Computation of transport timescales to support water quality and ecological diagnosis, simple modeling, and aquatic resource management
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Diagnostic timescales in fluid flows: from partial differential equations to simple models

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Diagnostic timescales: what are they good for?

• Nowadays numerical models of geophysical and environmental flows routinely produce **huge output files**. **Making sense** of all these real numbers (i.e. identifying **key processes** and establishing **causal relationships** between them) is no trivial task.

• Analysing **primitive variables** (velocity, pressure, temperature, concentrations, etc.) is not always conducive to the most fruitful interpretations. Examining **auxiliary variables** introduced for diagnostic purposes is an option worth considering.

• **Diagnostic timescales** (e.g., age, residence/exposure time, etc.) may help build **simple models** aimed at **understanding** the results of **complex ones** (dimension reduction).

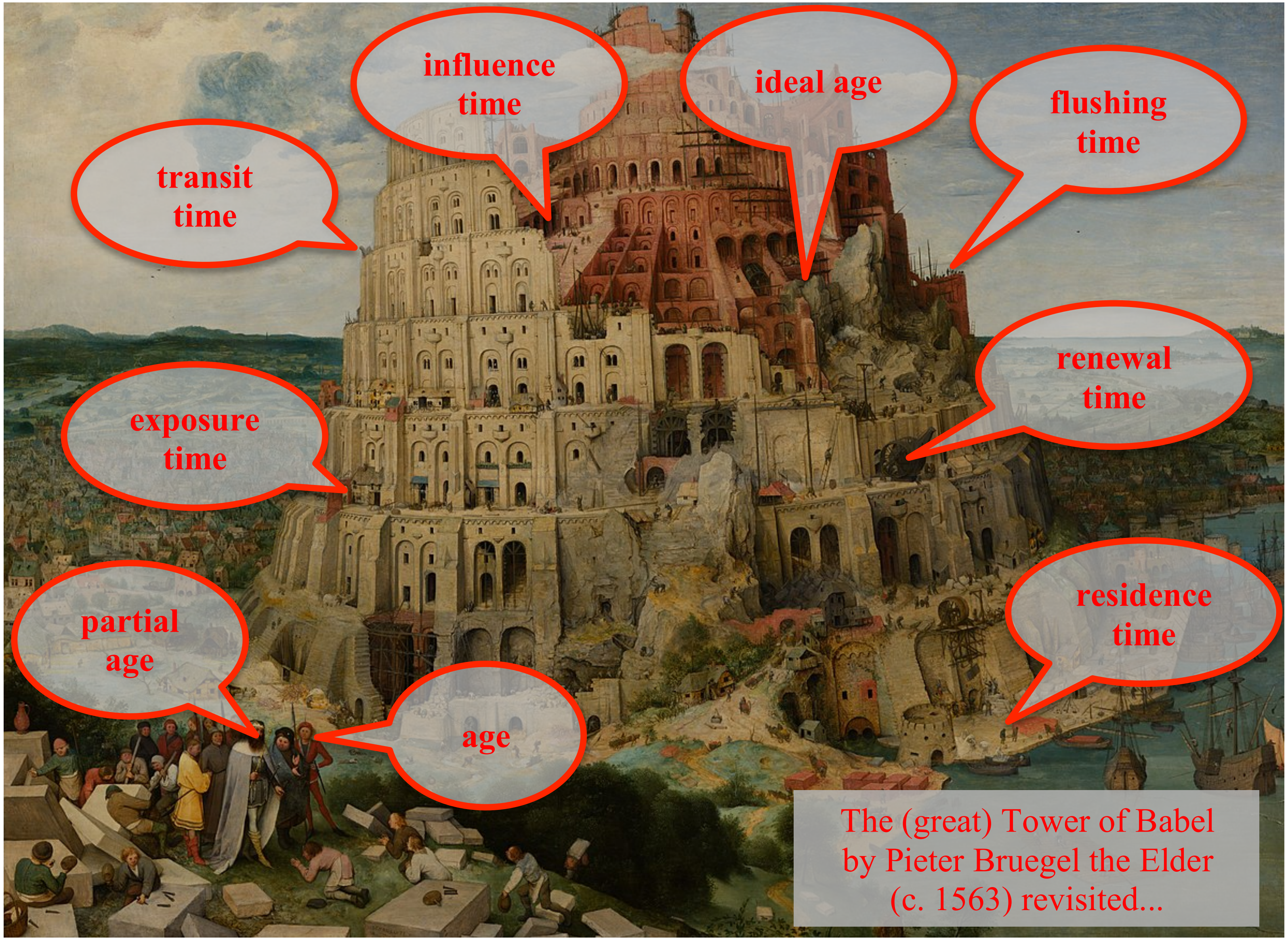
A wise piece of advice to begin with

- In their **seminal article** on diagnostic timescales, Bolin and Rodhe (*Tellus*, 1973) stated (what should have been) the **obvious**:

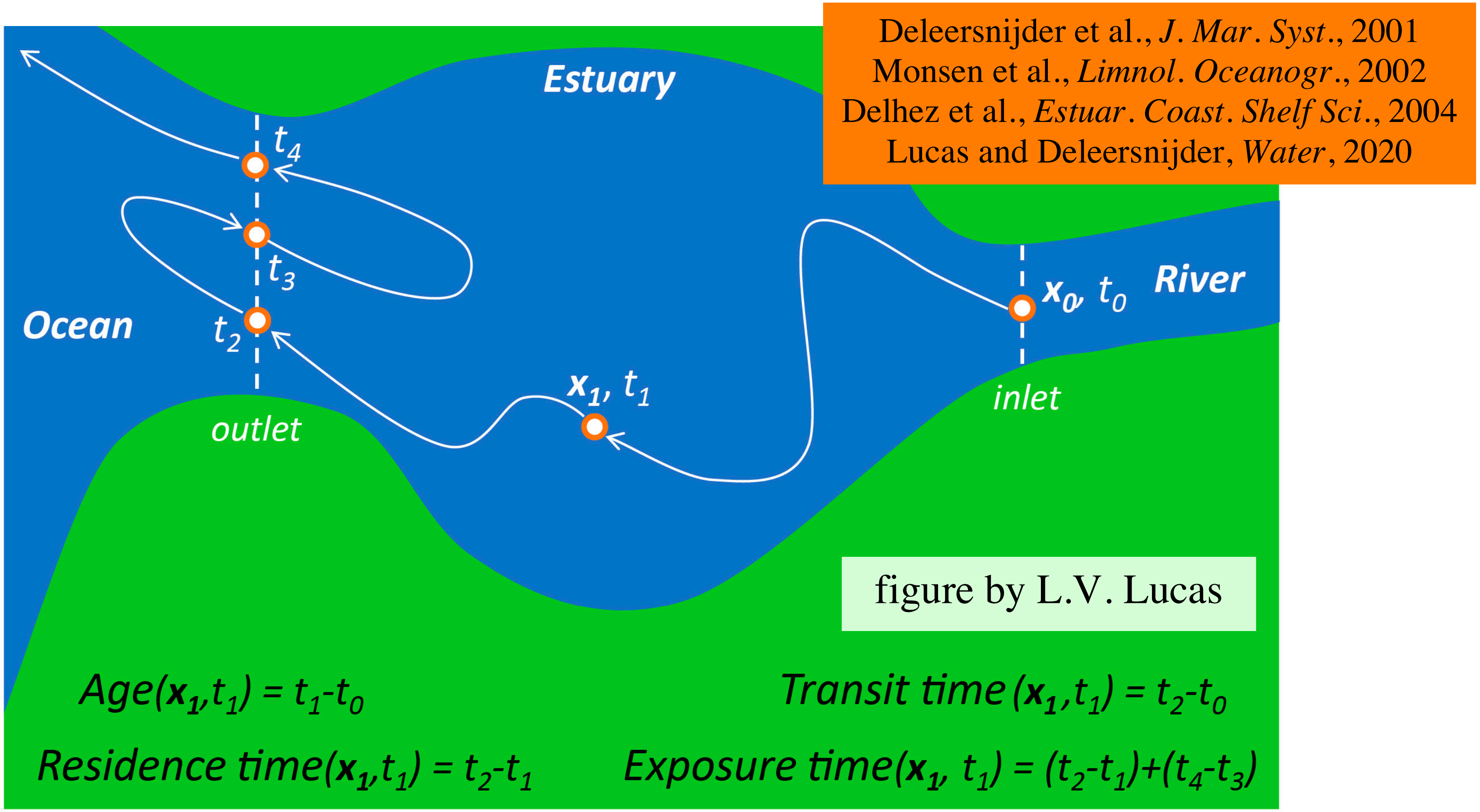
  To avoid misunderstandings and even erroneous conclusions it is important to introduce precise definitions and to use them with care.

