Effect of temperature and light on phytoplankton growth

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Olivier BERNARD, Francesca CASAGLI, Romain RANINI, Ignacio FIERRO, Jineth ARANGO, Kilian BURGI, David JEISON, Antoine SCIANDRA, Lionel GUIDI

BLUE EDGE ASSOCIATED TEAM

OCÉANIA IS AN INRIA CHALLENGE PROJECT

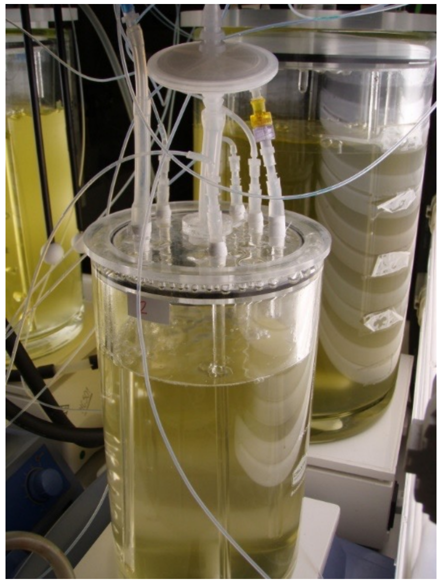
BIOCORE

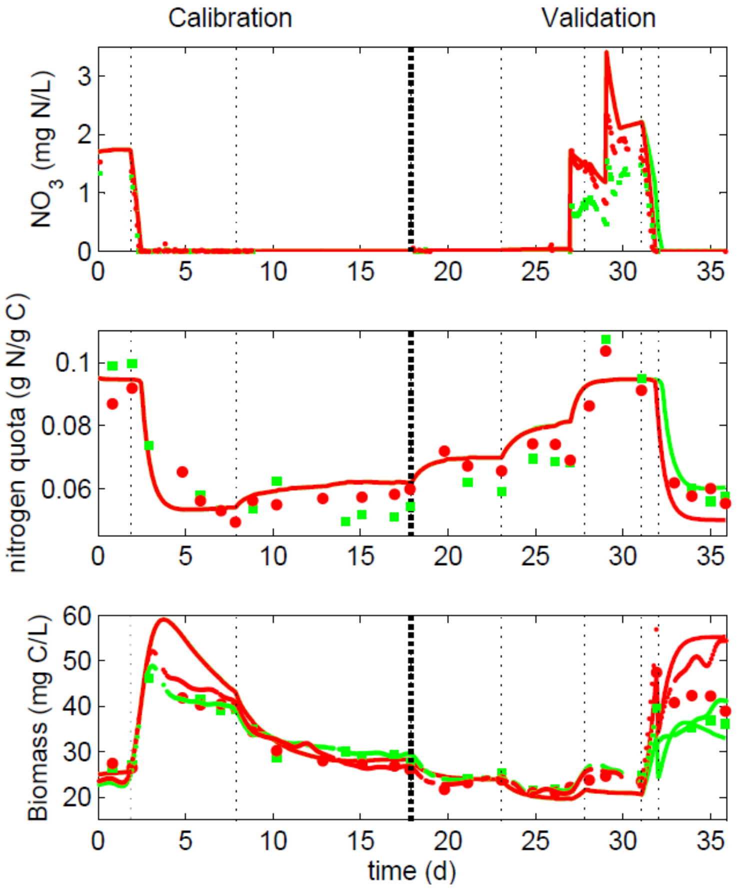
Biological control of artificial ecosystems:
modelling, control and optimization.
Focus on phytoplankton.

$$(D)\begin{cases}\dot{s} = Ds_{in} - \rho(s)x - Ds\\ \dot{q} = \rho(s) - \mu(q)q\\ \dot{x} = \mu(q)x - Dx\end{cases}$$

Uptake rate: $\rho(s) = \rho_m \frac{s}{s+K_s}$

Growth rate: $\mu(q) = \bar{\mu}(1 - \frac{Q_0}{q})$





BioCO_2re

Biocore: joined team with the Oceanographic Laboratory from Villefranche (LOV)

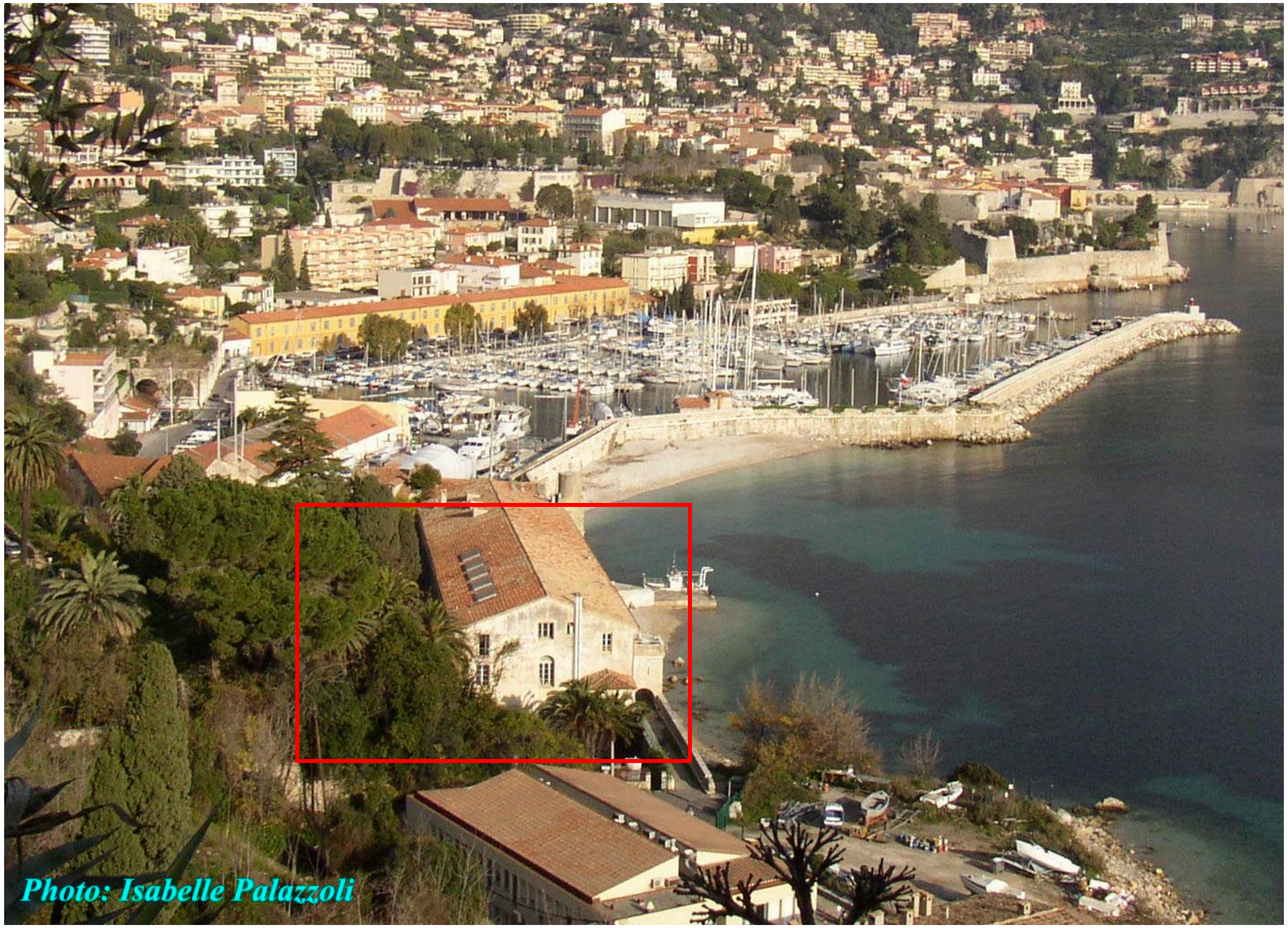
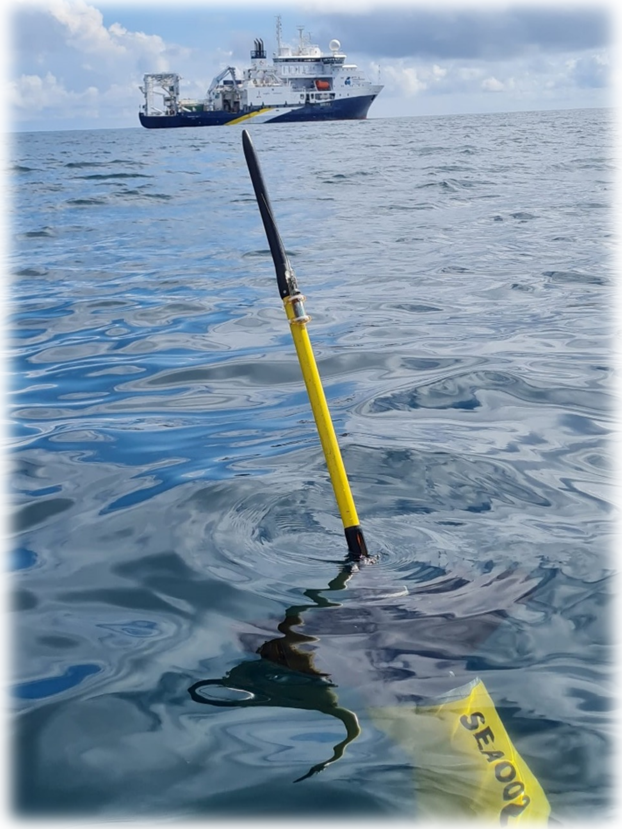


Photo: Isabelle Palazzoli

Link to in situ campaigns

Lionel GUIDI



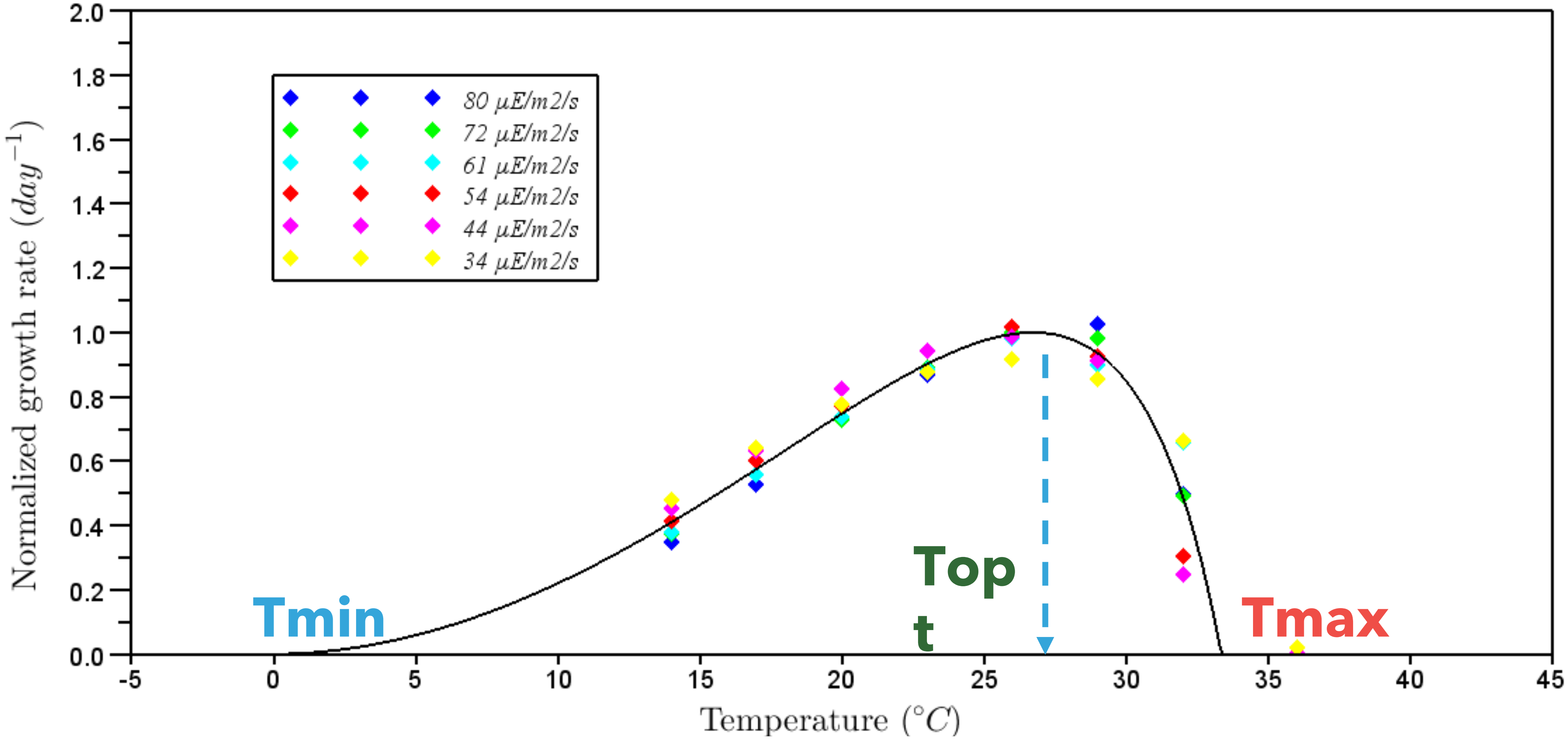
Biocore contribution

- **Understanding the rules driving response to temperature in phytoplankton (O. Bernard)**
- Neural ODE for representing phytoplankton growth driven my light (I. Fierro)
- Towards hybrid modelling of artificial microbial ecosystems (F. Casagli)
- Spatio-temporal high-resolution models of particulate organic matter abundance in the ocean (R. Ranini)

MICROBIAL RESPONSE TO TEMPERATURE

Temperature impact on growth at various light intensities

Temperature response for most of phytoplankton species



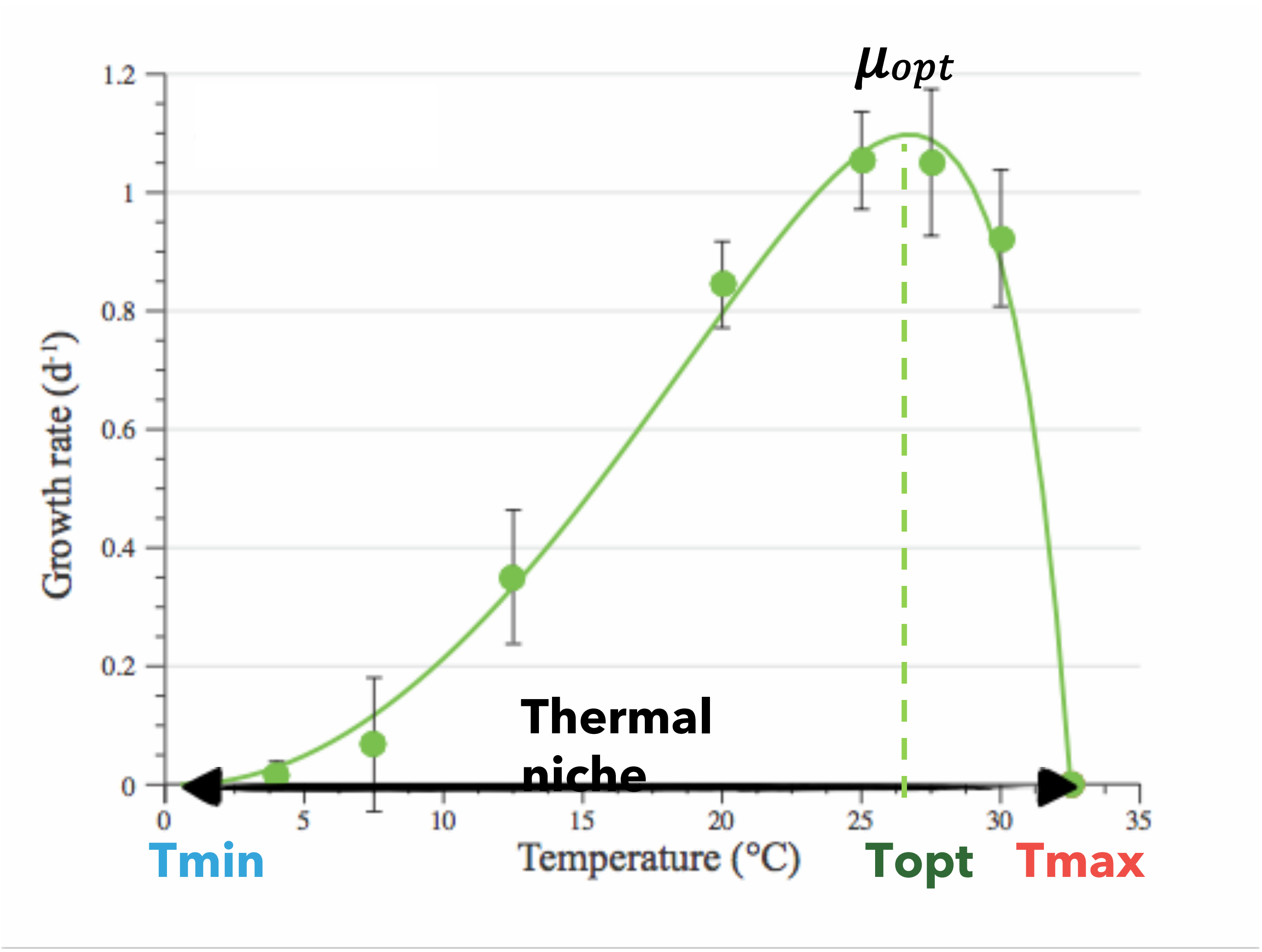
Nannochloropsis oceanica

Modelling growth response to temperature

BR model

Cardinal Parameters

Tmin **Topt** **Tmax** μ_{opt}



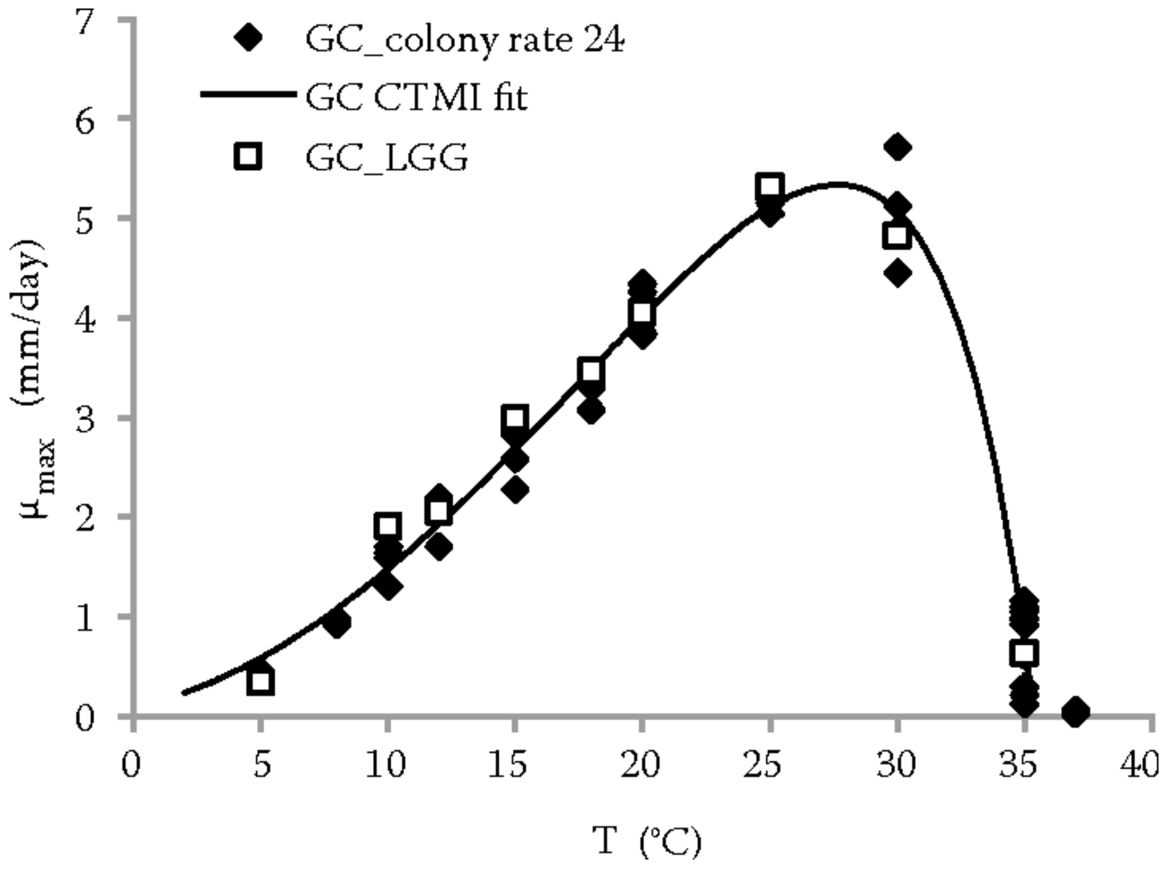
$$\mu_{\max} = \begin{cases} 0 \text{ for } T < T_{\min} \\ \mu_{\text{opt}} \cdot \phi(T) \text{ for } T_{\min} < T < T_{\max}, \\ 0 \text{ for } T > T_{\max}, \end{cases}$$

where

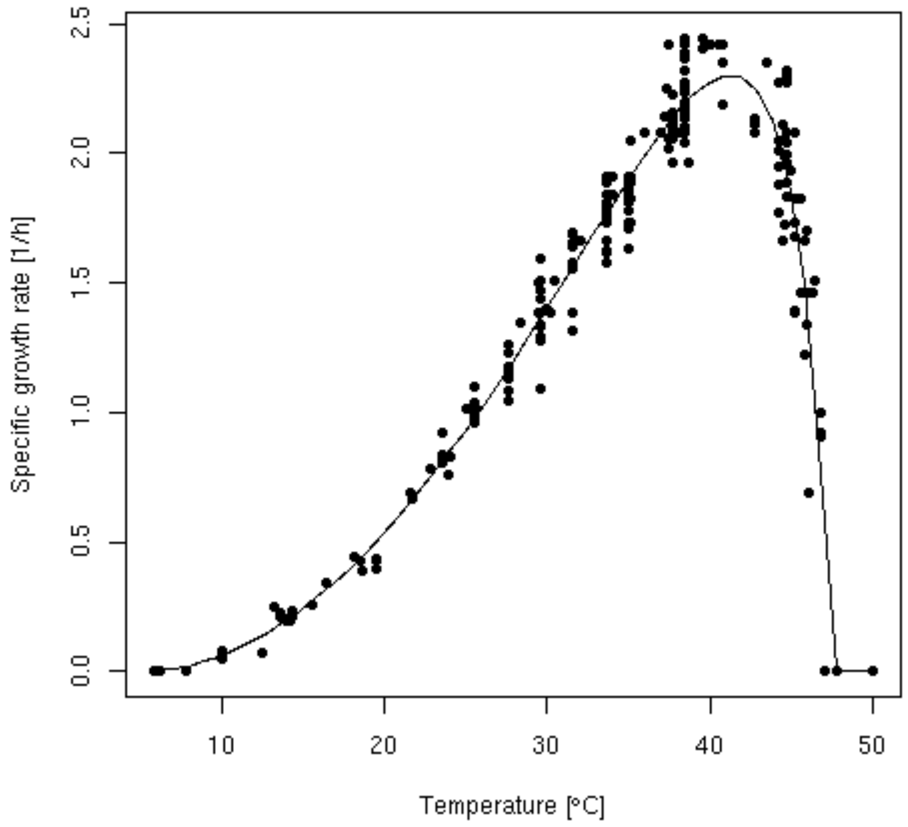
$$\phi(T) = \frac{(T - T_{\max})(T - T_{\min})^2}{(T_{\text{opt}} - T_{\min})[(T_{\text{opt}} - T_{\min})(T - T_{\text{opt}}) - (T_{\text{opt}} - T_{\max})(T_{\text{opt}} + T_{\min} - 2T)]}$$

