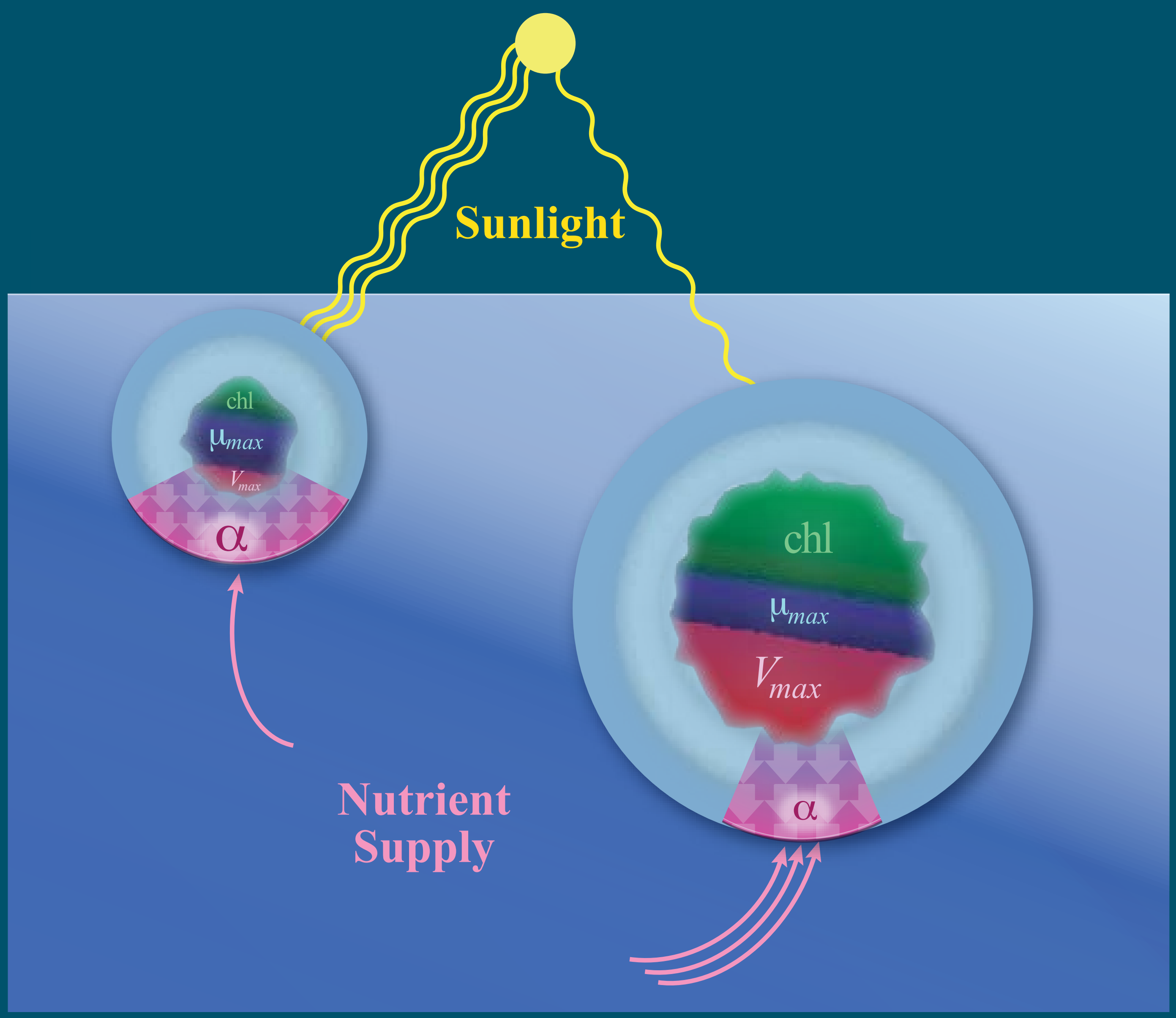
Optimality-based Modelling: from theory to implementation



It's all about combining
Traits & Trade-offs
(Smith et al. *L&O Review* 2011,
Smith et al. *JPR Horizons* 2014)

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CREST, Japan Science and Technology Agency, Tokyo, Japan

Trade-offs: apply to humans as well as plankton

体重

マラソン選手

一般的な体型の人

力士

走る速さ

マラソン選手は体重が少ないので力は強くないが速く走る事ができる

力士は体重が重いので力は強いが速く走ることはできない

Different body types perform *Optimally* for different goals.

Theory: Optimality-based models of plankton

Assumptions

- Natural Selection produces optimally adapted organisms
- Fitness = Growth Rate ← **Goal: Maximize Growth Rate**

Considerable success over the past decade

Recent Advances in:

- 'optimal foraging', Photoacclimation & Primary Production

Major Challenge

- D*ynamic* models consistent with Evolutionarily Stable Strategy (ESS)
  - ESS formulated in terms of steady state (John Maynard Smith)
- i.e., how to describe short-term dynamics, e.g., *acclimation*, consistent with *evolutionary adaptation* of the very ability to acclimate.

from the review by Smith et al. (*Limnology & Oceanography* 56, 2011)

'adaptive dynamics': modelling changing trait values

Trait *x* should change in proportion to its effect on fitness, *F*:

$$\frac{dx}{dt} = \delta_x \frac{\partial F(x,E)}{\partial x}$$

Different trait values are optimal under different environmental conditions.

δ_x: flexibility ~ diversity (trait distribution)
E: Environment (nutrients, light, temperature, etc.)

For plankton *F = Growth; dx/dt depends on E* (Smith et al. *L&O*, 2011)

Acclimation Rates depend on:

1. possible range of trait values (adaptive capacity),
2. environmental variability
3. current distribution of trait values

Remaining Challenge: modelled diversity tends to collapse

immigration required to maintain diversity (Bruggeman & Kooijman *L&O* 2007)

'Adaptive Dynamics': evolutionary changes
McGill and Brown (*An. Rev. Ecol. Evol. Syst.* 2007), Litchman et al. (*PNAS* 2009)

'adaptive dynamics': species succession, communities
Wirtz & Eckhardt (*Ecol. Modell.* 1996), Wirtz (*J. Biotech*. 2002), Abrams (*J. Evol. Biol.* 2005)

What can optimality be used to model?

What I do

Acclimation

short-term changes

e.g., seasonal change of a dog's coat of hair

changes in chl content of phytoplankton

Ecological Dynamics

species succession (changes in community composition)

Others also model

Adaptation

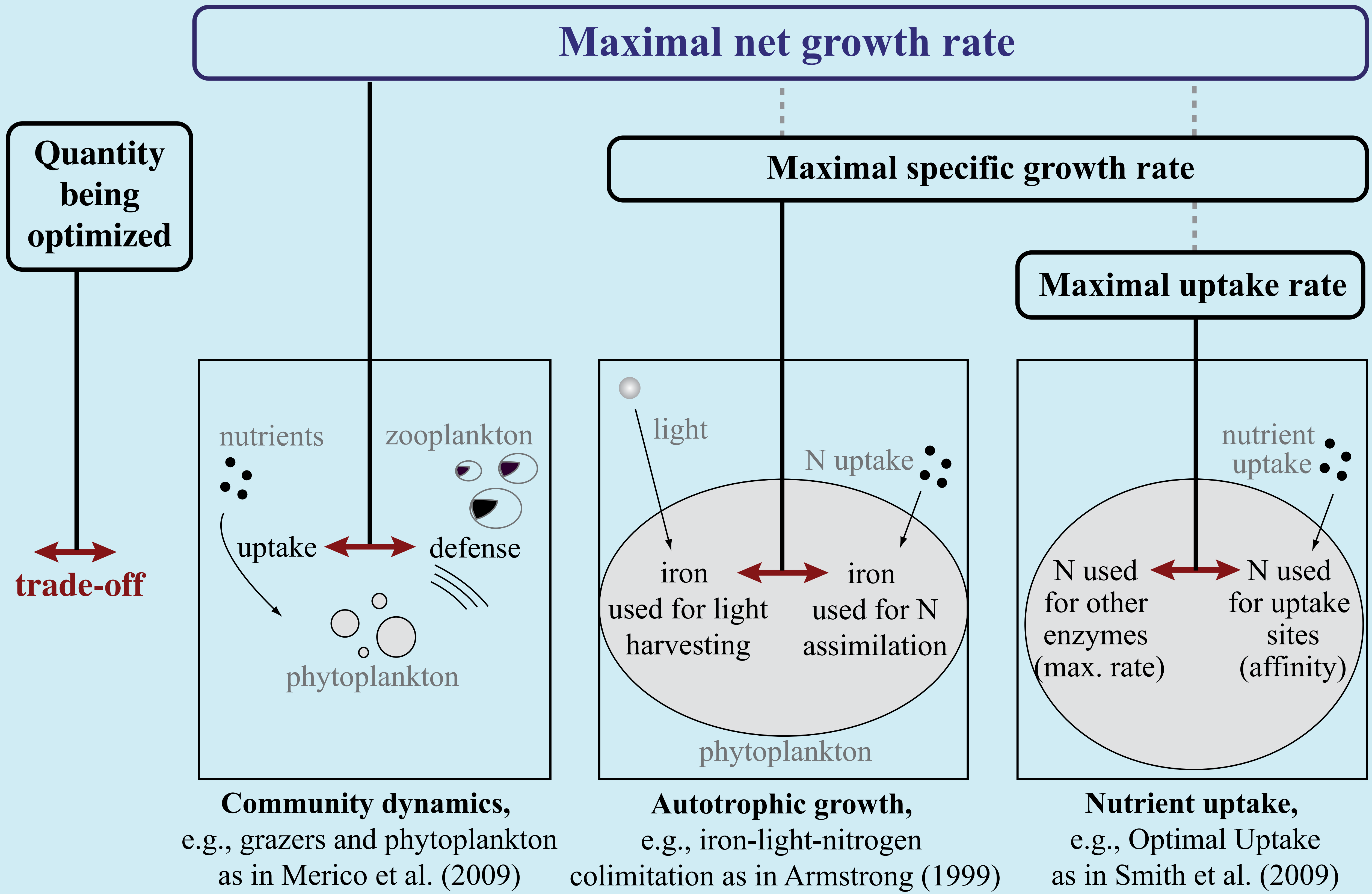
long(er)-term changes

evolution (genetic changes in a species)

The same approaches can be used to model all three.

e.g., Wirtz and Eckhardt (*Ecol. Mod.*, 1996), Merico et al. (*Ecol. Mod.*, 2009)

What to Optimize?



(Smith et al. *L&O* 2011, fig. 2)

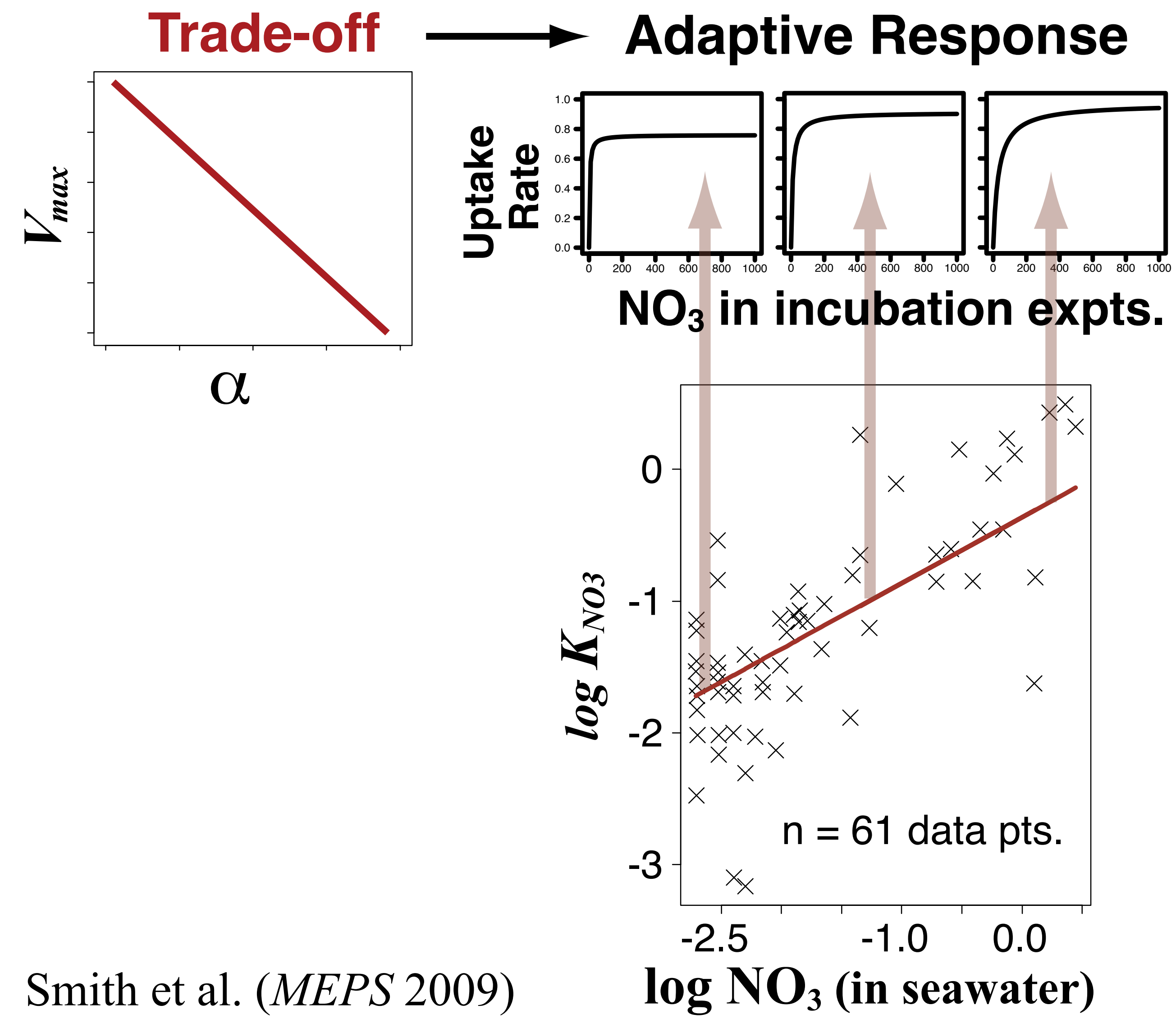
Trade-offs as ‘Hyper-Parameterizations’

‘Hyper-Parameters’ in hierarchical Bayesian modeling specify prior *distributions* of model parameters

(e.g., Gelman et al. *Bayesian Data Analysis*, 2nd edition, 2004)

