ML4Oceans summer school 2022 SCAI/SU - Paris 2nd of September 2022 Dynamic modelling

Marine ecosystem modelling





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How can we model marine ecosystems?

It's depend on your question....

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How can we model marine ecosystems?

Let's start by modelling one plankton population

Q: phytoplankton's dynamics in the surface ocean

Dynamical model



Differential equation

P(t): state variable

dP/dt = source - sink





Blackboard...

• Case #1: linear growth



This differential equation can be solved analytically

<u>Analytical solution:</u> $P(t) = P_0 \cdot e^{r \cdot t}$



Blackboard...

• Case #1: linear growth



This differential equation can be solved analytically

Analytical solution: $P(t) = P_0 \cdot e^{r \cdot t}$

NB: "Solving the equation":

- Find the analytical solution, when possible
- If not ? Compute an approximation
 ⇒ numerical integration!

ard...



NB: Numerical integration

- ≠ Finding the exact solution
- = Solving an equation using an approximation
- It requires to:
- \Rightarrow Discretize the time into time steps Δt
- \Rightarrow Estimate state at time P(t+ Δ t) from P(t)

Principle :

- Start from the initial condition
- Estimate the state after a very small time step, and so on (recursive)

On option is to use the Taylor's developments, e.g. at order 1 :

$$P(t+dt) \approx P(t) + \frac{dP(t)}{dt}$$
.dt

Making the hypothesis that the terms of higher order can be neglected

NB: Numerical integration

- ≠ Finding the exact solution
- = Solving an equation using an approximation
- It requires to:
- \Rightarrow Discretize the time into time steps Δt
- \Rightarrow Estimate state at time P(t+ Δ t) from P(t)

For the exponential growth of a population

$$\frac{d\mathbf{P}}{dt} = \mathbf{r} \cdot \mathbf{P}$$
$$\mathbf{P}(0) = \mathbf{P}_0$$

Numerical integration step by step: $P(t_1=t_0+\Delta t) =$ $P(t_2=t_2+\Delta t) =$ $P(t_3=t_3+\Delta t) =$ $P(t_4=t_4+\Delta t) =$...

<u>Nota bene</u>: This integration method is called Euler's integration, but many more (complex one) exist! E.g. Runge-Kutta...

NB: Numerical integration

- ≠ Finding the exact solution
- = Solving an equation using an approximation
- It requires to:
- \Rightarrow Discretize the time into time steps Δt
- \Rightarrow Estimate state at time P(t+ Δ t) from P(t)

To keep in mind:

- \Rightarrow This is how dynamical model are simulated
- ⇒ Several integration methods exist (more or less costly/precise)
- \Rightarrow This can lead to numerical diffusion is the time step is too small

• Case #1: linear growth



P'(t) = r.P(t)

This differential equation can be solved analytically



<u>Analytical solution:</u> $P(t) = P_0 \cdot e^{r \cdot t}$

<u>Malthus model</u> If r >1: Exponential growth is unlimited... Which is unrealistic.... !

Let's add a limitation term...

Blackboard...



<u>Case #2: density-dependant mortality</u>

Limiting term to avoid unlimited growth:

The growth is negative when the concentration becomes too high

P'(t) = r.P(t).[1 - P(t)/k]

Solution:

$$P(t) = \frac{k}{1 + (k/P_0 - 1).e^{-r.t}}$$

Logistic growth (Verhulst's model)



<u>Case #2: density-dependant mortality</u>

Limiting term to avoid unlimited growth:

The growth is negative when the concentration becomes too high

P'(t) = r.P(t).[1 - P(t)/k]

Much more realistic !





How can we model marine ecosystems?

Now, let's have two populations interacting



Modelling two populations



Predatory-prey relationships

Again, constructing the model step by step! From the most simple assumptions...



r: growth rate a: grazing rate e: efficiency of biomass/energy conversion m: mortality rate Blackboard...



