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Report on IOCCG Workshop

Phytoplankton Composition from Space: Towards a validation strategy for satellite algorithms

Astrid Bracher, Nick Hardman-Mountford, Takafumi Hirata, Stewart Bernard, Emmanuel Boss, Robert Brewin, Annick Bricaud, Vanda Brotas, Alison Chase, Aurea Ciotti, Jong-Kuk Choi, Lesley Clementson, Emmanuel Devred, Paul DiGiacomo, Cécile Dupouy, Toru Hirawake, Wonkook Kim, Tihomir Kostadinov, Ewa Kwiatkowska, Samantha Lavender, Tiffany Moisan, Colleen Mouw, Seunghyun Son, Heidi Sosik, Julia Uitz, Jeremy Werdell, and Guangming Zheng

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Goddard Space Flight Center
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Executive Summary

The IOCCG-supported workshop "Phytoplankton Composition from Space: towards a validation strategy for satellite algorithms" was organized as a follow-up to the Phytoplankton Functional Types from Space splinter session, held at the International Ocean Colour Science Meeting (Germany, 2013). The specific goals of the workshop were to:

1. Provide a summary of the status of activities from relevant IOCCG working groups, the 2nd PFT intercomparison working group, PFT validation data sets and other research developments.
2. Provide a PFT validation strategy that considers the different applications of PFT products: and seeks community consensus on datasets and analysis protocols.
3. Discuss possibilities for sustaining ongoing PFT algorithm validation and intercomparison activities.

The workshop included 15 talks, breakout sessions and plenary discussions. Talks covered community algorithm intercomparison activity updates, review of established and novel methods for PFT validation, validation activities for specific applications and space-agency requirements for PFT products and validation. These were followed by general discussions on (a) major recommendations for global intercomparison initiative in respect to validation, intercomparison and user's guide; (b) developing a community consensus on which data sets for validation are optimal and which measurement and analysis protocols should be followed to support sustained validation of PFT products considering different applications; (c) the status of different validation data bases and measurement protocols for different PFT applications, and (d) engagement of the various user communities for PFT algorithms in developing PFT product specifications.

From these discussions, two breakout groups provided in depth discussion and recommendations on (1) validation of current algorithms and (2) work plan to prepare for validation of future missions. Breakout group 1 provided an action list for progressing the current international community validation and intercomparison activity. Breakout group 2 provided the following recommendations towards developing a future validation strategy for satellite PFT products:

1. Establish a number of validation sites that maintain measurements of a key set of variables.
2. This set of variables should include:
    - Phytoplankton pigments from HPLC, phycobilins from spectrofluorometry
    - Phytoplankton cell counts and ID, volume / carbon estimation and imaging (e.g. from flow cytometry, FlowCam, FlowCytobot type technologies)
    - Inherent optical properties (e.g. absorption, backscattering, VSF)
    - Hyperspectral radiometry (both above and in-water)
    - Particle size distribution
    - Size-fractionated measurements of pigments and absorption
    - Genetic / -omics data
3. Undertake an intercomparison of methods / instruments over several years at a few sites to understand our capabilities to fully characterize the phytoplankton community.
4. Organise workshops to address the following topics:
    - Techniques for particle analysis, characterization and classification
    - Engagement with modellers and understanding end-user requirements
    - Data storage and management, standards for data contributors, data challenges

In conclusion, the workshop was assessed to have fulfilled its goals. A follow-on meeting will be organized during the International Ocean Colour Science Meeting 2015 in San Francisco. Specific follow-on actions are listed at the end of the report.

Content

Workshop Agenda

First day - 25 October 2014

7:30-9:00 Workshop breakfast

9:00-9:25 Session 1: Introduction

9:00-9:10 Astrid Bracher: Welcome, overall organization and schedule, welcome round

9:10-9:25 Astrid Bracher: Introduction and background information on workshop scope and goal; Attendees: introduce themselves

9:25-9:40 Session 2: IOCCG PFT report and intercomparison update (towards GOAL 1 "Progress update on global 2nd PFT intercomparison initiative"); chair: Takafumi Hirata, rapporteur: Coleen Mouw

9:25-9:40 Robert Brewin: "IOCCG PFT report in support to satellite PFT validation- lessons learned" and 10 min. discussion

