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Diagnostic timescales in fluid flows: from the Tower of Babel to partial differential problems

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Diagnostic timescales: what are they for?

• Nowadays numerical fluid flow models 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, concentration, 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 understand complex **reactive transport processes**. They are **holistic** in that all of the results are taken into account.

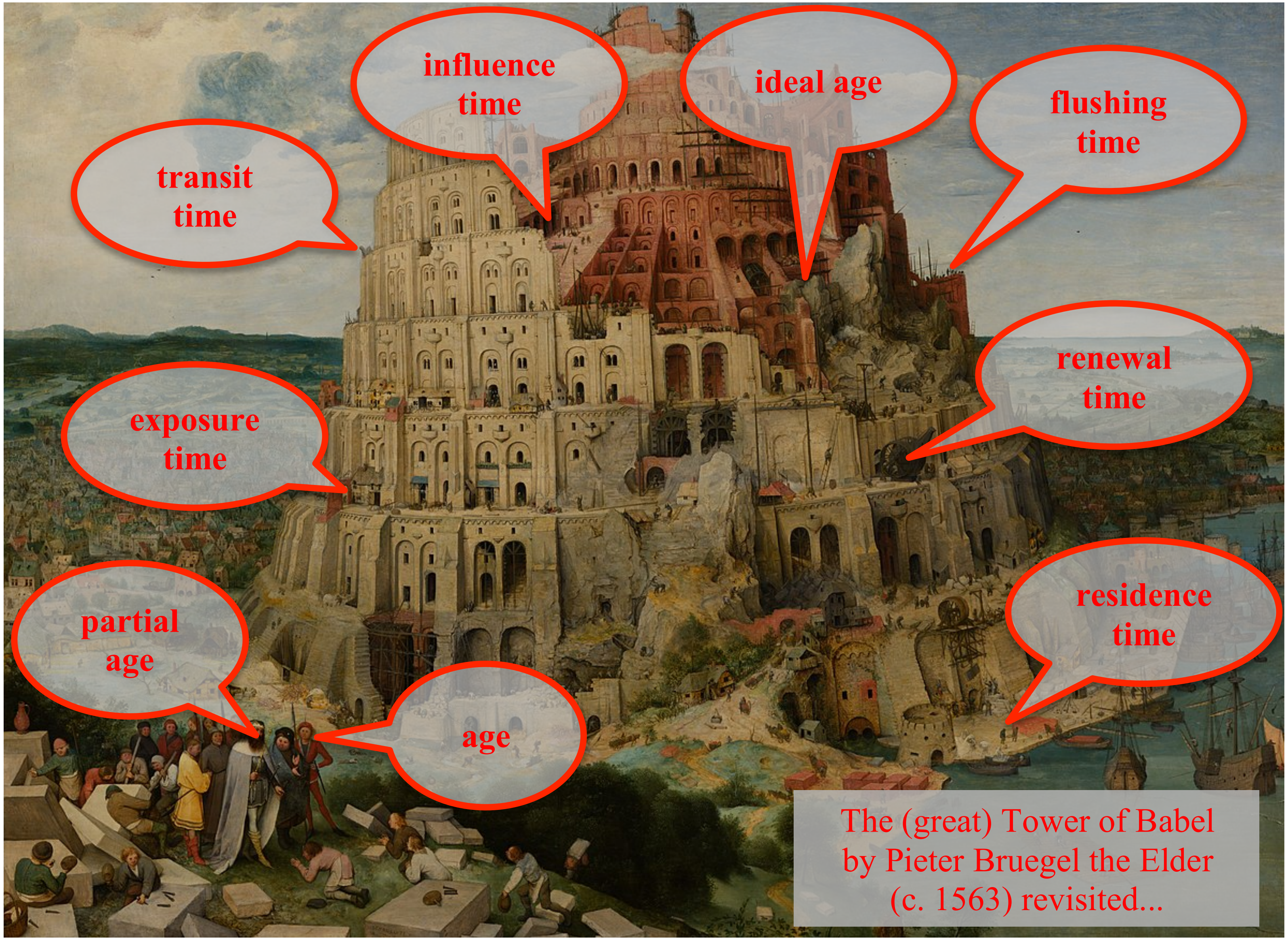
A wise piece of advice to begin with

• 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 needed

Age: forward/direct approach

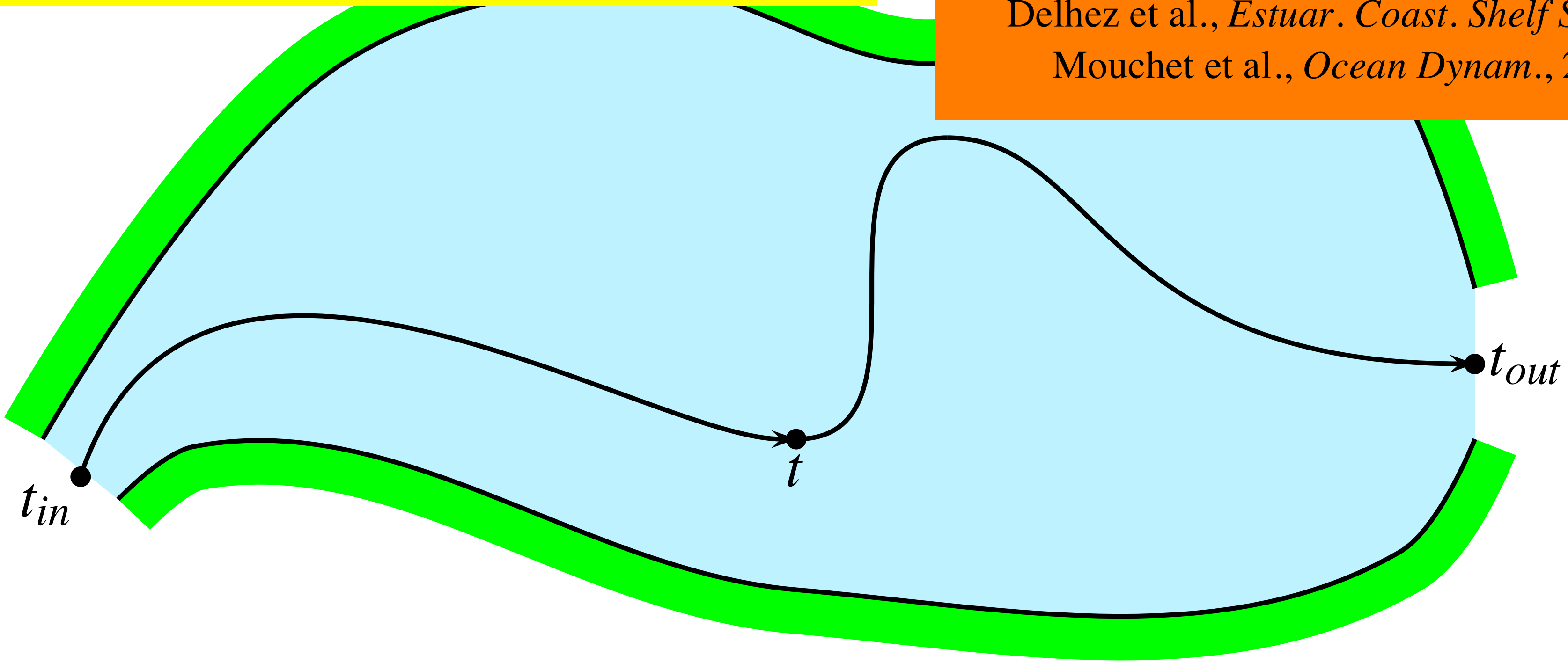
Residence time: backward/adjoint approach