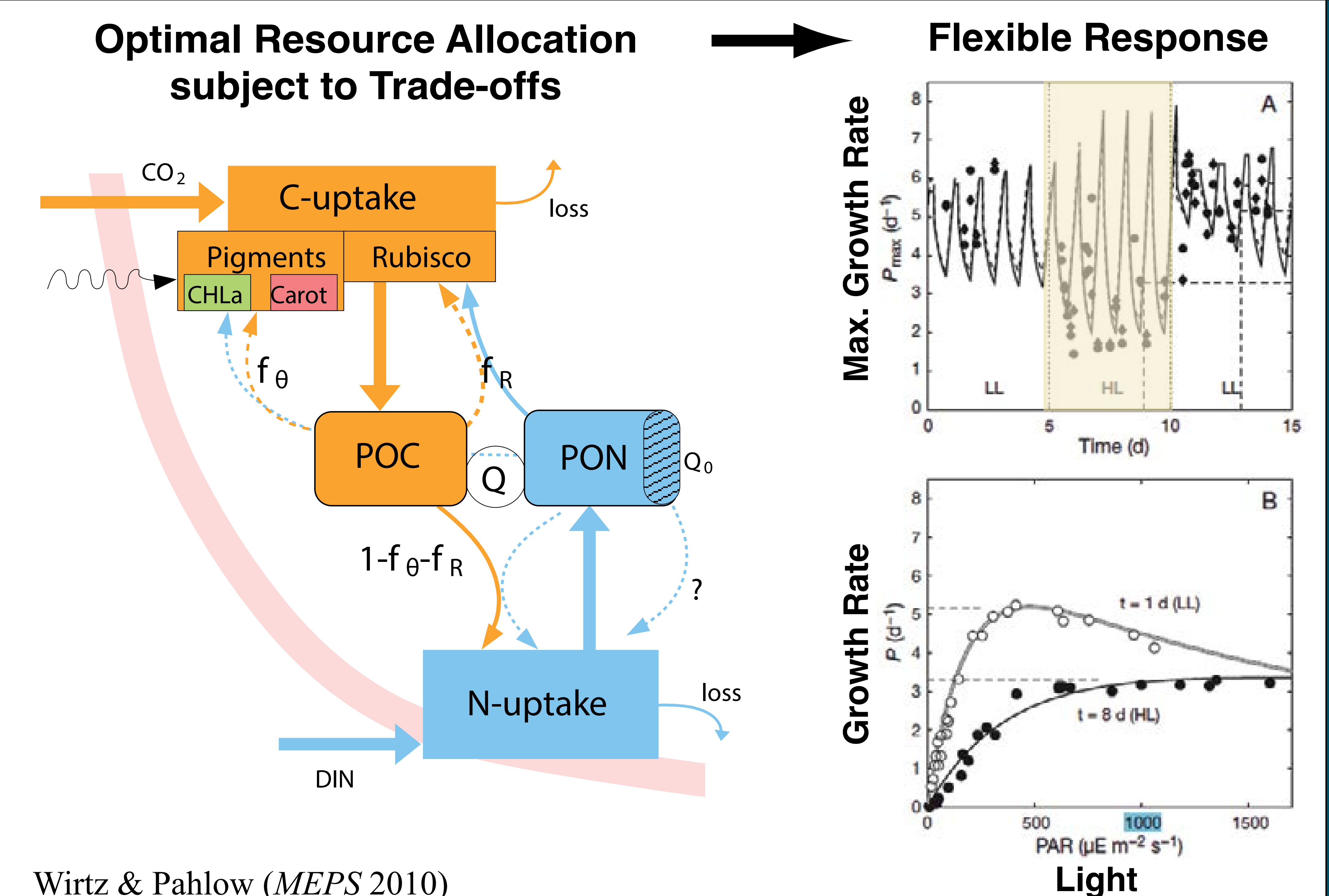
Trade-offs specify how the shapes of functional relationships may change, rather than fixing their shapes.

Optimal Uptake kinetics



Smith et al. (*MEPS* 2009)

Shape-shifting of the Growth vs. Irradiance curve

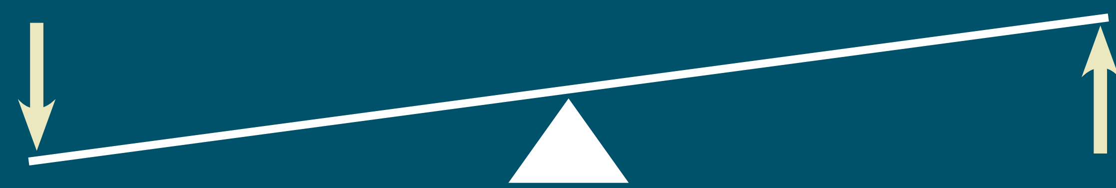


Wirtz & Pahlow (*MEPS* 2010)

Optimality-based Photoacclimation models have advantages compared to empirically-based functions (Smith & Yamanaka. *Ecol. Modell.* 2007)

Selected Examples of Trade-offs for Plankton

Costs vs. benefits
in allocating limited resources (energy, nutrients)



Affinity for nutrient vs. **Maximum Uptake Rate**

Pahlow (*MEPS* 2005), Smith et al. (*MEPS* 2009, 2014)

Light Harvesting vs. **Nutrient Uptake**

Pahlow (*MEPS* 2005, 2009, 2013), Wirtz and Pahlow (*MEPS* 2010)
and effectively all "photo-acclimation" models
*although many (e.g. Geider type) do not *explicity* employ trade-offs

Ingestion of Prey vs. **Cost of Foraging**

Pahlow and Prowe (*MEPS* 2010)

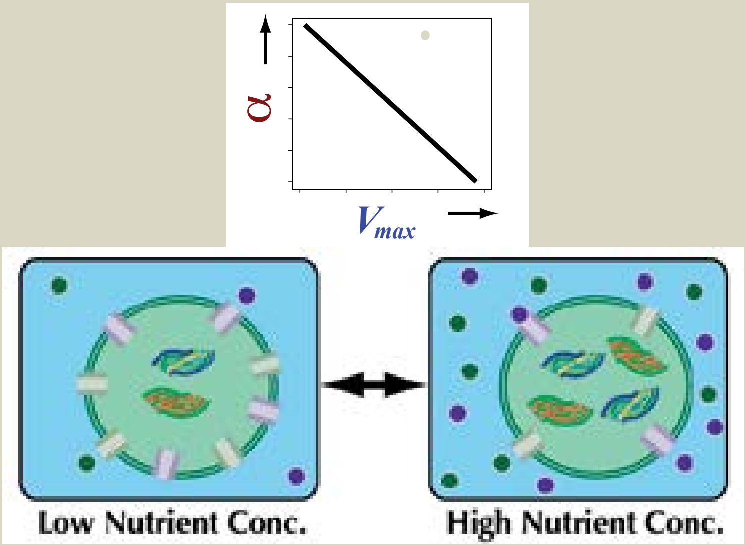
a few examples from Smith et al. (*L&O*, 2011)

Trade-offs allow simple models to Represent Flexible Response

Optimal Uptake kinetics
(Pahlow. *MEPS*, 2005; Smith et al. *MEPS*, 2009)

affinity (α) vs. max. uptake rate (V_{max})

$\propto f_A$ vs. $\propto (1 - f_A)$

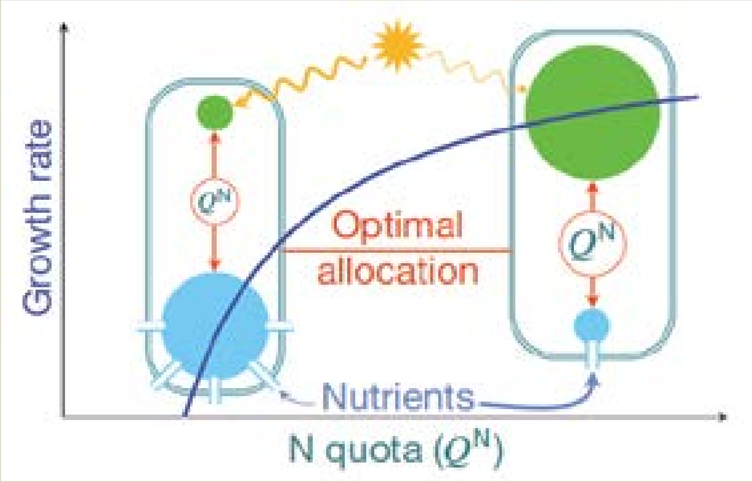


1 ← f_A 0

Optimal Growth model
(Pahlow and Oschlies. *MEPS*, 2013)

N uptake ($\hat{V}$) vs. C fixation ($\hat{\mu}^I$)

$\propto f_V$ $\propto (1 - \frac{Q_s}{Q^N} - f_V)$



0.5 ← f_V 0

submitted with revisions to *JPR* (March, 2015)

Just 1 diff. eqn. for dynamics of C biomass.

+ simple calc`ns for **chl:C & N:C**

Balanced Growth Assumption
(Burmaster *Am. Nat.* 1979)

$V = \mu Q$

A single, explicit equation:

$\mu = f(N, I)$

including adaptive response*

*assuming instantaneous optimal resource allocation

0-D (box) model of the mixed layer at stns. K2 & S1

Inflexible PFT vs. FlexPFT

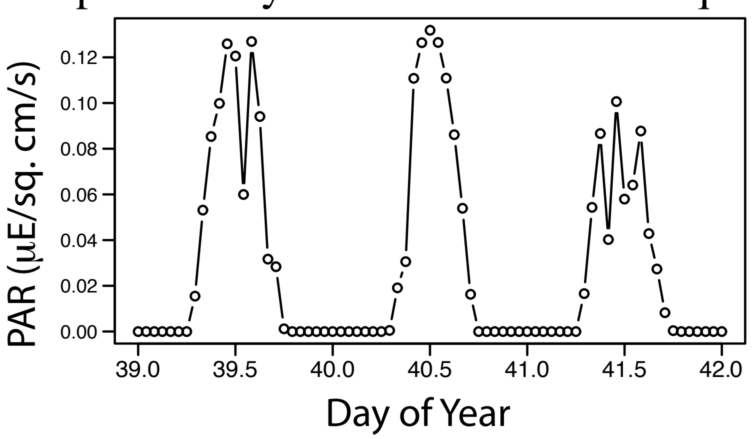
a single PFT for each (NPD model), respectively

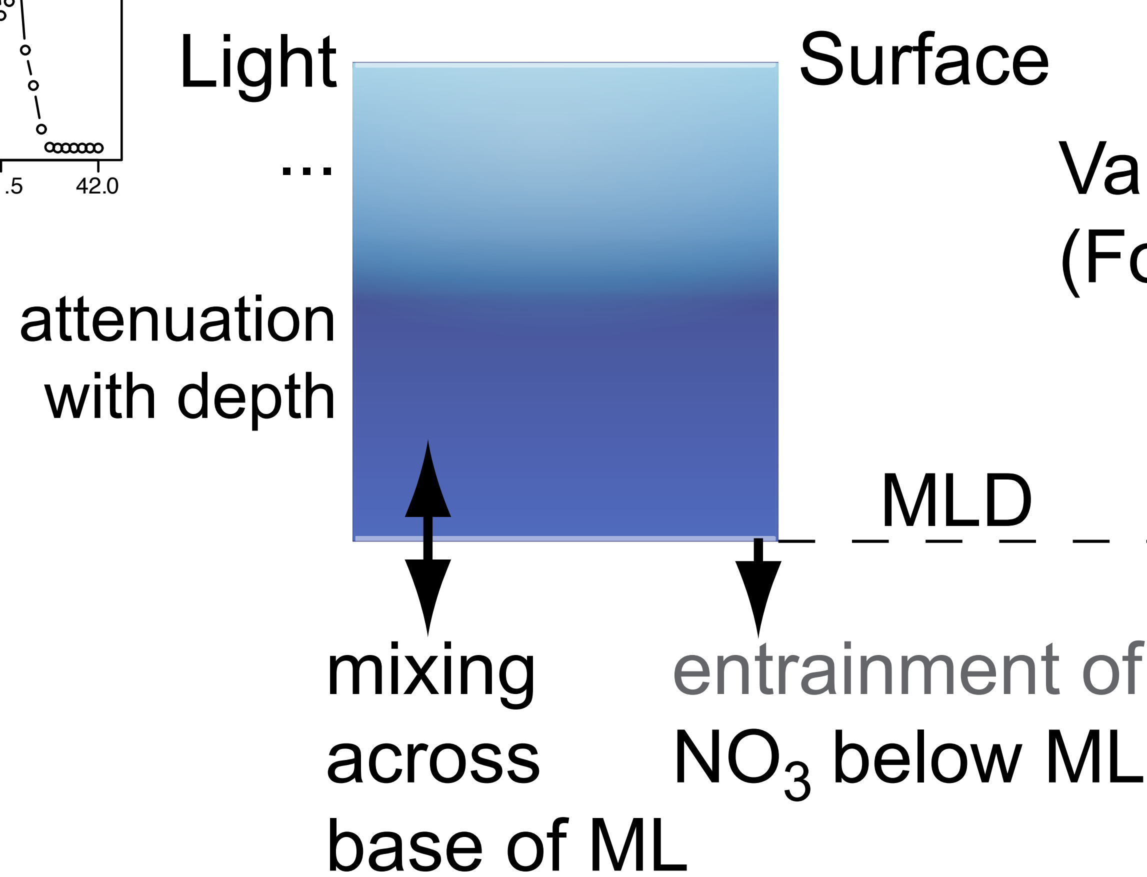
embedded in the same physical model

Fitted to Obs. Data for NO3, chl and PP

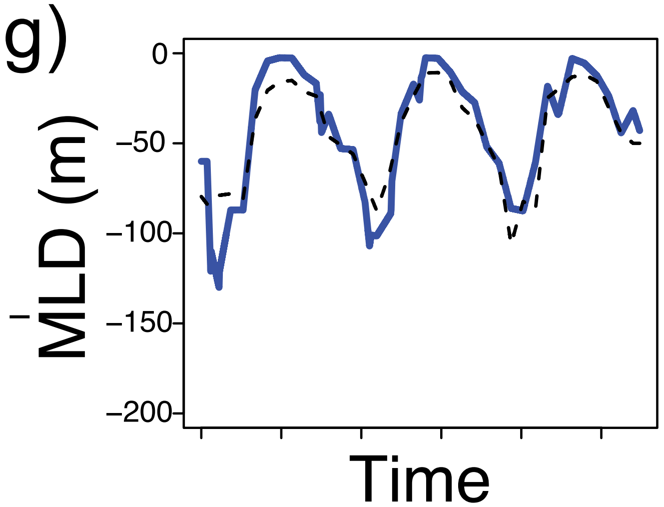
PAR Forcing:

Cruise Obs. when available +
interpolation by Ideal Astronomical Eqn.