- Surprisingly (or not), this wise piece of advice was **ignored** by many. This led to a situation half-jokingly referred to as the Tower of Babel by Viero and Defina (IAHR, 2016), i.e. a wealth of poorly defined diagnostic timescales used rather carelessly, eventually causing **misleading interpretations** and **conclusions** to be produced.

How to bring some order in this chaos?



Only two basic timescales are believed to be needed



The **age** looks into the **past**, whilst the **residence/exposure time** looks into the **future**.

Simple models for diagnosing complex ones (I)

• If **mixing** inside the domain is **much faster** than the **export processes**, which is usually the case in semi or nearly enclosed domains, then the outgoing mass flux is likely to be of the form

$$\phi^{out}(t) \approx \frac{m(t)}{\theta} \quad \Rightarrow \quad \frac{dm}{dt} \approx -\frac{m}{\theta} \quad \Rightarrow \quad m(t) = m(0)e^{-t/\theta}$$

where θ is the **domain-averaged residence time**. This idealised model is usually referred to as the **well-mixed box model** or **continuous stirred-tank reactor** (CSTR) in chemical engineering.

• Deleersnijder et al. (*Appl. Math. Lett.*, 1997) applied this concept to the **Mururoa atoll lagoon**, reproducing tracer transport results of a three-dimensional model (Tartinville et al., *Coral Reefs*, 1997) with an error of the order of 10%.

Simple models for diagnosing complex ones (II)

• The **plug flow model** is akin to a flow in a pipe with no longitudinal mixing. Therefore, the key parameter is the **transit time**, i.e., the time needed to travel from the inlet to the outlet.

• Deleersnijder et al. (*Cont. Shelf Res.*, 1998) built a simple model consisting of a **well-mixed box** and a **pipe** (plug flow) arranged in **parallel** to diagnose tracer transport results from a three-dimensional model of **Prince William Sound** (Alaska, USA) (Mooers et al., *Cont. Shelf Res.*, 1998) under different wind forcings. The discrepancies between the two models were smaller than 15%.

• These **old**, **easy-to-use** diagnostic methods are applicable only to those flows that satisfy the **key underlying assumptions**. Otherwise, a more sophisticated approach must be resorted to.

CART's age: basic variables and equations (I)

• Seawater is a mixture of constituents (freshwater, solutes, etc.). In an elemental control volume, every particle of each constituent has had a different history and, hence, has a different age. Therefore, the **histogram** of the ages has to be introduced, i.e., $c_i(t,\mathbf{x},\tau)$, the **concentration distribution function** of the "*i*" constituent (where τ is the age, as an independent variable). The corresponding **concentration** $C_i(t,\mathbf{x})$, age concentration $\alpha_i(t,\mathbf{x})$ and mean age $a_i(t,\mathbf{x})$ are (Delhez et al., *Ocean Model*., 1999):

$$C_i(t,\mathbf{x}) = \int_0^\infty c_i(t,\mathbf{x},\tau)\,d\tau \quad \bullet \quad \alpha_i(t,\mathbf{x}) = \int_0^\infty \tau c_i(t,\mathbf{x},\tau)\,d\tau$$

$$\text{age-averaging hypothesis} \quad \Rightarrow \quad a_i(t,\mathbf{x}) = \frac{\alpha_i(t,\mathbf{x})}{C_i(t,\mathbf{x})}$$

CART's age: basic variables and equations (II)

• Simple **mass budget** considerations yield

$$\frac{\partial c_i}{\partial t} = \underbrace{p_i - d_i}_{\text{source - sink}} - \nabla \bullet \underbrace{(\mathbf{u}c_i - \mathbf{K} \bullet \nabla c_i)}_{\text{advection + diffusion}} - \underbrace{\frac{\partial c_i}{\partial \tau}}_{\text{ageing}}$$

To derive this equation **no arbitrary hypothesis** has been resorted to. However, it was assumed that advective and diffusive transport proceed independently of the age of every particle of every constituent. These assumptions have not been challenged thus far.

• The equation for the distribution function is not easy to solve (e.g., Delhez and Deleersnijder, *J. Mar Syst.*, 2002) since c_i depends on 5 independent variables (time, 3 space coordinates, age). However, the mean age can be obtained without solving the above equation.

CART's age: basic variables and equations (III)

• Evaluating the **zeroth and first order moments** of the equation for the distribution function leads to equations easier to deal with:

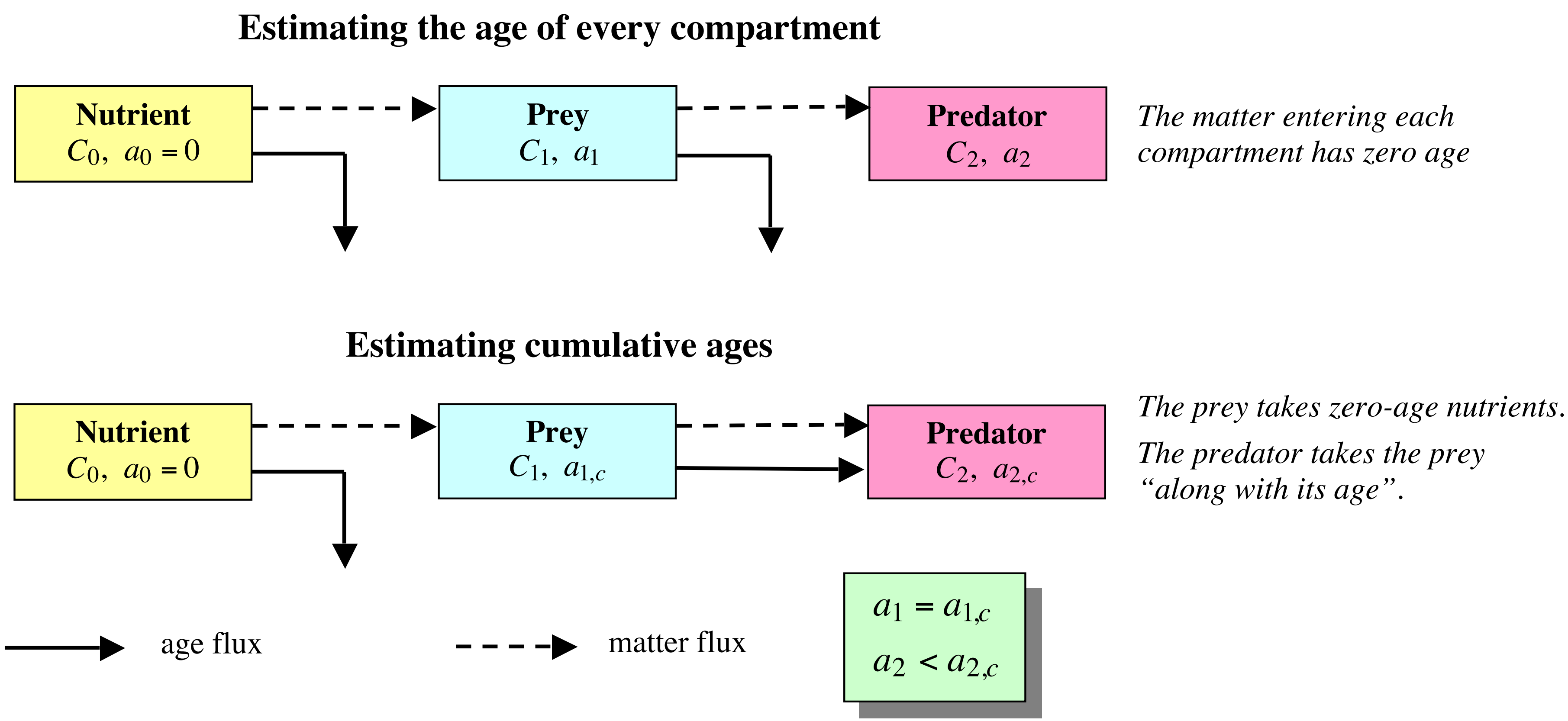
$$\int_0^\infty \left(\frac{\partial c_i}{\partial t} = \ldots \right) d\tau \quad \Rightarrow \quad \frac{\partial C_i}{\partial t} = \underbrace{P_i - D_i}_{\text{source - sink}} - \nabla \bullet \underbrace{(\mathbf{u} C_i - \mathbf{K} \bullet \nabla C_i)}_{\text{advection + diffusion}}$$

