

Age structure of well-mixed compartmental systems

Department Biogeochemical Processes

Overview

We find general formulas for the transit time and age distributions in well-mixed compartmental systems. As an example we consider a simple three-pool global carbon model with nonlinearities in two different scenarios:

- steady state** pre-industrial system before 1765
- perturbed** adding fossil fuels to the atmosphere, considering land use change, 1765-2500

Main quantities of interest

- transit time** time that a particle needs 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

Mathematical description

Well-mixed compartmental systems can be described by a system of generally **nonlinear** ordinary differential equations of the form

$$\frac{d}{dt} \mathbf{x}(t) = \mathbf{A}(\mathbf{x}(t), t) \mathbf{x}(t) + \mathbf{u}(t), \quad t > t_0, \quad (1)$$

with a given initial value \mathbf{x}_0 .

Reduction to linear nonautonomous systems

We assume to know (at least numerically) the unique solution of (1) and denote it by \mathbf{x} . We then plug it into $\mathbf{A}(\mathbf{x}, t)$ and obtain the **linear** system of ordinary differential equations.

$$\frac{d}{dt} \mathbf{x}(t) = \mathbf{A}(t) \mathbf{x}(t) + \mathbf{u}(t), \quad t > t_0$$

This equation has the general solution formula

$$\mathbf{x}(t) = \underbrace{\Phi(t, t_0) \mathbf{x}_0}_{\text{age}(t)=t-t_0+\text{initial age}} + \int_{t_0}^t \underbrace{\Phi(t, \tau) \mathbf{u}(\tau) d\tau}_{\text{age}(t)=t-\tau},$$

where Φ is the so-called state transition matrix. This leads immediately to the **vector of age densities**

$$\rho(a, t) = \begin{cases} \Phi(t, t_0) \rho_0(a - (t - t_0)), & a \geq t - t_0, \\ \Phi(t, t - a) \mathbf{u}(t - a), & a < t - t_0, \end{cases}$$

where ρ_0 is the initial age distribution.

Pre-industrial (<1765), system in steady state

Transit time density

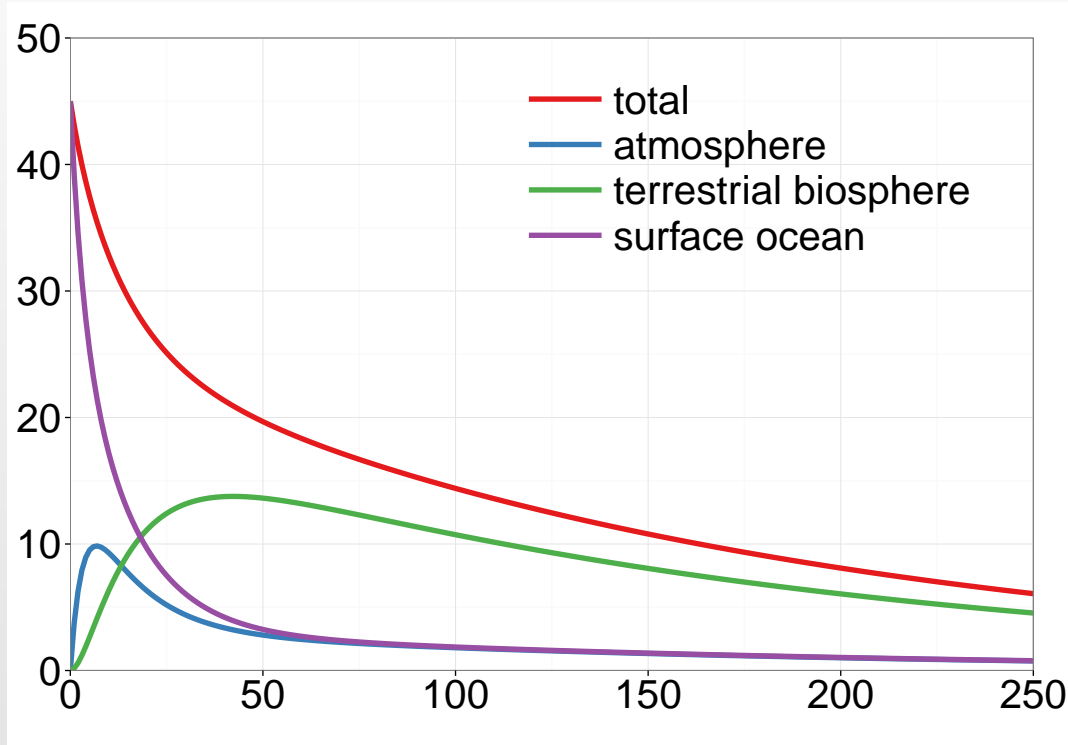
$$p_T(t) = \mathbf{z}^T e^{t\mathbf{A}} \mathbf{u}$$