<u>C</u>onstituent-oriented <u>A</u>ge and <u>R</u>esidence time <u>T</u>heory (CART, www.climate.be/cart)

Deleersnijder et al., *J. Mar. Syst.*, 2001

Delhez et al., *Estuar. Coast. Shelf S.*, 2004

Mouchet et al., *Ocean Dynam.*, 2016



$$age = t - t_{in}, \quad residence\ time = t_{out} - t$$

$$transit\ time = age + residence\ time$$

Age: basic variables and equations

- $\rho c_i(t,\mathbf{x},\tau)\delta V\delta\tau$: mass of the *i*-th constituent in δV, whose age lies in the interval $[\tau-\delta\tau/2,\tau+\delta\tau/2]$ $(\delta\tau\to 0)$, where $c_i(t,\mathbf{x},\tau)$ is the **concentration distribution function**.

- Concentration: $C_i(t,\mathbf{x}) = \int_0^\infty c_i(t,\mathbf{x},\tau)\,d\tau$

- Age concentration: $\alpha_i(t,\mathbf{x}) = \int_0^\infty \tau c_i(t,\mathbf{x},\tau)\,d\tau$

- Mean age: $a_i(t,\mathbf{x}) = \dfrac{\alpha_i(t,\mathbf{x})}{C_i(t,\mathbf{x})}$

Delhez et al., *Ocean Model*., 1999
Deleersnijder et al., *J. Mar Syst*., 2001

Age: basic variables and equations (continued)

- Simple **mass budget** considerations yield:

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

$$\frac{\partial C_i}{\partial t} = \underbrace{P_i - D_i}_{\text{source - sink}} - \nabla \bullet \underbrace{(\mathbf{u}C_i - \mathbf{K} \bullet \nabla C_i)}_{\text{advection + diffusion}}$$

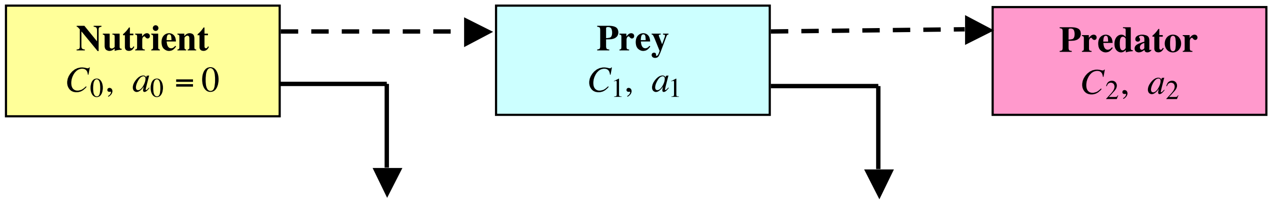
$$\frac{\partial \alpha_i}{\partial t} = \underbrace{C_i}_{\text{ageing}} + \underbrace{\pi_i - \delta_i}_{\text{source - sink}} - \nabla \bullet \underbrace{(\mathbf{u}\alpha_i - \mathbf{K} \bullet \nabla \alpha_i)}_{\text{advection + diffusion}}$$

- **Reactive** and **transport** (advection + diffusion) processes are properly **taken into account**. All transport terms are similar.

Diagnosing reactive processes (I)

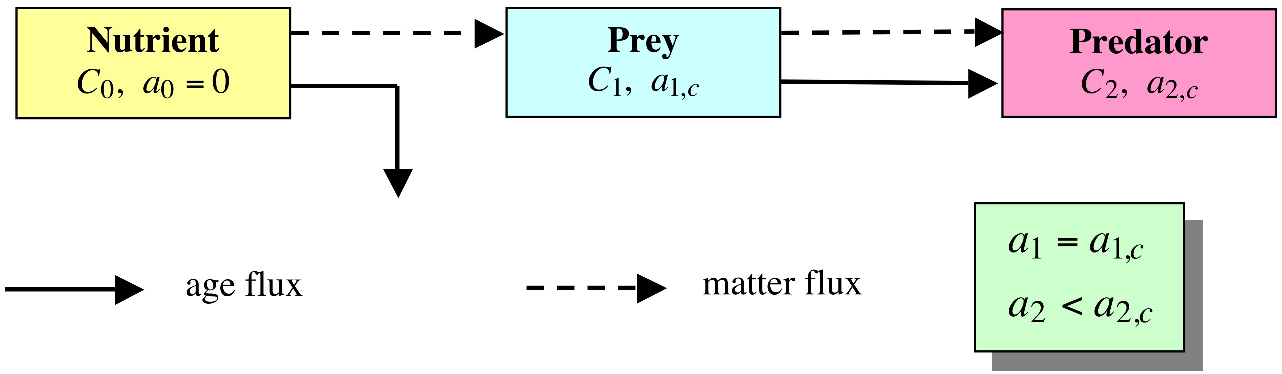
- The example of a simple **prey-predator** (Lotka-Volterra) model, with two options for the age.

