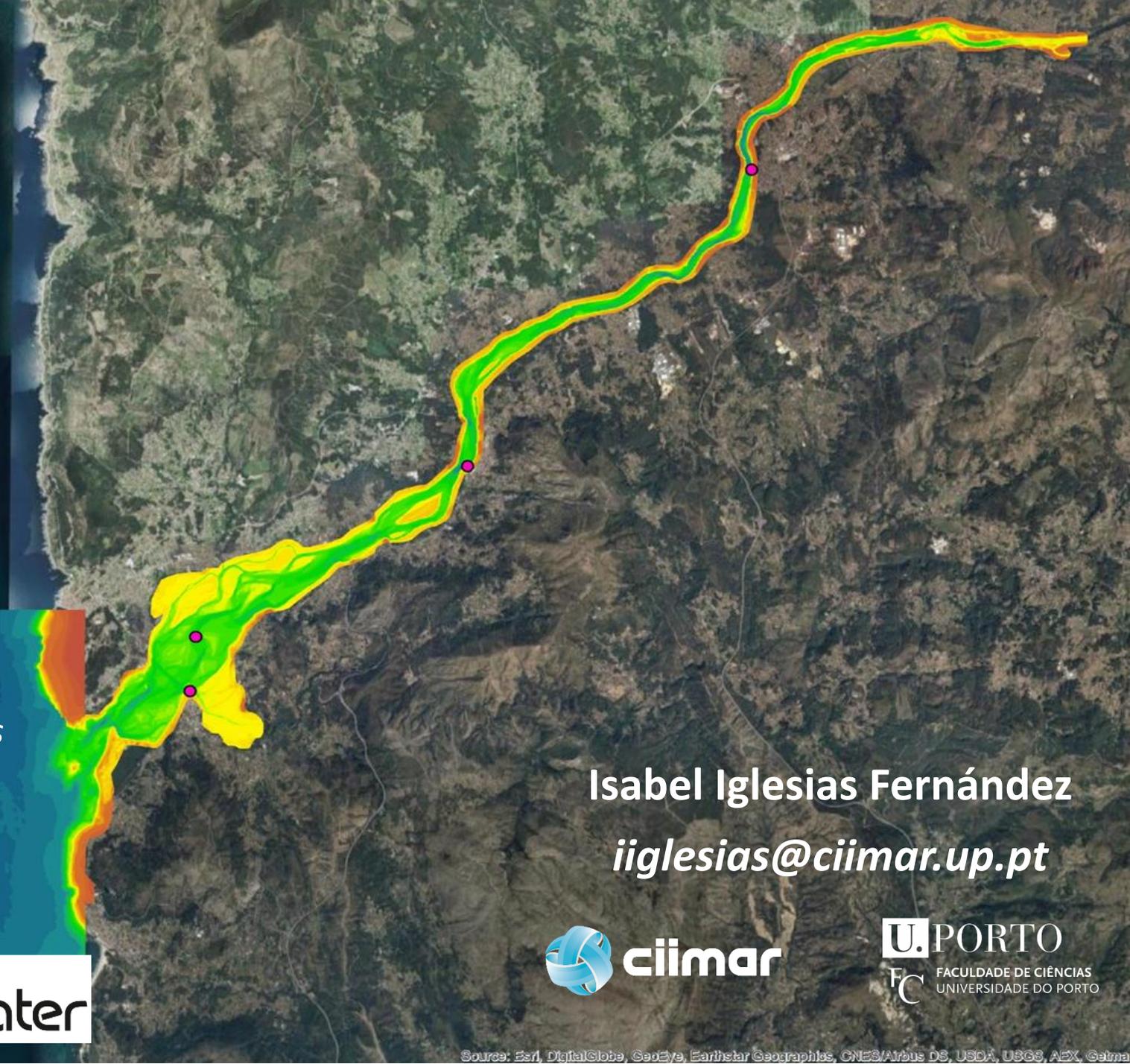


# A modelação numérica como ferramenta de apoio à avaliação de risco ambiental: modelos hidrodinâmicos e ecológicos

*Workshop*

*Risco ambiental de contaminantes de  
preocupação emergente em águas residuais  
urbanas: ferramentas de monitorização  
biológica, química e métodos avançados de  
tratamento e de modelação*



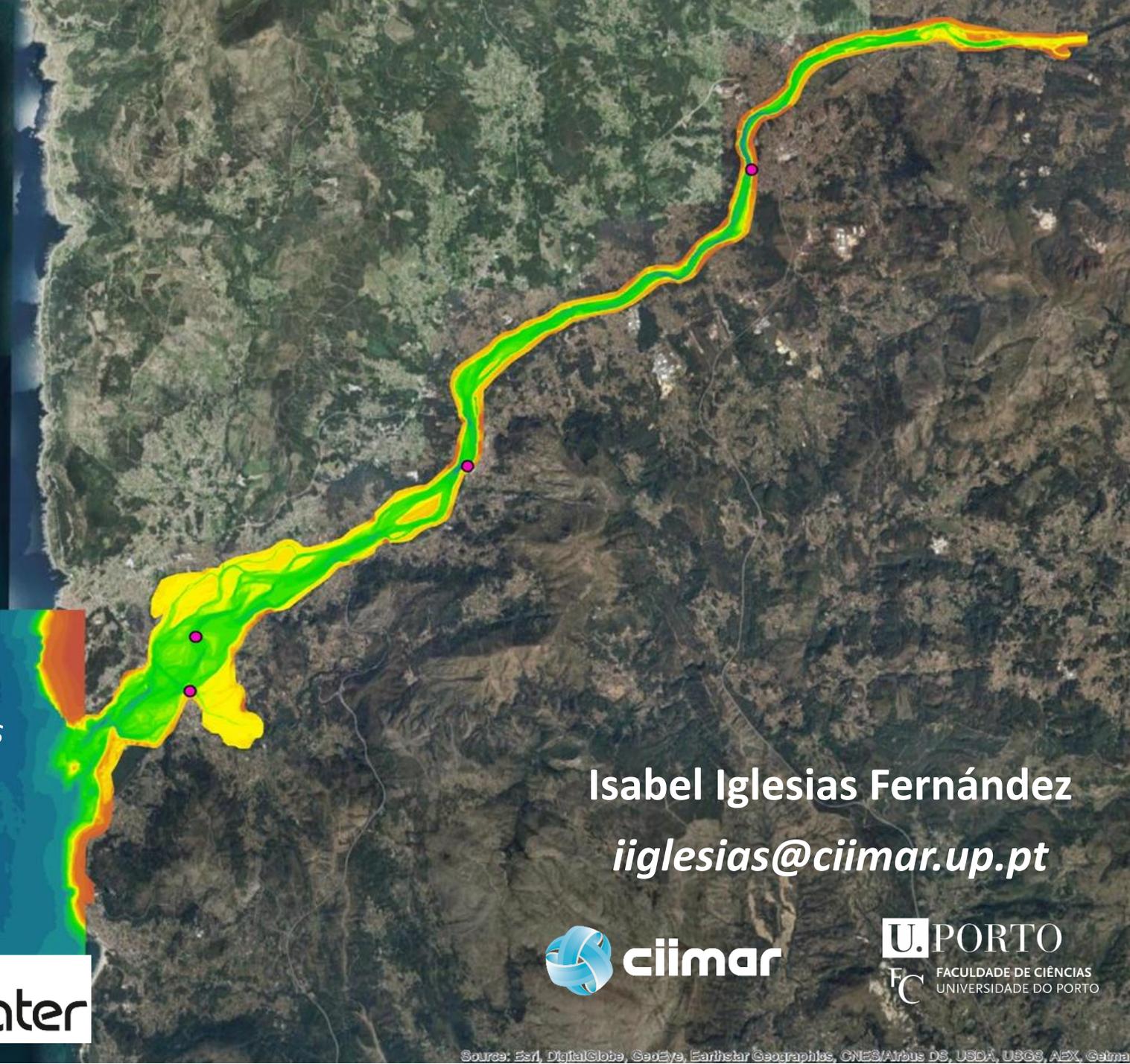
**Isabel Iglesias Fernández**  
[iiglesias@ciimar.up.pt](mailto:iiglesias@ciimar.up.pt)



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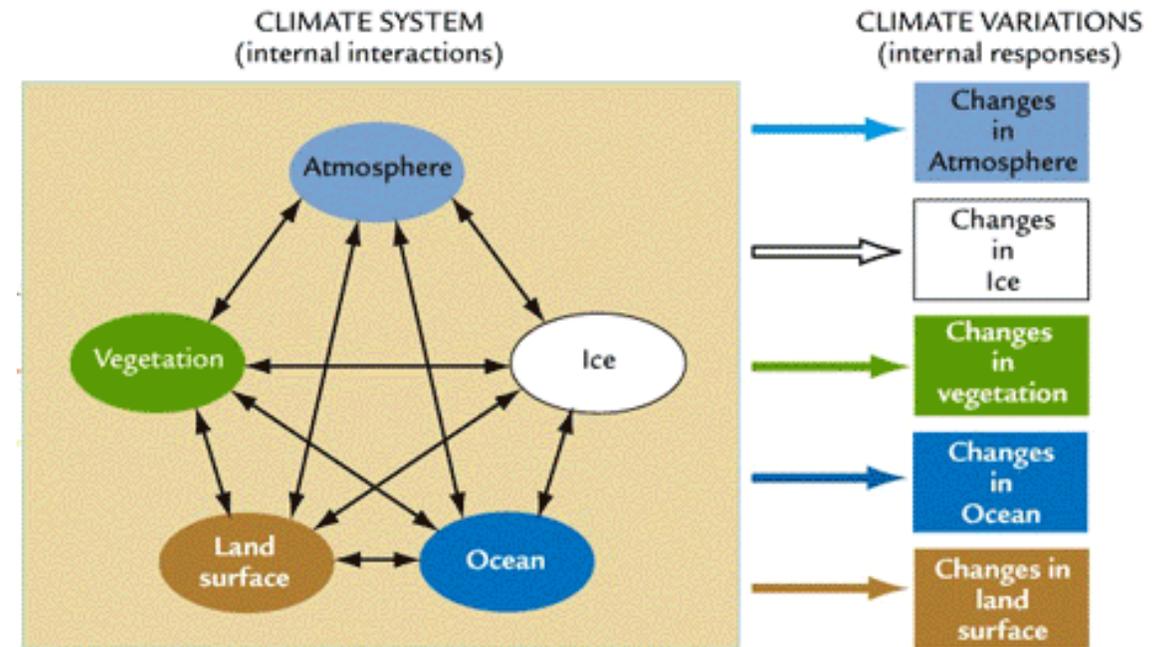
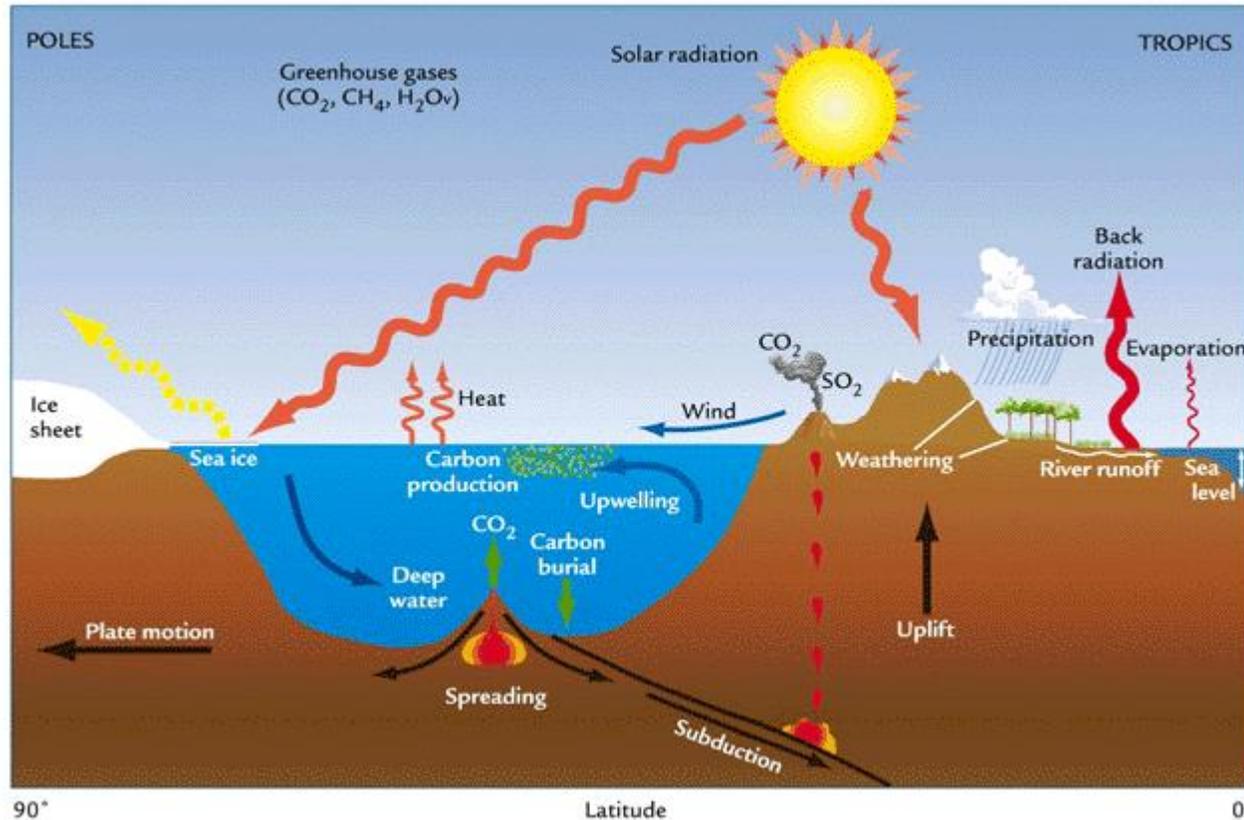


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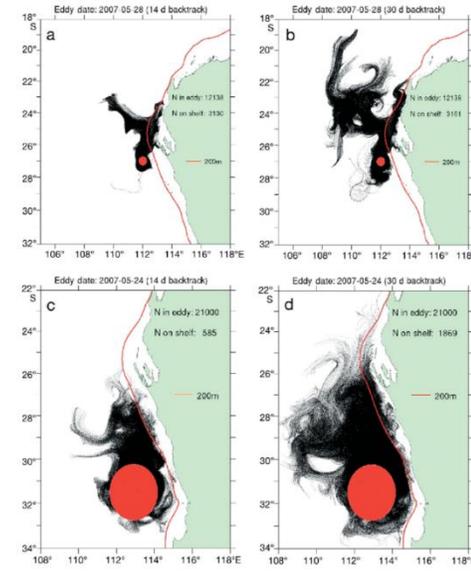
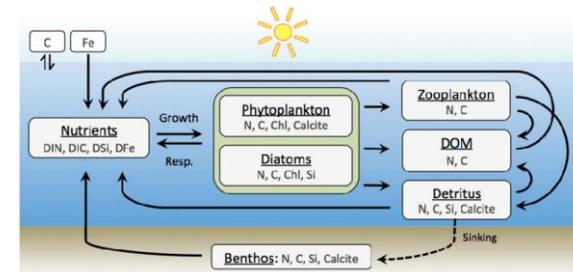
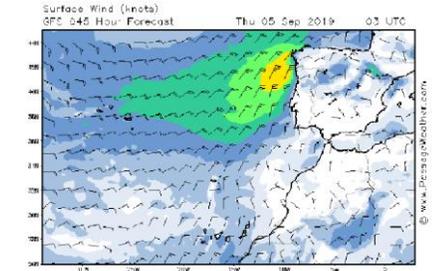
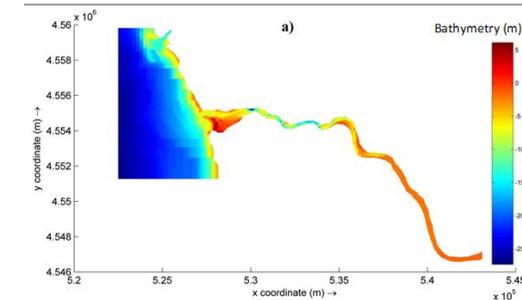
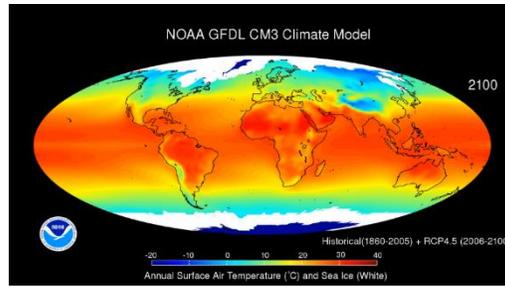
# Numerical models

- Simulators of the terrestrial system
- Solve the equations that govern the laws and principles associated with the processes between different components of the climate system, as well as energy and mass exchanges.