Bernard & Rémond (2012)

Idem for most of the microorganisms



Geotrichum candidum.(Hudecova et al., 2018)



E. Coli (Lobry& Chessel, 2003)

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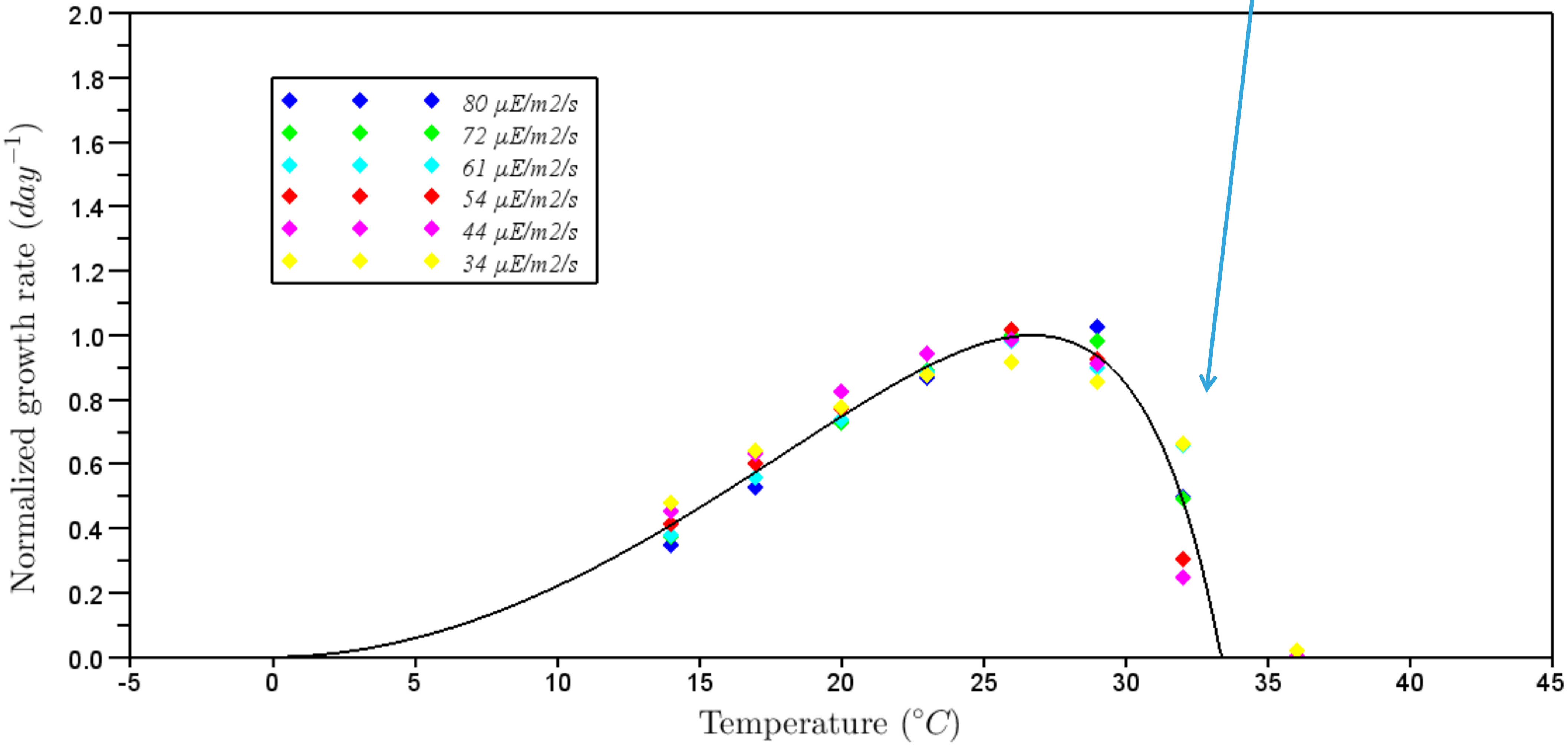
WHICH BIOLOGICAL MECHANISMS INVOLVED?

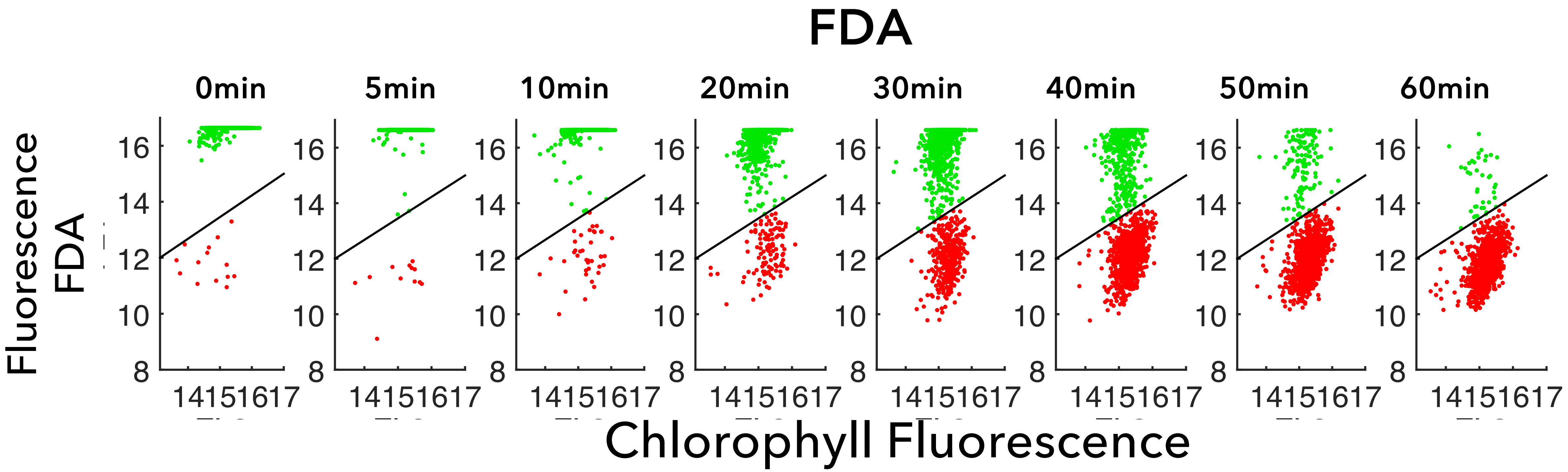
What happens at high temperature?

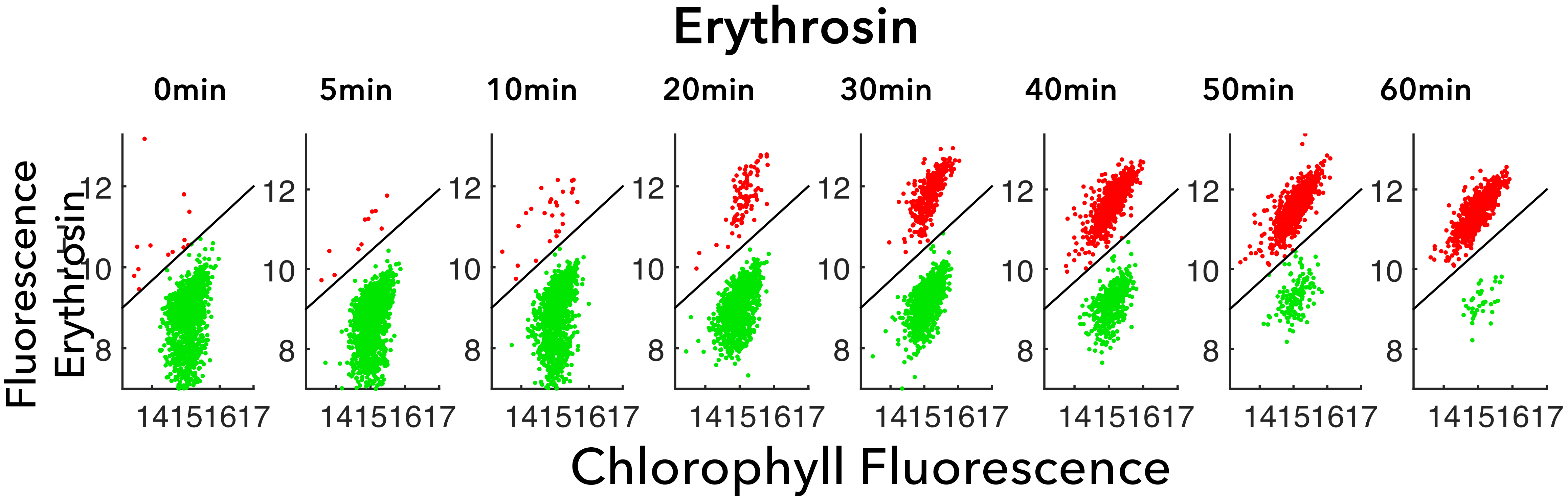
Why is the temperature response droping?



Nannochloropsis oceanica

Kinetics examples at 45°c





Dunaliella salina

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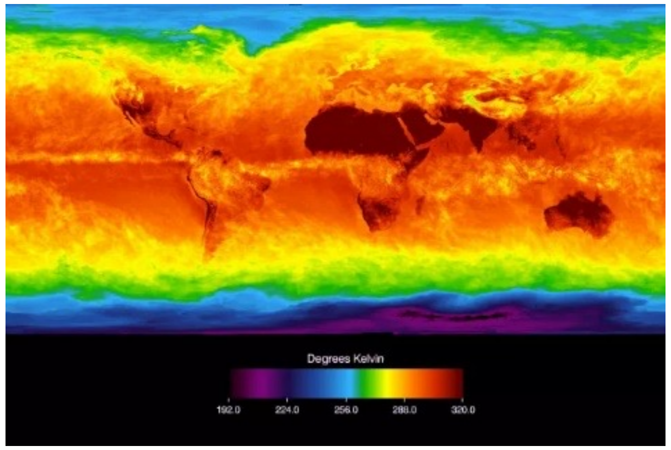
ARE THERE SOME GENERAL PATTERNS HIDDEN BEHIND TEMPERATURE RESPONSE?

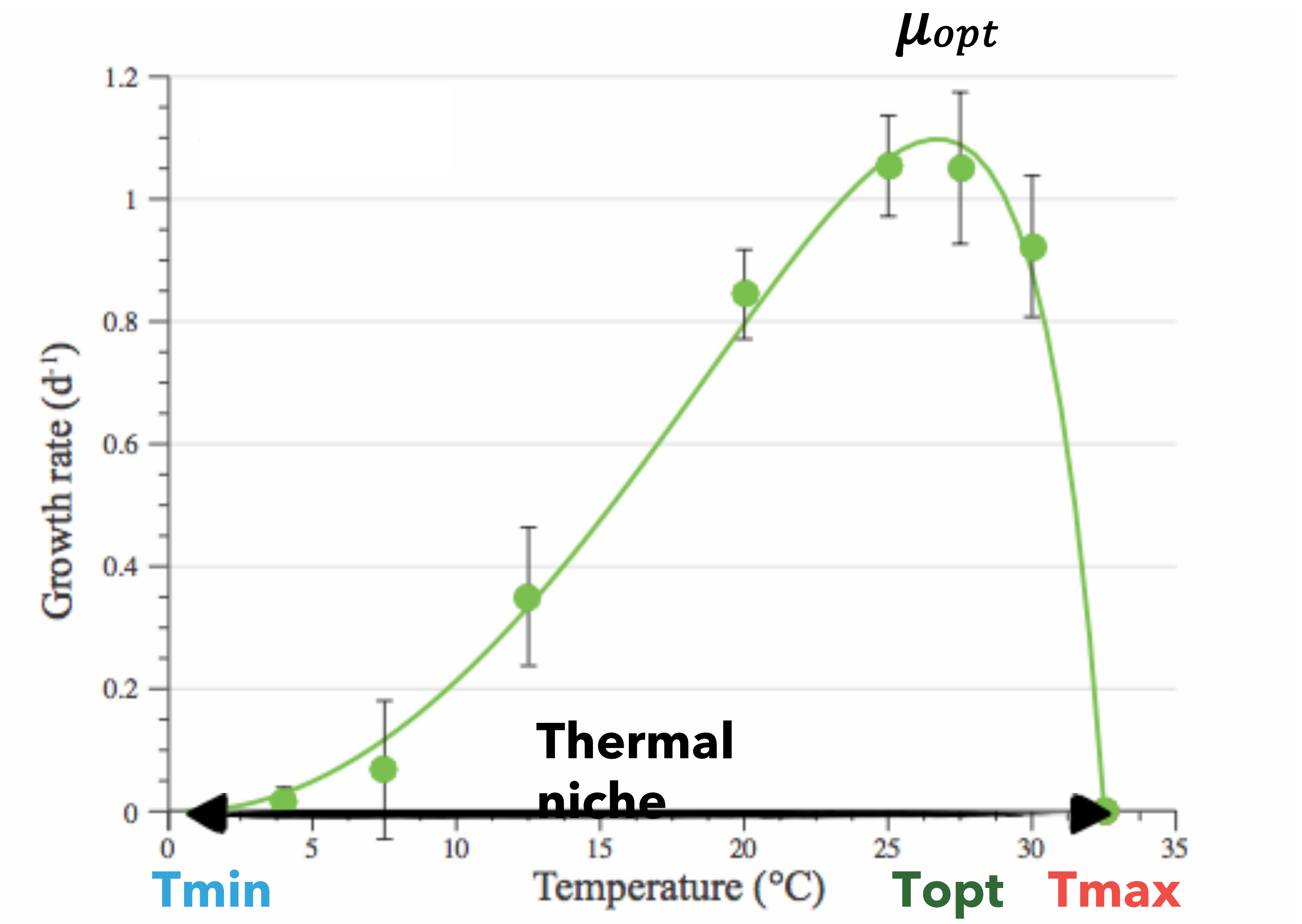
Can we predict the evolution of the Temperature Respon

Link between isolation temperature and the cardinal parameters?

Cardinal Parameters

Tmin **Topt** **Tmax** μ_{opt}





Analysis of 2240 experimental growth rates (merging 3 data bases)

(Thomas, 2016; Corkrey, 2019; Homemade 2020)

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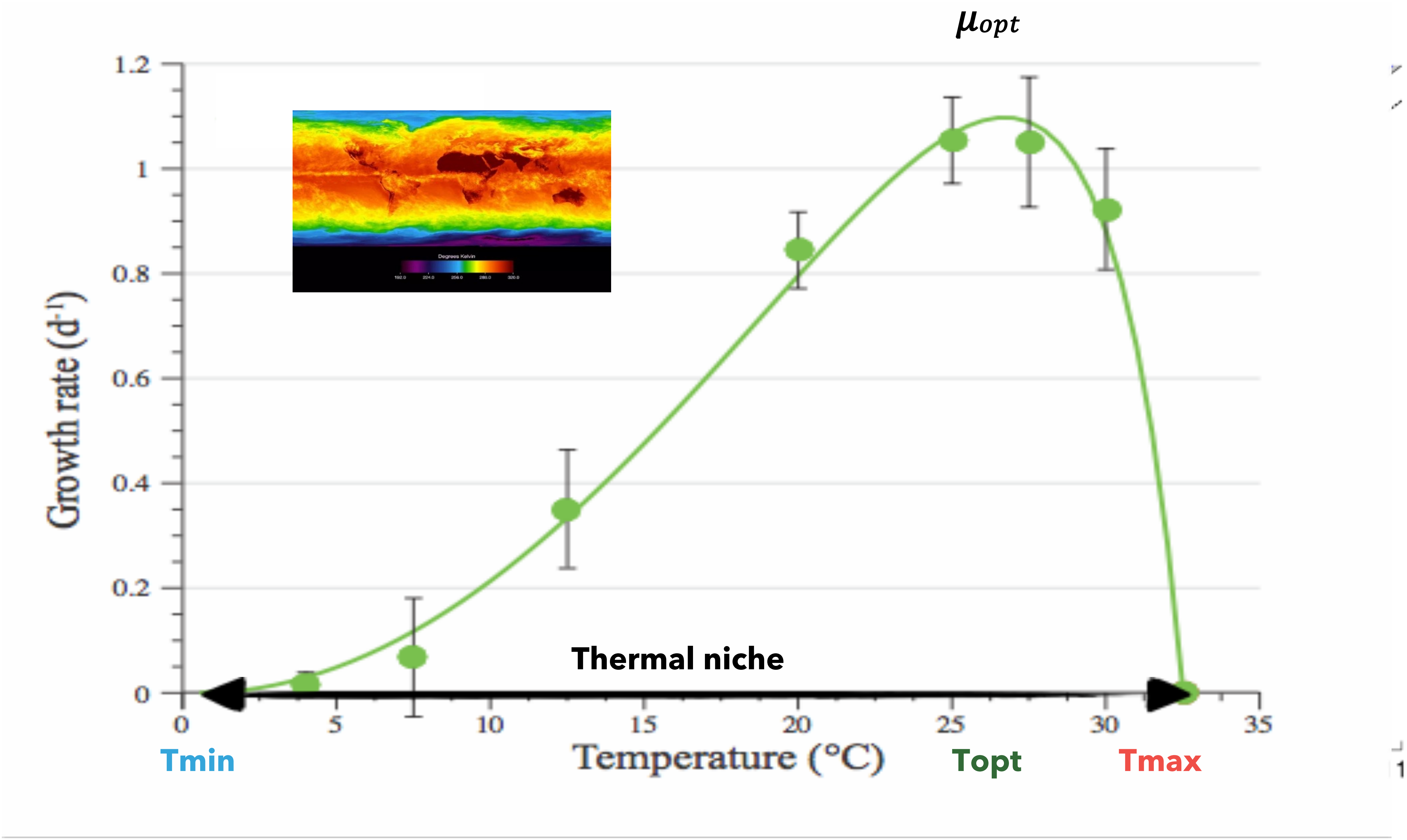
Bernard & Rémond (2012)

Relationship between cardinal parameters



μ_{opt}

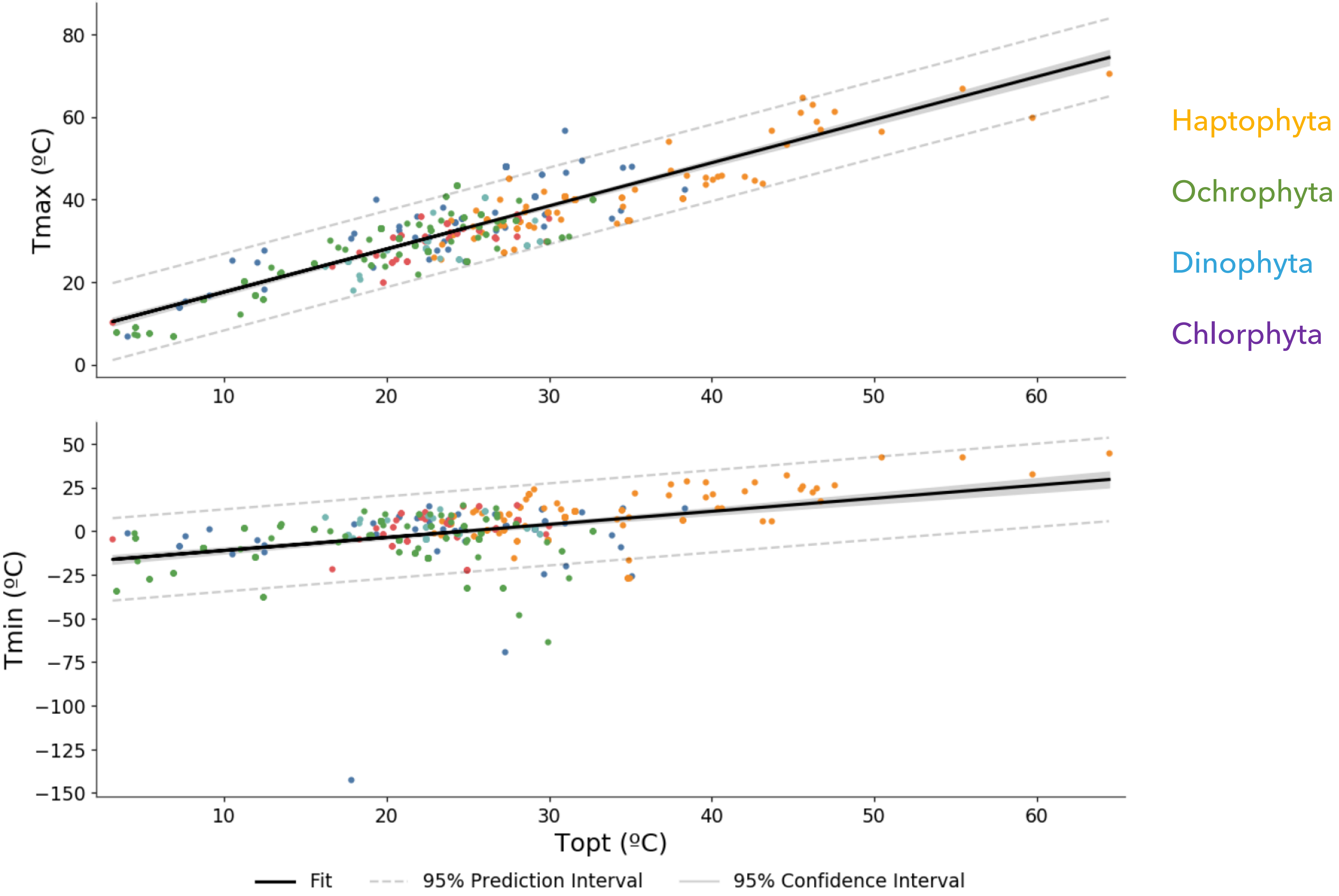
Thermal niche

Tmin

Topt

Tmax

Link between T_{min}, T_{max} and T_{opt}



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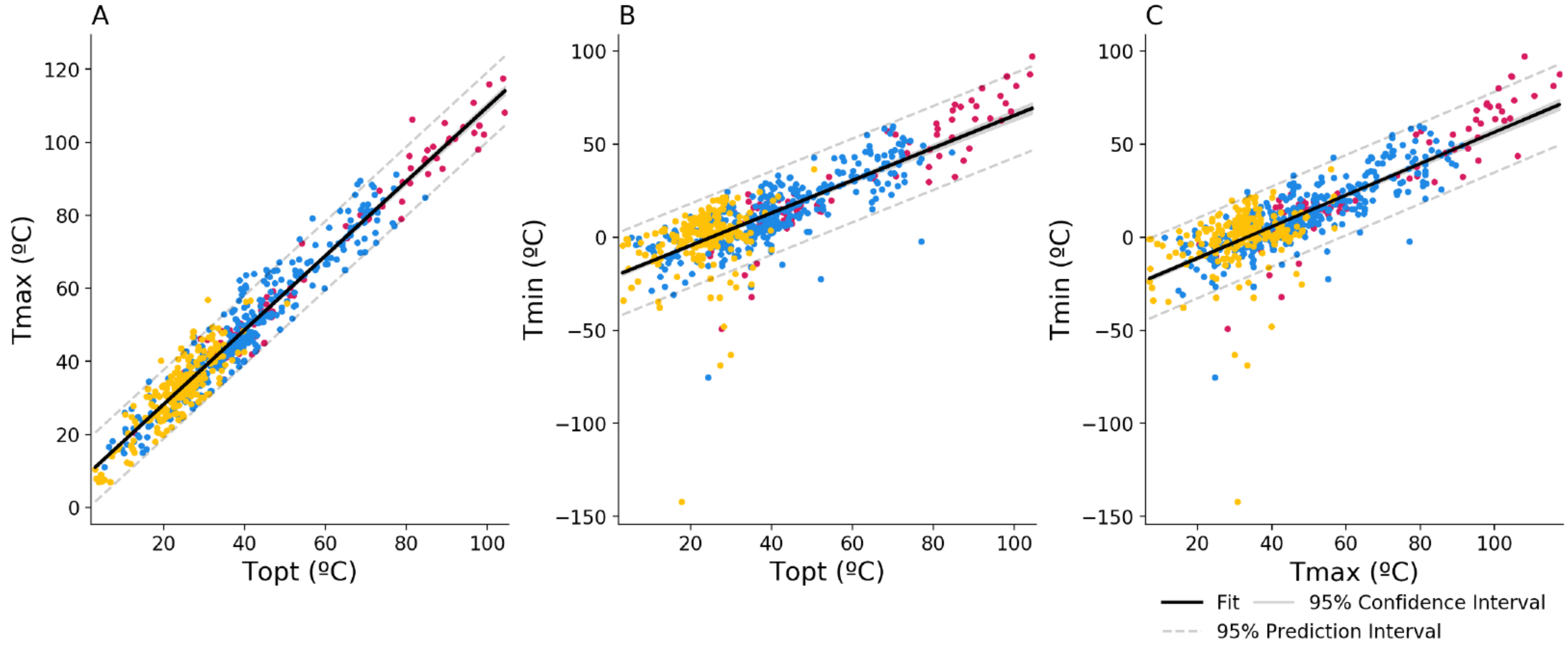
Cardinal temperature links among microorganisms