Estimating the age of every compartment



The matter entering each compartment has zero age

Estimating cumulative ages

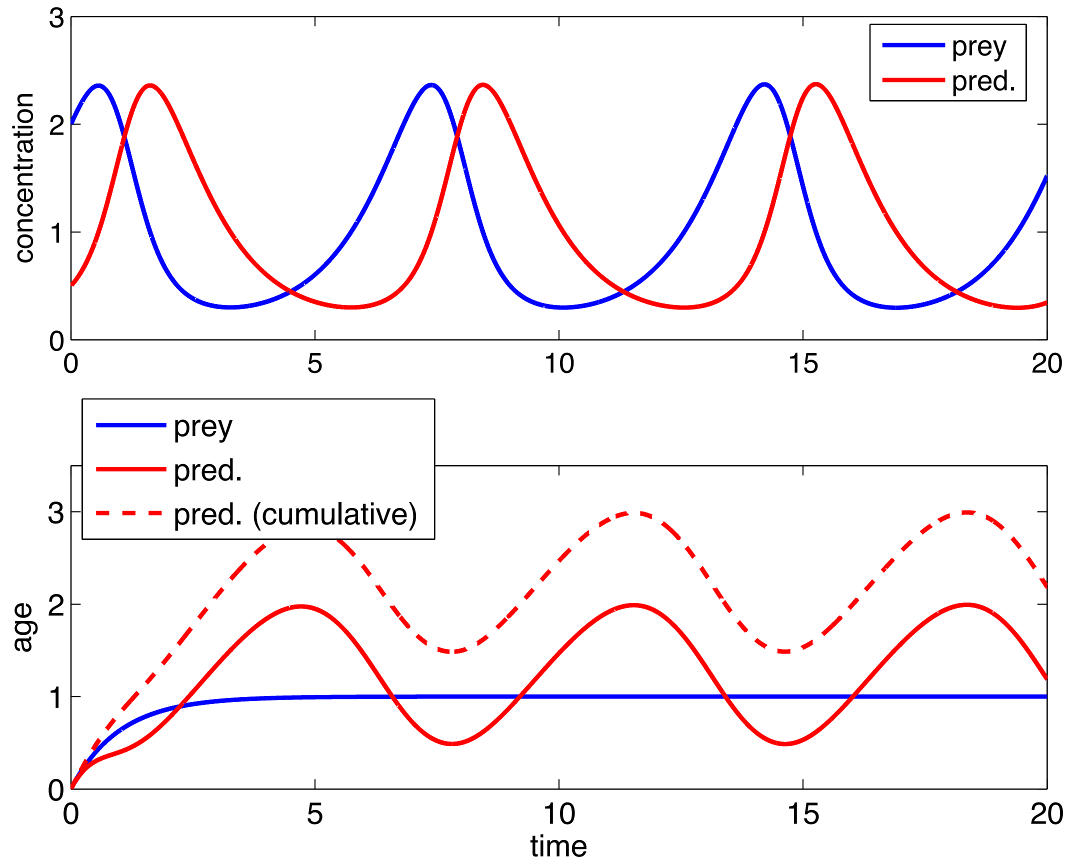


The prey takes zero-age nutrients.

The predator takes the prey "along with its age".

Diagnosing reactive processes (II)

• Assuming an infinite stock of nutrients (no nutrient-related limitation to growth), the solutions of a classical two-equation prey-predator model are illustrated using dimensionless variables.



• The prey and predator populations exhibit periodic oscillations and, yet, the age of the preys tends to a constant! Is this realistic?

Diagnosing reactive processes (III)

- The equations for the prey concentration and age are:

$$\frac{dC_1}{dt} = \underbrace{\frac{C_1}{\theta}}_{\substack{nutrient\\uptake}} - \underbrace{\frac{C_2}{\theta^*}C_1}_{predation} \quad , \quad \frac{d\alpha_1}{dt} = \underbrace{0}_{\substack{nutrient\\uptake}} - \underbrace{\left(\frac{C_2}{\theta^*}C_1\right)a_1}_{predation} + \underbrace{C_1}_{ageing}$$

$$\Rightarrow \quad \frac{da_1}{dt} = \underbrace{-\frac{a_1}{\theta}}_{\substack{nutrient\\uptake}} + \underbrace{1}_{ageing} \quad \Rightarrow \quad a_1(t) = \underbrace{[a_1(0) - \theta]e^{-t/\theta}}_{\to 0 \ as \ t/\theta \to \infty} + \theta$$

The prey's age tends to the nutrient uptake timescale, θ, because the predation term is age-independent, implying that the **probability that a prey is killed** by a predator is **independent of its age**, which is a **questionable** working **hypothesis** (Delhez et al., *Ocean Dynam*., 2004). Valid for any predation term of the form $f(t, C_1, C_2)C_1$.

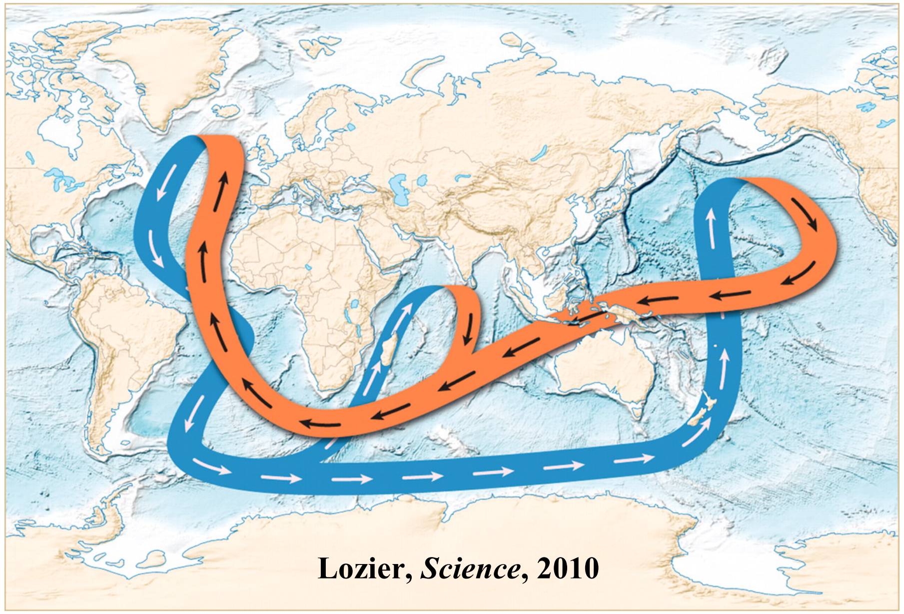
Constructing a reduced-dimension model (I)

• 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.

