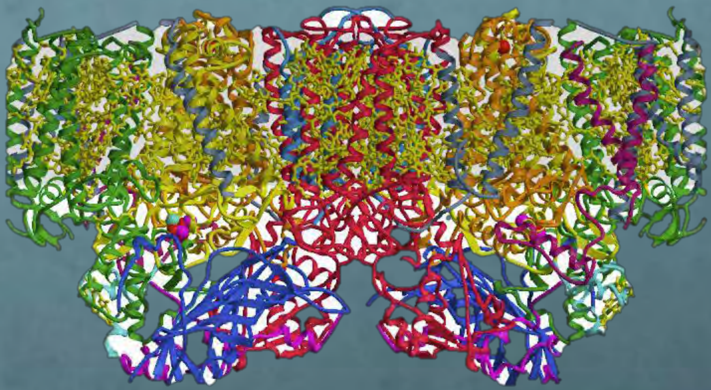
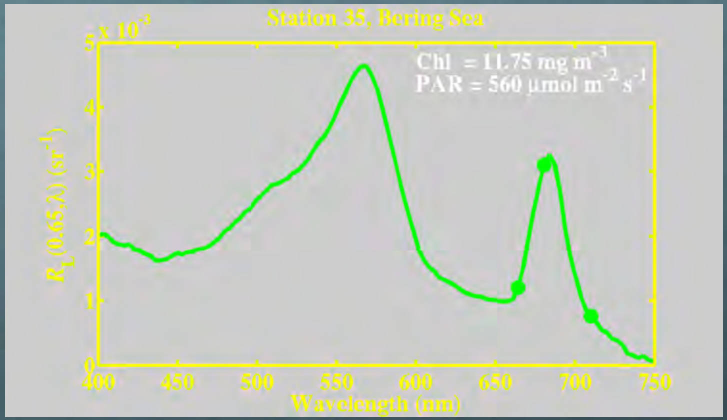




Remote sensing of Sun-induced fluorescence.

Part 2: from FLH to chl, Φ_f and beyond.

Yannick Huot
Centre d'applications et de recherches en télédétection (CARTEL)
Département de Géomatique
Université de Sherbrooke

How do current chl-based Φ_f satellite algorithms work?

Measured by ocean color satellites (FLH)

What we want

Modeled

$$L_{uf} \propto \phi_f^{app} \cdot \mathring{E}_{PAR} \cdot a_{\varphi} \cdot Q_a^{*} \frac{1}{a_f + K_{dPAR}}$$

Retrieved by OC algorithm

Estimated based on a_{φ} or K_d algorithm and known relationships

Morel, A. and S. Maritorena (2001), Journal of Geophysical Research **106**(C4): 7163-7180.
Bricaud, A., M. Babin, et al. (1995). Journal of Geophysical Research **100**(C7): 13321-13332.

Original idea for this type of algorithm originates from : Babin, M, A Morel, and B Gentili. "Remote Sensing of Sea Surface Sun-induced Chlorophyll Fluorescence: Consequences of Natural Variations in the Optical Characteristics of Phytoplankton and the Quantum Yield of Chlorophyll a Fluorescence." *International Journal of Remote Sensing* 17, no. 12 (1996): 2417-2448

In its simplest form

After a few assumptions a surprisingly compact form is obtained.

$$\phi_f^{app} = 0.68 \cdot 1.19 \cdot \frac{FLH_{nLw}}{Chl^{0.684}}$$

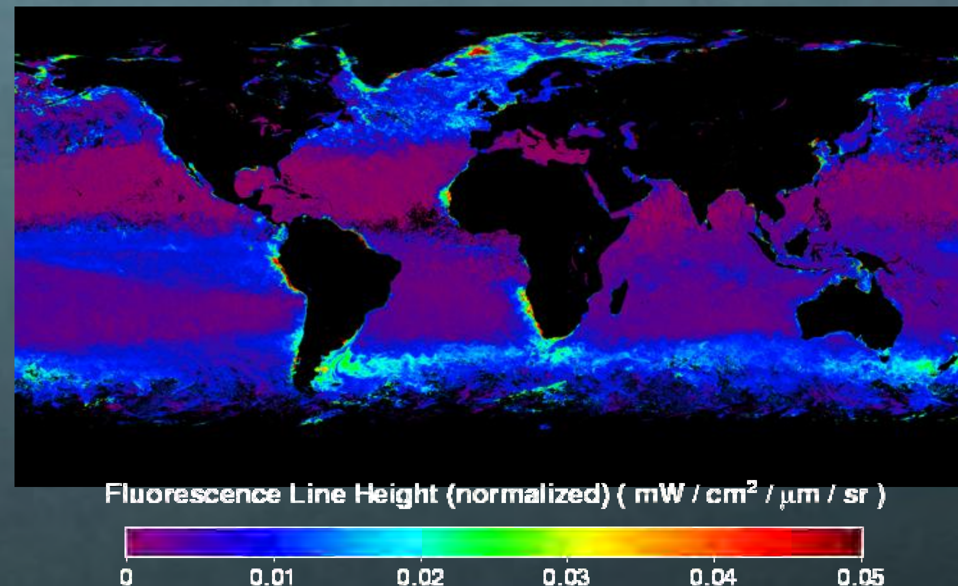
Where FLH_{nLw} is the FLH measured on the normalized water leaving radiance spectrum

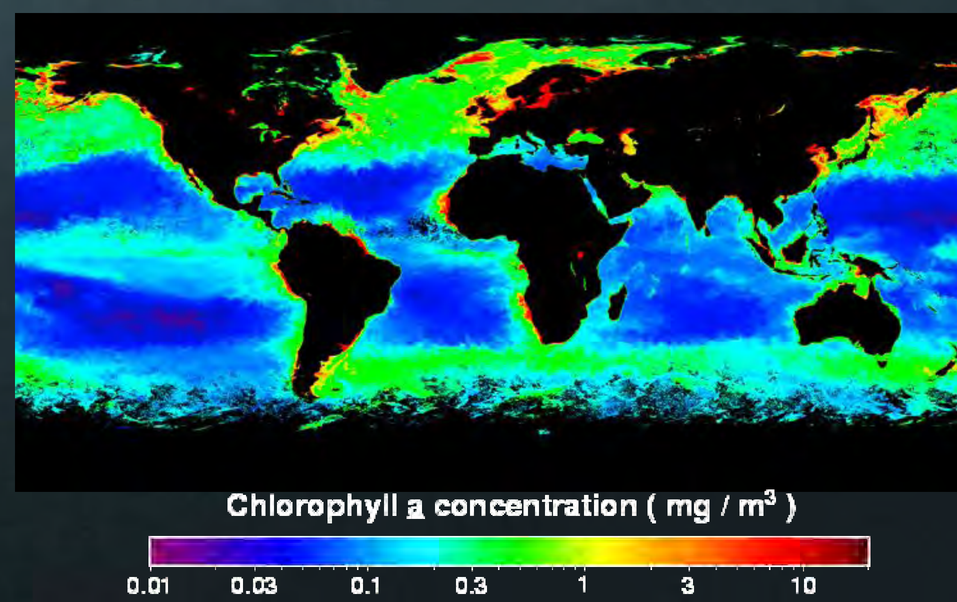
Behrenfeld, M J, T K Westberry, E S Boss, R T O'Malley, D A Siegel, J D Wiggert, B A Franz, *and others.* "Satellite-detected Fluorescence Reveals Global Physiology of Ocean Phytoplankton." *Biogeosciences* 6 (2009): 779-794

Sun-induced fluorescence

Spring 2007

FLH$_{nLw}$ looks like chlorophyll

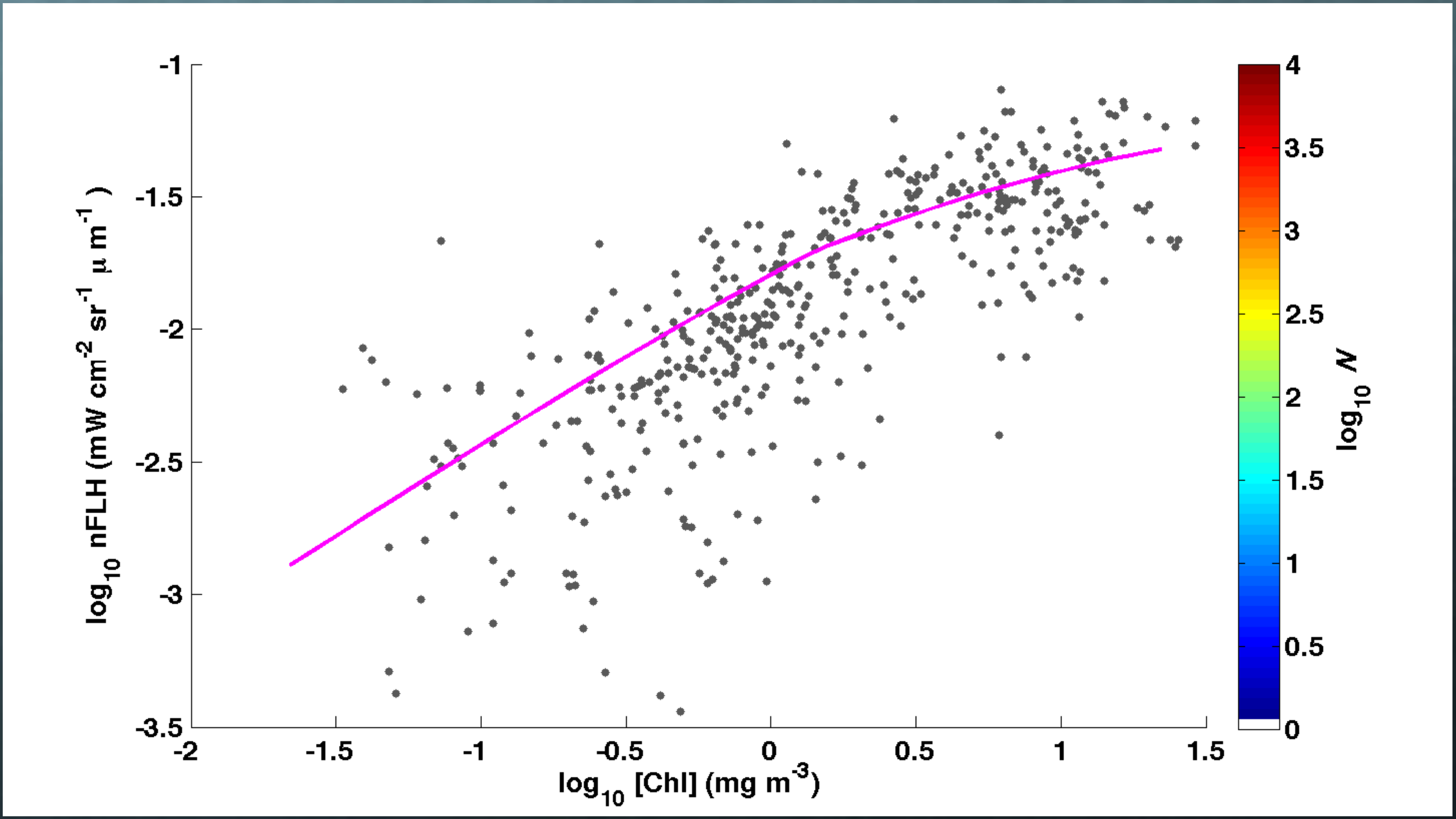




A detour to look at Chl from FLH

$$Chl = \left[0.81 \cdot \frac{FLH_{nLw}}{\phi_f^{app}} \right]^{\frac{1}{0.684}}$$

FLH_{Lwn} vs chlorophyll



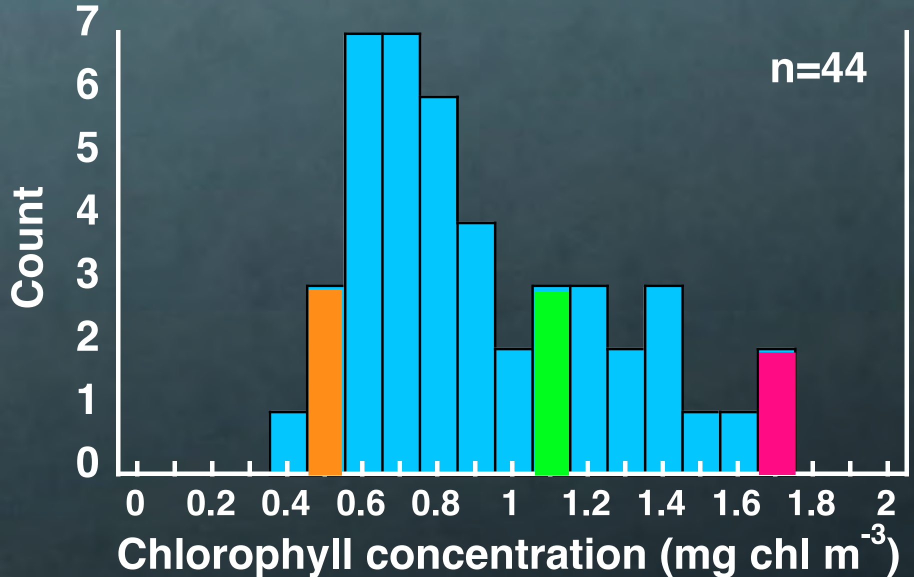
Not promising… but perhaps good enough in coastal waters

Coastal waters

Two challenges in Lunenburg Bay (Nova-Scotia, Canada)

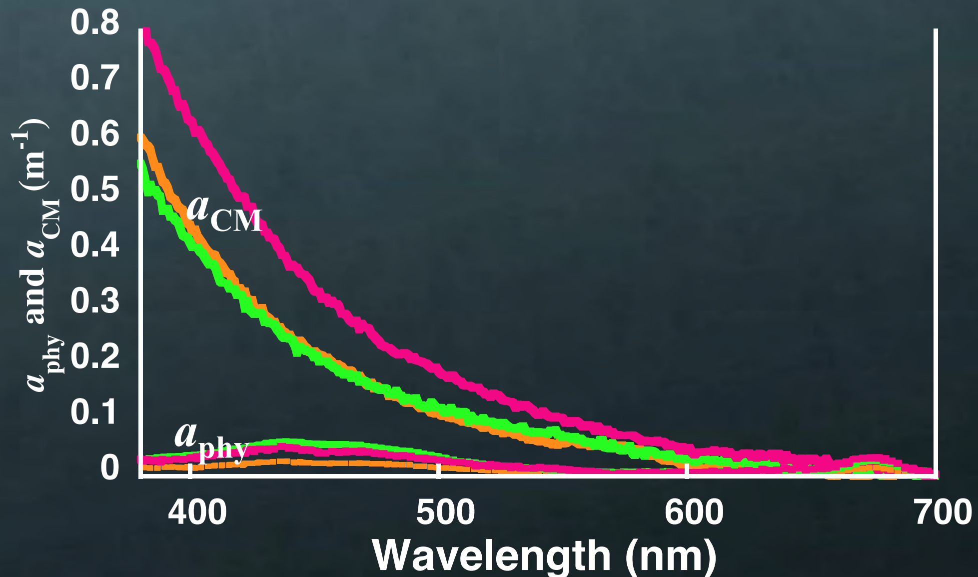
Not much variability in the chlorophyll concentration (Factor ~ 4-5)

Surface chlorophyll at LMB1 buoy, May 25 - Nov. 22, 2004



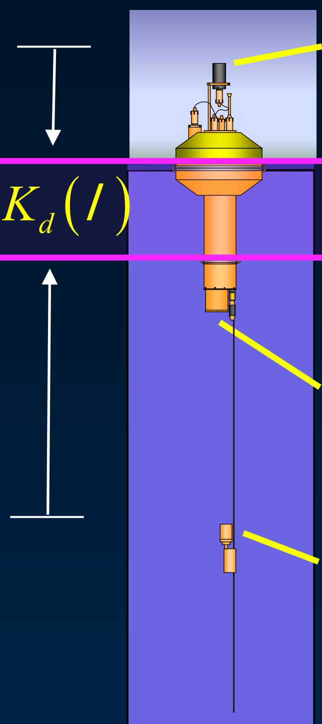
Algorithmes using band ratios do not work

Phytoplankton absorption is small compared to CDOM absorption



Measurements

AOPs



$E_d(\lambda, 0^+)$

$K_d(\lambda)$

$R_L(\lambda, 0.65)$

$L_u(\lambda, 0.65)$

$E_d(\lambda, 2.75)$

IOPs

- Scattering (ac-9)
- Backscattering (Hydroscat-6)
- Phytoplankton absorption
- CDOM absorption

Range of variability

Validation

Forward and inverse models

Minimize the difference between model and measurements

$$K_d(\lambda) - K_d^{\mathrm{mod}}(\lambda)$$

$$R_L(\lambda) - R_L^{\mathrm{mod}}(\lambda)$$

By changing the amplitudes and shapes of the IOPs

To obtain

$$a_\phi\ ,\ a_{CDOM}\ ,\ b_b$$

Radiative transfer simulations

Creation of look up tables

Simplified optical models

$$R_L^{\mathrm{mod}} = R_{Lb}^{mod} + R_{Lf}^{mod}$$

$$K_d^{\mathrm{mod}}$$

Analytical fluorescence model

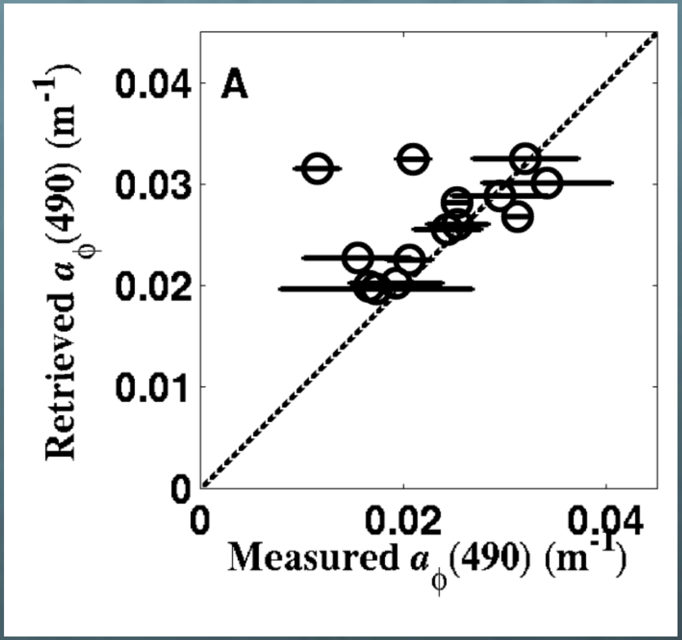
$$R_{Lf}^{mod}(\lambda, 0.65, a, b_b, \theta_s, \phi)$$