Eukayota

Bacteria

Archae

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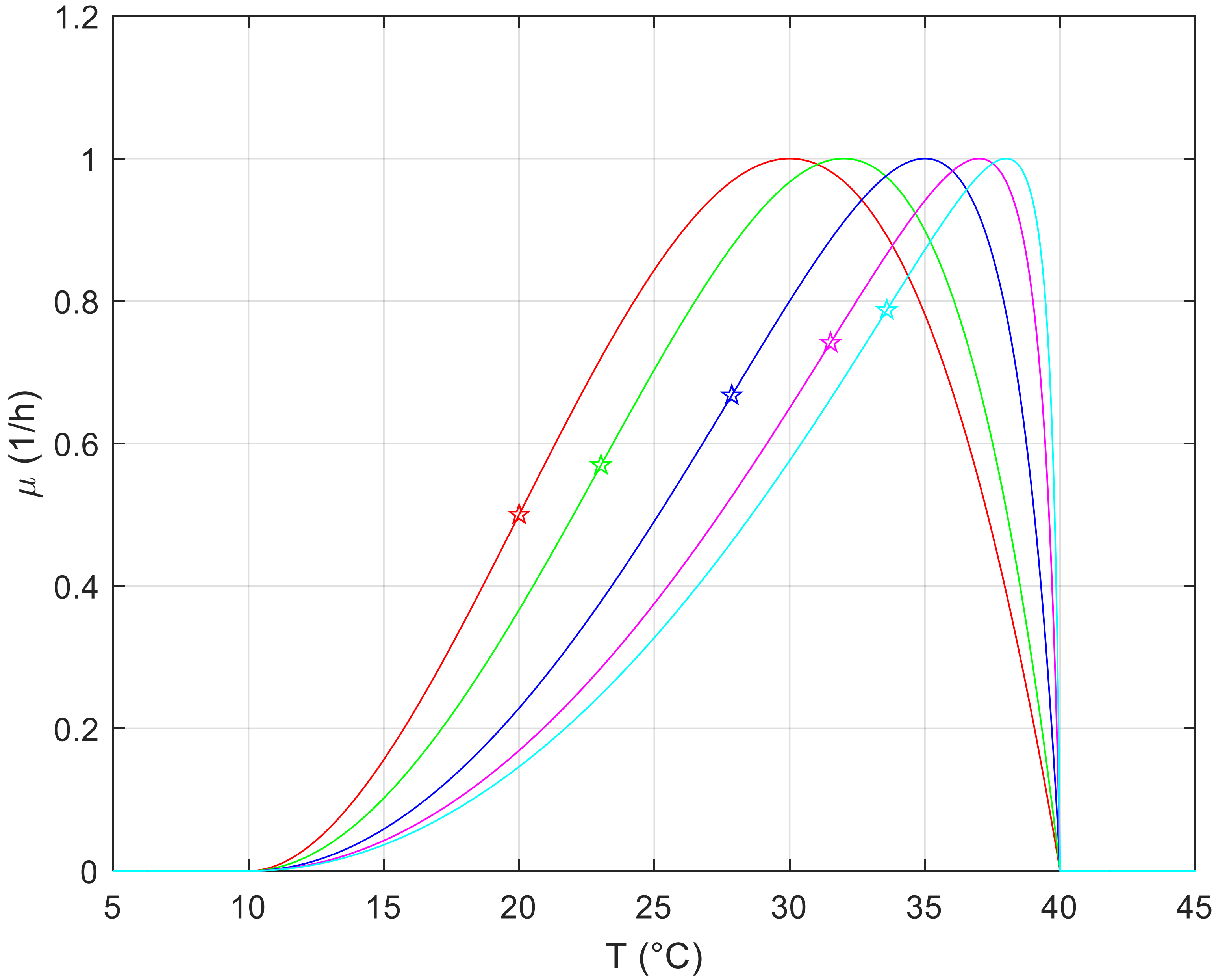
Which of these growth curves is realistic?



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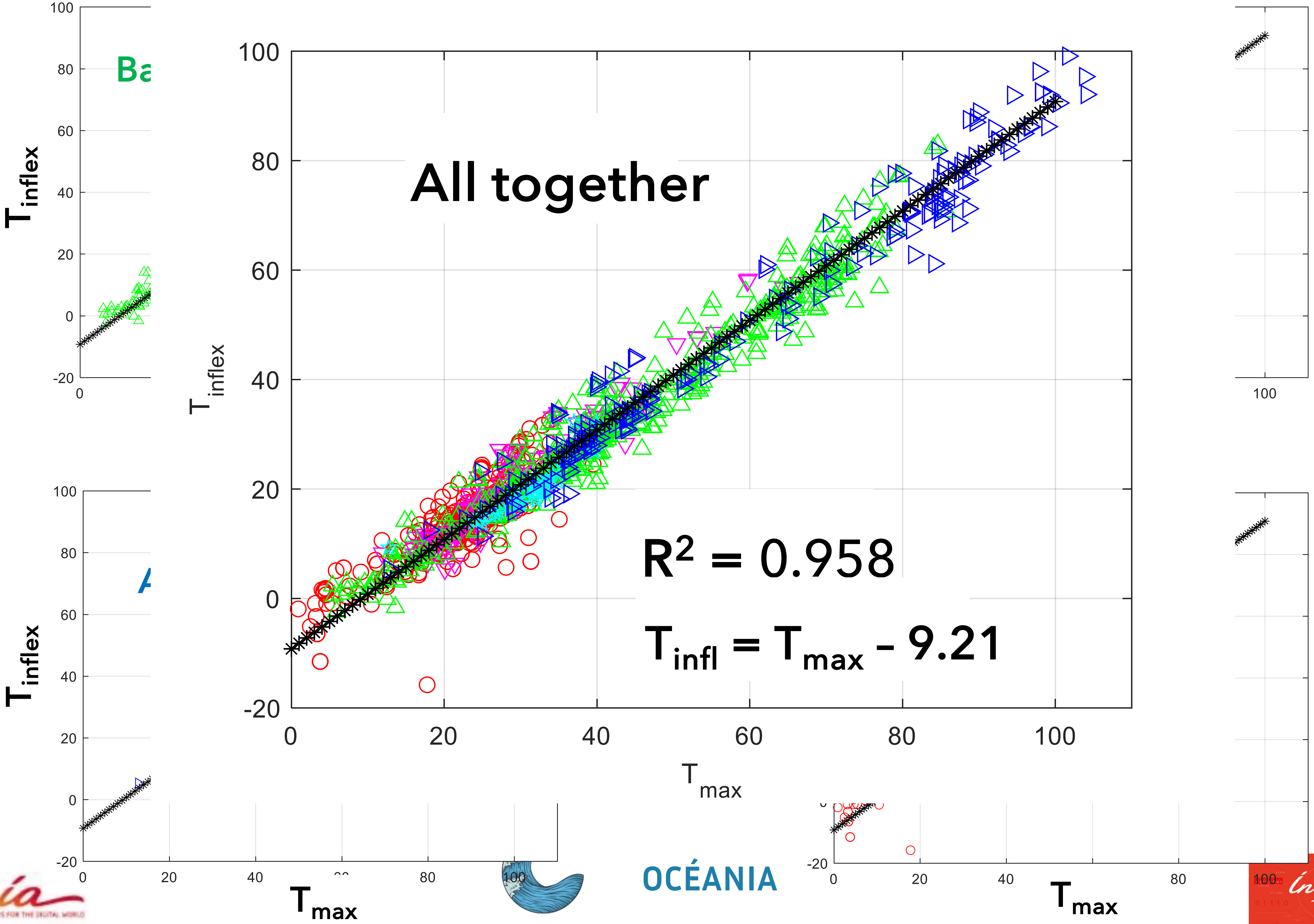
There is a link with the inflexion point!



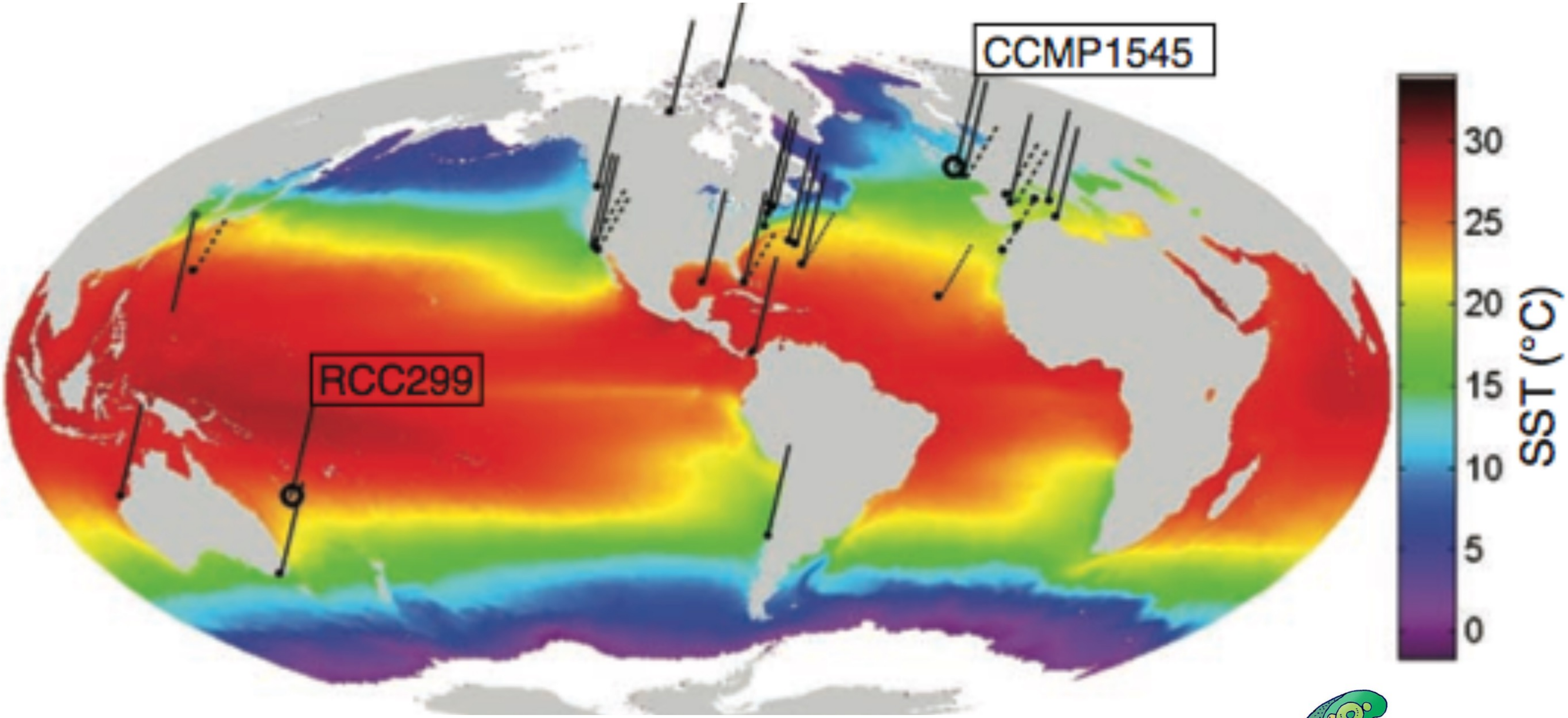
All together

$R^2 = 0.958$

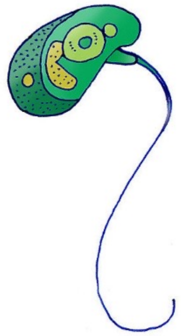
$T_{infl} = T_{max} - 9.21$

LINK BETWEEN LOCAL ENVIRONMENT AND TEMPERATURE RESPONSE

Micromonas temperature response in present and future oceans



Micromonas: **pico eucaryote** (*Mamiellaceae*)

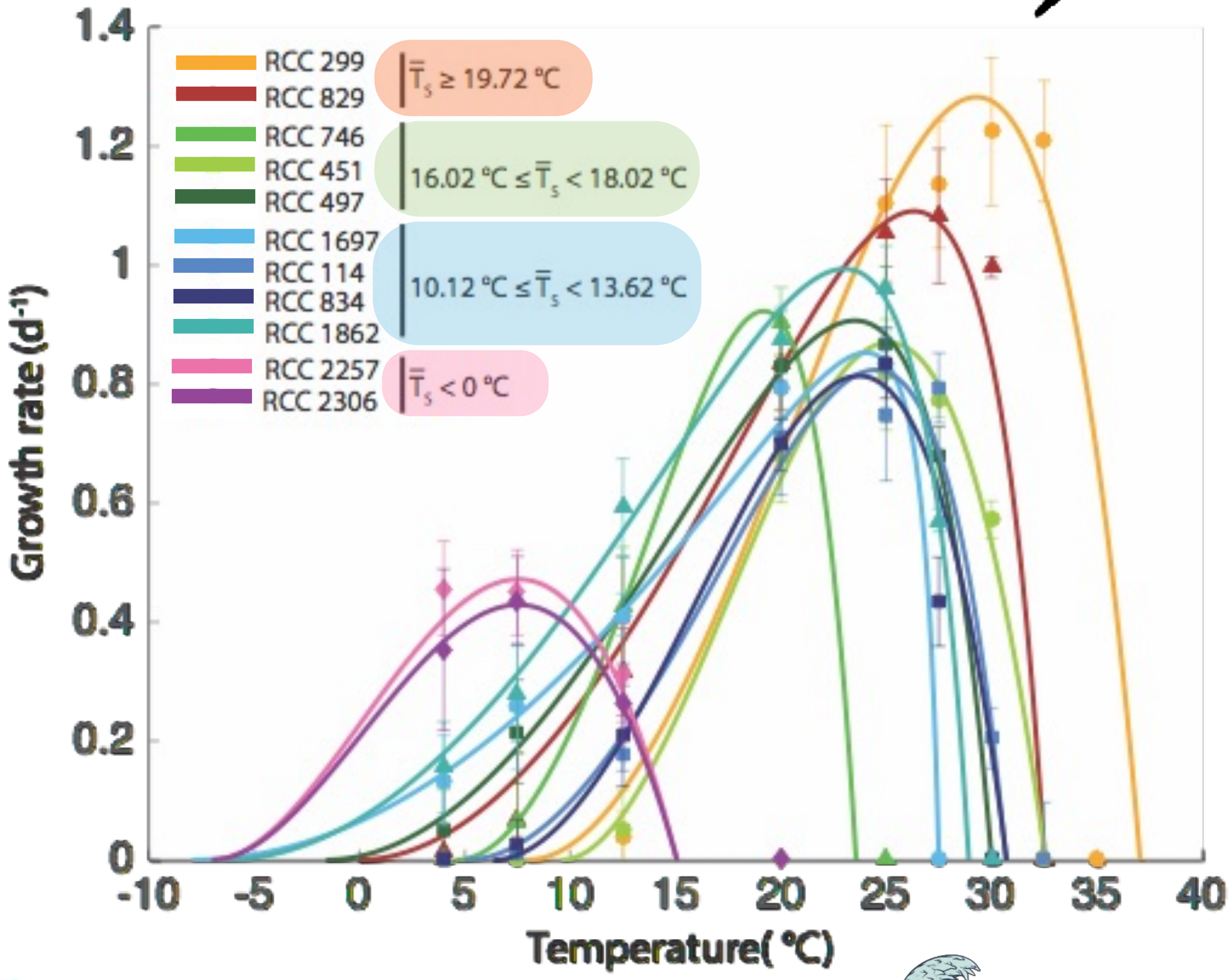


Worden et al., Green Evolution and Dynamic Adaptations Revealed by Genomes of the Marine Picoeukaryotes Micromonas, Science 2009

Link environment with thermal response

Thermal response

11 *Micromonas* strains



BR model

Thermal response data base

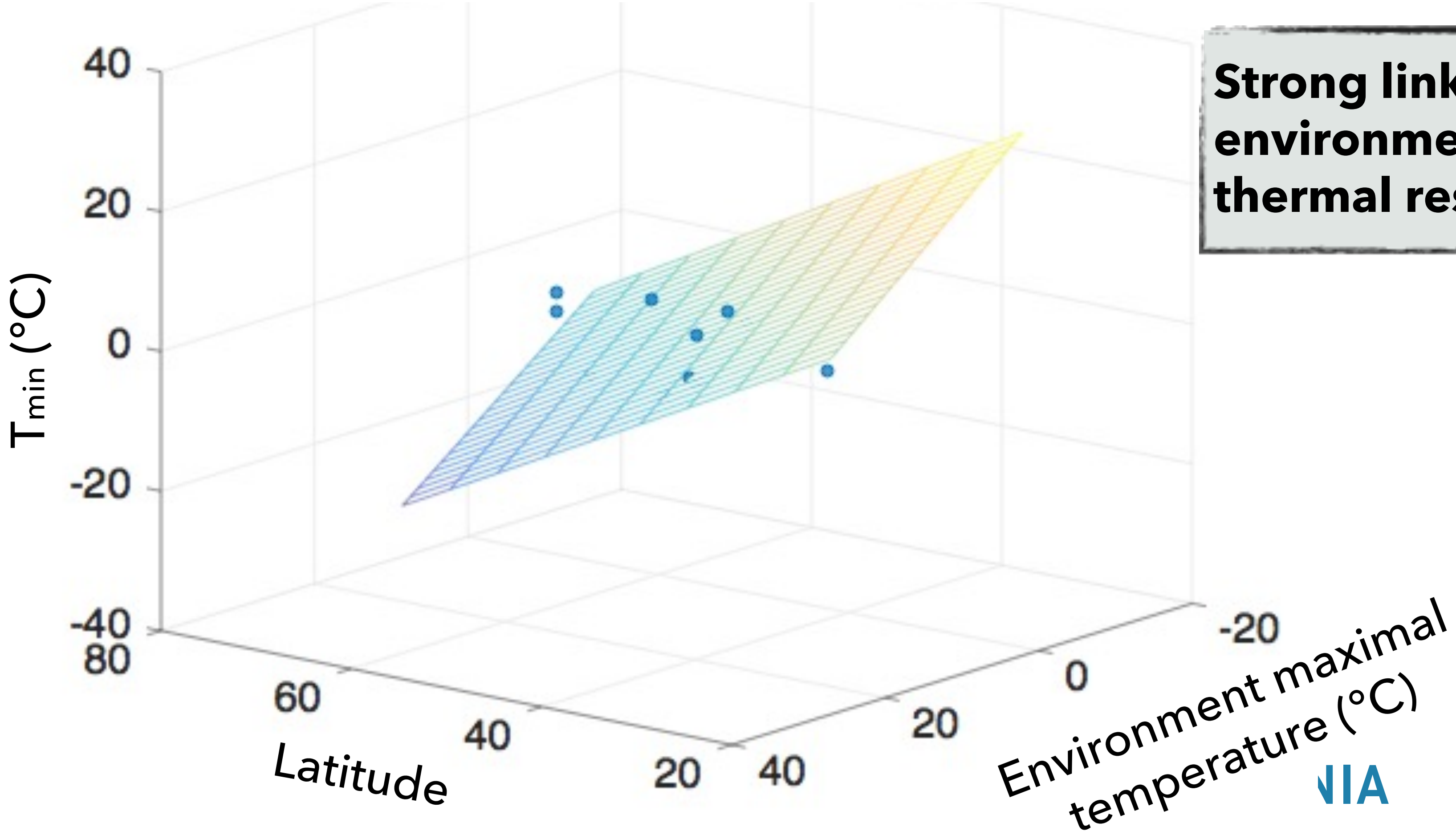
	°C			d^{-1}
Strains	**Tmin**	**Topt**	**Tmax**	**muopt**
RCC299	7.94	29.29	37.05	1.28
RCC829	-0.08	26.33	32.51	1.09
RCC746	4.60	19.18	23.57	0.92
RCC451	9.59	25.13	32.56	0.87
RCC497	-1.59	23.51	30.00	0.91
RCC1697	-16.04	24.04	27.5	0.85
RCC114	1.01	24.49	30.68	0.82
RCC834	6.34	23.71	30.71	0.81
RCC1862	-11.64	23.01	28.92	0.99
RCC2257	-14.12	7.03	16.91	0.45
RCC2306	-9.74	7.60	15.35	0.44

Link environment with thermal response

Linear model

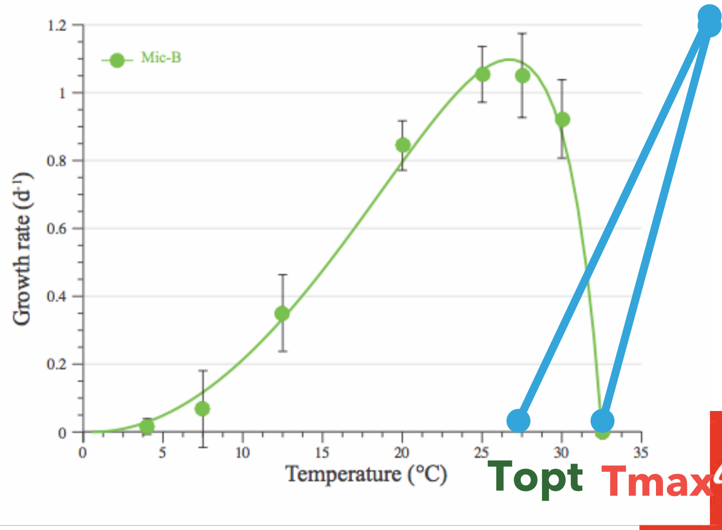
Demory et al. 2019, 2021

Cardinal Parameter	Model	R^2 adjusted	*p*-value
μ_{opt}	$\mu_{opt} = 0.03\ \overline{T}_S + 0.47$	0.90	$5.68\ 10^{-6}$
T_{max}	$T_{max} = 0.73\ T_S^+ + 14.46$	0.84	$4.29\ 10^{-5}$
T_{opt}	$T_{opt} = 0.81\ T_S^+ + 6.5642$	0.85	$3.22\ 10^{-5}$
T_{min}	$T_{min} = -0.76\ Lat - 0.92\ \overline{T}_S + 49.33$	0.47	0.03



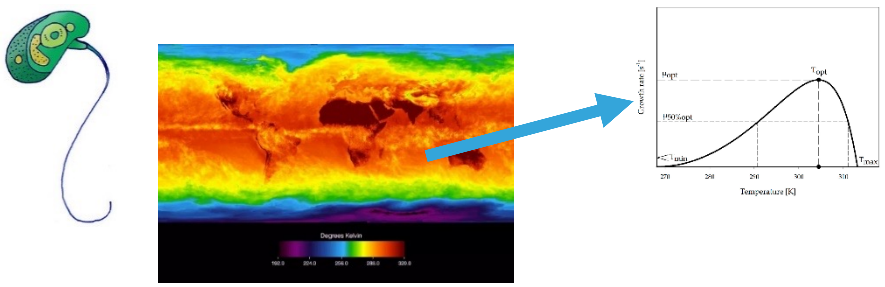
Strong link between environmental temperature and thermal response

Related to SST max temperature!