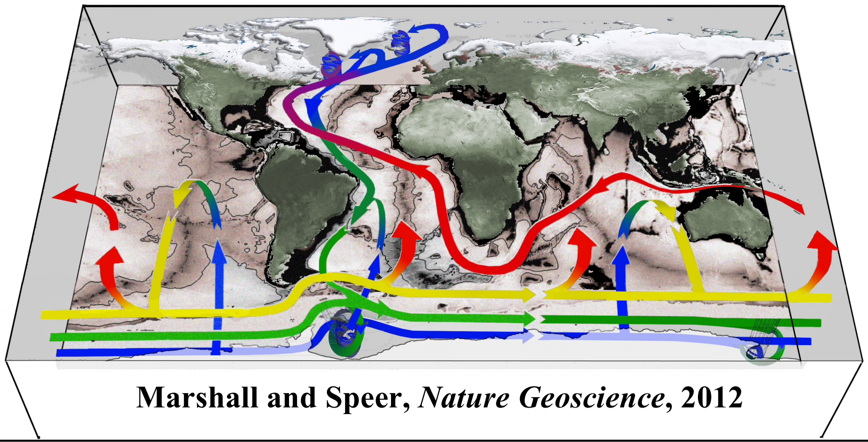
=> movie1
MITgcm results

• 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, **quantive** model?

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



Lozier, *Science*, 2010



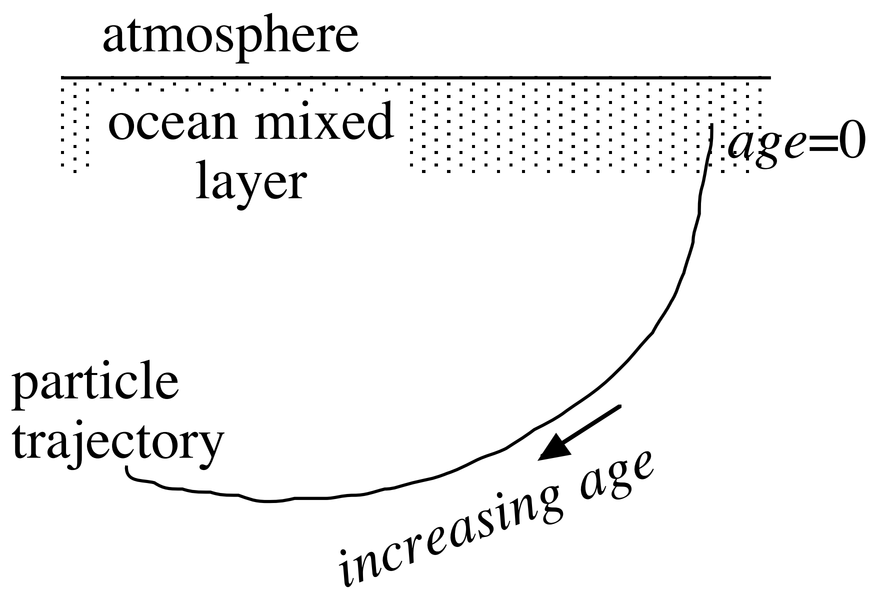
Marshall and Speer, *Nature Geoscience*, 2012

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

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

with τ = the age, Γ = the ocean surface and Ω = 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

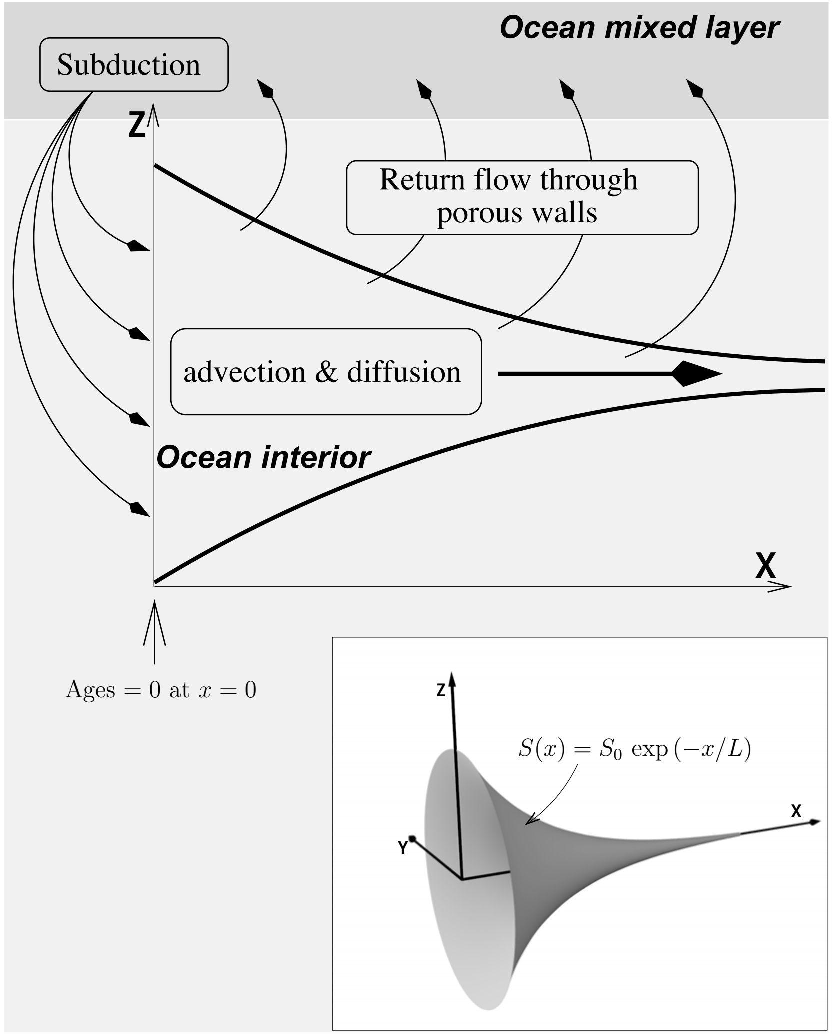
$$\mu(\tau) = \frac{1}{\Omega}\int_{\Omega} c(\mathbf{x},\tau)\, d\mathbf{x} \quad \Rightarrow \quad \int_0^{\infty} \mu(\tau)\, d\tau = 1$$

