1 Problem statement

2 Our proposed solution
- Definitions
- Algorithms
- Comparison to standard theory

3 Example
- Results

Dynamic transit times and mean ages

Applications to non steady state scenarios

Markus Müller, Carlos Sierra

August 5, 2019

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Outline

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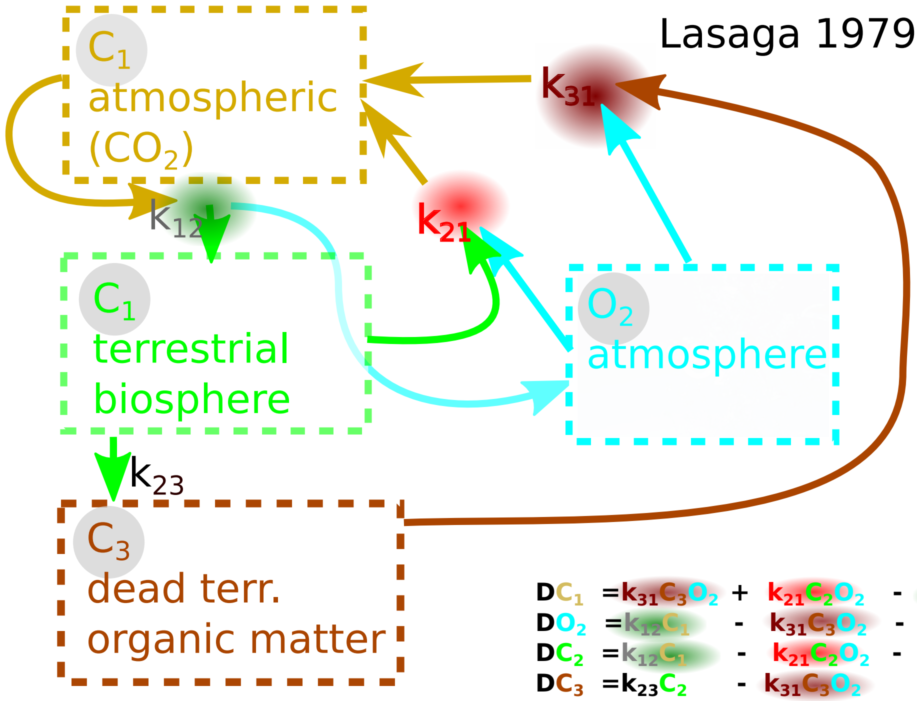
Example Model



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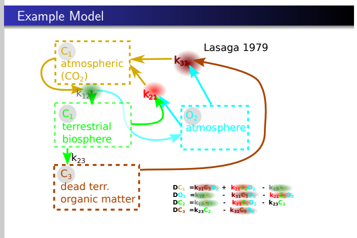

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To raise your interest we have chosen an example of an old global Carbon cycle model, that has some of the features we are interested in.

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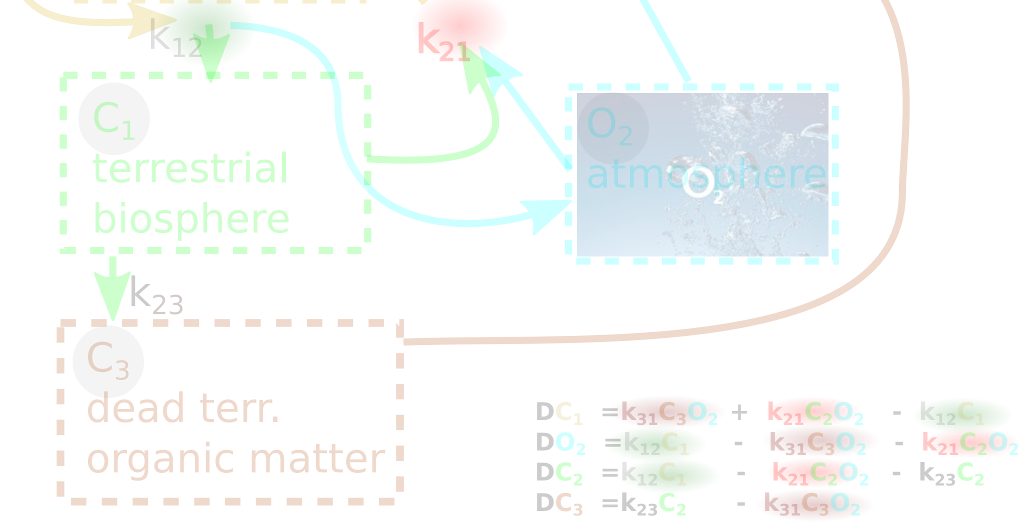
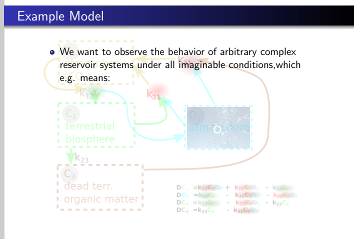


2019-08-05

Dynamic transit times and mean ages
└─Problem statement
└─Example Model



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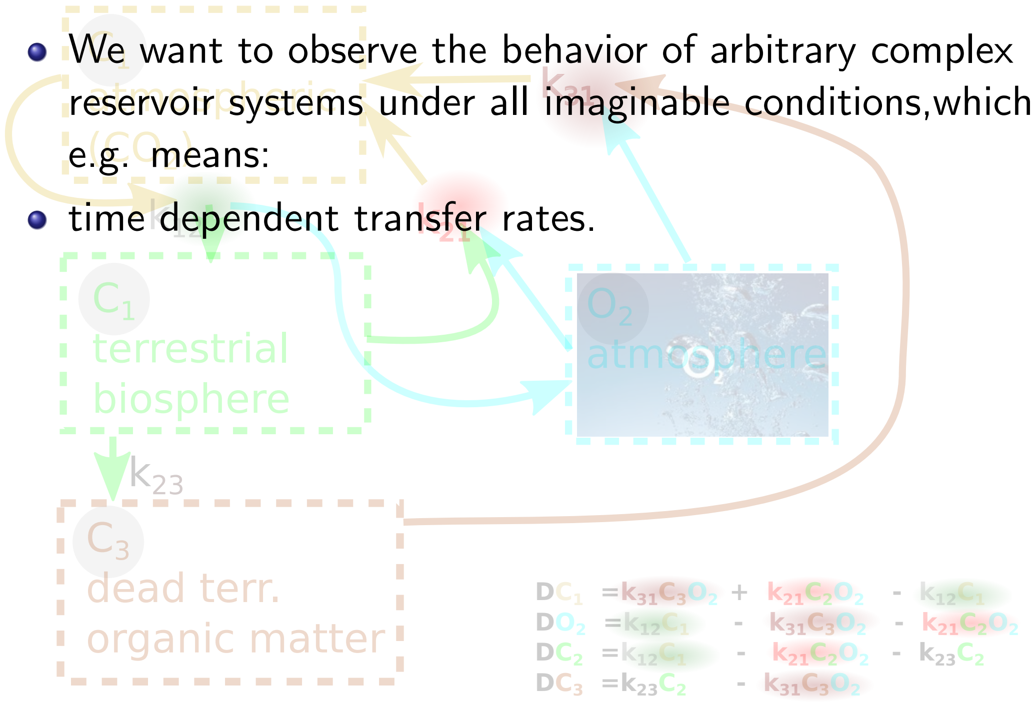

