite end
      $\rightarrow$ no ∞

The general concept of a reservoir



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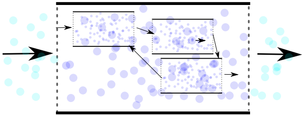

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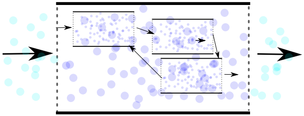

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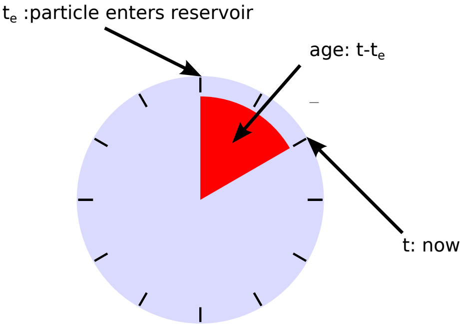
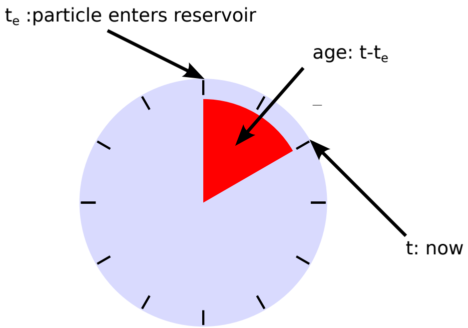
2. "Flows" do not necessarily involve "movement"
   In and out flow "channels" do not always have to be defined physically or spatially
3. reservoirs can have arbitrary complex subsctructures
4. reservoirs can be mixed or not

age of a particle

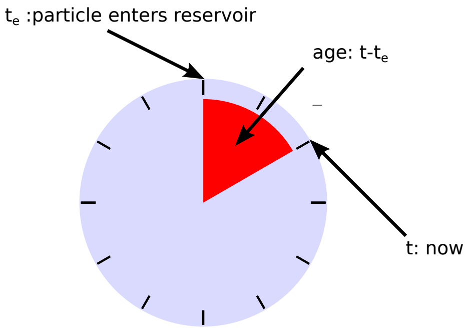


age of a particle



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

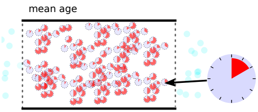
age of a particle



- The “age ” can not be negative!

Mean age

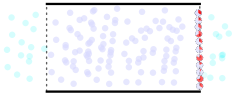
- Which set of particles to use for the average?
  proposition: *all* particles that are in the reservoir at the given time.
  $\rightarrow$ usually depends on input rates as well as the dynamics of the system.



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

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

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

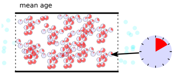
Mean transit time

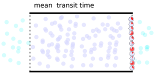
$$\bar{t}_r(t) = \frac{a_1 + a_2 + \cdots + a_{n_o}}{n_o}$$

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 particle and compute the average of their ages.

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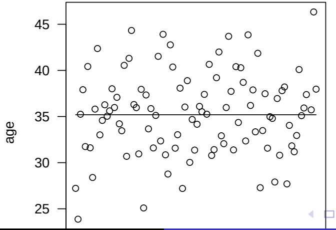
With $n_o = n_o(t)$ the number of particles just leaving at time t



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

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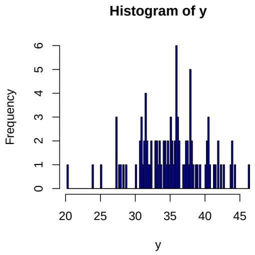
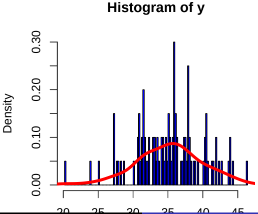
$$\bar{t}_r(t) = \frac{a_1 n_{a_1} + a_2 n_{a_2} + \cdots + a_n n_{a_n}}{n_o}$$

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

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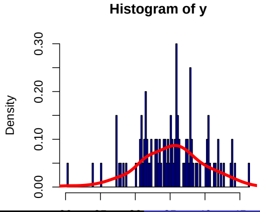
\end{aligned}
$$



Computation of the mean age, overview

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1. describe the rate of change for the stuff inside the system in the form inputrate - outputrate which is possible for all reservoir systems: $\dot{C} = F(C,t) = I(C,t) - O(C,t)$