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

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

Constructing a reduced-dimension model (VI)

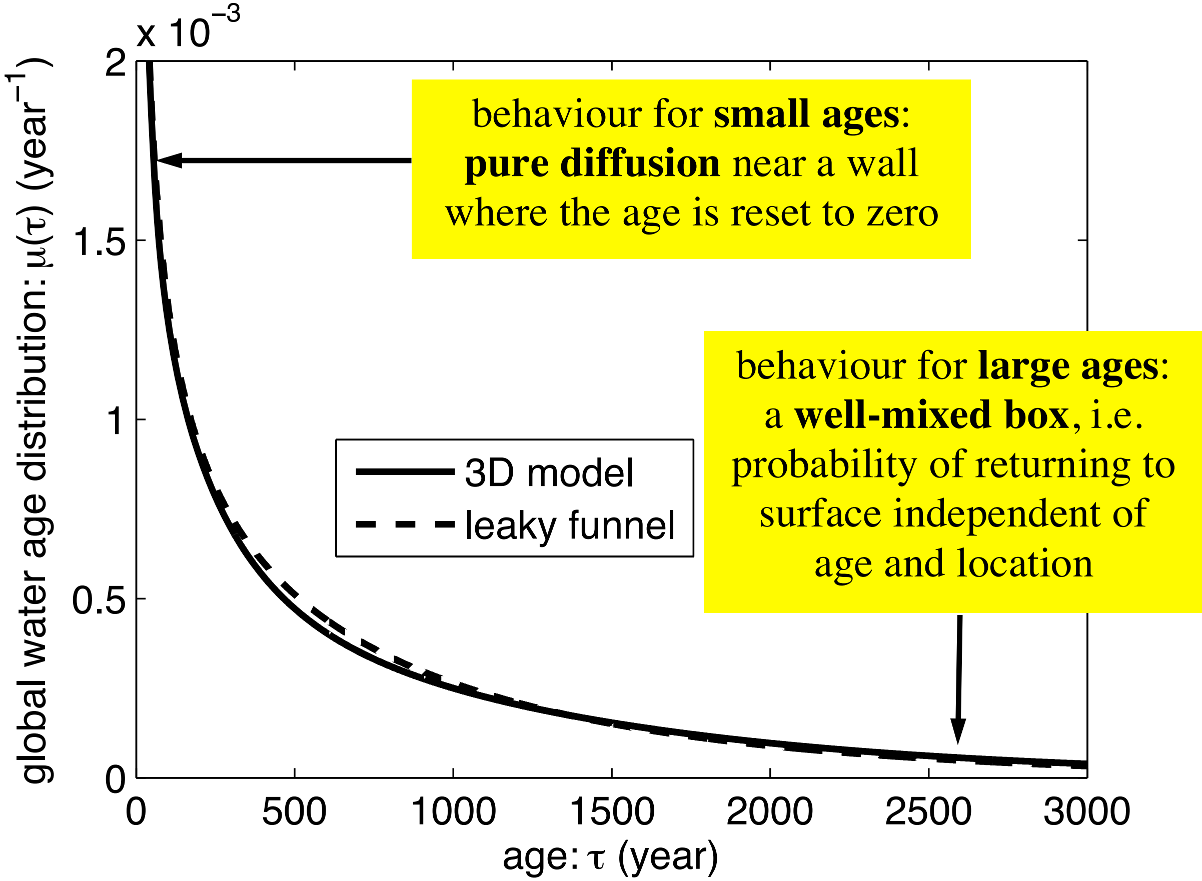
• The leaky funnel provides a neat illustration of the effectiveness and usefulness of model dimension reduction based on the age.

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

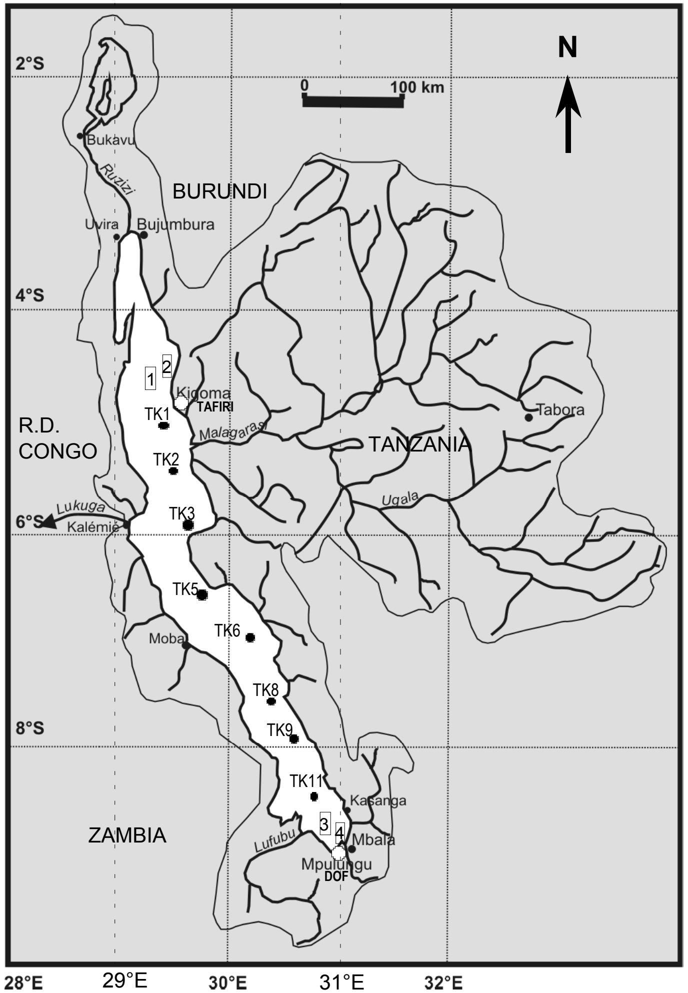
$$U \approx 3\times10^{-3}\,\mathrm{ms}^{-1}\ ,\quad L \approx 10^{8}\,\mathrm{m}$$

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

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



Primitive versus diagnostic variables (I)



