Update on IOCCG Working Group:

~~Ocean Colour Applications for Biogeochemical, Ecosystem and Climate Modeling~~

~~The Role of Ocean Colour in Biogeochemical, Ecosystem and Climate Modelling~~

Synergy between ocean colour and biogeochemical/ecosystem models

Stephanie Dutkiewicz and WG members (Mar 2019)

Update on IOCCG Working Group:

Synergy between ocean colour and biogeochemical/ecosystem models

NOTE: In this report, the word "model" refers to process-based three-dimensional biogeochemical/ecosystem computer models at large regional or global scales.

Update on IOCCG Working Group: **Synergy between ocean colour and biogeochemical/ecosystem models**

NOTE: In this report, the word "model" refers to process-based three-dimensional biogeochemical/ecosystem computer models at large regional or global scales.

"All models are wrong, but some models are useful"

George Box, 1976

Time Line:

July 2015:	WG approved
Feb 2016:	**Kick-Off Meeting (Ocean Sciences, New Orleans)– 2 days**
Jul 2016:	**MEAP-TT meeting (California)** – ch 6
Sep 2016:	**CLEO meeting (Rome)** – ch 4
Dec 2016:	Outline all chapters (except 5)
26 Feb 2017:	**WG meeting (ASLO, Hawaii) – 1 day**
3 Mar 2017:	**ASLO session (Hawaii)**
Apr 2017:	**EGU session (Vienna)**
May 2017-Feb 2018:	multiple internet meetings
Feb 2018:	**WG meeting (Ocean Sciences, Portland) – lunch**
Mar 2018-Sep 2018:	multiple internet meetings
2-3 Oct 2018:	**WG meeting (Boston) – 2 days**
Oct 2018-Mar 2019:	full draft completion, several internet meetings

<u>Full Draft of Report</u>

Editor: Stephanie Dutkiewicz

Working Group: Mark Baird, Fei Chai, Stefano Ciavatta, Stephanie Dutkiewicz, Marion Gehlen, Stephanie Henson, Anna Hickman, Cecile Rousseaux, Charles Stock, Jerry Wiggert

Contributions from: Mark Baird, Fei Chai, Stefano Ciavatta, Stephanie Dutkiewicz, Chris Edwards, Hayley Evers-King, Marjy Friedrichs, Sergey Frolov, Marion Gehlen, Stephanie Henson, Anna Hickman, Amir Ibrahim, Emlyn Jones, Daniel Kaufman, Frédéric Mélin, Barbara Muhling, Cecile Rousseaux, Igor Shulman, Charles Stock, Jeremy Werdell, Jerry Wiggert

Reviewers (external to the working group): Emmanuel Boss, John Dunne, Laura Lorenzoni, Xiao Liu, Tim Malthus, Galen McKinley, Matt Oliver, Cara Wilson

Chapter 1: Bridging Satellite Ocean Colour Remote Sensing and Biogeochemical/Ecosystem Modelling

Chapter 2: Ocean Colour Remote Sensing Overview

Chapter 3: Biogeochemical and ecosystem models: What are they and how can they be used?

Chapter 4: The (mis)match between biogeochemical/ecosystem model variables and ocean colour products

Chapter 5: Ocean Colour for Model Skill Assessment

Chapter 6: Assimilation of Ocean Colour

Chapter 7: Synergistic use of ocean colour data and models to understand marine biogeochemical processes

Chapter 8: Using Models to Inform Ocean Colour Science

Chapter 9: Summary and Recommendations

Appendix 1: Table of ocean colour notation, acronymns, and sensors
Appendix 2: Table of satellite imagery terminology
Appendix 3: Table of model terminology and acronyms

Chapter 1: Bridging Satellite Ocean Colour Remote Sensing and Biogeochemical/Ecosystem Modelling

Authors: Stephanie Dutkiewicz, Mark Baird, Stefano Ciavatta, Stephanie Henson, Anna Hickman, Cecile Rousseaux, Charles Stock

Chapter 2: Ocean Colour Remote Sensing Overview

Authors: Colleen Mouw, Cecile Rousseaux, Frédéric Mélin, Hayley Evers-King, Amir Ibrahim, Jeremy Werdell

Reviewers: Anna Hickman, Tim Malthus

2.1 What does a satellite radiometer "see"?
2.2. Historical and Current Instruments
2.3. Imagery Products
2.4. Uncertainty
2.5. Future Capability
2.6. Recommendations

In revision after second round reviews

Chapter 2: **Ocean Colour Remote Sensing Overview**

Authors: Colleen Mouw, Cecile Rousseaux, Frédéric Mélin, Hayley Evers-King, Amir Ibrahim, Jeremy Werdell