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4. for every t and every $a : 0 < a < t$ compute $\psi(a,t)$
5. for every t compute the expected value of a by integrating over the product:

$$E(t) = \int_0^t \psi(a,t)\; a \; da$$

Transforming the system I

inject the solution into the operator

$$
\begin{aligned}
\dot{\vec{F}} &= \dot{\vec{C}}(\vec{C}, t) \\
&= \begin{pmatrix} \dot{F}_1(C_1, \ldots, C_n, t) \\ \vdots \\ \dot{F}_n(C_1, \ldots, C_n, t) \end{pmatrix} \\
&= \begin{pmatrix} \dot{I}_1(C_1, \ldots, C_n, t) \\ \vdots \\ \dot{I}_n(C_1, \ldots, C_n, t) \end{pmatrix} + \begin{pmatrix} \dot{O}_1(C_1, \ldots, C_n, t) \\ \vdots \\ \dot{O}_n(C_1, \ldots, C_n, t) \end{pmatrix}
\end{aligned}
$$

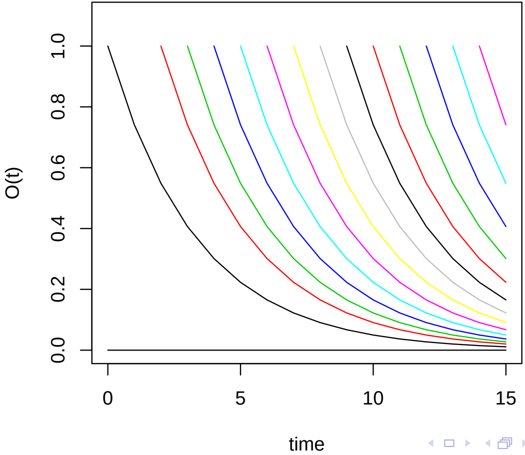
Transforming the system II

For every component F_i do:

$$\begin{aligned}
\dot{F}_i(t) &= \frac{I_i(C_1(t),\dots,C_n(t),t)}{C_i(t)}C_i(t) - \frac{O_i(C_1(t),\dots,C_n(t),t)}{C_i(t)}C_i(t) \\
&= I_{i_{lin}}(t)C_i(t) - O_{i_{lin}}(t)C_i(t) \\
&= F_{i_{lin}}(t)C_i(t)
\end{aligned}$$

Now the equations are uncoupled and linear.

Accumulating previous inputs



Compute $\psi(a, t)$

for every possible age $0 < a < t$ (nested loop) compute the probability density $\psi(a, t)$ as follows:

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5. compute the derivative with respect to a

Conceptual example

- Input(rate): impulsive only at the start $\dot{I} = C_0 \delta(0)$
- Output(rate): $\dot{O}(C,t) = -kC(t)$
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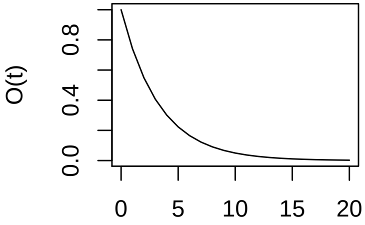
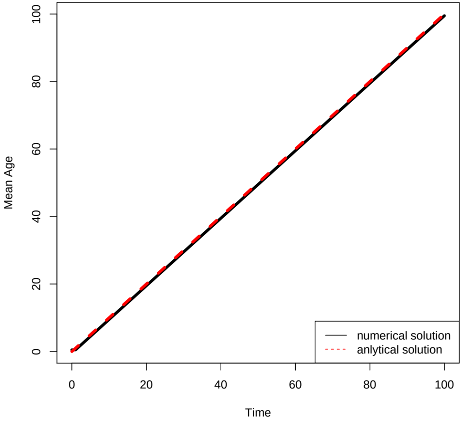


Intuitive solution for the example



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Manzoni,Katul,Porporato 2009:
"for any linear systems the transit time distribution is the output flow resulting from an impulsive unitary input."