$$\int_0^\infty \left(\frac{\partial c_i}{\partial t} = \ldots \right) \tau \, d\tau \quad \Rightarrow \quad \frac{\partial \alpha_i}{\partial t} = \underbrace{C_i}_{\text{ageing}} + \underbrace{\pi_i - \delta_i}_{\text{source - sink}} - \nabla \bullet \underbrace{(\mathbf{u} \alpha_i - \mathbf{K} \bullet \nabla \alpha_i)}_{\text{advection + diffusion}}$$

• Similar equations can be derived for **groups of constituents**, including the seawater itself. The **boundary conditions** must be derived from those applying to c_i (Deleersnijder et al., *Water*, 2020).

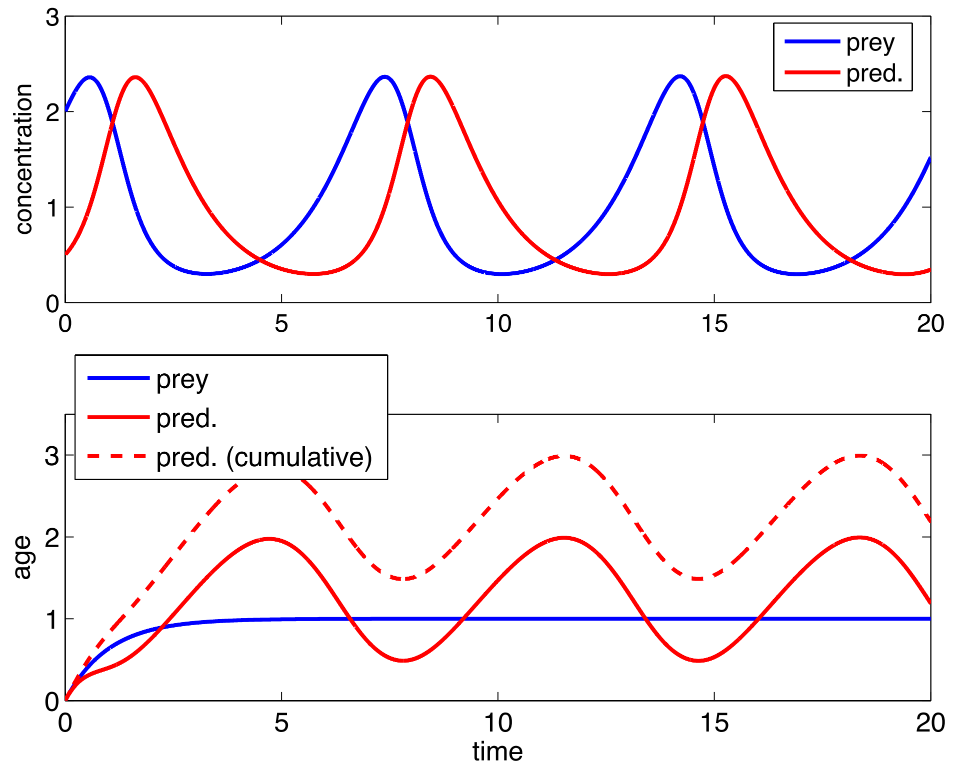
Diagnosing reactive processes (I)

- Delhez et al. (*Ocean Dyn.*, 2004) considered the simplest **prey-predator** (Lotka-Volterra) model, with two options for the age.



Diagnosing reactive processes (II)

• As is well known, the prey and predator populations exhibit periodic oscillations, but the age of the preys tends to a constant. This is because, in this model, the **predation term** is **independent of the age of the preys**. This property may be generalised to a wide class of sink terms.



• Delhez et al. (*J. Mar. Syst.*, 2003) compared the water age, the age of decaying tracers and the related radio-ages in the World Ocean, and established novel inequalities about these ages.

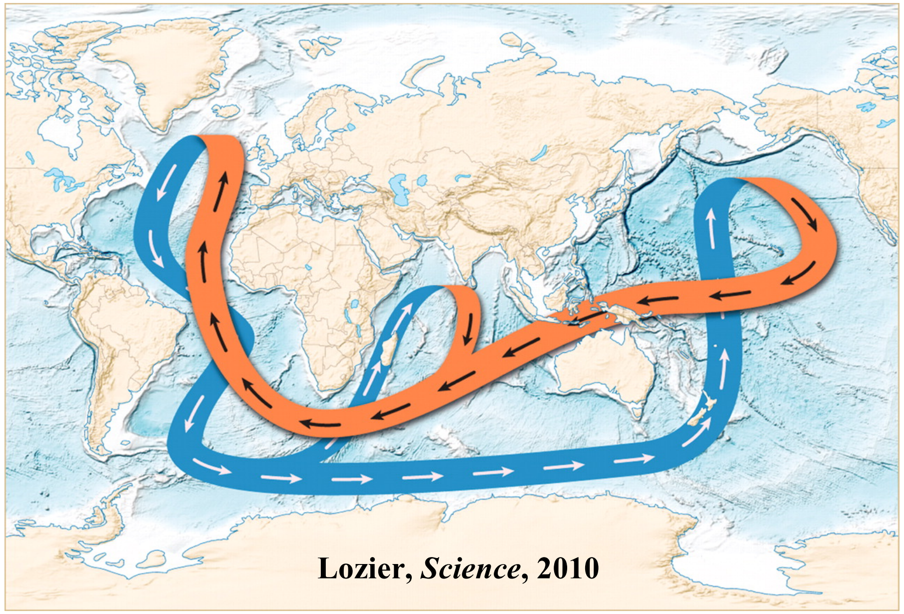
Constructing a reduced-dimension model (I)

• The flow in the **World Ocean** exhibits a **wide range** of **time** and **space scales**, i.e. 1 s to 10^3 y and 1 mm to 10^4 km. Clearly, this unsteady flow is a very complex one.