Modelling two populations

<u>Predatory-prey relationships</u>

Lotka-Volterra model

- Linear growth of the prey P (growth rate r)
- Linear predation by the predator Z (predation rate a)
- Growth of the predator proportional to the predation (factor e)
- Linear mortality of the predator Z (mortality rate m)

$$\begin{bmatrix} \bullet & \frac{dP}{dt} \\ \bullet & \frac{dZ}{dt} \end{bmatrix} = \text{Linear growth} - \text{linear death by predation} = \mathbf{r.P} - \mathbf{a.P.Z} = \mathbf{f}(\mathbf{P,Z})$$
$$\begin{bmatrix} \bullet & \frac{dZ}{dt} \\ \bullet & \frac{dZ}{dt} \end{bmatrix} = \text{Growth by predation} - \text{linear mortality} = \mathbf{e.a.P.Z} - \mathbf{m.Z} = \mathbf{g}(\mathbf{P,Z})$$

 \Rightarrow Analytical study of the model





Modelling two populations

Analytical study of the Lotka-Volterra model

Two equilibriums



Ζ **P*.Z***) r/a Р (0,0) m/(ea) Phase portrait



Cf. this afternoon with Redouane

BUT: Biological/ecological processes are usually NOT linear

For instance:

Phytoplankton growth is limited, especially by light and nutrient availability







Most of the time, more complex functions are needed!

How do we chose them?

"Functional responses" For instance: Holling-type I, II, III...

How can we model marine ecosystems?

3D ocean!



How can we model marine ecosystems?

3D ocean!

How to represent space in marine ecosystem models? How to take into account physical forcing?

Representing space in models

Spatiotemporal scales



Representing space in models

Example of zooplankton in the austral ocean

Spatiotemporal scales



Horizontal spatial scales

Time scales and spatial scales of oceanic processes

Representing space in models

Spatiotemporal scales



Example: modelling phytoplankton growth in the ocean

Example: modelling phytoplankton growth in the oceanOD: homogeneous mixed layer (box model)



Concentration of phytoplankton in the mixed layer in a OD model

Example: modelling phytoplankton growth in the ocean

• 1D: vertical model of the water column



Example: modelling phytoplankton growth in the ocean • Example of results from a 3D ocean model



Depth (z)

Ayata et al. 2014

Discrete vs continuous spatial models

How can we discretize space?

Horizontal grid in ocean models

Several gridding type along the horizontal



Horizontal grid in ocean models

Several mesh sizes, with smaller grid cells close to the coast



NOAA / PMEL

Non-rectangular adaptive grids

Horizontal grid for calculus

Arakawa horizontal grids for calculus



Vertical dimension

Several coordinates systems along the vertical

Constant layer depth

• Z-coordinates



Z vertical coordinate system

Vertical dimension

Several coordinates systems along the vertical

σ-coordinates (sigma)





Sigma vertical coordinate system

Vertical dimension in the ocean

Several coordinates systems along the vertical

Along density lines

Isopycnal-coordinates



Density-layer (or isopycnal) vertical coordinate system

NB: hydrid models using different types of vertical coordinates exist...

3D modelling in the ocean

3D grid combining 1D vertical grid and 2D horizontal grid



Example of a 3D grid in the ocean
3D modelling in the ocean

Realistic regional circulation models are available



Examples of realistic regional circulation models

Dynamical equations in biophysical models

General equation in 1D

The variable C varies with time t and space x: C(x,t)

The evolution of C(x,t) with time depends on physics and biogeochemistry

$$\frac{\partial C(x,t)}{\partial t} = P(C,x,t) + J(C,x,t)$$
Temporal evolution of
the concentration of
variable C (dye, plankton...)
Physical transport
(advection + diffusion)
Biogeochemical source/
sink transformation
processes

Equations for physical transport?