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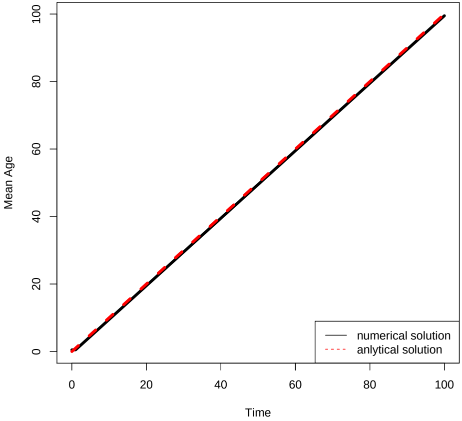
Intuitive Solution to the Example



Conceptual example II

- Input(rate): constant $I_0 = C_0 k$
- Output(rate): $\dot{O}(C, t) = -kC(t)$
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Conceptual example II

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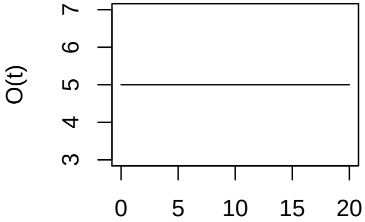
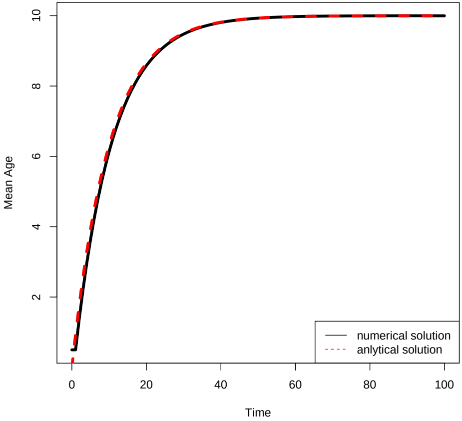
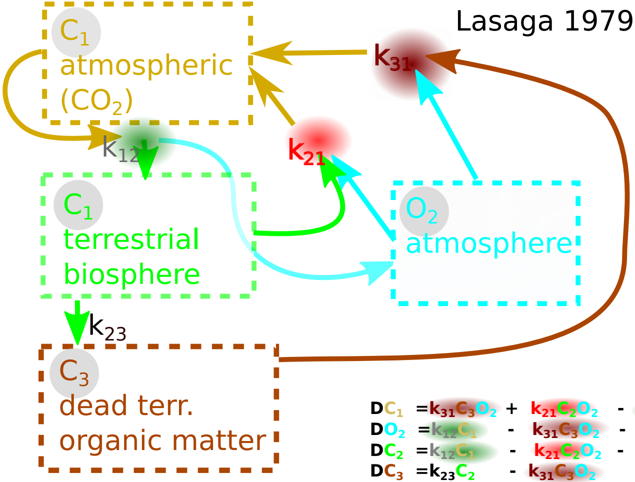
- solution:
  - $C(t) = C_0$



Intuitive Solution to the Example in steady state



Example Model



$$
\begin{aligned}
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 \\
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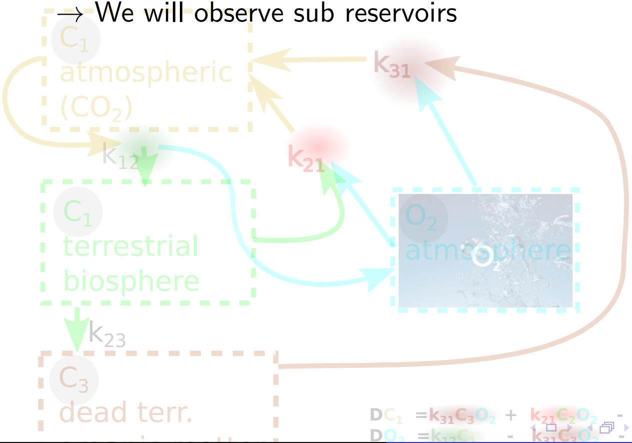
Didactical Considerations

- The system is a *cycle*.
  - $\rightarrow$ Nothing leaves the system as a whole.
  - $\rightarrow$ Transit times for the whole system do not make sense.
  - $\rightarrow$ We will observe sub reservoirs



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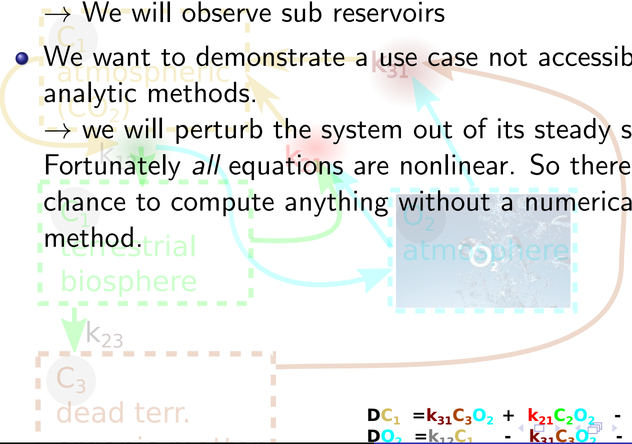
  Fortunately *all* equations are nonlinear. So there is no chance to compute anything without a numerical method.