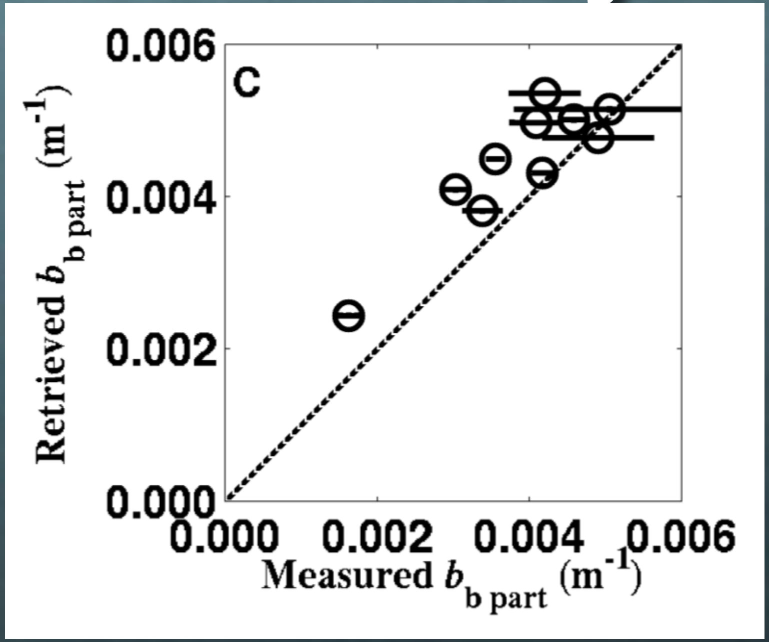
+

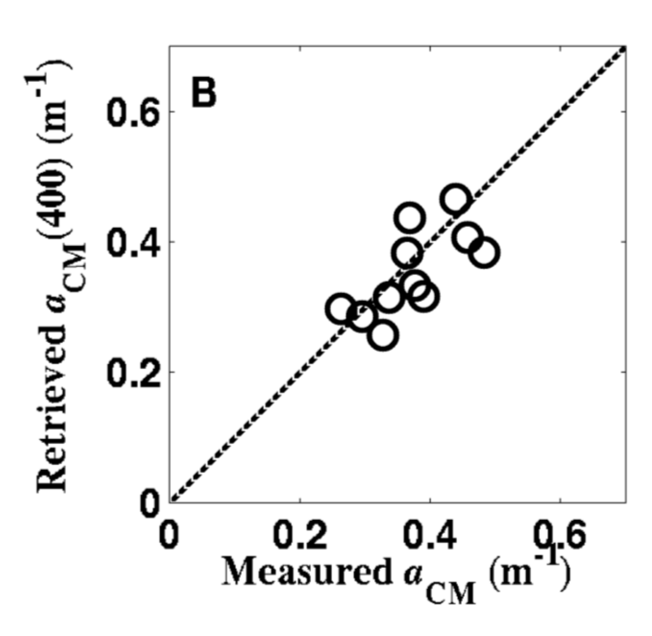
$$R_{Lb}^{mod}(\lambda, 0.65, a, b_b, \theta_s)$$

$$K_d^{\mathrm{mod}}(\lambda, a, b_b, \theta_s)$$

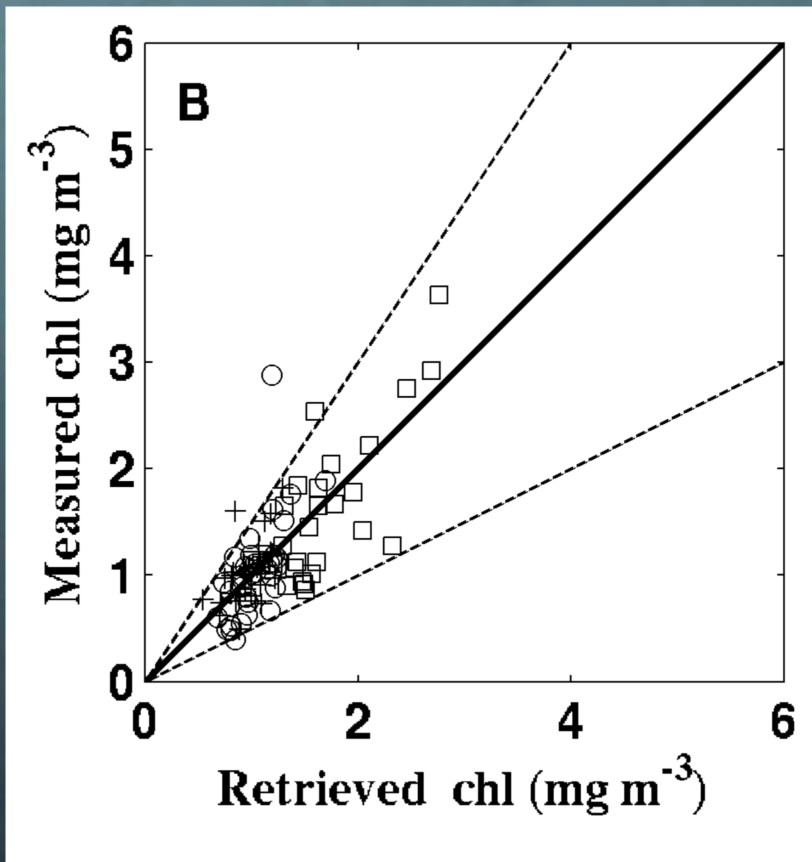
Summer 2001 at one buoy

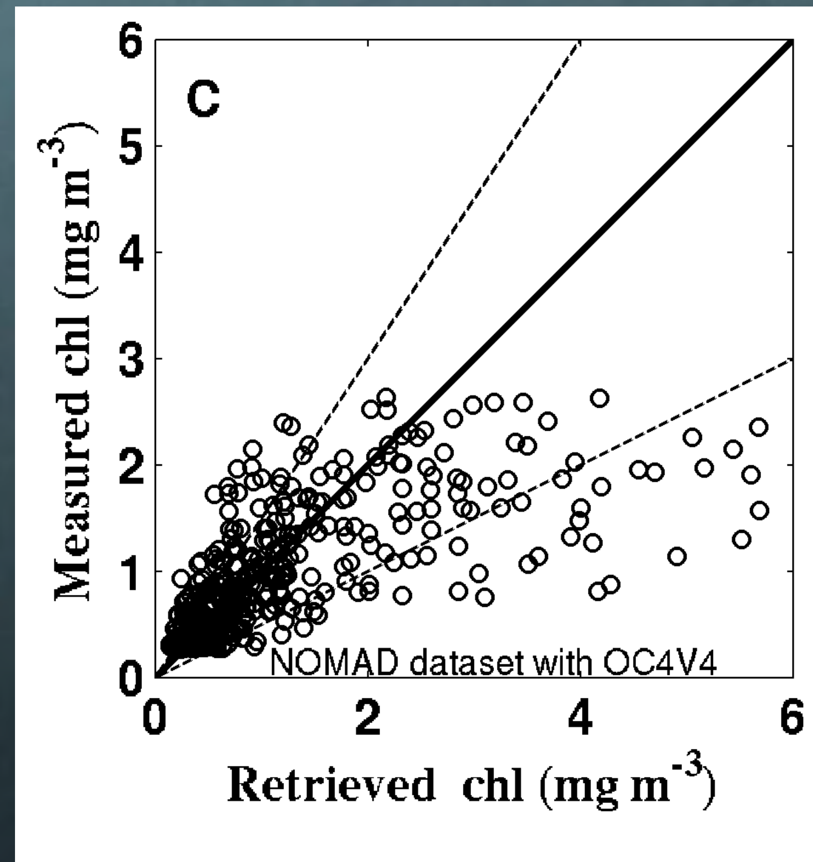






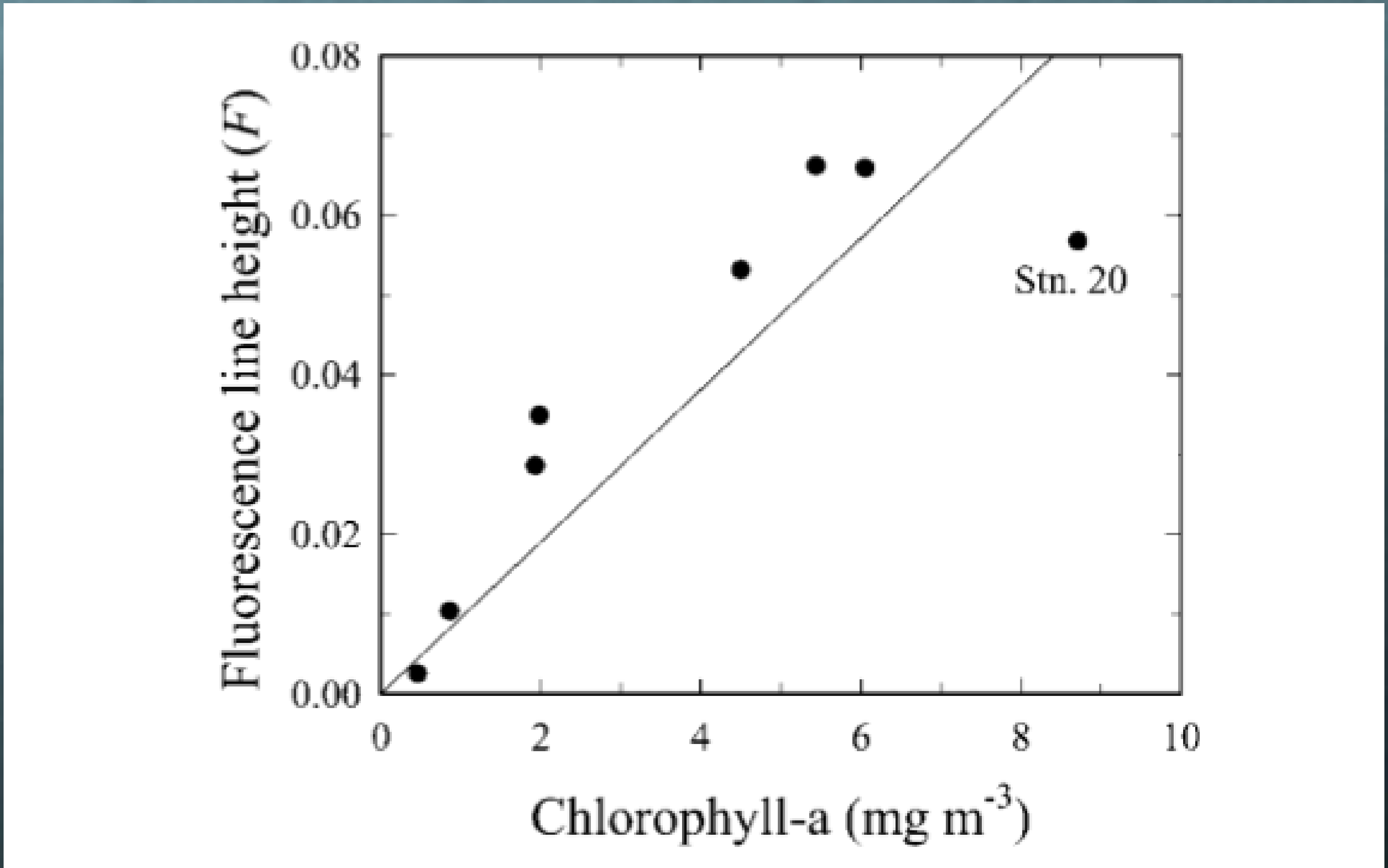
Validation in 2004 for three buoys





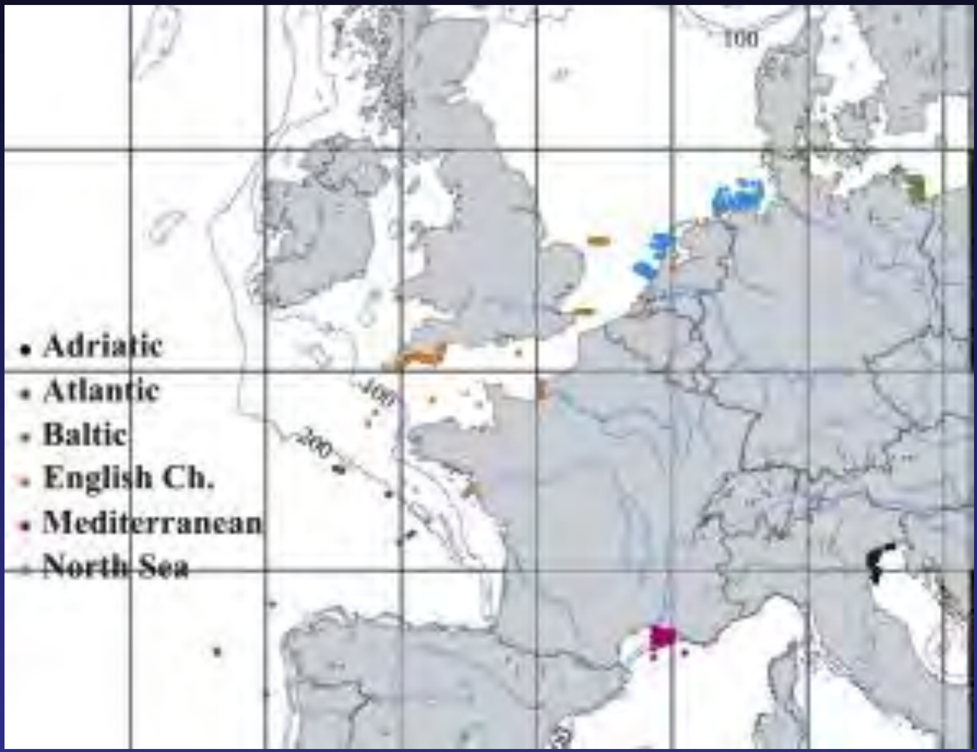
Huot, Y, C A Brown, and J J Cullen. "Retrieval of Phytoplankton Biomass From Simultaneous Inversion of Reflectance, the Diffuse Attenuation Coefficient, and Sun-induced Fluorescence in Coastal Waters." *Journal of Geophysical Research* 112 (2007): doi:10.1029/2006JC003794

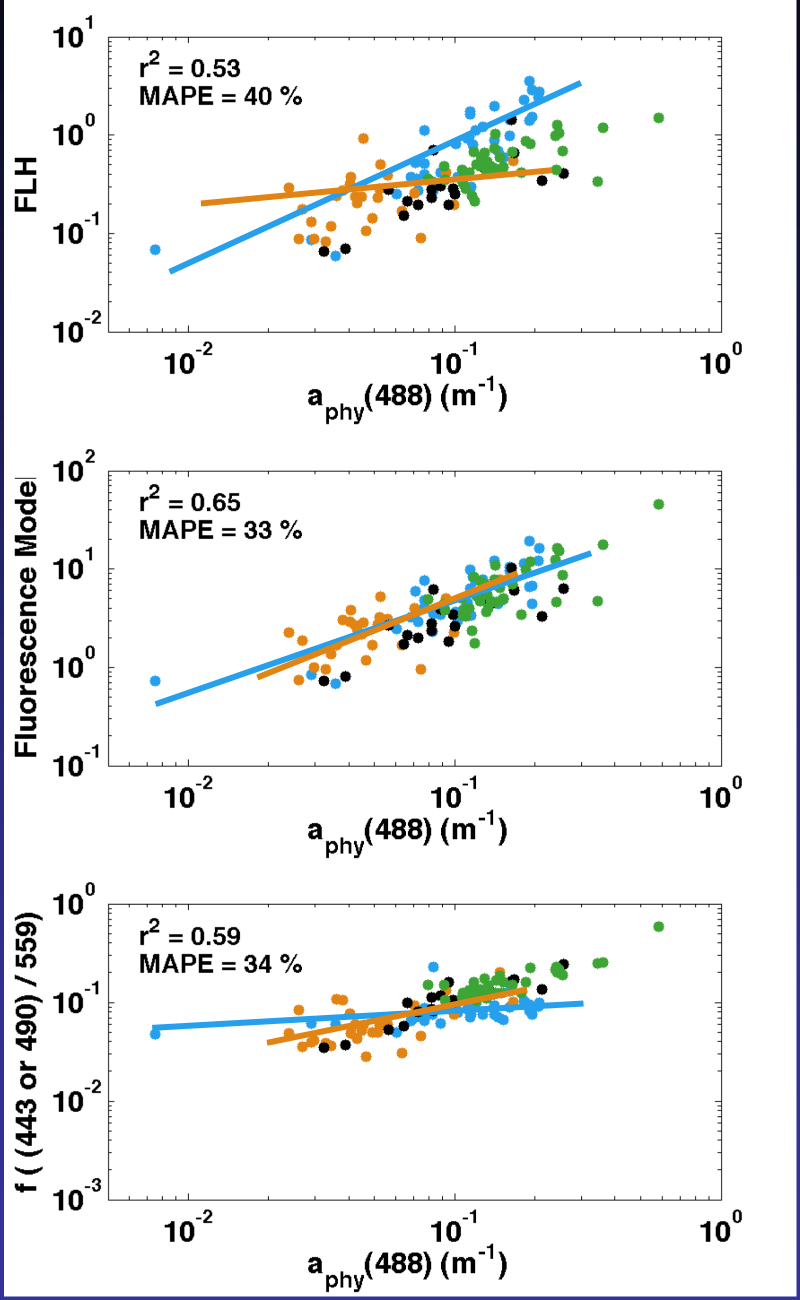
Similar results in Saanich inlet



Sathyendranath, Shubha,, T Platt, B Irwin, E Horne, G A Borstad, V Stuart, L Payzant, *and others.* "A Multispectral Remote Sensing Study of Coastal Waters Off Vancouver Island." *International Journal of Remote Sensing* 25, no. 5 (2004): 893-919

Coastal waters only



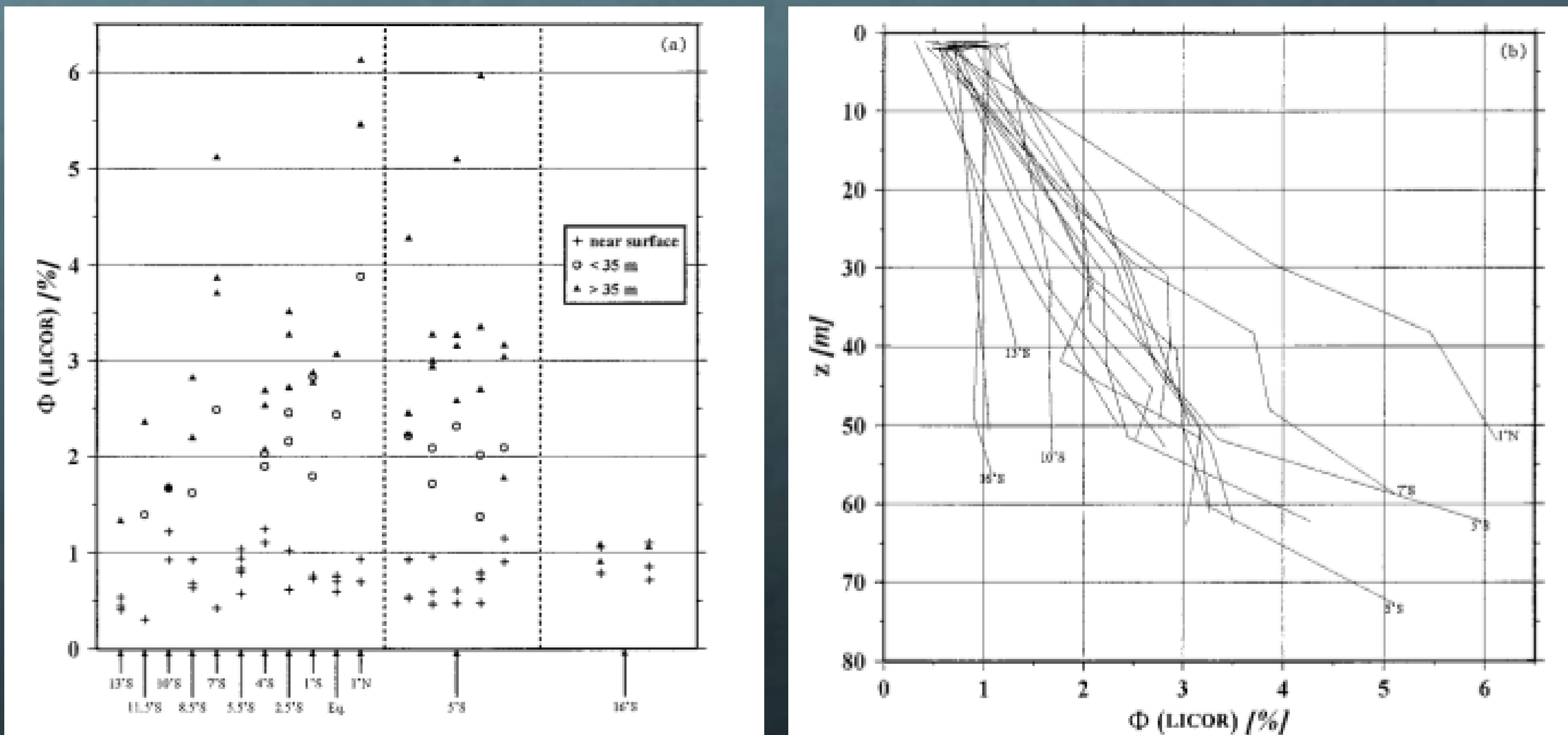


Similar or slightly better than a blue to green ratio algorithm

E. Devred is pursing this work…

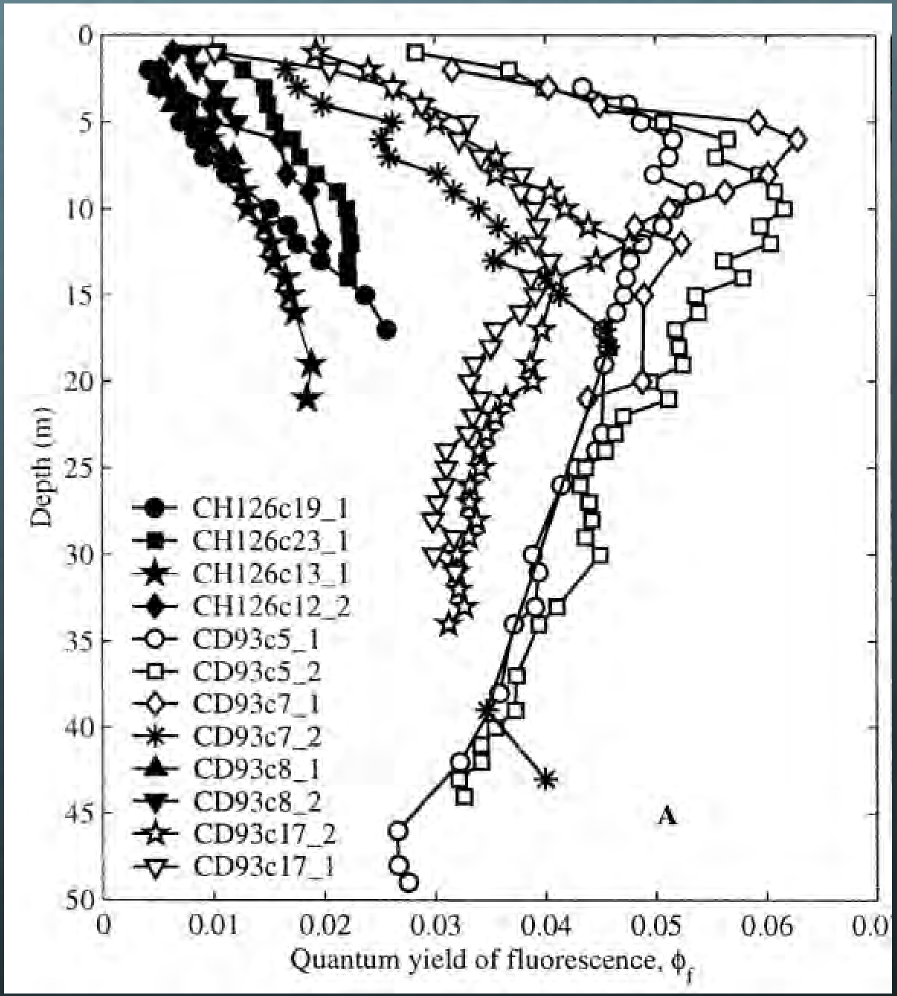
The quantum yield of fluorescence

In situ estimates



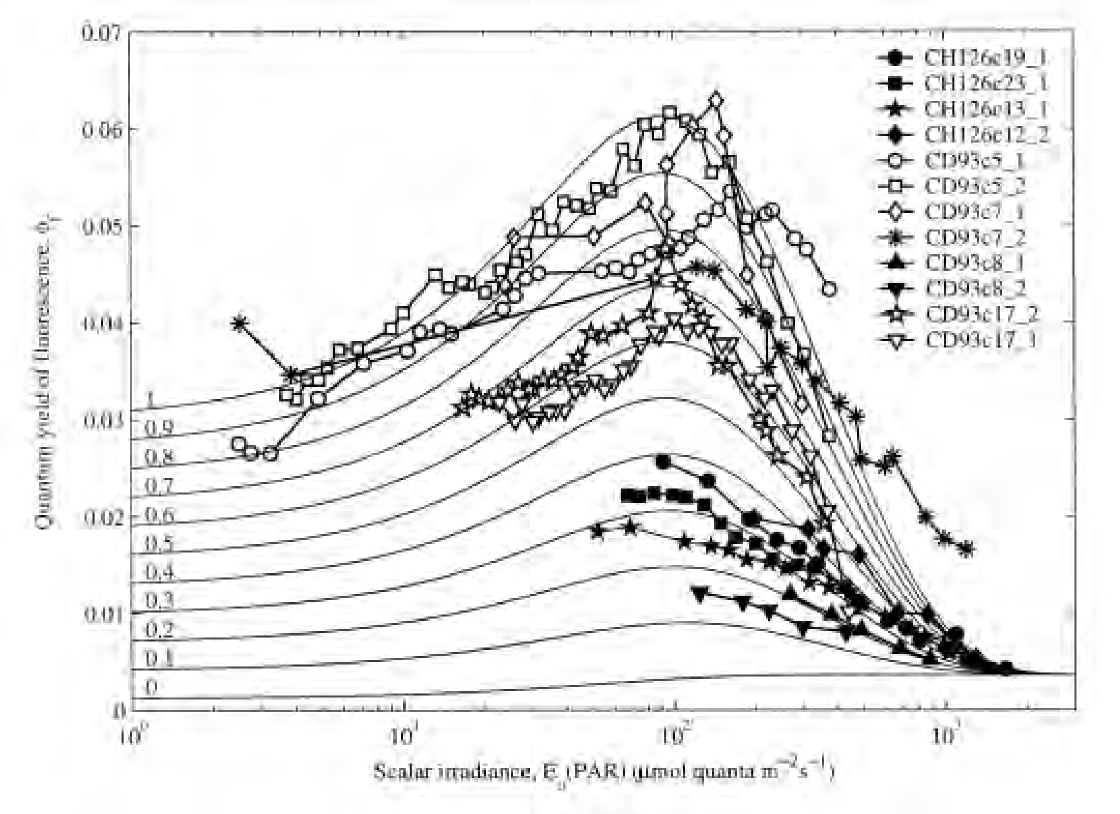
Maritorena, Stéphane, A Morel, and Bernard Gentili. "Determination of the Fluorescence Quantum Yield by Oceanic Phytoplankton in Their Natural Habitat." *Applied Optics 39, no. 36 (2000): 6725-6737*