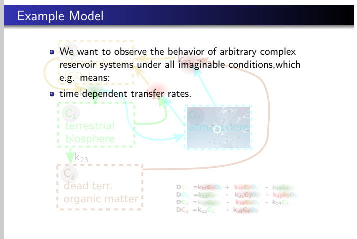

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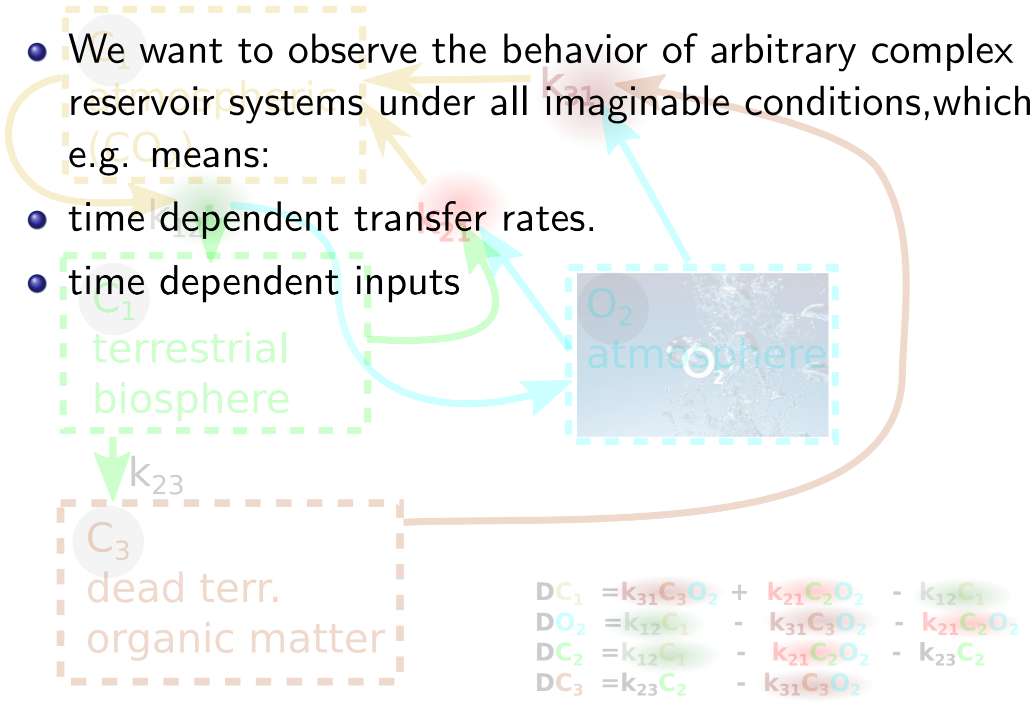

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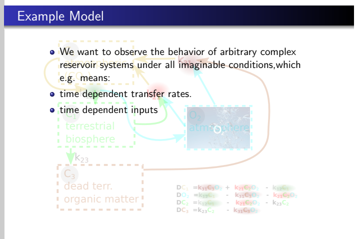

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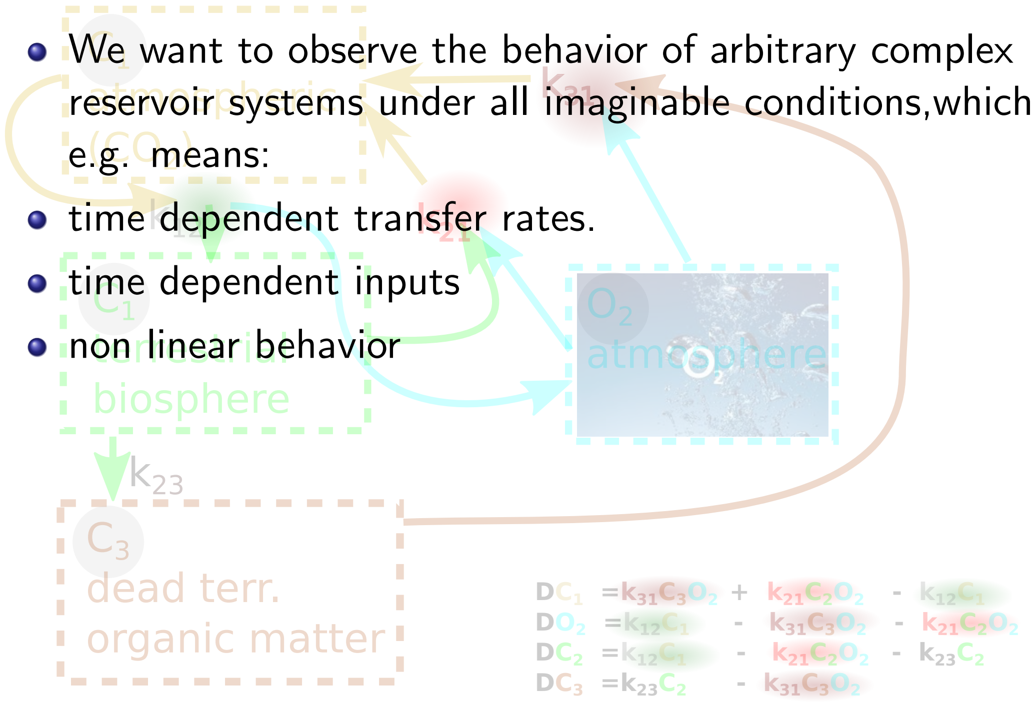