Reviewers: Anna Hickman, Tim Malthus

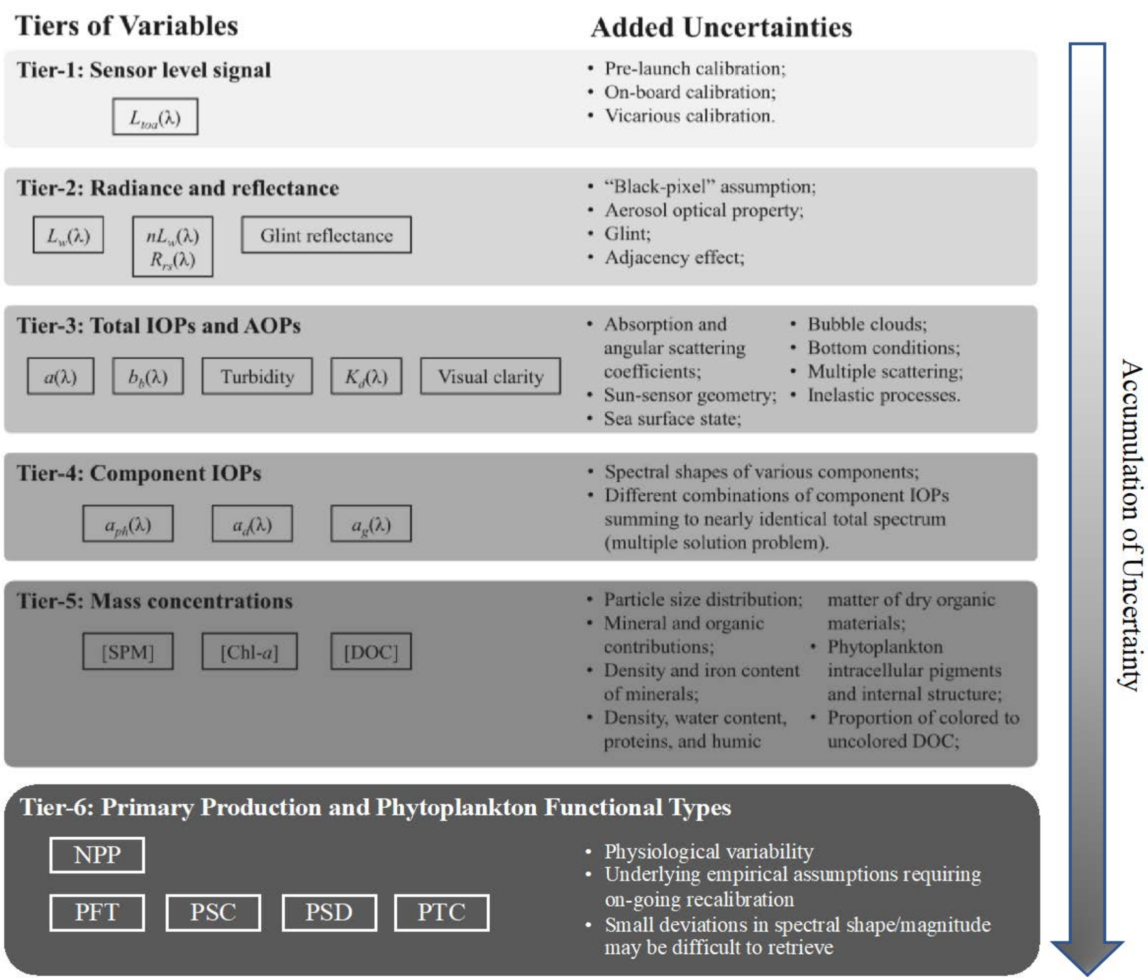

Figure 2.8. *Tiers of satellite-derived products and associated uncertainties introduced at each tier. The list of products is representative, but not exhaustive. Adapted from Zheng and DiGiacomo (2017).*

Authors: Colleen Mouw, Cecile Rousseaux, Frédéric Mélin, Hayley Evers-King, Amir Ibrahim, Jeremy Werdell
Reviewers: Anna Hickman, Tim Malthus

Table 2.3. *Imagery Online Access*
Note: IOCCG has mission specific data access links at: http://ioccg.org/resources/data/

Agency	Data Distribution	
NASA	Ocean Colour Web	https://oceancolour.gsfc.nasa.gov/
	Ocean Productivity	https://www.science.oregonstate.edu/ocean.productivity/
NOAA	Comprehensive Large-Array Data Stewardship System (CLASS)	https://www.class.ncdc.noaa.gov
EUMETSAT	EUMETSAT broadcast delivery system (EUMETCast)	https://www.eumetsat.int/website/home/Data/DataDelivery/EUMETCast/
EUMETSAT	EUMETSAT Data Centre	https://www.eumetsat.int/website/home/Data/DataDelivery/EUMETSATDataCentre
EUMETSAT and ESA	Copernicus Online Data Access (CODA) and SciHub	https://coda.eumetsat.int https://scihub.copernicus.eu/
European Commission	Copernicus Marine Environmental Monitoring Service	http://marine.copernicus.eu/
ESA and PML	Ocean Colour – Climate Change Initiative (OC-CCI)	https://www.oceancolour.org/
ACRI-ST	GlobColour	http://globcolour.info/

Chapter 2: Ocean Colour Remote Sensing Overview

Authors: Colleen Mouw, Cecile Rousseaux, Frédéric Mélin, Hayley Evers-King, Amir Ibrahim, Jeremy Werdell

Reviewers: Anna Hickman, Tim Malthus

Summary and Recommendations:

- Product selection
- Uncertainties

- Provide greater transparency on the products through more documentation.
- Provide additional information on data product uncertainties.

- Expand merged products to not only merge products in time, but also in space

- Improve the ease of access of the imagery through the use of Unidata's Thematic Real-time Environmental Distributed Data Services (THREDDS)
- Encourage greater sharing of community-derived custom data products through open data principles and services.
- Develop ocean colour methods and algorithms that employ additional hydrographic and biogeophysical information on environmental conditions.

<u>Chapter 3:</u> Biogeochemical and ecosystem models: What are they and how can they be used?

<u>Authors</u>: Stephanie Dutkiewicz, Cecile Rousseaux, Stefano Ciavatta, Charles Stock, Mark Baird, Fei Chai, Barbara Muhling, Marion Gehlen

<u>Reviewers</u>: Colleen Mouw, Cara Wilson, Laura Lorenzoni

3.1 Introducing the theory, practicalities of implementation and uses of biogeochemical models

3.2. Concepts, Equations, Code and Computers

3.3 Treatment of Light

3.4 Different models for different Applications

3.5 Model and Model Output Selection

In revision after second round reviews

<u>Chapter 3:</u> Biogeochemical and ecosystem models: What are they and how can they be used?