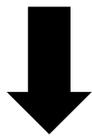


# Numerical models

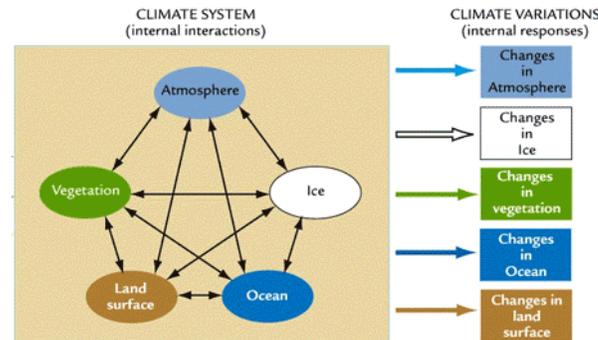
- Depending on the simulated processes and the climate system component that we want to investigate, we can have different numerical models:
- Meteorological
- Climatological
- Oceanic
- Estuarine
- Geological
- Biogeochemical
- ...



Increasing number of interactions

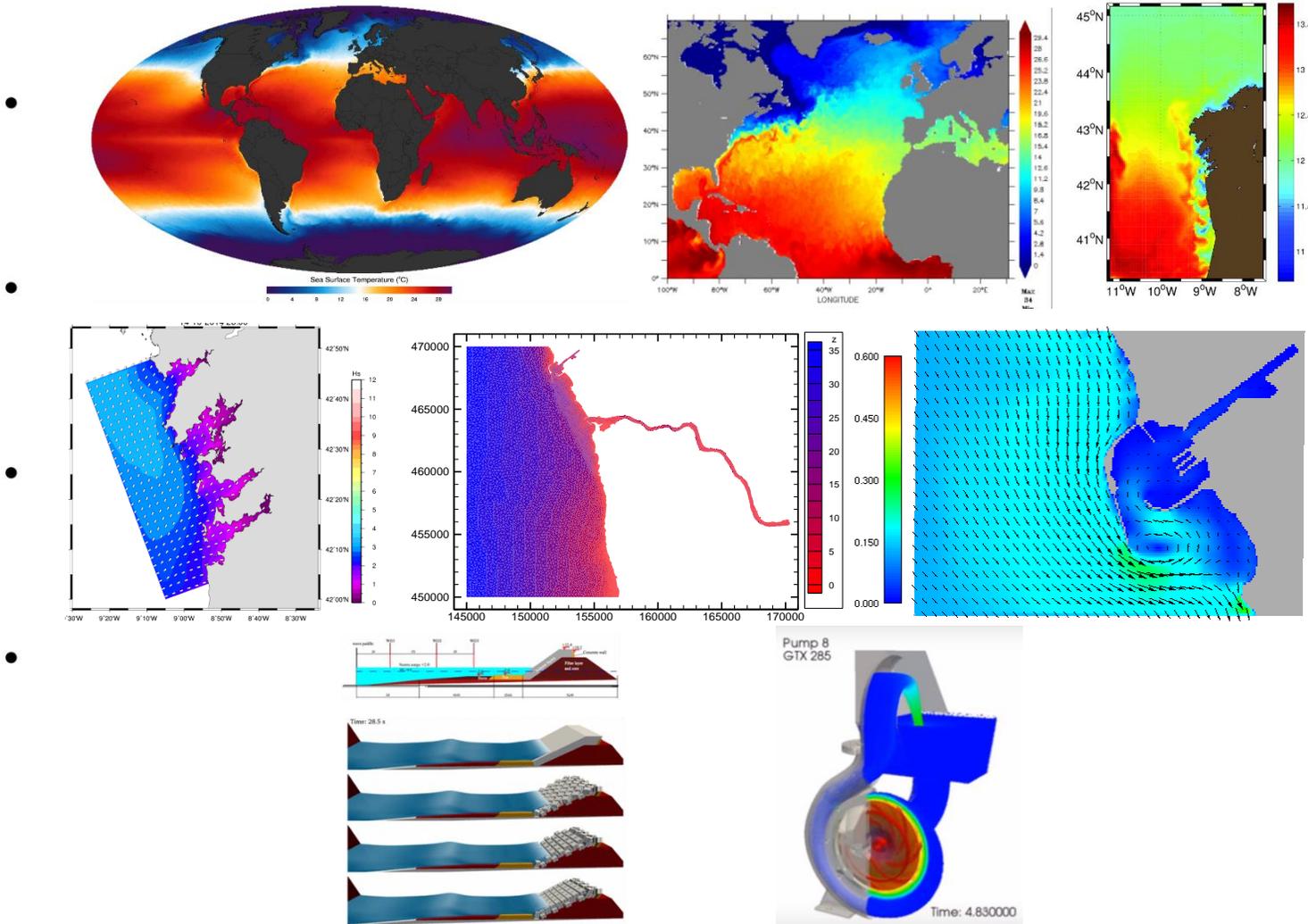
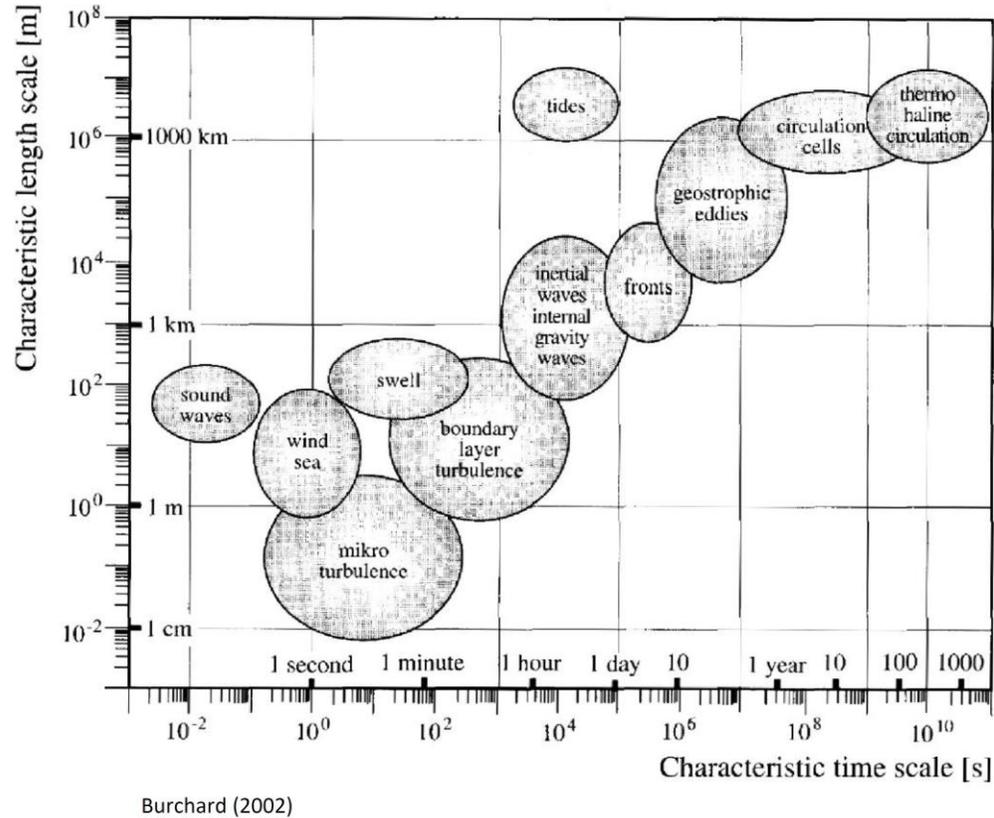


Increases the complexity of the model



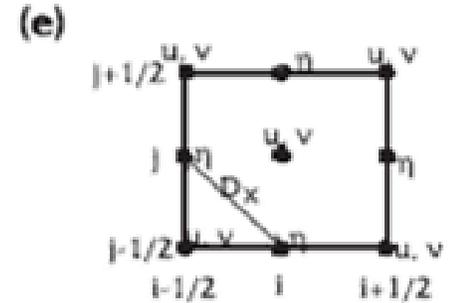
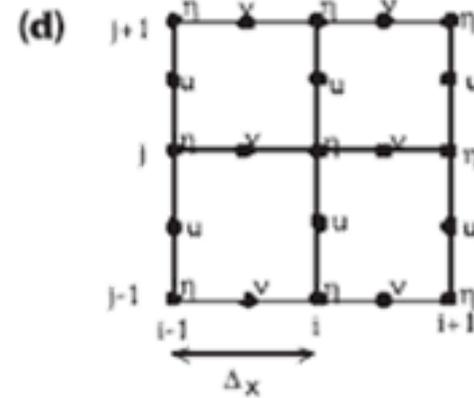
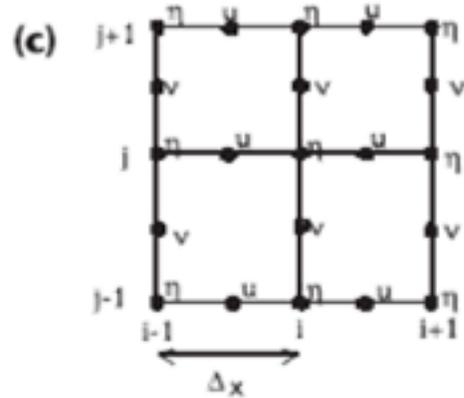
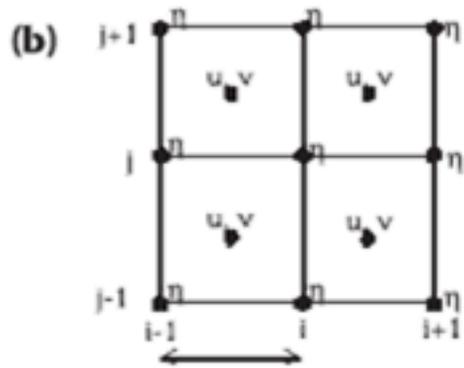
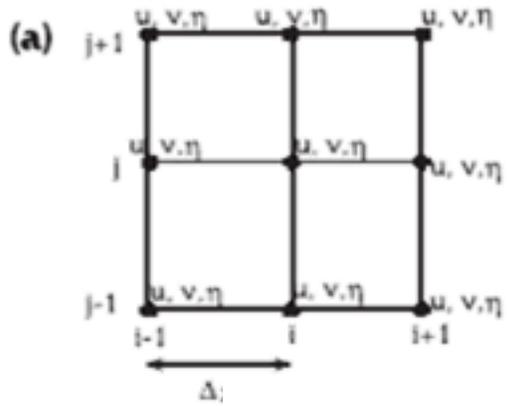
# Numerical models

- Temporal and spatial resolution: Define the problem to be solved

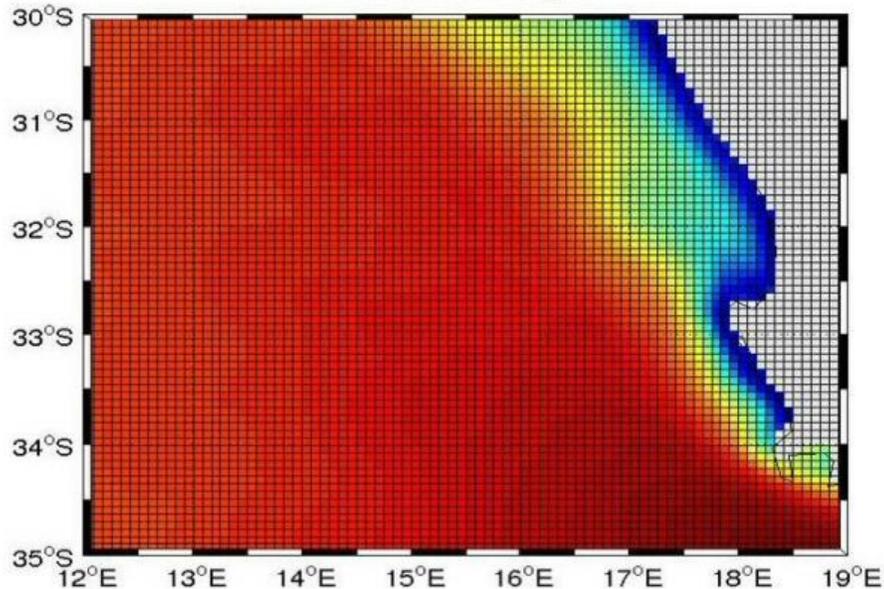


# Numerical models

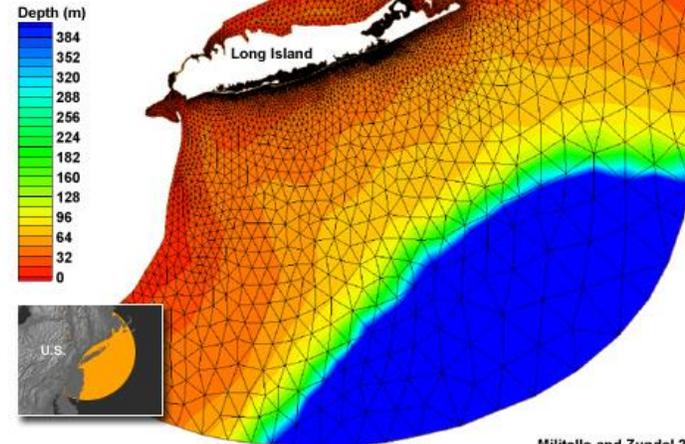
- Grids and parametrizations



The horizontal grid



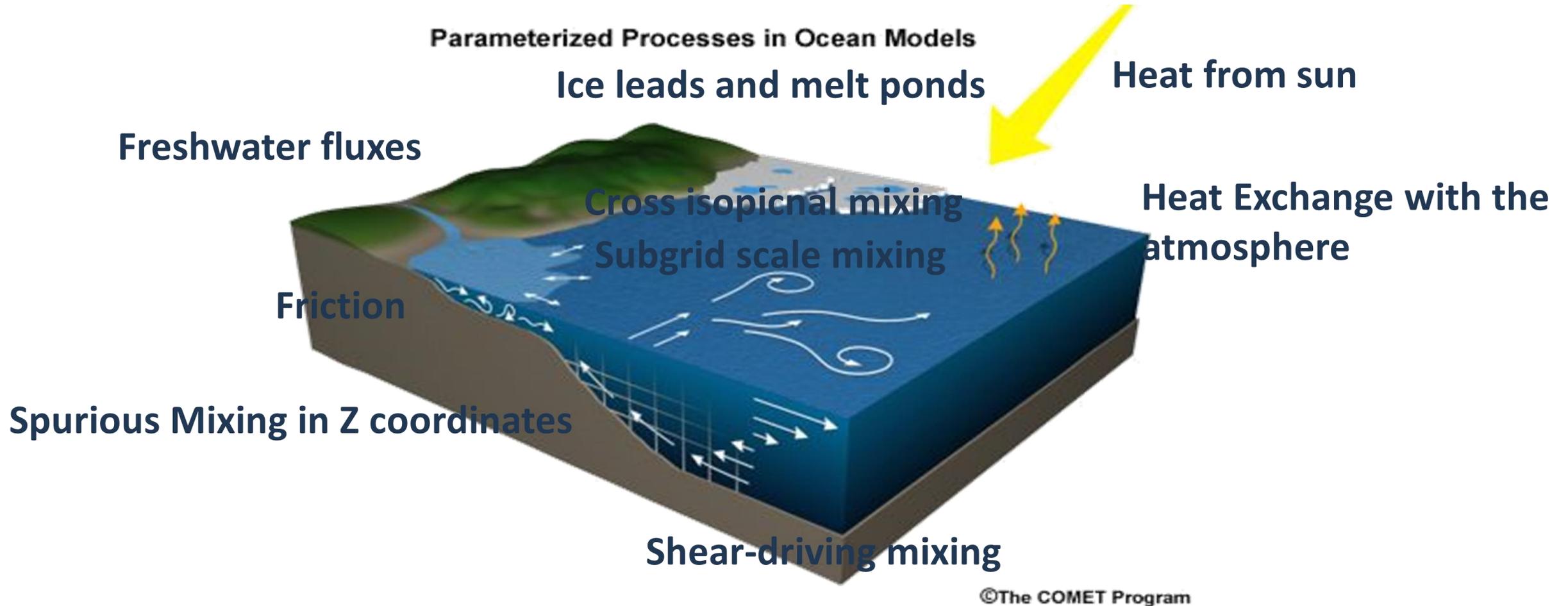
Finite Element Grid for the ADCIRC Model Domain, Long Island Sound