Variable Mixed Layer Depth (Forcing)



Intracellular Resource Allocation

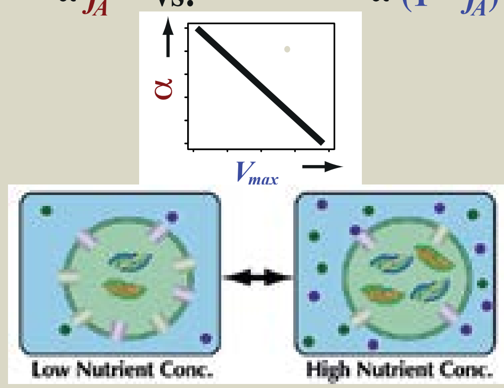
Inflexible Control:

Turn off Optimization:

constant f_A

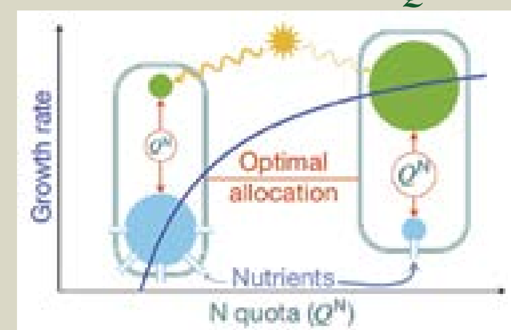
constant f_V

Optimal Uptake kinetics
(Pahlow 2005; Smith et al. 2009)
affinity (α) vs. max. uptake rate (V_{max})
$\propto f_A$ vs. $\propto (1 - f_A)$



1 ← f_A 0

Optimal Growth model
(Pahlow and Oschlies 2013)
N uptake ($\hat{V}$) vs. C fixation ($\hat{\mu}^I$)
$\propto f_V$ $\propto (1 - \frac{Q_s}{Q^N} - f_V)$



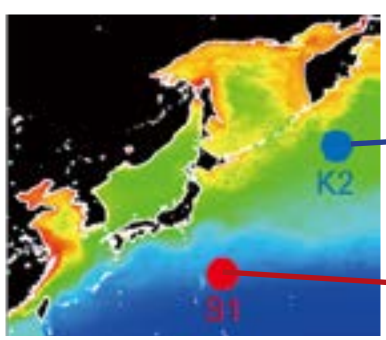
0.5 ← f_V 0

FlexPFT model

Optimal Allocation

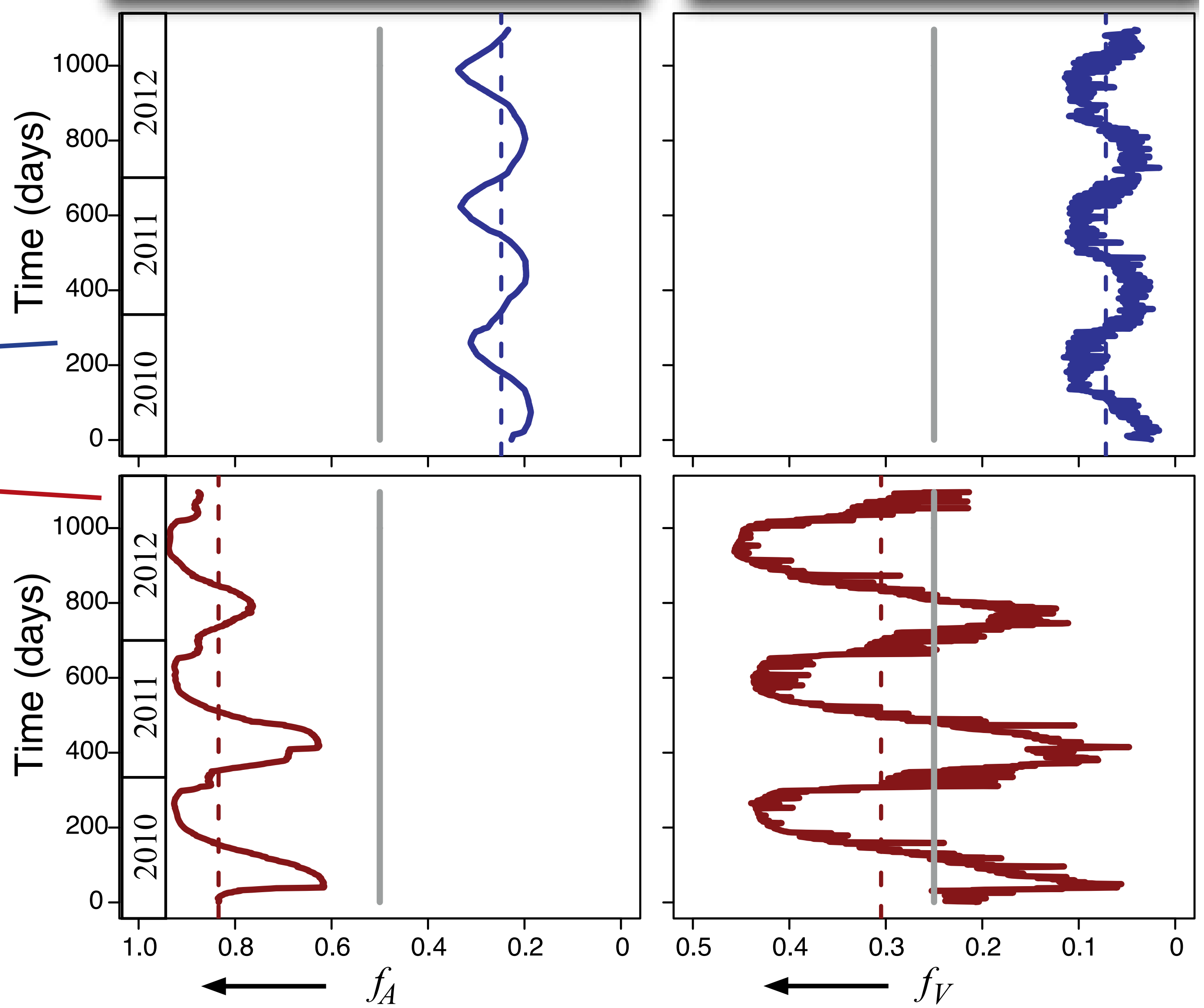
optimize f_A | N

optimize f_V | N, I



stn. K2

stn. S1



more allocation to light gathering at stn. K2

=> lower f_A & f_V

(lower in winter)

more allocation to nutrient uptake at stn. K2

higher f_A & f_V <=

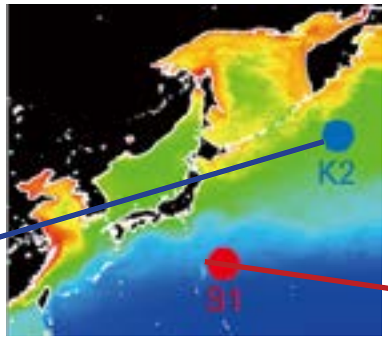
(higher in summer)

Applied in a 0-D (box) model of the mixed layer for two time-series stns.

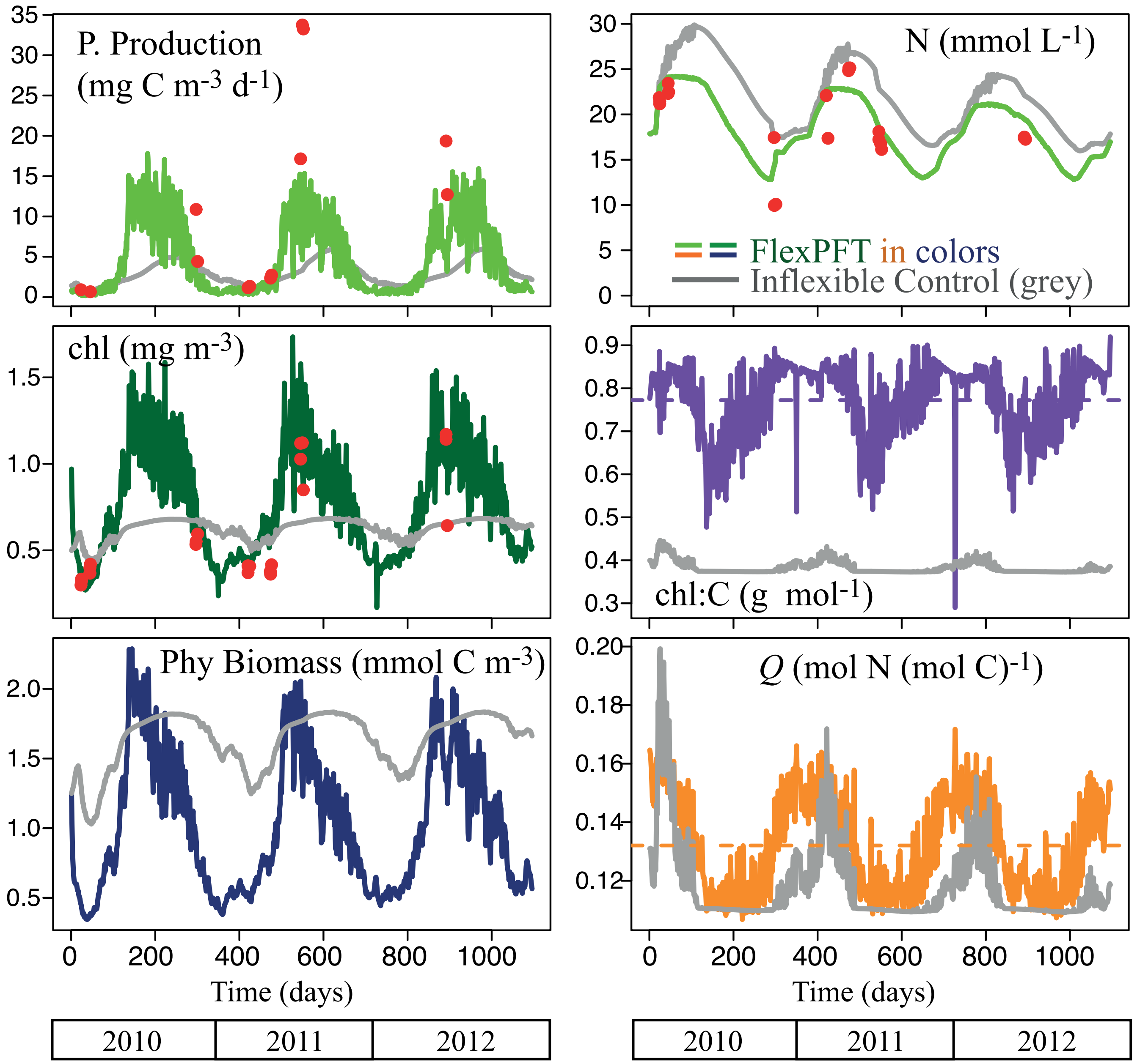
Inflexible PFT vs. FlexPFT applied to stns. K2 & S1

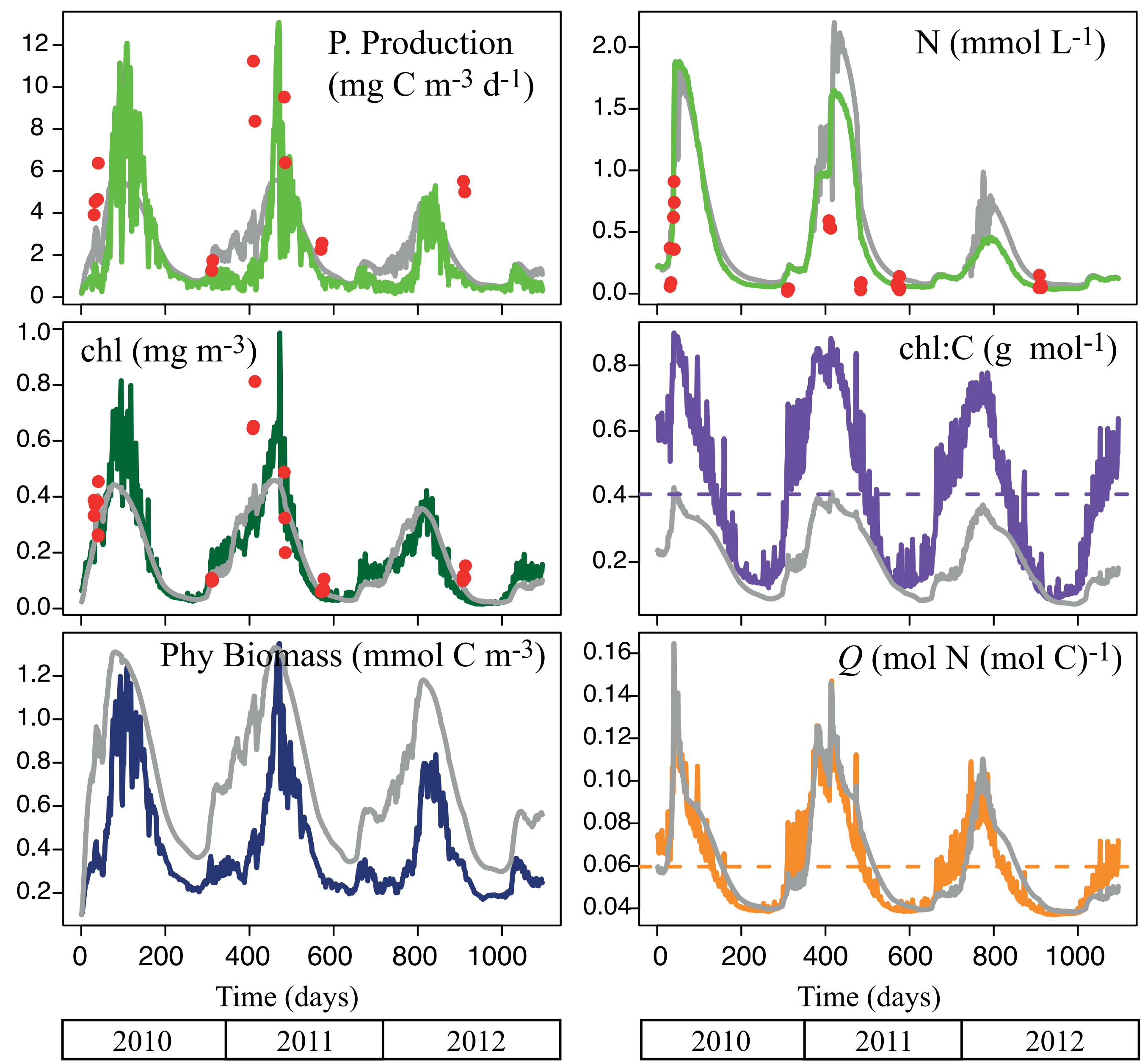
At N-rich stn. K2

Seasonal cycle of chl differs greatly



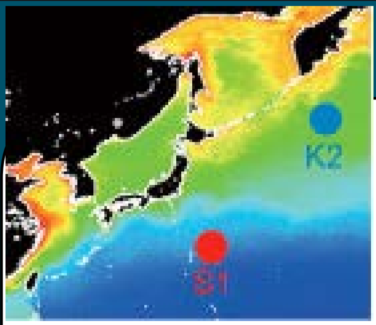
Less Difference at N-poor stn. S1 only





Each model was fitted to data (red dots) using the Adaptive Metropolis algorithm (Smith JGR 2011)

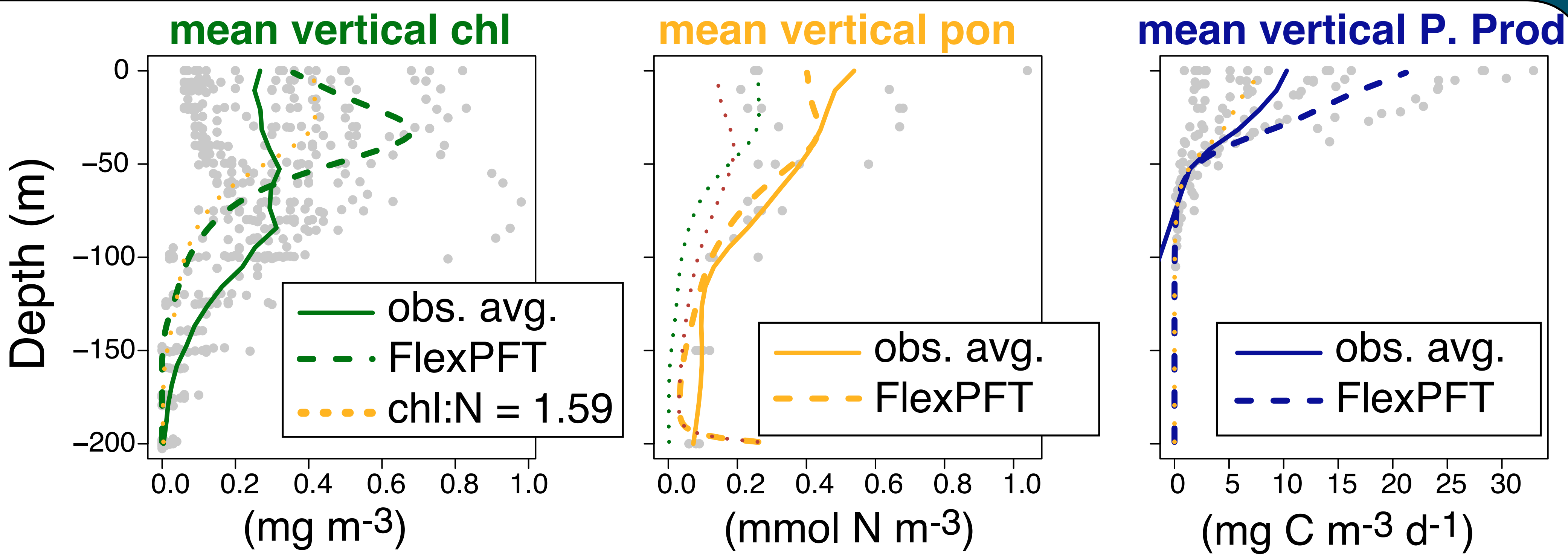
FlexPFT gives different vertical dist. for chl vs. N biomass, PP



stn. S1

most recent results 2015.01

1-D GOTM model, 3 year simulation of subtropical stn. S1.