Quantum yields vs depth



Morrison, J R. "In Situ Determination of the Quantum Yield of Phytoplankton Chlorophyll a Fluorescence: A Simple Algorithm, Observations, and a Model." *Limnology and Oceanography* 48, no. 2 (2003): 618-631

Describing irradiance vs quantum yield function



$$\phi_f^{app} = \left(q_I e^{-\overset{o}{E}/E_T} \right) \left(\phi_{f\min} A + \phi_{f\max} \left[1 - A \right] \right)$$

$$A = e^{-\overset{o}{E}/E_k}$$

Version of the model adopted in :Morrison, J R, and D S Goodwin. "Phytoplankton Photocompensation From Space-based Fluorescence Measurements." *Geophysical Research Letters* 37, no. 6 (2010): doi:10.1029/2009GL041799

Comparison of QY descriptions

From Part 1:

$$\phi_f^{app} = \phi_f \frac{{}^{PS}\overline{a}_{PSII}}{\left({}^{PS}\overline{a}_{PSII} + {}^{PS}\overline{a}_{PSI} + {}^{PP}\overline{a}_{PSII} + {}^{PP}\overline{a}_{PSI}\right)}$$

$$= \frac{k_f}{k_f + Ak_p + k_H + Zk_{NPQ} + Ck_{qI}} \frac{{}^{PS}\overline{a}_{PSII}}{\left({}^{PS}\overline{a}_{PSII} + {}^{PS}\overline{a}_{PSI} + {}^{PP}\overline{a}_{PSII} + {}^{PP}\overline{a}_{PSI}\right)}$$

From Morrison :

$$\phi_f = \left(q_I e^{-\overset{o}{E}/E_T} \right)\left(\phi_{f\,\min} A + \phi_{f\,\max}\left[1 - A\right]\right)$$

$$A = e^{-\overset{o}{E}/E_k}$$

Comparison of QY descriptions

From Part 1:

$$\boldsymbol{f}_f^{app} = \boldsymbol{f}_f \frac{{}^{PS}\overline{a}_{PSII}}{\left({}^{PS}\overline{a}_{PSII} + {}^{PS}\overline{a}_{PSI} + {}^{PP}\overline{a}_{PSII} + {}^{PP}\overline{a}_{PSI}\right)}$$

$$= \frac{k_f}{k_f + Ak_p + k_H + Zk_{NPQ} + Ck_{qI}} \frac{{}^{PS}\overline{a}_{PSII}}{\left({}^{PS}\overline{a}_{PSII} + {}^{PS}\overline{a}_{PSI} + {}^{PP}\overline{a}_{PSII} + {}^{PP}\overline{a}_{PSI}\right)}$$

From Morrison :

$$\boldsymbol{f}_f = \left(q_I e^{-\mathring{E}/E_T}\right)\left(\boldsymbol{f}_{f\,\min} A + \boldsymbol{f}_{f\,\max}\left[1 - A\right]\right)$$

$$\neq \boldsymbol{f}_f^{app}$$

$$A = e^{-\mathring{E}/E_k}$$

Morrison described the variability in the inherent quantum yield not in the apparent quantum yield of fluorescence

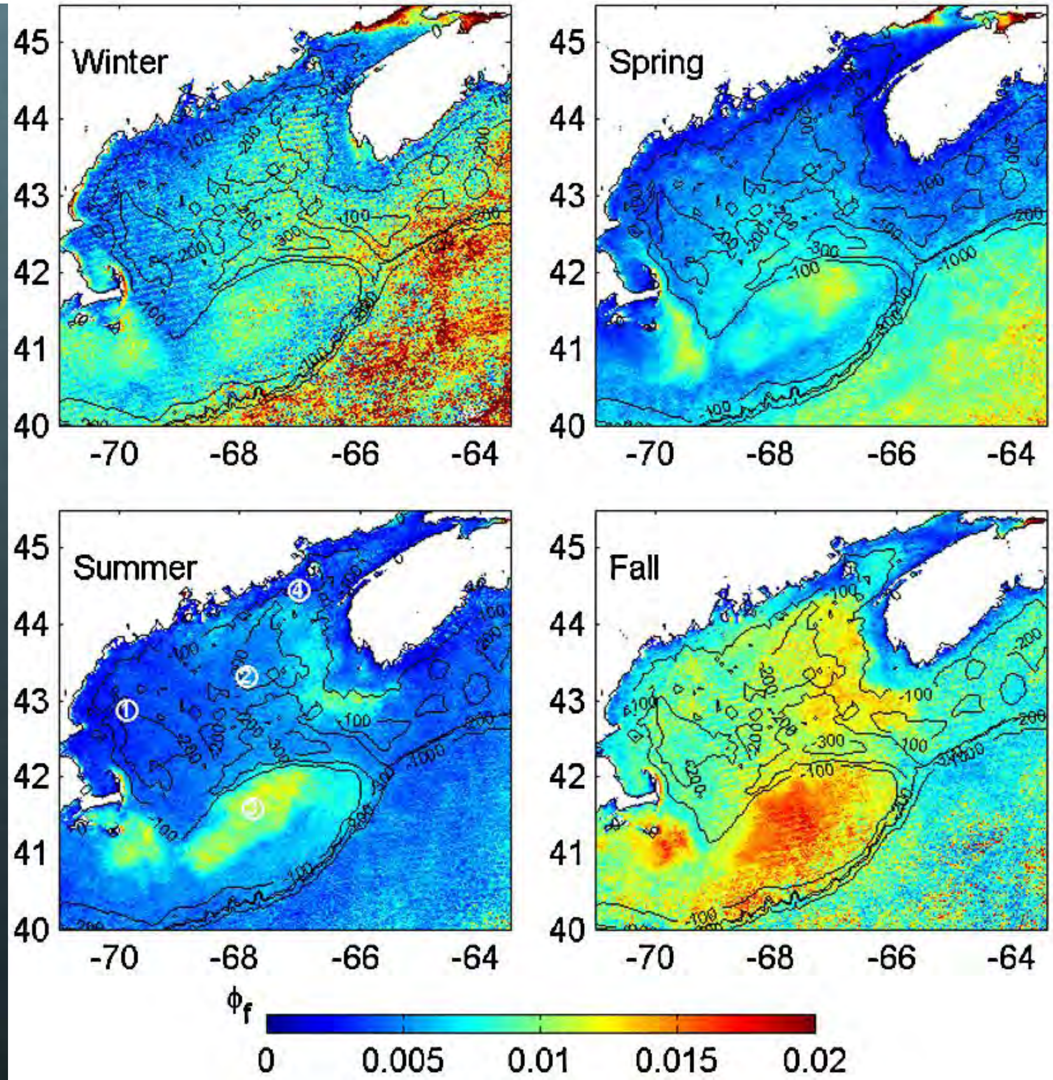
Interpreting variability in Φ_f

GEOPHYSICAL RESEARCH LETTERS, VOL. 37, L06603, doi:10.1029/2009GL041799, 2010

Click

Phytoplankton photocompensation from space-based fluorescence measurements

J. Ruairidh Morrison[1] and Deborah S. Goodwin[2]



GEOPHYSICAL RESEARCH LETTERS, VOL. 37, L06603, doi:10.1029/2009GL041799, 2010

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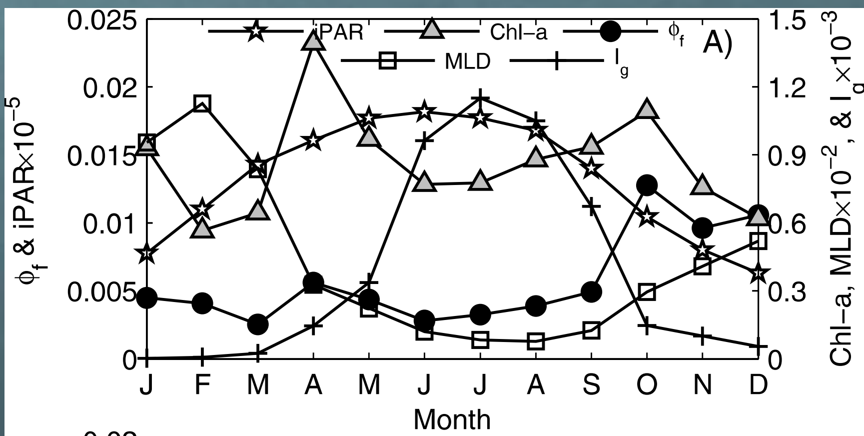
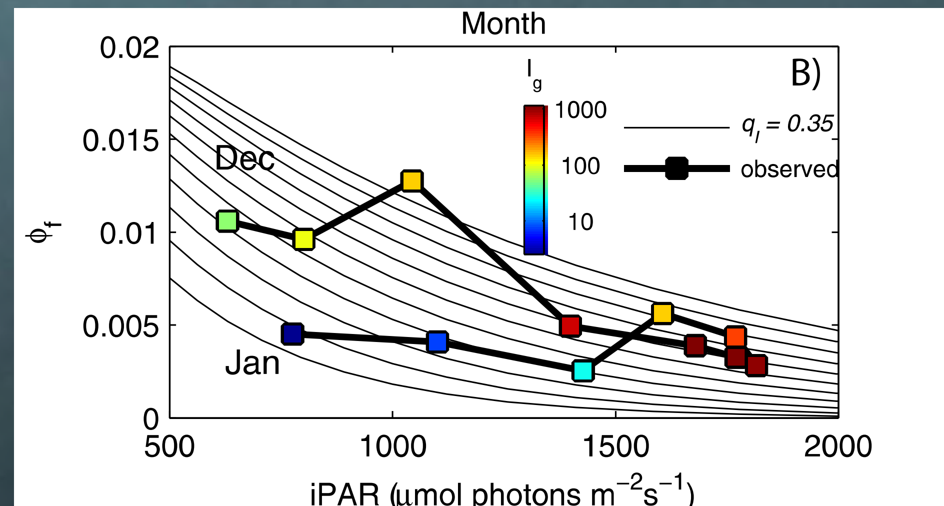




0.35   0

$$\phi_f = \left(q_I e^{-\overset{o}{E}/E_T}\right)\left(\phi_{f\min} A + \phi_{f\max}\left[1 - A\right]\right)$$

1

0

$$A = e^{-\overset{o}{E}/E_k}$$

Assume $\overset{o}{E} >> E_k$ leads to A=0

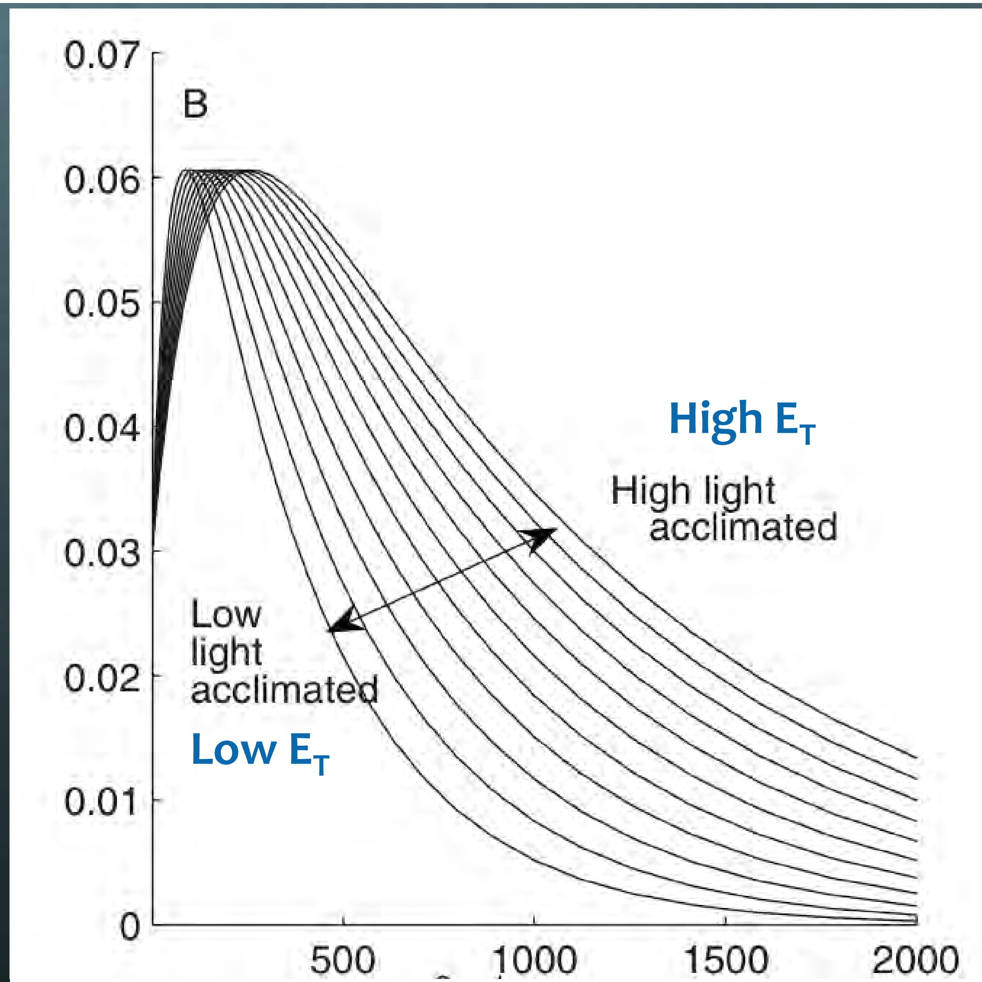
Assume qI is constant =0.35

GEOPHYSICAL RESEARCH LETTERS, VOL. 37, L06603, doi:10.1029/2009GL041799, 2010

Phytoplankton photocompensation from space-based fluorescence measurements

J. Ruairidh Morrison[1] and Deborah S. Goodwin[2]

$$\phi_f = 0.032e^{-\overset{o}{E}/E_T}$$



Presented in the supplementary material

GEOPHYSICAL RESEARCH LETTERS, VOL. 37, L06603, doi:10.1029/2009GL041799, 2010

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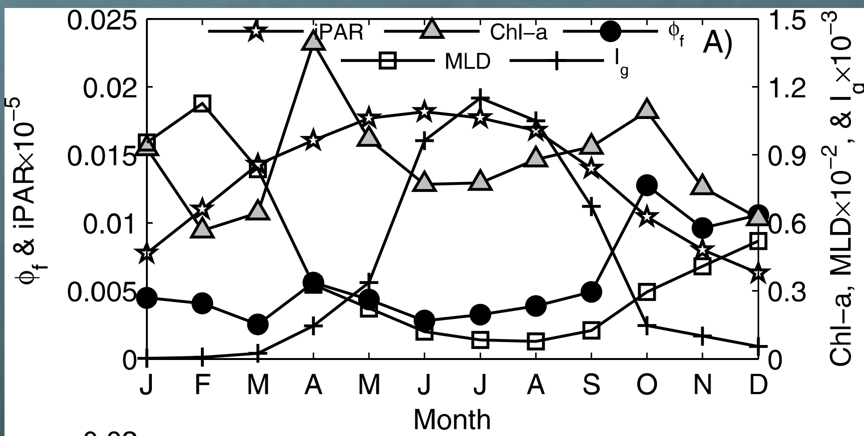
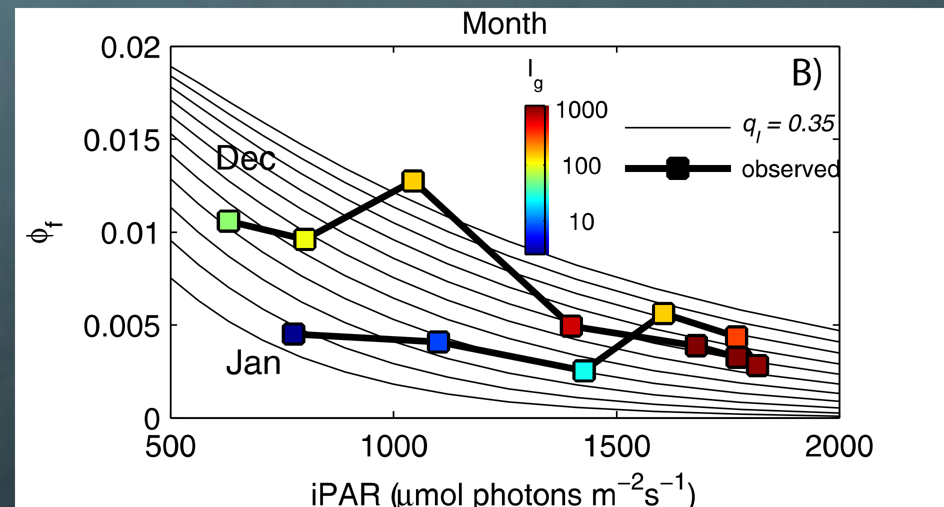
Phytoplankton photocompensation from space-based fluorescence measurements

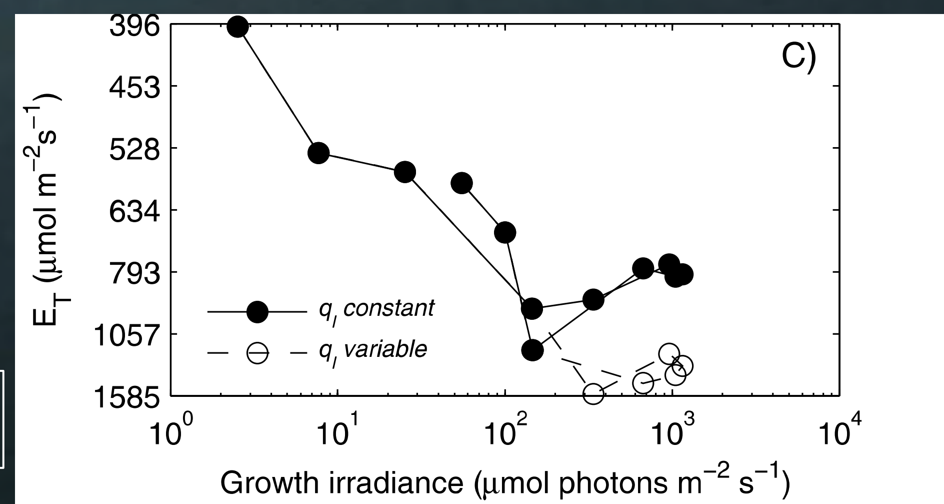
J. Ruairidh Morrison[1] and Deborah S. Goodwin[2]





$$\phi_f = 0.032e^{-\overset{o}{E}/E_T}$$

This allows them to retrieve E_T.