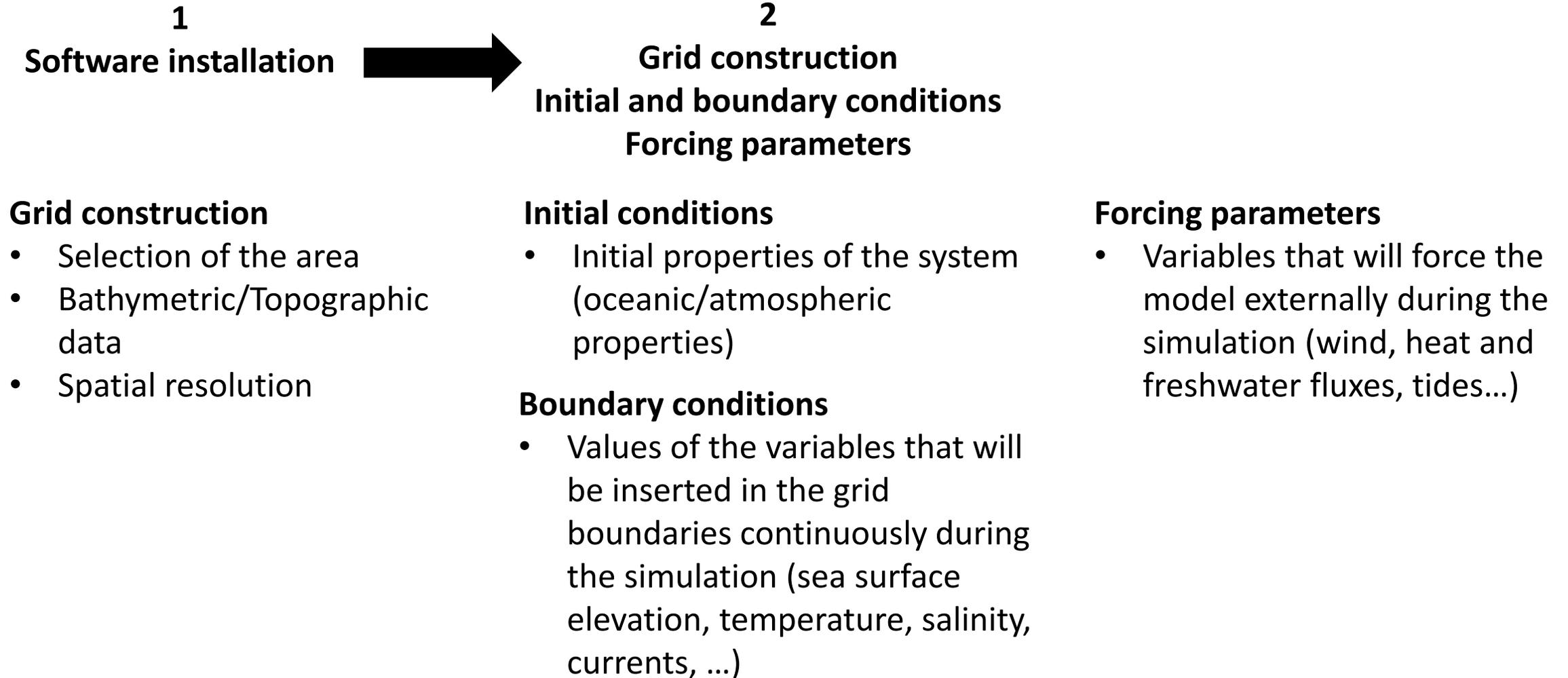
Militello and Zundel 2002

# Numerical models

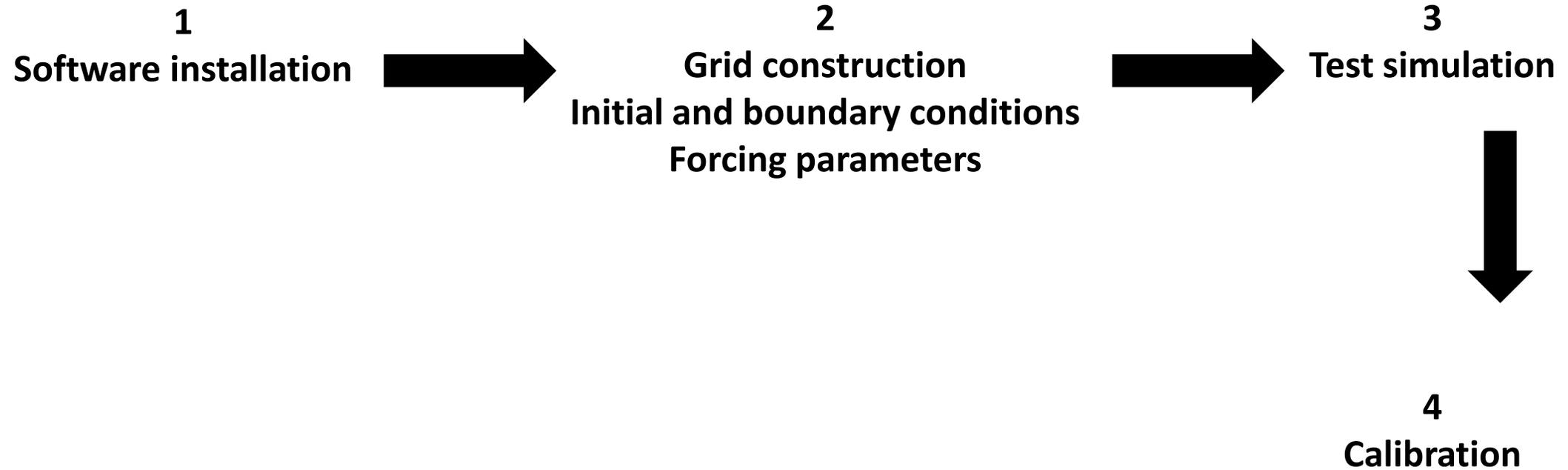
- Grids and parametrizations



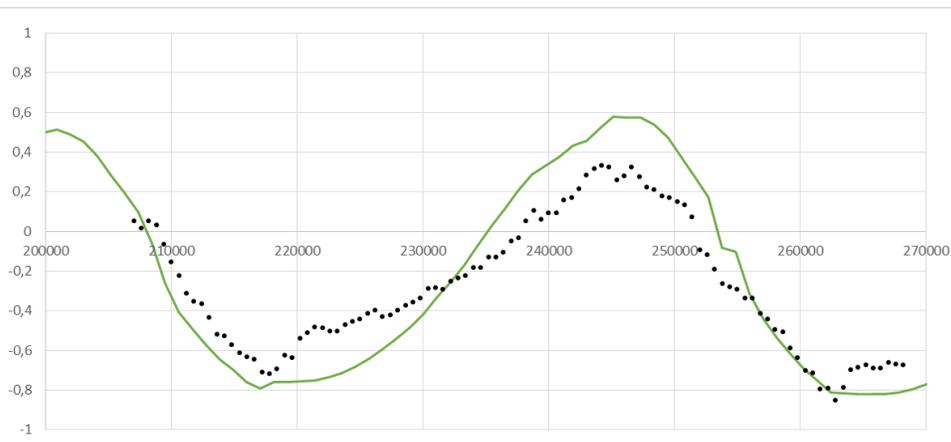
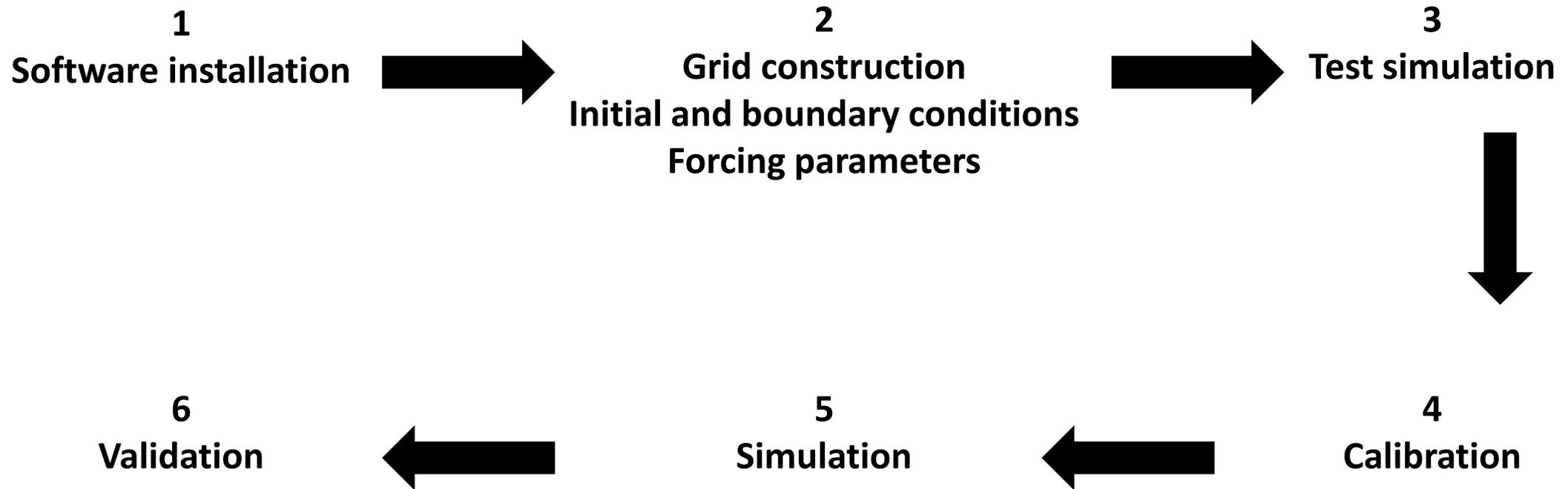
# Numerical models



# Numerical models

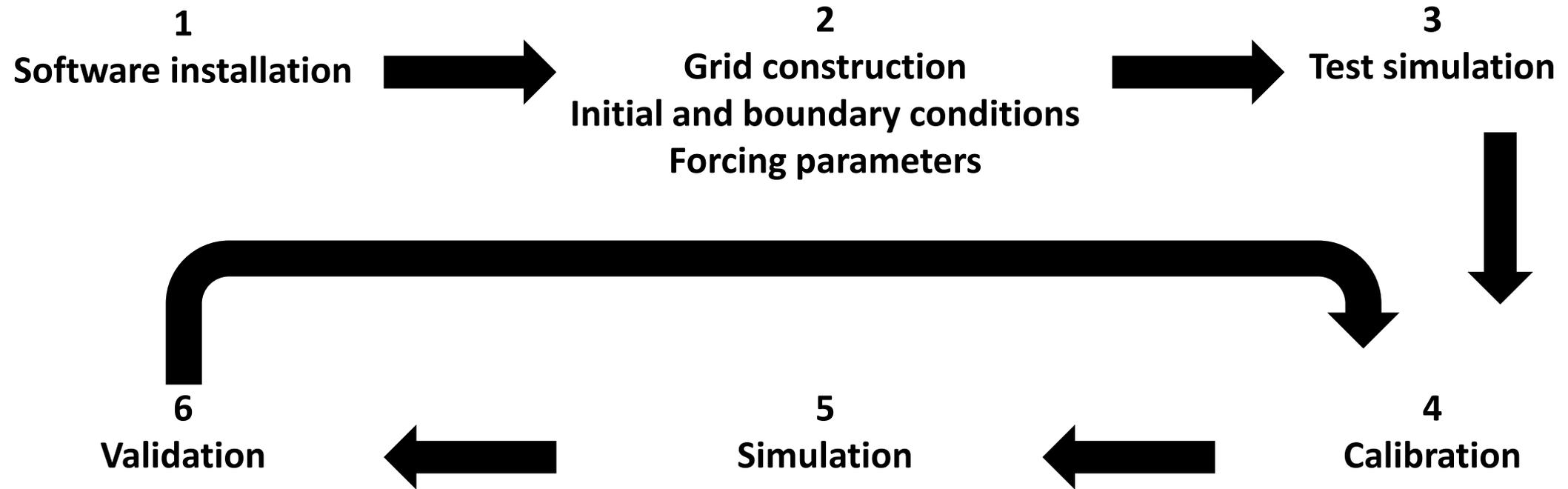


# Numerical models



upação emergente em águas residuais urbanas:  
odos avançados de tratamento e de modelação

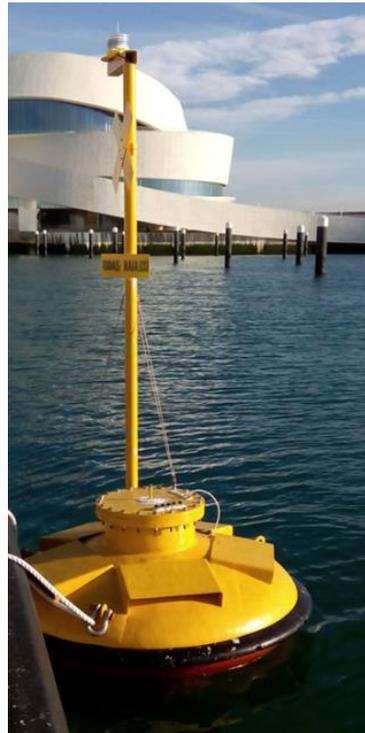
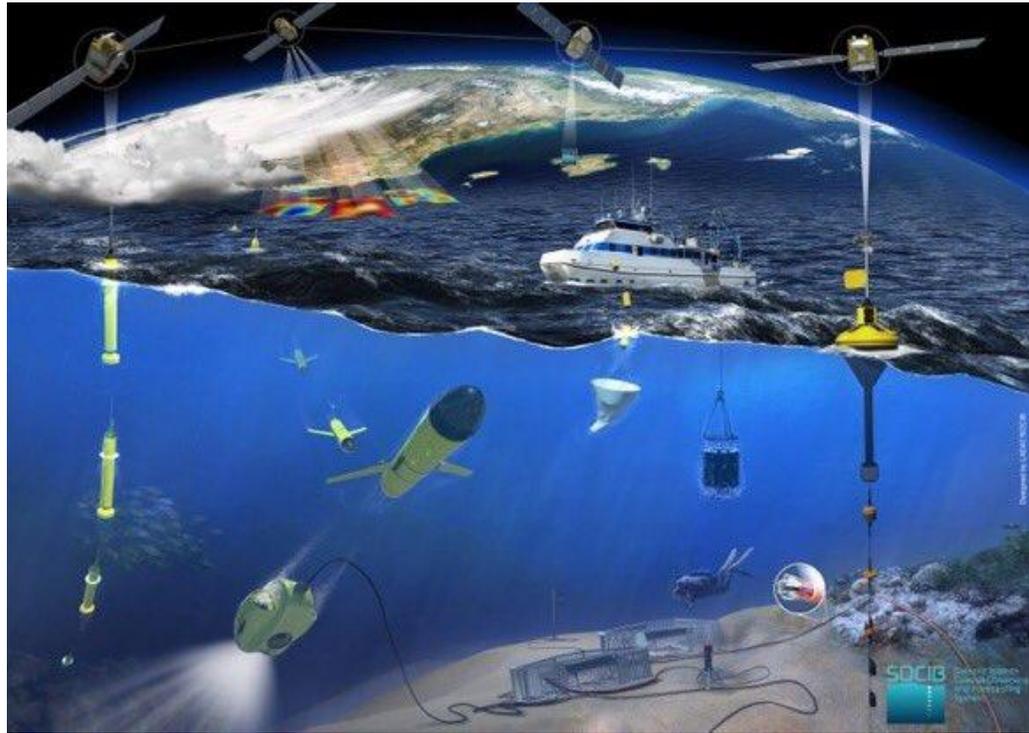
# Numerical models