Transport model in 1D or more

Physical processes affecting the transport: advection and diffusion



(transport due to mean flow)

Horizontal dimension (x)



Flow in a river



Depth (z)

Sinking of particles in a water column

Transport model in 1D or more

Physical processes affecting the transport: advection and diffusion

Diffusion

(transport due to flow's variability)



Diffusion



Molecular diffusion induced by random motion of particles



Eddy diffusion caused by turbulent mixing of particles

Conservation of mass of a tracer C (here in 1D)

 $\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x} (uC) + \frac{\partial}{\partial x} \left(D \frac{\partial C}{\partial x} \right) + J$

Biogeochemical source or sink processes

Temporal evolution of C

Advective flux divergence

Diffusive flux divergence

Contribution due to fluid flow (advection) u: velocity of the flow C: concentration

Conservation of mass of a tracer C (here in 1D)

 $\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}(uC) + \left[\frac{\partial}{\partial x}\left(D\frac{\partial C}{\partial x}\right) + J\right]$

Biogeochemical source or sink processes

Temporal evolution of C

Advective flux divergence

Diffusive flux divergence

Diffusion

D: molecular diffusivity (or K: eddy diffusivity) (of the order of 10⁻⁹m²s⁻¹ for most substances in the ocean)

Follows the gradient of concentration → Second derivative!

Conservation of mass of a tracer C (here in 1D)

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}(uC) + \frac{\partial}{\partial x}\left(D\frac{\partial C}{\partial x}\right) + J$$

Temporal evolution of C

Advective flux divergence

Diffusive flux divergence

Biogeochemical source or sink processes

Biological production or consumption, Radioactive production or decay, ...



NB: Eulerian framework

 $\frac{\partial}{\partial t}$ This equation is cast in terms of fixed-space frame of reference. It is equivalent to sitting in a particular spot in the ocean and making measurements over time, such as moorings and shipbased time series, or numerical models constructed on a fix geographic grid.

Temporal evolution in 3D

Let us consider the advection-diffusion equation in 3 spatial dimensions:

$$\frac{\partial C}{\partial t} = -\nabla(\boldsymbol{u}C) + \nabla(\boldsymbol{\kappa}\nabla C) + J$$
3D velocity field 3D turbulent diffusivity tension

with the operator ∇ , the 3D gradient operator, given by:

$$abla=\hat{x}rac{\partial}{\partial x}+\hat{y}rac{\partial}{\partial y}+\hat{z}rac{\partial}{\partial z}$$
 wi $\hat{x}\hat{y}$, \hat{z} ,, z the unit-length vectors and x , y , z the directions

Numerical diffusion

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x} \left(uC \right) - \frac{\partial}{\partial x} \left(\kappa \frac{\partial C}{\partial x} \right) + J$$

Pay attention when doing numerical integration!!

Attention must be paid to the integration time Δt and space Δx !

Indeed, the advection-diffusion equation can be used only under the following condition. If the current **u** or the diffusivity **K** are too big, then the matter in a given grid of the model will be completely advected or diffused to the adjacent grids, and the initial grid will be totally emptied! This is called **numerical diffusion**. You can detect it if you model calculates negative or infinite values for concentration.

Numerical diffusion

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x} \left(uC \right) - \frac{\partial}{\partial x} \left(\kappa \frac{\partial C}{\partial x} \right) + J$$

Pay attention when doing numerical integration!!

Conditions on the time step Δt and on the spatial resolution Δx

To avoid numerical diffusion, the following constraints must be verified in all directions: $\Delta x = (\Delta x)^2$

$$u_x << \frac{\Delta x}{\Delta t} \qquad \qquad K_x << \frac{(\Delta x)^2}{\Delta t}$$
$$u_x \Delta t << \Delta x \qquad \qquad K_x \Delta t << (\Delta x)^2$$

Otherwise the biological tracer of concentration C will be advected or diffused artificially because of the grid and time step that you have chosen are to small and to large, respectively.

How can we model marine ecosystems?

Physical forcing

How to represent physical forcing? How to couple physical and biological models?

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Physical forcing

Which physical forcing should be considered to model the marine ecosystem?