<u>Authors</u>: Stephanie Dutkiewicz, Cecile Rousseaux, Stefano Ciavatta, Charles Stock, Mark Baird, Fei Chai, Barbara Muhling, Marion Gehlen

<u>Reviewers</u>: Colleen Mouw, Cara Wilson, Laura Lorenzoni

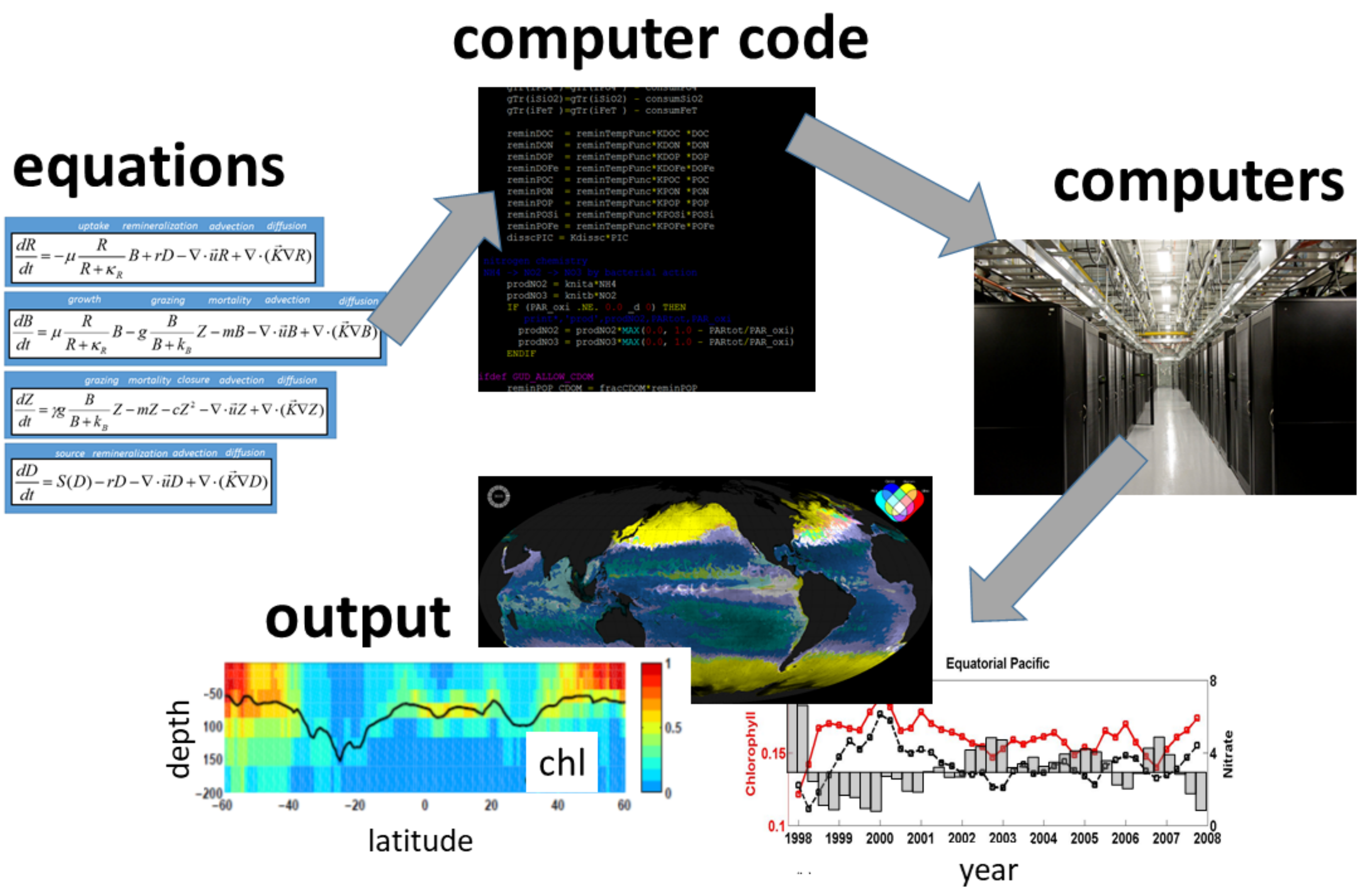

Figure 3.3: Schematic on developing and using a numerical model.

<u>Chapter 3:</u> Biogeochemical and ecosystem models: What are they and how can they be used?

<u>Authors</u>: Stephanie Dutkiewicz, Cecile Rousseaux, Stefano Ciavatta, Charles Stock, Mark Baird, Fei Chai, Barbara Muhling, Marion Gehlen

<u>Reviewers</u>: Colleen Mouw, Cara Wilson, Laura Lorenzoni

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In revision after second round reviews

<u>Chapter 4:</u> The (mis)match between biogeochemical/ecosystem model variables and ocean colour products

<u>Authors:</u> Stephanie Dutkiewicz, Anna Hickman, Colleen Mouw, Cecile Rousseaux, Stefano Ciavatta, Mark Baird, Charles Stock, Fei Chai

<u>Reviewers:</u> Stephanie Henson, Emmanuel Boss

4.1. Same Name, Different "Measurement"

4.1.1. Water Leaving Irradiance and Reflectance

4.1.2 Optical Properties

4.1.3. Chlorophyll-a

4.1.4 Carbon Pools

4.1.5. Phytoplankton Types/Groups

4.1.6. Primary Production

4.2. Temporal and spatial mis-match of model outputs and ocean colour products.

4.2.1. Temporal gaps in ocean colour measurements: "mean" and "climatology"

4.2.2. Matching in time

4.3 Summary and Recommendations

4.3.1. Questions to consider when comparing model and satellite output

4.3.2. Should we bring model output closer to ocean colour or ocean colour products closer to model outputs?

4.3.3. Recommendation

In revision after second round reviews

<u>Chapter 4:</u> The (mis)match between biogeochemical/ecosystem model variables and ocean colour products