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

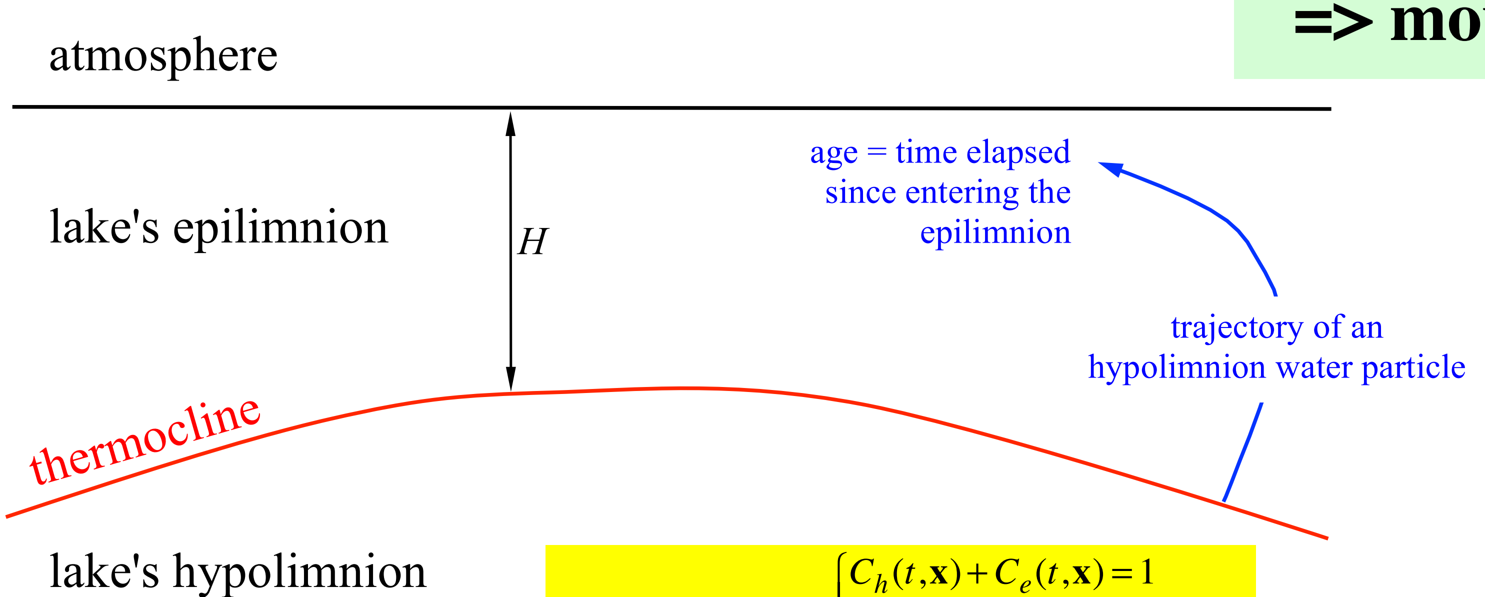
The water fluxes through the permanent thermocline are the main source of **renewing** water and **nutrients** for the **epilimnion**.

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

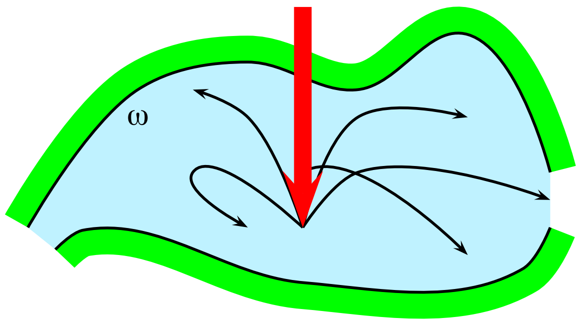


In the epilimnion: $\begin{cases} C_h(t,\mathbf{x}) + C_e(t,\mathbf{x}) = 1 \\ C_h(0,\mathbf{x}) = 0\ ,\quad C_e(0,\mathbf{x}) = 1 \\ C_h(\infty,\mathbf{x}) = 1\ ,\quad C_e(\infty,\mathbf{x}) = 0 \end{cases}$

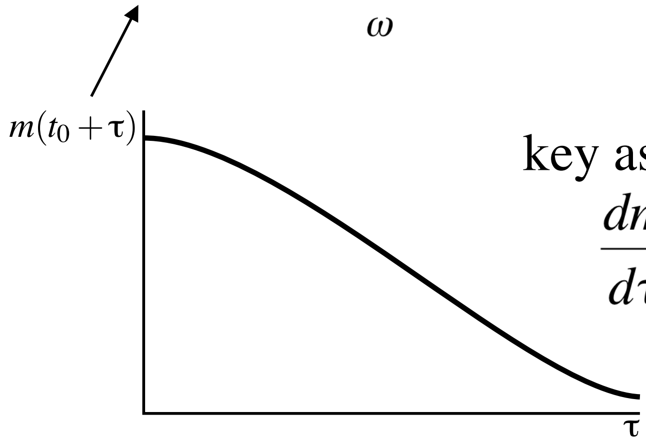
Gourgue et al., *Estuar. Coast. Shelf S.*, 2007