CAN WE PREDICT PHYTOPLANKTON BIODIVERSITY FROM SST?

Predicting micromonas diversity response to temperature = representative of phytoplan

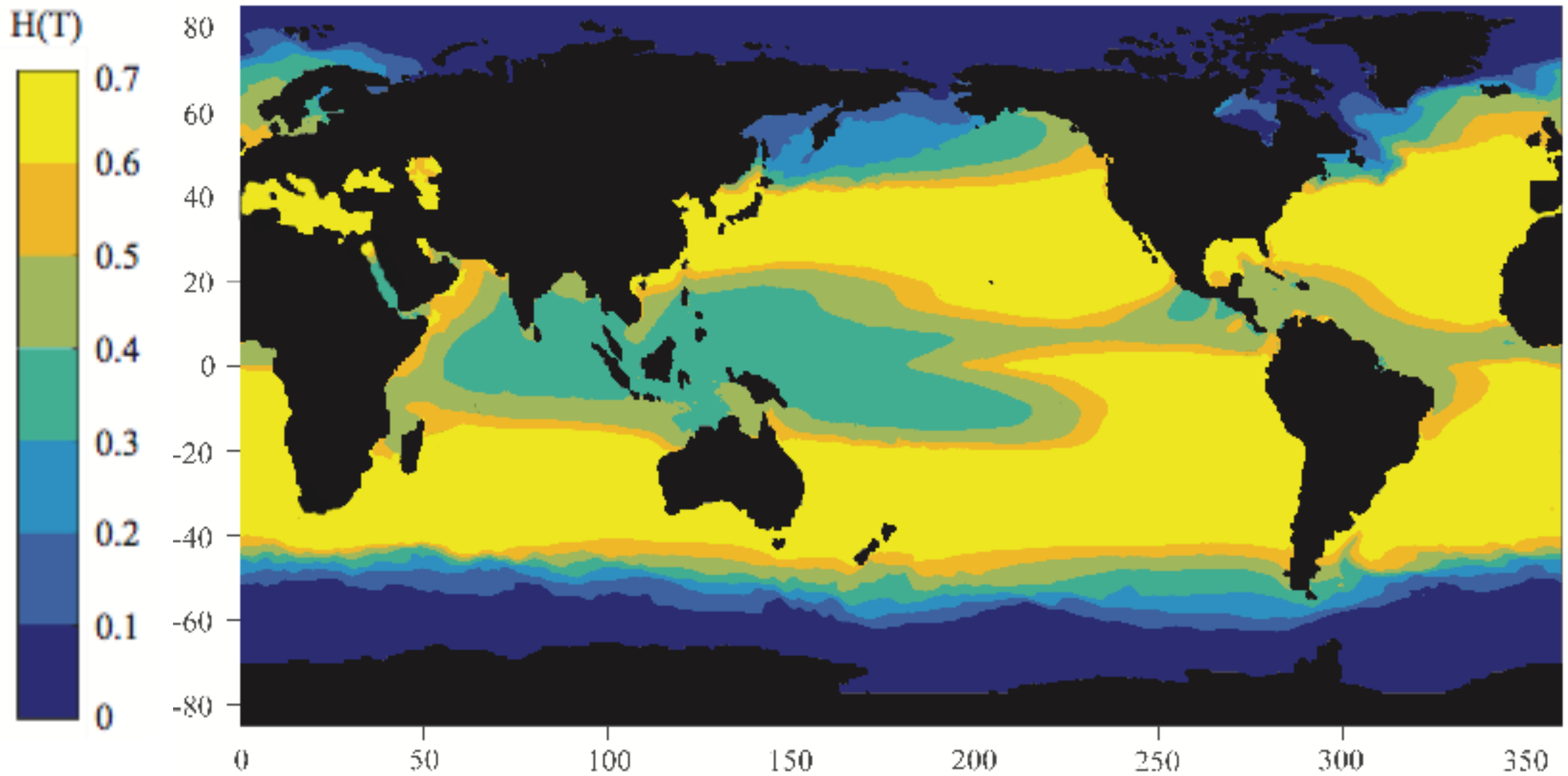


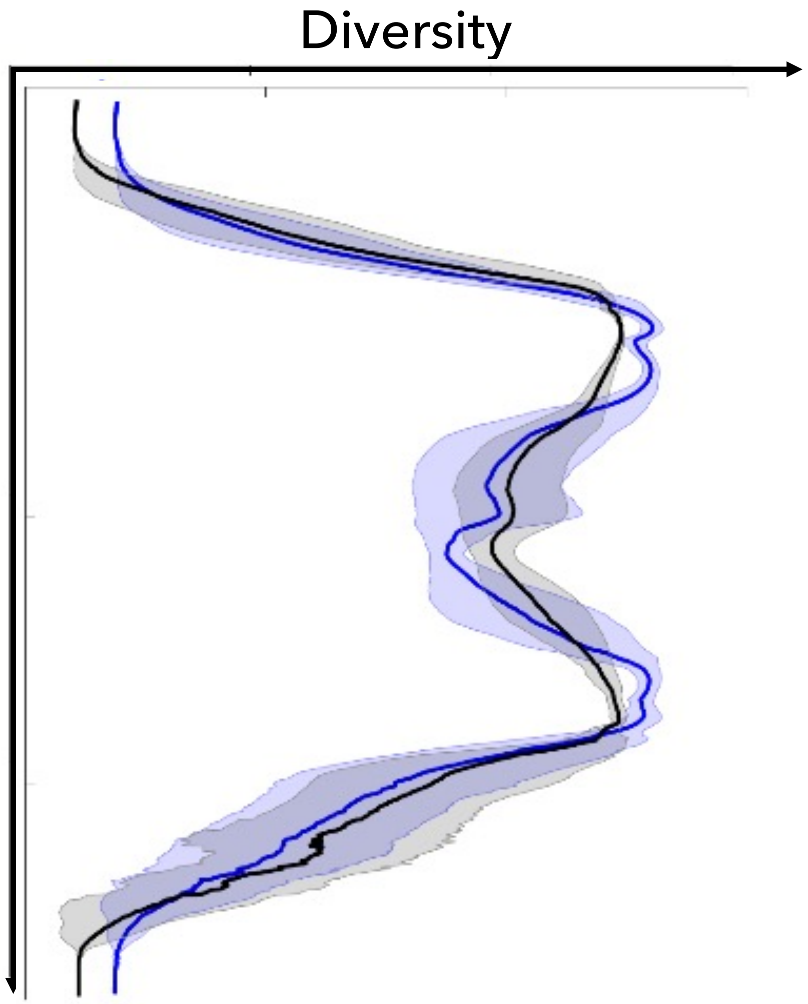
Micromonas: a phytoplankton sentinel

— Phytoplankton Diversity from Thomas *et al.* 2012

— *Micromonas* Diversity

Average from 1993 to 2012





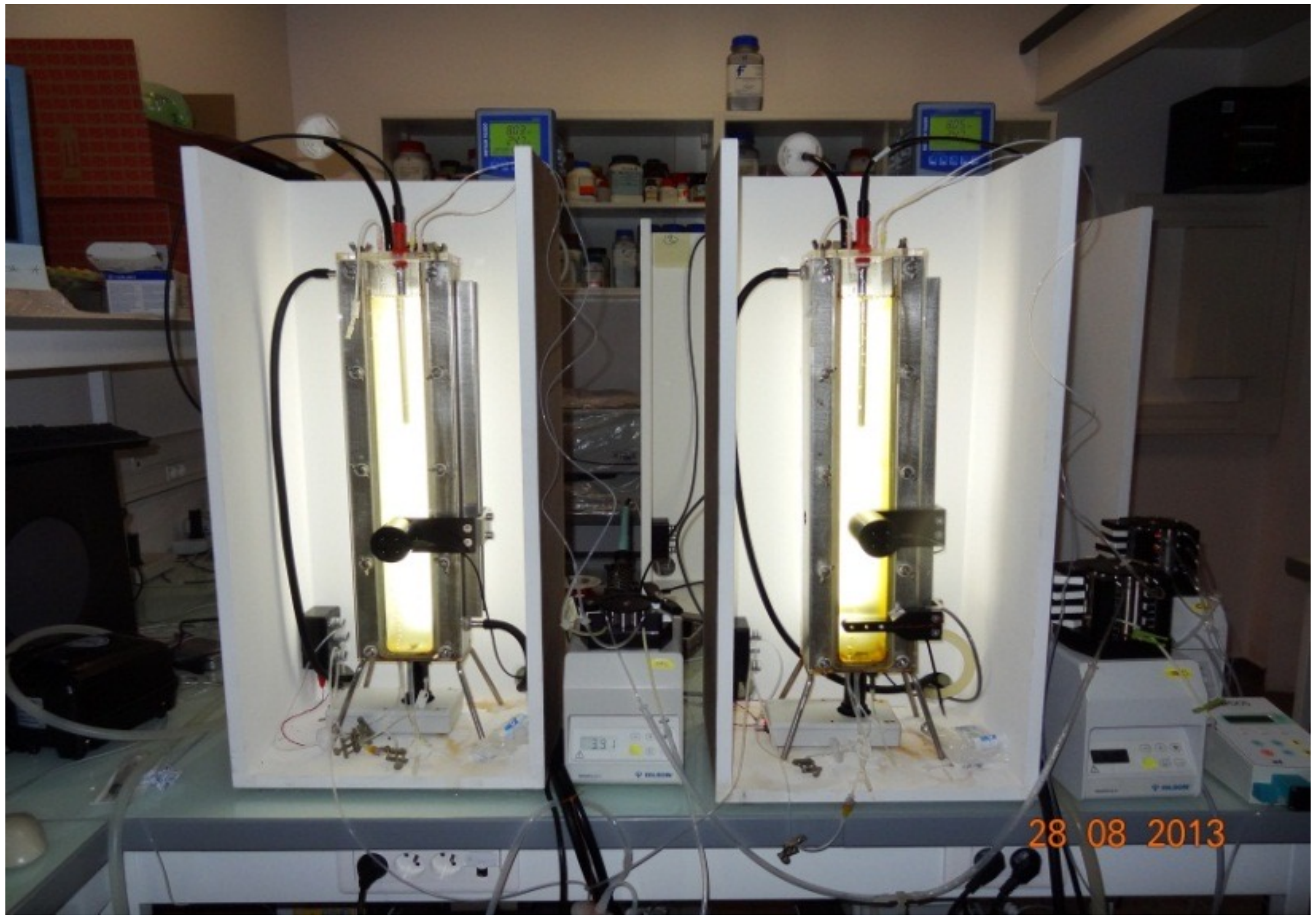
Demory et al. 2019

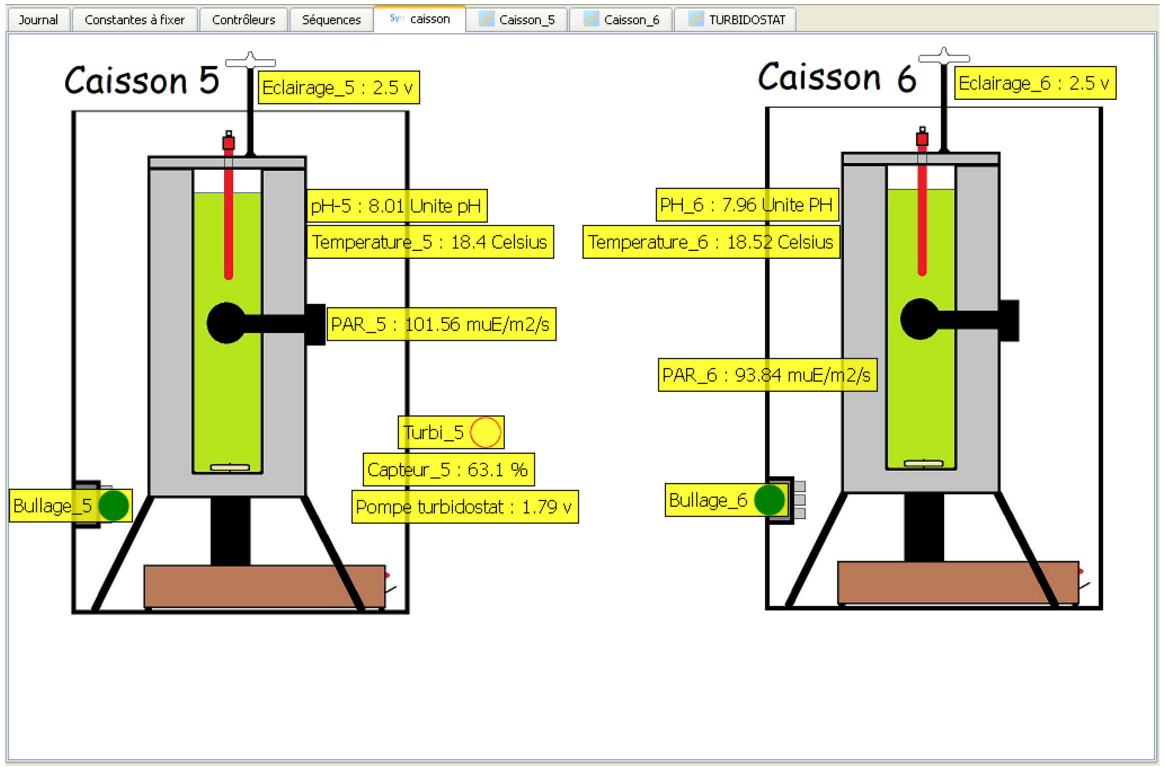
SST data from: Copernicus Marine Environment Monitoring Service

CAN WE PREDICT THE EVOLUTION OF THE TEMPERATURE RESPONSE?

The selectiostat principle

Computer controlled devices to trigger adaptation on the long term in a dynamical realistic envirnment





Eclairage_5 : 2.5 v

pH-5 : 8.01 Unite pH

Temperature_5 : 18.4 Celsius

PAR_5 : 101.56 muE/m2/s

Turbi_5 ○

Capteur_5 : 63.1 %

Pompe turbidostat : 1.79 v

Bullage_5 ●

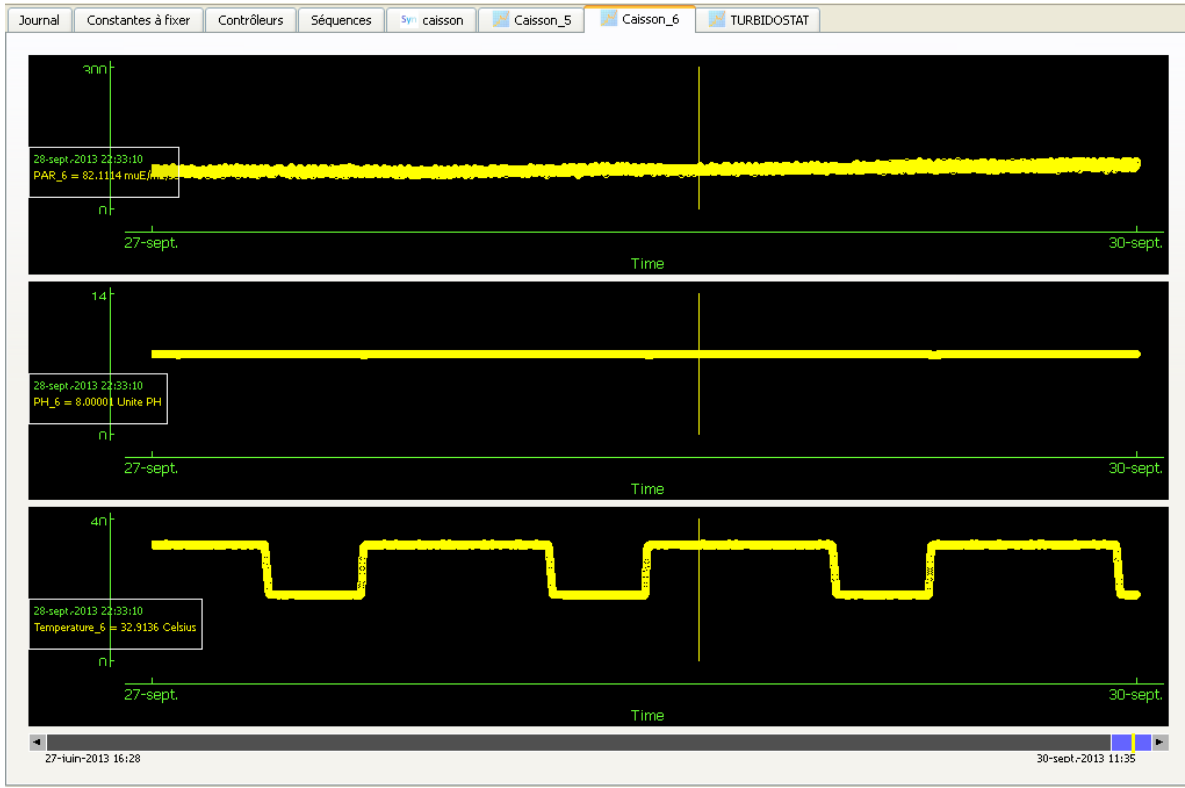
Eclairage_6 : 2.5 v

PH_6 : 7.96 Unite PH

Temperature_6 : 18.52 Celsius

PAR_6 : 93.84 muE/m2/s

Bullage_6 ●



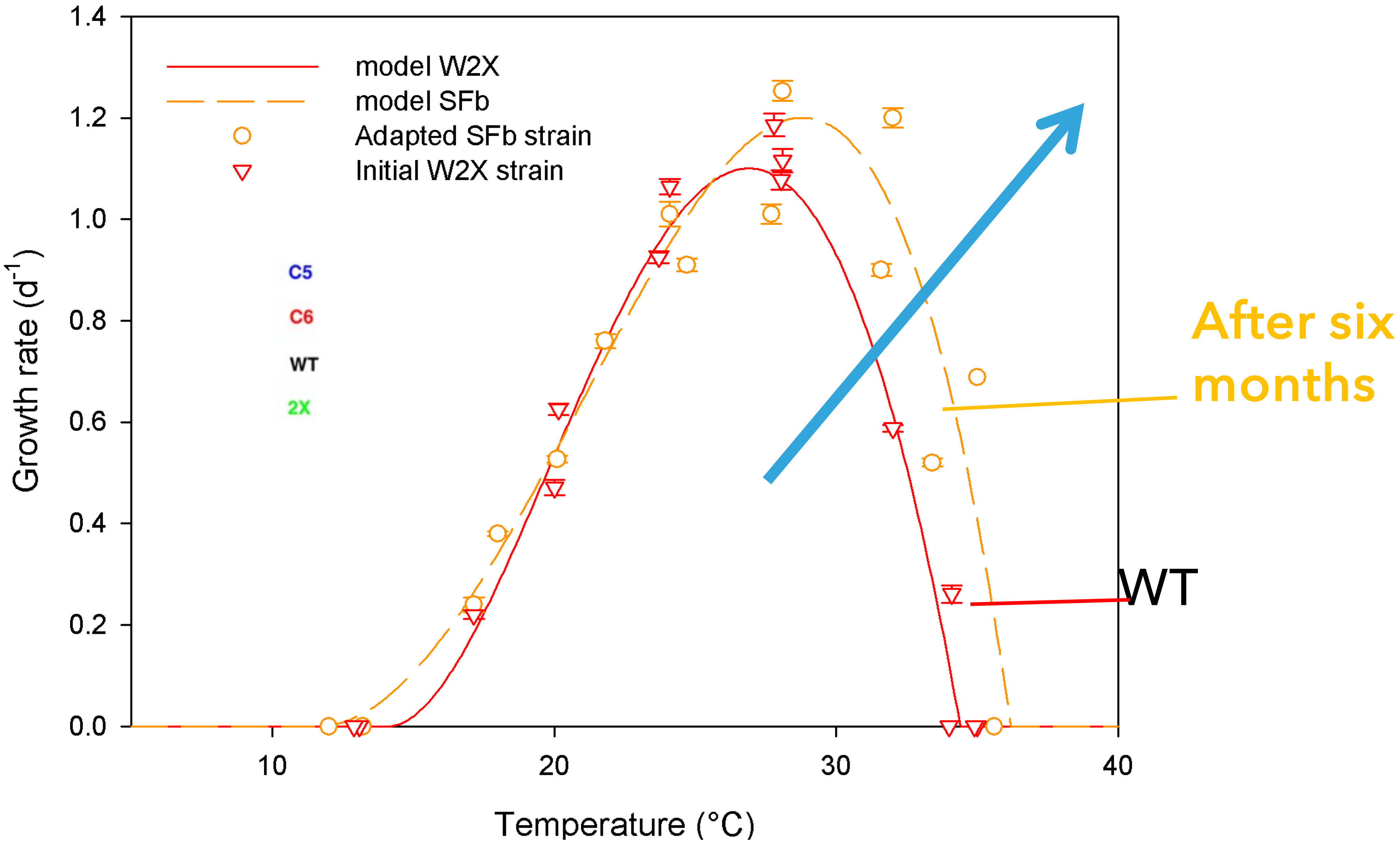
28-sept.-2013 22:33:10
PAR_6 = 82.1114 muE/m2/s