System age density

$$p_A(a) = \sum_j (e^{a\mathbf{A}} \mathbf{u})_j$$

Compartmental age density

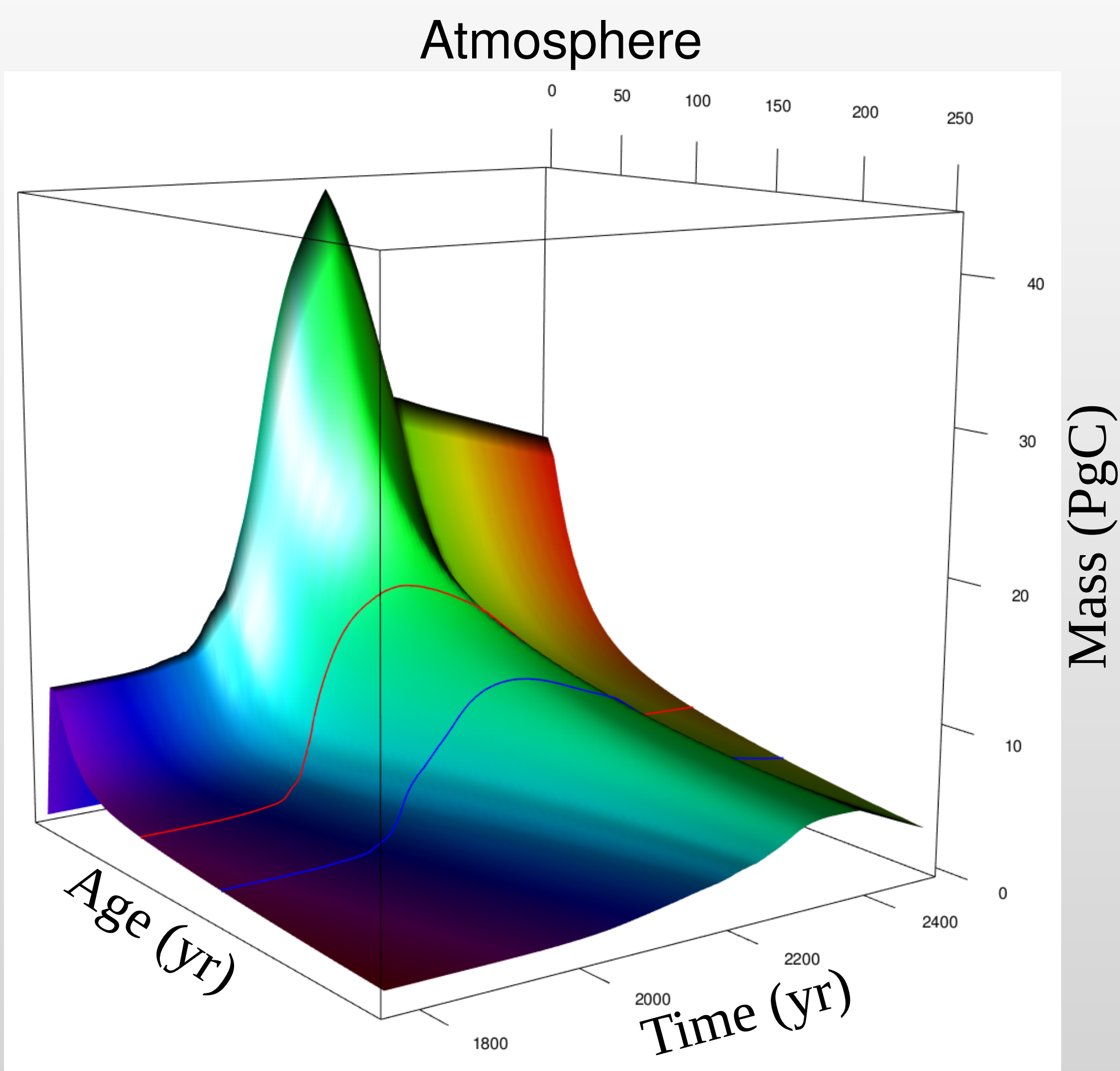
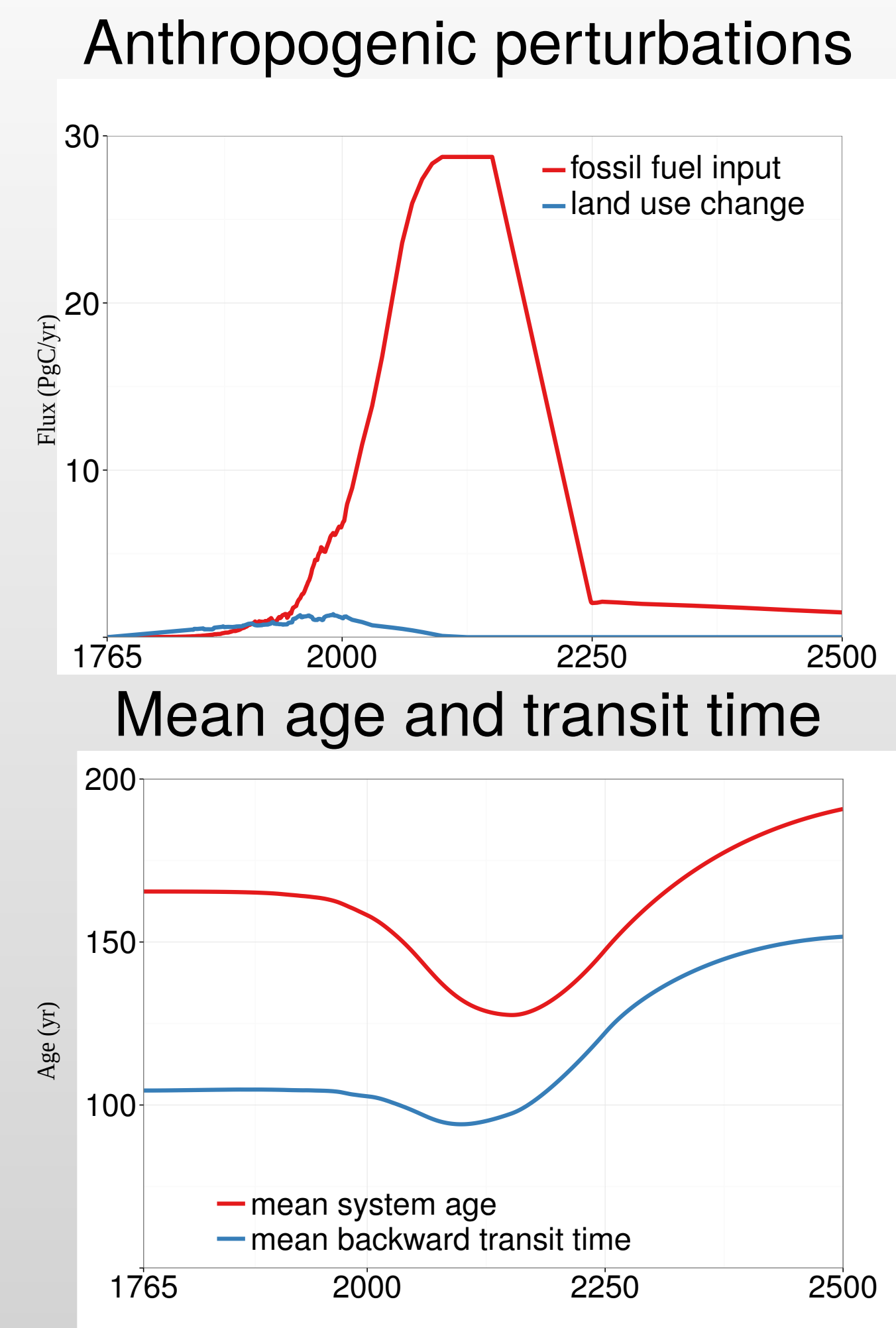
$$p_j(a) = (e^{a\mathbf{A}} \mathbf{u})_j$$