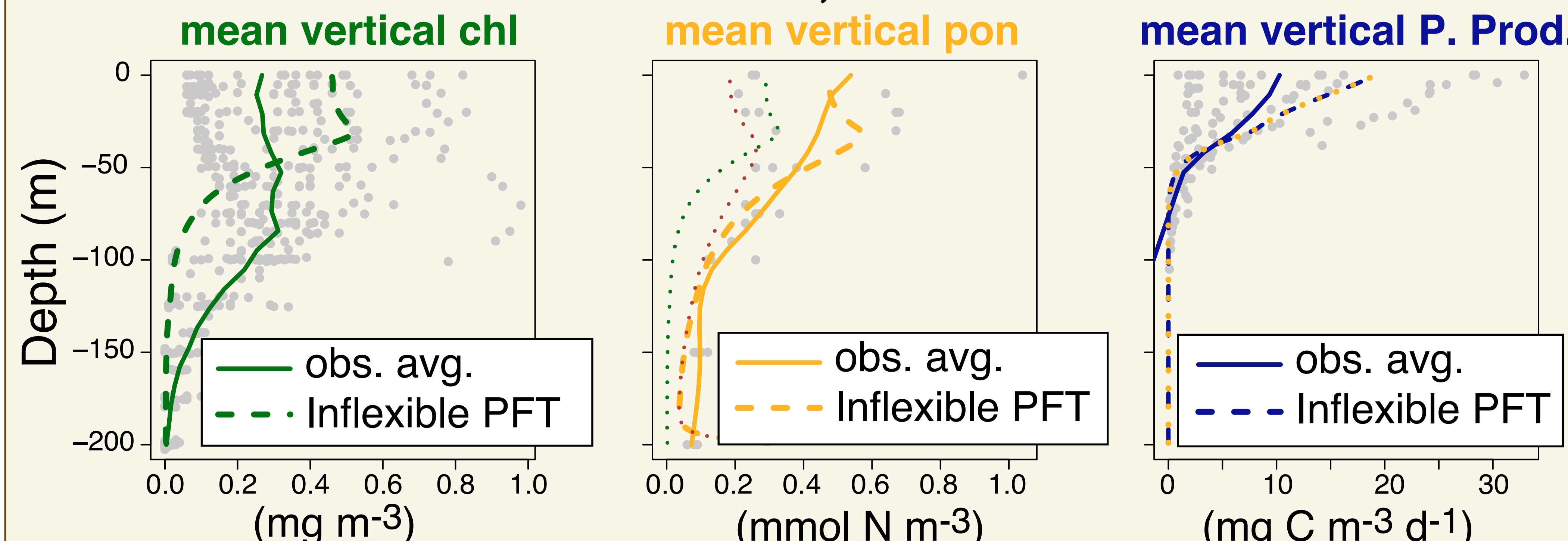


Here the two models perform similarly.

In both, chl decreases too steeply with depth.

Need to add DON to the model to stop 'nutrient trapping'.

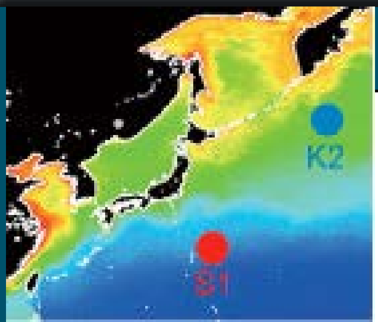
An Inflexible Control Model, chl:N:C ratios



Importance of 'Photo-acclimation' is well known for subtropics (Ayata et al. *JMS* 2013)

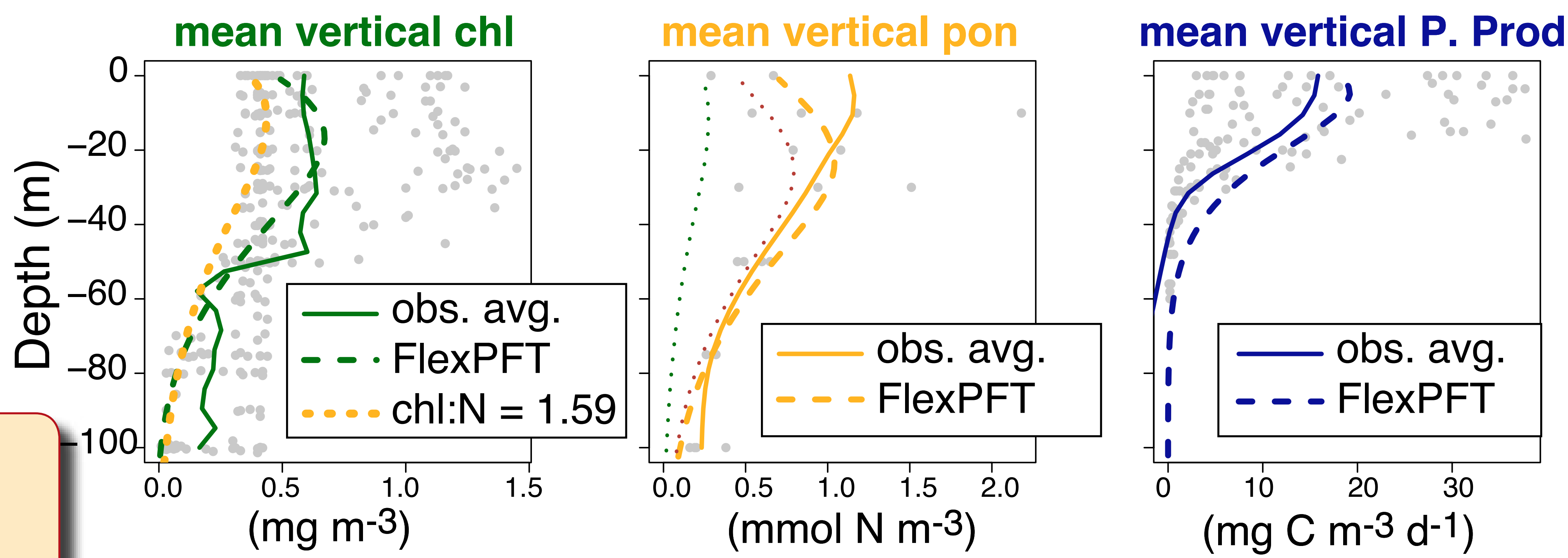
FlexPFT gives different vertical dist. for chl vs. N biomass, PP

1-D GOTM model, 3 year simulation of subarctic stn. K2



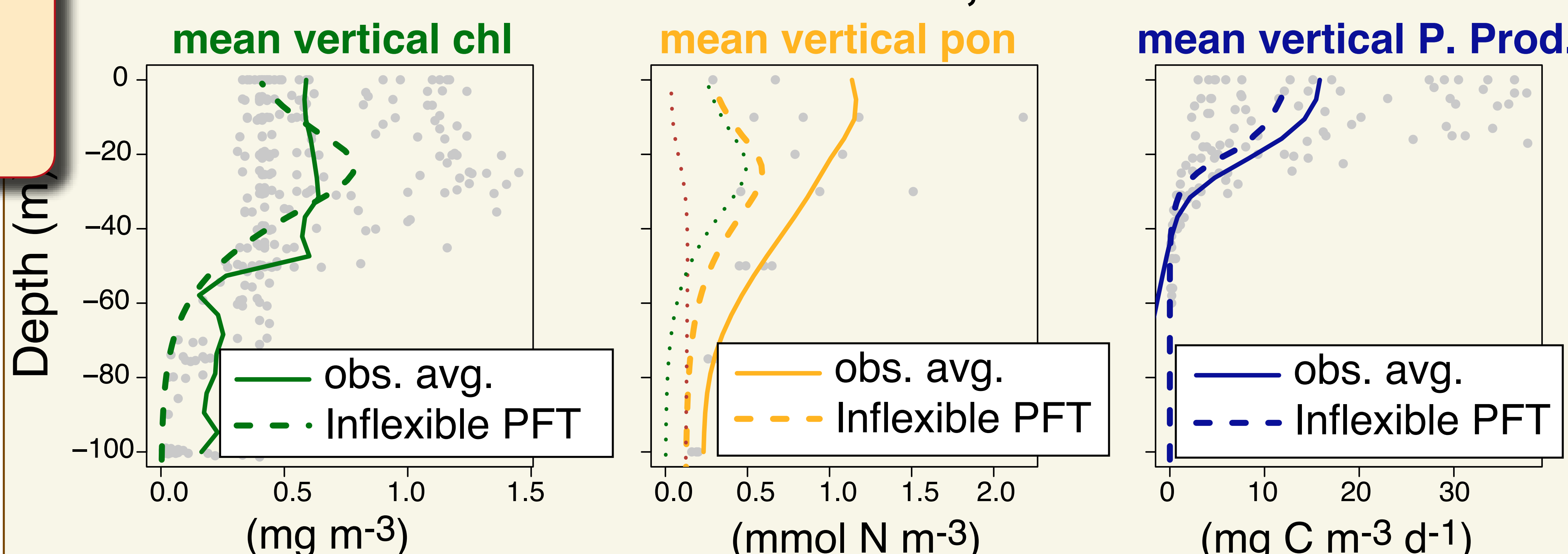
stn. K2

most recent results 2015.01



Flexible chl:N:C is important at subarctic stn. K2 & likely over much of the ocean -- NOT only at low latitudes.

An Inflexible Control Model, chl:N:C ratios

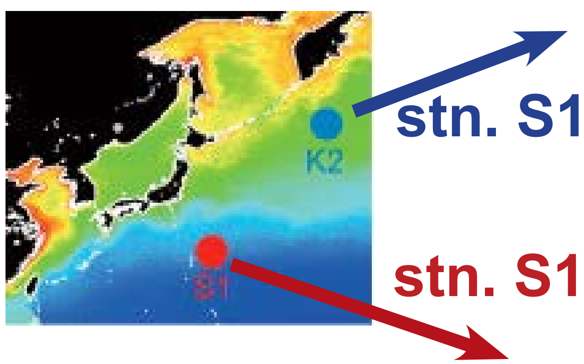


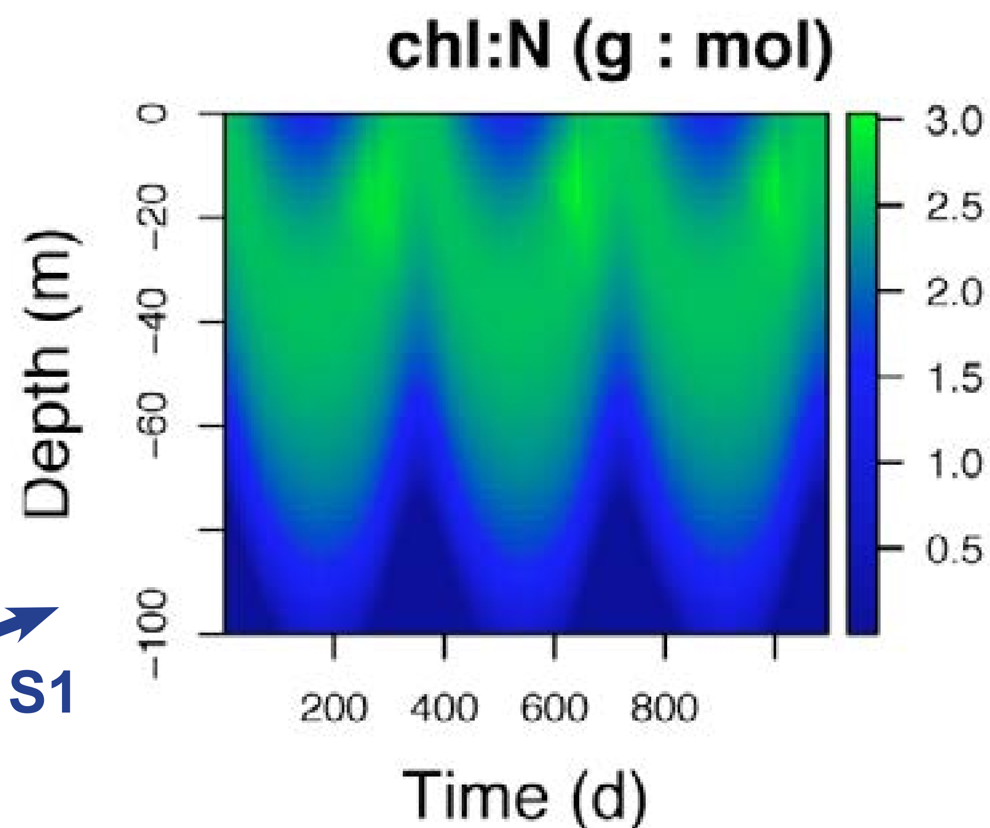
The inflexible model cannot consistently reproduce both chl & PON.