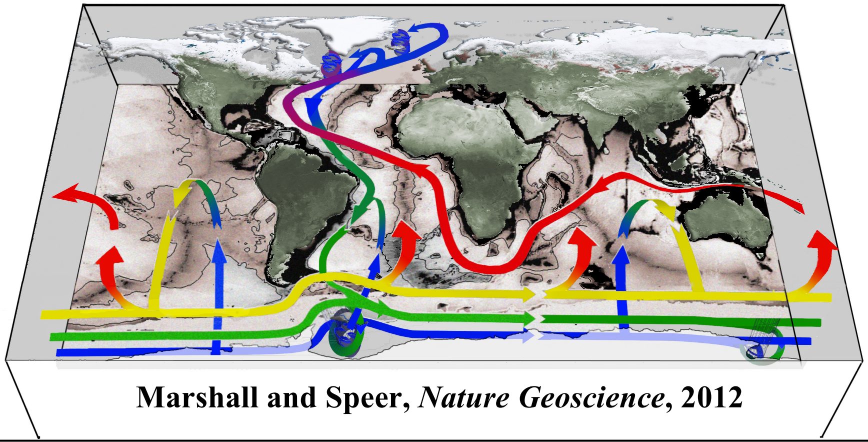
=> movie1 MITgcm results

• Many simple, **qualitative** representations of this flow exist, focusing on the **largest scales**, which are believed to be the most relevant in Earth climate studies. Is it possible to produce a **simple** and, yet, **quantitative** model?

Schematic representations of the 3D World Ocean circulation at the largest scales



Lozier, *Science*, 2010



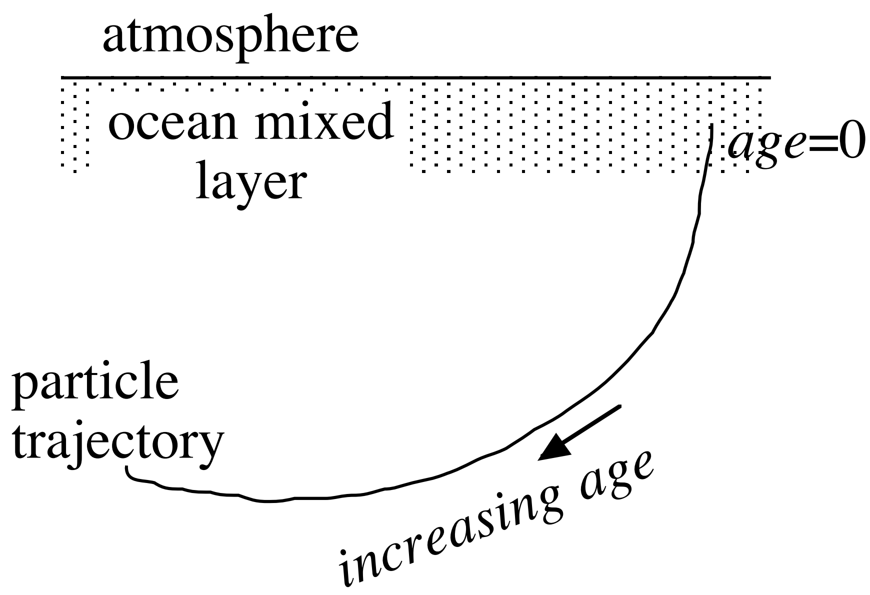
Marshall and Speer, *Nature Geoscience*, 2012

Constructing a reduced-dimension model (II)

At the largest scales, the World Ocean circulation "can be thought of as a **gradual renewal** or **ventilation** of the deep ocean by water that was once at the sea surface" (England, *Journal of Physical Oceanography*, 1995)

Therefore, the **age**, a measure of the **time since leaving the ocean upper mixed layer**, is a popular diagnostic tool in the World Ocean.

estimating ocean ventilation rate



age = time elapsed since leaving surface mixed layer

Constructing a reduced-dimension model (III)

- At a steady state, the **water age distribution** $c(\mathbf{x},\tau)$ is satisfies

$$\frac{\partial c}{\partial \tau} = -\nabla \bullet (\mathbf{u}c - \mathbf{K} \bullet \nabla c)\,,\ \left[c(\mathbf{x},\tau)\right]_{\Gamma} = \delta(\tau - 0)\,,\ \left[c(\mathbf{x},0)\right]_{\Omega} = 0$$

with $\tau =$ the age, $\Gamma =$ the ocean surface and $\Omega =$ the ocean interior.

- **Global water age distribution** $\mu(\tau)$: the volume of the water whose age lies in the interval $[\tau, \tau + \Delta\tau]$ $(\Delta\tau \to 0)$ is $\Omega\mu(\tau)\Delta\tau$, with

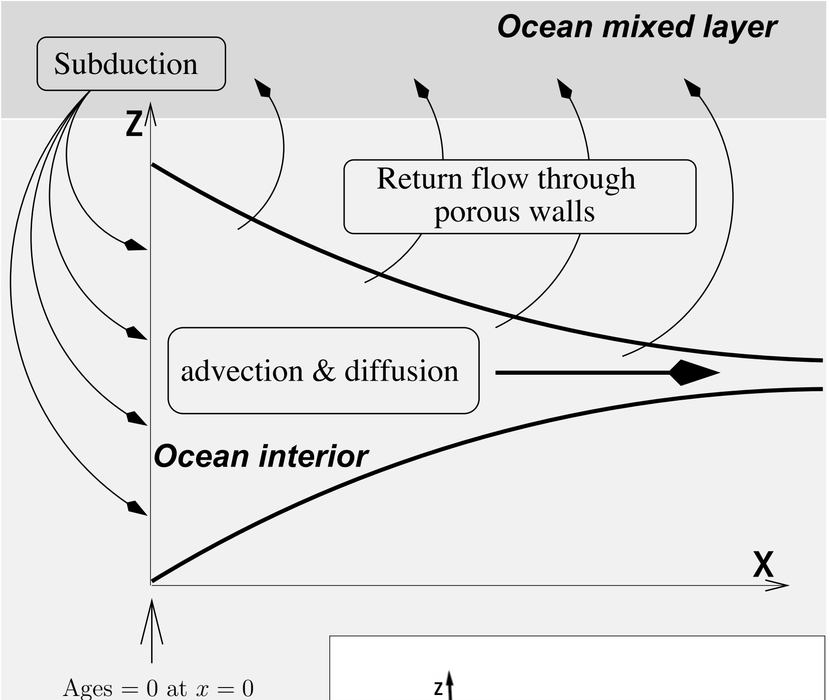
$$\mu(\tau) = \frac{1}{\Omega}\int_{\Omega} c(\mathbf{x},\tau)\,d\mathbf{x} \quad \Rightarrow \quad \int_{0}^{\infty} \mu(\tau)\,d\tau = 1$$

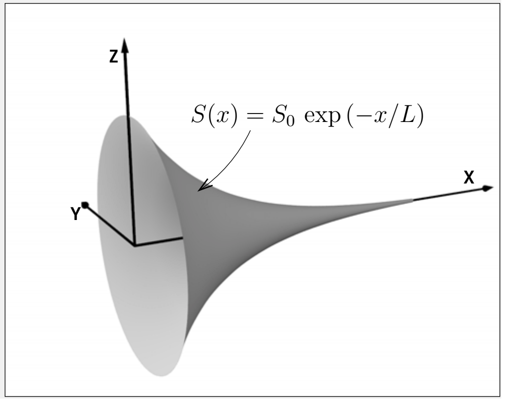
- **Global mean water age**: $\bar{a} = \int_{0}^{\infty} \tau\,\mu(\tau)\,d\tau = \frac{1}{\Omega}\int_{0}^{\infty}\int_{\Omega} \tau\,c(\mathbf{x},\tau)\,d\mathbf{x}\,d\tau$