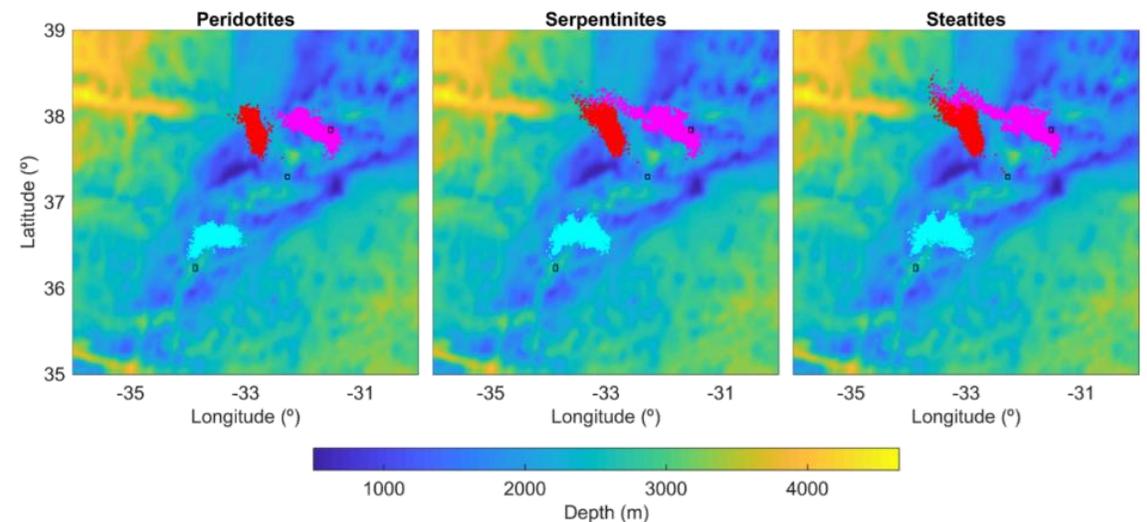
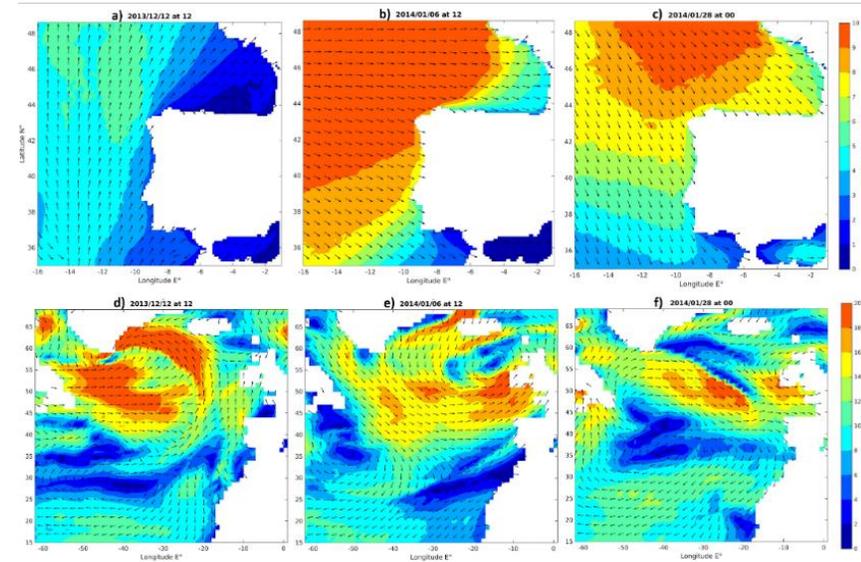
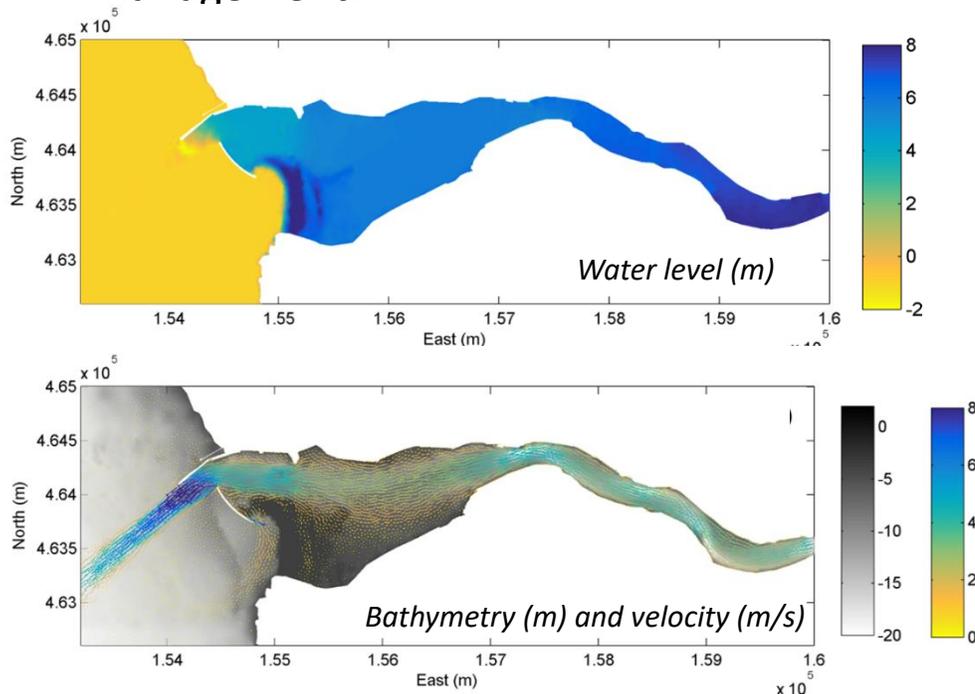
# Numerical models

- Importance of ocean observations for numerical models:
  - Define the initial conditions, the bathymetry of the grid, the forcing conditions.
  - Comparing model results with the reality of the system.
- Data used:
  - Space: Sensors on satellites
  - Marine: Buoys, drifting buoys, gliders, ships, platforms, autonomous vehicles
  - Aerial: Drones, airplanes, hyperspectral cameras, Lidar, GNSS, etc...



# Importance of numerical models

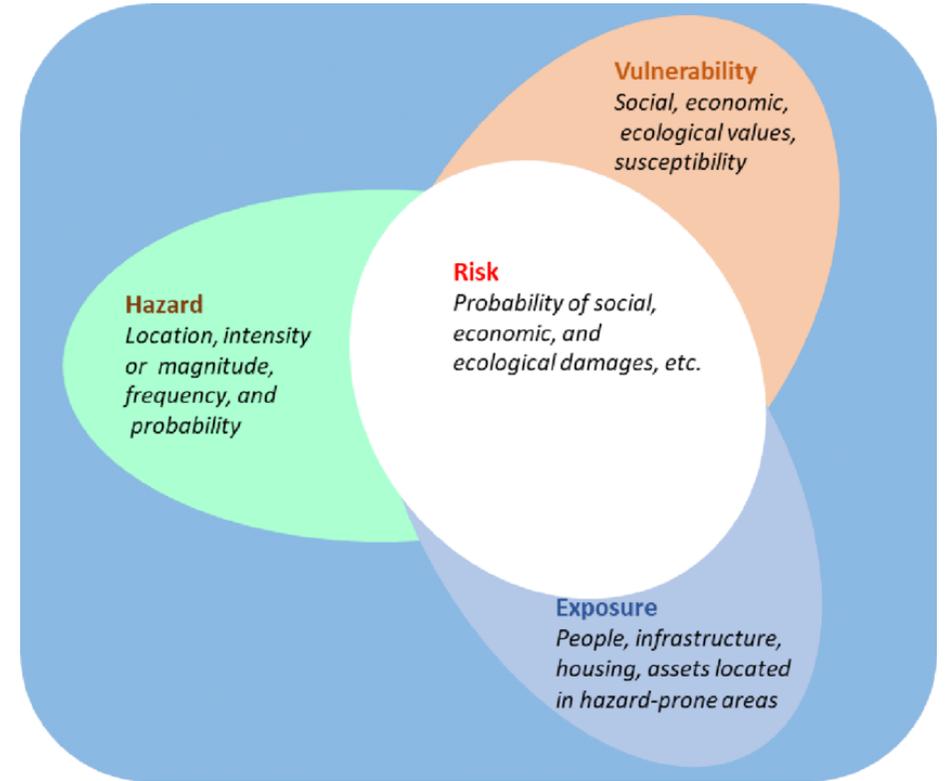
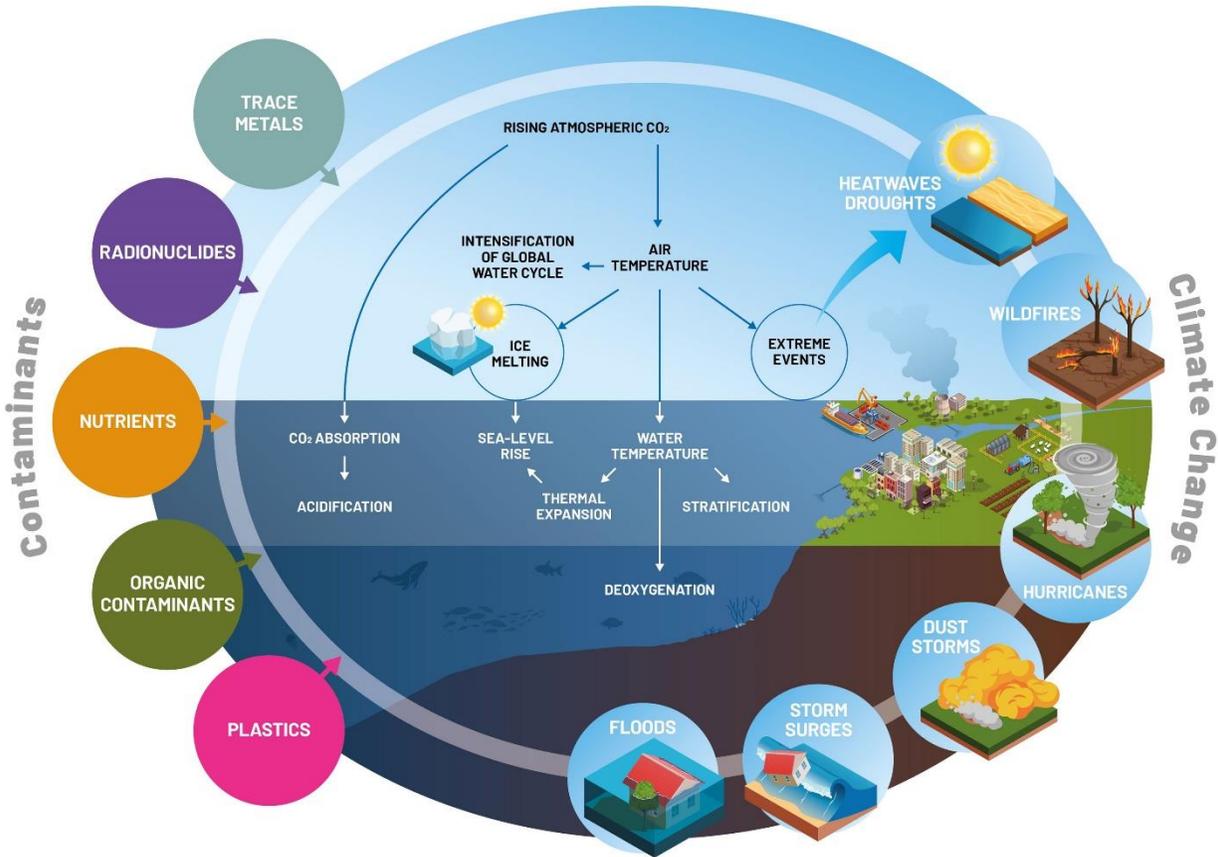
- It is impossible to monitor every point => Lack of continuous, long-term observations.
- Numerical models help to overcome this lack of observation, characterise the behaviour of these areas and anticipate the effects of extreme events, anthropogenic activities or climate change.
- Valuable information for population's safety and ecosystems' sustainability
- Essential decision-making support tools for effective and integrated management.



# Importance of numerical models

- Uses:
  - **Interpretation of** physical and biogeochemical oceanographic **data**.
  - Representing and **understanding** ocean, coastal and estuarine **processes**.
  - **Isolate** phenomena.
  - **Analytical** applications (test cases).
  - Linking different subsystems of the **climate system**.
  - Representation of **past** (reanalysis) and **future** (forecast) states, and the the **hydro-morphodynamical evolution** of an estuary for short- and long-term periods.
  - Understand the main **circulation patterns** and scenarios.
  - Potential of the region for wave or hydrokinetic **energy** production.
  - Projections of **sea level rise**.
  - Representation of the **effects** on systems (ecosystems, migration patterns, urban settlements, etc.) of:
    - Sea states
    - Extreme events (waves, floods, ...)
    - Climate change
    - Man-made interventions (dams, margins alterations, dredging activities, breakwaters, NBS)
    - Trends and evolutions (SST, SSS, currents, nutrients, Chl-A, ...)
    - Pollutants, sediments, larvae, plastics (macro and micro)
  - Key tools for coastal/estuarine management and **risk assessment**.

# Numerical models for risk analysis

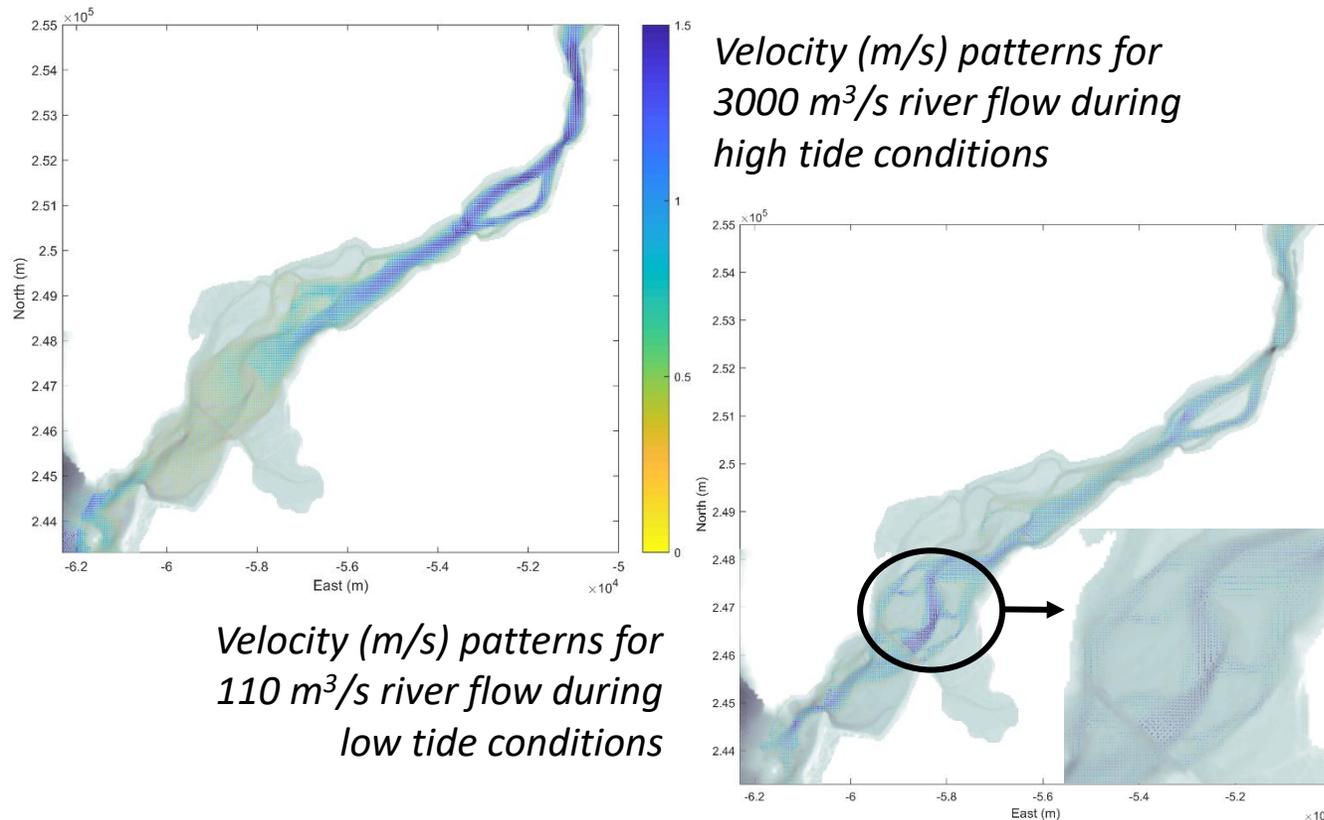


# Numerical models for risk analysis

- Hydrodynamic and lagrangian models for contamination risk analysis at oceanic, coastal and estuarine locations:

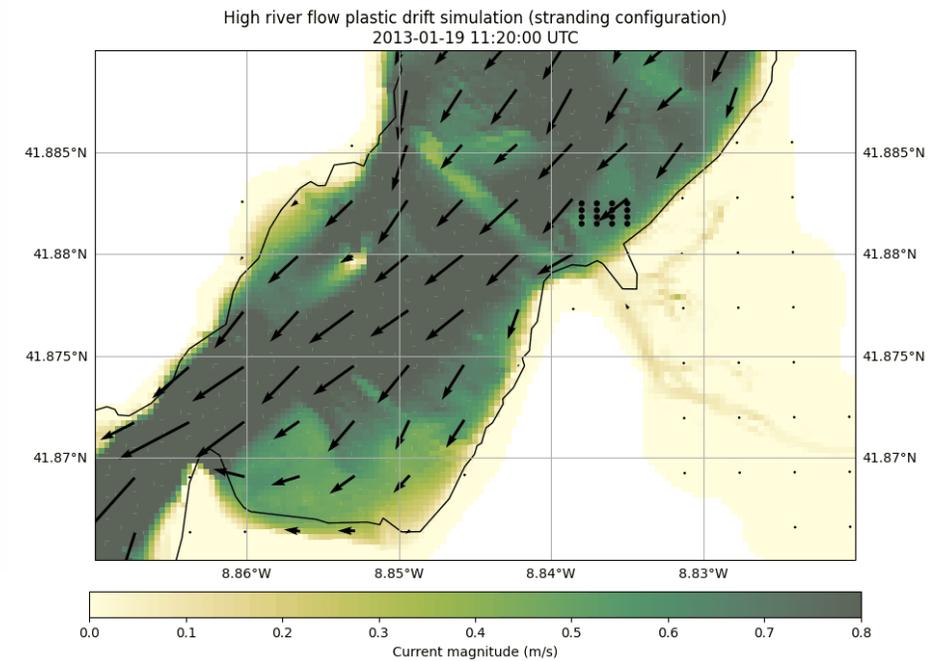
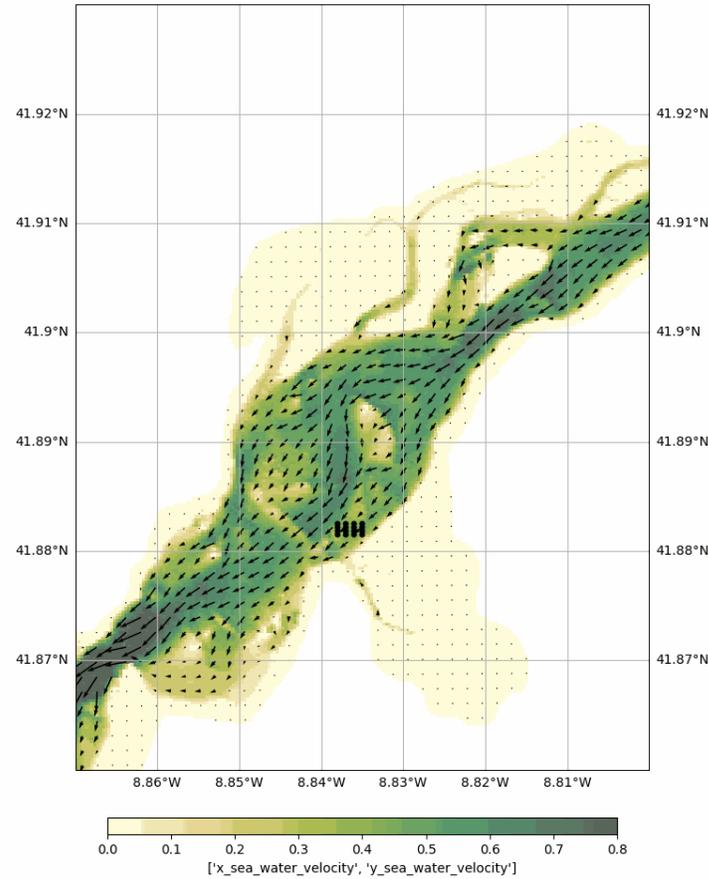
	S1	S2	S3
Time	20 February–9 March 2006	1–13 December 2012	16–26 January 2013
Tide level	TPXO.2	TPXO.2	TPXO.2
River flow ( $\text{m}^3 \text{s}^{-1}$ )	Daily mean	Hourly mean	Hourly mean
Run length (days)	18	13	11

Numerical simulations	Return period (years)	River flow ( $\text{m}^3/\text{s}$ )		Scenario	Oceanic elevation (m)
		Minho	Douro		
S1	100	6038	17634	Historic	3.0
S2		6038	17634	RCP 4.5 2100	3.5
S3		6038	17634	RCP 8.5 2100	3.7
S4	1000	8262	24629	Historic	3.3
S5		8262	24629	RCP 4.5 2100	3.7
S6		8262	24629	RCP 8.5 2100	4



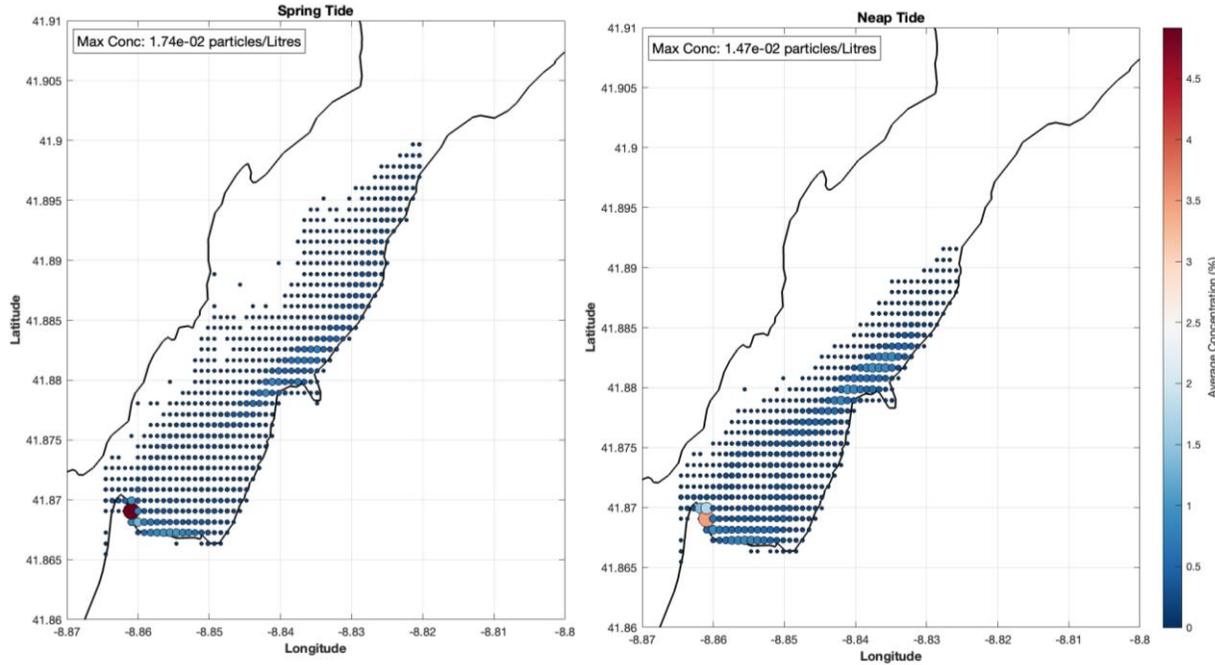
# Numerical models for risk analysis

- Hydrodynamic and lagrangian models for contamination risk analysis at oceanic, coastal and estuarine locations:



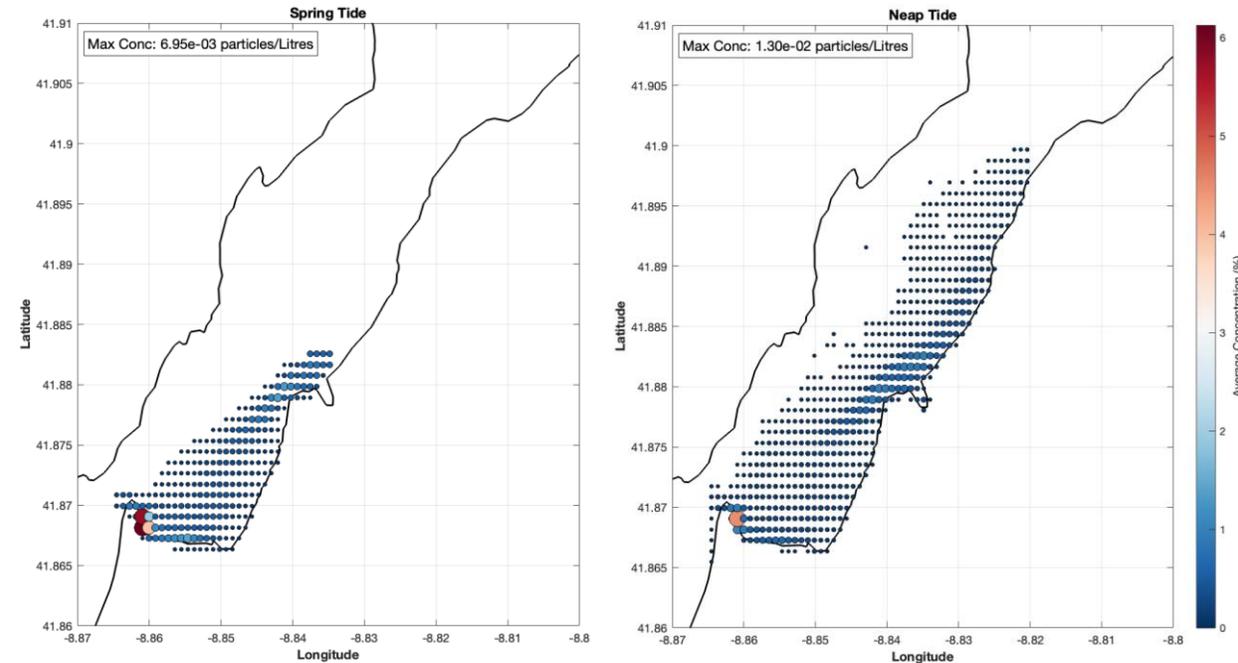
# Numerical models for risk analysis

- Hydrodynamic and lagrangian models for contamination risk analysis at oceanic, coastal and estuarine locations:



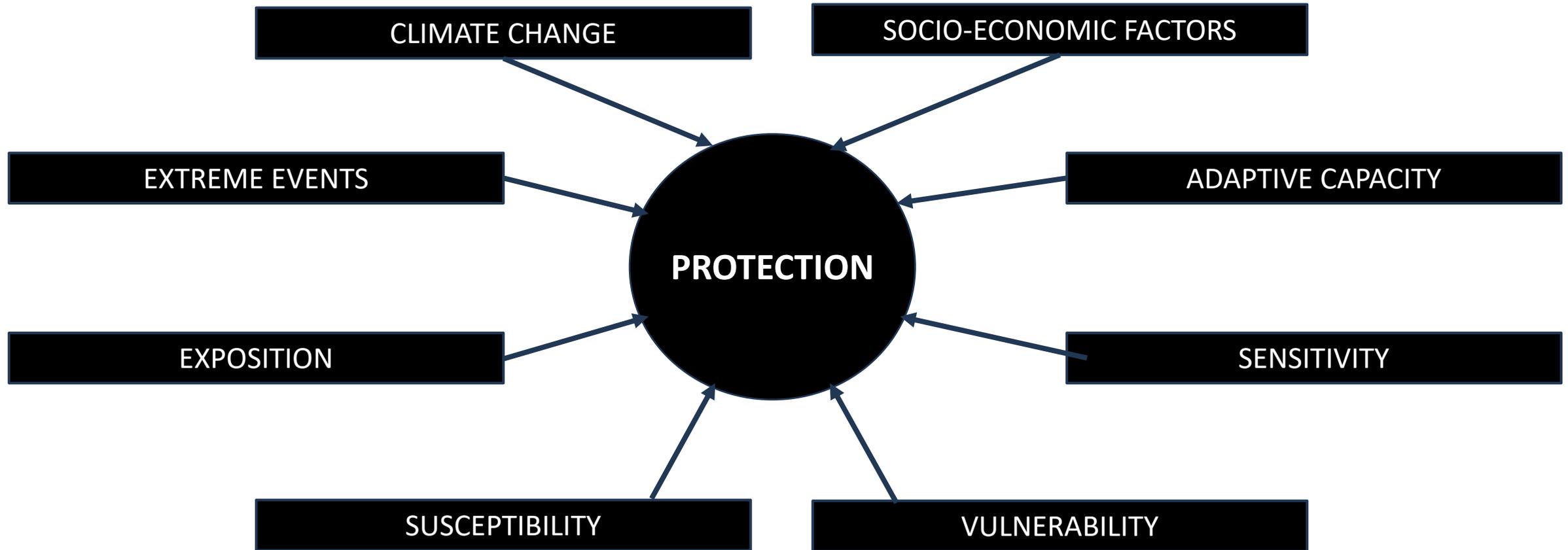
Accumulation zones in 'Summer' scenario: Neap tides vs. Spring tides

Accumulation zones in 'Winter' scenario: Neap tides vs. Spring tides



# Numerical models for risk analysis

- But modelling is just another tool.
- A complete study needs to characterise the vulnerability, susceptibility, exposure, adaptive capacity, sensitivity and economic factors of a system in order to protect the community and the environment.



# Thank you!

*Workshop*  
*Risco ambiental de contaminantes de preocupação emergente em águas residuais urbanas: ferramentas de monitorização biológica, química e métodos avançados de tratamento e de modelação*

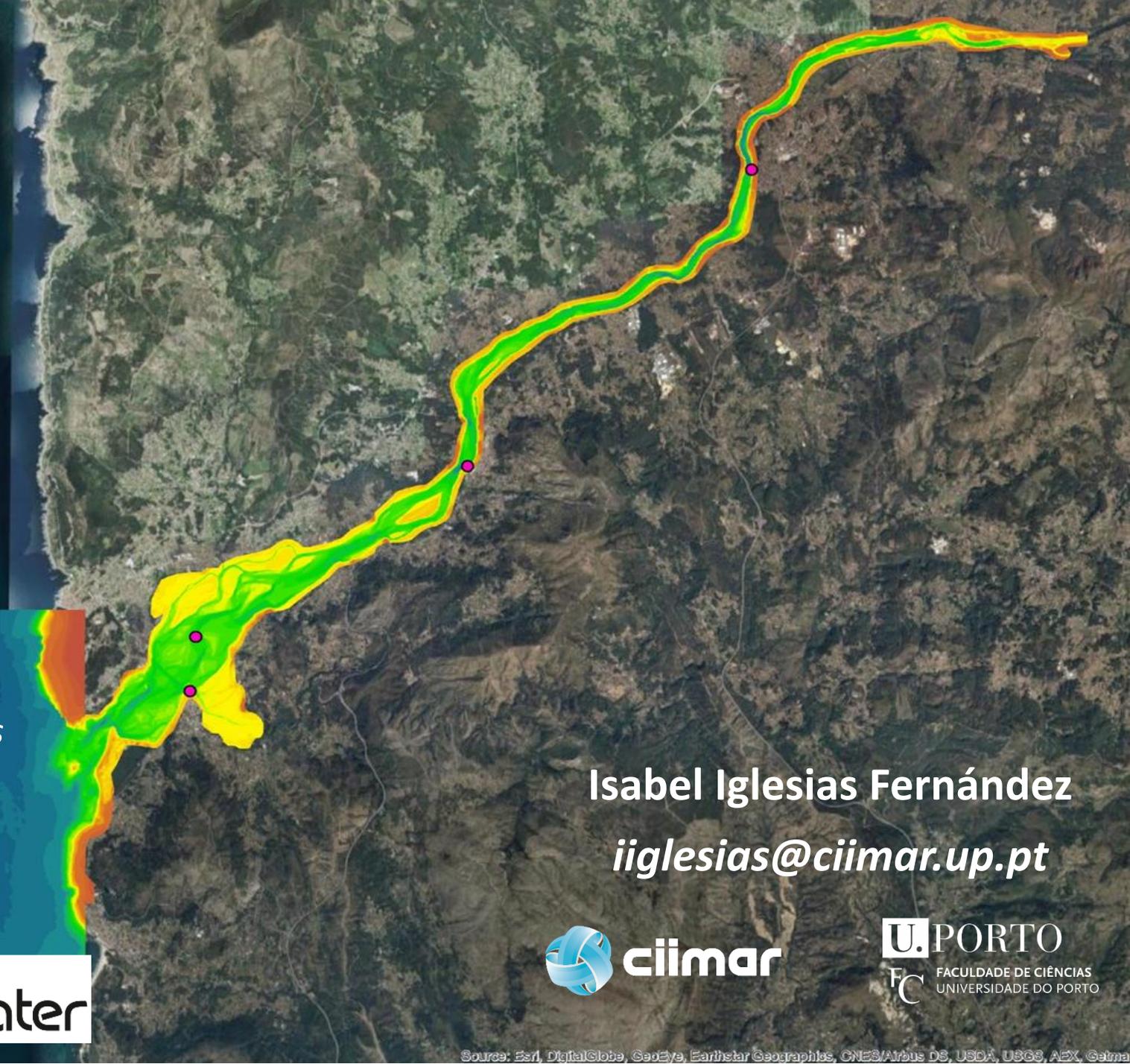
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# A modelação numérica como ferramenta de apoio à avaliação de risco ambiental: modelos hidrodinâmicos e ecológicos