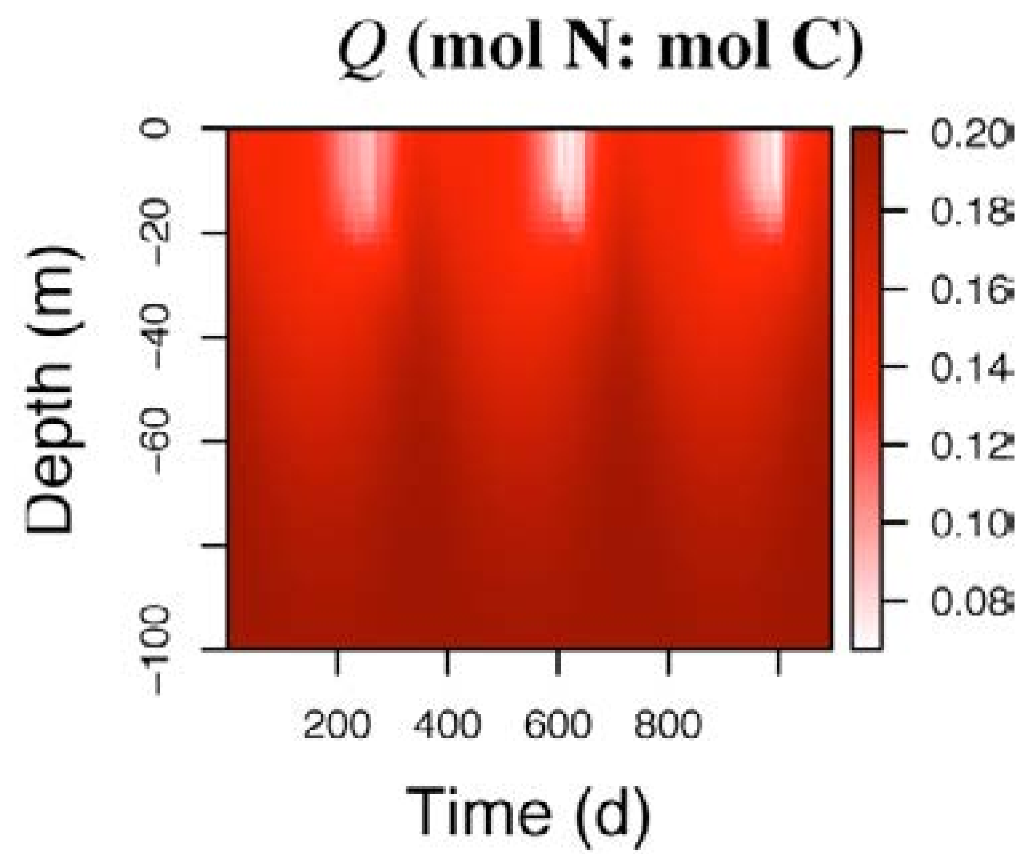
FlexPFT gives dynamic vertical distr. for chl:N and Q

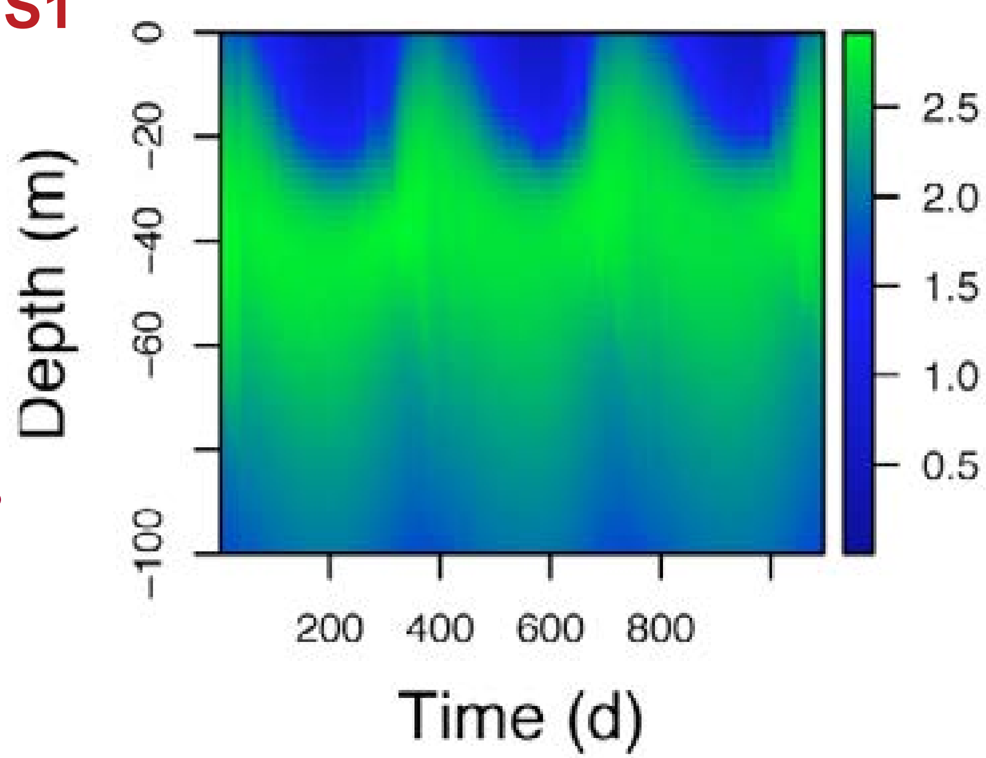
1-D GOTM model, 3 year simulations of stns. S1 & K2.

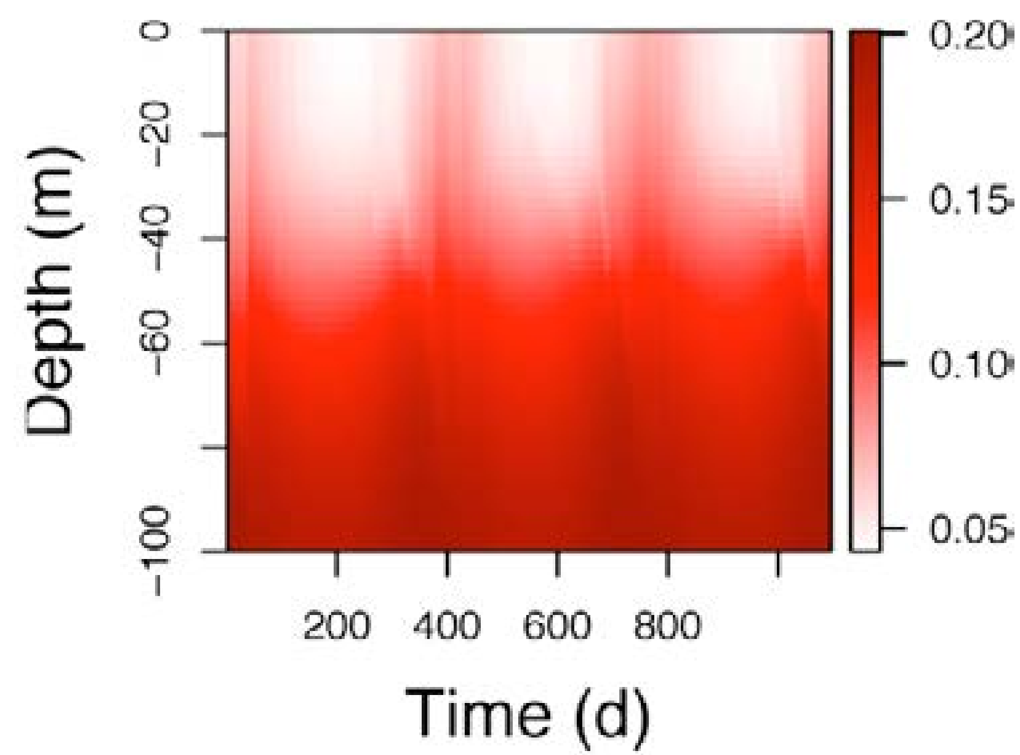
most
recent
results
2015.01











The Importance of 'Photo-acclimation' is well known for sub-tropics (Ayata et al. *JMS* 2013)

New Flexible ZooEFT model developed in FY2014

Sergio Vallina + PI Smith
Cooperative Researcher
(ICM-CSIC, Spain)
- Modelling Zooplankton
- Plankton Diversity

Based on the 'Kill-the-Winner' model
(Vallina et al. ***Nat. Comm.*** 2014;
Vallina et al. ***Prog. Oceanogr.*** 2014)

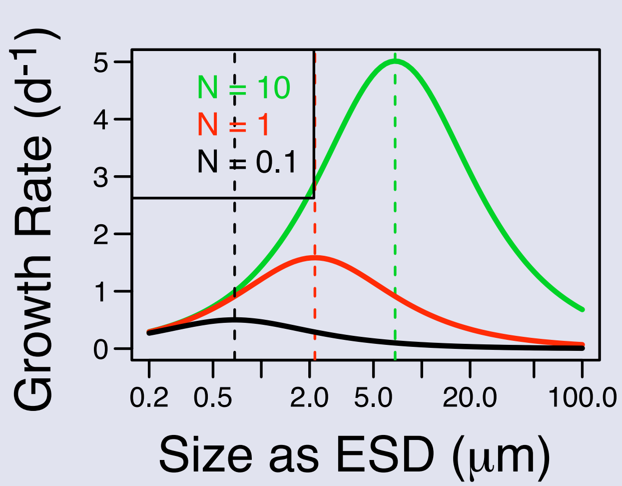
Results here are from a simple size-based model using Monod Growth kinetics.

We plan to publish this soon.

The ZooEFT model has also been coupled with our PhyEFT model in the 0-D setup for stns. K2 & S1.

Next step: try it in the 1-D setup.

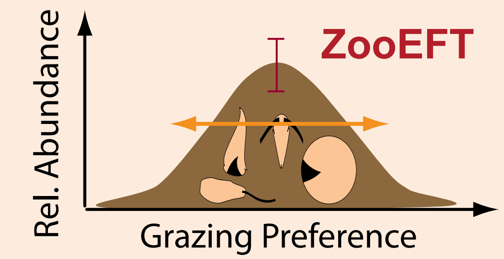
Simple Trade-off assumed for Phy:
Smaller is better at low Nutrient
Bigger is better at high Nutrient

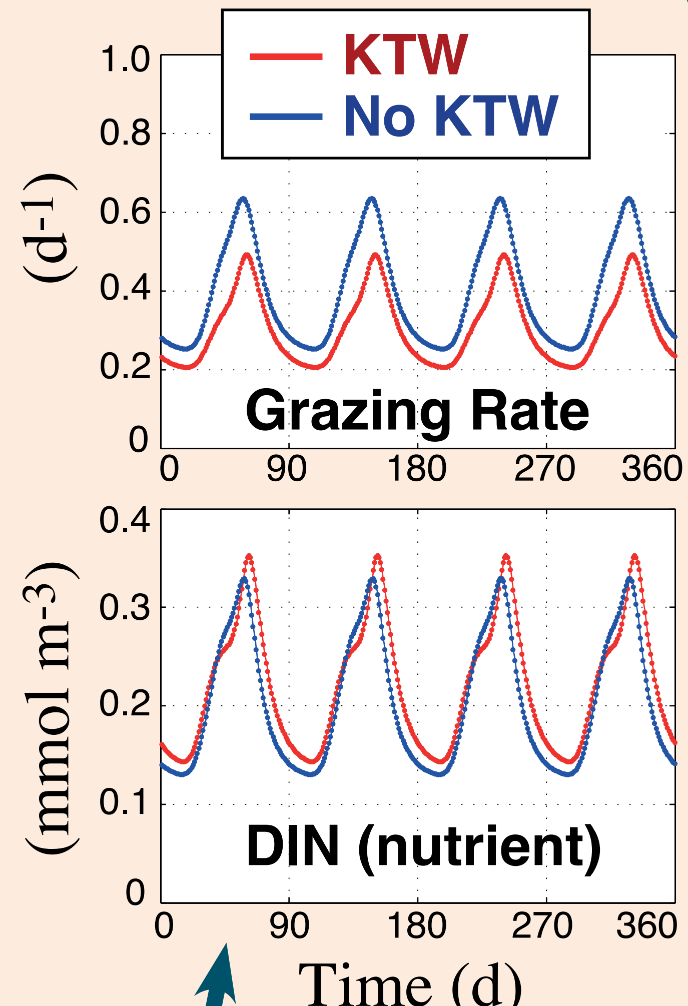


Emergent Trade-off

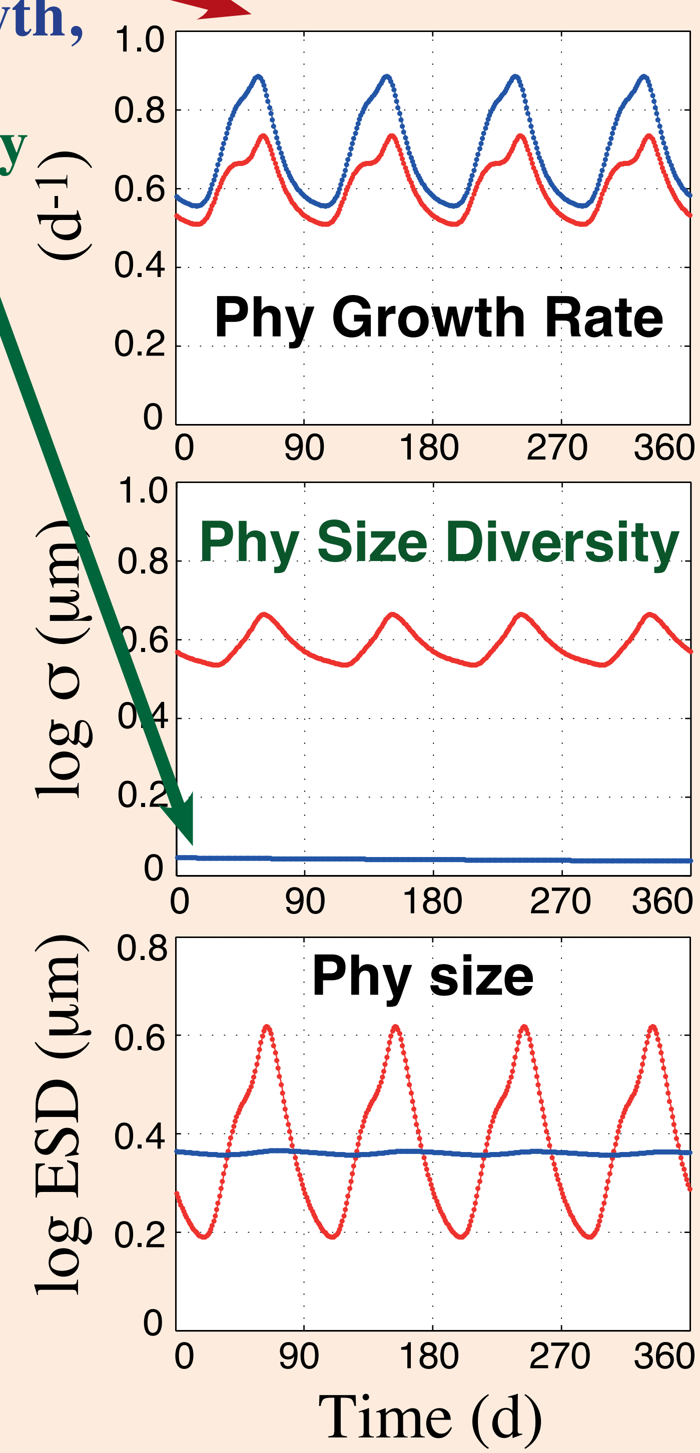
KTW: High Phy Size Diversity, more even Growth

No KTW: Faster Peak Growth, but more variable, Low Phy size diversity





Periodic Nutrient supply was imposed.

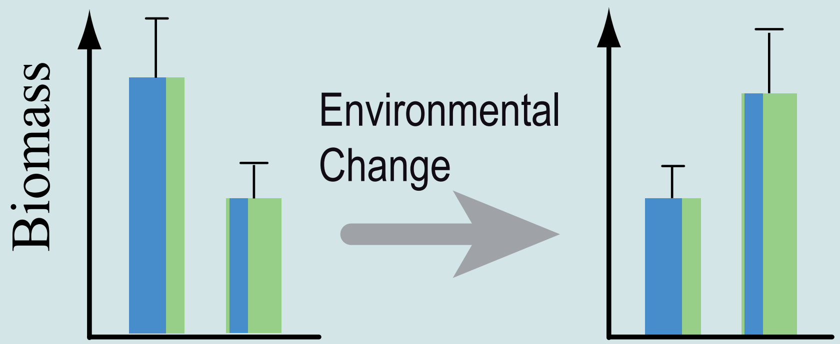


Non-Adaptive vs. Flexible models

(a) Existing PFT models

Plankton Functional Types (PFT)

Only the distribution of biomass can change.