Constructing a reduced-dimension model (IV)

The **leaky-funnel model**
a World Ocean **idealization**,
is based on the following
key assumption:

The horizontal circulation in the actual ocean may be thought to be a consequence of ***localized sinking*** *and* ***generalized upwelling***.
(Warren, 1981)





Mouchet and Deleersnijder, *Tellus*, 2008 — Mouchet et al., *Tellus*, 2012

Constructing a reduced-dimension model (V)

- Parameters of the leaky funnel model:

U = water velocity, K = diffusivity

L = e-folding length scale for the section: $S(x) = S_0\, e^{-x/L}$

L is also the mean length of the water parcel trajectories in the funnel

- The leaky funnel water age distribution is

$$\mu(\tau) = \sqrt{\frac{K}{\pi L^2 \tau}} \exp\left(-\frac{U'^2 \tau}{4K}\right) + \frac{1}{\theta}\left[1 + \mathrm{erf}\left(\frac{1}{\theta}\sqrt{\frac{L^2 \tau}{K}}\right)\right] \exp\left(-\frac{U\tau}{L}\right)$$

with $\frac{1}{\theta} = \frac{U'}{2L}\left(1 - \frac{2}{Pe'}\right)$, $Pe' = U'L/K$ and $U' = U + K/L$.

- The leaky funnel mean age is $\bar{a} = \frac{L}{U + K/L}$.

Constructing a reduced-dimension model (VI)

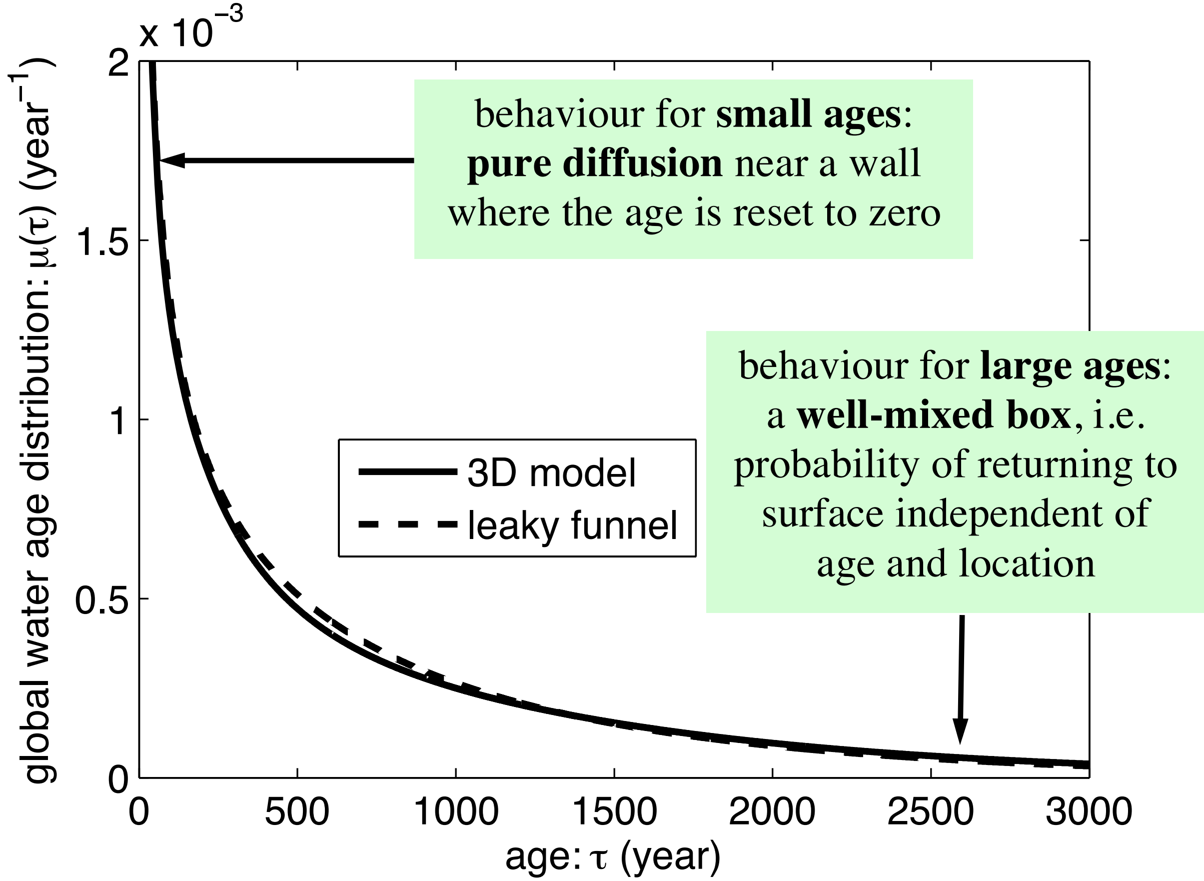
- The leaky funnel provides a neat illustration of the effectiveness and usefulness of model dimension reduction based on the age.

The parameters of the leaky funnel are optimised so as to minimise the difference between $\mu^{3D}(\tau)$ and $\mu(\tau)$

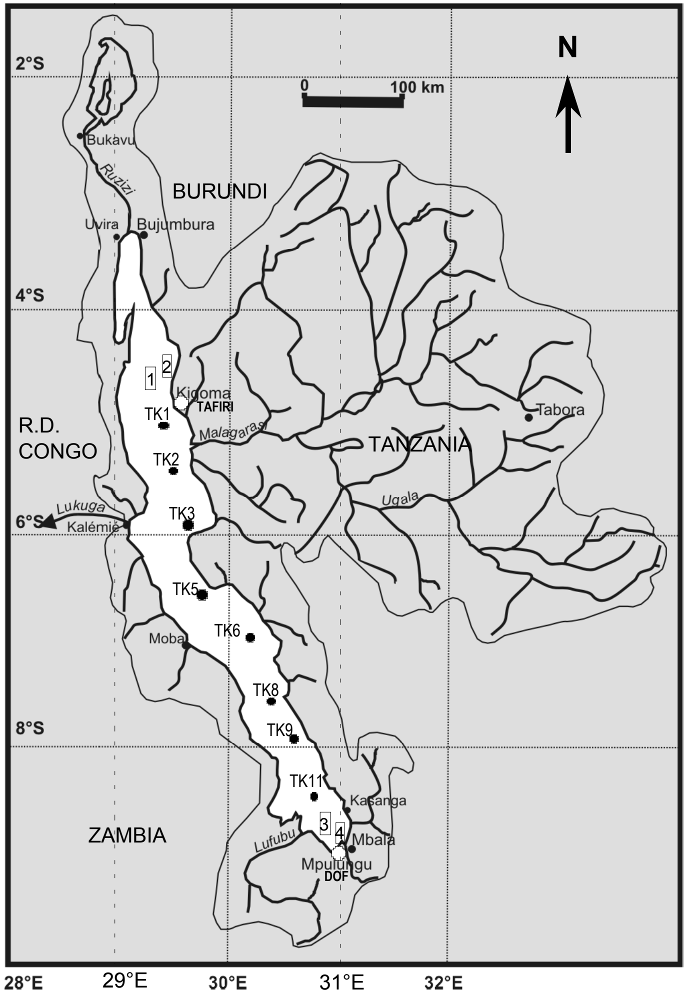
$$U \approx 3\times10^{-3}\,\mathrm{m\,s^{-1}} \;,\quad L \approx 10^{8}\,\mathrm{m}$$

$$K \approx 1.4\times10^{5}\,\mathrm{m^2\,s^{-1}}$$

$$\bar{a}^{3D} = 764\,\mathrm{y} \;,\quad \bar{a} = 721\,\mathrm{y}$$



Primitive versus diagnostic variables (I)



Lake Tanganyika: **two layers** of water separated by a **thermocline**, located at about 50 m from the surface.