<u>Authors:</u> Stephanie Dutkiewicz, Anna Hickman, Colleen Mouw, Cecile Rousseaux, Stefano Ciavatta, Mark Baird, Charles Stock, Fei Chai

<u>Reviewers:</u> Stephanie Henson, Emmanuel Boss

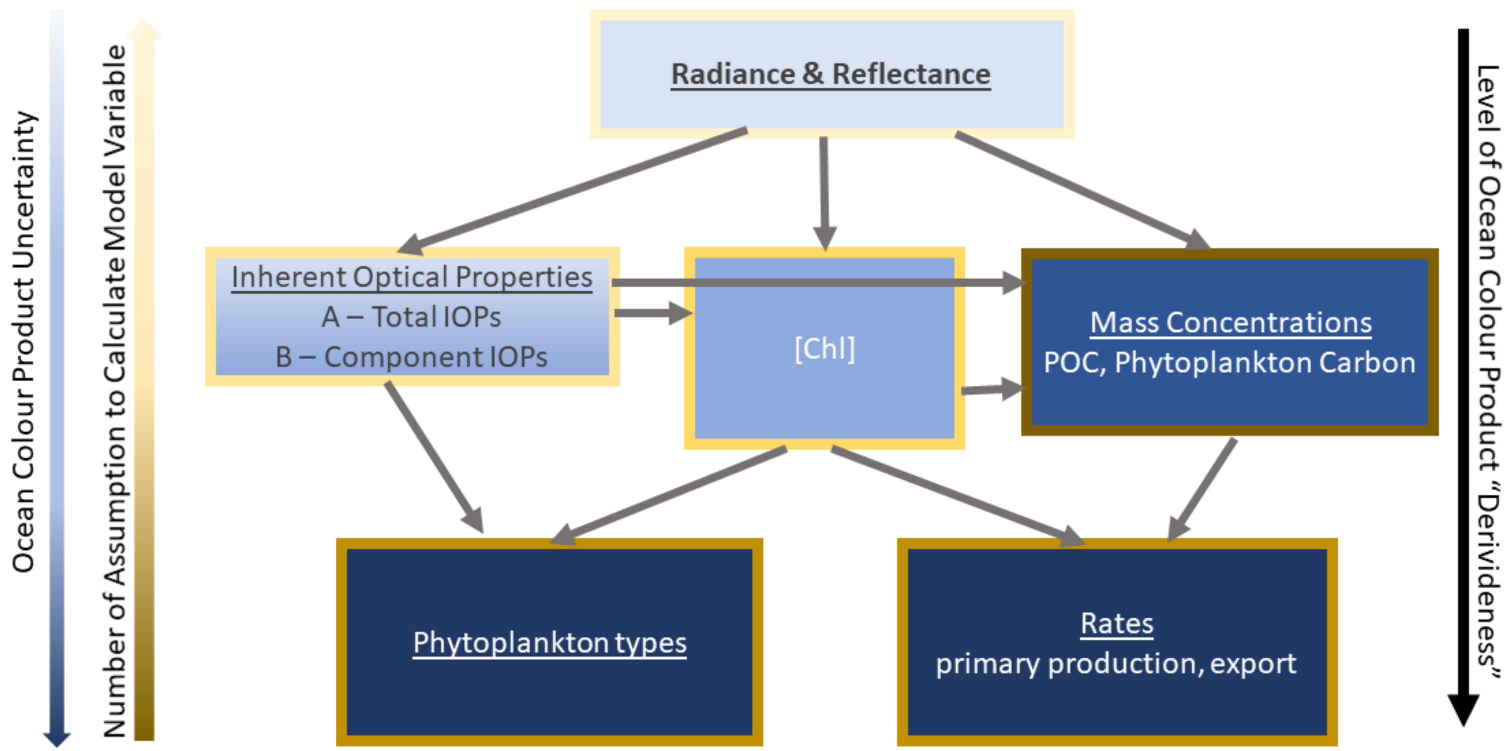

Figure 4.1. Schematic depicting uncertainties and level of "derivedness".

<u>Chapter 4:</u> The (mis)match between biogeochemical/ecosystem model variables and ocean colour products

<u>Authors:</u> Stephanie Dutkiewicz, Anna Hickman, Colleen Mouw, Cecile Rousseaux, Stefano Ciavatta, Mark Baird, Charles Stock, Fei Chai