Example of physical forcing in the ocean

Coupled bio-physical modelling



Example of ocean models

NEMO: Nucleus for European Modelling of the Ocean MARS-3D: Model for Application at Regional Scales ROMS: Regional Ocean Modeling System POM: Princeton Ocean Model HYCOM: Hybrid Coordinate Ocean Model

HYCOM Cean es

100

100

10



POM



...





Bio-physical coupling

Biophysical coupling through the advection-diffusion equation of transport and biogeochemical source/sink terms



Bio-physical coupling

Biophysical coupling act at every scales of the marine ecosystems



Bio-physical coupling

Biophysical models are systems of interconnected modules



Examples of a bio-physical model with interconnected modules

How can we model marine ecosystems?

Taking into account biodiversity...



Simple view of planktonic ecosystem



Irradiance

Nutrient

Getting into more details...

Plankton Functional Groups



Different equations for each type of phytoplankton! (Le Quéré et al, 2005)

 \Rightarrow Traits of each PFT

Global Change Biology (2005) 11, 2016–2040, doi: 10.1111/j.1365-2486.2005.01004.x

Ecosystem dynamics based on plankton functional types for global ocean biogeochemistry models

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Table 1 Biomass and size distribution of Plankton Functional Types (PFT)

Size class	Biomass (PgC)	PFT name	Cell Size (µm)	
Bacteria				
Pico	0.35*	Pico-heterotrophs	0.3–1.0	
Phytoplankton		-		
Pico	0.28^{\dagger}	Pico-autotrophs	0.7-2.0	
		Phytoplankton N_2 -fixers	$0.5 - 2.0^{\ddagger}$	
Nano	0.39 [†]	Phytoplankton calcifiers	5–10	
		Phytoplankton DMS-producers	5 [§]	
		Mixed-Phytoplankton	2-200	
Micro	0.11^{\dagger}	Phytoplankton silicifiers	20-200	
Zooplankton				
Proto	0.16 [¶]	Proto-zooplankton	5-200	
Meso	0.10	Meso-zooplankton	200-2000	
Macro	Unknown	Macro-zooplankton	>2000	

Different equations for each type of phytoplankton! (Le Quéré et al, 2005)

⇒Parameters for each PFT



 Table 2
 Traits that characterize different Plankton Functional Types

		Max mortality rate [†] (day ⁻¹)	Light		Half-saturation			
	Max growth rate at $0^{\circ}C^*$ (day ⁻¹)		Affinity [‡]	Stress [§] 0 to 1	P¶ (nM)	Fe [∥] (aM)	Si** (µм)	Other nutritional source ^{††}
Bacteria								
Pico-heterotrophs	2.1	No data						5 (DOM)
Phytoplankton								
Pico-autotrophs	0.6	0.05	3.2	0	19	No data		
Phytoplankton N ₂ -fixers	0.04	0.05	1.6	No data	75	120		0 (N ₂)
Phytoplankton calcifiers	0.2	0.05	1.6	1	4	20		1.9 (DOP)
Phytoplankton DMS producers	0.6	0.05	1.6	No data	700	20		
Phytoplankton silicifiers	0.6	0.05	5.1	0	75	120	4	
Mixed-phytoplankton	0.6	0.05	1.6	0.5	19	20		
Zooplankton								
Proto-zooplankton	0.6	1e [¶] -proto						18
Meso-zooplankton	0.24	0.058						0.29
Macro-zooplankton	No data	No data						No data

Fig. 2 Example of productivity vs. irradiance at 15-25 °C for different phytoplankton groups (Geider *et al.*, 1997). The diatoms

Example of results from PFT global models (Le Quéré et al, 2005)



Fig. 4 Zonal average of the contribution of different phytoplankton plankton functional types to the total chl*a* (in mg Chl m⁻³) for the (top) micro-, nano-, and pico-size classes estimated using the combination of the statistical analysis of an HPLC pigment database and monthly composite SeaWiFS scenes of the year 2000 (Uitz *et al.*, 2005) and (bottom) silicifiers, calcifiers, and mixedphytoplankton estimated using a Dynamic Green Ocean Model.