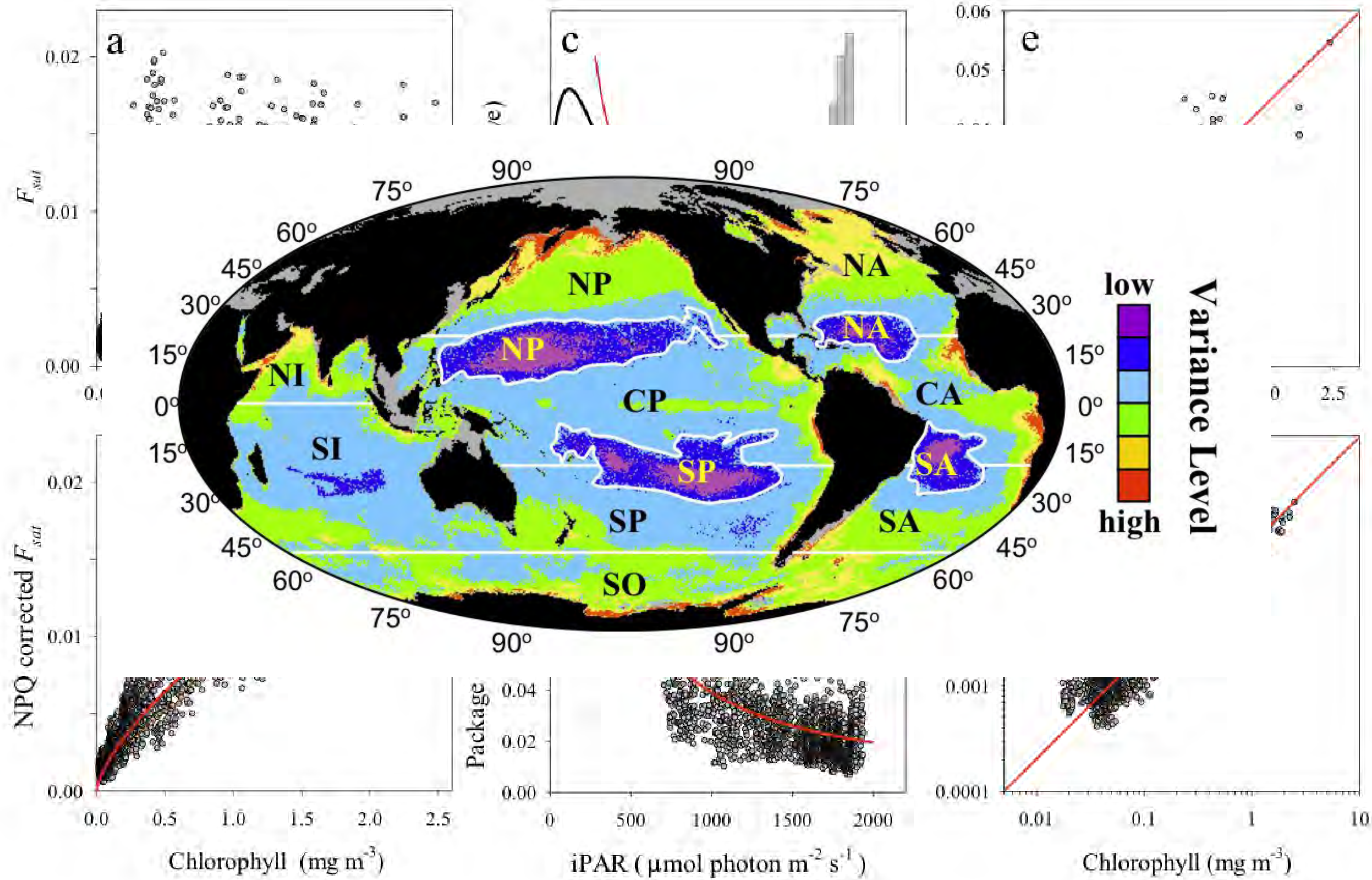


E_T varies with growth irradiance

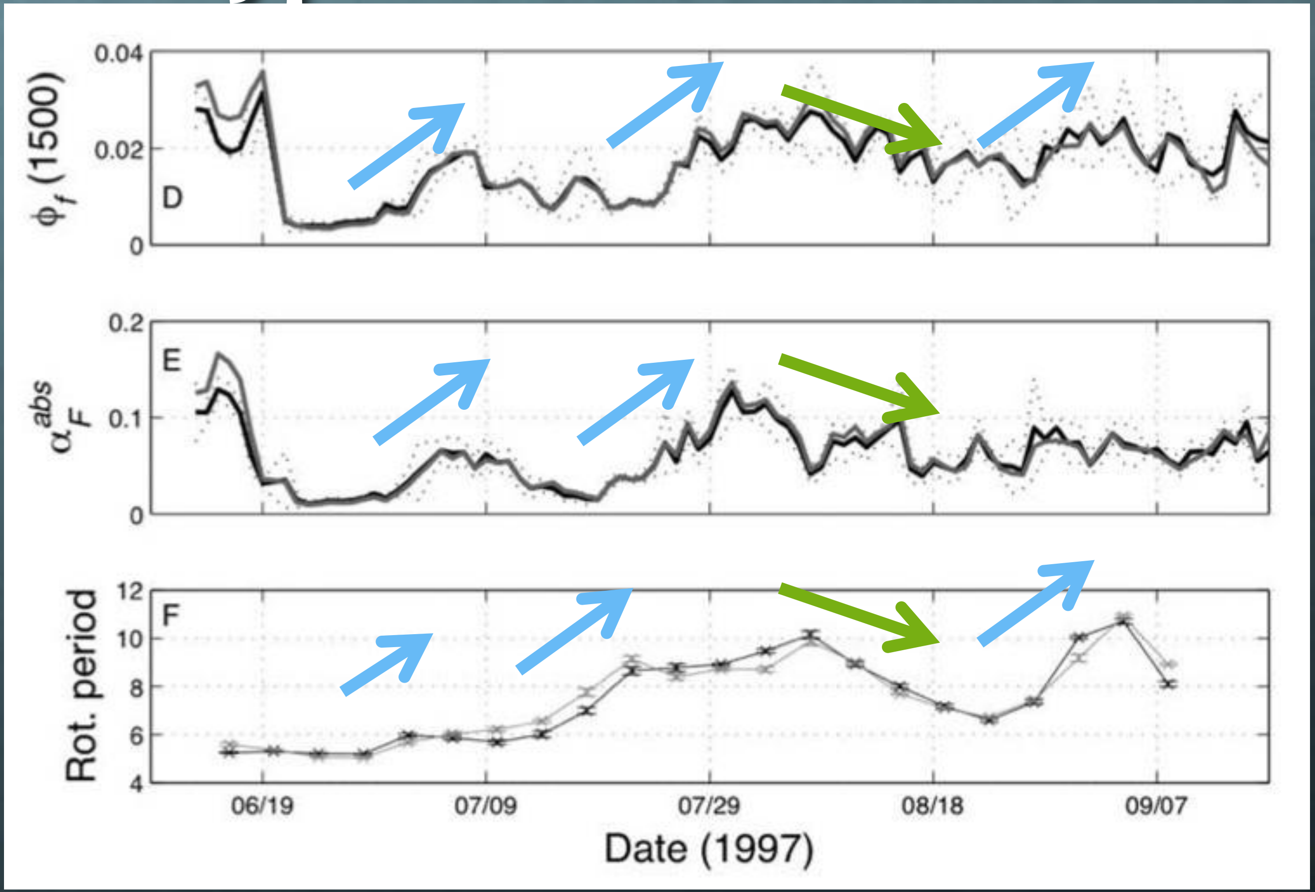
Biogeosciences, 6, 779–794, 2009
www.biogeosciences.net/6/779/2009/

Biogeosciences

Satellite-detected fluorescence reveals global physiology of ocean



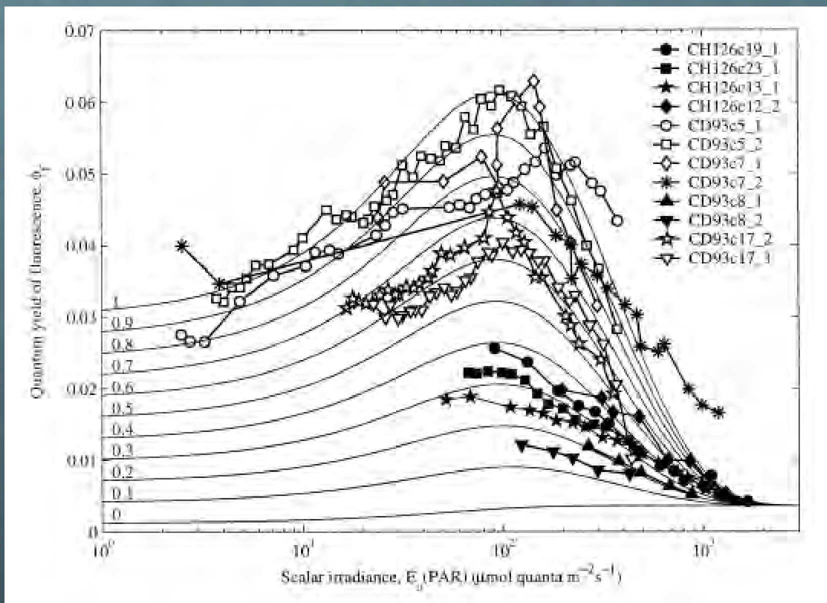
Similar results, a different hypothesized cause

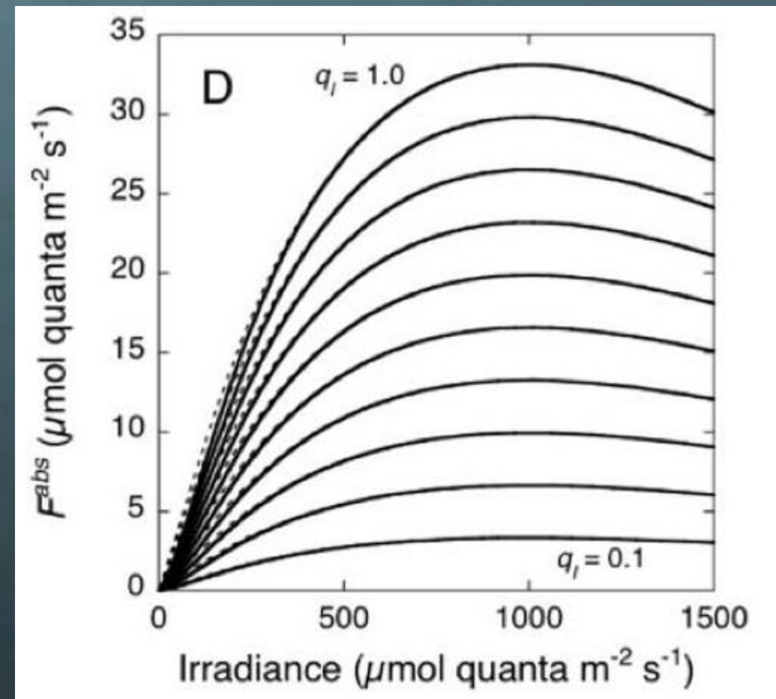


When the eddy slows (period increases) qI quenching is reduced by nutrient stress and this leads to an increase in Φ_f.

Schallenberg, Christina, M R Lewis, D E Kelley, and J J Cullen. "The Inferred Influence of Nutrient Availability on the Relationship Between Sun-induced Fluorescence and Incident Irradiance in the Bering Sea." *Journal of Geophysical Research* 113 (2008): doi:10.1029/2007JC004355

One current hypothesis: reduced qI quenching or downregulation under nutrient stress accounts for most of the variability?





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Biogeosciences, 6, 779–794, 2009
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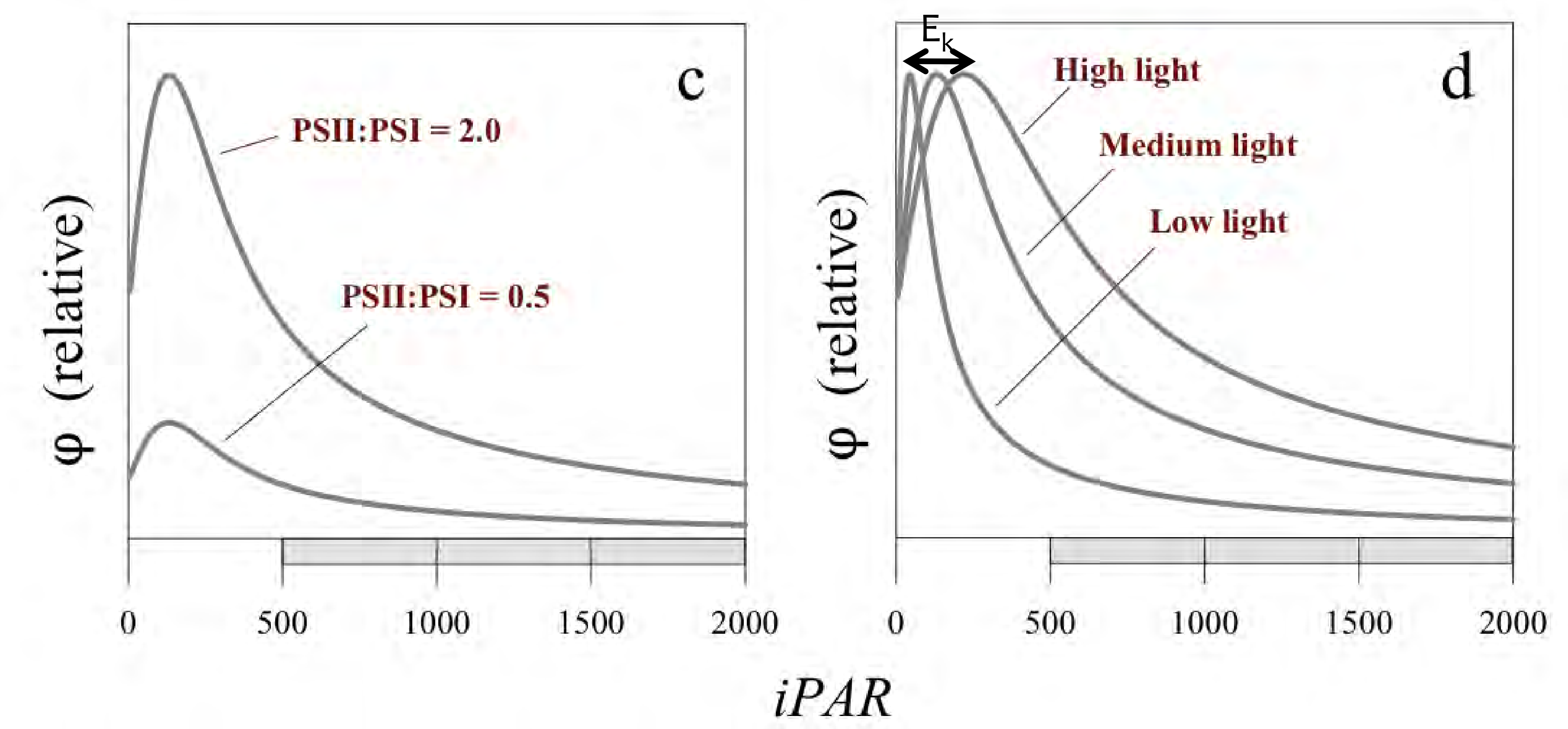
Satellite-detected fluorescence reveals global physiology of ocean phytoplankton

M. J. Behrenfeld[1], T. K. Westberry[1], E. S. Boss[2], R. T. O'Malley[1], D. A. Siegel[3], J. D. Wiggert[4], B. A. Franz[5], C. R. McClain[5], G. C. Feldman[5], S. C. Doney[6], J. K. Moore[7], G. Dall'Olmo[1], A. J. Milligan[1], I. Lima[6], and N. Mahowald[8]



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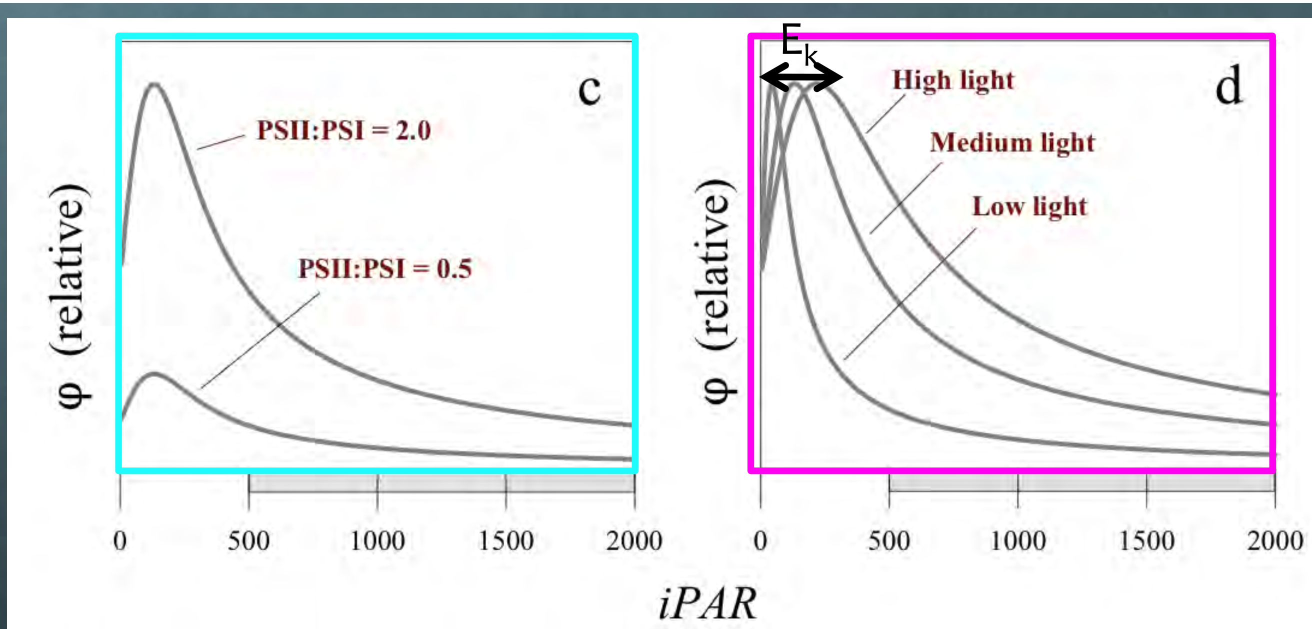

$$f_f^{app} = \frac{k_f}{k_f + Ak_p + k_H + Zk_{NPQ} + Ck_{qI}} \frac{{}^{PS}\bar{a}_{PSII}}{\left({}^{PS}\bar{a}_{PSII} + {}^{PS}\bar{a}_{PSI} + {}^{PP}\bar{a}_{PSII} + {}^{PP}\bar{a}_{PSI}\right)}$$

In the text they also discuss how iron stress could decrease qI and increase the PSII photosynthetic absorption cross-section (in high macronutrient regions).

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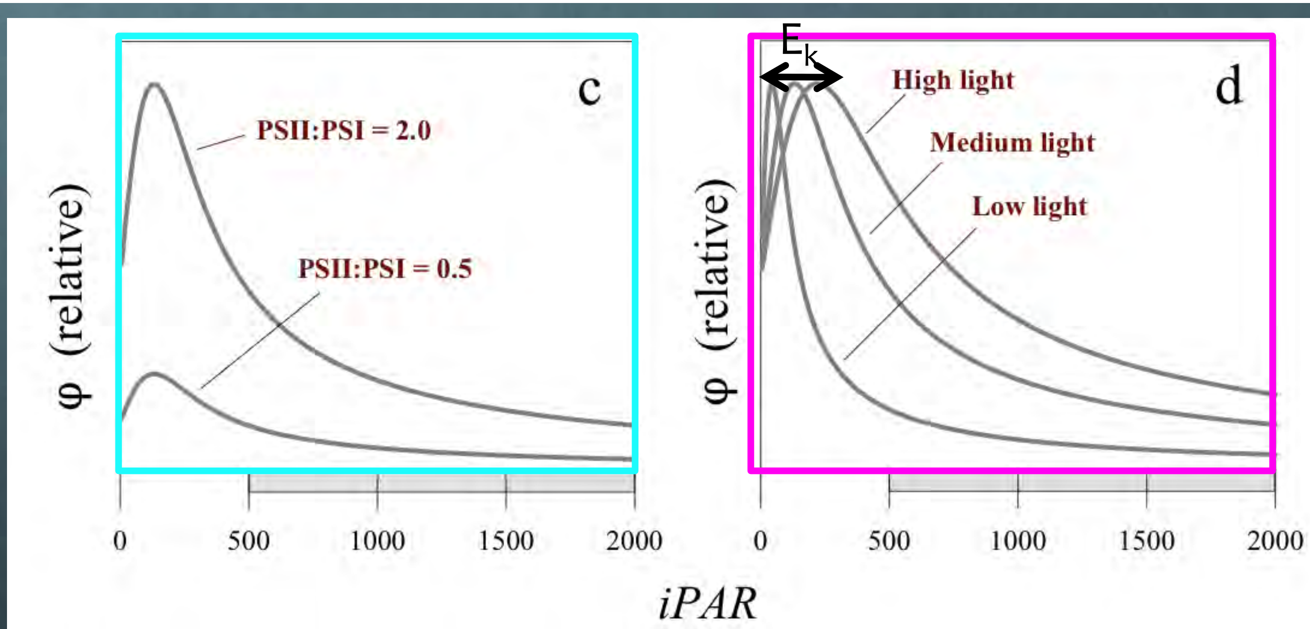

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In summary, according to them, whatever the process, **iron stress is expected to increase the apparent quantum yield of fluorescence.**