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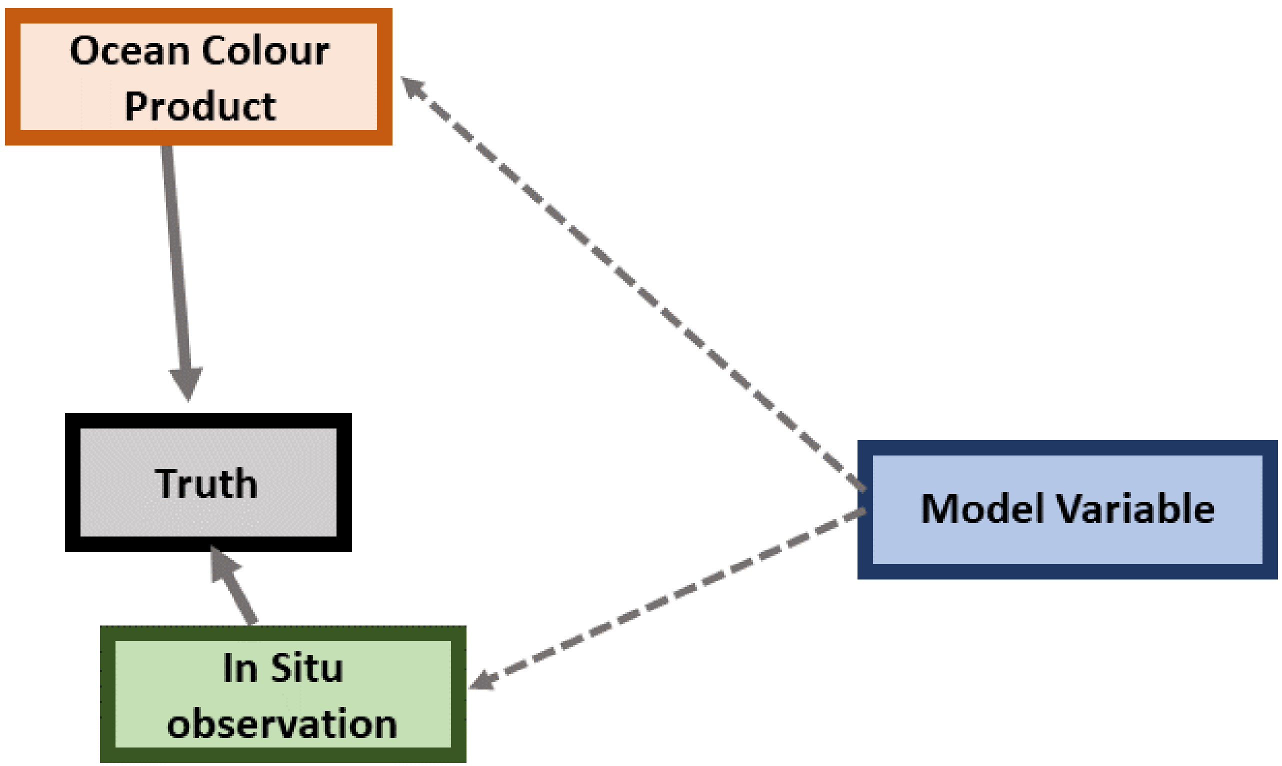

Fig 4.2. Schematic of uncertainties in in situ and ocean colour products.

Chapter 4: **The (mis)match between biogeochemical/ecosystem model variables and ocean colour products**

Authors: Stephanie Dutkiewicz, Anna Hickman, Colleen Mouw, Cecile Rousseaux, Stefano Ciavatta, Mark Baird, Charles Stock, Fei Chai

Reviewers: Stephanie Henson, Emmanuel Boss

4.1. Same Name, Different "Measurement"

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In revision after second round reviews

Chapter 4: **The (mis)match between biogeochemical/ecosystem model variables and ocean colour products**

Authors: Stephanie Dutkiewicz, Anna Hickman, Colleen Mouw, Cecile Rousseaux, Stefano Ciavatta, Mark Baird, Charles Stock, Fei Chai

Reviewers: Stephanie Henson, Emmanuel Boss

Summary and Recommendations:

Models, in situ observations and ocean colour products are different tools to help us understand the ecological and biogeochemical processes in the ocean. Integrated results will need a multi-way discussion.

- modellers should have better information about using satellite data and new approaches.
- agencies should examine and explore how additional information can be presented alongside satellite products to help modellers make informed choices and interpretations.
- Other ways to inform modelling community: e.g. this report

<u>Chapter 5:</u> Ocean Colour for Model Skill Assessment

<u>Authors:</u> Charles Stock, Stefano Ciavatta
<u>Reviewers:</u> Mark Baird, John Dunne, Xiao Liu

5.1. Introduction
5.2. Model skill assessment metrics
5.3. Ocean chlorophyll comparisons across scales
5.3.1: Regional biases in satellite chlorophyll measurements
5.3.2:* Challenges of *point-to-point comparisons in a heterogenous ocean
5.3.3: Making the space and time scales of skill assessments "fit to purpose"

5.4. Beyond chlorophyll: assessing skill against other satellite-derived ecosystem properties
5.5. Conclusions

In revision after second round reviews

Chapter 5: Ocean Colour for Model Skill Assessment
Authors: Charles Stock, Stefano Ciavatta
Reviewers: Mark Baird, John Dunne, Xiao Liu