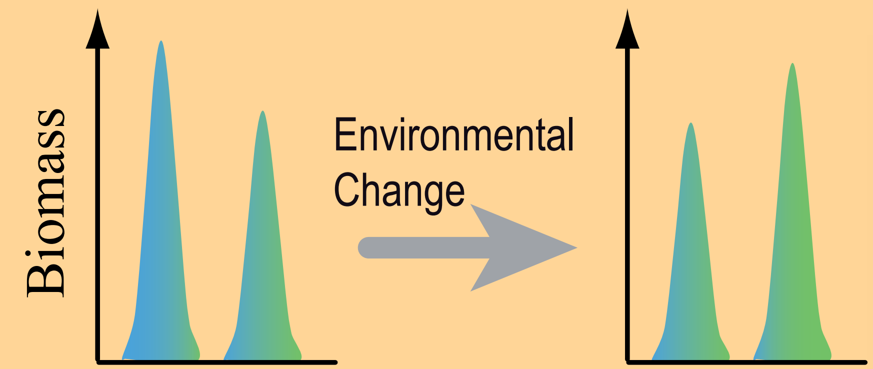
Different PFTs,
each having different abilities

Competitive abilities remain fixed for each PFT

N uptake ability	C fix'n ability

(b) New Flexible FlexPFT model

- Each FlexPFT adapts to changing environment (e.g., light, nutrients).



Different AdaPFTs,
each having different ***flexible*** abilities

Both the biomass & response of each FlexPFT can change.

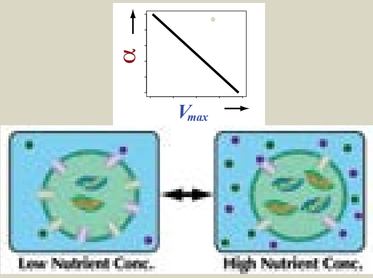
How do changing env. conditions impact:

Overal ecosystem response to, e.g., climate change or human nutrient inputs?

Biodiversity?

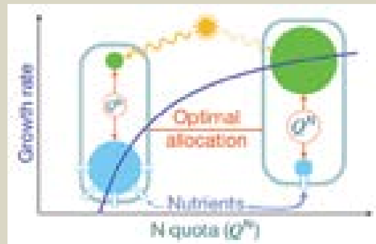
New size-based PhyEFT model

Optimal Uptake kinetics
(Pahlow. *MEPS*, 2005; Smith et al. *MEPS*, 2009)
affinity (α) vs. max. uptake rate (V_{max})
$\propto f_A$ vs. $\propto (1 - f_A)$



1 ← f_A 0

Optimal Growth model
(Pahlow and Oschlies. *MEPS*, 2013)
N uptake ($\hat{V}$) vs. C fixation ($\hat{\mu}^I$)
$\propto f_V$ $\propto (1 - \frac{Q_s}{Q^N} - f_V)$



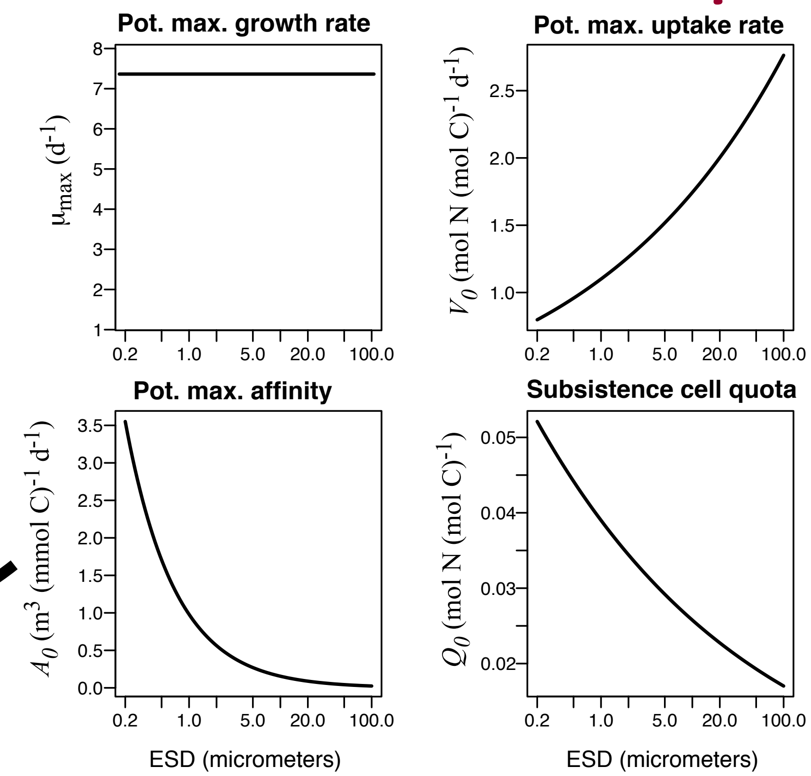
0.5 ← f_V 0

Balanced Growth Assumption
(Burmaster *Am. Nat.* 1979)
$V = \mu Q$

A single, explicit equation:
$\mu = f(N, I)$
including adaptive response*

*assuming instantaneous optimal resource allocation

Size scaling of Traits (input parameters)



empirical allometries

Litchman et al. (*Ecol. Lett.* 2007)

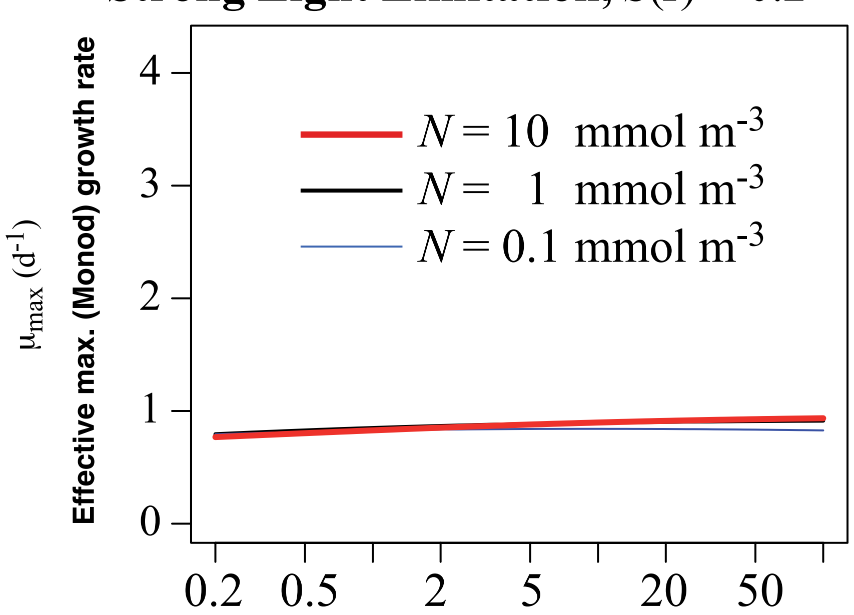
Edwards et al. (*L&O* 2007)

Marañon et al. (*Ecol. Lett.* 2013)

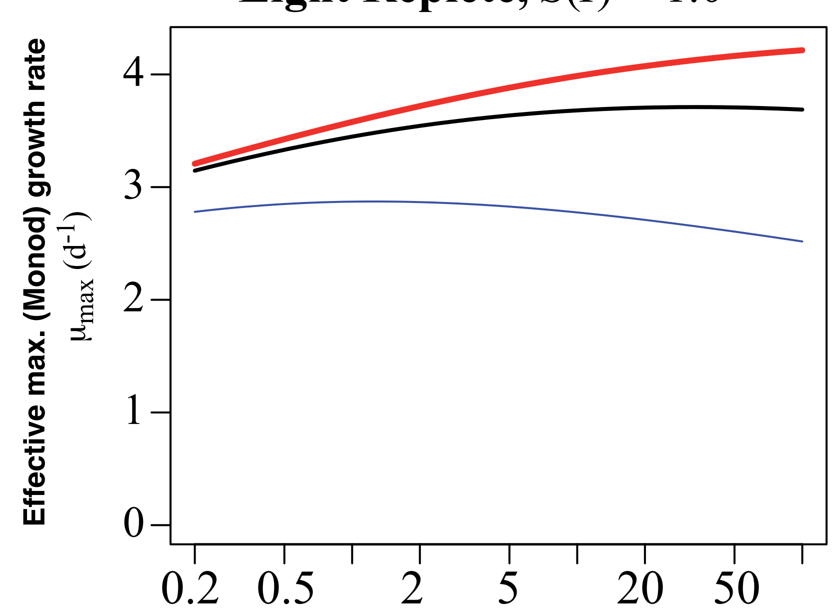
as in Wirtz (*Mar. Biol.* 2013)

Dark ⟷ Light

Strong Light Limitation, $S(I) = 0.2$



Light Replete, $S(I) = 1.0$



Adaptive Response to env. (light & N)

Big is better at high N

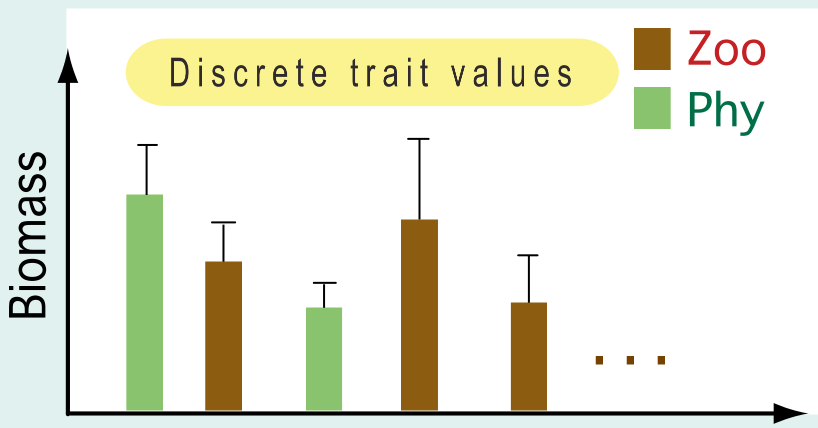
Small is better at low N (esp. at high light)

Old NPZD approach vs. New Ecologically Flexible Types

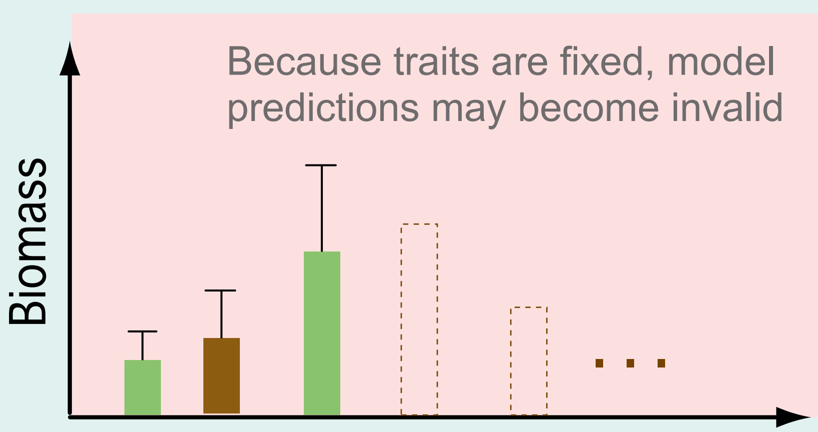
(a) Existing NPZD models

Plankton Functional Types (PFT)

- separate differential eqs. for each PFT
- traits are fixed (constant) for each PFT



Environmental Change



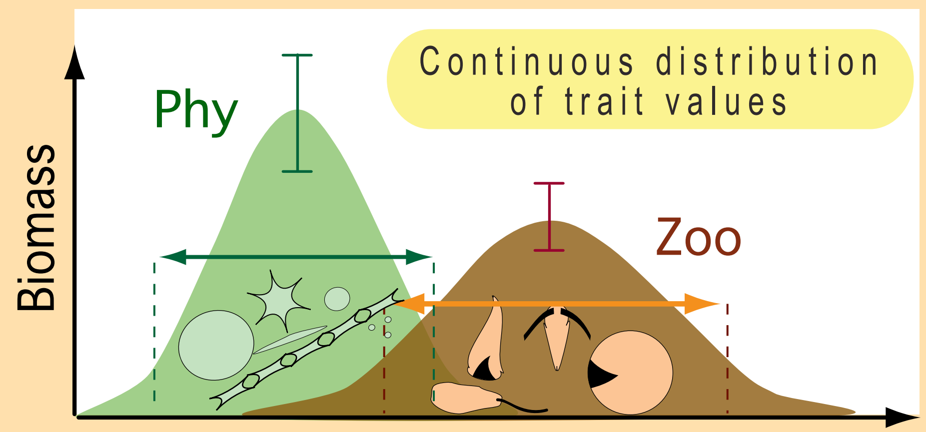
Trait value

*e.g., affinity, V_{max}, size

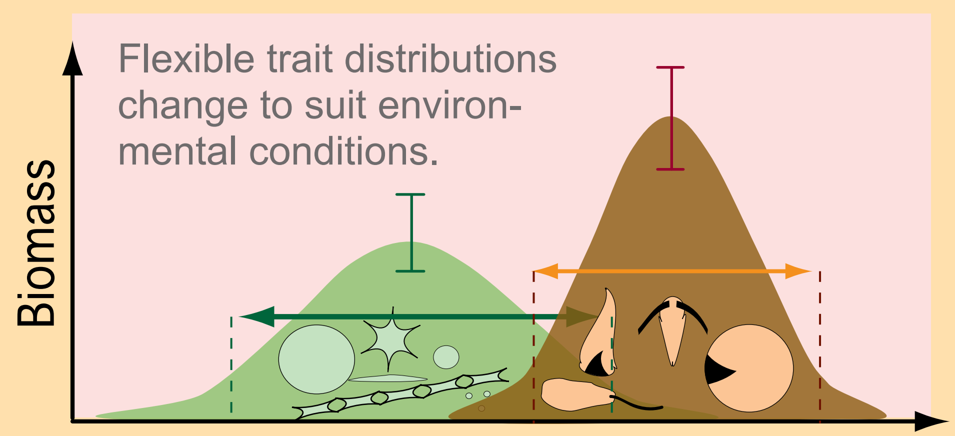
(b) EFT-model to be developed

Ecologically Flexible Types

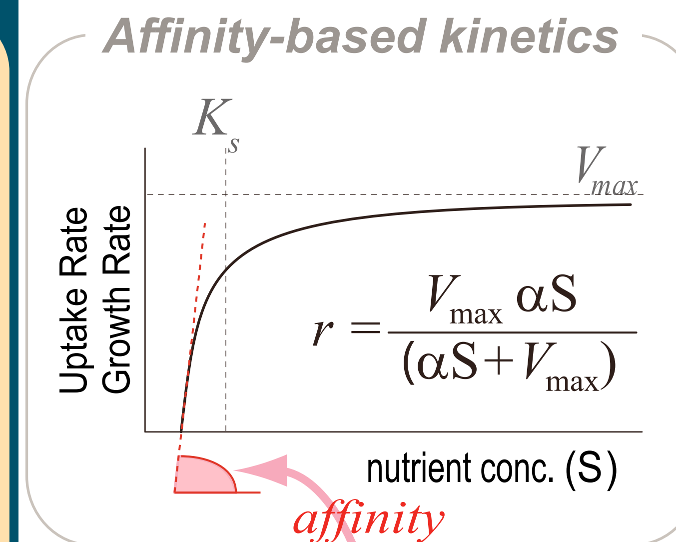
'adaptive dynamics' can represent the dynamics of the trait distribution ($\bar{\alpha}$,σ) using only two differential equations per EFT.