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

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

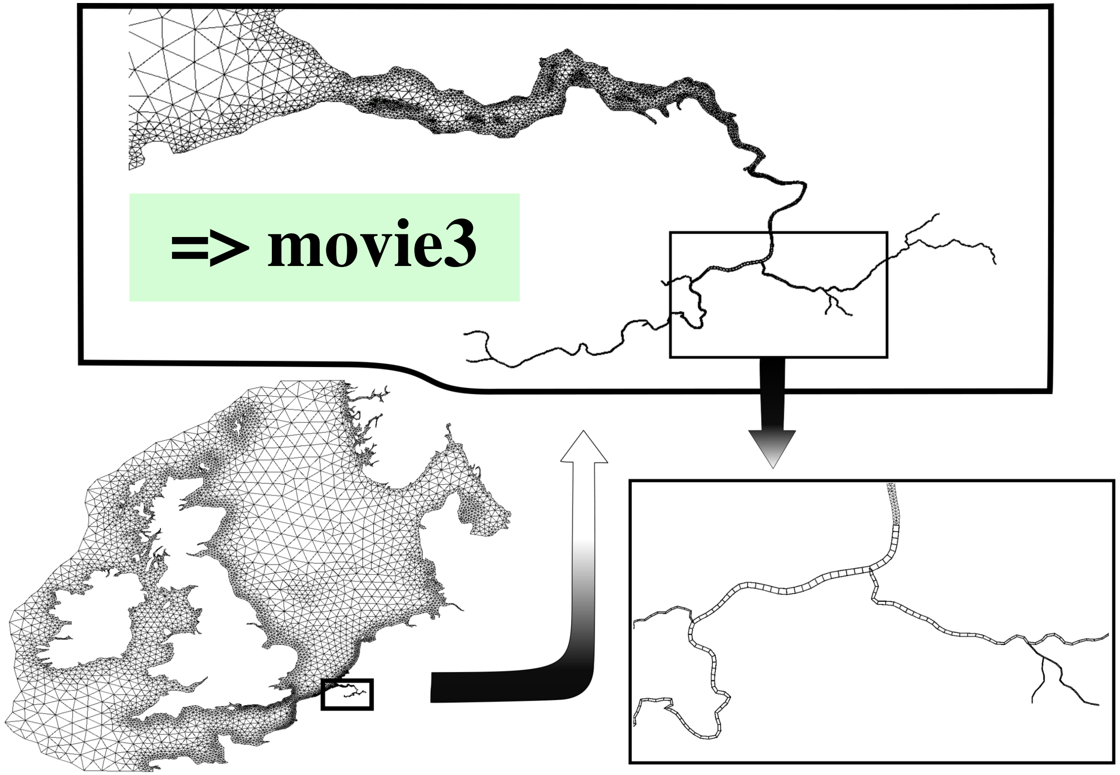
This equation is to be integrated backward in time from $t = T$, with $\theta(T,\mathbf{x}) = 0$ and $T \rightarrow \infty$.

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.

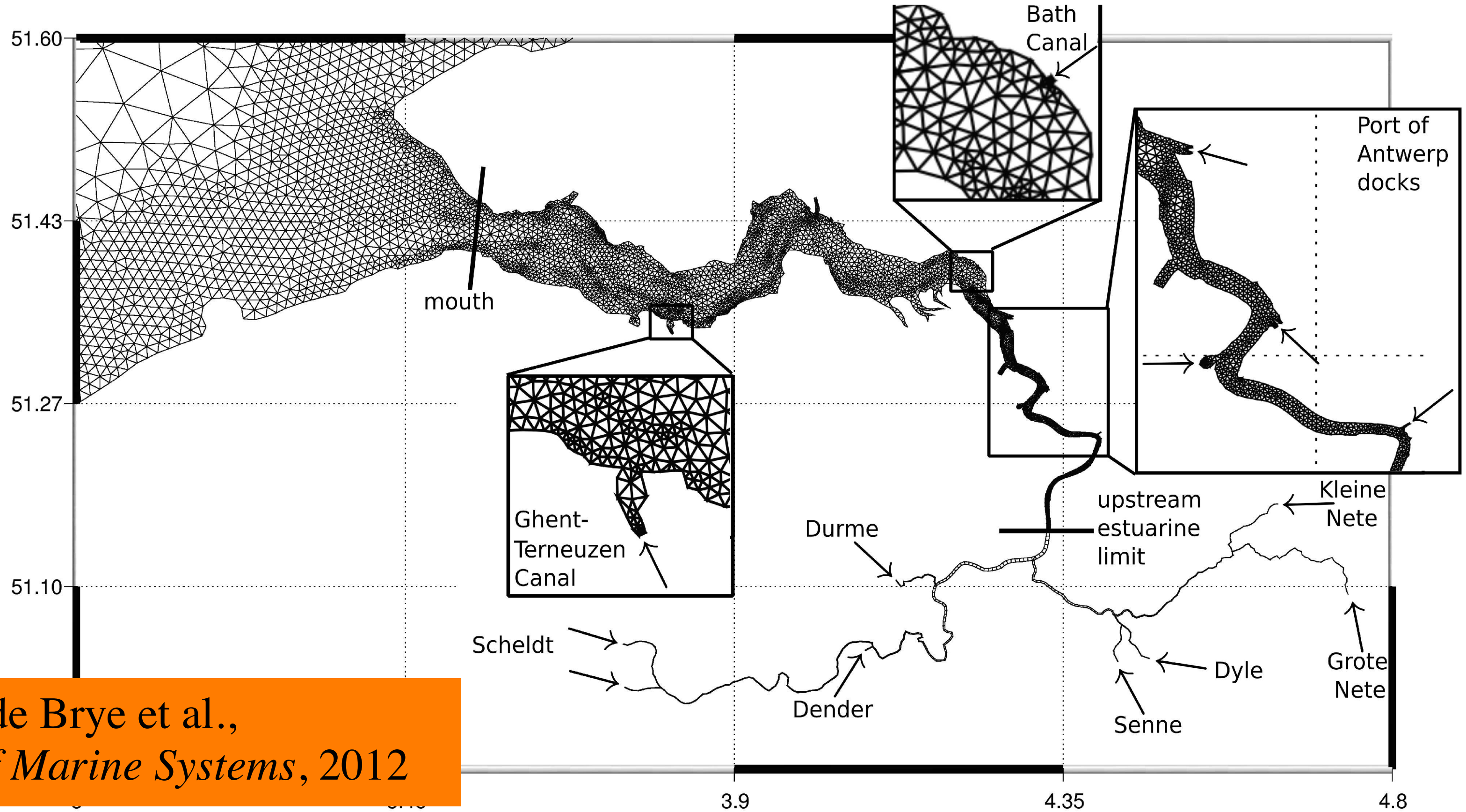
• No major problem with open boundary conditions (for tides, storms, river discharge).



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**.