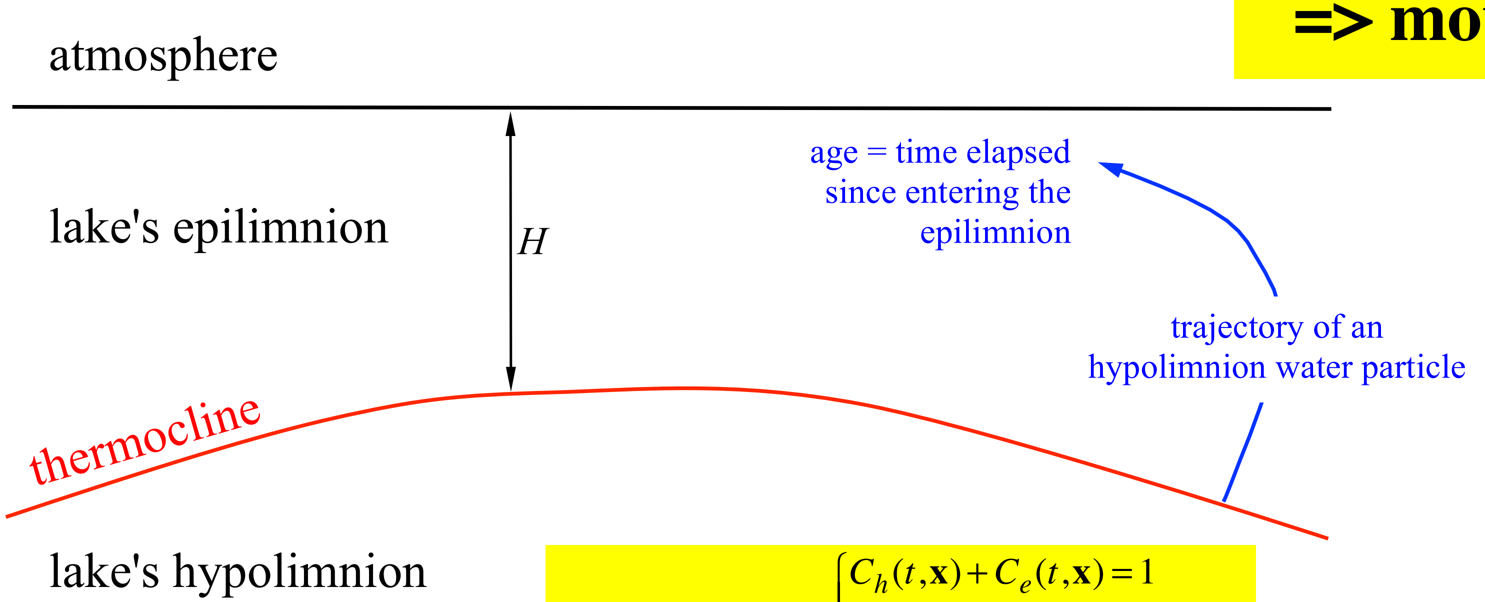
The water fluxes through the permanent thermocline are the main source of **renewing** water and **nutrients** for the **epilimnion**.

A reduced-gravity model calculated the **depth** of the thermocline, the **velocity** in the epilimnion, the epilimnion **concentration** of water originating from the lower layer and its **age**.

Primitive versus diagnostic variables (II)

• As for the **renewing** of **epilimnion's** water, the **age** is a relevant diagnosis, allowing one to clearly distinguish the **wet** season regime (old water) from the **dry** (young water) season one.

=> movie2

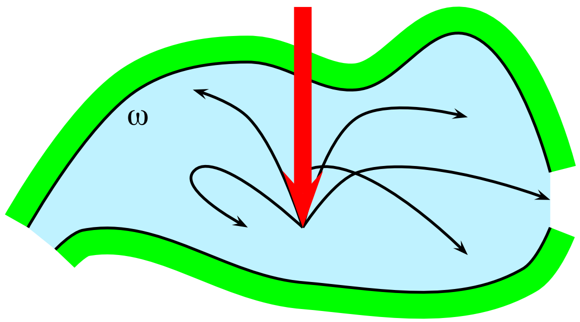


In the epilimnion: $\begin{cases} C_h(t,\mathbf{x}) + C_e(t,\mathbf{x}) = 1 \\ C_h(0,\mathbf{x}) = 0\ ,\quad C_e(0,\mathbf{x}) = 1 \\ C_h(\infty,\mathbf{x}) = 1\ ,\quad C_e(\infty,\mathbf{x}) = 0 \end{cases}$

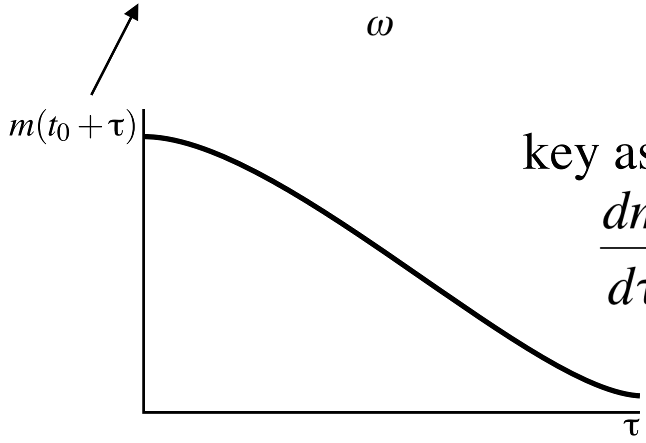
Gourgue et al.,
Estuar. Coast. Shelf S., 2007

Residence time: the forward/direct procedure

unit mass released
at $(t_0, \mathbf{x}_0)$



$$m(t_0+\tau) = \int_\omega C(t_0+\tau, \mathbf{x})\, d\mathbf{x}$$



key assumption:

$$\frac{dm}{d\tau} \leq 0$$

1. Introduce unit mass of **passive tracer** at time t_0 and location $\mathbf{x}_0$;
2. Calculate the mass $m(t_0+\tau)$ of the tracer in the domain ω;
3. Residence time: $\theta(t_0, \mathbf{x}_0) = -\int_1^0 \tau\, dm = \int_0^\infty m(t_0+\tau)\, d\tau$.

Tartinville et al., *Coral Reefs*, 1997 — Deleersnijder et al., *Applied Mathematics Letters*, 1997

Deleersnijder et al., *Continental Shelf Research*, 1998

Residence time: the backward/adjoint procedure

- Using the direct procedure, the number of model runs that are needed is equal to the number of t_0 and $\mathbf{x}_0$ at which the residence time is to be estimated. The **CPU** cost can be **prohibitive**!

- Delhez et al. (*Estuarine, Costal and Shelf Science*, 2004) developed an **adjoint** model that is potentially much **more efficient**, but requires **backward integration in time**.