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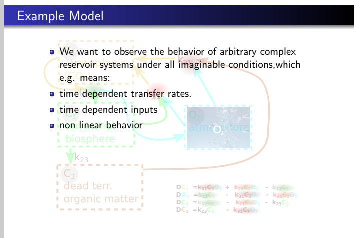

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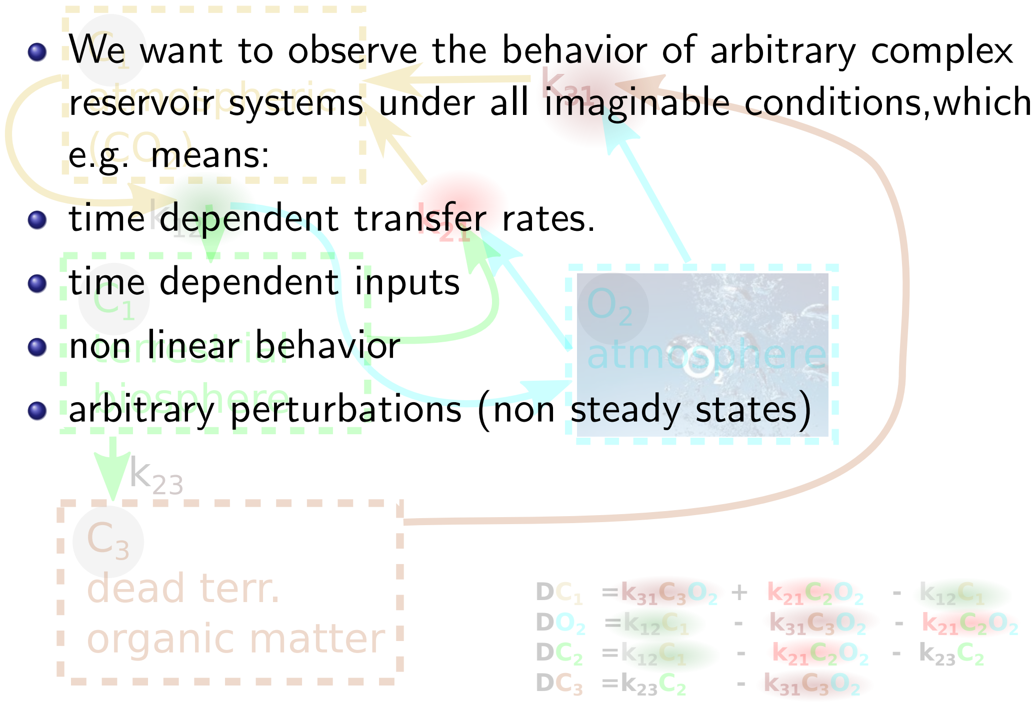

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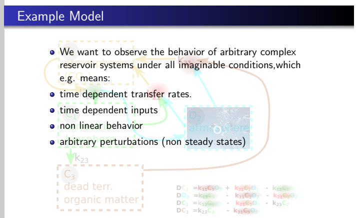

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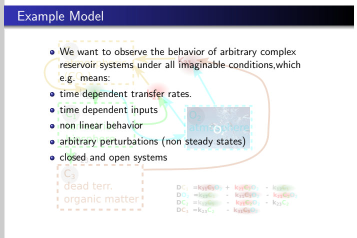

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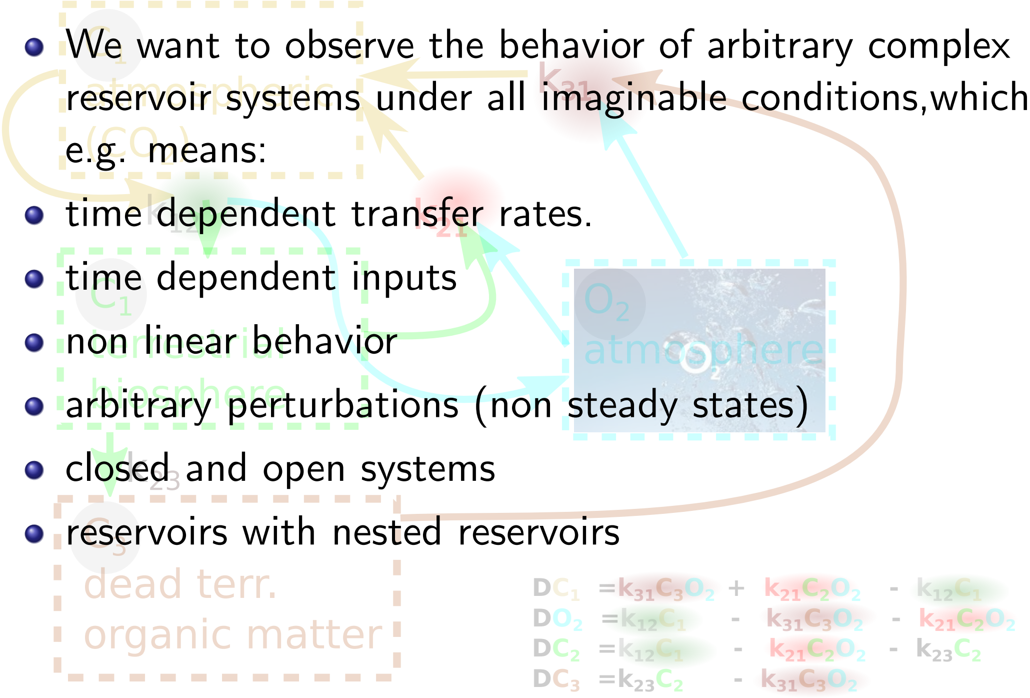

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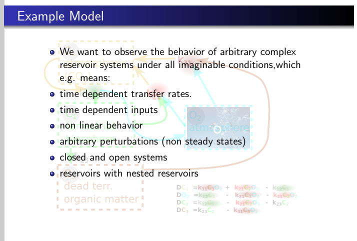

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  $\rightarrow$ motivation for a numerical counterpart where all the assumptions (if any) should be intuitive and obvious.

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Assume that we want to run a particle simulation, that we want to "observe" So all features used should be observable in the real world too. To formulate the problem in a numerical way we need to define the basic concepts precisely and in a way that a computer would understand. This means that we should avoid infinities. While the definitions are clear in some cases, there are subtle differences in details that may change the interpretations considerably.