Examples of Plankton Functional Type models









HAMOCC (Maier-Reimer et al, 2005) Figure from Ilyina et al (2013)

Solving Plankton Functional Type models

Interests of modelling PFTs:

 Even more mechanistic because resolving key functional groups and processes

BUT

- May require hundreds of empirical parameters!



Figure from B. Ward



Growth rates of PFTs

Still significant variability of traits within groups!

Trait-based models

Taking into account the variability of the "traits"

Defining traits for each component:



- Need to find ways to **reduce dimensionality** of traits that describe interactions **between trophic levels**
- Use scaling relationships and stoichiometry to define traits

Trait-based models

Trait-based biogeography of plankton

Global size-structured plankton community model



Figure 2 Size-spectral slope in a global size-structured plankton community model (data from Ward *et al.* 2012). 'A' indicates a subtropical location with relatively few large cells present (more negative slope), whereas 'B' indicates a subpolar location with a greater representation of large cells in the community (less negative slope).

Trait-based and adaptive dynamic approach

May the best one win!



Adaptive dynamic approach & Trait evolution

Example: biogeography of plankton communities

Modeling plankton communities using size-classes (trait-based approach + competition)



Fig. 2. Schematic representation of the ecosystem model. Not all size classes and not all predator-prey interactions are shown.

Size-classes

Competition for limited resources

Predator-prey interactions

Model structure : n times (NPZD) with quota

- \Rightarrow About 60 biogeochemical parameters
- \Rightarrow About 50 "species"
- ⇒ About 300 state variables

Trait evolution

Example: biogeography of plankton communities

Modeling plankton communities using size-classes (trait-based approach + competition)



Example of results

Nitrate, chl a & primary production

Cf. DARWIN's model (developed at MIT)

Trait evolution

Example: biogeography of plankton communities

Modeling plankton communities using size-classes (trait-based approach + competition)

a) Pico-eukaryotes, prokaryotes and Prochlorococcus



b) Modeled pico-eukaryotes, Synechococcus and Prochlorococcus



c) Prymnesiophytes and green algae



e) Diatoms and dinoflagellates



d) Modeled small eukaryotes



f) Modeled diatoms and other large eukaryotes



Example of results

Phytoplankton types' distribution

Adaptive model

Other examples of adaptive dynamic approach

www.sciencemag.org SCIENCE VOL 315 30 MARCH 2007

Emergent Biogeography of Microbial Communities in a Model Ocean

• Bruggeman and Kooijman (2007) L&O

Michael J. Follows,¹* Stephanie Dutkiewicz,¹ Scott Grant,^{1,2} Sallie W. Chisholm³

Light vs nutrient competitive ability in a seasonal 1D water column

• Clark et al. (2013) L&O

Cell size in a global ocean model

• Follows et al. (2007) Science

Optimum temperature and irradiance in a global ocean model

• Dutkiewicz et al. (2013) Global Biogeochemical Cycles

Ecological and biogeochemical consequences of global warming

• Sauterey et al. (2015)

When everything is not everywhere but species evolve

=> Emergent properties

Adaptive model

Going beyond the size axis...



⇒ Considering continuous trophic strategy

⇒ A way for solving the mixotroph problem!

End-to-end model



End-to-end model

Expending the NPZD model to fish



- Stock sizes and magnitude of change well simulated
- Responses time and phases of the variations not well reproduced



Fennel, 2008;2009;2010


Available online at www.sciencedirect.cor

ScienceDirect

Progress in

Oceanography

- Aims to represent the entire food web and the associated abiotic environment
 - Multiple species or functional groups are represented at each of the key trophic levels
 - Top predators in the system are also included •
- Requires the integration of **physical** and **biological** processes at different **scales**
- Implements two-way interactions between ecosystem components (from higher to lower trophic levels and from lower to higher trophic levels)
- Accounts for the dynamic forcing effect of climate and human impacts at **multiple trophic levels** (represented in a dynamical manner)