28-sept.-2013 22:33:10
PH_6 = 8.00001 Unite PH

28-sept.-2013 22:33:10
Temperature_6 = 32.9136 Celsius

Designed by E. Pruvost

Temperature adaptation experiments



- **Increase of max growth rate**
- **Increase of max temperature**

Bonnefond et al. 2017, Plos On

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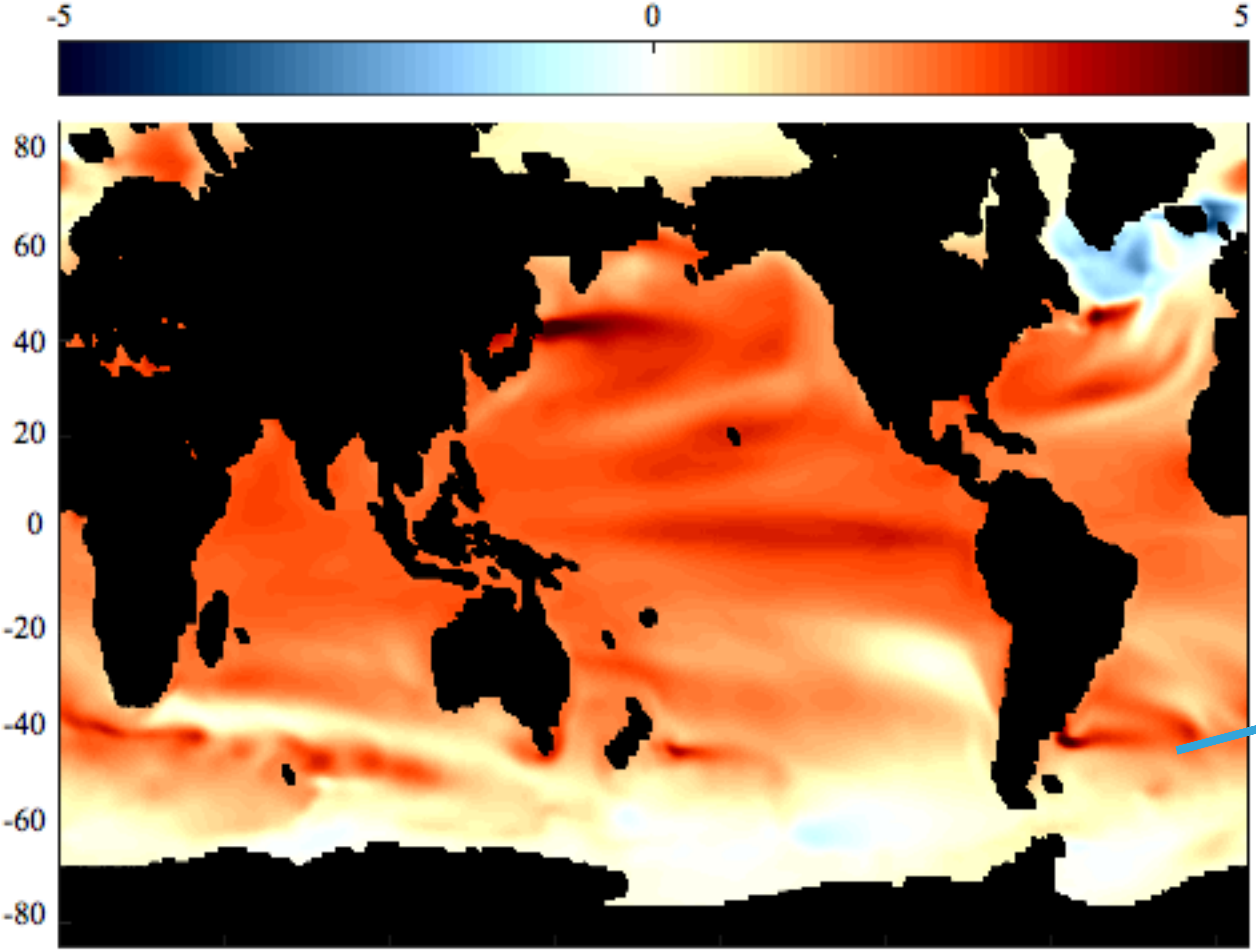
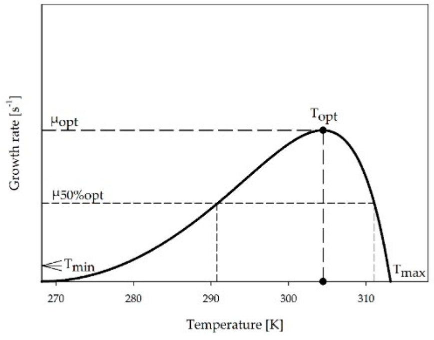
Evolution of ocean temperature

SST anomalies (2001 – 2100)



Global warming



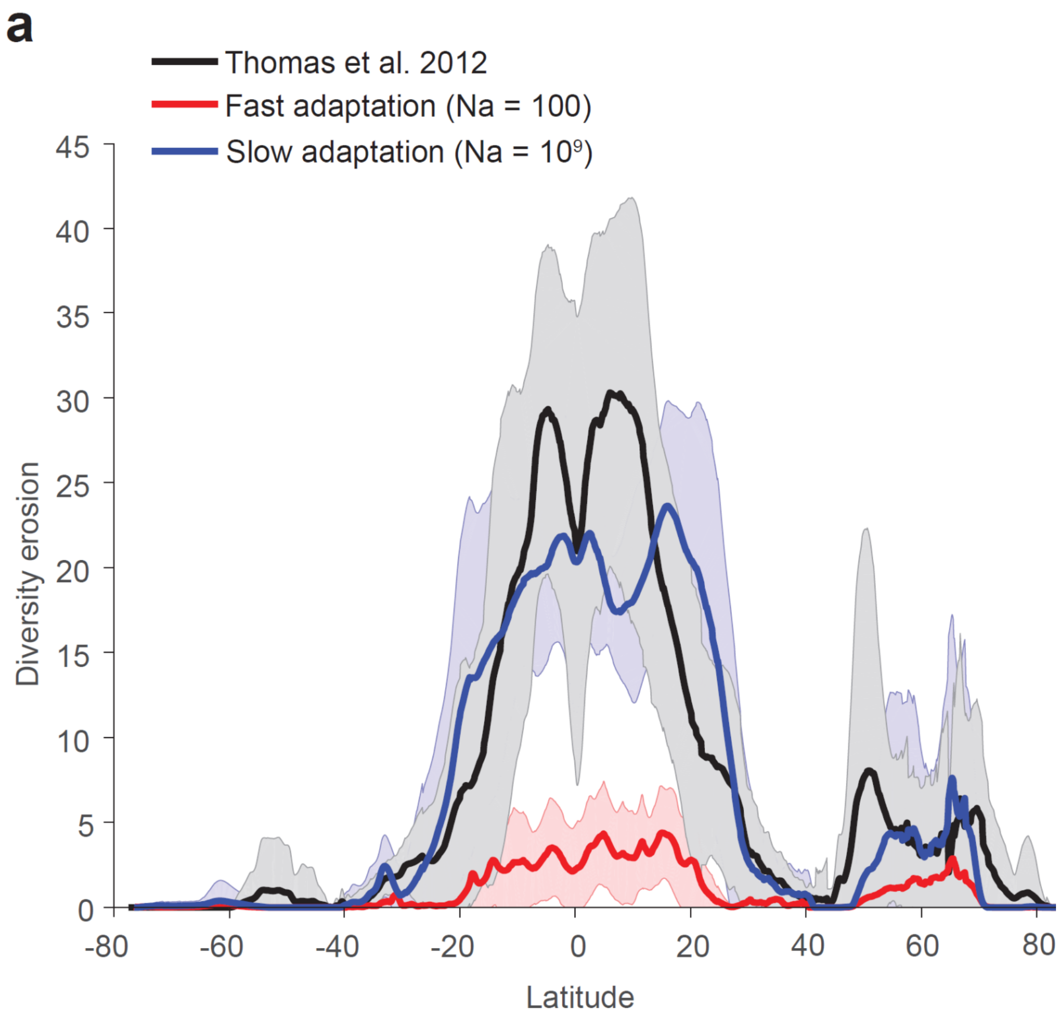
Climate projections from: NOAA GFDL329 CM2.1 driven with the SRES A2 scenario (Griffies *et al.* 2005; Delworth *et al.* 2006)

How fast can phytoplankton adapt?

➡ **Importance of the adaptation time scale**

?

Phytoplankton from Thomas *et al.* 2012



Demory et al. 2019

Conclusion – challenges

- Temperature plays a key role (as light) on phytoplankton: but it has not been studied and understood with the same details!

- Much remains to be done to understand and represent in models acclimation to temperature

- Understand and include adaptation to temperature change in the models

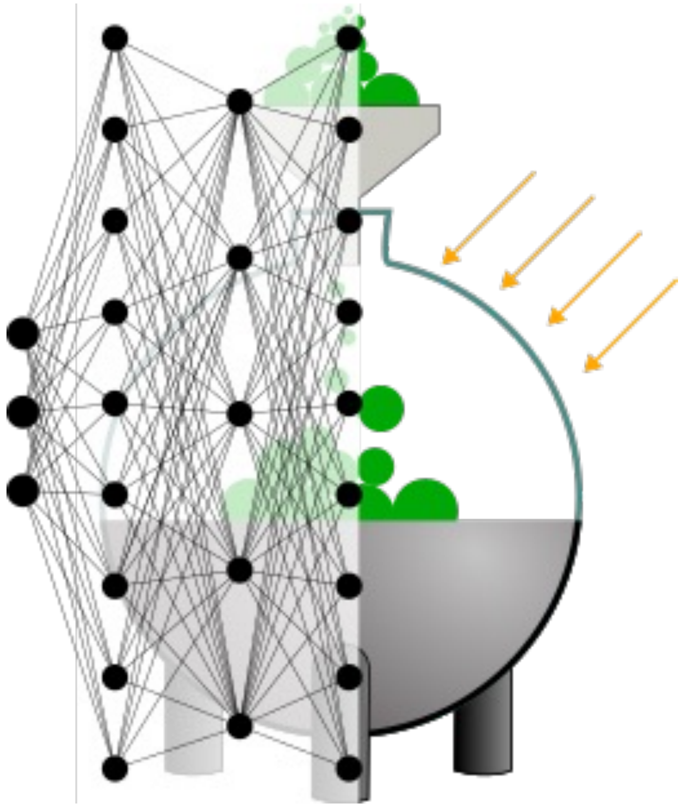
- Key question to predict the impact of global changes!

Biocore contribution

- Understanding the rules driving response to temperature in phytoplankton (O. Bernard)
- **Neural ODE for representing phytoplankton growth driven my light (I. Fierro)**
- Towards hybrid modelling of artificial microbial ecosystems (F. Casagli)
- Spatio-temporal high-resolution models of particulate organic matter abundance in the ocean (R. Ranini)

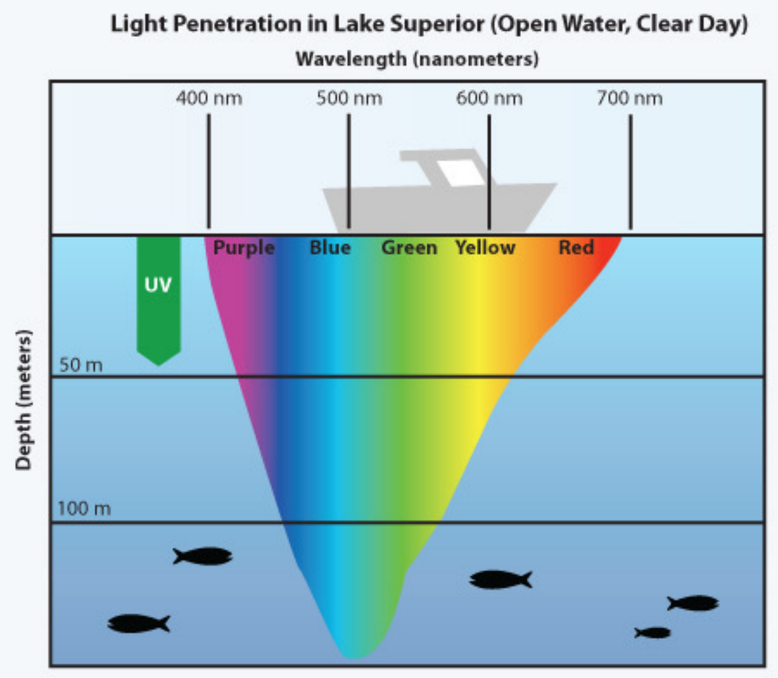
NEURAL ODES FOR PHYTOPLANKTON MODELING

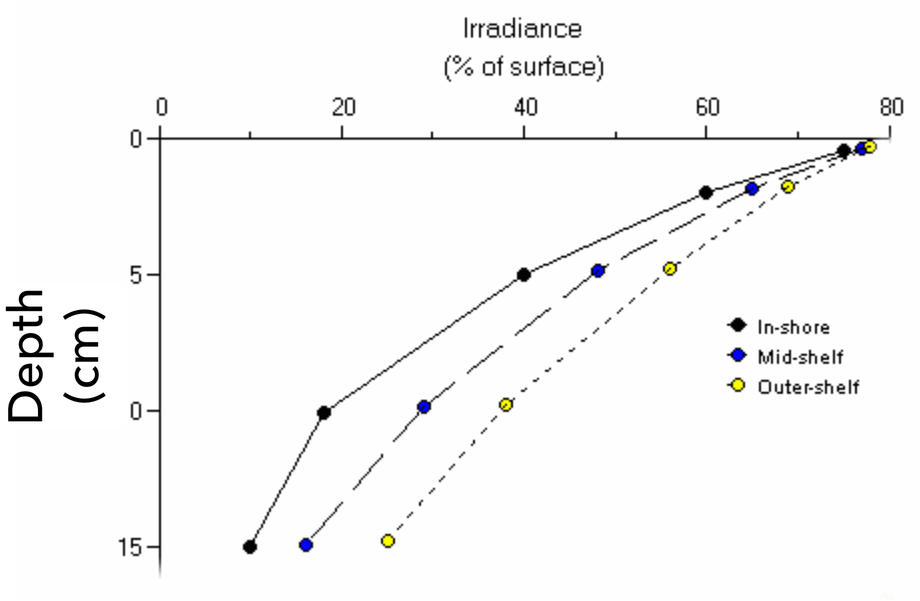
Combining first order principles and neural networks

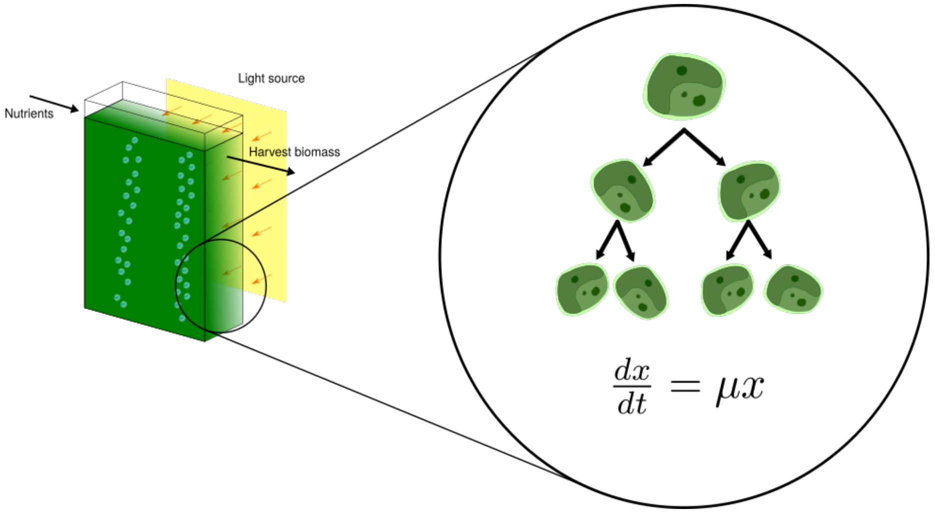


J. Ignacio Fierro U. & Olivier Bernard

Modeling phytoplankton evolution in a light gradient







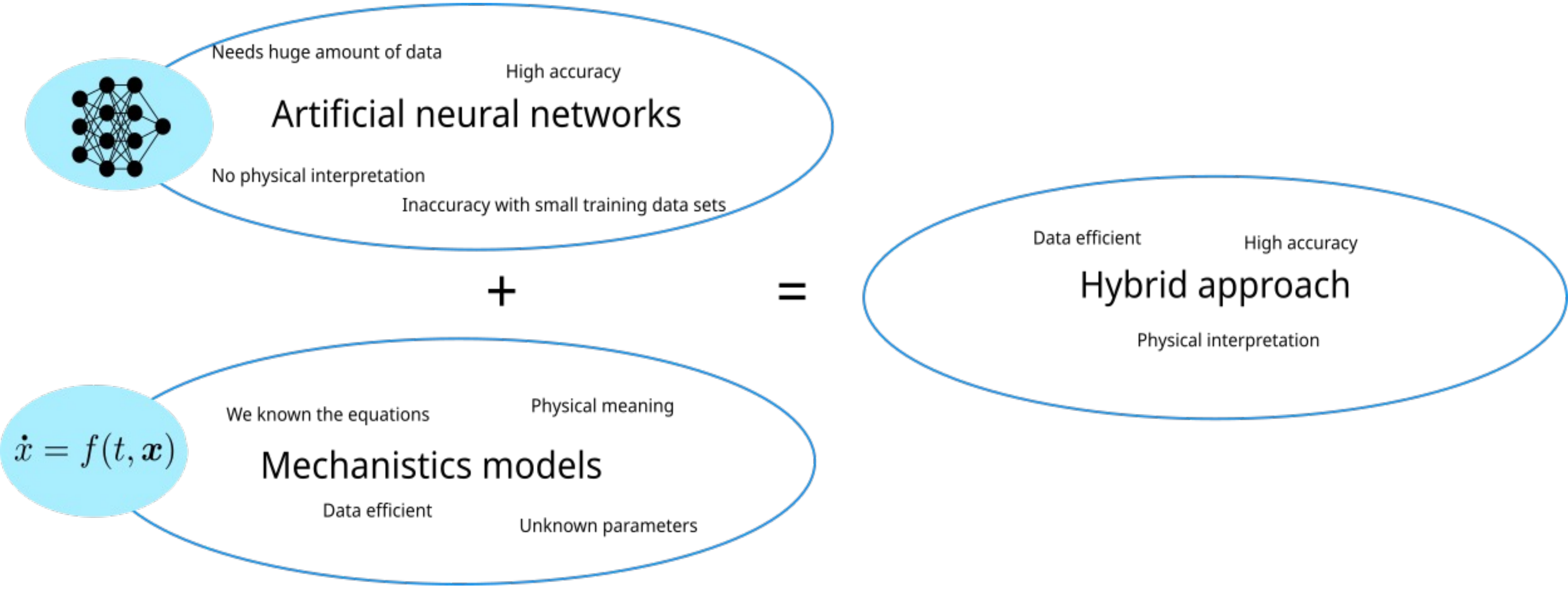
Ocean

Light availability

Photobioreactors

Growth rate is affected by: Temperature, pH, nutrients, **light**, etc.

Neural Ordinary Differential Equations



Needs huge amount of data

High accuracy

Artificial neural networks

No physical interpretation

Inaccuracy with small training data sets

+

$\dot{x} = f(t, \boldsymbol{x})$

We known the equations

Physical meaning

Mechanistics models

Data efficient

Unknown parameters

=

Data efficient

High accuracy

Hybrid approach

Physical interpretation

Diatoms growing in photobioreactor

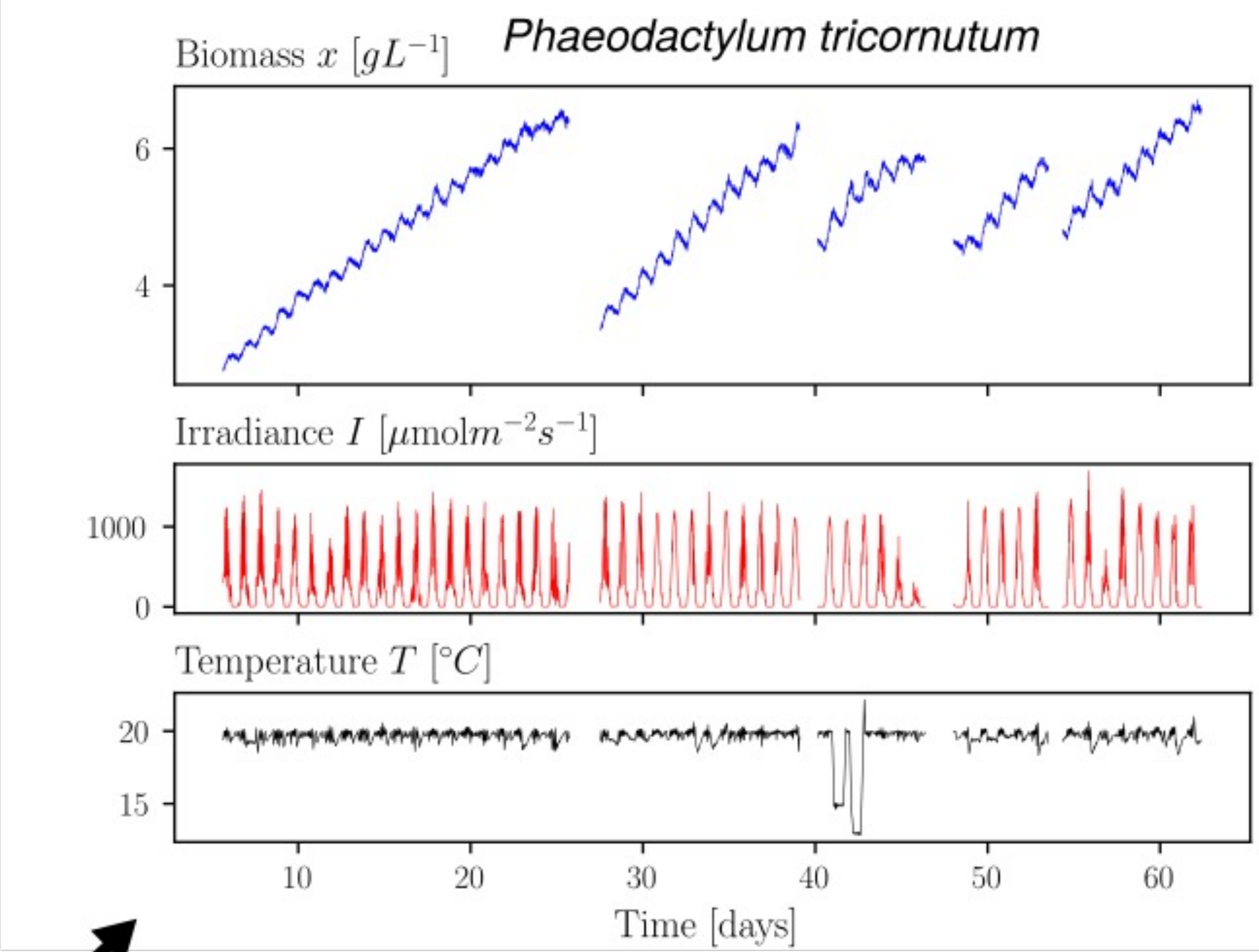
Phaeodactylum tricornutum cultivated under natural light in a 180L flat-panel airlift in a greenhouse (Leuna, Germany, July - September 2015).