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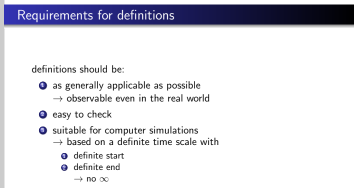
   $\rightarrow$ no ∞



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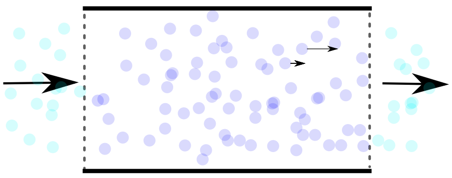
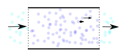
The general concept of a reservoir



1. In and out "flows" must be unambiguously defined

The general concept of a reservoir



1. In and out "flows" must be unambiguously defined

Imagine a reservoir of particles with an input and an output channel. Particles will enter the system through some input channel, will stay there for a while and eventually leave the system through an output stream. Here Only the dark blue particles are "in" the reservoir.

The general concept of a reservoir

1. In and out "flows" must be unambiguously defined
2. "Flows" do not necessarily involve "movement"
   In and out flow "channels" do not always have to be defined physically or spatially

The general concept of a reservoir
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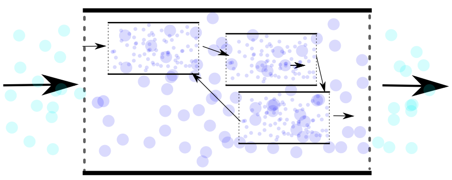
Although the concept of a reservoir is usually intuitively attached to some kind of a pool with fluid moving trough it the idea is more general.
An example that shows how generally this idea can be applied is the human population of the world. A particle here refers to a human being that is born, lives and dies.

The inflow and outflow boundaries are not spatially defined in this case

The general concept of a reservoir



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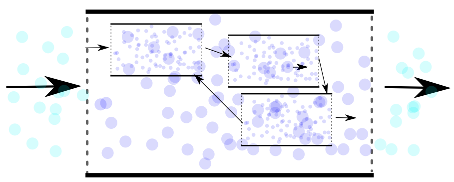

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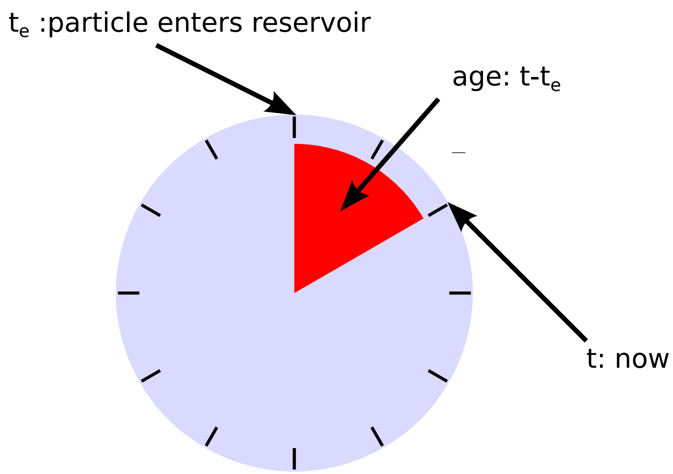
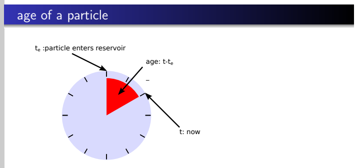
4. reservoirs can be mixed or not

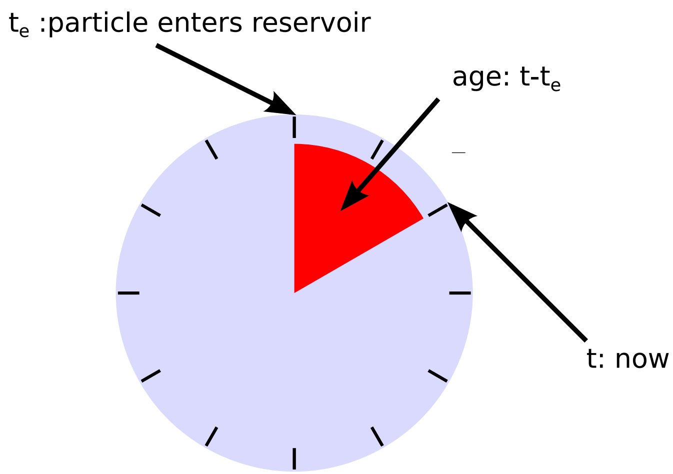
age of a particle





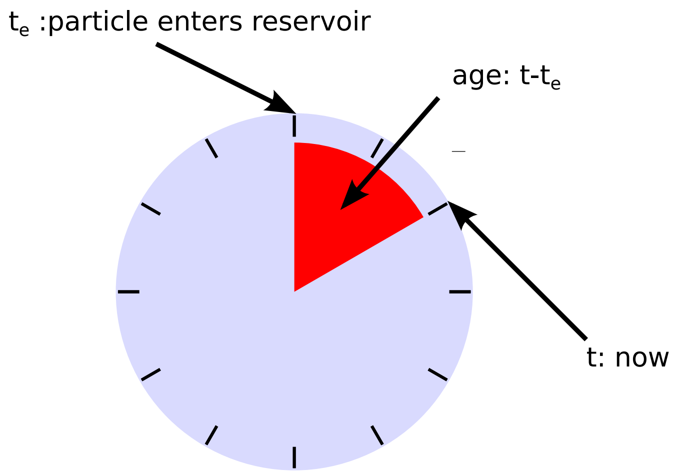
We can define the age of a particle with respect to the reservoir as the time it has spent in it. In the case of the human population this refers to the age in common sense. But in general the age refers not to the time of creation but to the time the reservoir was entered. If the reservoir in question 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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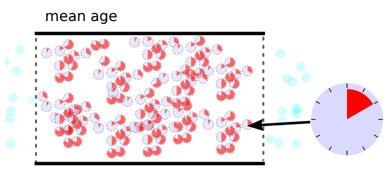
Mean age

- 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.