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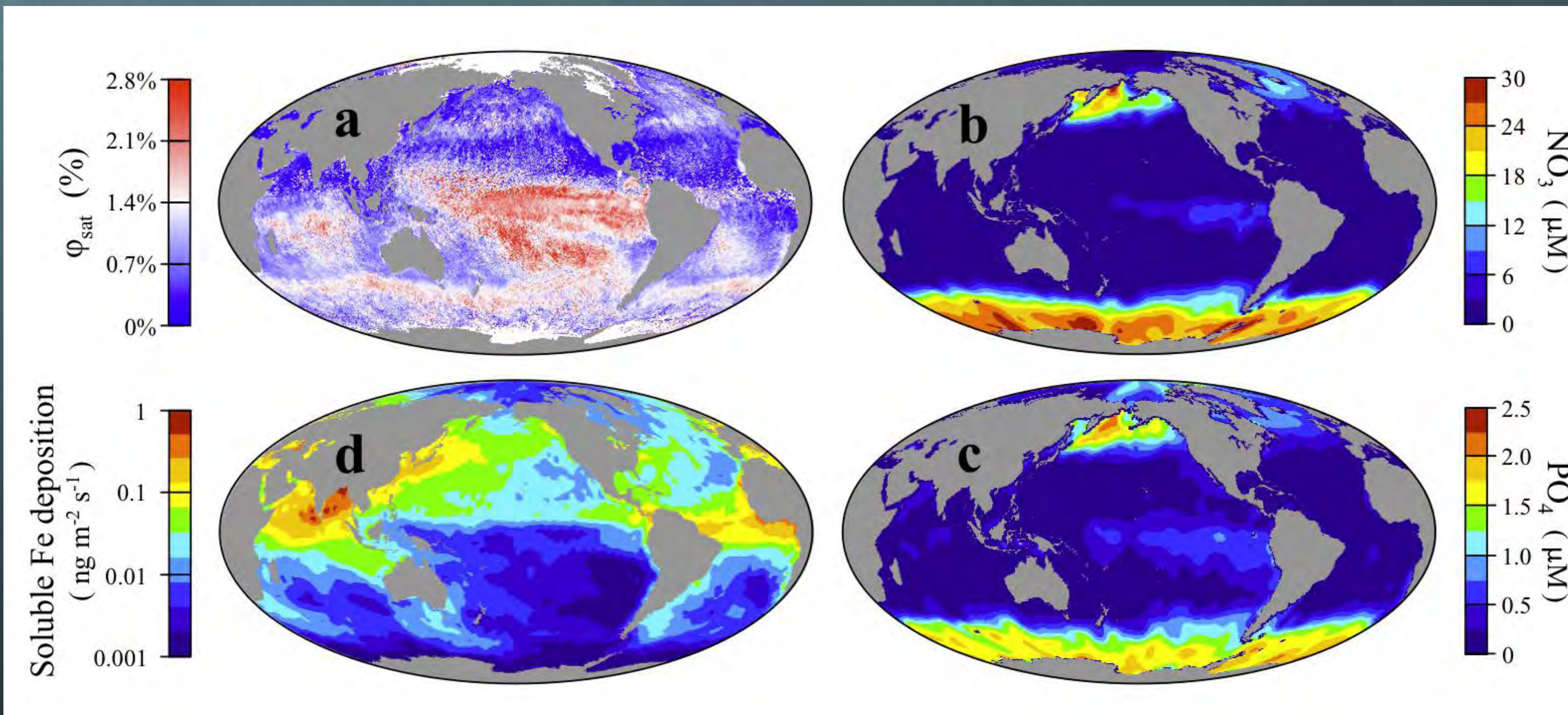

Observed quantum yield did not show clear relationship with macronutrient concentration

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Biogeosciences

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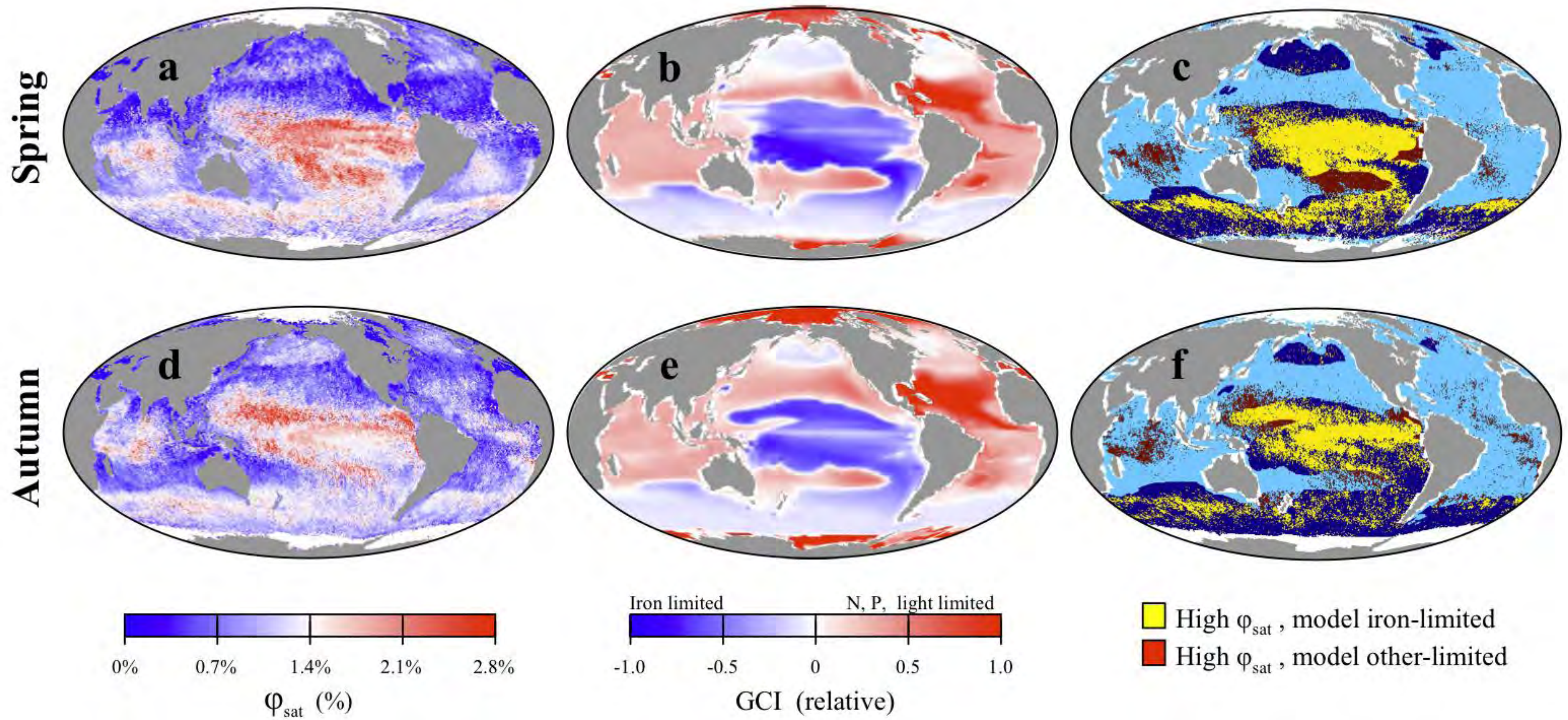


Two general hypotheses

1. Growth irradiance is responsible for much of the variability in the quantum yield of Sun-induced fluorescence - Morisson and Goodwin

2. Nutrient limitation is responsible for much of the limitation in the quantum yield of Sun-induced fluorescence
    a. Macro-Nutrient - Schallenberget al. (effect on qI), Letelier and Abbott (effect on PQ)
    b. Iron - Behrenfeld and others

Others possible?

Physiology vs ecology: species composition another possibility?

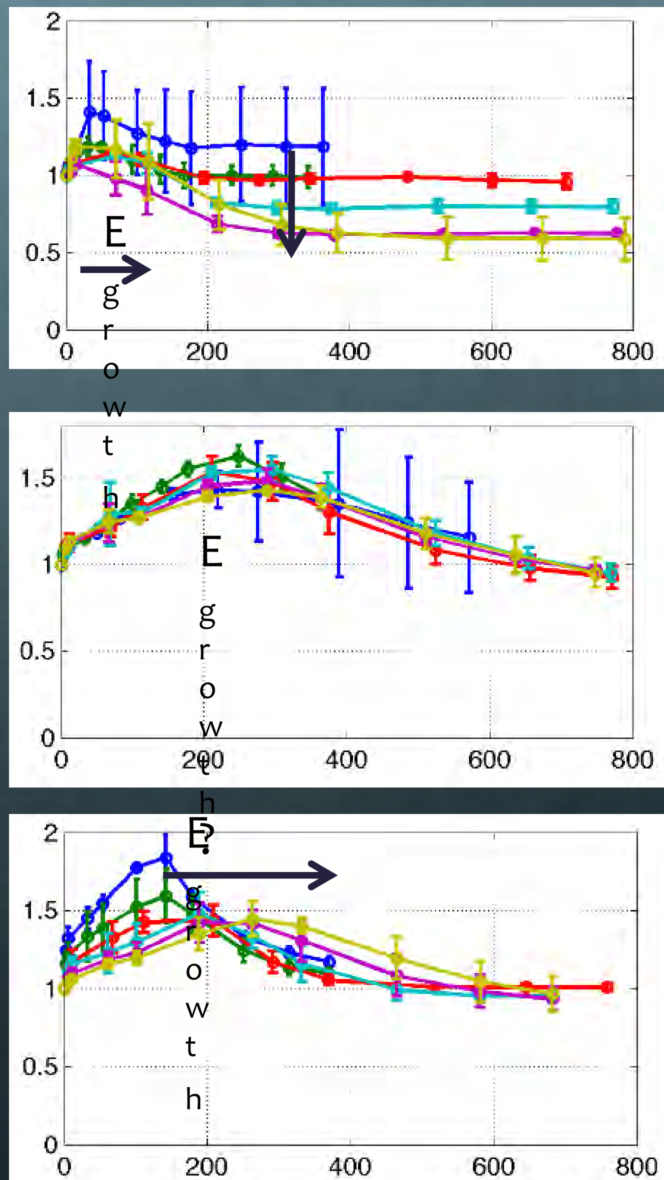
3 species, 6 growth irradiances

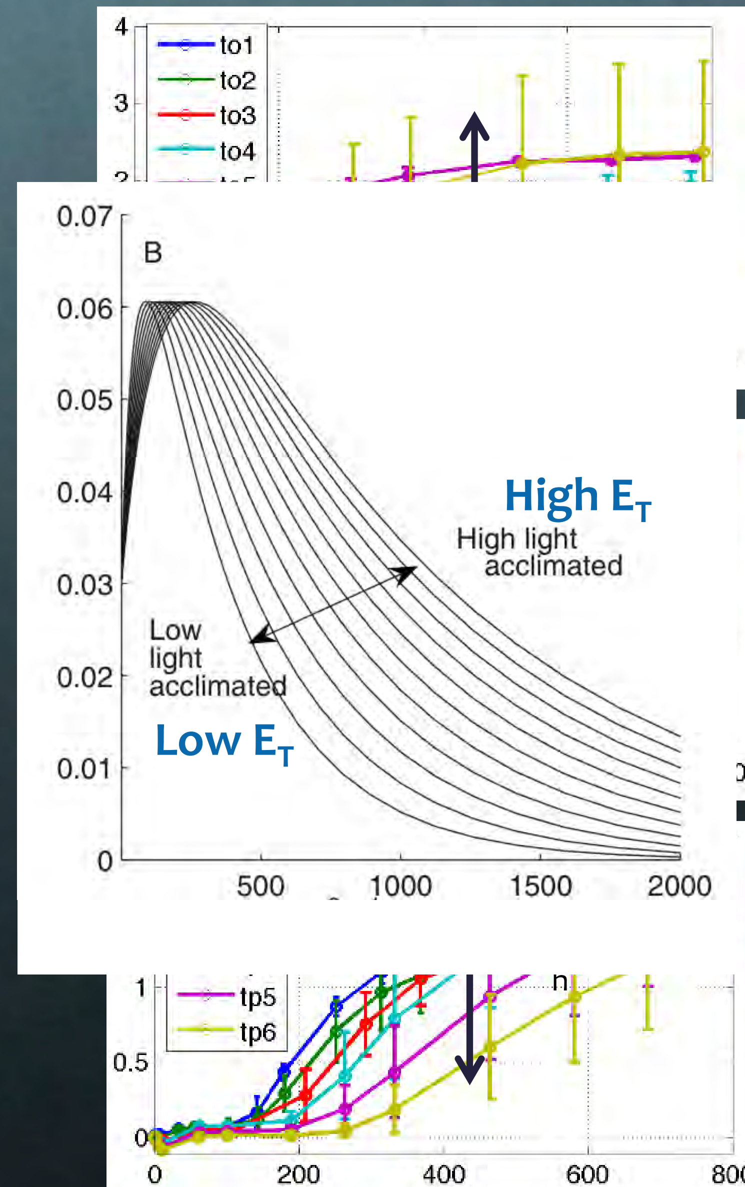
F_s — *NPQ*

T. oceanica

T. weissflogii

T. pseudonana





Three general hypotheses

1. Growth irradiance is responsible for much of the variability in the quantum yield of Sun-induced fluorescence (Morisson and others)
2. Nutrient limitation is responsible for much of the limitation in the quantum yield of Sun-induced fluorescence
   a. Macro-Nutrient (Schallenberg, Letelier and others)
   b. Iron (Behrenfeld and others)
3. Species composition

Four general hypotheses

1. Growth irradiance is responsible for much of the variability in the quantum yield of Sun-induced fluorescence (Morisson and others)
2. Nutrient limitation is responsible for much of the limitation in in the quantum yield of Sun-induced fluorescence
   a. Macro-nutrient (Schallenberg, Letelier and others)
   b. Iron (Behrenfeld and others)
3. Species composition
4. We are not measuring the quantum yield of fluorescence…
   a. Biases prevent us from observing real global distributions

How do current chl-based φ_f satellite algorithms work?

Measured by ocean color satellites

What we want

Modeled

$$L_{uf} \propto \varphi_f \times \mathring{E}_{PAR} \times a_{\varphi} \times Q_a^* \frac{1}{a_{\varphi} + K_{dPAR}}$$

Retrieved by OC algorithm

Estimated based on a_φ or K_d algorithm and known relationships

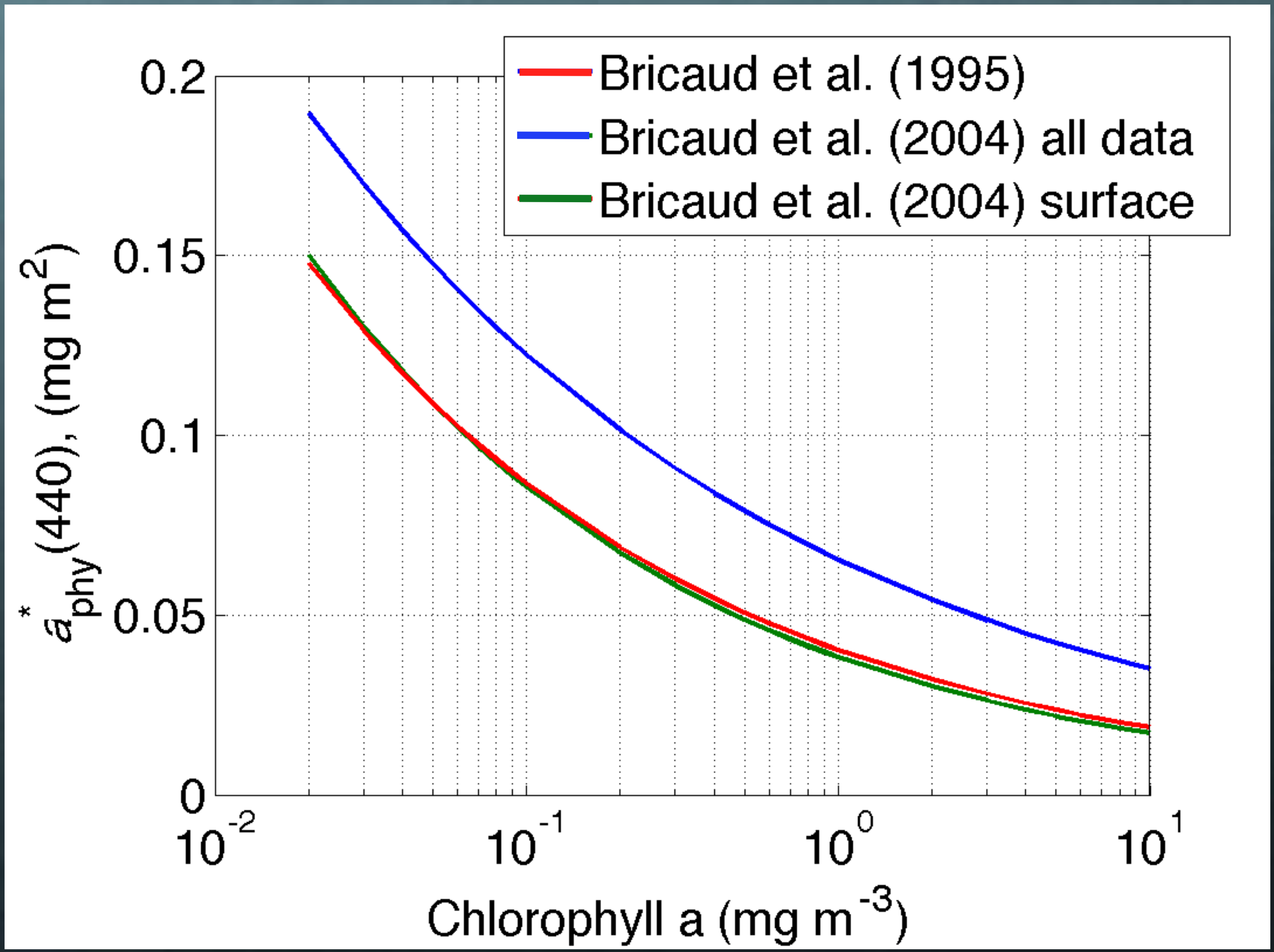
Morel, A. and S. Maritorena (2001), Journal of Geophysical Research **106**(C4): 7163-7180.
Bricaud, A., M. Babin, et al. (1995). Journal of Geophysical Research **100**(C7): 13321-13332.

Errors in a_φ (or chl) estimated by ocean color algorithms thus propagate directly to estimates of φ_f.

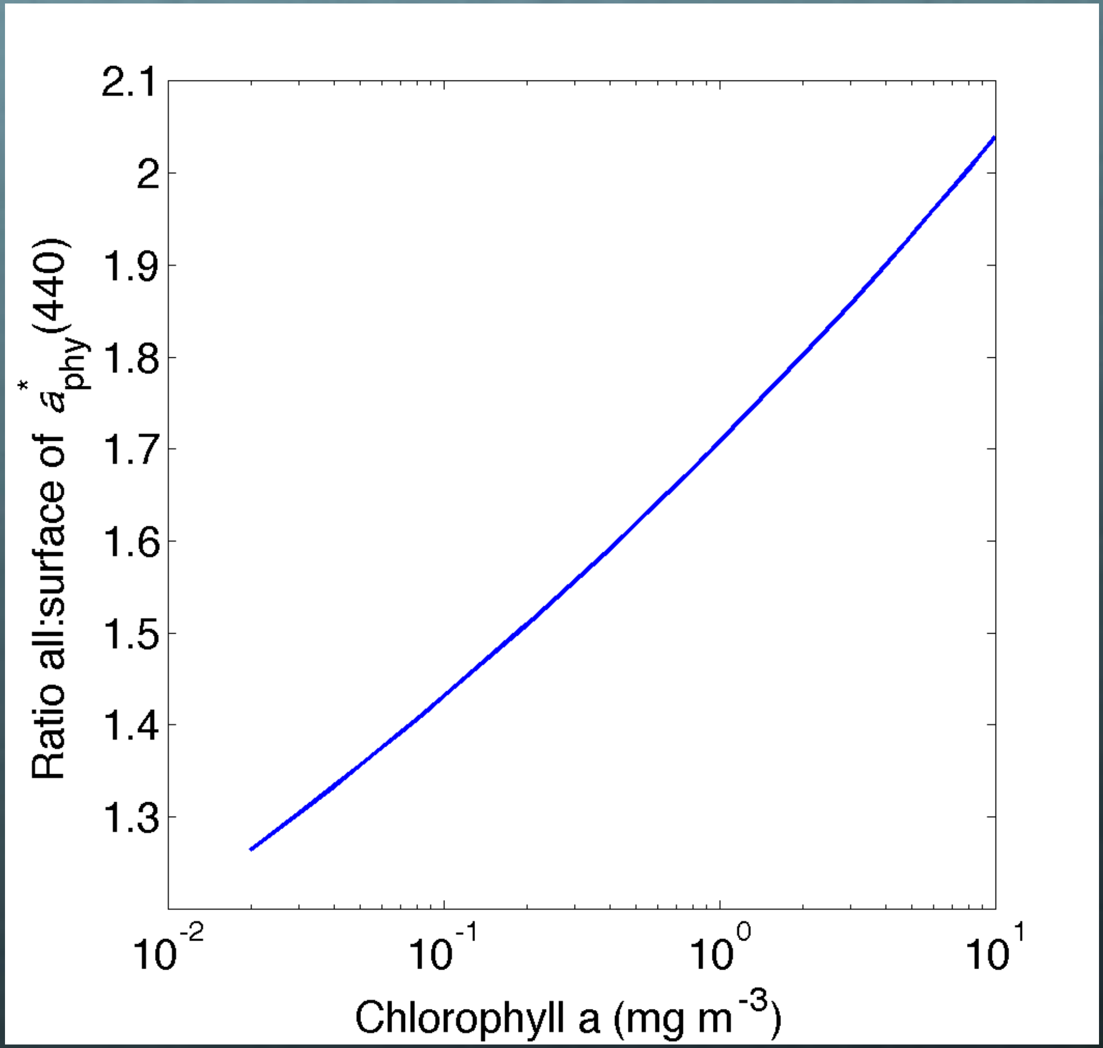
An overestimate of a_φ leads to an underestimate of the quantum yield.