Online measurements recorded every 10 minutes.

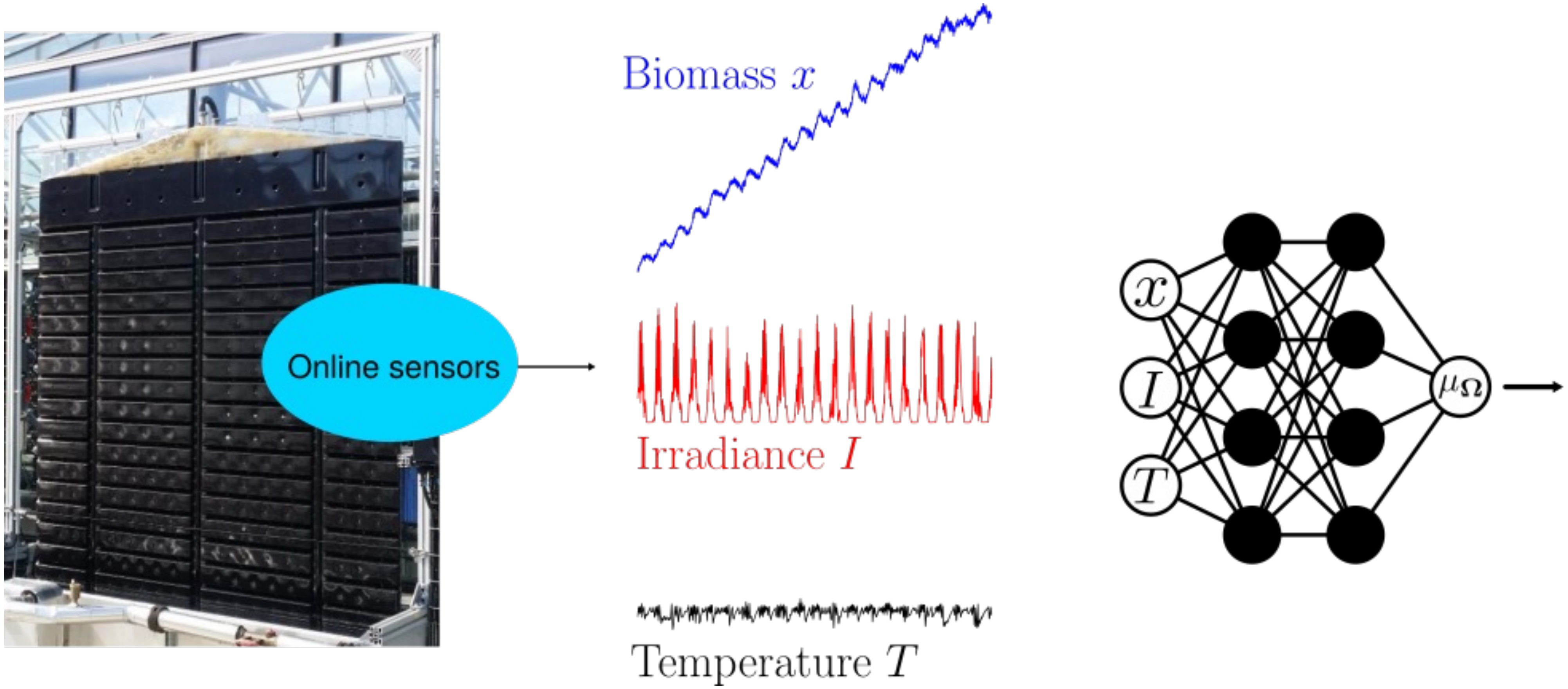
Fraunhofer Center for Chemical-Biotechnological Processes.

Diatoms growing in photobioreactor

Online sensors

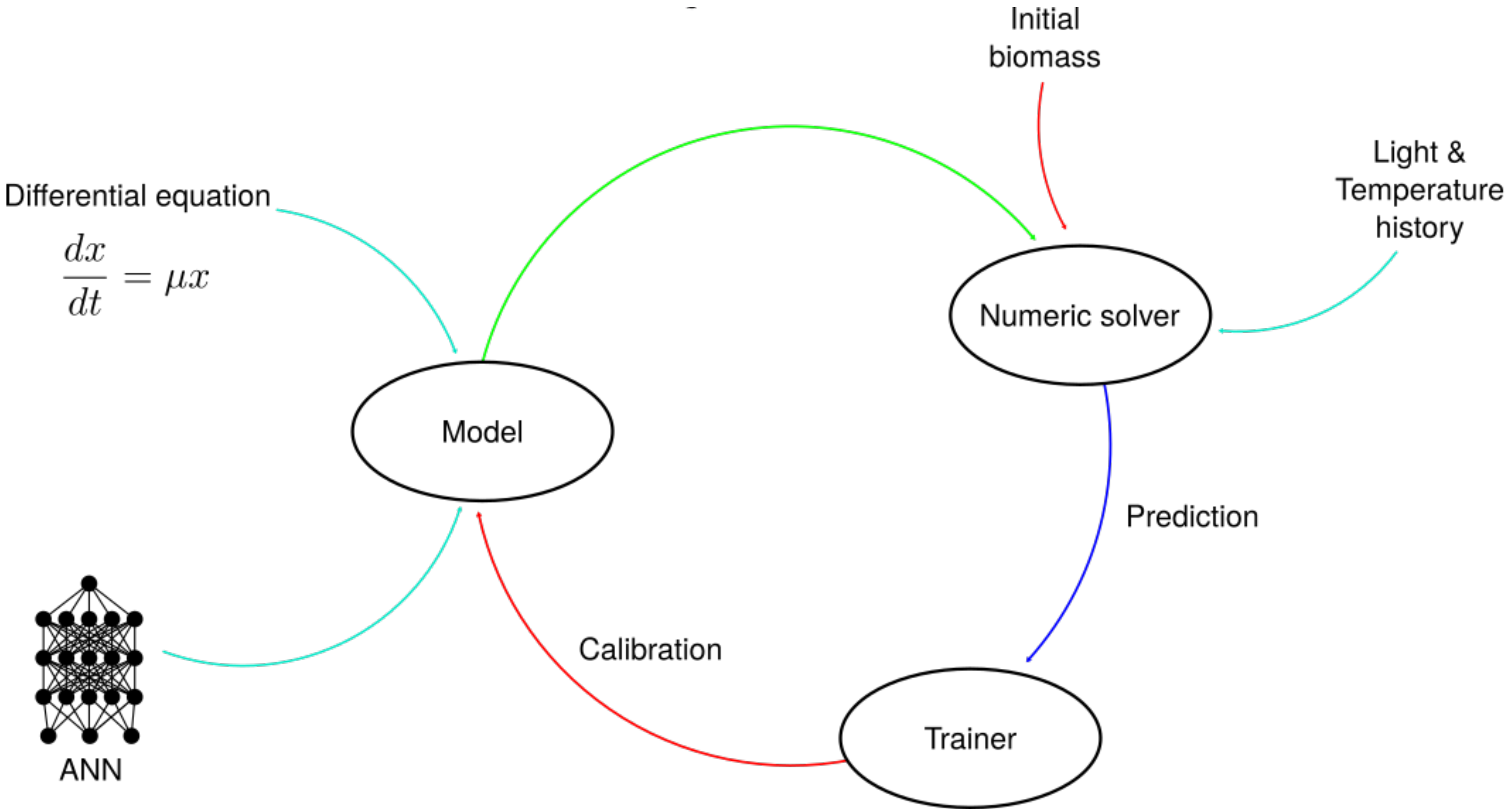


Neural ODE



$$\frac{dx}{dt} = \mu_{\mathbf{\Omega}}(x, I, T)x$$

Implementation of the model in PyTorch

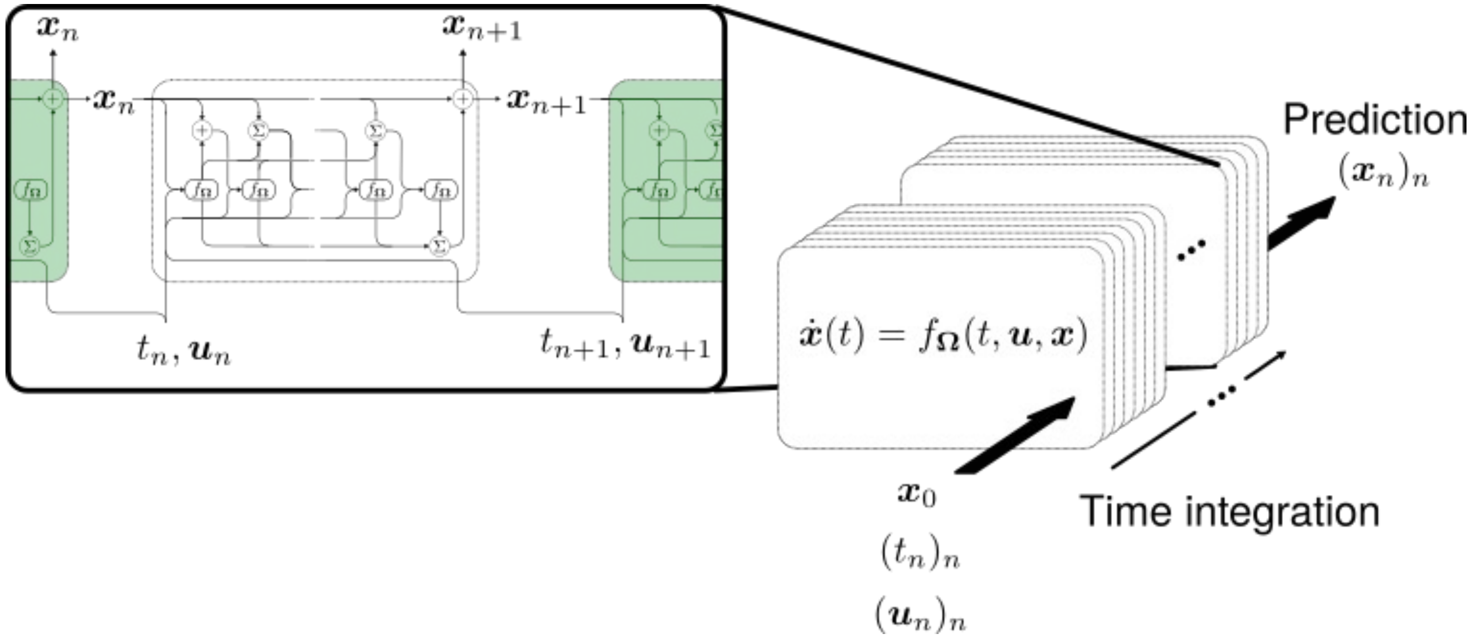


Numeric solver

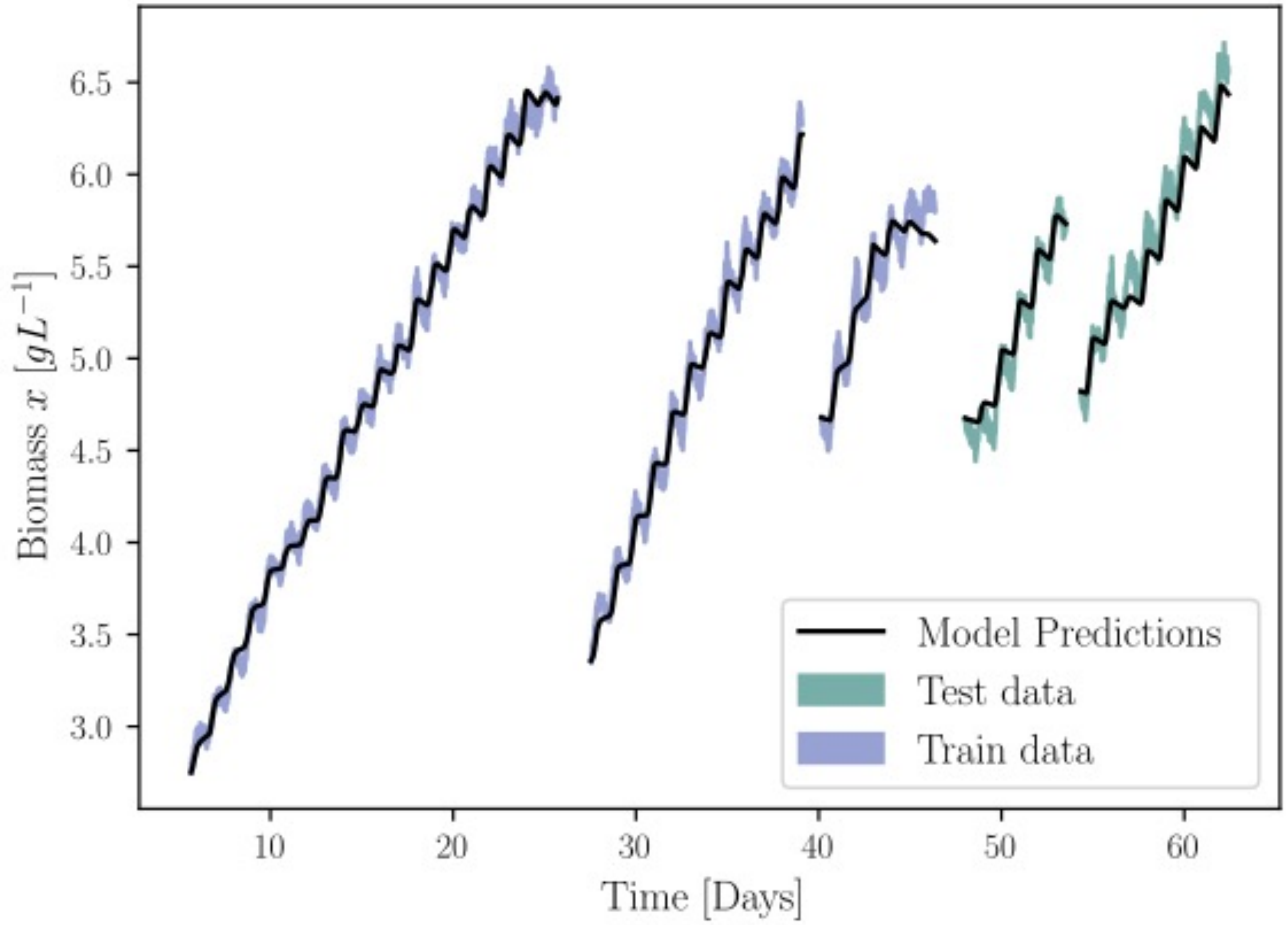
We code our own Runge-Kutta method as recurrent neural network to allow backpropagation.

Solving in batch: several equations can be solved at the same time.

Light and temperature are interpolated at the same time the equations are solved.



Results

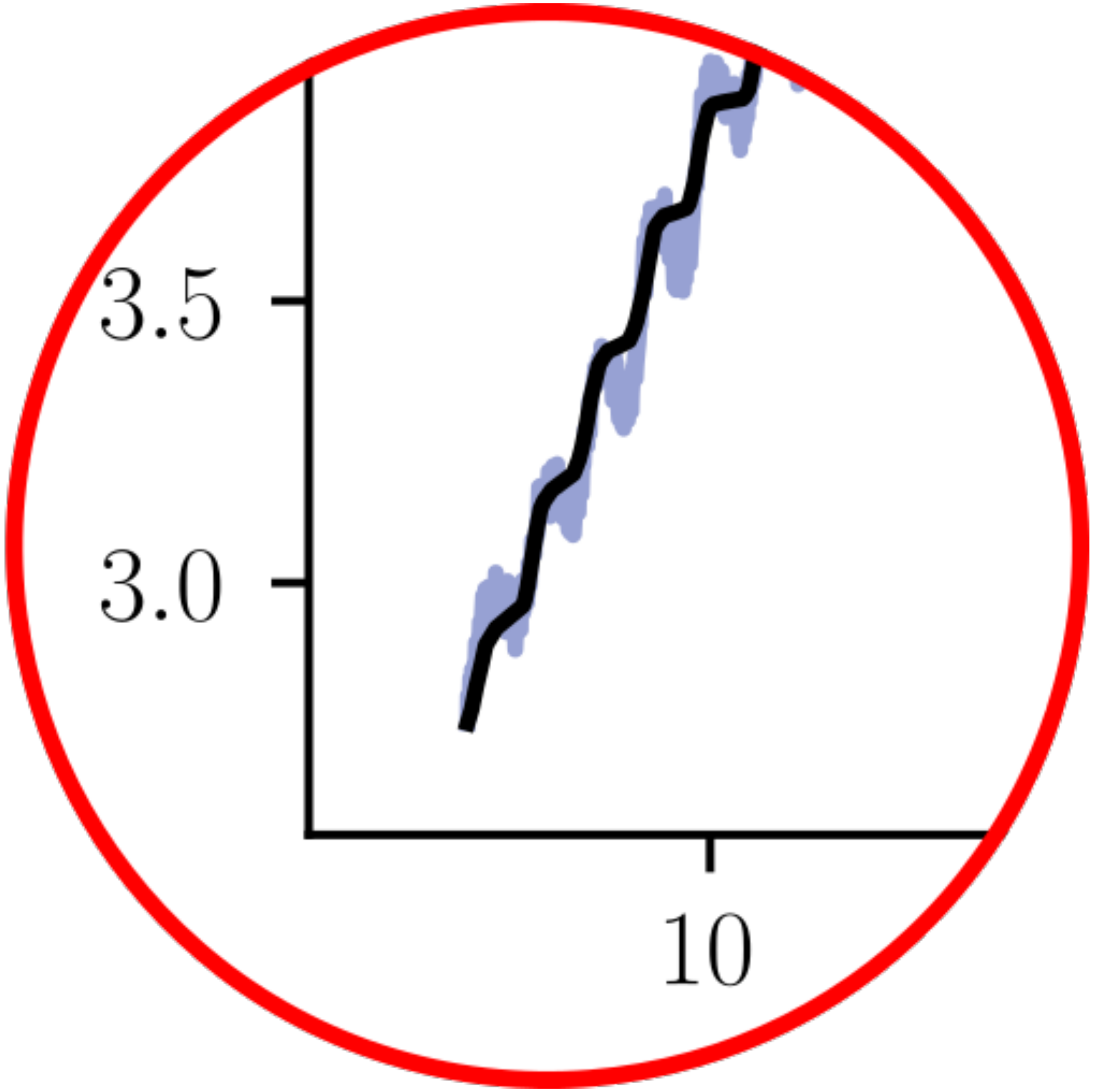


Error	Training dataset			Test dataset	
	Batch 1	Batch 2	Batch 3	Batch 4	Batch 5
RMSE	0.059	0.075	0.108	0.078	0.114
Percentage	1.037	1.318	1.648	1.247	1.697