Example: Sardine & anchovy in the California current

- Coupling of four models:
 - 1) Physical model: 3-dimensional ROMS
 - 2) Plankton model: NEMURO
 - 3) Fish model: multiple-species individual-based model
 - 4) Fishing fleet dynamics

Example: Sardine & anchovy in the California current

1) Physical model: 3-dimensional ROMS





Vertical layers 42 sigma levels

Run duration: 40 years (1958-2007)

Example: Sardine & anchovy in the California current

2) Plankton model: NEMURO

NPZD-type model



Fig. 1 – Schematic view of the NEMURO lower trophic level ecosystem model. Solid black arrows indicate nitrogen flows and dashed blue arrows indicate silicon. Dotted black arrows represent the exchange or sinking of the materials between the modeled box below the mixed layer depth.

Example: Sardine & anchovy in the California current

3) Fish model: multiple-species individual-based model (IBM)



Sardine



Anchovy

Both sardine and anchovy are fully modelled:

- Reproduction (T-dependant)
- Growth (T- and Plankton-dependant)
- Mortality: constant, starvation, predation, fishing
- Movement (T-dependant + transport + swimming)
- Competition (for food and space)
- Predators



Migratory predators

Migratory predators are not fully modelled:

- Enter and exit the grid,
- Movement
- Consumption of sardine and anchovy only
- Typically : albacore tuna

Example: Sardine & anchovy in the California current

4) Fishing fleet dynamics



Fishing fleet:

- 100 boats and 5 ports for fishing the sardine
- Day boats so complete a trip in 24 hours
- Daily evaluation
- Compute expected net revenue (ENR) based on:
 - Perceived CPUE (10-day average)
 - Price per pound
 - Cost per km
 - Return to nearest port



Example: Sardine & anchovy in the California current

Examples of results







2000

-200. ----

1970

1980

1990

Figure from K. Rose

Numerical challenges...

- Solving everything simultaneously
- Code is thousands of lines
- Computing speed
- Two-way coupling between fish and zooplankton
- Mass balance
- Eulerian with Lagrangian
- Full life cycle of fishes
- ...

How can we model marine ecosystems?

And the machine learning in all of this?



Data assimilation in marine ecosystem models

Traditional methods:

e.g. using ocean color data, time-series data… ⇒ Parameter optimization, e.g. microgenetic algorithm (Ayata et al. 2013) ⇒Gradient descent/ variational methods (3D-VAR)

ML-based methods?

⇒ Used for physical models so far (e.g. high resolution)
⇒ Cf. Patrick Gallinari's lecture and Rédouane Lguensat's lab

An open field of research!

Using ML for marine ecosystem modelling

Examples of recent articles...??

Conference paper

Artificial Intelligence, Machine Learning and Modeling for Understanding the Oceans and Climate Change

Nayat Sanchez-Pi¹, Luis Marti¹, André Abreu², Olivier Bernard³, Colomban de Vargas⁴, Damien Eveillard^{5, 6}, Alejandro Maass⁷, Pablo A. Marquet⁸, Jacques Sainte-Marie⁹, Julien Salomon⁹, Marc Schoenauer¹⁰, Michele Sebag¹⁰ Détails



Ecological Modelling Volume 451, 1 July 2021, 109578



Global assessment of marine phytoplankton primary production: Integrating machine learning and environmental accounting models

F. Mattei ^{a, c, d} $\stackrel{\otimes}{\sim}$ $\stackrel{\boxtimes}{\sim}$, E. Buonocore ^{b, c}, P.P. Franzese ^{b, c}, M. Scardi ^{a, c}

Still a lot of opportunities!

Using ML for marine ecosystem modelling

Perspectives?

- Combining ML-based prediction with dynamical models
 - cf. Jean-Olivier Irisson's lecture and TD of Tuesday
- Using ML to represent unresolved process
 - cf. sub-grid dynamics in AI-informed physical models (next lecture)
- Symbolic AI? Hybrid AI?
 - cf. the ongoing ANR IA-Biodiv Challenge...



Thank you for your attention!