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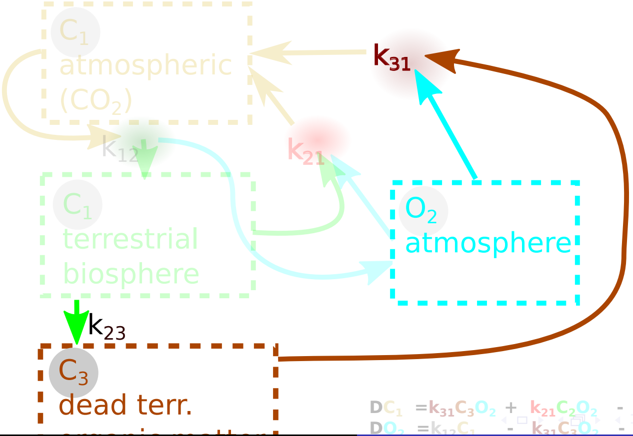
  Fortunately *all* equations are nonlinear. So there is no chance to compute anything without a numerical method.
- We do not want to complicate matters unnecessarily.
  $\rightarrow$ We will go for the simplest equation.
  $\rightarrow$ observe the last pool.

Didactical Considerations



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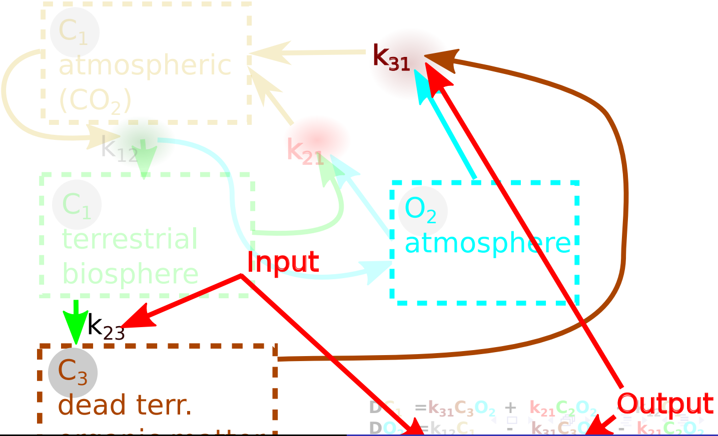
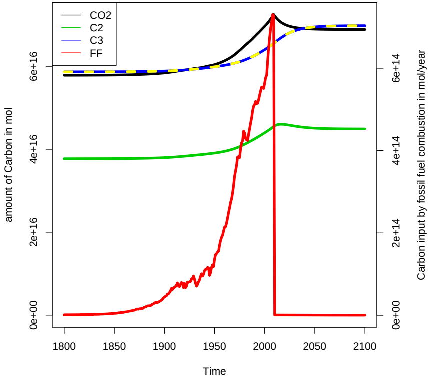
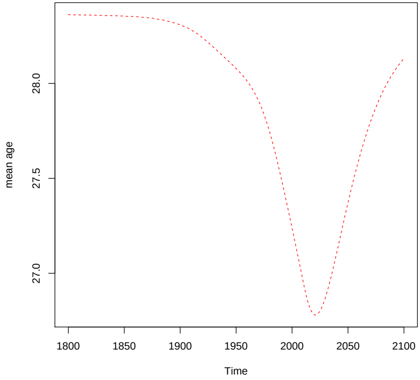


Solution


CO2
C2
C3
FF
0e+00
2e+16
4e+16
6e+16
amount of Carbon in mol
0e+00
2e+14
4e+14
6e+14
Carbon input by fossil fuel combustion in mol/year
1800
1850
1900
1950
2000
2050
2100
Time

Mean age as function of time



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- One more generally applicable set of definitions has been proposed.
- A numerical method has been (partly) developed to obtain the desired values for nonlinear, coupled, time variant systems.
- The method has to be applied to coupled open systems
- Other definitions of mean age and transit times could be evaluated for suitability.

Thank you for your attention