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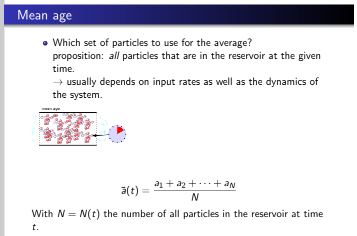
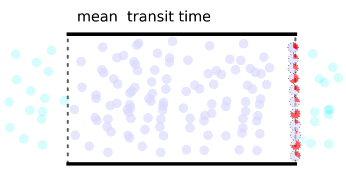
Dynamic transit times and mean ages



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

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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- 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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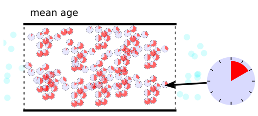
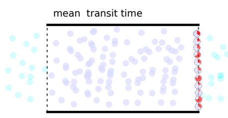
Differences between mean age and mean transit time





- 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 particle and compute the average of their ages.

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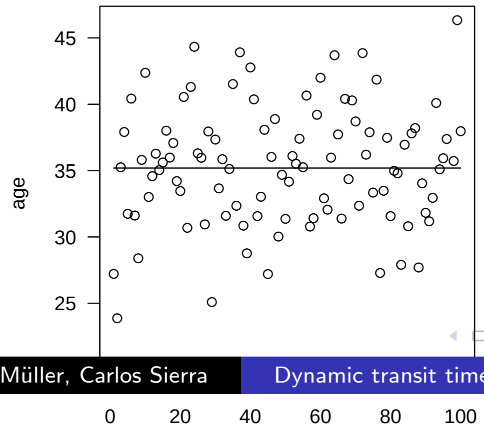

Iteration over all ages

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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Iteration over all ages

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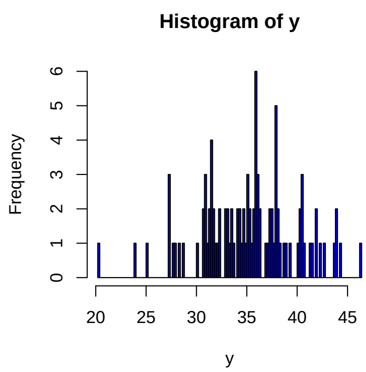
3. iterate over all ages and compute their weighted average

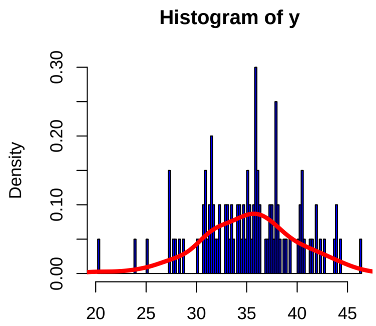
$$\bar{t}_r(t) = \frac{a_1 n_{a_1} + a_2 n_{a_2} + \cdots + a_n n_{a_n}}{n_o}$$

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



Integration over a density

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



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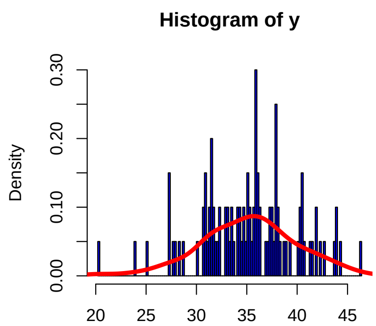
Same procedure for age density

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



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Dynamic transit times and mean ages

Computation of the mean age, overview

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3. use the solution to transform it to a linear uncoupled system with exactly the same solution
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

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

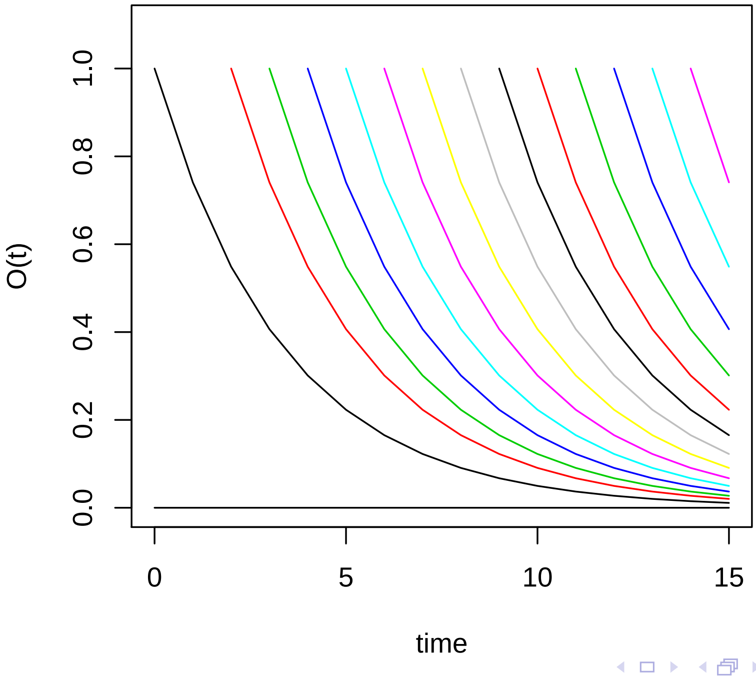
Transforming the system II

For every component F_i do:

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

Now the equations are uncoupled and linear.

Accumulating previous inputs



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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): $\dot{O}(C, t) = -kC(t)$
- wanted: $C(t), \phi(t), \psi(t), \bar{t}_r, \bar{a}$

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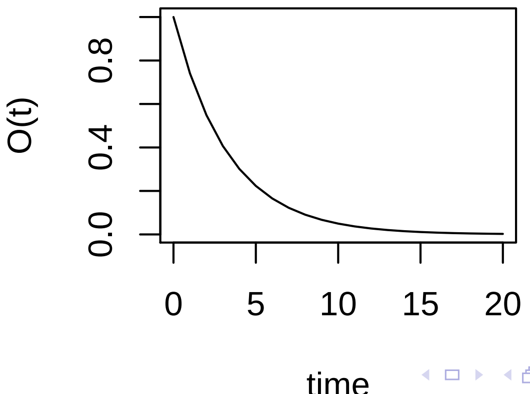
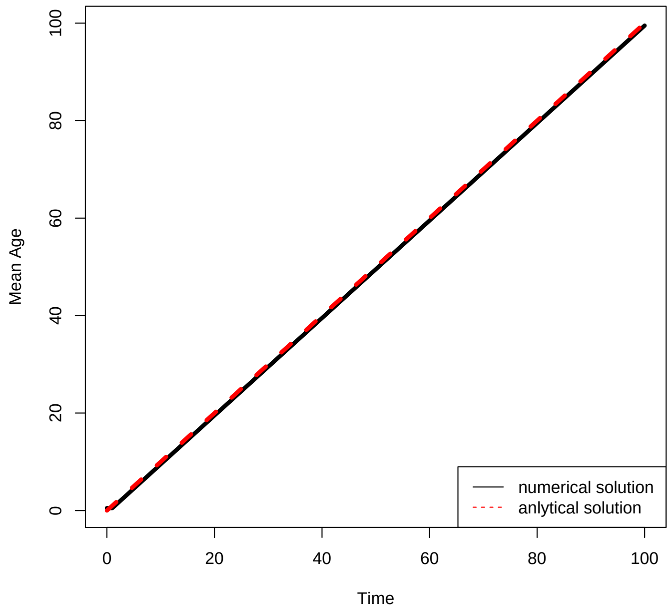
- solution:
  - $C(t) = C_0 e^{-kt}$