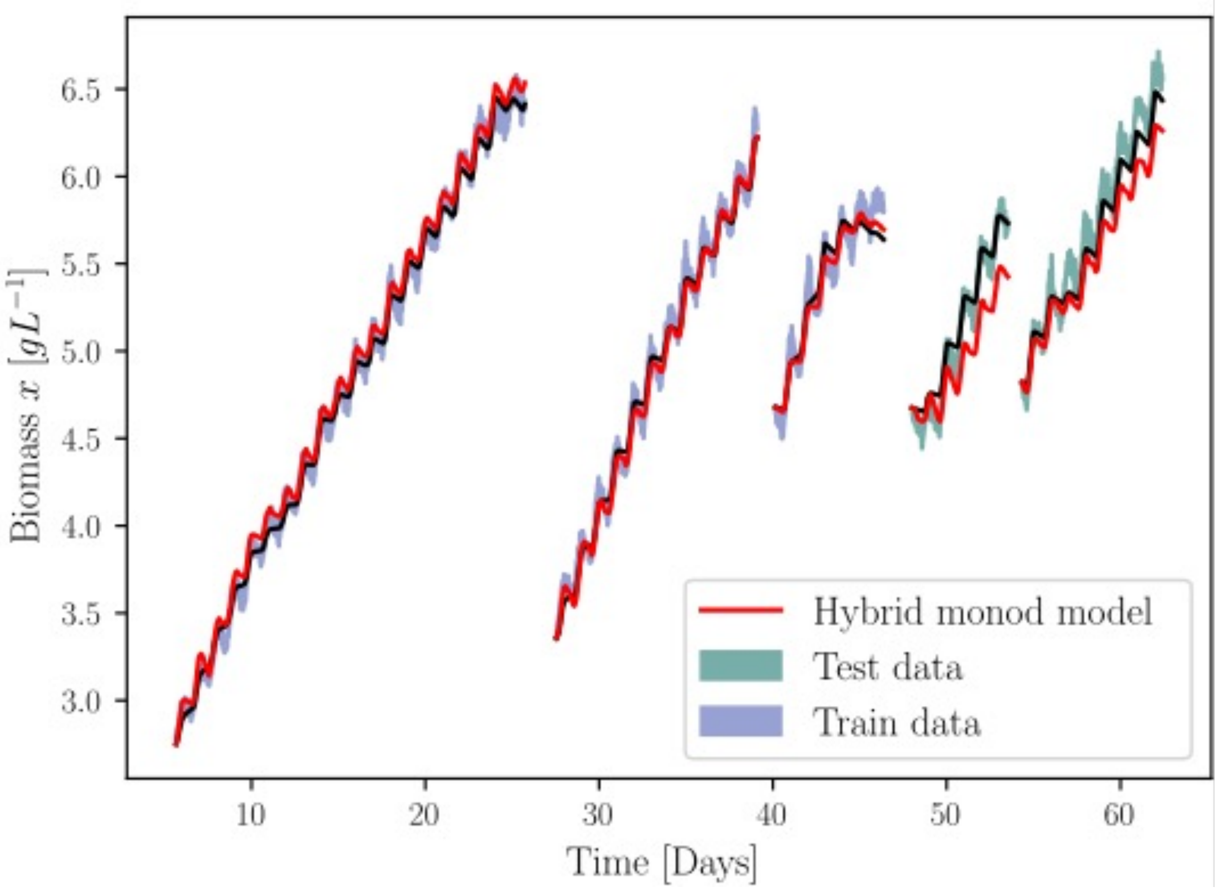
Low error

Some Issues

Local inaccuracy



Solution: informed differential equation



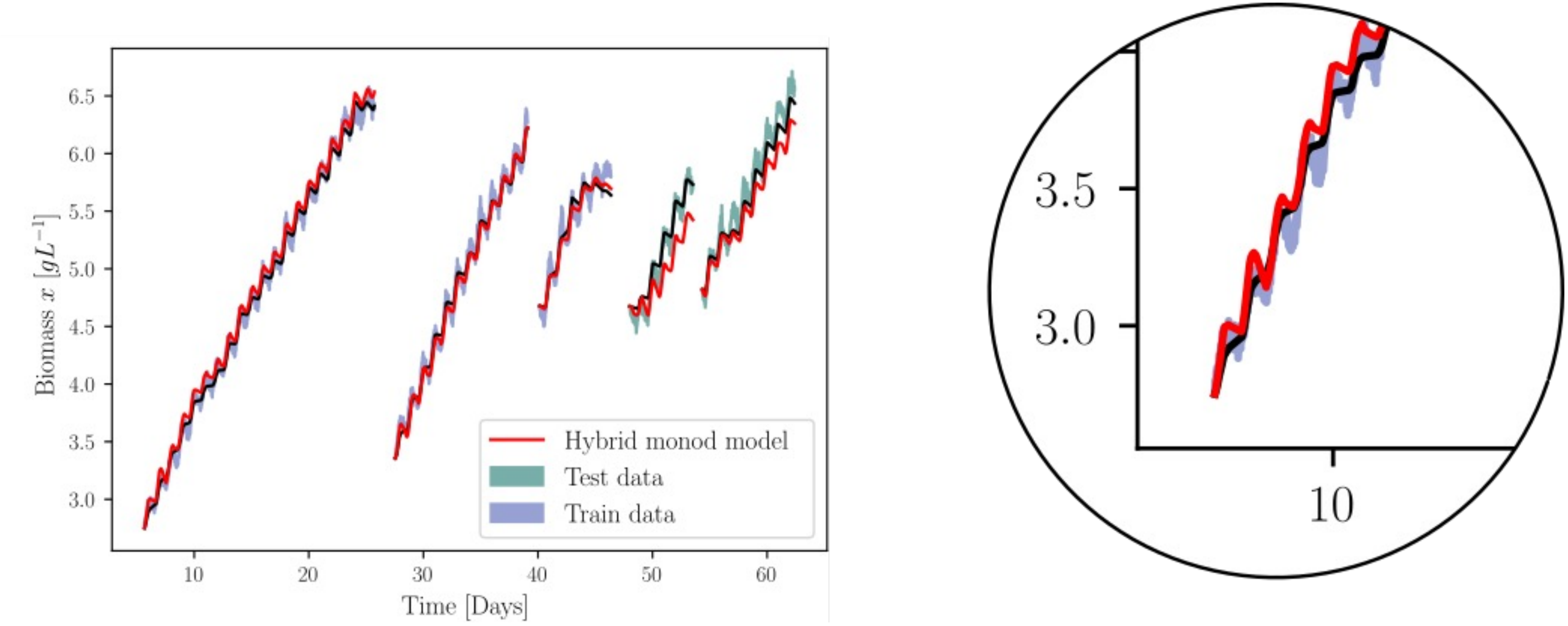
$$\frac{dx}{dt} = \frac{\mu_{\max}}{kx^bL} \ln\left(\frac{I + K_I}{Ie^{-kx^bL} + K_I}\right) x - Rx + NN_{\boldsymbol{\theta}}(I, T, x)$$

Monod kinetics
+
Beer - Lambert law

Respiration rate

Neural Network

Solution: informed differential equation



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FROM MECHANISTIC TO HYBRID MODELLING OF ALGAE-BACTERIA SYSTEMS

Francesca Casagli, Morgan Scalabrino, Joel Ignacio Fierro Ulloa, Olivier Bernard

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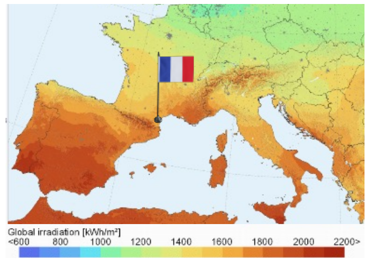
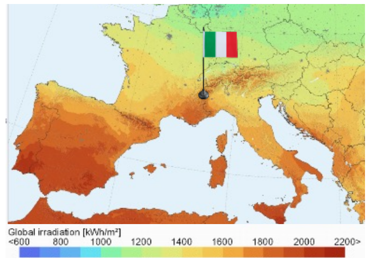
STARTING POINT: THE ALBA MODEL

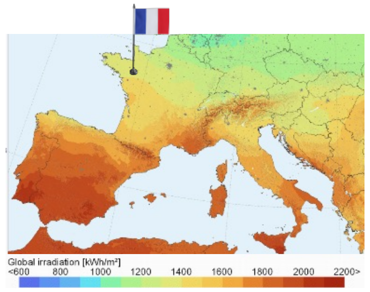
Narbonne

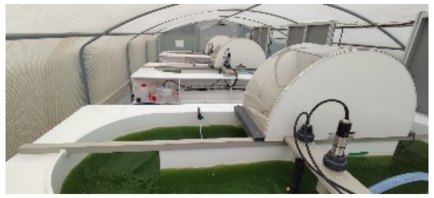


Milan



Rennes





Synthetic WW

443 days

CALIBRATION + VALIDATION

Piggery digestate

189 days

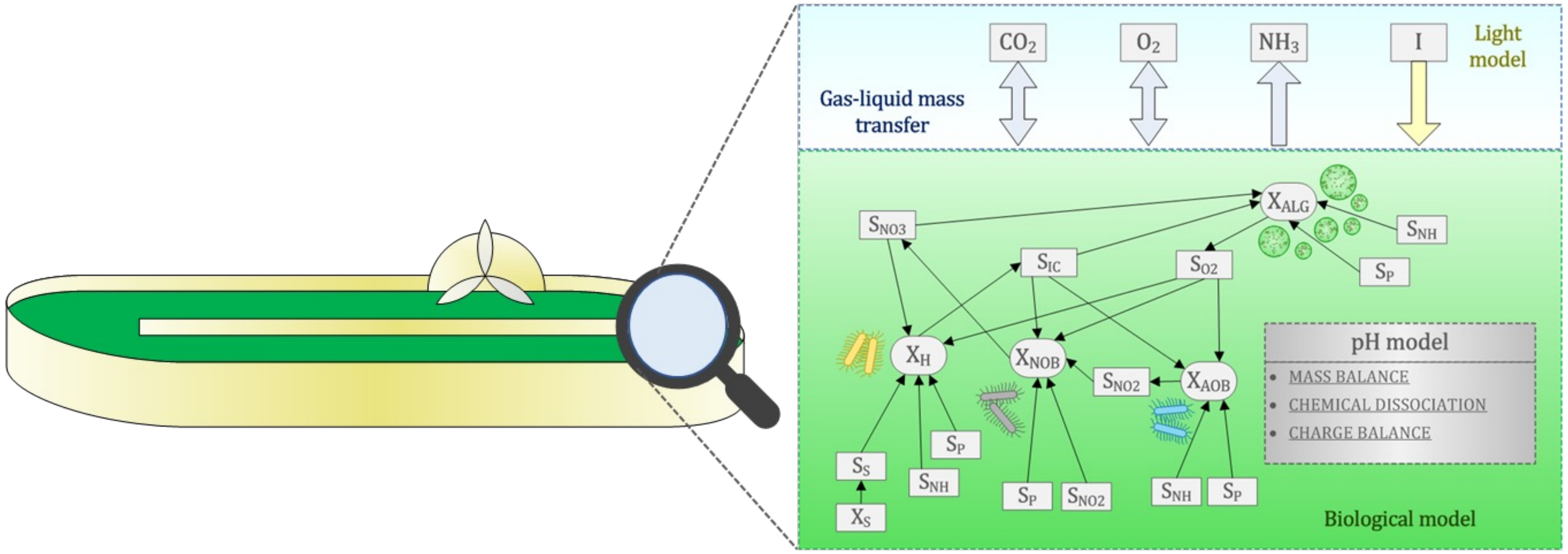
VALIDATION

Piggery digestate

14 days

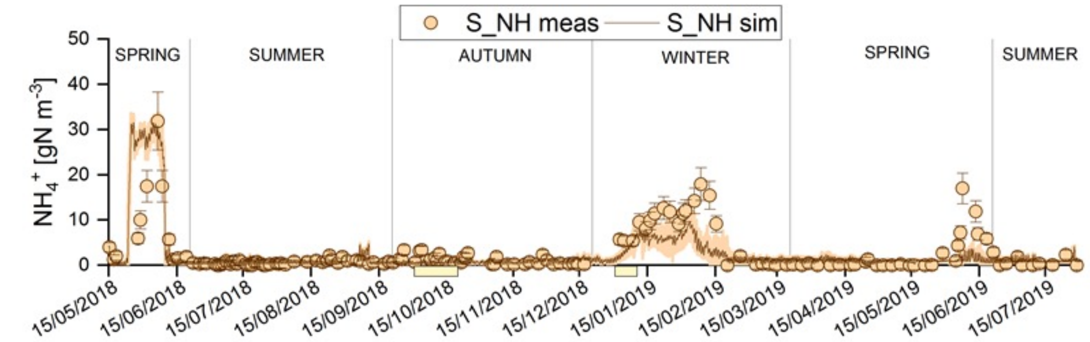
VALIDATION

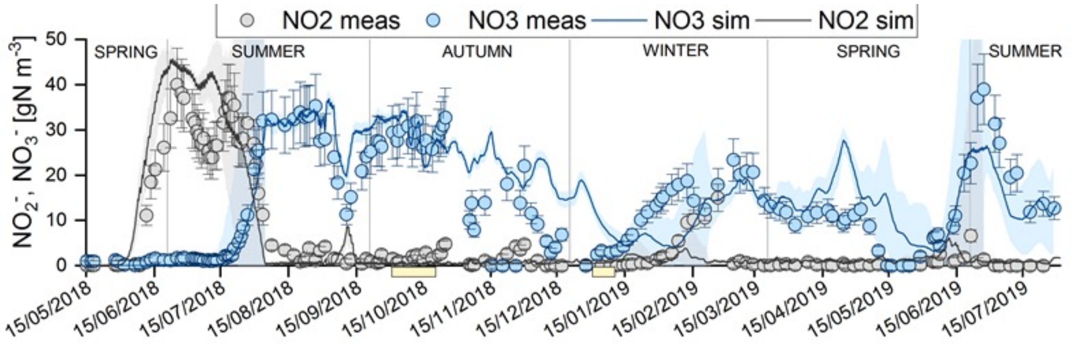
$$
\begin{aligned}
\dot{\xi} &= K \cdot \rho(\xi, T, \theta, \hat{H}^{+}) + \Delta(\xi, \xi_{in}, T, \hat{H}^{+}) \\
\dot{V} &= Q_{in} - Q_{out} + Q_{rain} - Q_{evap}
\end{aligned}
$$

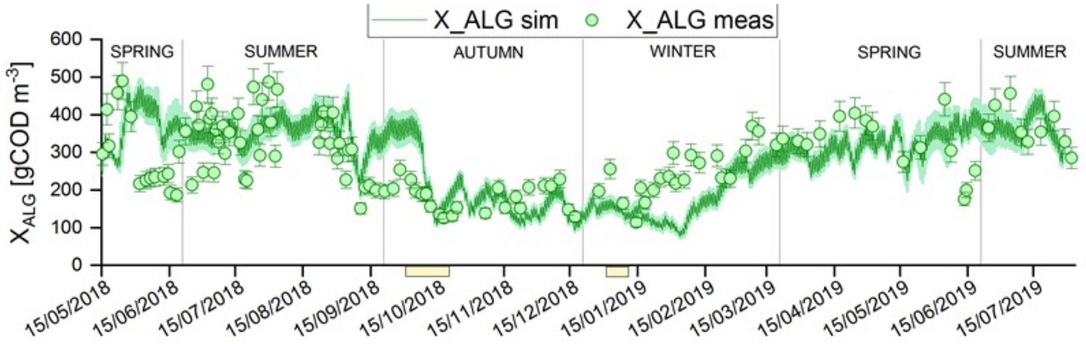


MECHANISTIC MODEL VALIDATION

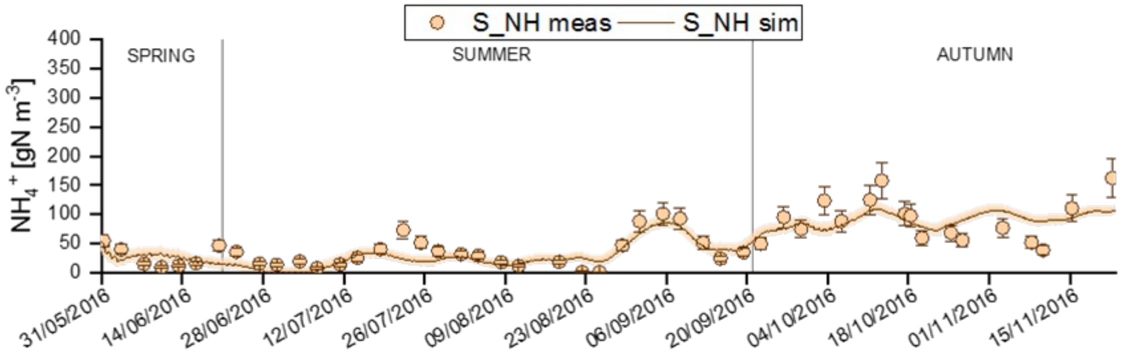
Calibration – Validation

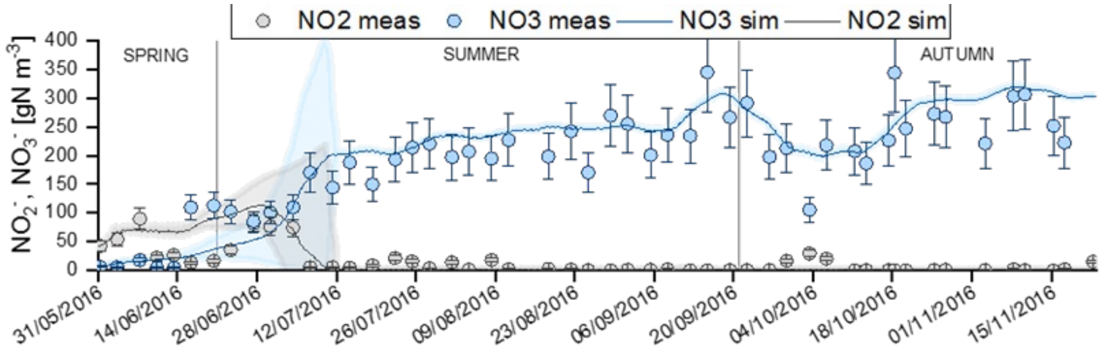


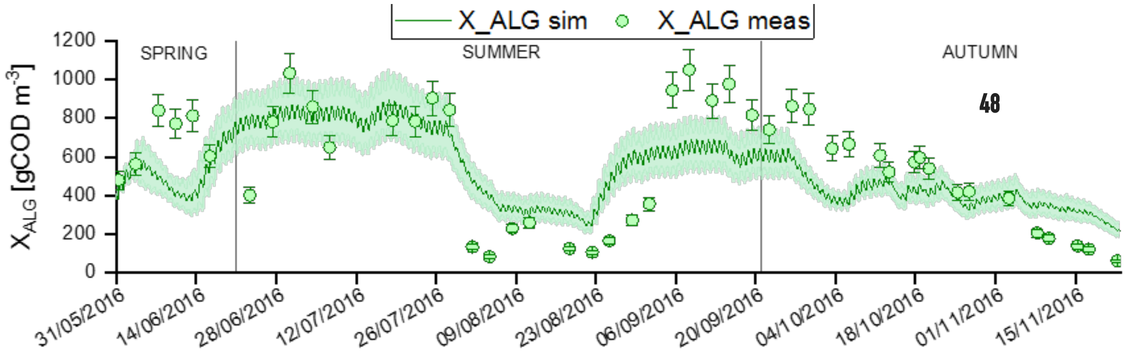




Validation







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HYBRIDIZATION APPROACH: FROM MECHANISTIC MODELS TO PINNS

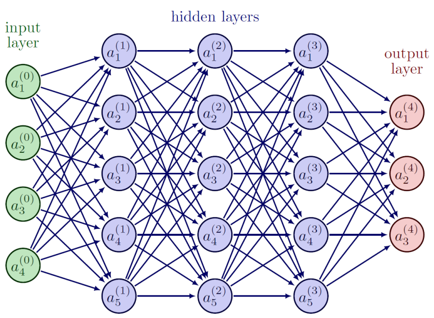
Strategy:

- Replace the part most affected by uncertainty by neural networks
- General formulation applying specific constrains
- Example of application to a mass balance model: the ALBA model

Application:

- Pre-training neural network: determining a first set of parameters ⟶ **static approach**
- Training techniques based on back propagation: closing the gap between model and real data ⟶ **dynamic approach**

$$\dot{\xi} = \underbrace{K \cdot \rho(\xi, T, \theta, \hat{H}^+)} + \Delta(\xi, \xi_{in}, T, \hat{H}^+)$$

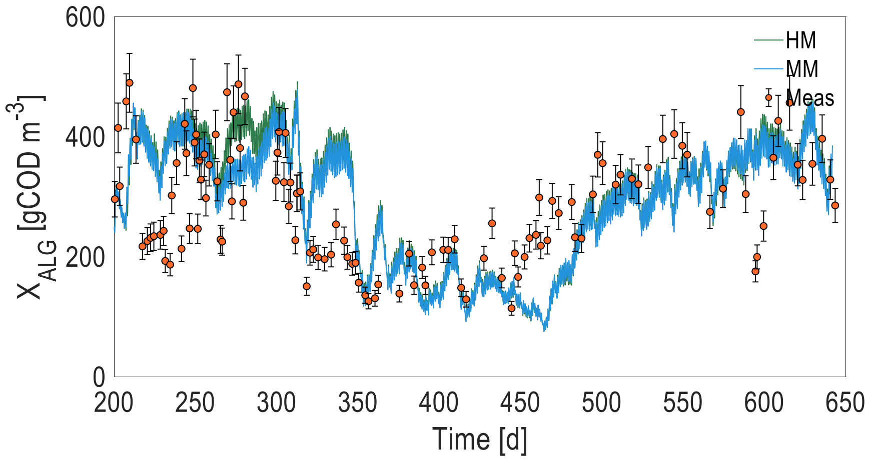


<u>Mass conservation</u>

$$\forall\ \eta \in \{C, N, P, O, H\}\ \ \exists \lambda_\eta > 0 \in\ Ker(K^T)\ |\ \lambda_\eta^T K = 0$$

$\Psi = \lambda_\eta^T \xi$ → *mass of the total element η in the system*

$$\dot{\Psi} = \cancel{\lambda_\eta^T K}\ \rho(\xi, T, \theta, \hat{H}^+) + \lambda_\eta^T\ \Delta(\xi, \xi_{in}, T, \hat{H}^+)$$



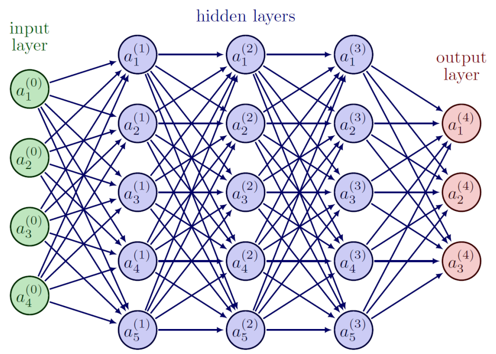
1ST PHASE: CONSTRAINED STATE BOUNDARY

First level of hybridization

$$\frac{d\xi}{dt} = Kr(\xi, u) + D(\xi_{in} - \xi) - Q(\xi, u)$$

Which structure for the kinetics would guaranty the trajectory to respect

- physical positivity of the concentrations
- causality (i.e. no substrate: no reaction)



$$r_i(\xi, u) = \mathcal{C}(\xi)\,\omega(\xi, u)$$

Unknown part given by the NN

$$\omega_i(\xi, u) = \sigma\left(\sum_{i=1}^{n} w_{1,i} a_i^{(L)} + b_1^{(0)}\right)$$

Constrain function (containing) $\Pi_k \xi_k$

Such that: $\xi_i = 0 \Rightarrow \dot{\xi}_i \geq 0$

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2ND PHASE: KINETIC IDENTIFICATION

Second level of hybridization

Computing the **target functions** from the trajectories of the mechanistic model:

$$\omega_i^{MM}(\xi^{MM}, u) = \frac{\rho_i^{MM}}{\mathcal{C}_i(\xi^{MM})}$$

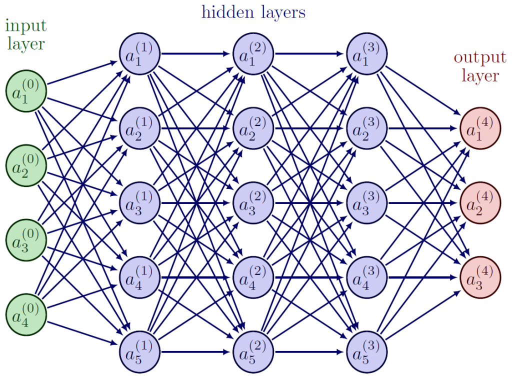
Generated by the mechanistic model

Chosen constrain function

Static problem: Loss function (Ω: parameters of the Neural Network)

$$\mathcal{L}_i(\Omega) = \sum_j \left(\omega_i^{NN}\underbrace{(\Omega, \xi^{MM}(t_j), u)}_{} - \omega_i^{MM}(\xi^{MM}(t_j), u)\right)^2$$

$$\sigma\left(\sum_{i=1}^{n} w_{L+1,i}\, a_i^{(L+1)} + b_1^{(L+1)}\right)$$



$$= \sigma\left(w_{1,0}a_0^{(0)} + w_{1,1}a_1^{(0)} + \ldots + w_{1,n}a_n^{(0)} + b_1^{(0)}\right)$$

$$= \sigma\left(\sum_{i=1}^{n} w_{1,i}a_i^{(0)} + b_1^{(0)}\right)$$

$$\begin{pmatrix} a_1^{(1)} \\ a_2^{(1)} \\ \vdots \\ a_m^{(1)} \end{pmatrix} = \sigma\left[\begin{pmatrix} w_{1,0} & w_{1,1} & \ldots & w_{1,n} \\ w_{2,0} & w_{2,1} & \ldots & w_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ w_{m,0} & w_{m,1} & \ldots & w_{m,n} \end{pmatrix}\begin{pmatrix} a_1^{(0)} \\ a_2^{(0)} \\ \vdots \\ a_n^{(0)} \end{pmatrix} + \begin{pmatrix} b_1^{(0)} \\ b_2^{(0)} \\ \vdots \\ b_m^{(0)} \end{pmatrix}\right]$$

$$a^{(1)} = \sigma\left(\mathbf{W}^{(0)}a^{(0)} + \mathbf{b}^{(0)}\right)$$

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2ND PHASE: KINETIC IDENTIFICATION