- The residence time $\theta(t,\mathbf{x})$ of a passive tracer is the solution of

$$\frac{\partial\theta}{\partial t} = -1 - \nabla\bullet(\mathbf{u}\theta + \mathbf{K}\bullet\nabla\theta)$$

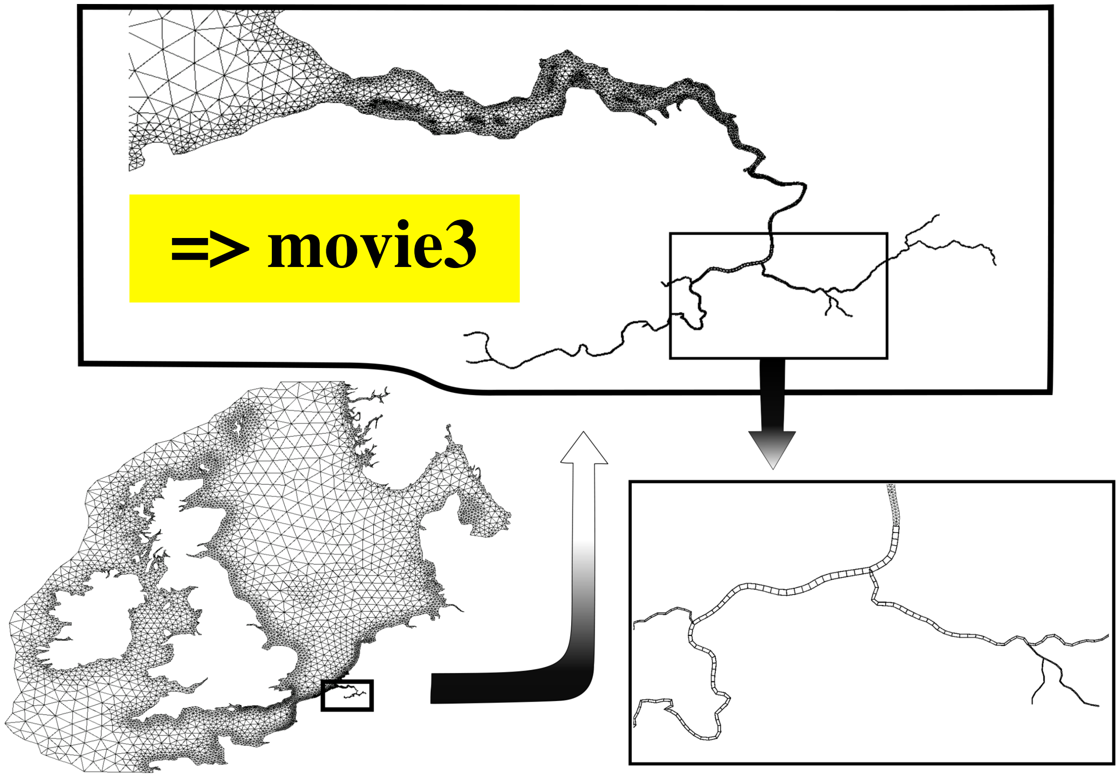
This equation is to be integrated backward in time from $t = T$, with $\theta(T,\mathbf{x}) = 0$ and $T \rightarrow \infty$.

Residence time in an unsteady flow (I)

• SLIM (www.climate.be/slim), a finite-element, unstructured-mesh, depth-averaged model of the Scheldt tributaries, River and Estuary.

• 40% of the meshes in the estuary, which represents 0.3% of the computational domain.

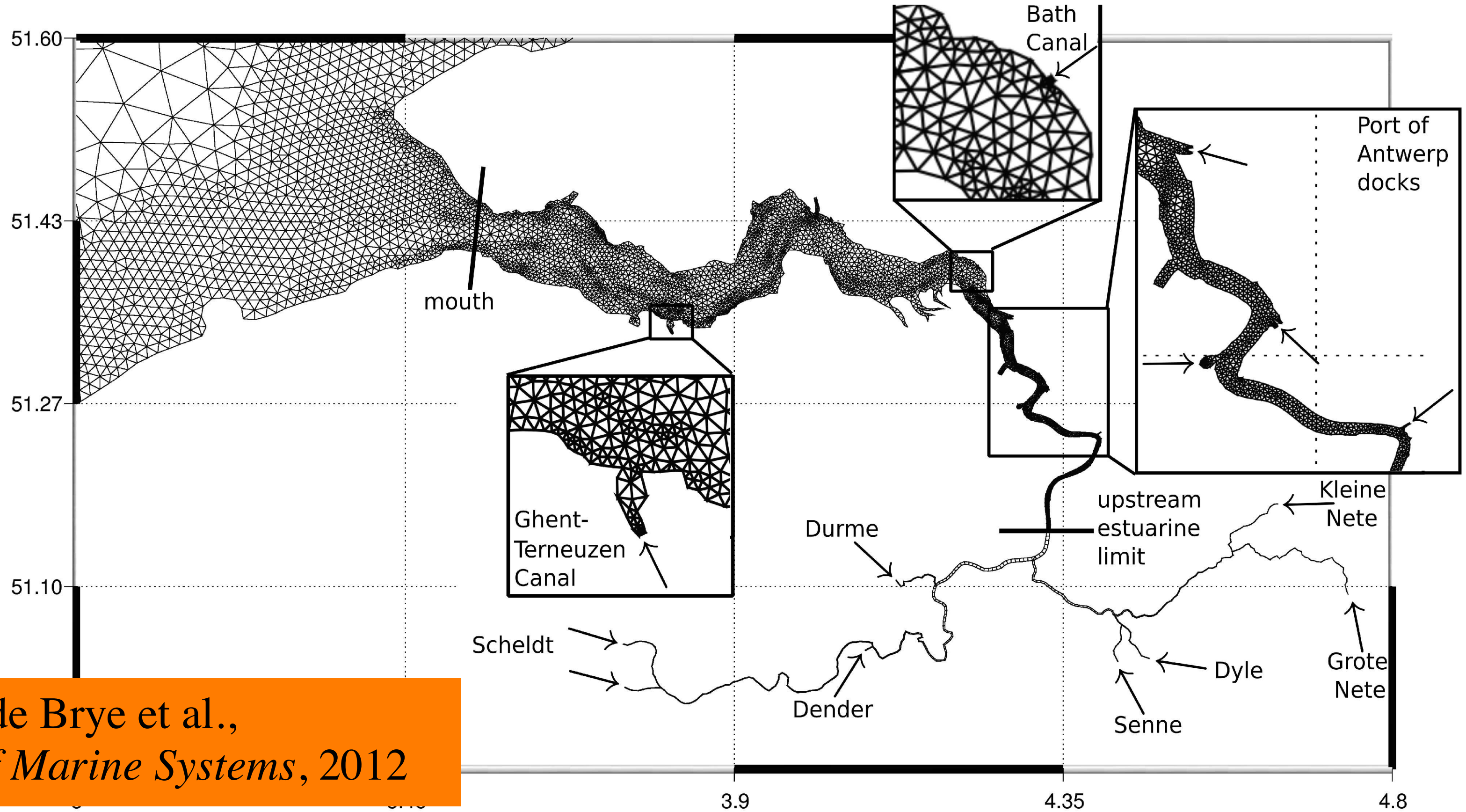
• No major problem with open boundary conditions (for tides, storms, river discharge).