Intuitive solution for the example



Theory for the example

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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\begin{aligned}
O(t) &= \int_0^\infty \psi(T) I(t-T) dT \\
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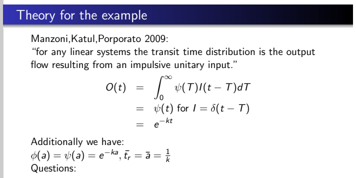

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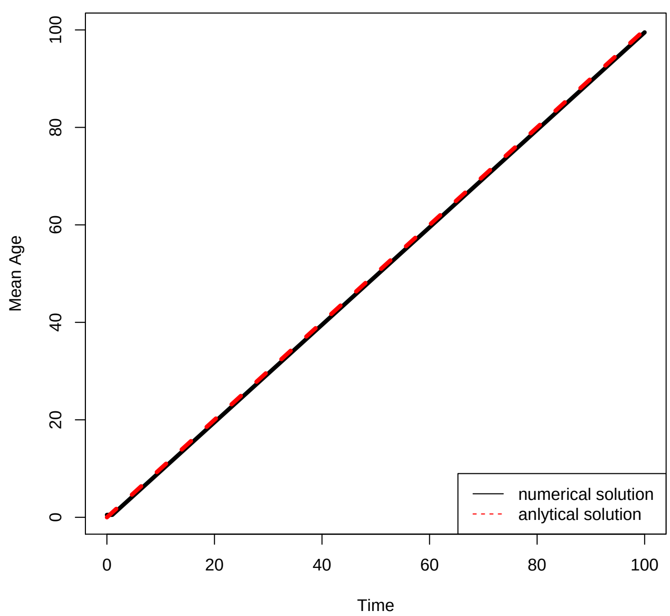

Conceptual example II

- Input(rate): constant $I_0 = C_0 k$
- Output(rate): $\dot{O}(C, t) = -kC(t)$
- wanted: $C(t), \phi(t), \psi(t), \bar{t}_r, \bar{a}$

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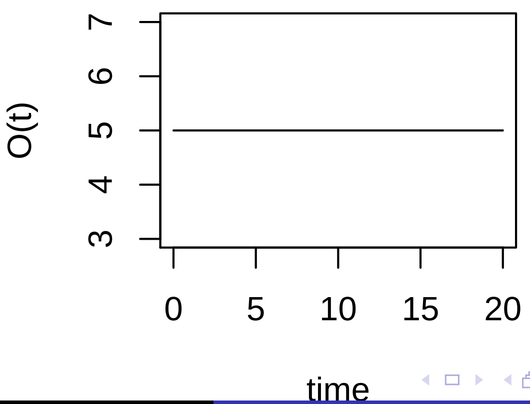
- solution:
  - $C(t) = C_0$



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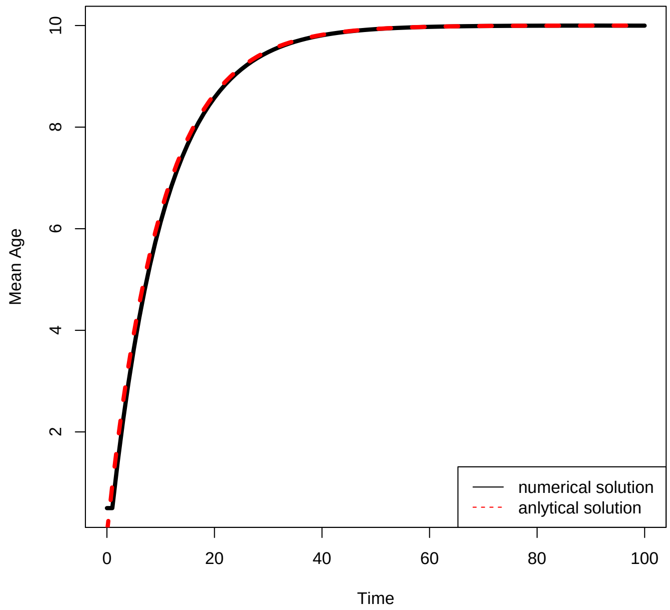
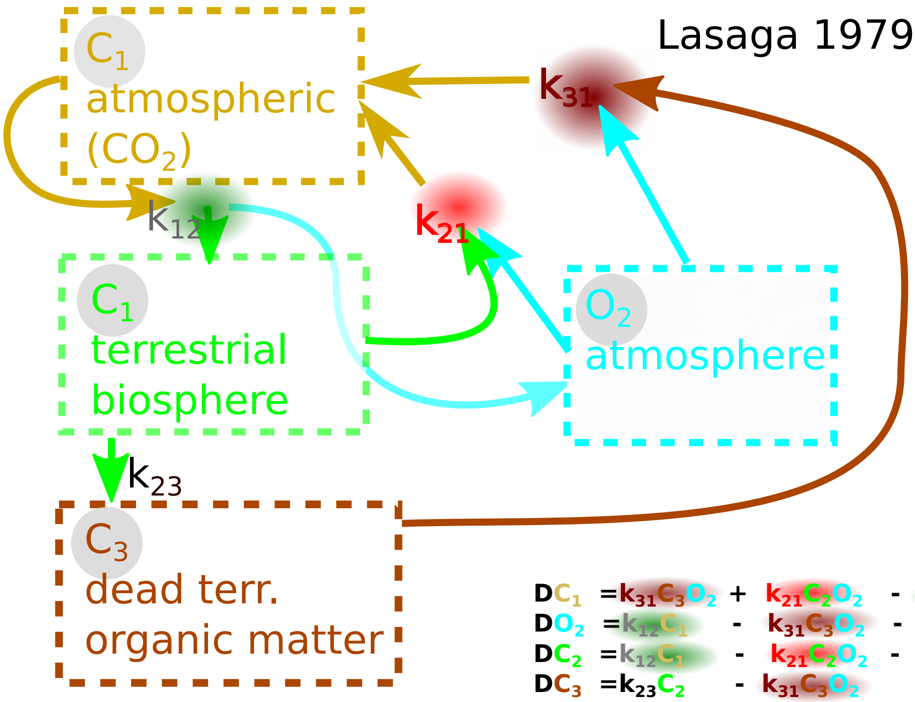
Intuitive Solution to the Example in steady state