State transition matrix

- one-dimensional $\Phi(t, t_0) = \exp[(t - t_0)A(t)]$ exponential function
- multi-dimensional, $\Phi(t, t_0) = \exp[(t - t_0)A(t)]$ matrix exponential
- autonomous
- multi-dimensional, $\frac{d}{dt} \Phi(t, t_0) = A\Phi(t, t_0)$ only numerical solution
- nonautonomous

Perturbed (1765-2500)



Transit time

If we define the (backward) transit time of a particle as the age of the particle at the time when it exits the system, we can easily derive explicit formulas for its distribution from the age distribution. The simple approach stock/flux for the transit time is valid only for a system in steady state. **Out of steady state, stock(t)/flux(t) cannot be interpreted as a transit time.**

Evolution

Year	Author	System	Quantity	Geometric structure	Example
1983	Anderson	steady state	mean	point	
2009	Manzoni et al.	steady state (simple structure)	density	curve over age	
2016	Rasmussen et al.	linear time dependent	mean	curve over time	
2016	Metzler & Sierra	steady state (all structures)	density	curve over age	
2017	Metzler et al.	linear/nonlinear time dependent	density	surface over age and time	

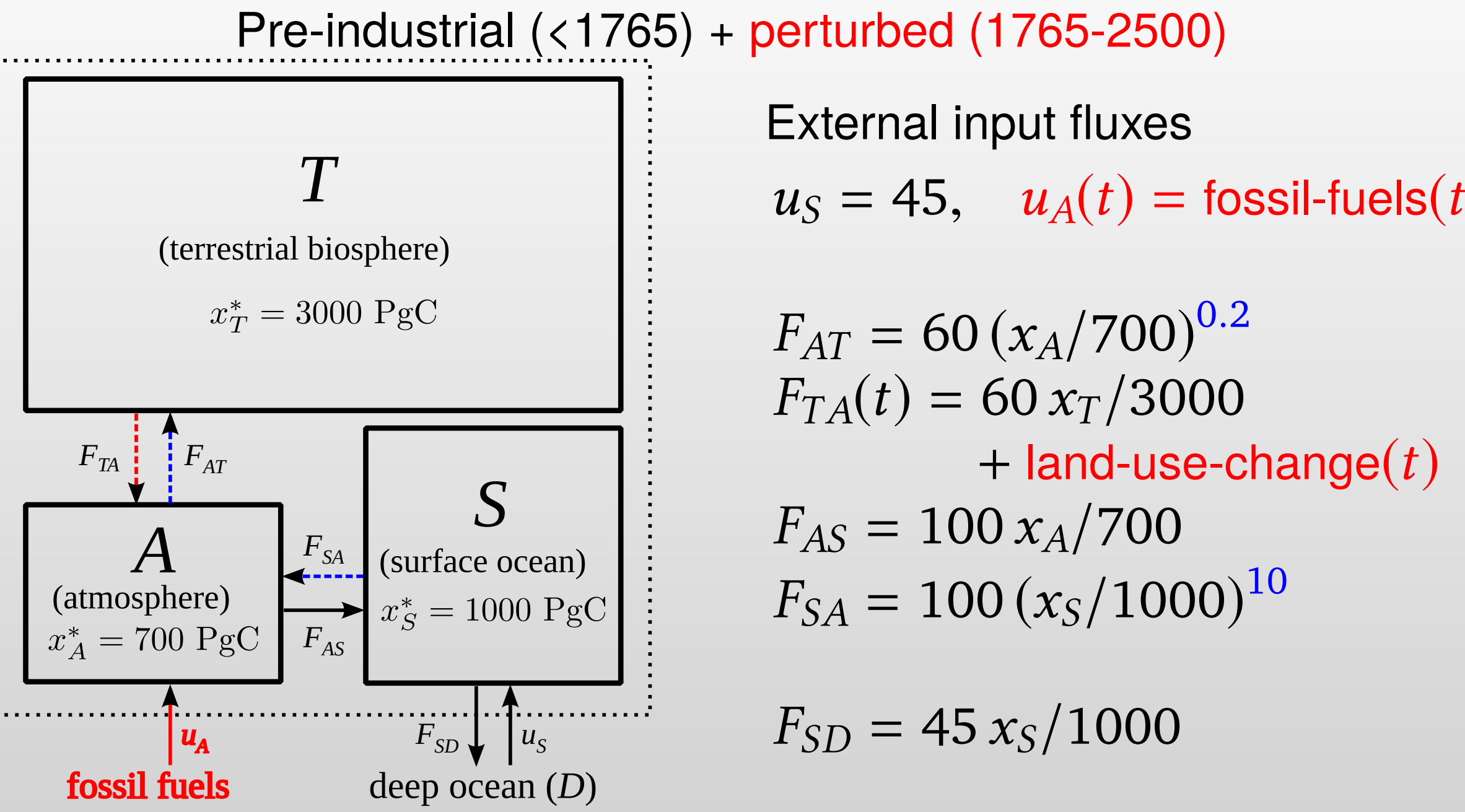
increasing information

Classification

- $\mathbf{A}(\mathbf{x}(t), t)$ nonlinear,
- $\mathbf{A}(\mathbf{x}(t)), \mathbf{u}(t)$ nonautonomous
- $\mathbf{A}(\mathbf{x}(t)), \mathbf{u}$ nonlinear, autonomous