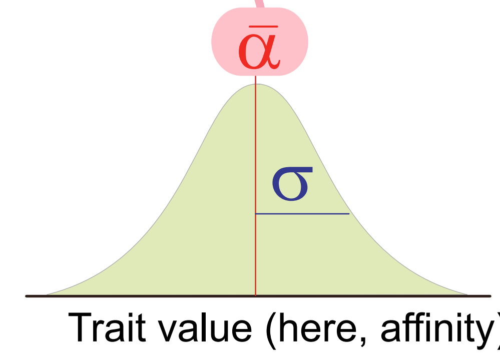


Environmental Change



Trait value





mean trait value:

$$\frac{d\bar{\alpha}}{dt} \approx \sigma \frac{\partial g(\bar{\alpha})}{\partial \alpha}$$

std. dev. of trait value:

$$\frac{d\sigma}{dt} \approx \sigma^2 \frac{\partial^2 g(\bar{\alpha})}{\partial a^2}$$

g: net growth rate

$g = r(\alpha) - m(\delta^{-1})$

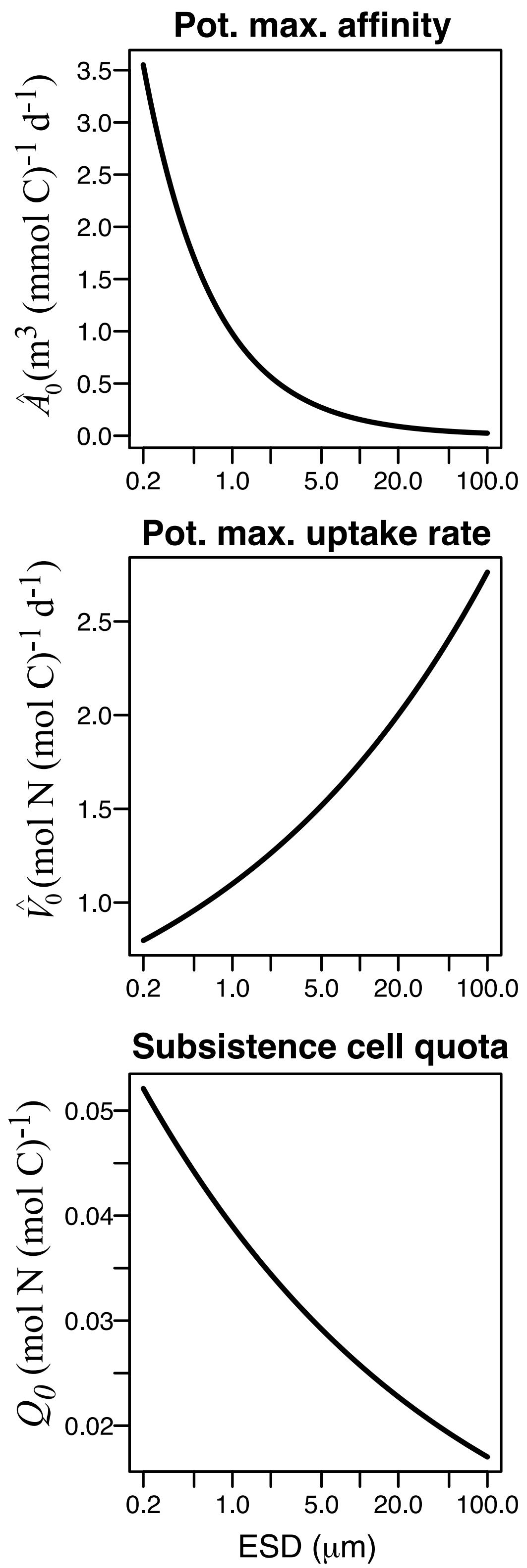
m: mortality by grazing

δ: defense ~ $(\delta_0 - \alpha)$

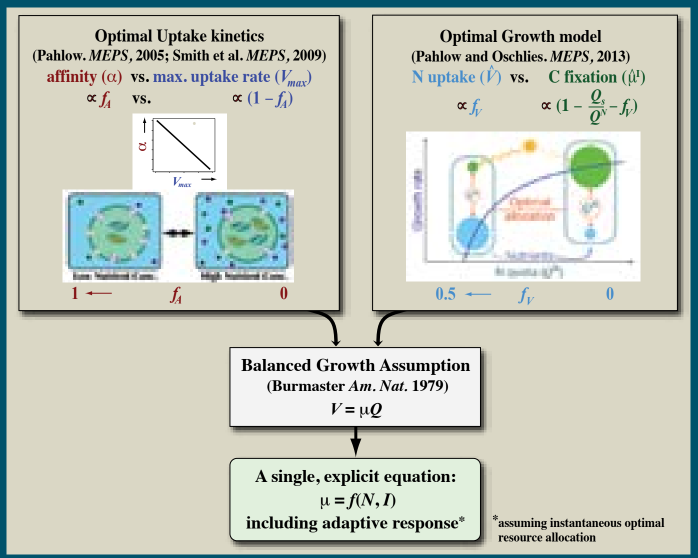
Trade off

Size-Scaling of Traits => Size-Scaling of Growth

Empirical Size-scalings



New modelling framework to relate lab. measurements to the dynamic response of phytoplankton communities.



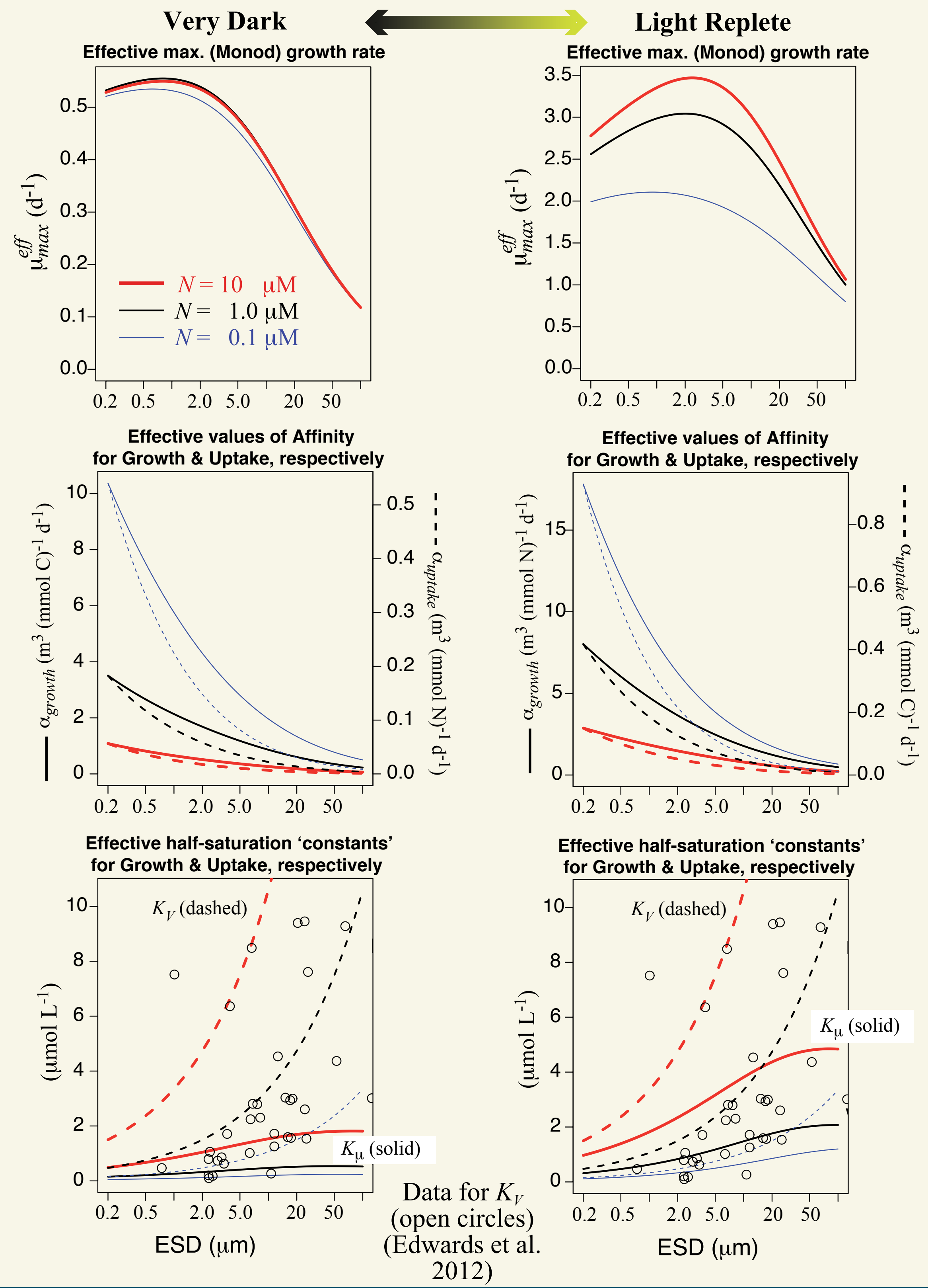
K_μ < K_V

(growth) (uptake)

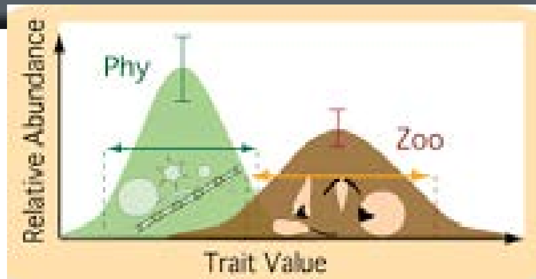
Morel (*J. Phycol.* 1987)

Here size-scaling for K_μ depends on light and nutrient environment.

Response depends on both cell size and Environment



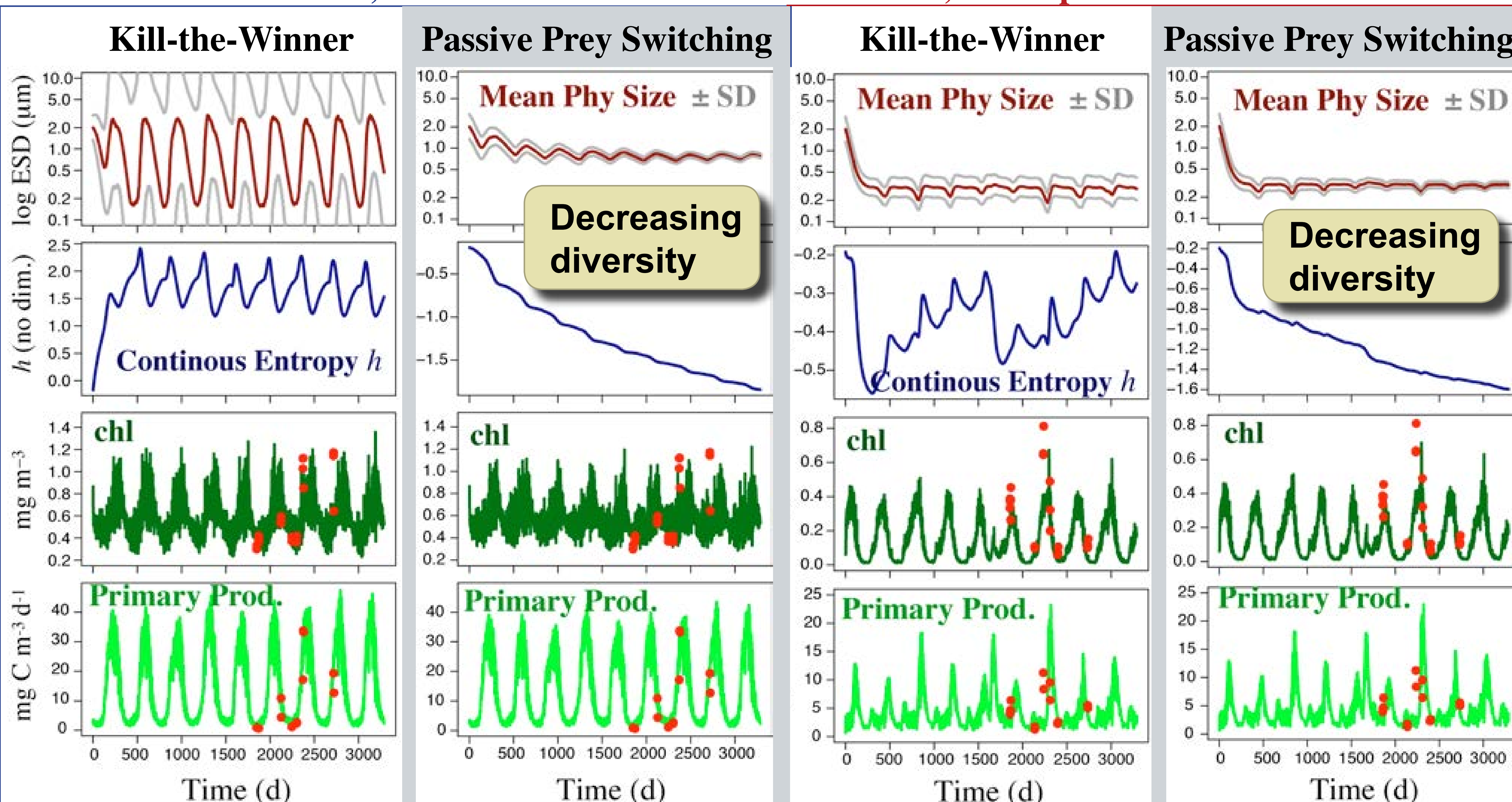
Phy+ZooEFT in 0-D model of stns. K2 & S1 (9 yr. sim.)



KTW sustains Phy diversity, & its seasonality with modest effects on chl, PP

Next: Examine how diversity relates to function
Compare to Obs. size distr.

stn. K2, subarctic | **stn. S1, subtropical**



Summary & Conclusions

Optimality-based modelling has well established theory.
and is recently being applied to model plankton in the ocean.

Flexible Phytoplankton Functional Type: FlexPFT developed

Optimizes specific growth rate w.r.t. to 2 trade-offs:

1. **Optimal Uptake (OU) kinetics**
2. **C (energy) vs. N aquisition**

Only 1 diff. eq. per PFT

Trait-based => can Directly use reported size-scalings

Framework for modelling Size Diversity of phy.

Flexible models respond quite differently vs. Inflexible PFTs

e.g., Variable chl & N content => more dynamic

Some models of optimal Grazing developed,

Much more work needed ...

Biodiversity: beyond coarse large-scale patterns

May impact dynamic functioning & resilience of ecosystems

e.g., predator-prey feedbacks (Tirok et al. *PLoS One* 6, 2011)

Major Challenge: How to model realistic biodiversity in dynamic, heterogenous environments?