Parameterization "errors"

$$a_j = a_j^* \times Chla$$



Parameterization “errors”

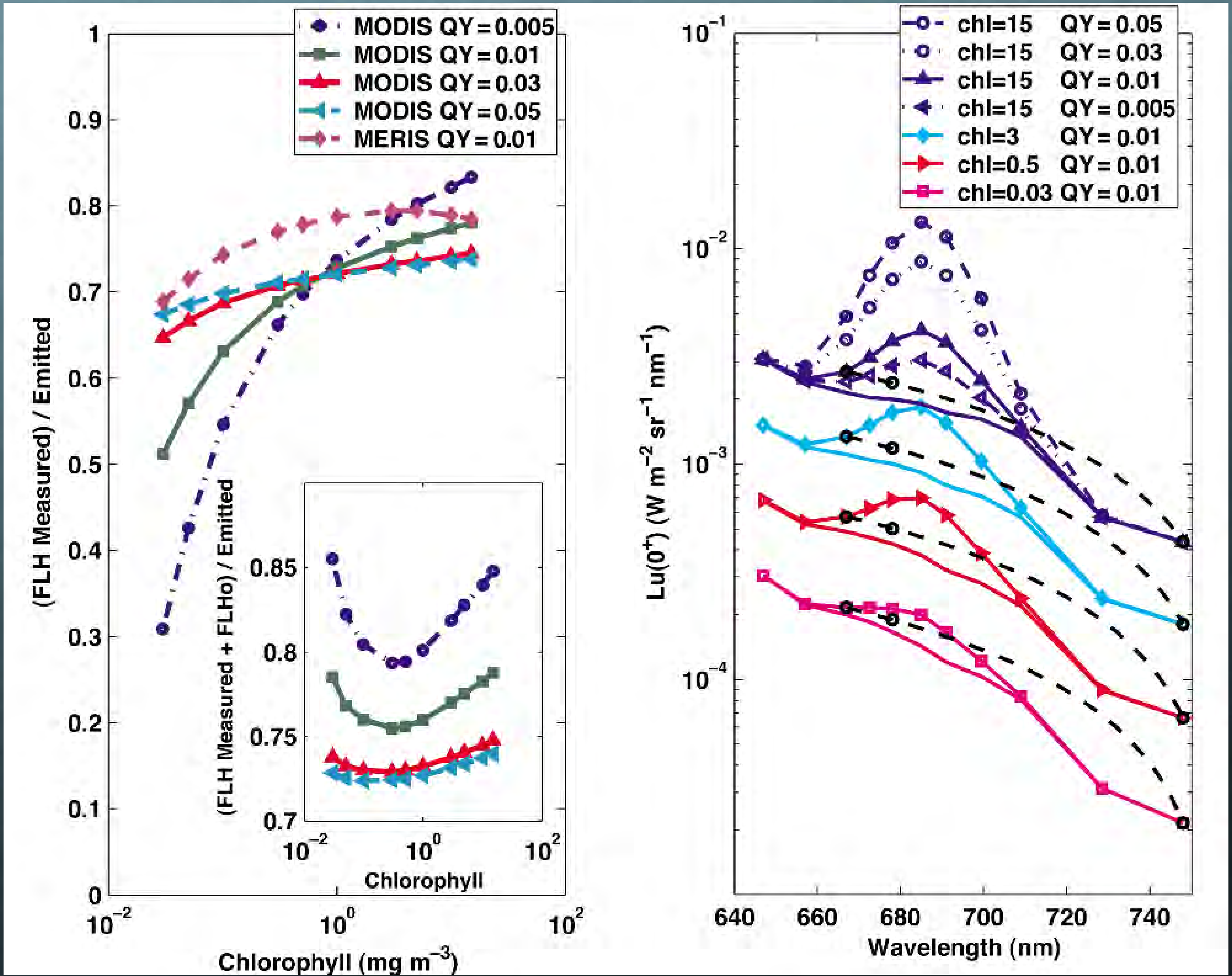


$$f_f^{app} = 0.81 \times \frac{FLH_{Lwn}}{Chl^{0.684}}$$

The exact exponent matters over three orders of magnitudes

Current algorithms are likely biased across Chla gradient because of such parameterization errors (error likely also in Q_a* vs Chla and K_{dPAR} vs Chla)

FLH is a biased estimate of fluorescence



Huot, Y, C A Brown, and J J Cullen. "New Algorithms for MODIS Sun-induced Chlorophyll Fluorescence and a Comparison with Present Data Products." *Limnology and Oceanography: Methods 3 (2005): 108-130*

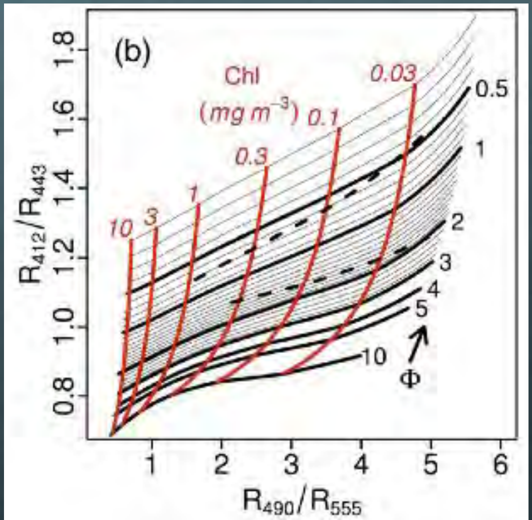
Biases in a_φ: main source and potential corrections

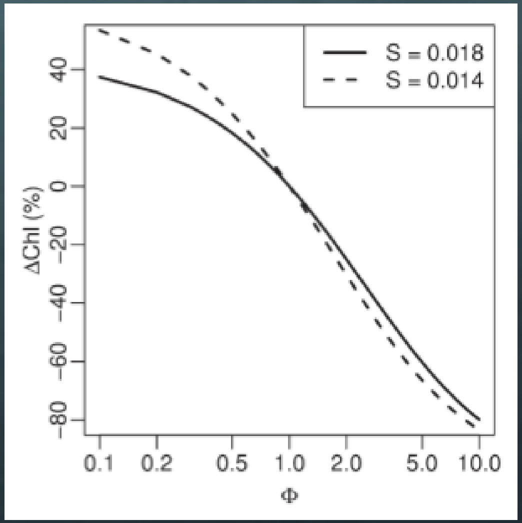
The absorption by colored dissolved organic matter (CDOM) appears to be the largest bias in the estimate of phytoplankton absorption from space using empirical algorithms.

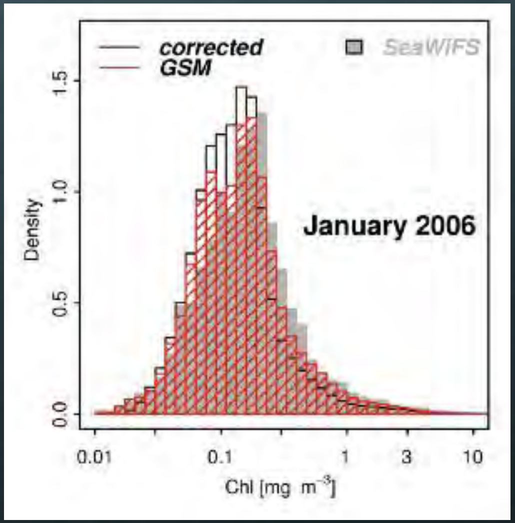
Two approaches to resolve this issue…

1) Empirical corrections (e.g. Φ-correction)

2) Semi-analytical approaches (e.g. GSM or QAA algorithms)





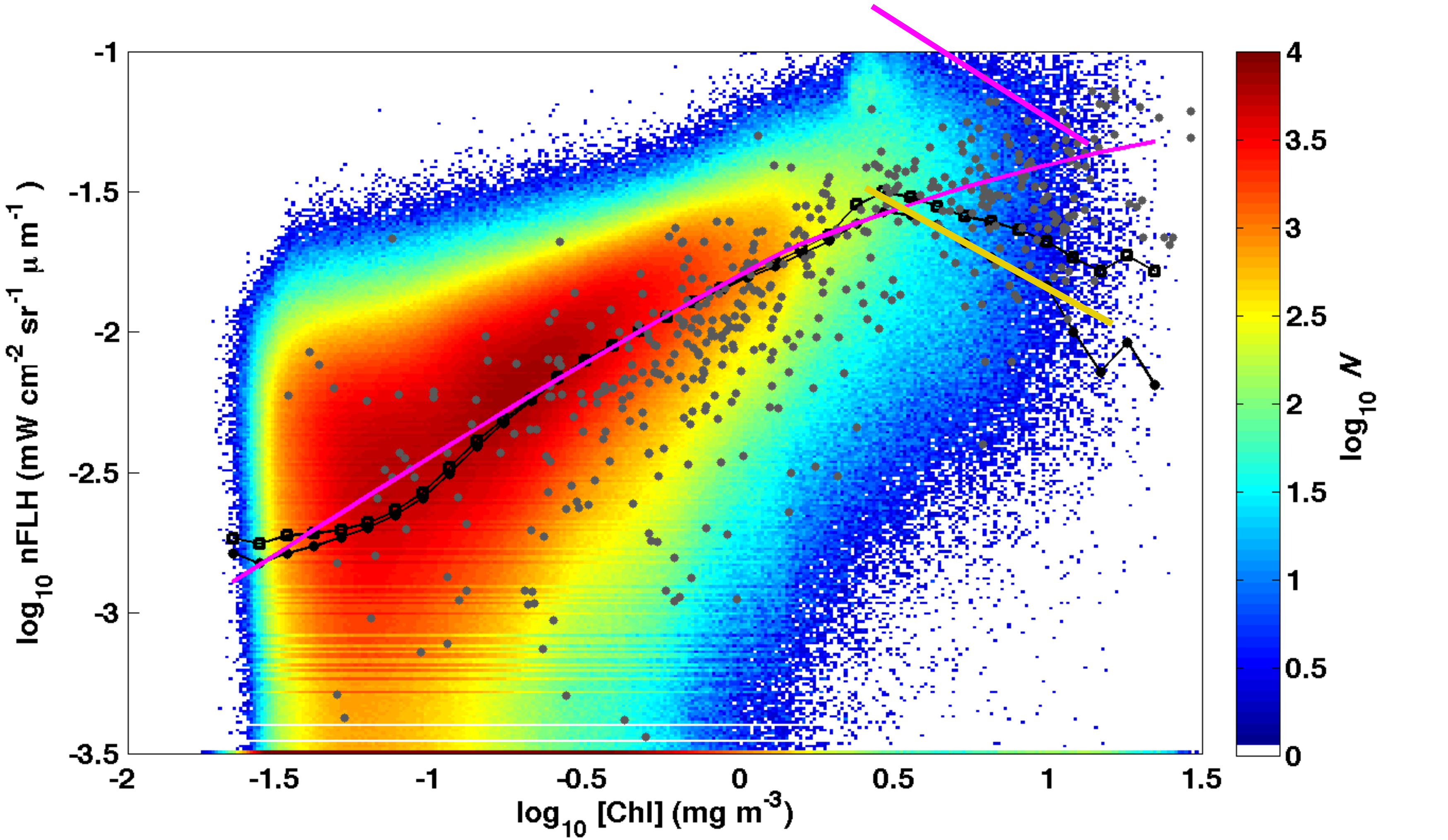


Both approaches also allow an estimate of CDOM absorption

Figures from : Morel, A. & Gentili, B. (2009). A simple band ratio technique to quantify the colored dissolved and detrital organic material from ocean color remotely sensed data. *Remote Sensing of Environment*, *113*(5), 998-1011.

Fluorescence vs chlorophyll OC2M

Scaled theoretical line (Huot et al. 2005)

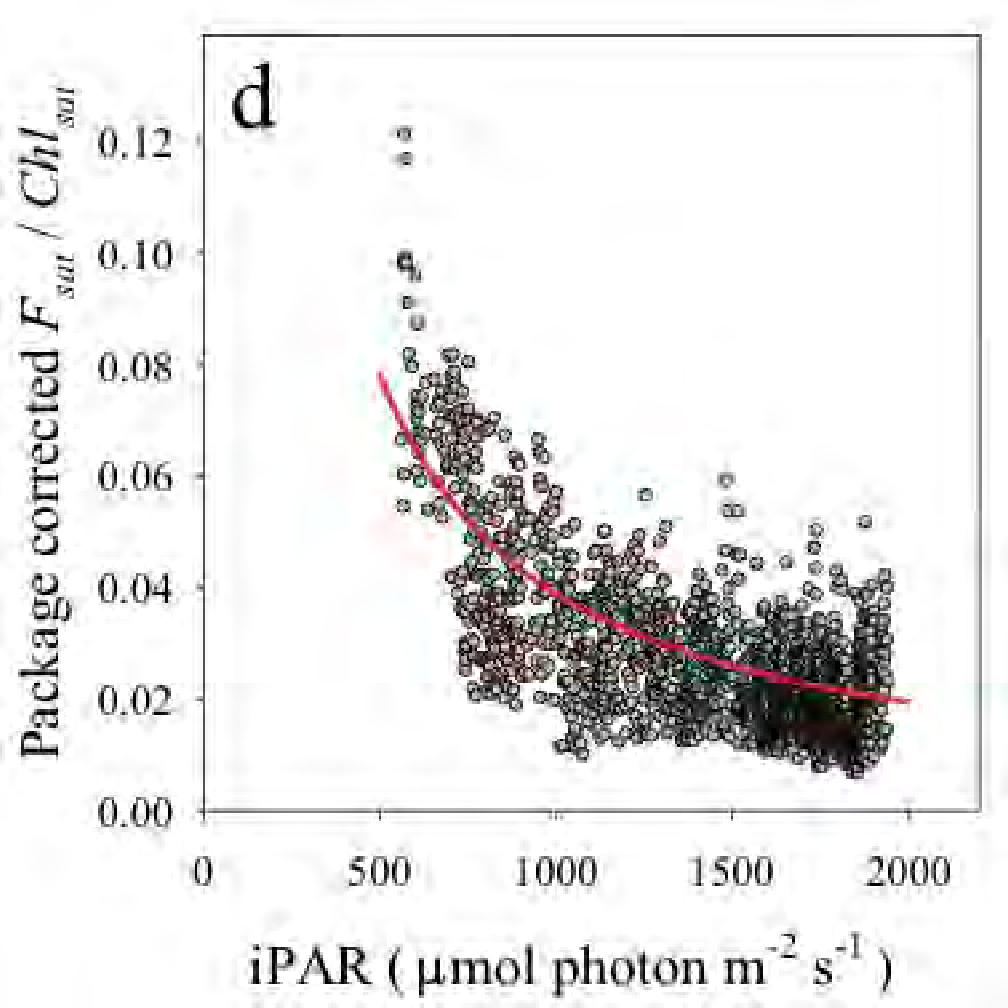


nFLH is the fluorescence line height on nLw:

$$nFLH \approx \frac{L_{uf}}{\mathring{E}_{PAR}} \mu \varphi_f \times a_f \times Q_a^* \frac{1}{a_f + K_{dPAR}}$$

Correction for "average" effect of PAR.

$\sim\varphi_f$



$\mu\ iPAR^{-1}$

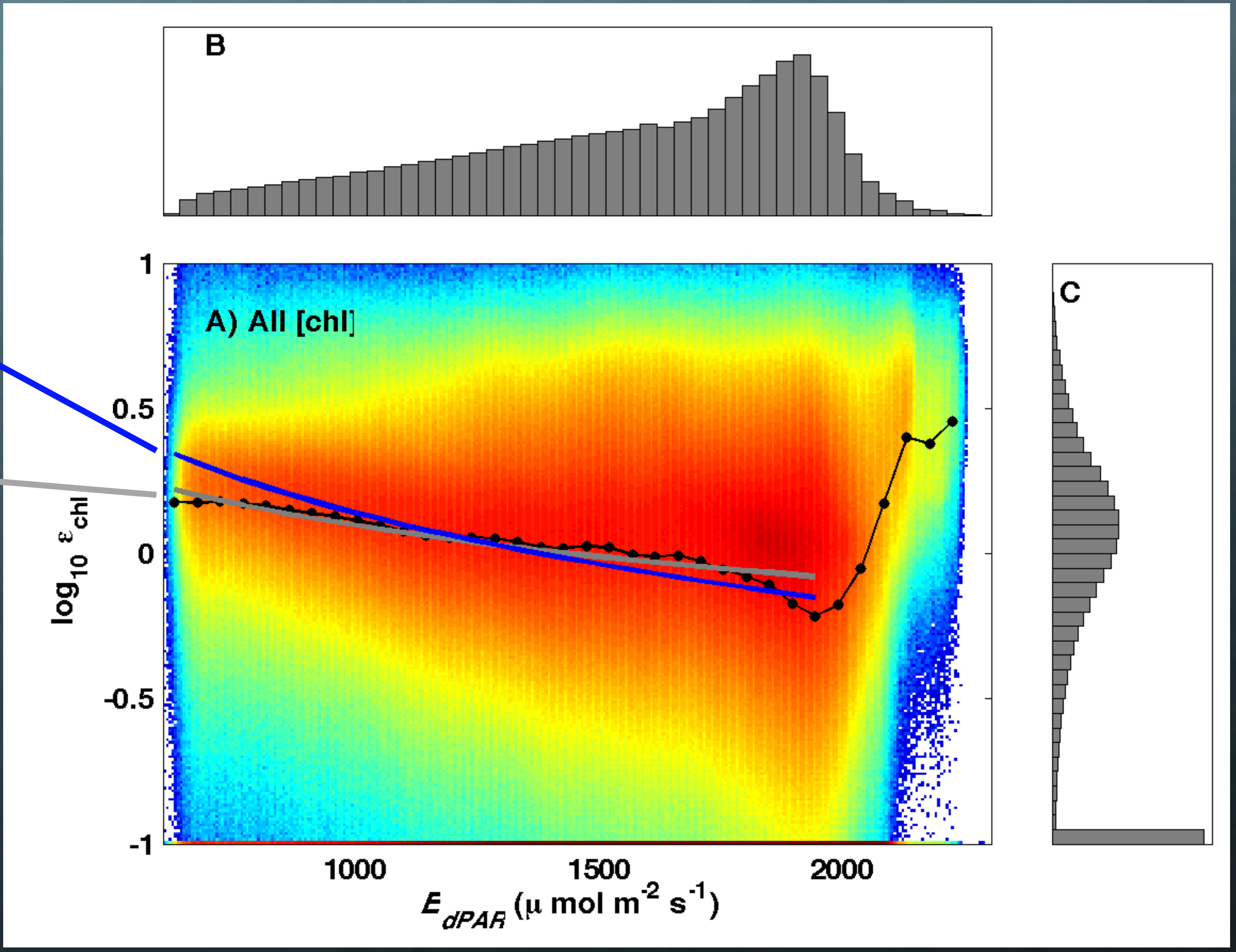
Figure from: Behrenfeld, M J, T K Westberry, E S Boss, R T O'Malley, D A Siegel, J D Wiggert, B A Franz, *and others.* "Satellite-Detected Fluorescence Reveals Global Physiology of Ocean Phytoplankton." *Biogeosciences* 6 (2009): 779-794

Effect of irradiance

Behrenfeld et al. 2009 $(E_{dPAR})^{-1}$

Best fit to median points

$$e_{chl} = \frac{nFLH}{\hat{y}_{median}}$$

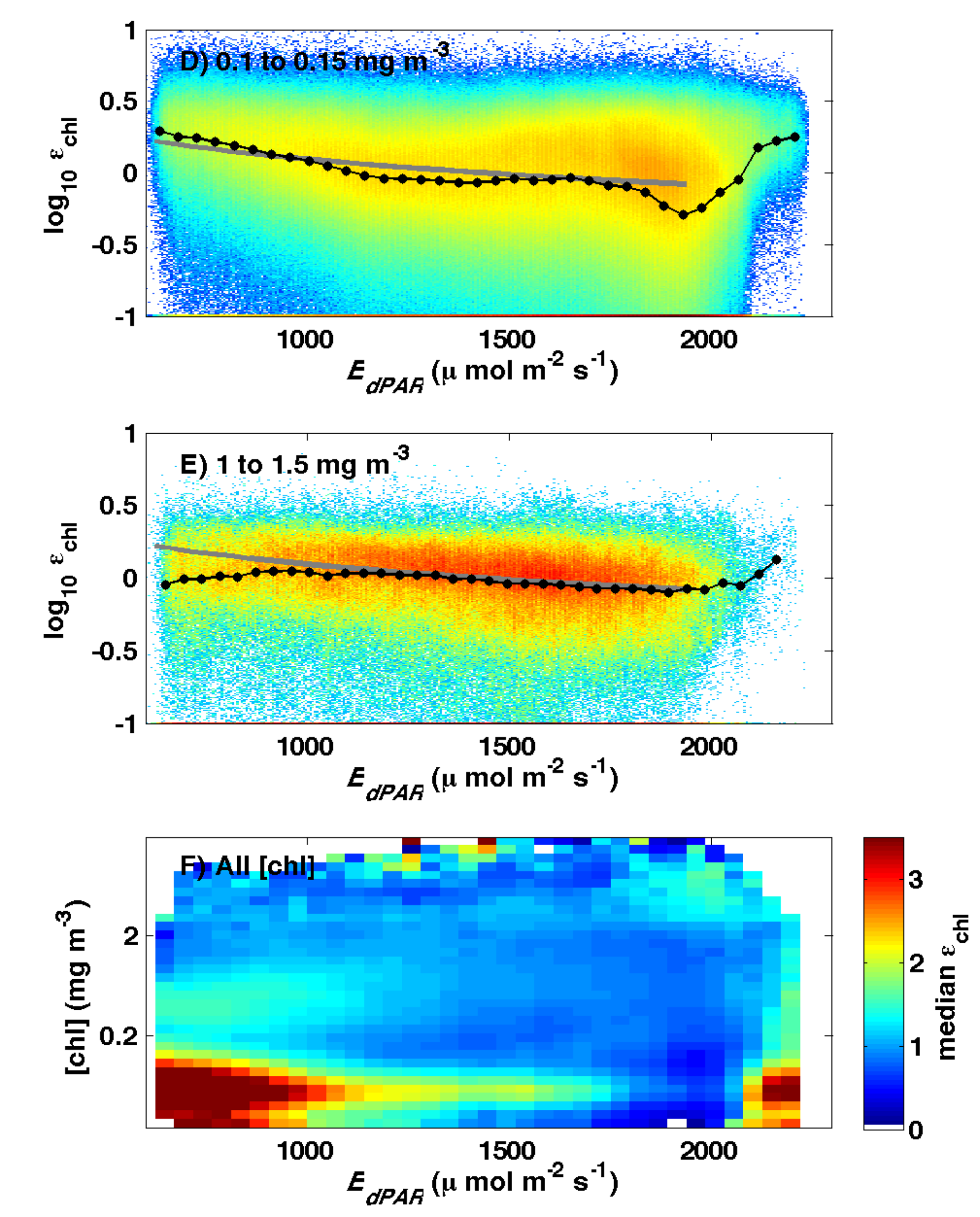


Further dependence on chlorophyll

$$e_{chl} = \frac{nFLH}{\hat{y}_{median}}$$

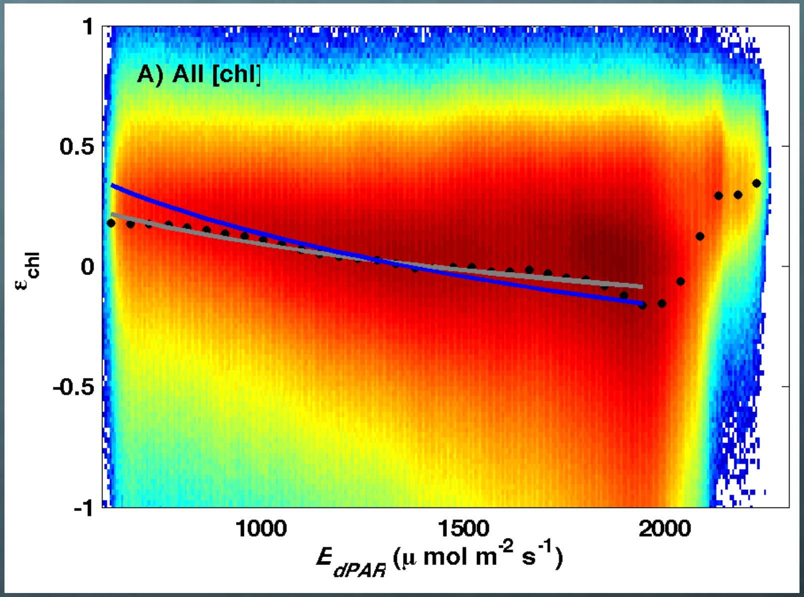
Median trends vary with chlorophyll concentration

We can represent those trends for all [chl] with a “median surface ”.