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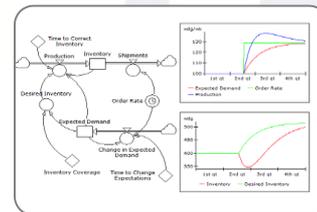
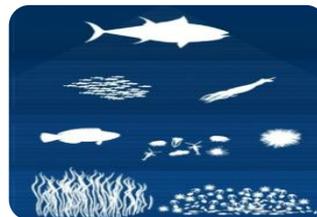
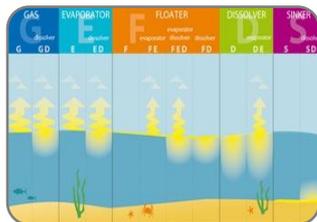




# A modelação numérica como ferramenta de apoio à avaliação de risco ambiental: modelos ecológicos

IRENE MARTINS  
ALEXANDRA GUERRA  
ALESSIA AMANCAI RUSSO



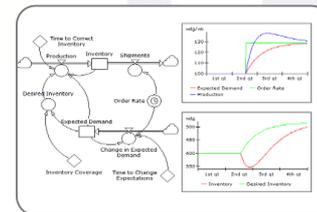
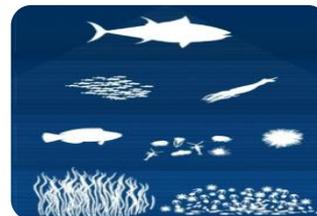
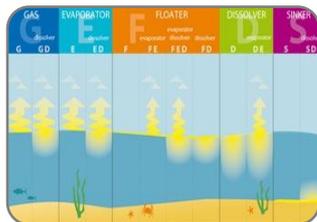


1. Seleção de contaminantes

2. Modelos hidrodinâmicos e de dispersão de contaminantes

3. Modelos de teia trófica e de ecossistema

4. Simulações e análise de cenários para avaliação de risco ambiental



1. Seleção de contaminantes

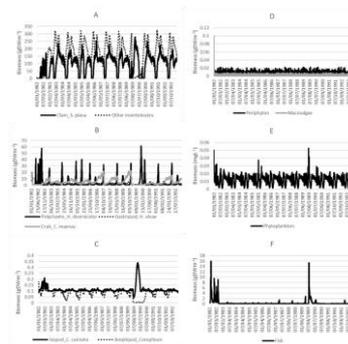
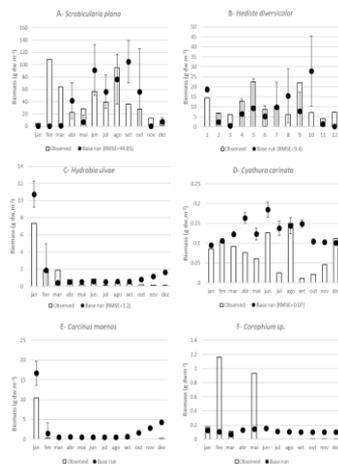
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- Modelo de teia trófica do estuário do Rio Minho
- Calibrado e validado para zona estuarina próxima da embocadura do estuário



**toxics** MDPI

**Article**  
**Prioritizing the Effects of Emerging Contaminants on Estuarine Production under Global Warming Scenarios**

Inês Martins <sup>1,2</sup>, Joana Soares <sup>1,4</sup>, Teresa Neuparth <sup>1,5</sup>, Aldo F. Barreiros <sup>1</sup>, Cândido Xavier <sup>2,6</sup>, Carlos Antunes <sup>1,7,8</sup> and Miguel M. Santos <sup>1,2,4</sup>

<sup>1</sup> CIMAR/CIIMAR—Interdisciplinary Centre of Marine and Environmental Research, University of Porto, Av. General Norton de Matos S/N, 4450-208 Matosinhos, Portugal; pmartins@ciimar.up.pt (I.M.); joanasoares@ciimar.up.pt (J.S.); tneuparth@ciimar.up.pt (T.N.); miguel@ciimar.up.pt (M.M.S.); carlosantunes@ciimar.up.pt (C.A.)  
<sup>2</sup> FCUP—Faculty of Sciences, University of Porto, Rua do Campo Alegre S/N, 4169-007 Porto, Portugal; candido@ciimar.up.pt  
<sup>3</sup> Aquário de Bio Mar, Parque de Casilhões, 4520-290 Vila Nova de Conde, Portugal  
<sup>4</sup> Correspondence: imartins@ciimar.up.pt (I.M.); miguel@ciimar.up.pt (M.M.S.)  
<sup>5</sup> Present address: AIR Centro, TERINCO—Parque de Ciência e Tecnologia da Bica Teófilo, Castelo de Bode S/N, Serra Cha, 9700-702 Azaga do Hermoso, Portugal.

**Abstract:** Due to non-linear interactions, the effects of contaminant mixtures on aquatic ecosystems are difficult to assess, especially under temperature rise that will likely exacerbate the complexity of the responses. Yet, under the current climatic crisis, assessing the effects of some contaminants and temperature is paramount to understanding the biological impacts of mixtures of stressors on aquatic ecosystems. Here, we use an ecosystem model followed by global sensitivity analysis (GSA) to prioritize the effects of four single-emerging contaminants (ECUs) and their mixture, combined with

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Journal homepage: [www.elsevier.com/locate/ecolind](http://www.elsevier.com/locate/ecolind)

**Antagonistic effects of multiple stressors on macroinvertebrate biomass from a temperate estuary (Minho estuary, NW Iberian Peninsula)**

Inês Martins<sup>a,\*</sup>, Ester Dias<sup>a</sup>, Mariana I. Irti<sup>a</sup>, Francisco J. Campuzano<sup>a</sup>, Lígia Pinho<sup>b</sup>, Miguel M. Santos<sup>a,c</sup>, Carlos Antunes<sup>a,d,e</sup>

<sup>a</sup> CIMAR/CIIMAR—Interdisciplinary Centre of Marine and Environmental Research, University of Porto, Rua do Campo Alegre S/N, 4169-007 Porto, Portugal  
<sup>b</sup> ICMAR/CIIMAR—Interdisciplinary Centre of Marine and Environmental Research, University of Porto, Rua do Campo Alegre S/N, 4169-007 Porto, Portugal  
<sup>c</sup> MAREC/CIIMAR—Interdisciplinary Centre of Marine and Environmental Research, University of Porto, Rua do Campo Alegre S/N, 4169-007 Porto, Portugal  
<sup>d</sup> Aquário de Bio Mar, Parque de Casilhões, 4520-290 Vila Nova de Conde, Portugal

**ARTICLE INFO**

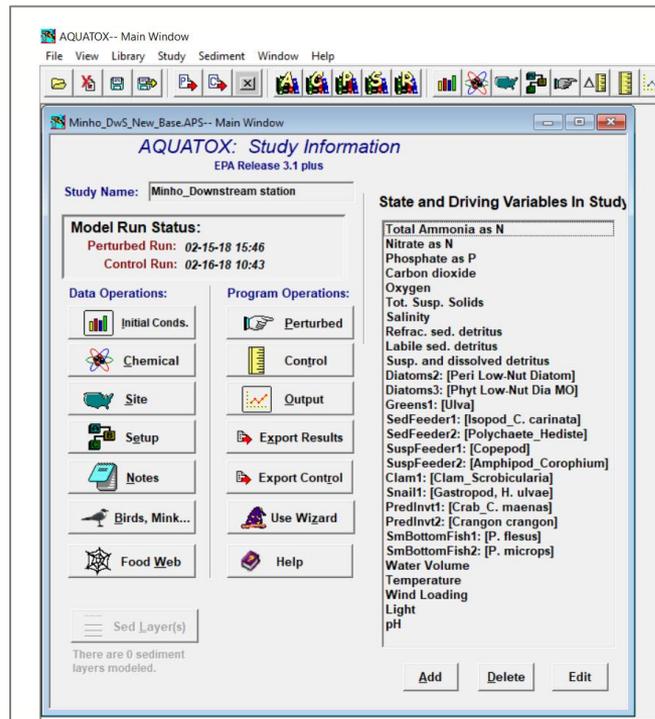
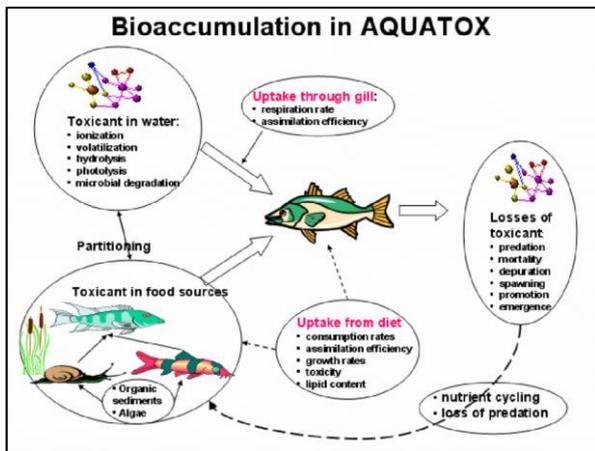
**ABSTRACT**

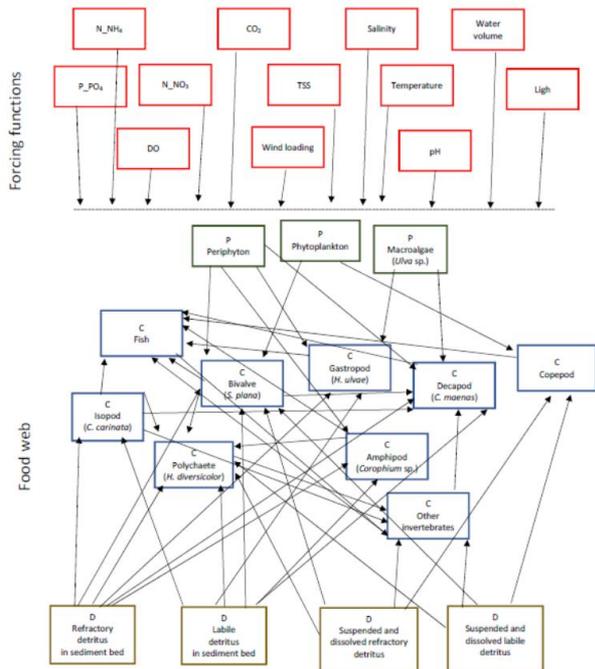
An ecosystem model of the Minho estuary (NW coast of Iberian Peninsula) was implemented in AQUASIM 1.1 (3D-EPA) to check whether the effects of temperature rise, six years, only warm and river flow decrease adding isolated (single stressor) or combined (multiple stressor) would be the same type of response on macroinvertebrate biomass variables and to identify the type of stressor interactions. The model was parameterized with site-specific and species-specific data and assessed for a food web with primary producers, herbivores, omnivores, fish and detritus, with 12 biotic groups, 9 groups of detritus and 12 living functions.

Results showed that macroinvertebrate biomass responded differently to single stressor and multiple stressor scenarios and interactions among the tested stressors were antagonistic. During medium-term simulations



- Modelo de ecosistema
  - . Sub-modelo da teia trófica
  - . Sub-modelo toxicológico





• **3 primary producers groups**  
Periphyton, Phytoplankton, Macroalgae

• **9 consumers groups**  
Isopod, Amphipod, Polychaete, Bivalve, Gastropod, Decapod  
Copepod, Other invertebrates, Fish

• **4 detritus groups**  
Refract. detritus in sediment, Labile detritus in sediment, Suspended and dissolved refract. detritus, Suspended and Dissolved labile detritus

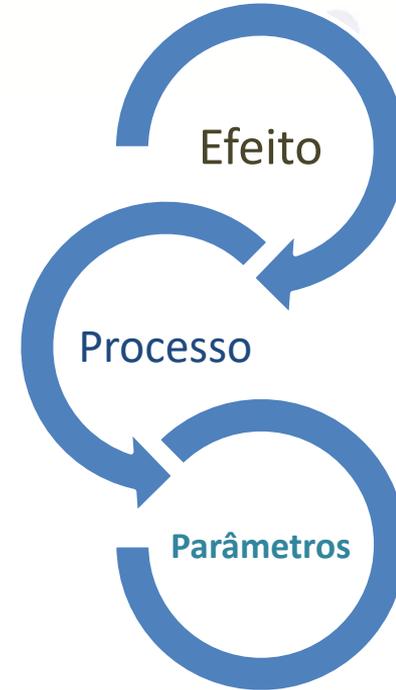
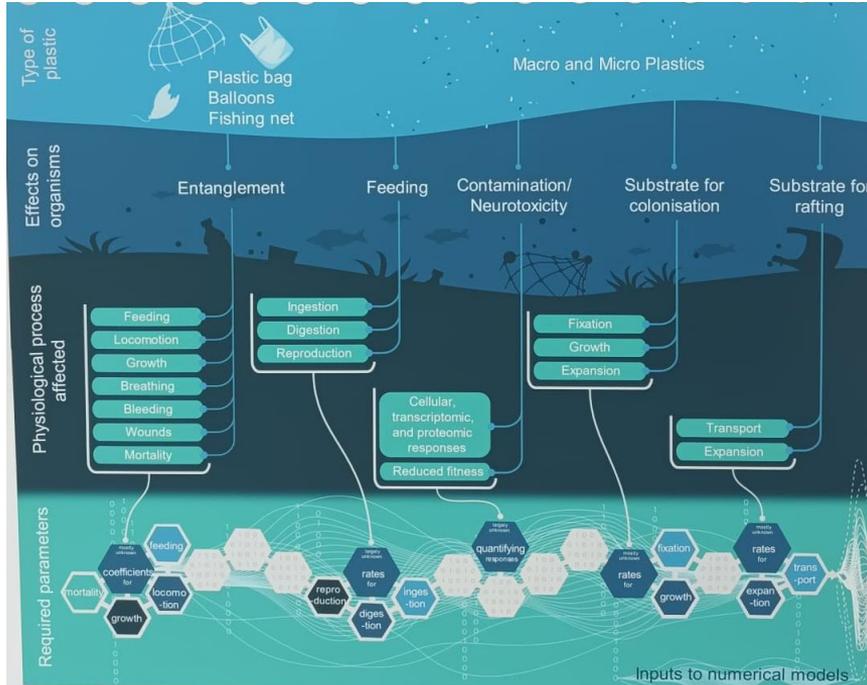


## Simulação base: controlo

# Efeitos dos MP em organismos



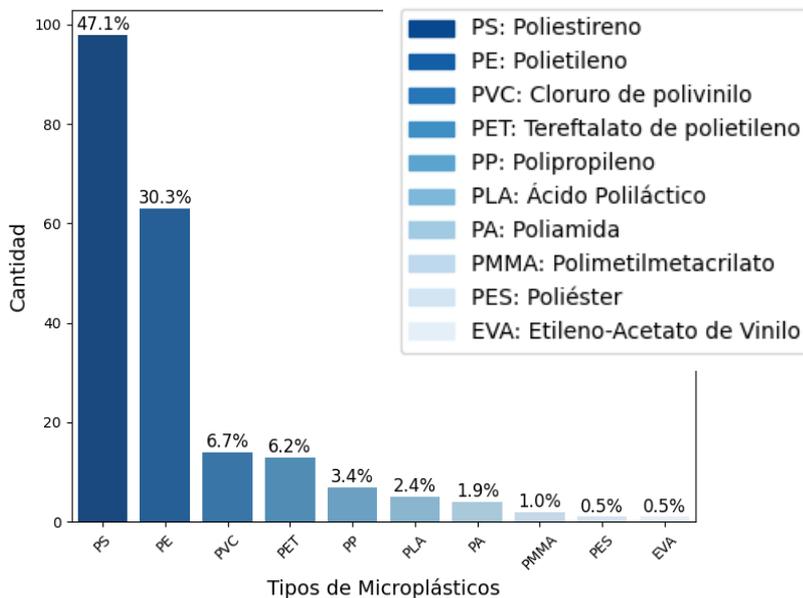
- Incorporação dos efeitos de MP em modelos ecológicos