Easiest → More Difficult

Simplistic → More Realistic

1. Add more species

competitive displacement of many species

e.g., Moisan et al. (*Ecol. Modell.*, 2002)

2. Resolve traits better

differentiate strategies more precisely

e.g., Litchman and Klausmeier (*Am. Naturalist* 157, 2001)

3. 'adaptive dynamics'

acclimation within species

competitive displacement between species

& trait evolution

(Wirtz. *J. Biotechnol.* 97, 2002; Smith et al. *L&O.* 56, 2011; Tirok et al. *PLoS One* 6, 2011)

Effective Monod (growth) params. vs. MM params.

Burmaster (Am. Nat. 1979)

MM kinetics (uptake) + Droop model (Growth) => Monod kinetics (growth)

Similarly, we combine

OU kinetics (uptake) + Optimal Growth (OG) model => Effective Monod Params.

$$\mu = \frac{\mu_{\max}^{eff} N}{K_{\mu}^{eff} + N}$$

where

$$\mu_{\max}^{eff} = \frac{\mu_{\infty}(1 - f_A)V_0}{\mu_{\infty}Q_0 + (1 - f_A)V_0}$$

$$K_{\mu}^{eff} = \frac{\mu_{\infty}Q_0(1 - f_A)V_0}{f_A A_0[\mu_{\infty}Q_0 + (1 - f_A)V_0]} = \frac{Q_0}{f_A A_0}\mu_{\max}^{eff}$$

or, equivalently

$$K_{\mu}^{eff} = \left[1 + \frac{V_{\max}}{\mu_{\max}Q_{\max}}\left(\frac{Q_{\max} - Q_0}{Q_0}\right)\right]^{-1} K_V^{eff}$$

Now, observed size-scalings for MM & Droop parameters can be used to predict size-scalings for Monod parameters.

Diversity Index: Discrete vs. Continuous

Shannon Diversity Index
for N discrete Obs. *or* PFTs

$$H = -\sum_{i}^{N} p_i \, ln(p_i)$$

where p_i is the probability of belonging to the i-th class

depends on 'binning' choice
and on N, which is arbitrary

Differential entropy
for log-normal distribution (model)

$$h = \frac{1}{2} + ln(\sigma\sqrt{2\pi}) + \mu$$

where μ is mean (in log space)
σ is the std. deviation

depends on the assumed distr'n.
log-normal is reasonable for plankton

(Quintana et al. 2008, Schartau et al. 2010)

Instead, for obs. & PFT models

Non-parametric estimate of h from discrete data (y_i)

$$h = \bar{y} - \frac{1}{n}\sum_{k=1}^{n} \ln\left[\frac{1}{n\sqrt{2\pi}\,\sigma}\sum_{j=1}^{n}\exp\left(-\frac{1}{2}\frac{(y_k - y_j)^2}{\sigma^2}\right)\right]$$

Qintana et al. (*L&O. Methods* 2008)
who denote diff. entropy as μ
applied to obs. by Schartau et al. (*JPR* 2010)

Advantages of h

Consistently quantifies diversity despite different # of obs.

or different # of PFTs (in models)

Dis-advantages of h

not bounded: can be < 0

not as intuitive for intrepretation

Comparing *h* vs. *H*

h **is independent of *N* (# of PFTs), whereas *H* increases with *N***

Only slight difference between FlexPFT vs. control

3 yr. simulation for stn. K2

h **is better for obs.-model & model-model comparsions**

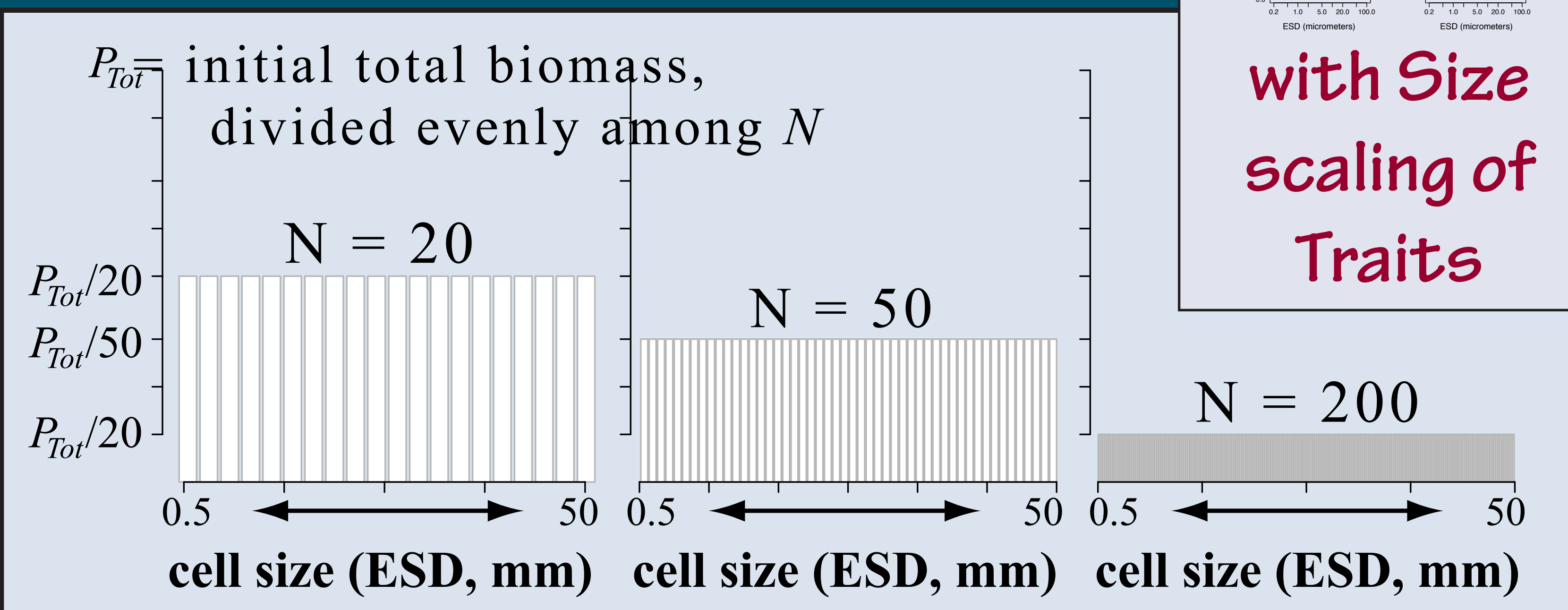
Model Set-up for different number, *N* of either PFTs, or AdaPFTs

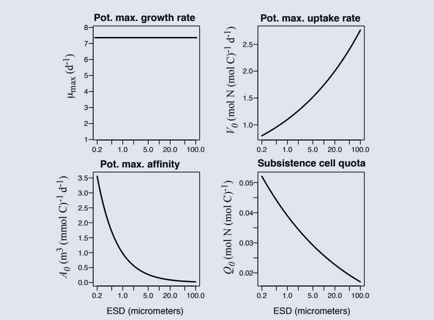
in a simple NO_3 - P_{xN} - D model (no Zoo)

mortality for $m_i = m_0 P_{avg} P_i$

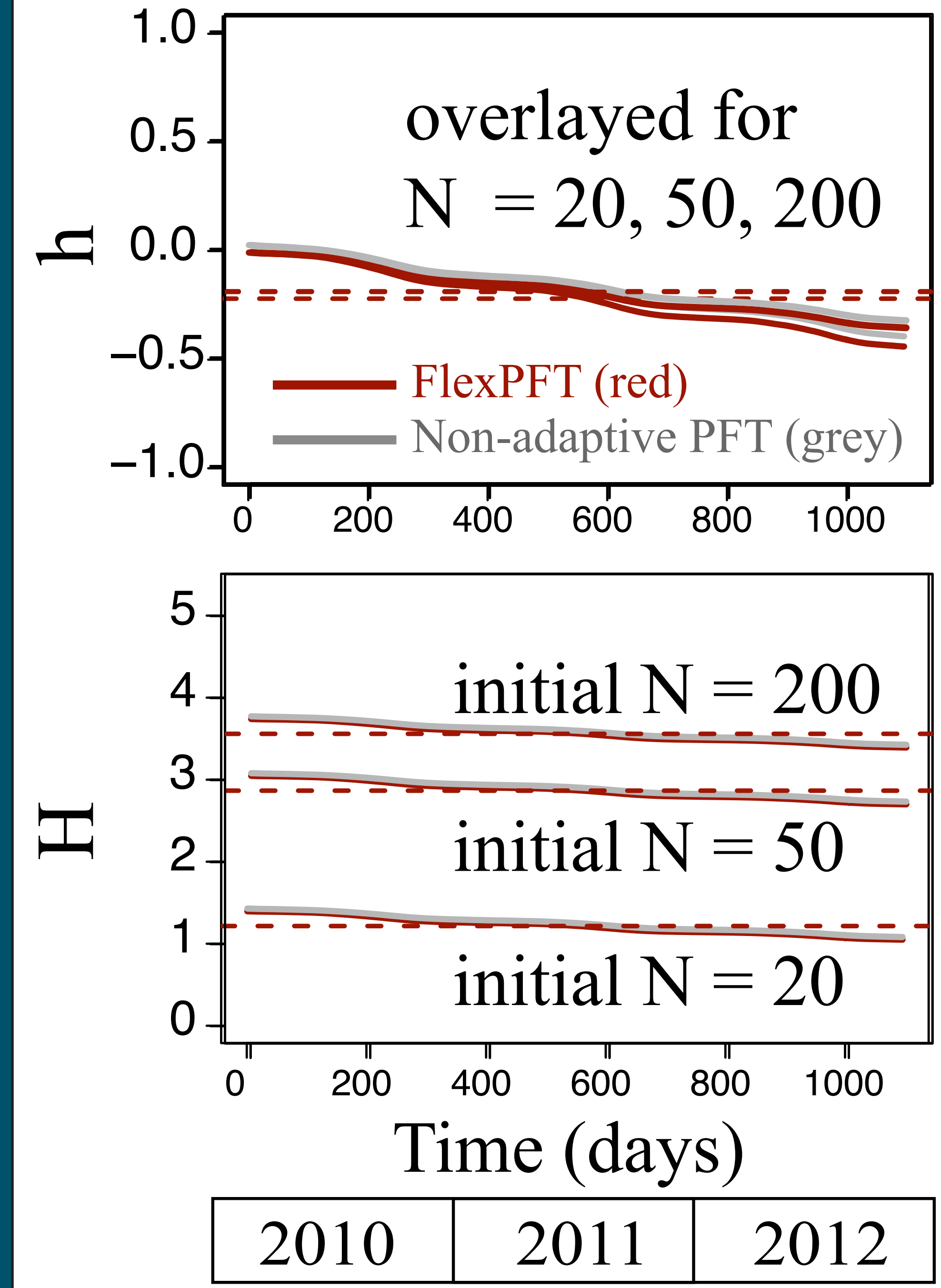
which maintains biodiversity

(Record et al. *ICES J. Mar. Sci.* 2013)





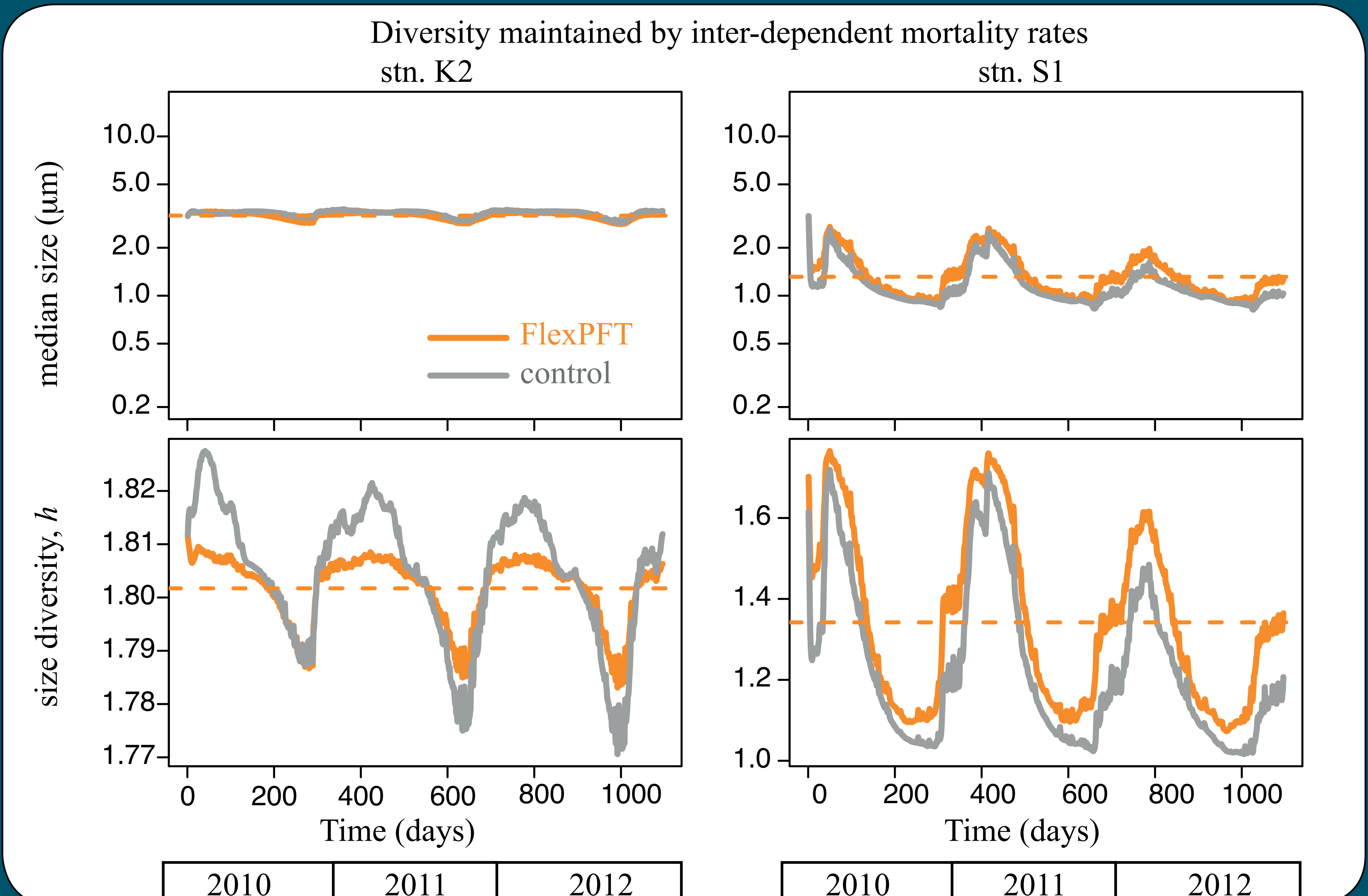
with Size scaling of Traits



Comparing *h:* FlexPFT vs. Inflexible Control

200 PFTs in a simple 0-D model: NO_3 - P_x - D model (no Zoo)

simplified Kill-the-Winner mortality, $m_{P_i} = m_0 P_{avg} P_i$, maintains biodiversity
(Record et al. *ICES J. Mar. Sci.* 2013)



Comparing *h:* FlexPFT vs. Inflexible Control

200 PFTs in a simple 0-D model: NO_3 - P_x - D model (no Zoo)

independent quadratic mortality, $m_{P_i} = m_0 P_i^2$, gives Competitive Exclusion

(Record et al. *ICES J. Mar. Sci.* 2013)