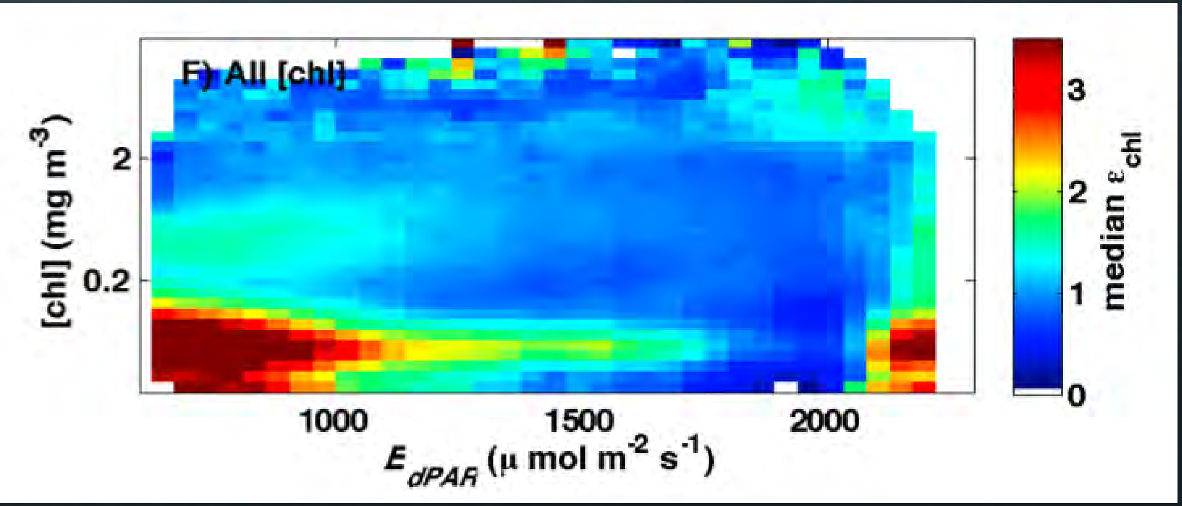


One step further...

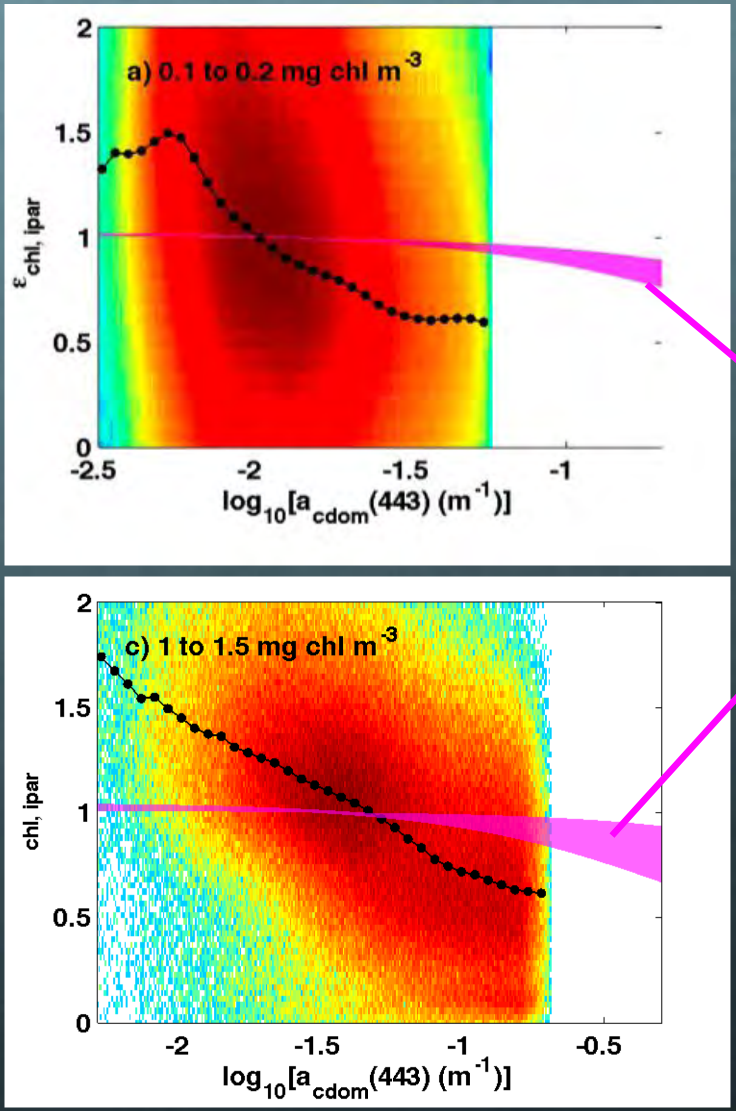
Lets divide the results from the previous graph...



by the « median surface »



…and plot the results as a function of CDOM absorption

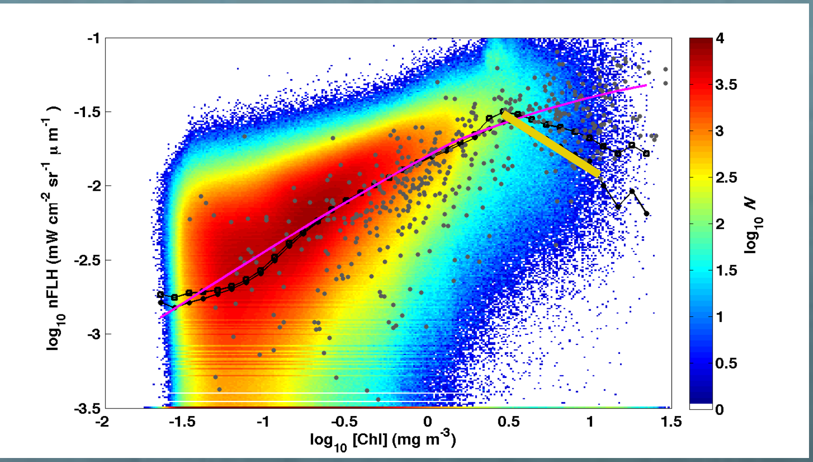


Theoretical "domain" if the attenuation of irradiance is the CDOM's only effect on chlorophyll fluorescence algorithms

<u>CDOM is not only causing an increased attenuation of irradiance</u>

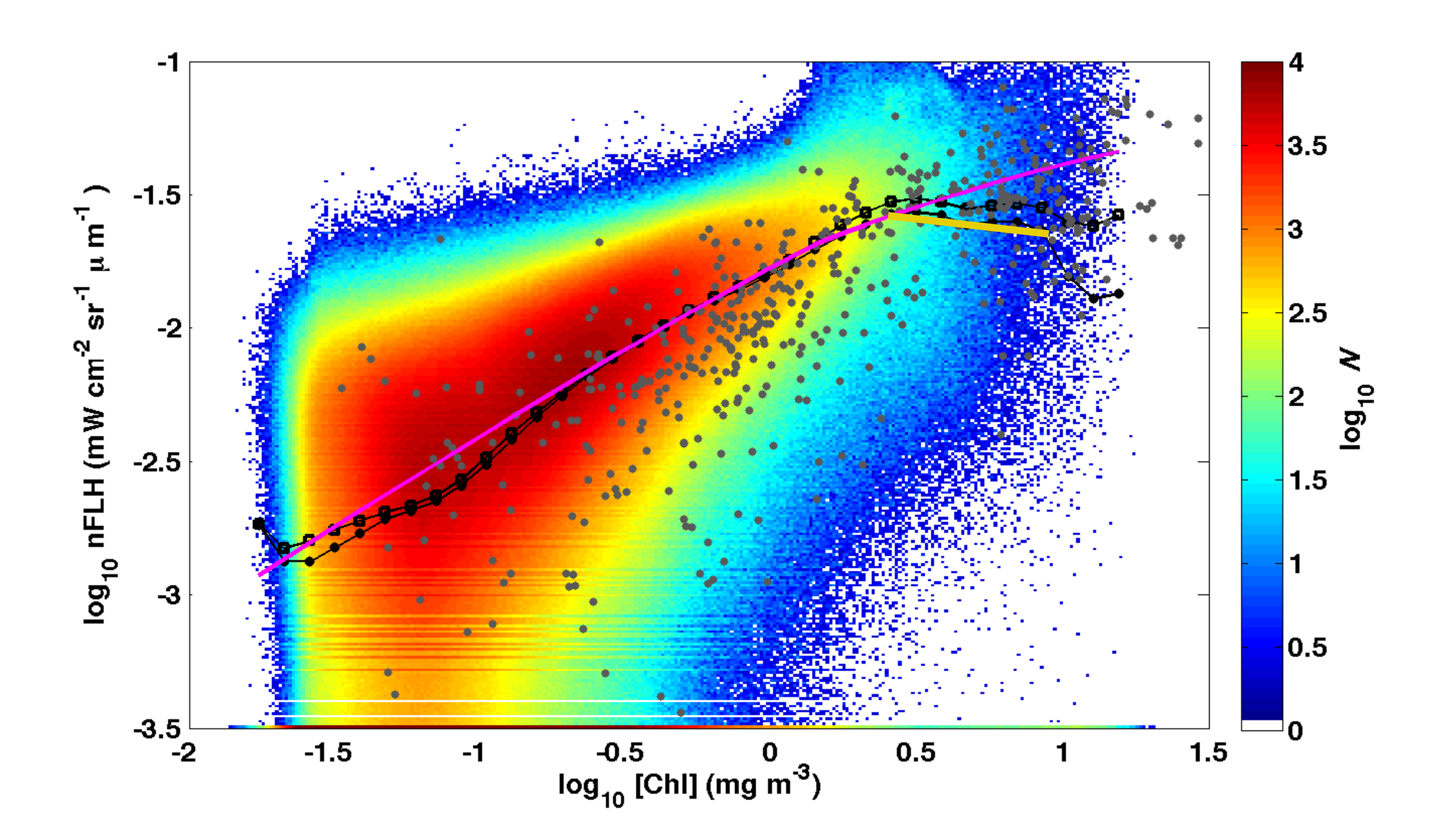
Most likely it is causing a bias in the estimates of chlorophyll - OC2M is biased by CDOM no surprise there!

What happens if we correct OC2M for CDOM using the Φ-correction?



Before (MARD=0.887)

After (MARD=0.815)

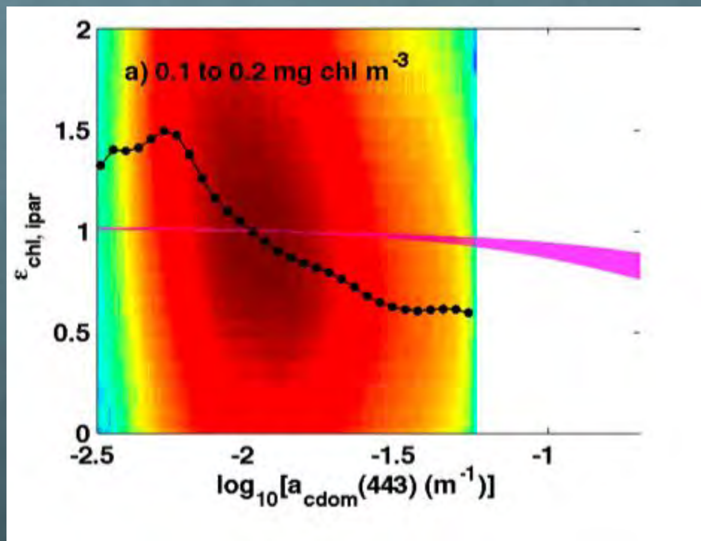


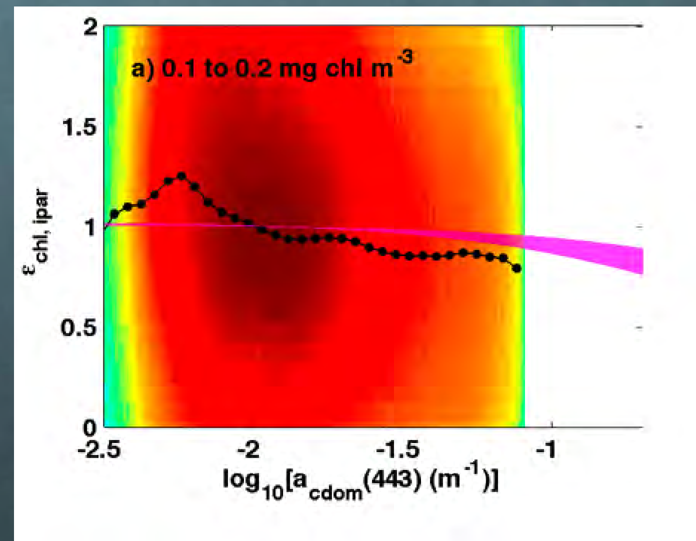
Effect of CDOM

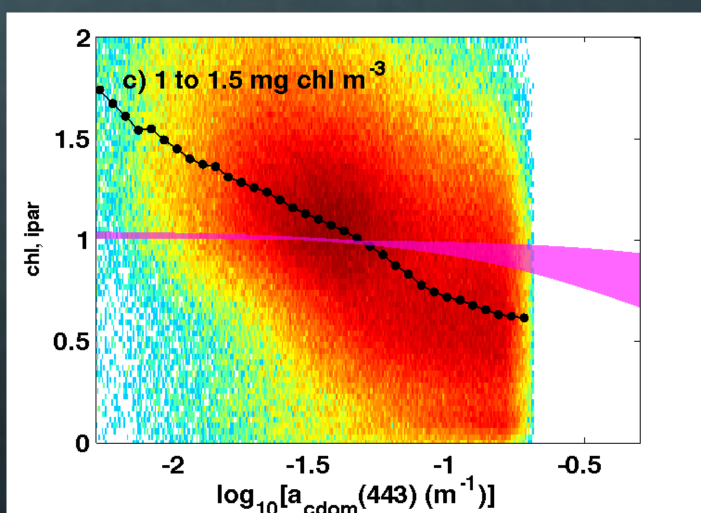
(Φ-corrected OC2M)