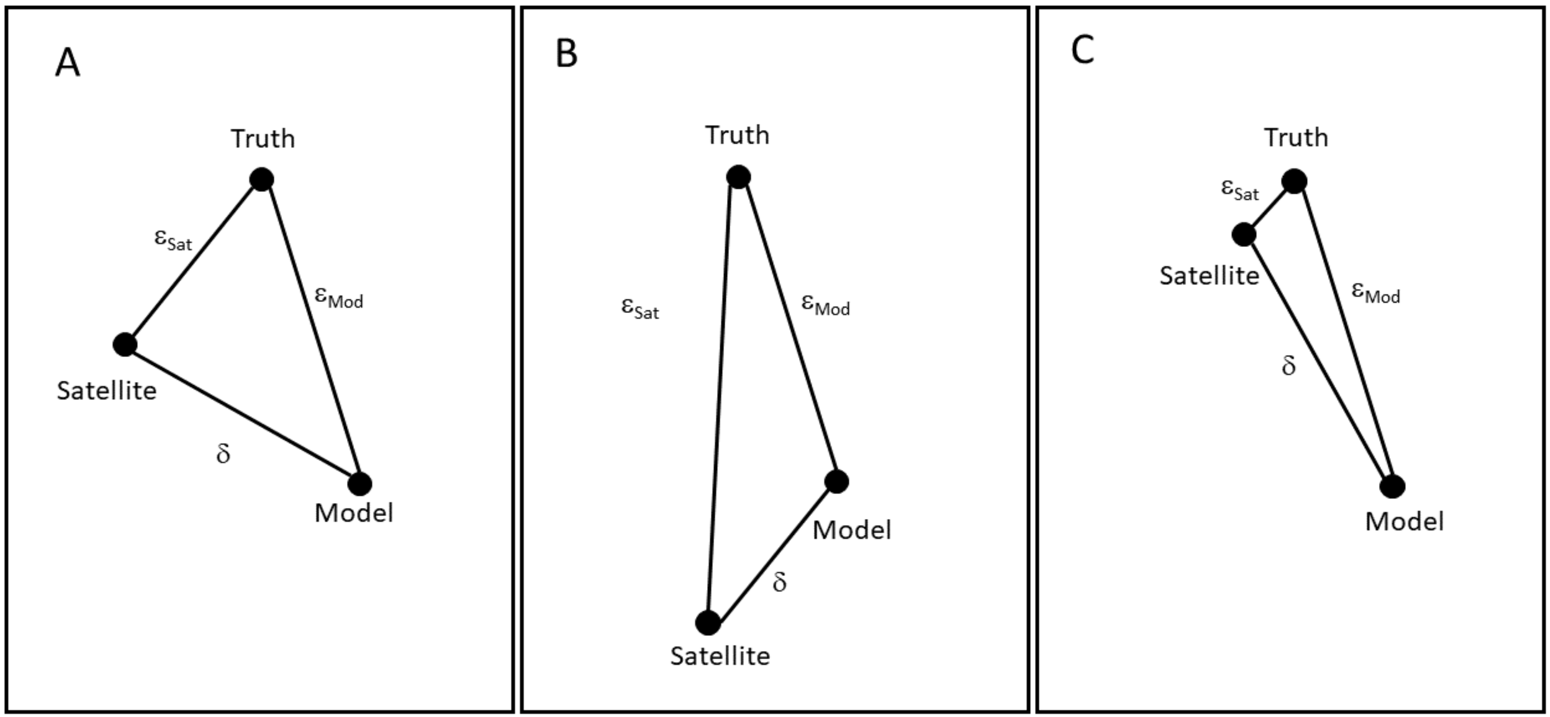

Figure 5.1: Truth, error and misfit in comparing ocean colour estimates and models (Following Lynch et al., (2009)).

Chapter 5: Ocean Colour for Model Skill Assessment

Authors: Charles Stock, Stefano Ciavatta

Reviewers: Mark Baird, John Dunne, Xiao Liu

Metric	Formula	Interpretation
Median absolute deviation (MAD)	$MAD = median\ (\lvert\delta\rvert)$	The dispersion of the model-satellite misfits
Robust bias (B*)	$B^* = median(\hat{y}) - median\ (y)$	The distance between model and satellite medians
Spearman's rank correlation coefficient (ρ)	$\rho = \frac{\frac{1}{n}\sum_{i=1}^{n}\left((\hat{y}_{r,i} - \bar{\hat{y}}_r)(y_{r,i} - \bar{y}_r)\right)}{\sigma_{\widehat{yr}}\sigma_{yr}}$	Normalized measure of monotonic consistency of relative spatiotemporal variations
Unbiased Median Absolute Deviation (MAD')	$MAD' = median(\lvert\delta - B^*\rvert)$	MAD after subtracting out the robust bias
Normalized interquartile range	$IQR^* = IQR_{\hat{y}}/IQR_y$	Ratio of variability in model to that of the comparison data

Table 5.2: Robust skill metrics used in comparing models with satellite data. In all cases, δ is the misfit between the model-based estimate (y) and the satellite-based estimate (y), and n is the number of comparison points. The interquartile ranges of the model and satellite data are indicated as $IQRy$ and $IQRy$, respectively. The ranked values of model and satellite data are indicated as yr and yr, and the standard deviation of the model and satellite data are indicated as σyr and σyr.

<u>Chapter 5:</u> Ocean Colour for Model Skill Assessment
<u>Authors:</u> Charles Stock, Stefano Ciavatta
<u>Reviewers:</u> Mark Baird, John Dunne, Xiao Liu

<u>Summary and Recommendations:</u>

- ocean colour measurements has played a crucial role in building confidence in marine ecosystem models: combination of spatial and temporal coverage
- challenges that still must be confronted by the modeling and ocean colour communities
- skill assessment metrics to be closely fit to the space and time scales of interest.
- the continued lengthening of the satellite time series will also enable more direct testing of climate change trends

Chapter 6: Assimilation of Ocean Colour

Authors: Mark Baird, Emlyn Jones, Stefano Ciavatta, Cecile Rousseaux, Marjy Friedrichs, Daniel Kaufman, Igor Shulman, Sergey Frolov, Chris Edwards

Reviewers: Charles Stock, ????

6.1. Basics of assimilation/Types of Assimilation Models:

6.1.1. Variational Methods

6.1.2. Sequential methods

6.1.3. Common Requirements of observational data sets

6.1.4. Parameter estimation

6.2 Role of ocean colour and model structural uncertainties

6.2.1. Model structure uncertainty

6.2.2. Ocean Colour data uncertainty

6.3. Examples Studies

6.3.1. Assimilating Chlorophyll

6.3.2. Assimilating remotely-sensed diffuse attenuation coefficient using a localized Ensemble Kalman Filter (EnKF)

6.3.3. Assimilating remote-sensing reflectance using a Deterministic Ensemble Kalman Filter (DEnKF)

6.3.4 Assimilating Phytoplankton Functional Type (PFTs) data

6.3.5. Assimilation of satellite derived bio-optical properties – impact on short-term model predictions

Seeking second reviewer

6.4. State estimates/Re-analysis

6.5. Available software that can be used for BGC data assimilation.

6.6. Recommendations

<u>Chapter 6:</u> Assimilation of Ocean Colour

<u>Authors</u>: Mark Baird, Emlyn Jones, Stefano Ciavatta, Cecile Rousseaux, Marjy Friedrichs, Daniel Kaufman, Igor Shulman, Sergey Frolov, Chris Edwards

<u>Reviewers</u>: Charles Stock, ????