- $\mathbf{A}(t), \mathbf{u}$ linear,
- $\mathbf{A}, \mathbf{u}(t)$ nonautonomous
- $\mathbf{A}(t), \mathbf{u}(t)$
- \mathbf{A}, \mathbf{u} linear, autonomous

- $\mathbf{x}(t)$ vector of compartment content (e.g. C) at time t
- \mathbf{A} compartmental matrix, describes fluxes between compartments
- $\mathbf{z}(t)$ external outflux vector at time t
- $\mathbf{u}(t)$ external input vector at time t

Model

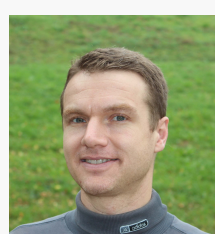


Bibliography

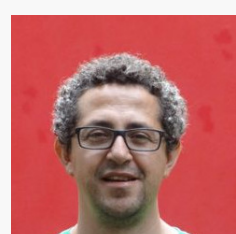
- Anderson DH (1983) Compartmental modeling and tracer kinetics, vol 50. Springer Science & Business Media
- Manzoni S, Katul GG, Porporato A (2009) Analysis of soil carbon transit times and age distributions using network theories. Journal of Geophysical Research 114(G4):1–14, DOI10.1029/2009JG001070
- Metzler H, Mäijller M, Sierra CA Age and transit time distributions of well-mixed compartmental systems, PNAS
- Metzler H, Sierra CA (2016, in review) Linear autonomous compartmental models as continuous-time Markov chains: transit time and system age distributions
- Rasmussen M, Hastings A, Smith MJ, Agosto FB, Chen-Charpentier BM, Hoffman FM, Jiang J, Todd-Brown KEO, Wang Y, Wang YP, Luo Y (2016) Transit times and mean ages for nonautonomous and autonomous compartmental systems. J Math Biol



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