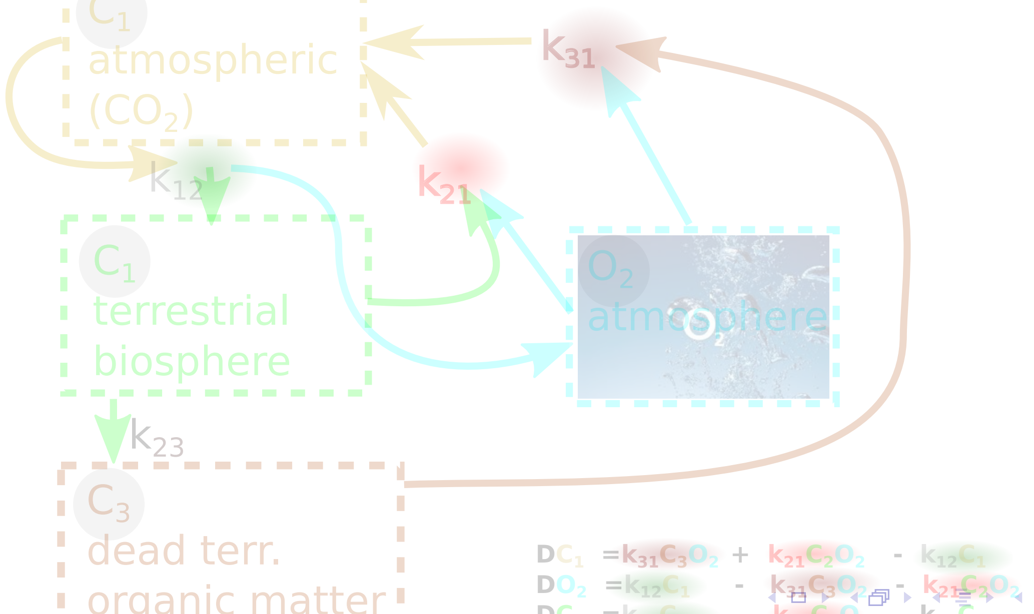
Example Model



$$
\begin{aligned}
DC_1 &= k_{31} C_3 O_2 + k_{21} C_2 O_2 - k_{12} C_1 \\
DO_2 &= k_{12} C_1 - k_{31} C_3 O_2 - k_{21} C_2 O_2 \\
DC_2 &= k_{12} C_1 - k_{21} C_2 O_2 - k_{23} C_2 \\
DC_3 &= k_{23} C_2 - k_{31} C_3 O_2
\end{aligned}
$$

Didactical Considerations

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



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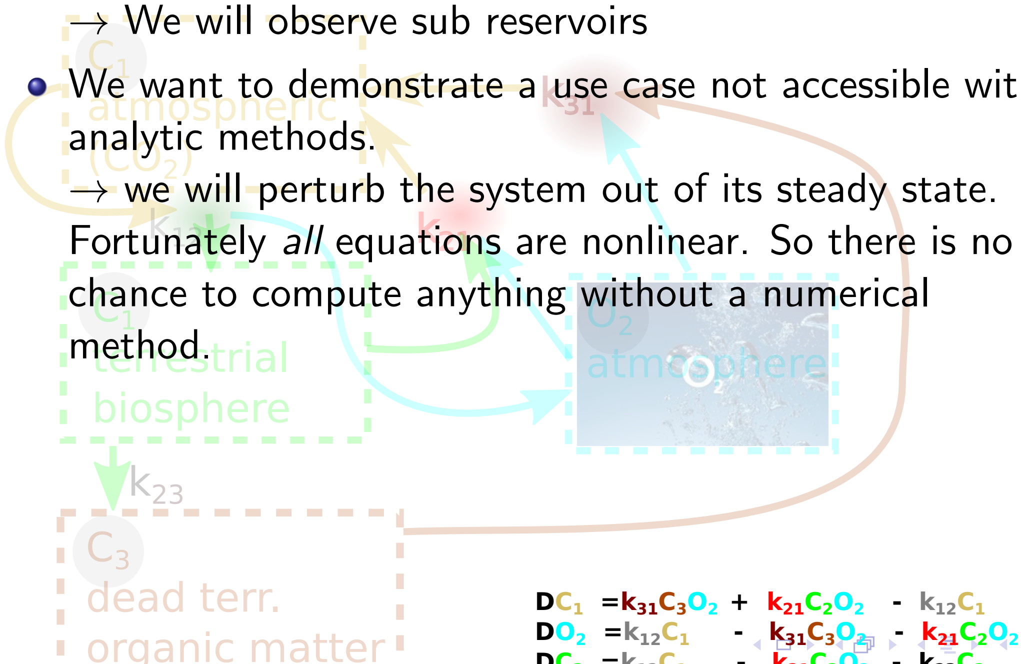
  Fortunately *all* equations are nonlinear. So there is no chance to compute anything without a numerical method.