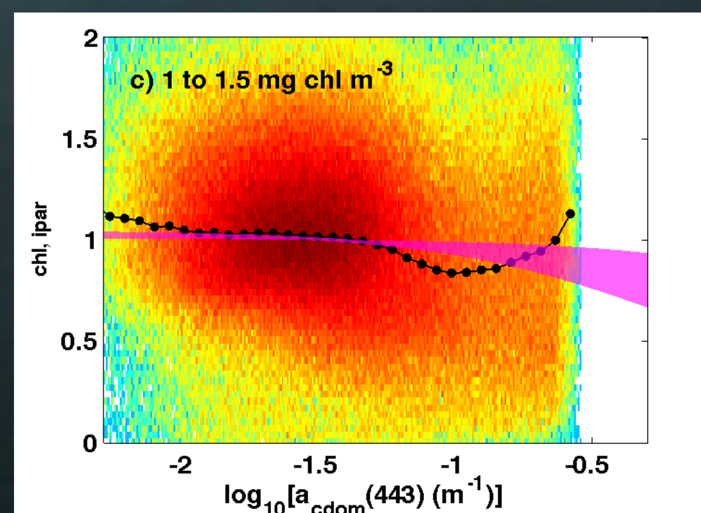
Before

After





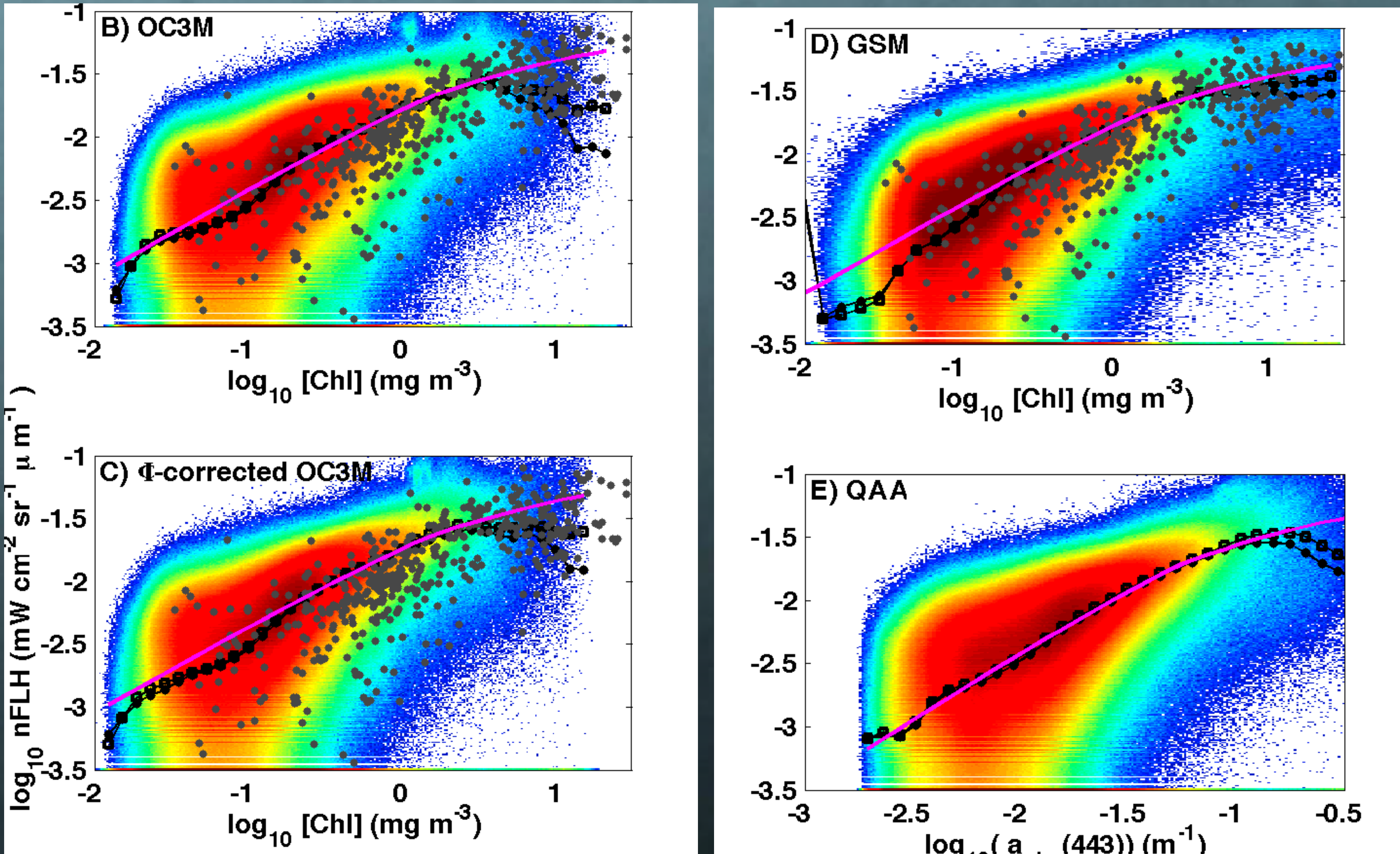




Other algorithms

MARD=0.826

MARD=0.792

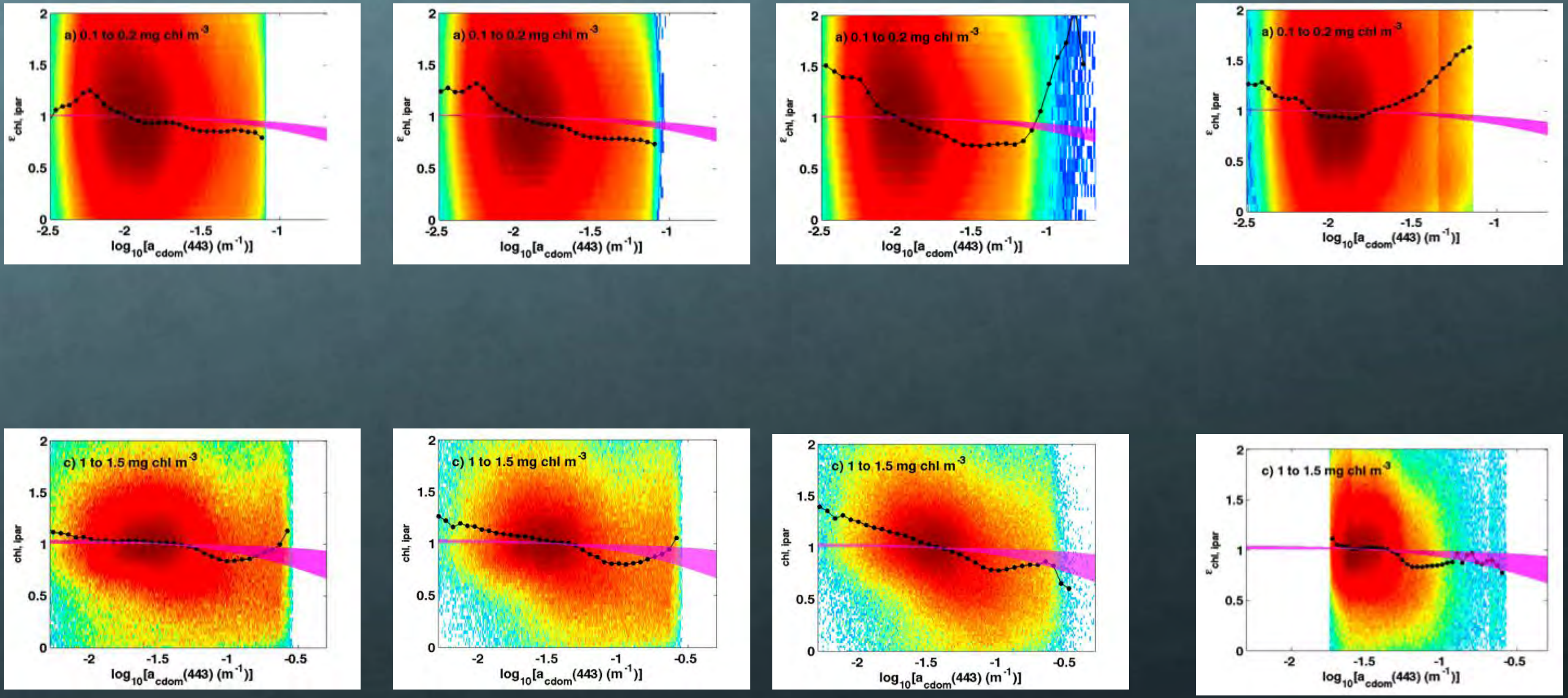


MARD=0.808

MARD=0.889

CDOM is a different story

Φ corrected –OC2M   Φ corrected –OC3M   GSM   QAA



Summing up so far…

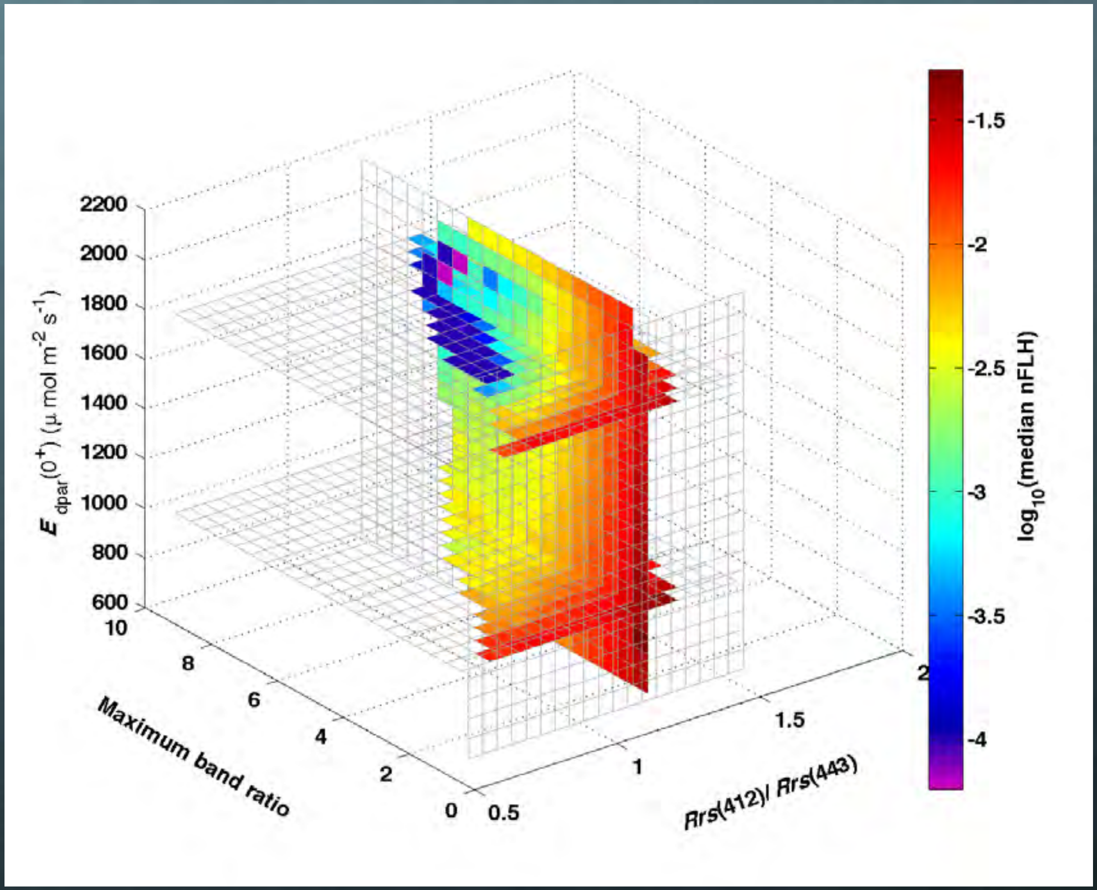
E_{dPAR} has a significant effect of *nFLH* which depends on the trophic level.

Φ-correction allows the best retrieval of CDOM trends and improves chl empirical algorithms significantly.

GSM performs very well for chl, less well for CDOM.

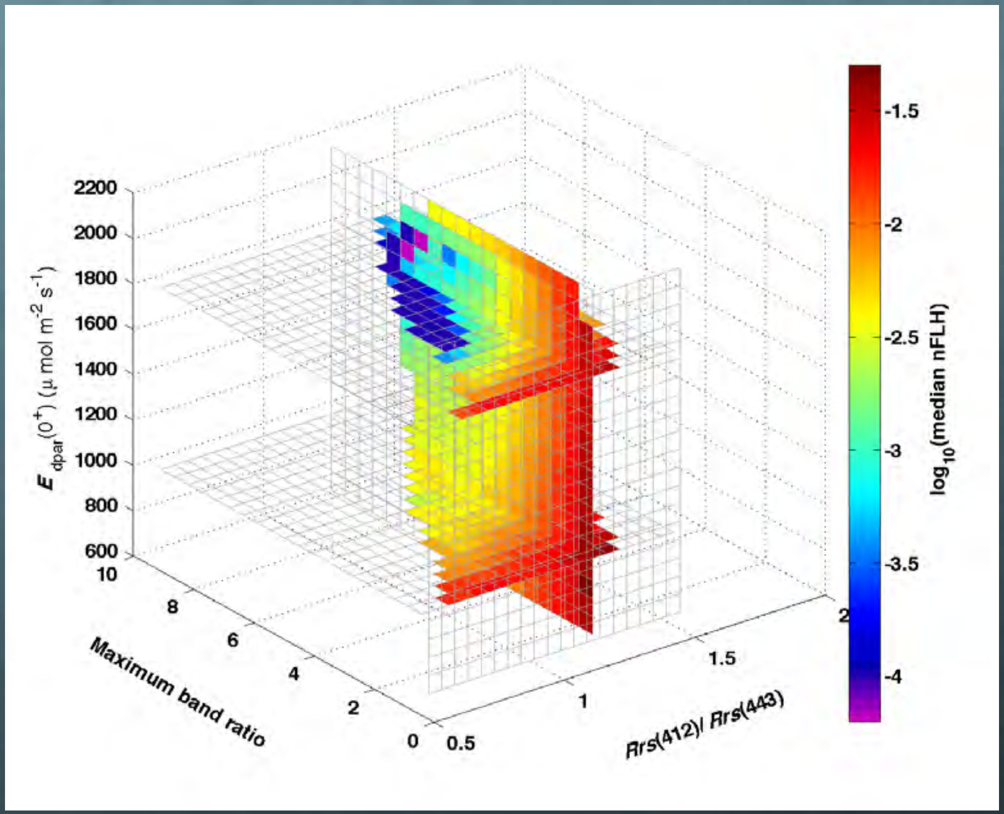
New algorithm for the quantum yield of fluorescence.

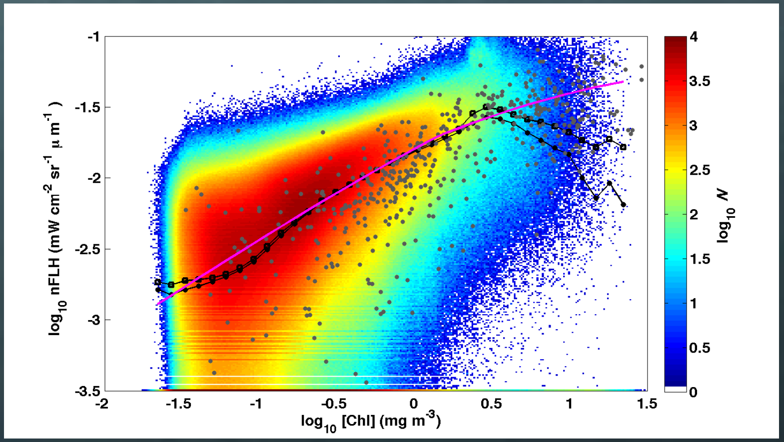
Objective: Removing the variability in nFLH arising from phytoplankton absorption, CDOM absorption and E_{dPAR} to observe variability caused by other factors.



Brown, C A, et al. "The Origin and Global Distribution of Second Order Variability in Satellite Ocean Color and Its Potential Applications to Algorithm Development." *Remote Sensing of Environment (2008): doi:10.1016/j.rse.2008.06.008*

Morel, A, and B Gentili. "A Simple Band Ratio Technique to Quantify the Colored Dissolved and Detrital Organic Material From Ocean Color Remotely Sensed Data." *Remote Sensing of Environment 113, no. 5 (2009): doi:10.1029/2008JC004803*





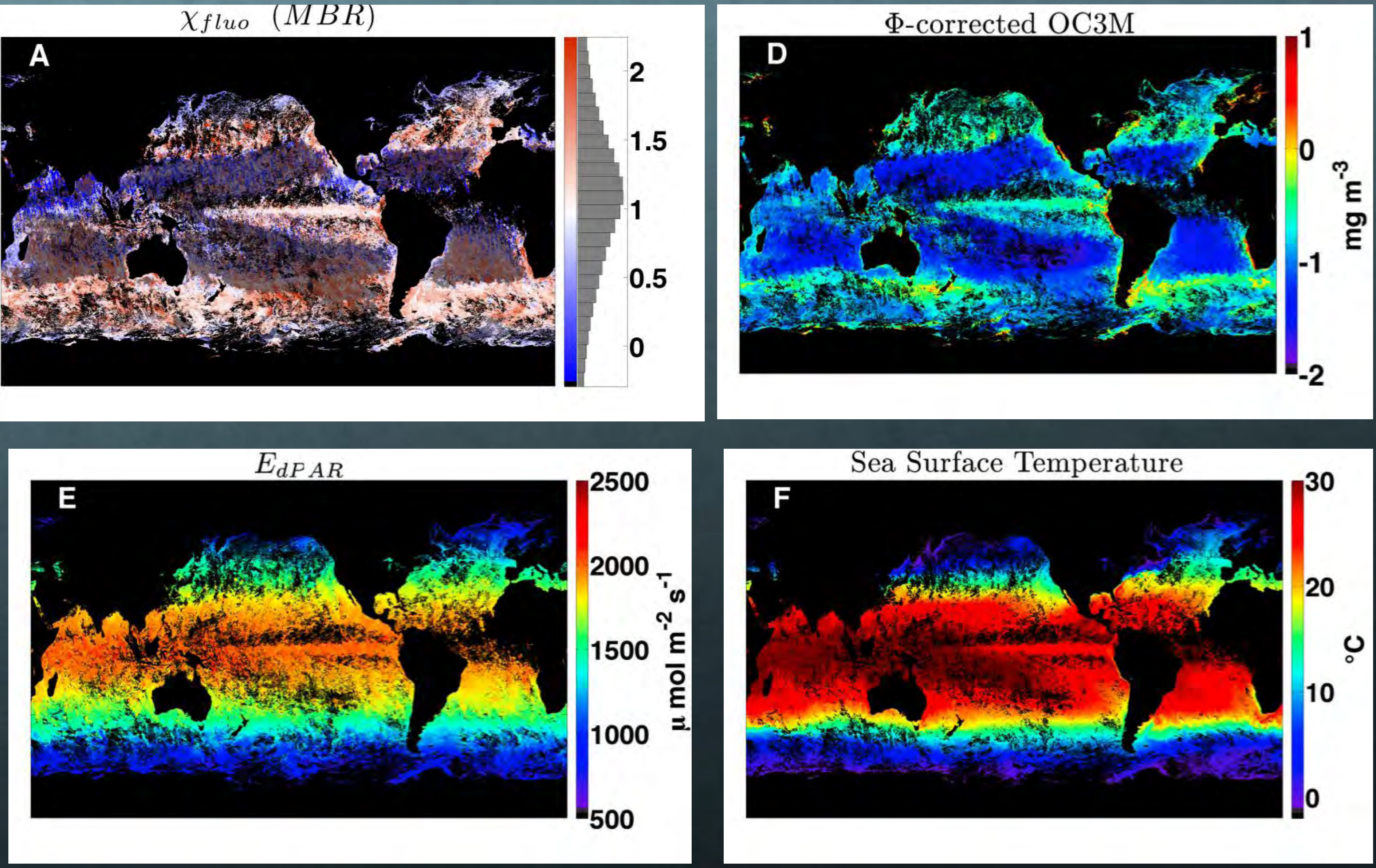
$$nFLH \approx \frac{L_{uf}}{\mathring{E}_{PAR}} \propto \varphi_f(\mathring{E}_{PAR}, chl) \cdot a_{\varphi} \cdot Q_a^* \frac{1}{a_f + K_{dPAR}}$$

The LUT "replaces" the magenta lines in current algorithms

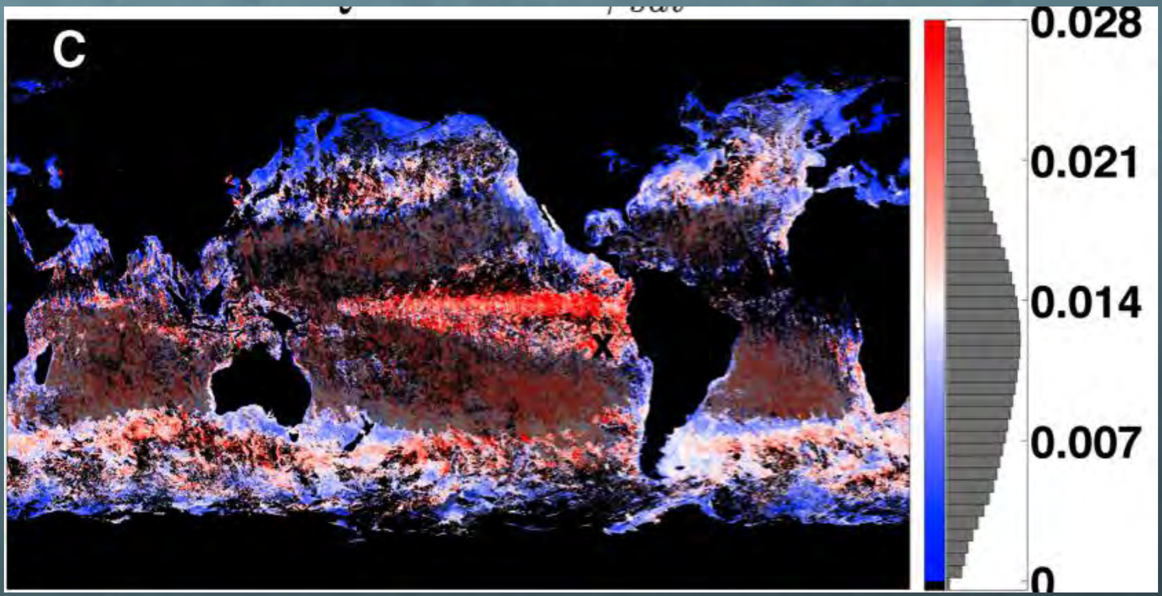
The χ_{fluo} index

$$\chi_{fluo} = \frac{FLH_{nLw}}{FLH_{LUT}}$$

Composite March 2007

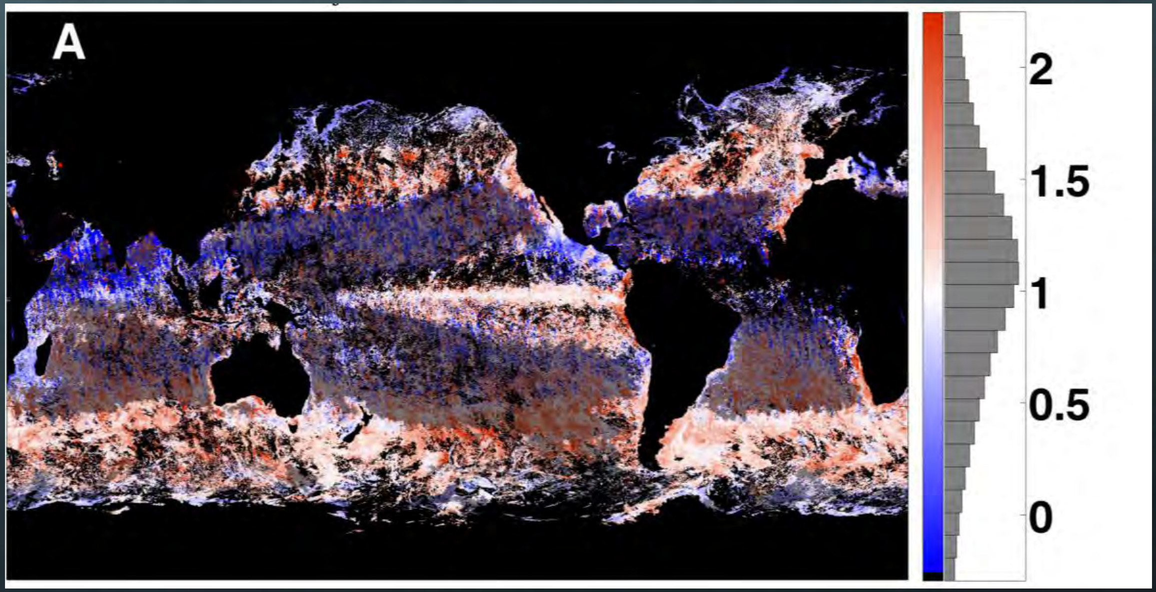


Algorithms comparison (March 2007)



Behrenfeld et al. 2009,(Φ_{sat}; equation A-12)

$$\phi_f^{app} = 0.68 \cdot 1.19 \cdot \frac{FLH_{nLw}}{Chl^{0.684}}$$



C_{fluo}

The new algorithm - Conclusions

Upside:

- Accounts for most of the variability in ocean color affecting *nFLH* that is not due to physiology or species composition (globally).
- Easy to tune the LUT for regional application; no need to know in situ optical properties.
- Independent of absolute calibration of the satellite (as long as it is stable).

Downside:

- The χ_{fluo} index provides only relative values of the quantum yield.

Thank you

Where do we go now?

Enhanced abilities to interpret Sun-induced fluorescence fields observed from space could provide unprecedented information about phytoplankton physiology at global scales.

- **The four testable hypotheses highlighted before provide good ground for future work.**
  - **Nutrient enrichment experiments coupled with measurements of Sun-induced fluorescence along (well chosen) transects could provide strong evidence into the nutrient-iron limitation hypothesis.**
  - **These experiments complemented with species composition (HPLC, flowcytometry) and average growth irradiance within the mixed layer should help identify the variable that explains the most variance.**
  - **Natural and anthropogenic iron enrichment areas are being studied at the moment and may help confirm the iron stress hypothesis.**
  - **The proposed algorithm just presented should reduce biases in current algorithms**