Gourgue et al., *Advances in Water Resources*, 2009 — de Brye et al., *Coastal Engineering*, 2010
Kärnä et al., *Computer Methods in Applied Mechanics and Engineering*, 2011

Residence time in an unsteady flow (II)

- The water **residence time** in the **estuary** is evaluated as a function of **time** and **position**.



de Brye et al.,
Journal of Marine Systems, 2012

Residence time in an unsteady flow (III)

- The time- and space-average of the residence time is of the order of 2 months. Surprisingly, the residence time varies by one to two weeks over a tidal cycle (period ≈ 0.5 day). So **high** a **variability** is simulated in other estuaries too (e.g. Andutta et al., *Cont. Shelf Res.*, 2016)

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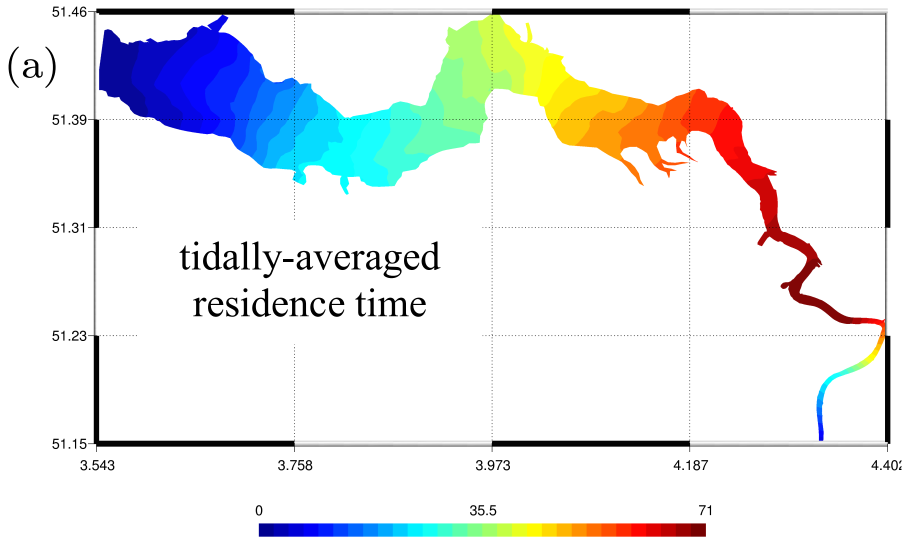
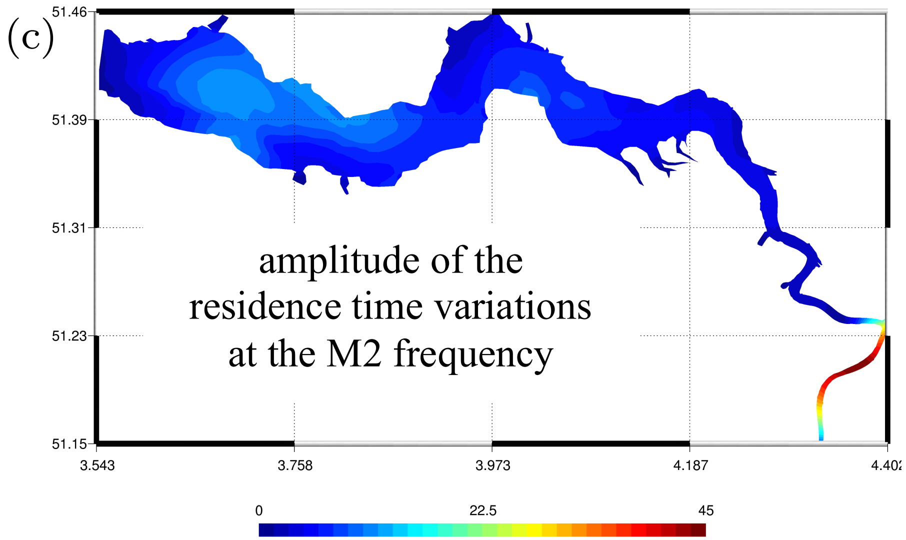
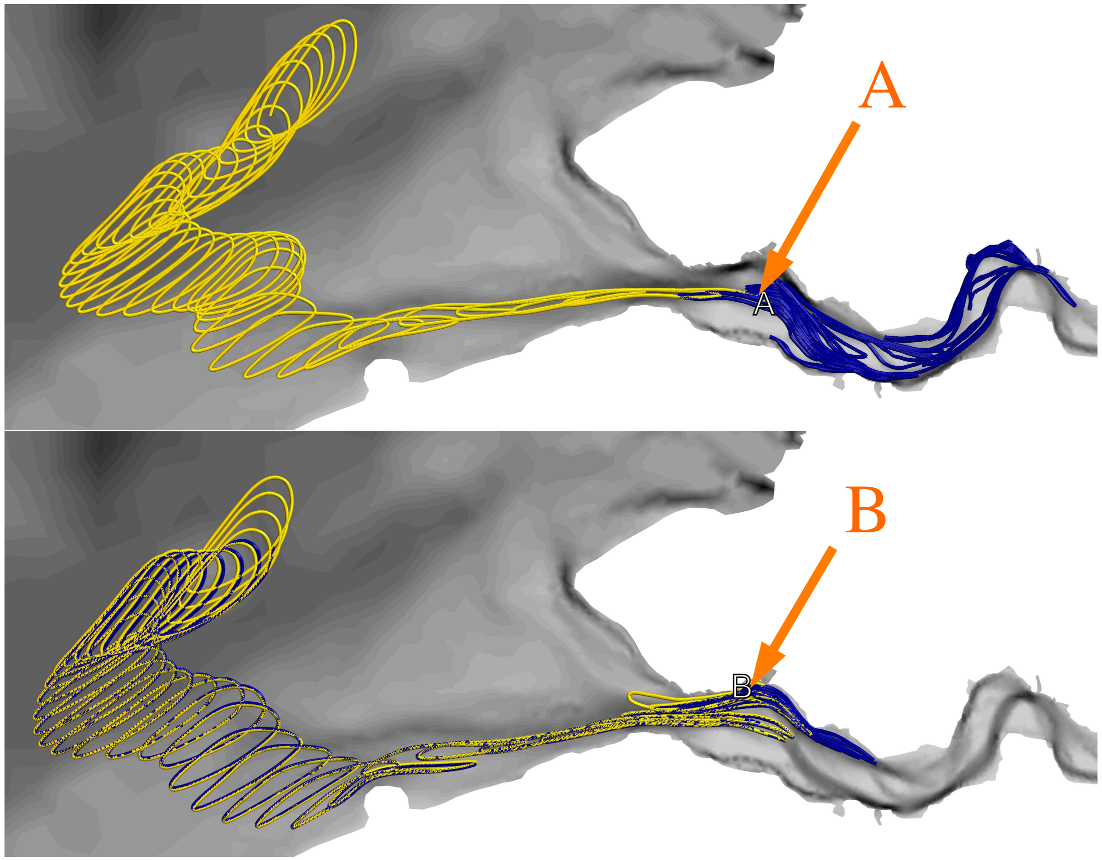




Residence time in an unsteady flow (IV)

- Trajectories of particles released at high tide (yellow) and low tide (blue) at points A (upper panel) and B (lower panel).

The trajectories displayed in the figure opposite are in accordance with the high space/time variability of the exposure time. However, the very reason thereof remains elusive.



Conclusion and outlook

- **Timescales** paint a **picture** of the functioning of (numerical models of) reactive transport phenomena that is different from that obtained by analysing **primitive variables**, i.e., velocity, surface elevation, temperature, concentration, etc.
- Timescales may help build **reduced-dimension models**, which may be of use to understand complex flows (e.g., the leaky funnel metaphor). See also http://hdl.handle.net/2078.1/154174
- Future developments might focus on constituents present in **various phases** (in relation with, e.g., **sediment**), **connectivity** diagnoses (e.g., **partial** ages or residence times, Mouchet et al., *Ocean Dyn*., 2016; Lin and Liu, *Ocean Dyn*., 2019), the development of **new boundary conditions** (for, e.g., **water renewal** studies), **benchmarks** for numerical models, etc.

For additional information, see

www.climate.be/cart