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- We want to demonstrate a use case not accessible with analytic methods.
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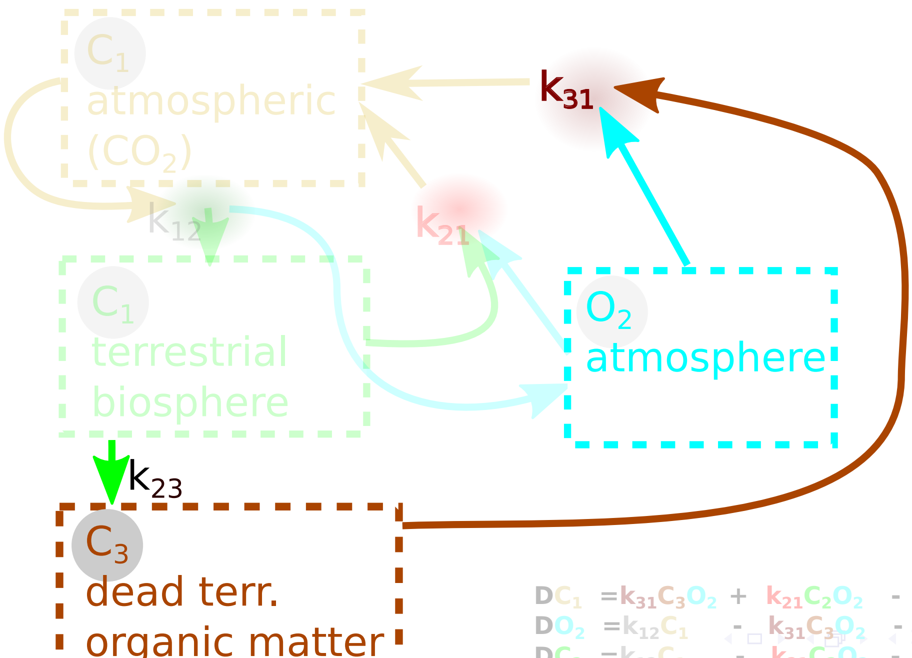
  Fortunately *all* equations are nonlinear. So there is no chance to compute anything without a numerical method.
- We do not want to complicate matters unnecessarily.
  → We will go for the simplest equation.
  → observe the last pool.

Didactical Considerations



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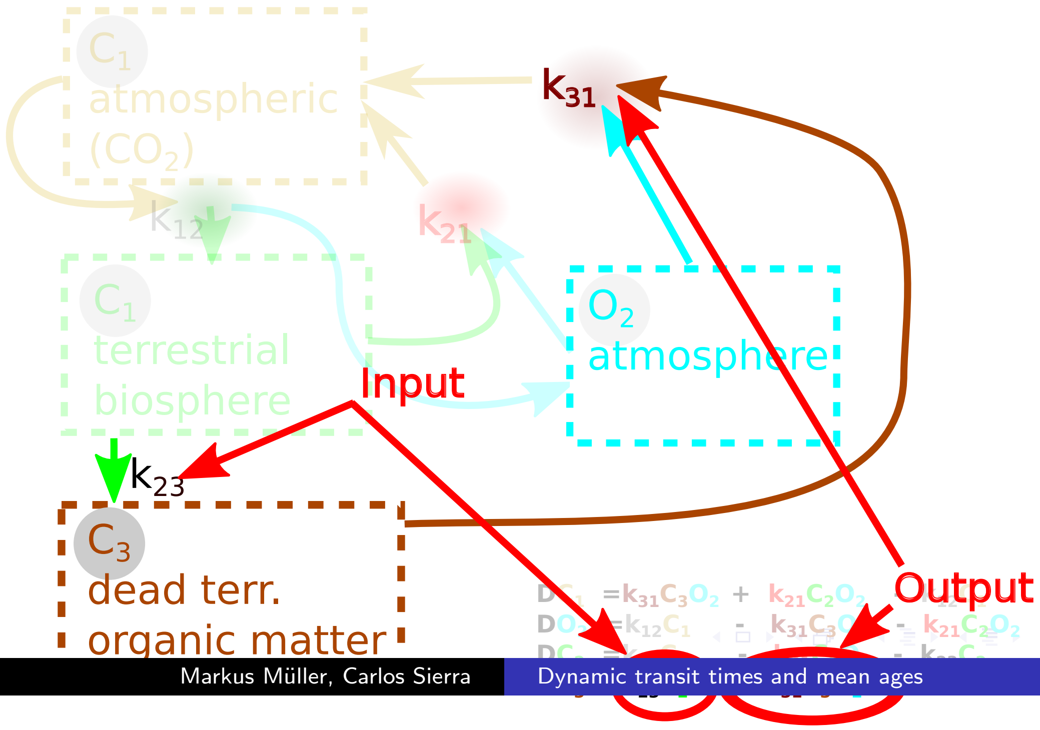
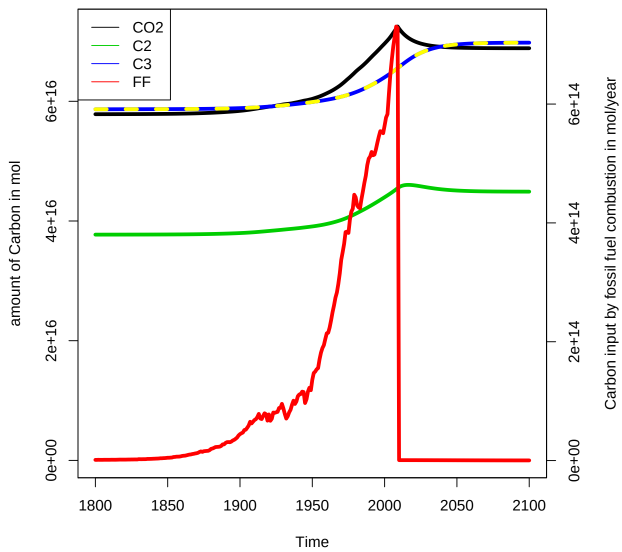
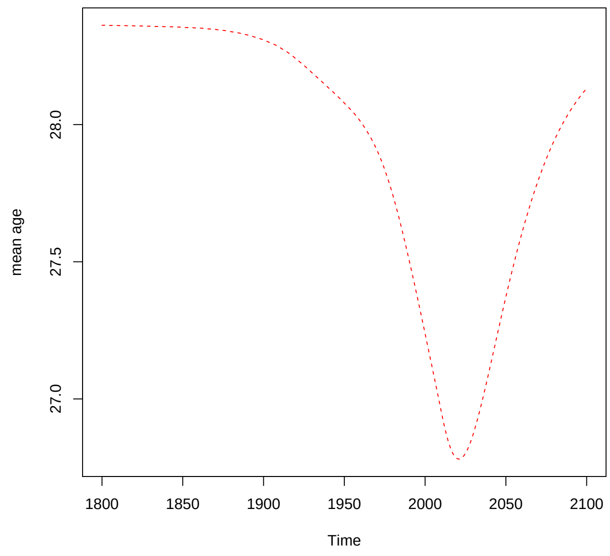


Solution



Mean age as function of time



Conclusions and outlook

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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