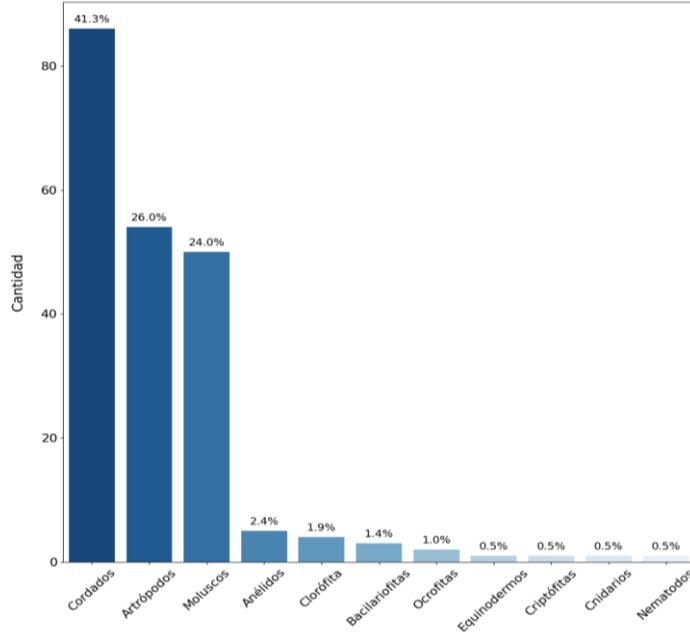
- Efeitos de MPs em organismos marinhos

- 
- 190 artigos científicos
  - 2012-2024

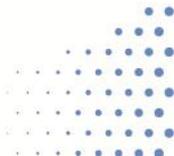
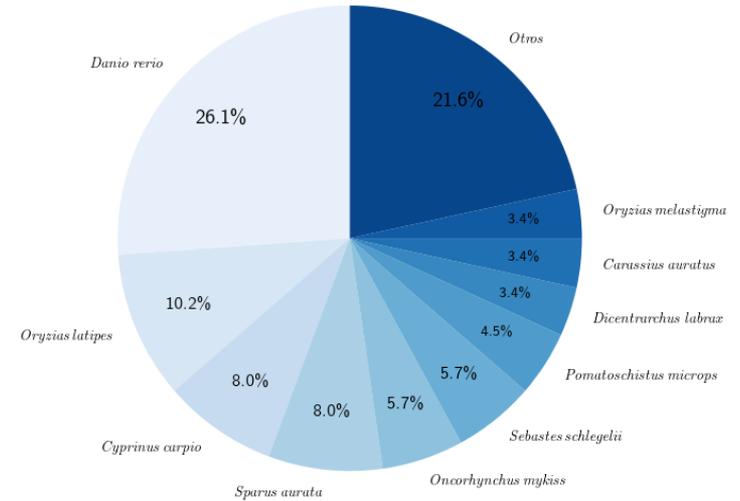


# Espécies mais estudadas

## Efeitos de MPs



Especies de Cordados

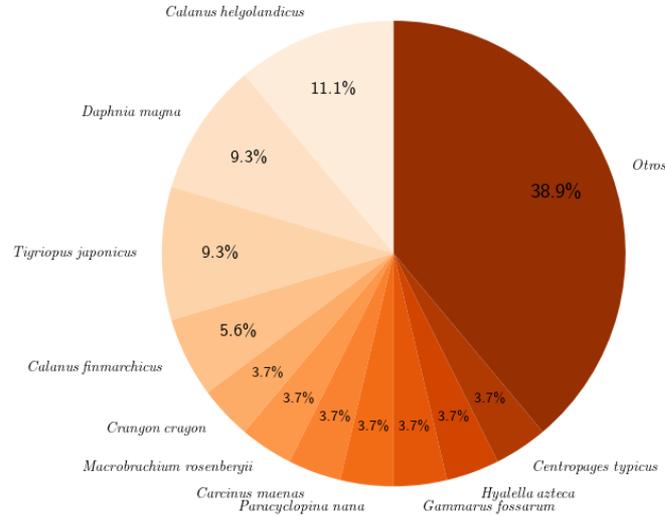


# Espécies mais estudadas

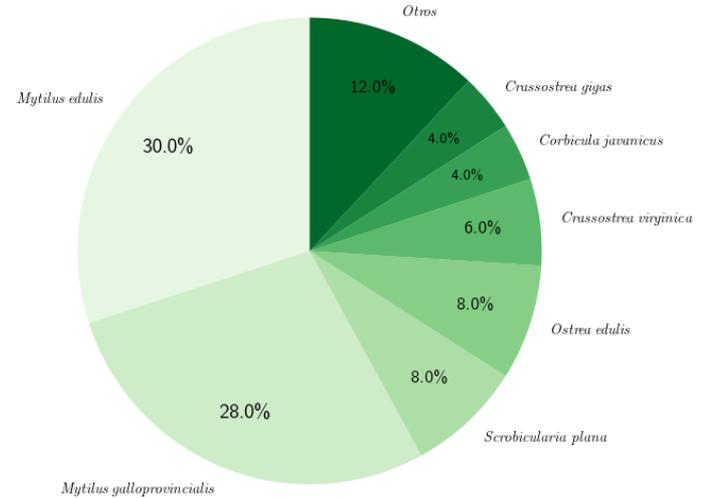
## Efeitos de MPs



Especies de Artrópodos

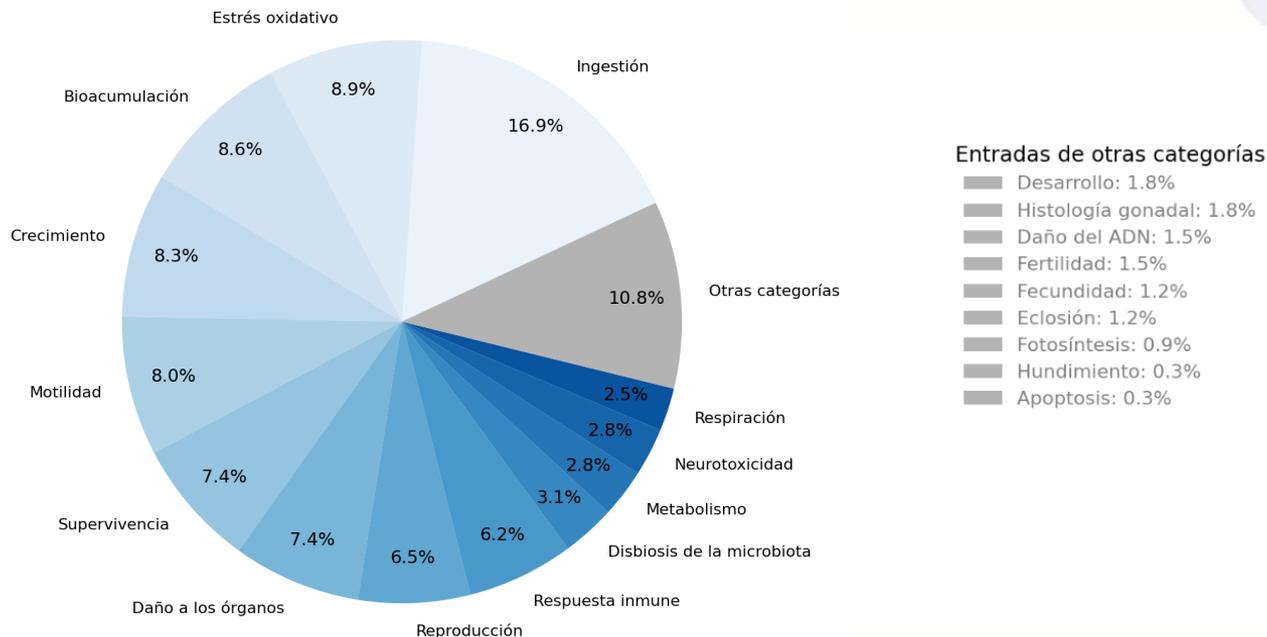


Especies de Moluscos



# End-points (efectos fisiológicos)

## Efeitos de MPs



# Incorporação de efeitos de MP- Critérios de seleção



“Experimental Studies on Microplastics lack Realism”

“... only 17% of concentrations used in laboratory experiments have been found in nature, and 80% of particle sizes used in experiments fall below the size range seen in the majority of environmental sampling”

Bucci et al. (2020)

## TIPO

Embora os MPs reais do ambiente sejam **maioritariamente microfibras**, as microesferas são mais práticas para estudos laboratoriais.

### ESFERAS

(sem dados para fibras)

## TAMANHO

- Mais frequentes: 20 – 5 000  $\mu\text{m}$
- Mais significativos: 20 – 1 000  $\mu\text{m}$

Tendência: Fragmentação contínua → **aumento das partículas mais pequenas**

[20 – 1 000  $\mu\text{m}$ ]

## CONCENTRAÇÃO

- Mar/rios: 0,0005–16 MPs/L
- Estudos realistas\*: efeitos para concentrações de 0,003–0,007; 0,025 e 25 MPs/mL.

\*Horn et al., 2020; Woods et al., 2020; Crump et al., 2020)

Tendência: Fragmentação contínua, aumento das partículas pequenas → **maior concentração**

[0,003–100 MPs/mL]

“worst case scenario” (hotspots urbanos)



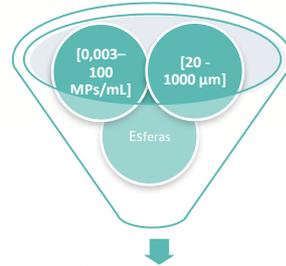
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# Incorporação de efeitos de MP- Critérios de seleção



grupo AQX	size (µm) MP [1 - 5000]		[MP] (MPs/mL)		Value	Effect	AQX parameters	original value	effective value
SuspFeeder5	20,00	20,00	75,000	75,000	--39%	Ingestão de (biomassa) de presas	Max Consumption Feed Half Sat	1,80 1,00	1,10 1,39
SuspFeeder5	20,00	20,00	75,000	75,000	--100%	Défice energético	Excretion : Respiration	0,170	0,340
SuspFeeder5	20,00	20,00	75,000	75,000	--20-30%	Sucesso de eclosão	Gamete mortality	0,00010	0,00013
DepFeeder1	65,60	102,60	0,002	0,433	-87,5%	Redução no recrutamento (nº de juvenis)	Gamete mortality	0,01	0,01875
DepFeeder2	8,00	12,00	100,000	100,000	+42%	Aumento da mortalidade	Mort Coeff	0,0007	0,00099
Clam1	11,00	60,00	10,000	10,000	-50%	redução da taxa de ingestao	Max Consumption Feed Half Sat	0,70 0,05	0,35 0,08
Snail1	65,60	102,60	0,149	0,433	-50%	redução do recrutamento	Gamete mortality	0,25	0,38
PredInv2	50,00	500,00	0,350	0,350	-20,63%	Redução da taxa de crescimento	Max Consumption Feed Half Sat	0,18 0,05	0,14 0,06
SmBottomFish1 e 2	0,50	15,00	53,900	$\frac{7279344}{900}$	-38 a 80%	Taxa de ganho de peso (WGR%)	CA RA	0,30 0,0028	0,19 0,0039
Greens1	10,00	10,00	7,500	7,500	-45%	Produção de clorofila	Max Photosynth Rate	1,08	0,59

# Incorporação de efeitos de MP no modelo base



Minho\_BR\_DEF\_base.aps - Main Window

**AQUATOX: Study Information**  
EPA Release 3.2

Study Name: Minho\_Downstream station

**Model Run Status:**  
Perturbed Run: 05-0-20 11:00  
Control Run: 05-31-21 12:33

**Data Operations:**  
Initial Conds.  
Chemical  
Site  
Setup  
Notes  
Birds, Mink...  
Food Web

**Program Operations:**  
Perturbed  
Control  
Output  
Export Results  
Export Control  
Use Wizard  
Help

**State and Driving Variables In Study**

Total Ammonia as N  
Nitrate as N  
Phosphate as P  
Carbon dioxide  
Oxygen  
Tot. Susp. Solids  
Salinity  
Refrac. sed. detritus  
Labile sed. detritus  
Susp. and dissolved detritus  
Diatoms2: [Peri Low-Nut Dia.]  
Diatoms3: [Plyt Low-Nut Dia./O]  
Greens1: [Jlva]  
SuspFeeder5: [Copepod]  
SuspFeeder6: [Amphipod\_Cyrophilum]  
DepFeeder1: [Isopod\_C. carinata]  
DepFeeder2: [Polychaete\_Hedote]  
Clam1: [Clam\_Scrobicularia]  
Snail1: [Gastropod\_H. ulvae]  
PredInv1: [Crab\_C. maenas]  
PredInv2: [Other benth.invert]  
SmBottomFish1: [P. leasus]  
SmBottomFish2: [P. microps]

Water Volume  
Temperature  
Wind Loading  
Light  
pH

Add Delete Edit

There are 0 sediment layers modeled.

Ingestão

Reprod.

**Animal Data:** Help

Animal:  Scientific Name:

Trophic Interactions

Animal Type:  Toxicity Record:  Edit All  
 Taxonomic Type or Guild:  Benthic Metric Designation:

**References:**

Half Saturation Feeding	1 mg/L	Leidy & Ploskey '80, p. 42 max.-4.2
Maximum Consumption	1.8 g/g d	Kiorboe et al. 1985
Min Prey for Feeding	0.25 mg/L	Gaudy et al. 2000
Sorting: degree to which there is selective feeding	1 unitless	Default - no sediment effect
Mean wet weight	0.0006 g wet	Thomann '89
Endogenous Respiration	0.01 1/d	Leidy & Ploskey, 198, p. D16 = 0.18; respiration increases when salinity c
Specific Dynamic Action	0.07 (unitless)	Kiorboe et al. 1985
Excretion : Respiration	0.17 ratio	Scavia and Park, 1976; excretion of NH3 used for osmoregulation (Gaud
N to Organics	0 frac. dry	
P to Organics	0 frac. dry	
Wet to Dry	5 ratio	
Gametes : Biomass	0.01 ratio	
Gamete Mortality	0.0001 1/d	
Mortality Coefficient	0.027 1/d	Kimmerer and McKinnon 1987 26 d ave.
Sensitivity to Sediment (lethal effects)	<input type="text" value="Zero Sensitivity"/>	<input type="text" value="Default - no sediment effect"/>
Mean lifespan	26 days	Kimmerer and McKinnon 1987
Fraction that is lipid	0.012 (wet wt.)	

Metabol.

Mort.

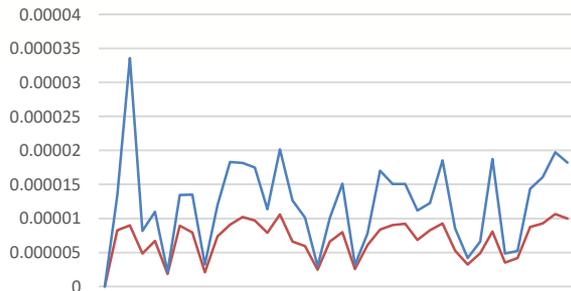
Alteração dos parâmetros específicos de cada espécie de referência, visando refletir os efeitos observados dos MPs.