<u>Case Studies:</u>

- Study region and model configuration.
- Data assimilation system.
- Skill improvement of the system.
- Lessons learnt

Chapter 6: Assimilation of Ocean Colour

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Authors: Mark Baird, Emlyn Jones, Stefano Ciavatta, Cecile Rousseaux, Marjy Friedrichs, Daniel Kaufman, Igor Shulman, Sergey Frolov, Chris Edwards
Reviewers: Charles Stock, ????

Summary and Recommendations:

- Data assimilation of ocean colour still new – need to continue method development
- Use of Argos float data to provide depth information will be important development

<u>Chapter 7:</u> Synergistic use of ocean colour data and models to understand marine biogeochemical processes

<u>Authors</u>: Stephanie Henson, Colleen Mouw, Cecile Rousseaux, Jerry Wiggert

<u>Reviewers</u>: Marion Gehlen, Matt Oliver

7.1 Use of hindcast simulations to explore processes that result in observed variability

Case Study 7.1.1: Elucidating the nutrient supply routes controlling primary production

Case study 7.1.2: Drivers of trends in phytoplankton community composition

Case study 7.1.3: Investigating the potential for iron limitation of primary production

7.2 Using hindcast models to extend satellite data into the recent past to explore decadal variability

Case Study 7.2.1: Exploring the response of the North Atlantic bloom to decadal variability

Case Study 7.2.2: Investigating the mechanisms of decadal variability in North Atlantic biomass

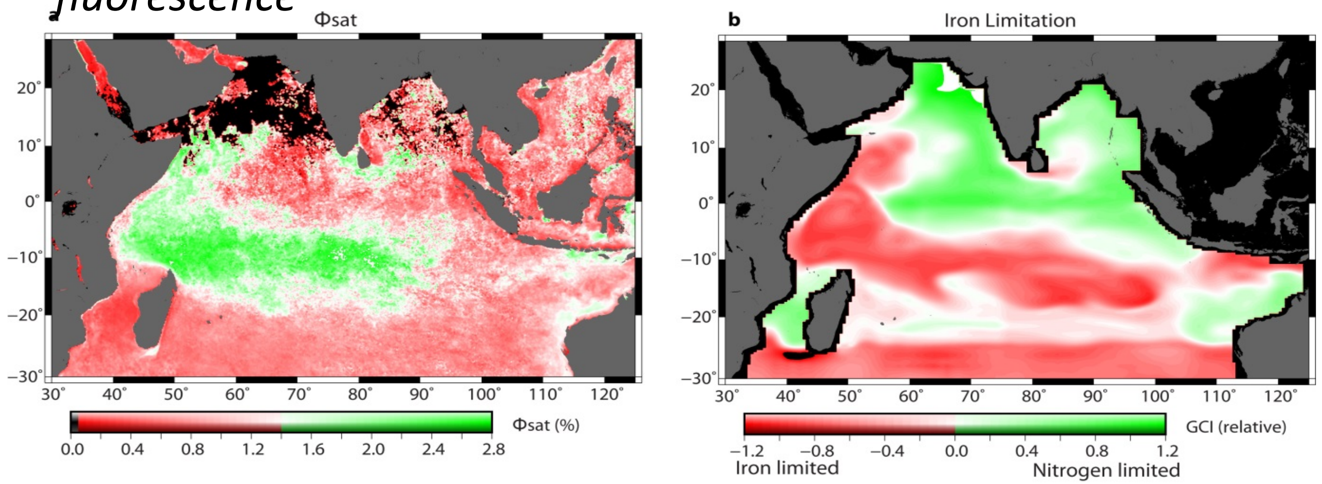
7.3 Caveats and Recommendations

Waiting second review

Case study 7.1.3: Investigating the potential for iron limitation of primary production

satellite-based quantum yield of fluorescence

model-based nutrient limitation



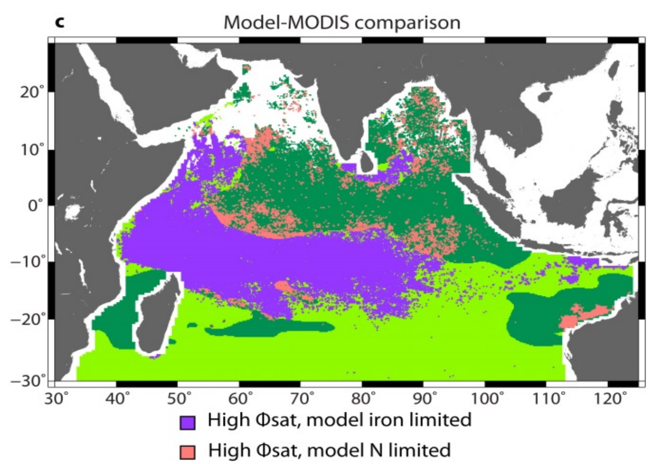


Figure 7.3: *(a) φ_{sat} and (b) model-based growth constraint index (GCI) (Wiggert et al., 2006) for boreal summer (June–August). (c) State-space comparison of φ_{sat} and GCI. (redrawn from Behrenfeld et al., 2009)*

Chapter 7: Synergistic use of ocean colour data and models to understand marine biogeochemical processes

Authors: Stephanie Henson, Colleen Mouw, Cecile Rousseaux, Jerry Wiggert
Reviewers: Marion Gehlen, Matt Oliver

Summary and Recommendations:

- Use of biogeochemical models in combination with satellite-derived ocean colour data provided information on the processes controlling observed phytoplankton variability

- Caveat: the model must be able to reproduce the observed variability
  models may miss some processes

- Recommend more such studies and collaborations:
  e.g. use model output to extend satellite data sub-surface.

Chapter 8: Using Models to Inform Ocean Colour Science

Authors: Stephanie Dutkiewicz, Stephanie Henson, Colleen Mouw, Cecile Rousseaux
Reviewers: Stefano Ciavatta, Anna Hickman, Galen McKinley

8.1 Exploring the consequences of missing data

Case Study 8.1.1: Effect of missing data on annual and monthly means

Case Study 8.1.2: How do gaps in satellite data affect phenology studies?