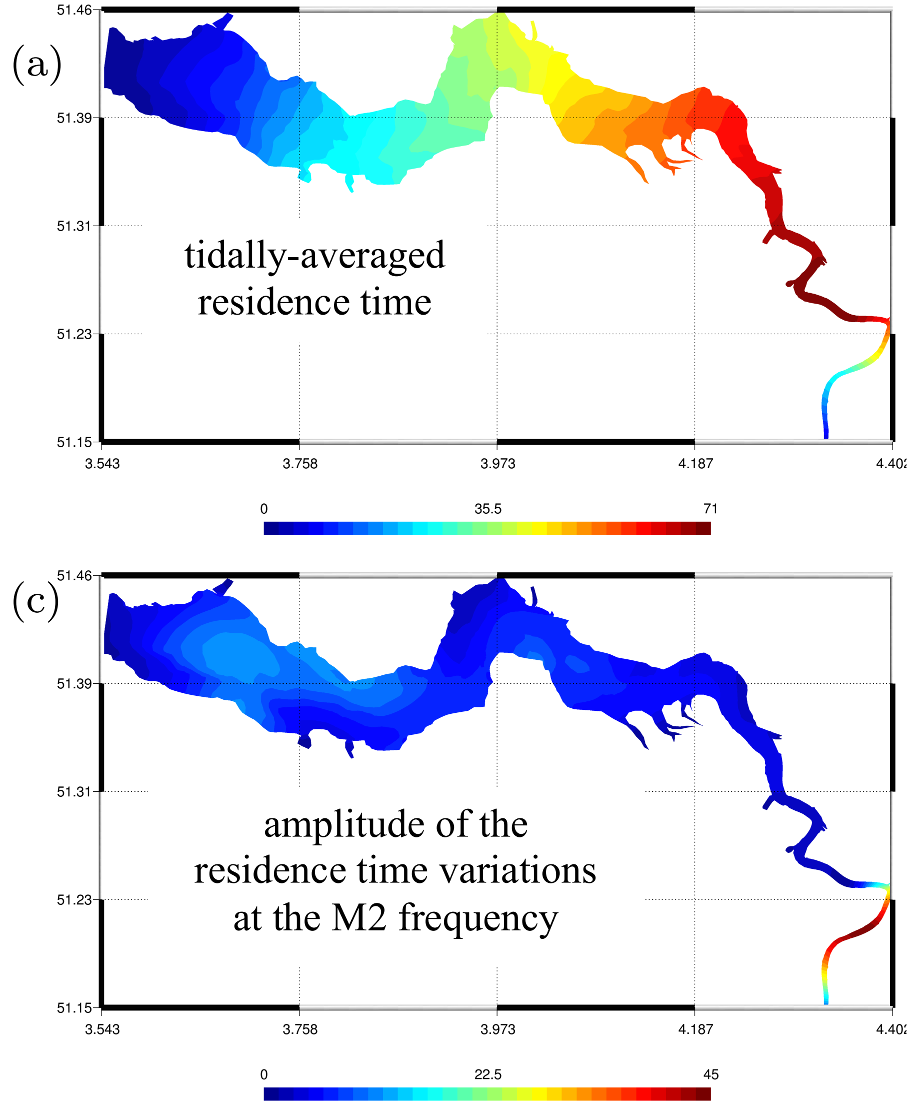


de Brye et al.,
Journal of Marine Systems, 2012

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)

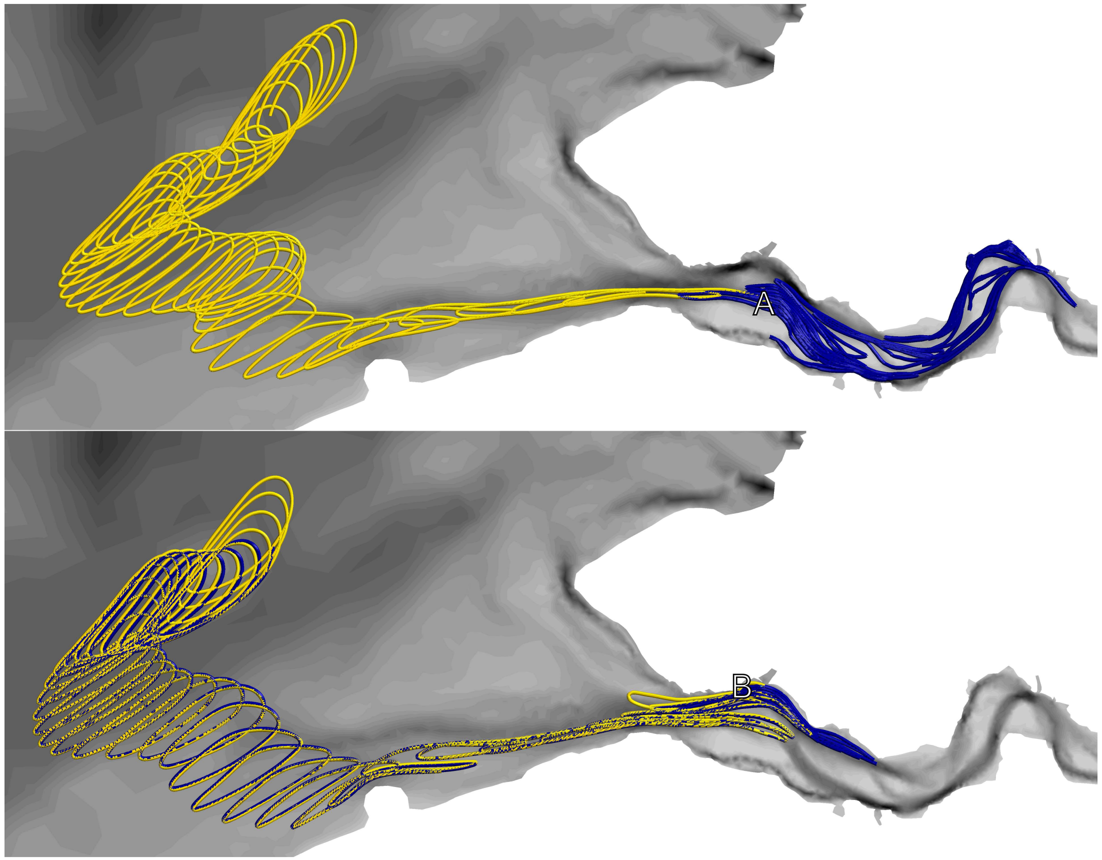
=> movie4



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 are of use for designing reduced-dimension models, thereby helping in the interpretation of complex flows (e.g. leaky funnel metaphor). See also http://hdl.handle.net/2078.1/154174
- Future developments should focus on reactive constituents rather than passive ones (e.g. water), constituents present in various phases (dissolved, attached on sediment particles, deposited on the seabed) and diagnoses relying on muliple clocks (partial ages).

For additional information, see

www.climate.be/cart