# Resultados das simulações: biomassa\_grupos funcionais

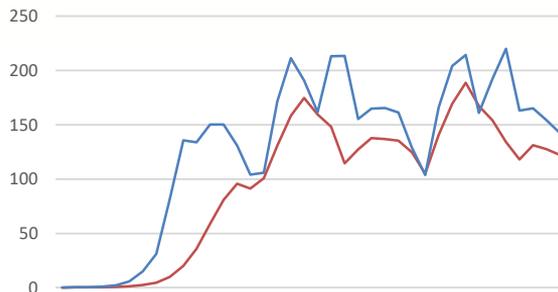


— MP  
— Base

### Copepods

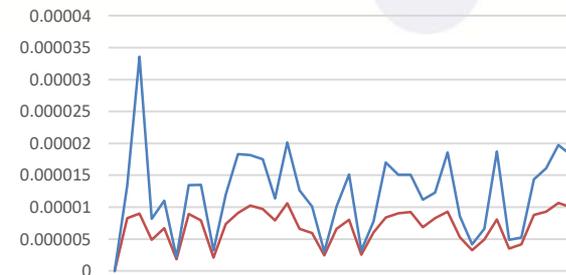


### Benthic invertebrates

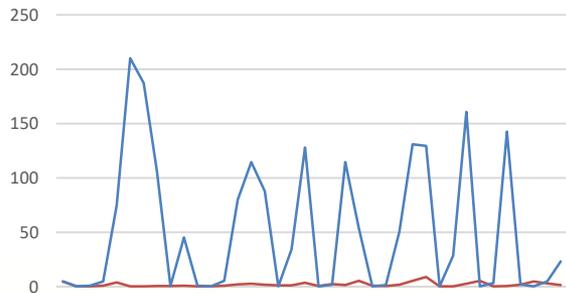


### Amphipods (g/m2 dry)

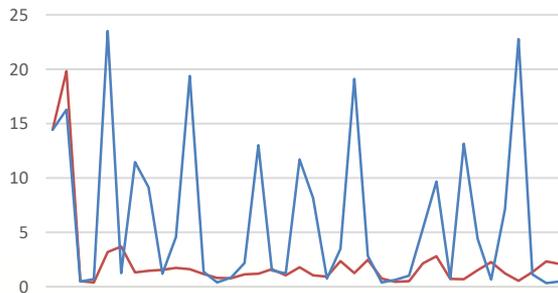
Sem efeito direto dos MPs



### Clams



### Polychaeta



**Copépodes e Anfípodes** → Redução moderada da biomassa com MPs. (Anfípodes, estão a sofrer efeitos indiretos - via teia trófica)

**Bivalves** → Colapso populacional evidente no cenário com MPs.

**Poliquetas** → Biomassa bastante reduzida e menos oscilatória com MPs.

**Invertebrados Bentónicos** → Queda consistente da biomassa com MPs.

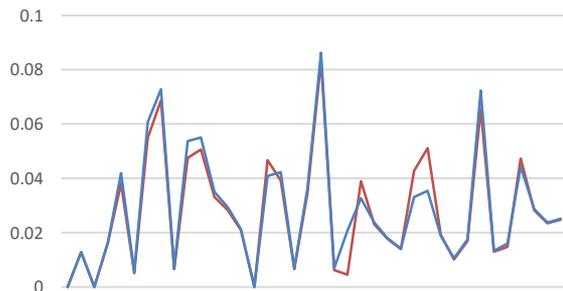


# Resultados das simulações: indicadores do sistema

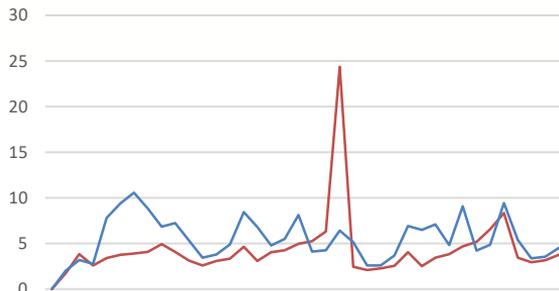


— MP  
— Base

GPP (gO<sub>2</sub>/m<sup>2</sup> d)



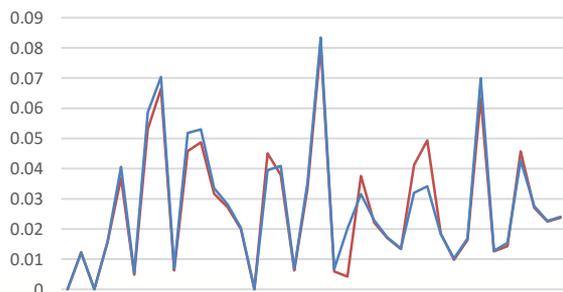
Community Resp. (gO<sub>2</sub>/m<sup>2</sup> d)



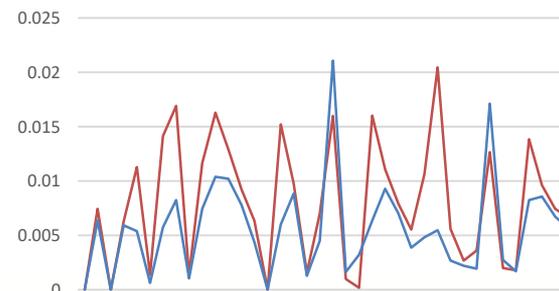
Turnover (B/P) (days)



NPP (gO<sub>2</sub>/m<sup>2</sup> d)



P/R (frac)



**GPP:** Quantidade total de oxigénio produzido pela fotossíntese → Sem efeito

**NPP:** Energia que sobra da fotossíntese depois da respiração dos produtores.

**Respiração Comunitária:** Oxigénio consumido por toda a comunidade → Picos atípicos no cenário MP.

**Turnover (B/P):** Tempo que a biomassa leva para se renovar.

**P/R:** Equilíbrio entre produção e consumo de energia no ecossistema.

# Conclusões preliminares: Efeitos de MPs



- Foram simulados os efeitos dos MPs em parâmetros fisiológicos de vários grupos funcionais (como filtradores, bivalves e predadores bentónicos), utilizando **intervalos de concentração baseados em estudos laboratoriais**, uma vez que não estão reportados efeitos em organismos marinhos para as baixas concentrações de MP medidas *in situ* (estuário do Minho).
- As simulações mostraram **reduções significativas nas biomassas** de alguns grupos, refletindo efeitos adversos de MPs.
- No entanto, os indicadores globais do estado do ecossistema (ex: produtividade primária líquida e bruta, turnover, etc) mantiveram-se estáveis ou com variações pouco relevantes.
- Estes resultados indicam uma **resiliência relativa do sistema** em relação aos efeitos dos MPs; os efeitos manifestam-se sobretudo de forma localizada e em alguns grupos funcionais, sem comprometer o funcionamento geral do ecossistema a curto/médio prazo.

**Os presentes resultados fornecem uma indicação útil sobre os possíveis impactos ecológicos dos MPs, mas devem ser interpretados com precaução.**

**O modelo pode ser melhorado caso surjam novos dados que permitam melhorar a sua parameterização.**

Interreg



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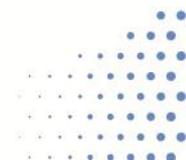


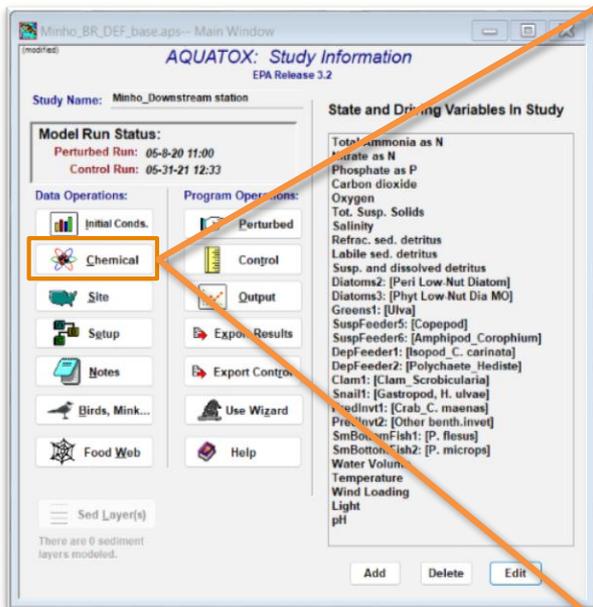
## Transposição de Dados Experimentais

- Muitos dos efeitos dos MPs foram retirados de ensaios laboratoriais que não refletem as concentrações de MPs quantificadas no ambiente.

## Limitações dos Parâmetros no AQUATOX

- O sub-modelo ecotoxicológico não contempla uma classe própria para MPs, sendo necessário ajustar parâmetros funcionais de forma indireta
- Nem todos os grupos funcionais foram parameterizados, por falta de dados quantitativos.
- Muitos efeitos foram estimados a partir de dados aproximados ou “proxies” (e.g. variações na taxa de crescimento)





Minho\_BR\_DEF\_base.apss - Main Window  
(modified) **AQUATOX: Study Information**  
EPA Release 3.2

Study Name: Minho\_Downstream station

**Model Run Status:**  
Perturbed Run: 06-8-20 11:00  
Control Run: 06-31-21 12:33

**Data Operations:**  
Initial Conds.  
**Chemical**  
Site  
Setup  
Notes  
Birds, Mink...  
Food Web

**Program Operations:**  
Perturbed  
Control  
Output  
Expos. Results  
Export Conto...  
Use Wizard  
Help

**State and Driving Variables In Study**

Total ammonia as N  
Nitrate as N  
Phosphate as P  
Carbon dioxide  
Oxygen  
Tot. Susp. Solids  
Salinity  
Refrac. sed. detritus  
Labile sed. detritus  
Susp. and dissolved detritus  
Diatoms2: [Pant Low Nut Diatom]  
Diatoms3: [Phyt Low Nut Dia MO]  
Greens1: [Ulva]  
SuspFeeder5: [Copepod]  
SuspFeeder6: [Amphipod\_Corophium]  
DepFeeder1: [Isopod\_C. carinata]  
DepFeeder2: [Polychaete\_Hediste]  
Clam1: [Clam\_Scrobicularia]  
Snail1: [Gastropod\_H. ulvae]  
InvetInvt1: [Crab\_C. maenas]  
PreInv2: [Other benth.invet]  
SmBottomFish1: [P. flesus]  
SmBottomFish2: [P. microps]  
Water Volume  
Temperature  
Wind Loading  
Light  
pH

There are 0 sediment layers modeled.

Add Delete Edit

### Chemical Properties and Fate Data:

**Toxicity Data**    **PFA Parameters**    Use BCF to Estimate Uptake   
Chemical is a Base

CAS Registry No: 80-05-7

Molecular Weight: 228.29

References:  
Dissociation Constant: 10.29 pKa  
set to zero to ignore ionization)    +-0.69; US-EPA, 2014- i

Knuth, U.S. E.P.A. pers. comm.

Henry's Law Constant: 4E-11 atm-m<sup>3</sup>/mol-Convert  
U.S. E.P.A. Ecotox Profile

Corrales et al., 2015- i

Octanol-Water Partition Coefficient: 3.64 (log)    +- 0.32; Corrales et al., 2015- i

Days to Reach Equilibrium: 5.65  
(Calculated Using Octanol-Water Partition Coefficient)

**Sed/Detritus to Water Partition Coefficient:** at pH 7, KPSED would be:  
Calc dynamically using pH, pKa and LogKOW  2.533E+0003 L/kg OC  
OR, Enter override value for KPSED: 794000 L/kg OC    John;50118, Isobe et al; 794000 Jonkers et al

**Refractory DOM to Water Partition Coefficient:** at pH 7, KDOM would be:  
Calc dynamically using pH, pKa and LogKOW  4.161E+0002 L/kg OM  
OR, Enter override value for KOM:RefrOM: 0 L/kg OM

**Uptake Rate (K1) Detritus:** 1.39 L/kg d    default

**Sorption to / Desorption from Inorganics: (if sediment submodel included)**

	K1 (L/kg dry d)	K2 (1/d)	Kd (L/kg dry)	References:
Cohesives: (<63 µm)	0	0	0	no sorp/desorp
Non-Cohesives: (63-250 µm)	0	0	0	no sorp/desorp
Non-Cohesives2: (>250 µm)	0	0	0	no sorp/desorp

**Activation Energy for Temperature:** 18000 cal/mol    default Lyman, Reehl, Rosenblatt, 1982; assumed; i

**Rate of Anaerobic Microbial Degradation:** 0 1/d    NA; i

**Max. Rate of Aerobic Microbial Degradation:** 0 1/d in water    NA; i

**Uncatalyzed heterolysis constant:** 0 1/d    negligible, Servos et al. 200; assumed; i

## Avaliação de múltiplos fatores de stress

Inclusão de contaminantes orgânicos (e.g. CE, nutrientes) no modelo, de forma a obter previsões (mais) integradas e realistas dos impactos cumulativos de vários "stressors" no ecossistema.



## Dependente de:

- Concentrações de contaminantes medidas *in situ*
- Existência de dados toxicológicos dos contaminantes considerados nos grupos funcionais do modelo

### Chemical Properties and Fate Data:

**Toxicity Data** **PFA Parameters** Use BCF to Estimate Uptake   
 Chemical is a Base

CAS Registry No. **80-05-7**

Molecular Weight **228.29**

Dissociation Constant (to zero to ignore ionization) **10.29 pKa**

Solubility **6.2 ppm**

Henry's Law Constant **4E-11 atm·m<sup>3</sup>/mol·Convert**

Vapor Pressure **8.04E-5 mm Hg**

Octanol-Water Partition Coefficient **3.64 (log)**

Days to Reach Equilibrium: **5.65**  
 (Calculated Using Octanol-Water Partition Coefficient)

**Sed/Detritus to Water Partition Coefficient:** at pH 7, KPSED would be **2.533E+0003 L/kg OC**  
 Calc dynamically using pH, pKa and LogKOW

OR, Enter override value for KPSED **794000 L/kg OC** John:50118, Isobe et al; 794000 John:ers et al

**Refractory DOM to Water Partition Coefficient:** at pH 7, KDOM would be **4.161E+0002 L/kg OM**  
 Calc dynamically using pH, pKa and LogKOW

OR, Enter override value for KOM refDOM **0 L/kg OM**

**Uptake Rate (K1) Detritus** **1.39 L/kg d** default

Sorption to / Desorption from Inorganics: (if sediment submodel included)

	K1 (L/kg dry d)	K2 (1/d)	Kp (L/kg dry)	References:
Cohesives: (<63 µm)	0	0	0	no sorp/desorp
Non-Cohesives: (63-250 µm)	0	0	0	no sorp/desorp
Non-Cohesives2: (>250 µm)	0	0	0	no sorp/desorp

Activation Energy for Temperature **18000 cal/mol** default Lyman, Reesh, Rosenblatt, 1982; assumed; i

Rate of Anaerobic Microbial Degradation **0 1/d** NA: i

Max. Rate of Aerobic Microbial Degradation **0 1/d in water** NA: i

Uncatalyzed hydrolysis constant **0 1/d** negligible, Servos et al. 200; assumed; i

### Animal Toxicity Data

Chemical name	Animal name	LC50 (µg/L)	LC50 exp. time (h)	LC50 comment	K2 Elim. rate const (1/d)	EC50 growth (µg/L)	Growth exp. (h)	EC50 repro (µg/L)	Repro exp (EC50 comment)	Ave. wet wt. (g)	Lipid Fac
Bisphenol-SPA	Clam	791	593	96 ICE Reg. on Freshw fish. n=5, c	1E-01	3.68	49	3.68	49 for Maklax galpov.	2.088	0.015
Bisphenol-SPA	Polychaete	5375	624	96 ICE Reg. on freshw crin. n=8, c	1E-01	11.4	96	11.4	1 for C. clopheta	0.19804	0.0075
Bisphenol-SPA	Gastropod	2100		96 Potencia letalis freshwwater gas	1E-01	1.82	96	1.02	96 for Haliotis demissicola	0.00079	0.0075
Bisphenol-SPA	Copepod	4320	96	96 Marcol et al. 2003	1E-01	550	96	550	96 for A. tonsa	0.001	0.012
Bisphenol-SPA	Amphipod	1100		96 Stamp, Alexandre et al. 1998	1E-01	2500	504	2500	96 for freshw isopod	0.5	0.078
Bisphenol-SPA	Fish	9400	96	96 Marine fish: Alexandre et al. 19K	1E-01	9103	96	9103	49 for Zebra fish: wendyey	1	0.02
Bisphenol-SPA	Freshw fish	4600	96	96 Alexander et al. 1998	3E-01	0	0	0	0	0	0.11
Bisphenol-SPA	Freshw crin	6800	96	96 Pascoe et al. 2002	1E-01	0	0	0	0	0	0
Bisphenol-SPA	Freshw snail	2240	96	96 Mitsu et al. 2009; at 25°C	1E-01	0	0	0	0	0	0
Bisphenol-SPA	Zebra fish larvae	6669	96	96 Thi et al. 2016	3E-01	0	0	0	0	0	0.11
Bisphenol-SPA	Daphnia magna	6000	96	96 Ministry Environm. Japan	1E-01	16000	0	0	0	0	0

Enter or Estimate K2, Calculate K1 and BCF (default behavior)  Enter K1 and K2, Calculate BCF  Enter K1 and BCF, Calculate K2  Enter K2 and BCF, Calculate K1  
 K1, BCF entered on a dry weight basis, lipid frac. is wet wt.

### Plant Toxicity Data

Chemical name	Plant name	EC50 (µg/L)	EC50 exp. time (h)	EC50 dislodge (µg/L)	EC50 comment	K2 Elim. rate const (1/d)	EC50 (µg/L)	EC50 exp. time (h)	Lipid Fac
Bisphenol-SPA	Green	2700	96	0	0	0.150	2700	96	0.0096
Bisphenol-SPA	Diatoms	1000	96	0	0	0.150	1000	96	0.0096
Bisphenol-SPA	Bluegill	1013	96	0	NA	0.150	1013	96	0.0096
Bisphenol-SPA	Maquitos	134	96	0	0	0.150	134	96	0.0096

Enter or Estimate K2, Calculate K1 and BCF (default behavior)  Enter K1 and K2, Calculate BCF  Enter K1 and BCF, Calculate K2  Enter K2 and BCF, Calculate K1  
 K1, BCF entered on a dry weight basis, lipid frac. is wet wt.

Estimate Animal K2's using Kow  Estimate Plant K2's using Kow  Interspecies Toxicity Correlation Models

Estimate plant LC50's using EC50 to LC50 ratio

Estimate animal EC50's using LC50 to EC50 ratio

Help  OK

- LC50 (µg/L)
- K2 Elim. rate const (1/d)
- K1 Uptake const (L/kg d)
- BCF (L/kg)
- Biotransfm. rate (1/d)
- EC50 growth (µg/L)
- Growth exp. (h)
- EC50 repro (µg/L)
- Ave. wet wt. (g)
- ...



**Obrigada!**

[imartins@ciimar.up.pt](mailto:imartins@ciimar.up.pt)

**Interreg**



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