8.2 Models can be used to inform on ocean colour signals and products

Case Study 8.2.1. Contribution of phytoplankton functional types to ocean colour product uncertainty

Case Study 8.2.2. Exploring Uncertainty in the remotely sensed Chl product derived from limited in situ observations.

8.3 Application of climate models to help inform the ocean colour community on trend detection and attribution

Case Study 8.3.1: Informing detection of climate change trends in satellite ocean colour records

Case Study 8.3.2: Exploring the effect of data record gaps on trend detection

Case Study 8.3.3. Comparing trends in multiple components of the system

8.4. Models informing future ocean colour products and missions

8.5. Summary and Recommendations

In revision after second round reviews

Chapter 8: Using Models to Inform Ocean Colour Science
Authors: Stephanie Dutkiewicz, Stephanie Henson, Colleen Mouw, Cecile Rousseaux
Reviewers: Stefano Ciavatta, Anna Hickman, Galen McKinley

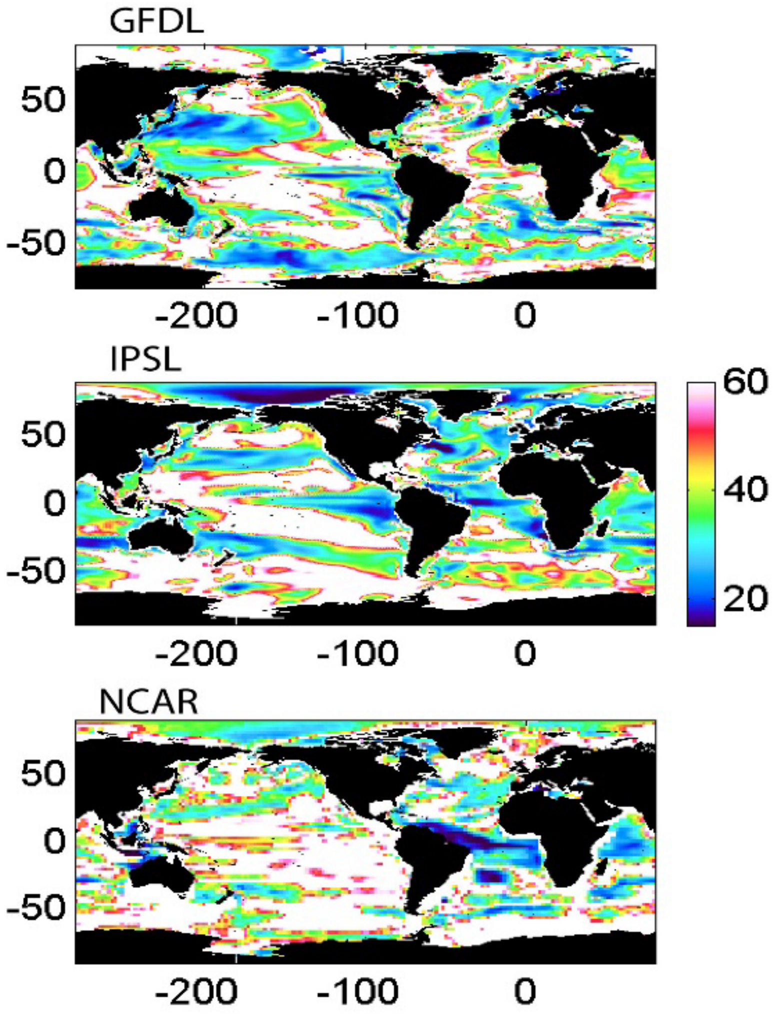


Figure 8.7: *Number of years of continuous data required to distinguish a climate change-driven trend in chlorophyll concentration from natural variability. (Modified from Henson et al., 2010).*

Chapter 8: Using Models to Inform Ocean Colour Science

Authors: Stephanie Dutkiewicz, Stephanie Henson, Colleen Mouw, Cecile Rousseaux
Reviewers: Stefano Ciavatta, Anna Hickman, Galen McKinley

Summary and Recommendations:

Numerical models can be used as laboratories
- Elucidate some of the limitations and uncertainties of ocean colour products,
- Inform future needs of ocean colour missions
- Assist in algorithm development.

Facilitate the full potential of these applications:
- collaboration between modellers and ocean colour communities
- continued development of models that include ocean optics
- comparison of uncertainties in ocean states derived from both model output and ocean-colour products.
- including models in mission and ocean monitoring design (e.g. OSSEs)

<u>Chapter 9:</u> Summary and Recommendations

<u>Authors:</u> Stephanie Dutkiewicz, Mark Baird, Stefano Caviatti, Stephanie Henson, Anna Hickman, Colleen Mouw, Cecile Rousseaux, Charles Stock

9.1. Using ocean colour products to evaluate models
9.2. Using models and ocean colour products together: Data assimilation
9.3. Using models and ocean colour products together: Process studies
9.4. Using models to inform ocean colour science
9.5 Recommendations for continued and new developments of ocean colour products.
9.6. Recommendations for choosing ocean colour products to use in model studies.
9.7 Recommendations for choosing model output for ocean colour/processes studies
9.8. Bridging Across Scientific Communities
9.9. Looking Forward

IOCCG committee: please review

<u>Appendix 1:</u> Table of ocean colour notation, acronymns, and sensors
<u>Appendix 2:</u> Table of satellite imagery terminology
<u>Appendix 3:</u> Table of model terminology and acronyms

Update on IOCCG Working Group:

Synergy between ocean colour and biogeochemical/ecosystem models

Stephanie Dutkiewicz and WG members (Mar 2019)

Plans:

- Finish revisions by early May 2019
- Finish recommendations
- (Formatting for report)

Issues:

- length