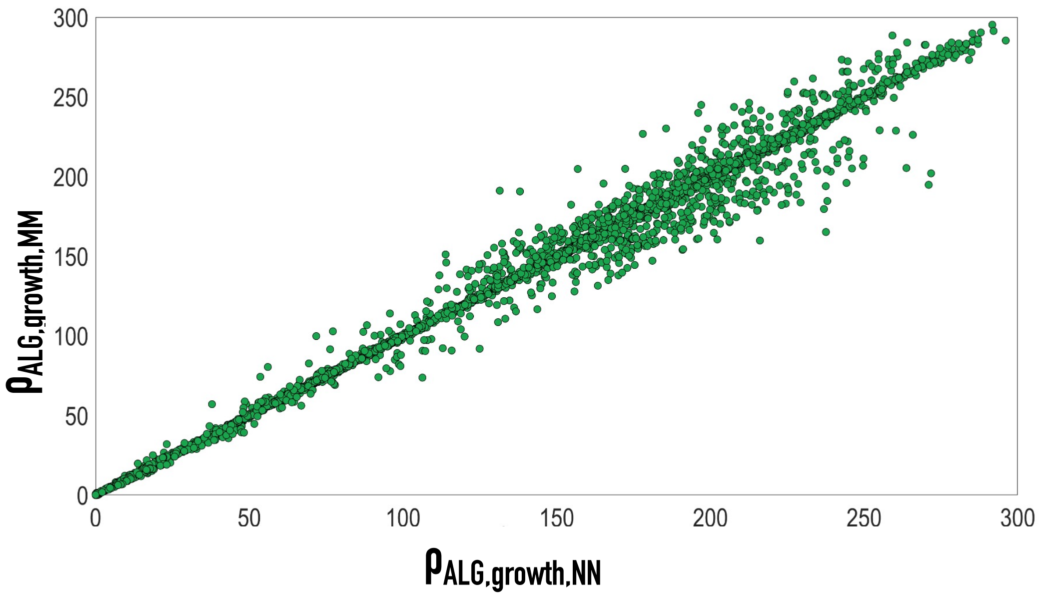
Application to the ALBA model

Identifying a neural network structure for every biological kinetic

Hidden layers structure	Parameters (weights for one kinetic)	Parameters (weights for all the kinetic)	Input	Target
7 - 7 - 7	252	4788	21	$\rho_{i,MM}$

Hidden layers structure	Mean error (10k iteration)	Performance test
5 - 3 - 2	0.0115	3.5e-04
7 - 7 - 7	0.0029	3.5e-04
7	0.0272	4.5e-04

Learning of function $\omega_1(\xi, u)$



- Training the neural network based on the simulated mechanistic kinetics
- Advantage: with the model we can generate a wide range of conditions and points!

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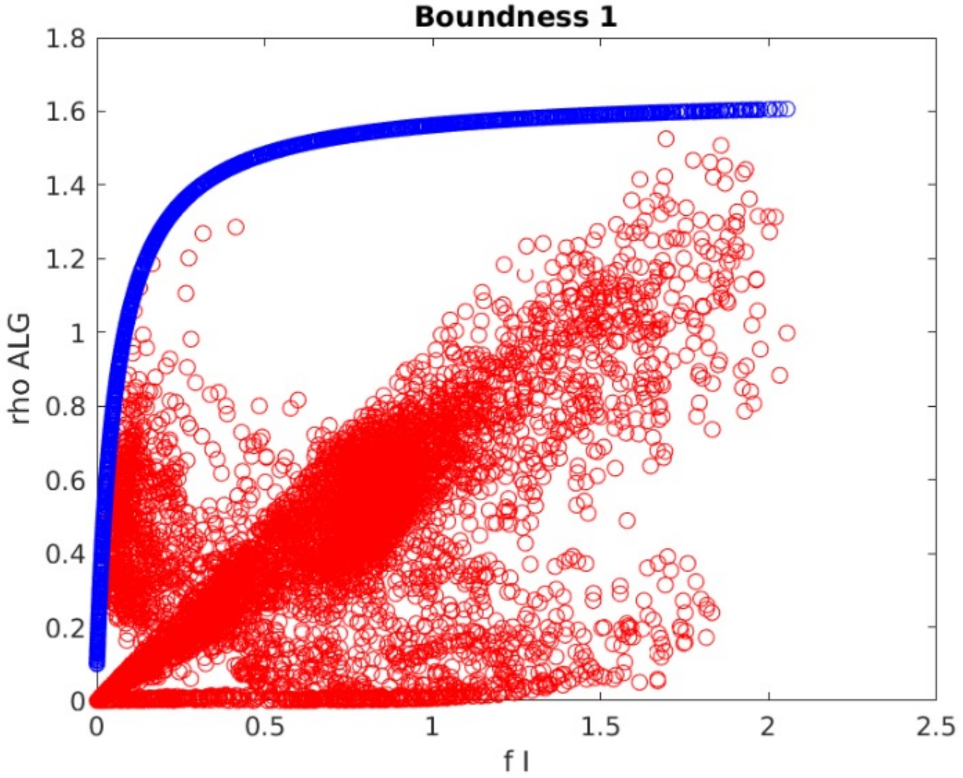
3RD PHASE : KINETIC BOUNDARIES

Creation of functions to bound the bio-kinetic rates (derived from the MM simulation):

- Non negative bio-kinetic reats (min boundary)
- Not too high values → not realistic (max boundary)
- Can also be derived by expert knowledge on the kinetics

$$\rho_i^{NN}(\Omega, \xi, u) \leq \mathcal{P}_i(\xi, u)$$



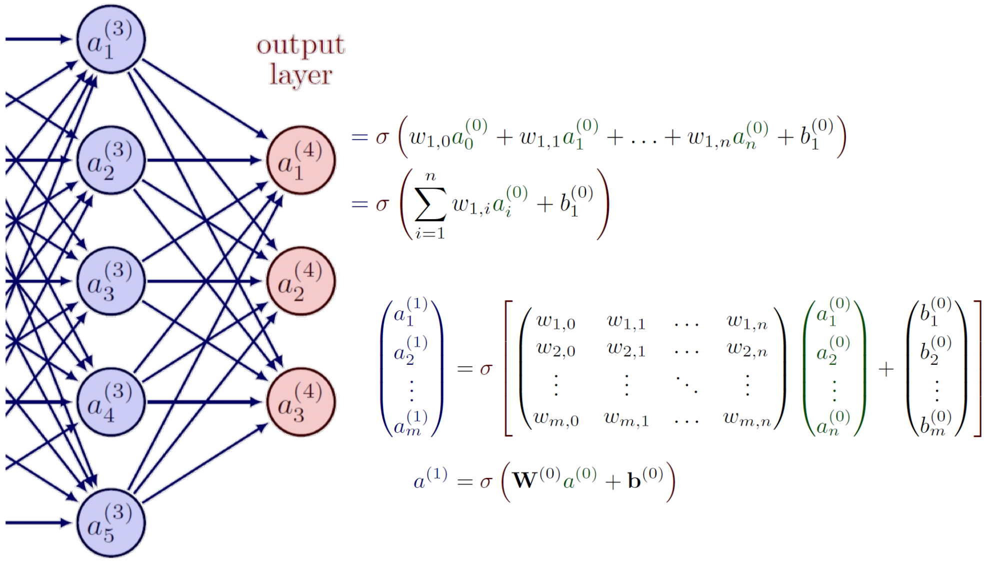
Saturation of the NN prediction: guarantees the predicted kinetics do not become weird far from the training data set.

4^{TH} PHASE : FINE TUNING

Fine tuning of a **subset** of the NN parameters **with the experimental data** using **dynamic backpropagation**

Loss function ($\tilde{\Omega}$: subset of the parameters Ω from the Neural Network):

$$\tilde{\mathcal{L}}(\tilde{\Omega}) = \sum_{i,j} \left(\xi_i^{NN}(t_j, \tilde{\Omega}) - \xi_i^{Meas}(t_j) \right)^2$$



$$= \sigma\left(w_{1,0}a_0^{(0)} + w_{1,1}a_1^{(0)} + \ldots + w_{1,n}a_n^{(0)} + b_1^{(0)}\right)$$

$$= \sigma\left(\sum_{i=1}^{n} w_{1,i}a_i^{(0)} + b_1^{(0)}\right)$$

$$\begin{pmatrix} a_1^{(1)} \\ a_2^{(1)} \\ \vdots \\ a_m^{(1)} \end{pmatrix} = \sigma\left[\begin{pmatrix} w_{1,0} & w_{1,1} & \ldots & w_{1,n} \\ w_{2,0} & w_{2,1} & \ldots & w_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ w_{m,0} & w_{m,1} & \ldots & w_{m,n} \end{pmatrix}\begin{pmatrix} a_1^{(0)} \\ a_2^{(0)} \\ \vdots \\ a_n^{(0)} \end{pmatrix} + \begin{pmatrix} b_1^{(0)} \\ b_2^{(0)} \\ \vdots \\ b_m^{(0)} \end{pmatrix}\right]$$

$$a^{(1)} = \sigma\left(\mathbf{W}^{(0)}a^{(0)} + \mathbf{b}^{(0)}\right)$$

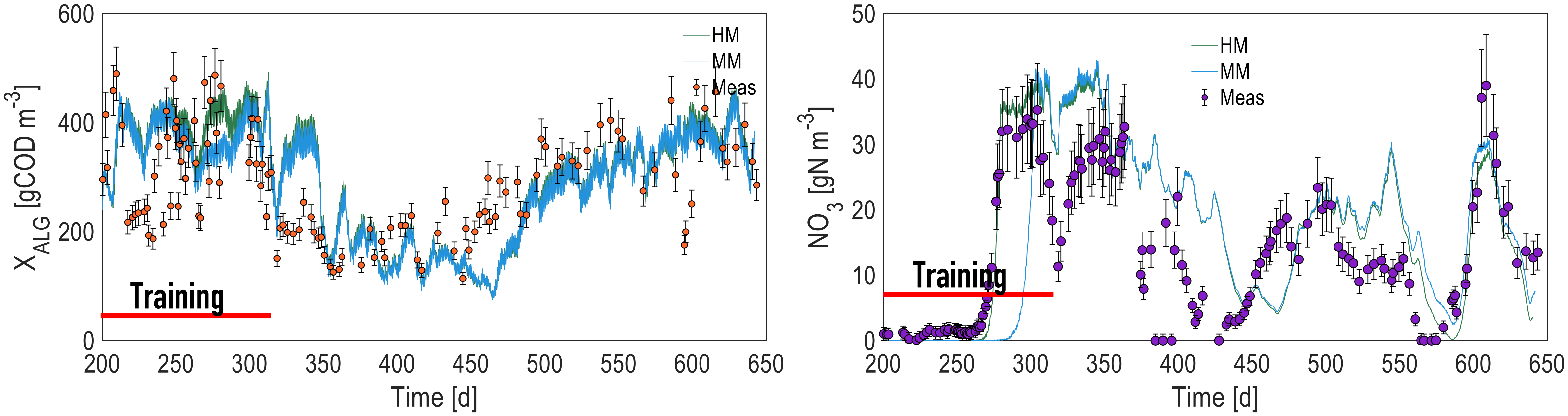
The gradient $\vec{\text{grad}}(\Omega) = \frac{\partial \mathcal{L}}{\partial \Omega}$ is computed with a backpropagation approach, based on an estimate of the sensitivity funct $\sigma_\Omega = \frac{\partial \xi}{\partial \Omega}$

The algorithm starts from the parameter Ω t estimated in phase 2.

4TH PHASE : FINE TUNING

Application to the ALBA model

Fine tuning using on-line O_2 and measurements of algal biomass and inorganic nitrogen



Fit improvement in the training period

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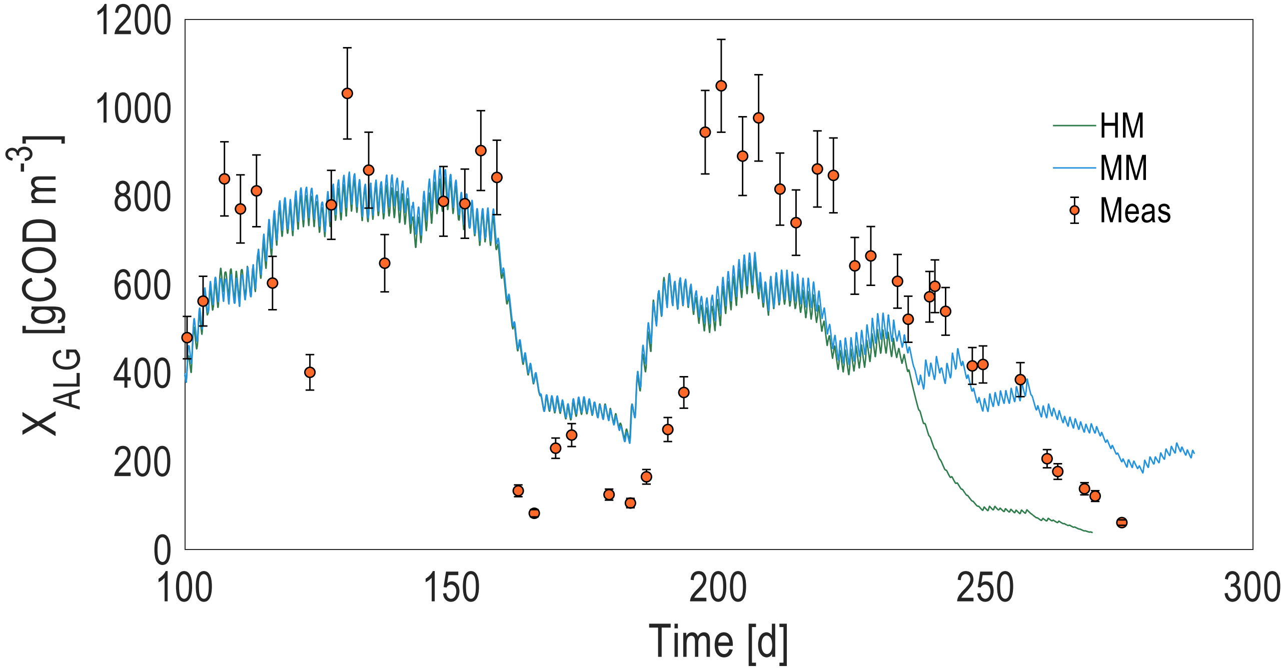
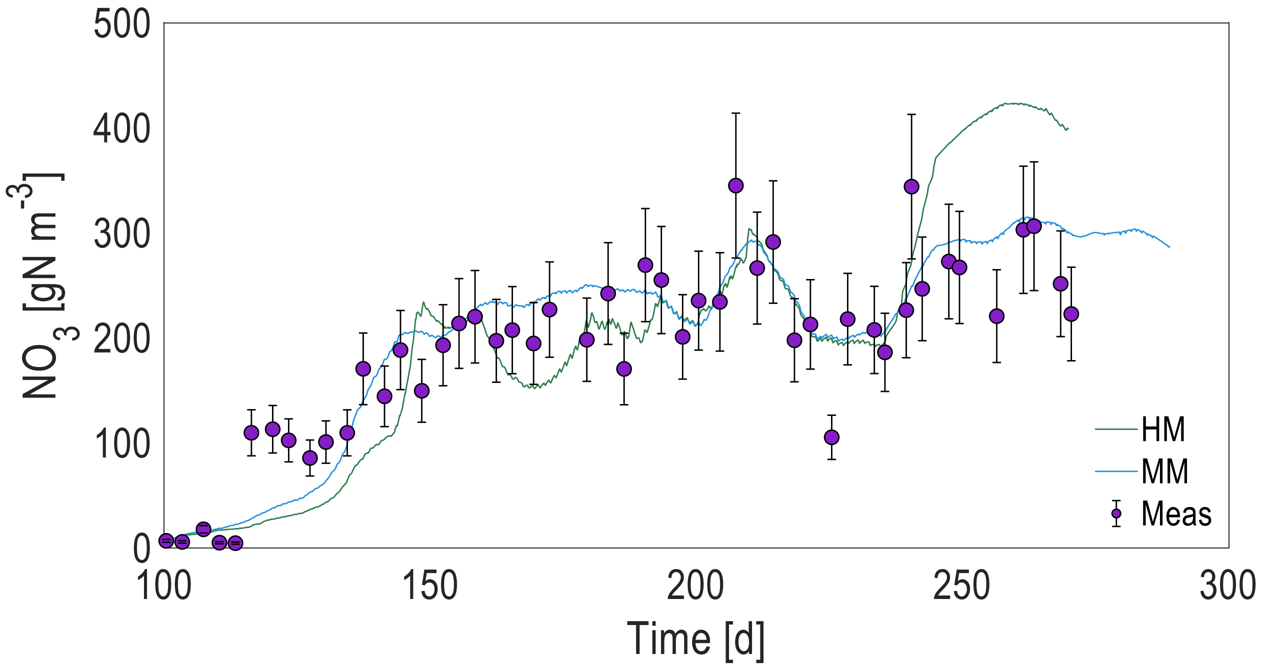
5TH PHASE: VALIDATION AND TEST

Application to the ALBA model for predicting another case (Milan)

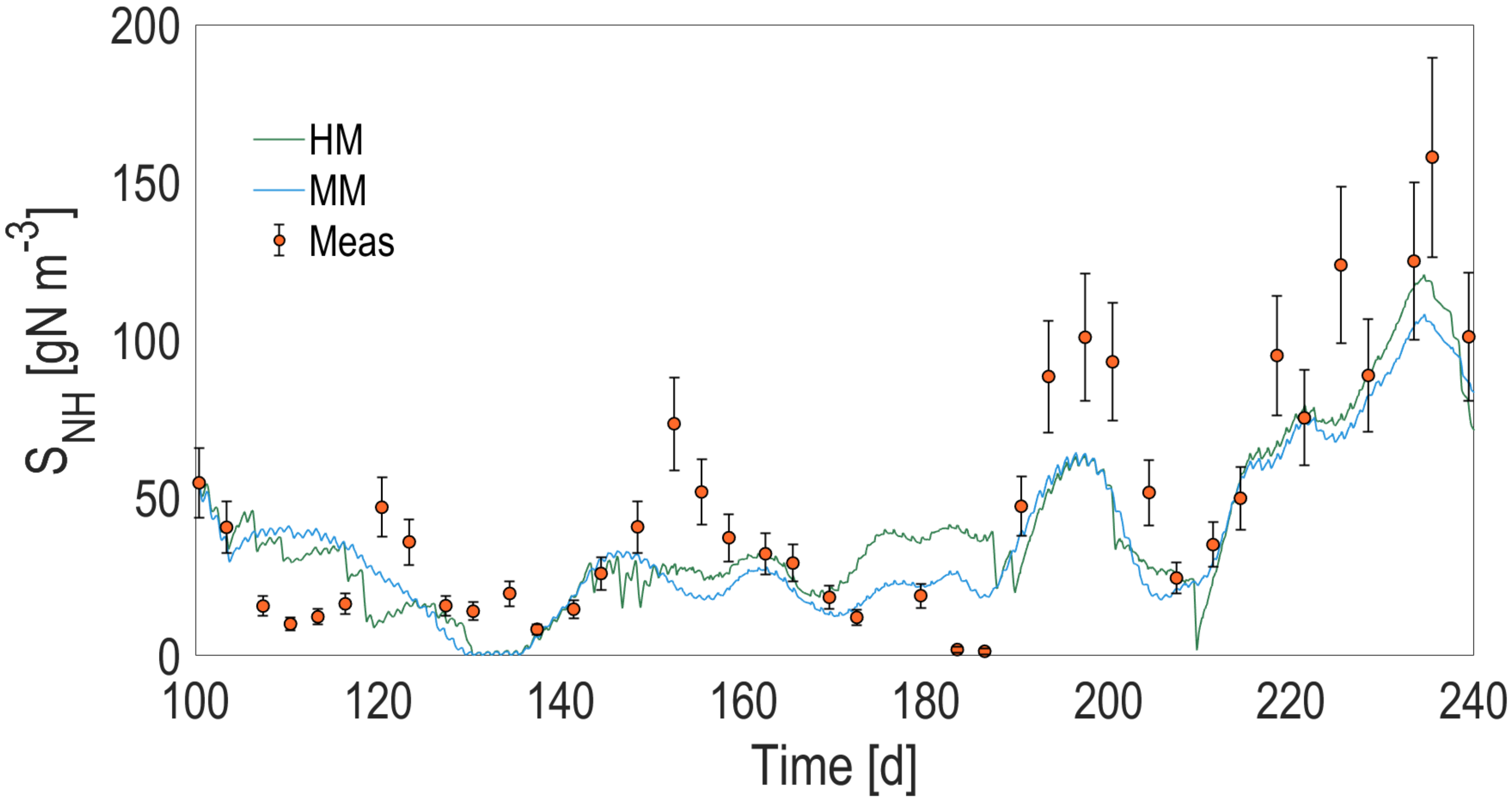




Test phase: different dataset not used for the training

5^{TH} PHASE: VALIDATION AND TEST

Application to the ALBA model for predicting another case (Milan)



NH_4^+ is very allenging to predict

Test phase: different dataset not used for the training

Biocore contribution

- Understanding the rules driving response to temperature in phytoplankton (O. Bernard)
- Neural ODE for representing phytoplankton growth driven my light (I. Fierro)
- Towards hybrid modelling of artificial microbial ecosystems (F. Casagli)
- **Spatio-temporal high-resolution models of particulate organic matter abundance in the ocean (R. Ranini)**

Effect of temperature and light on phytoplankton growth

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Olivier BERNARD, Francesca CASAGLI, Romain RANINI, Ignacio FIERRO, Jineth ARANGO, Kilian BURGI, David JEISON, Antoine SCIANDRA, Lionel GUIDI

INVENTEURS DU MONDE NUMÉRIQUE

OCÉANIA IS AN INRIA CHALLENGE PROJECT

Green Owl

OPTIMISATION OF WATER LIVING MICROORGANISMS FOR GENERATING RENEWABLE RESOURCES

Olivier BERNARD