9:40-9:55: Takafumi Hirata: "A brief introduction to PFT intercomparison"

9:55-10:15 Lesley Clementson: "Collection of *in-situ* data base for phytoplankton functional groups", and 5 min. discussion

10:15-10:35 Colleen Mouw: "A User's Guide for Satellite Remote Sensing of Phytoplankton Functional Types", and 5 min. discussion

10:35-11:00 Coffee break

11:00-11:30 Tihomir Kostadinov and Taka Hirata: "Phenology intercomparison in PFT algorithms & CMIP5 models via FFT", and 10 min. discussion

11:30-12:00 Robert Brewin: "PFT Algorithm Validation", and 10 min. discussion

12:00-12:30 Discussion on major recommendations for global intercomparison initiative in respect to validation, intercomparison and user's guide

12:30-13:30 Workshop lunch

13:30-15:00 Session 3: Validation strategies and moving beyond HPLC; chair: Robert Brewin, rapporteur: Alison Chase

13.30-14:00 Annick Bricaud: "Advances in optical methods for measuring phytoplankton size and functional type (from *in situ* IOPs)", and 10 min. discussion

14:00-14:30 Vanda Brotas: "Size-fractionation techniques", and 10 min. discussion

14:30-15:00 Heidi Sosik: "PFTs from microscopy, flow cytometry and genetic analyses ", and 10 min. discussions

15:00-15:30 Coffee break

15:30-17:00 Session 4: PFT validation activities with specific applications; chair: Astrid Bracher, rapporteur: Emmanuel Devred

15:30-16:00 Stewart Bernard: "Validation of phytoplankton functional type algorithms in coastal water, with a focus on harmful algal blooms", and 10 min. discussion

16:00-16:30 Cecile Dupouy: "PFT validation activities with special applications: Trichodesmium, and 10 min. discussion

16:30-17:00 Toru Hirawake: "Validation of diagnostic pigment analysis in polar waters and first results from using PFT satellite data in fish habitat modeling", and 10 min. discussion

17:00-17:30: Discussion towards GOAL 2: "Develop a community consensus on which data sets for validation are optimal and which measurement and analysis protocols should be followed to support the sustained validation of PFT products considering different applications"

19:00: Workshop dinner at GRACE Restaurant, Portland

Second day - 26 October 2014

7:30-8:30 Workshop breakfast

8:30-10:30 Session 5: Towards GOAL 2 "Community consensus on data sets for validation and analysis protocols"; chair: Lesley Clementson, rapporteur: Samantha Lavender

8:30-9:00 Jeremy Werdell: "(NASA) strategies for and challenges with PFT algorithm validation", and 10 min. discussion

9:00-10:30 Plenary discussion (chaired by Lesley Clementson) on the status of different validation data bases and measurement protocols for different PFT applications

10:30-11:00 Coffee break

11:00-15:45 Session 6: Break-out groups towards GOAL 2 "Community consensus on data sets for validation and analysis protocols" ; chair: Nick Hardman-Mountford, rapporteur: Samantha Lavender

11:00-11:30 Plenary: Definition of break-out groups (Lead by Nick Hardman-Mountford)

11:30-12:30 Break-out group 1 and break-out group 2 meet in separate rooms (approx. 10-14 participants each)

Break-out group 1 with chair: Samantha Lavender; rapporteur: Robert Brewin / Lesley Clementson

Break-out group 2 with chair: Aurea Ciotti; rapporteur: Alison Chase, other participants

Lunch 12:30-13:15

13:15-14:15 Break-out group 1 and 2 cont.

14:15-15:45 Presentation of outcome of breakout group 1 and 2 by their chairs; Discussion in plenary

15:45-16:00 coffee break

16:00-17:00 Session 7: Towards GOAL 3 "Possibilities for sustaining ongoing PFT algorithm validation and intercomparison activities"; chair: Nick Hardman-Mountford, rapporteur: Tiffany Moisan

16:00-16:10 Ewa Kwiatkowska: ESA/Eumetsat

16:10-16:15 Taka Hirata: JAXA

16:15-16:20 Jon-Kuk Choi: KIOST

16:20-16:30 Paul DiGiacomo: NOAA

16:30-16:55 Overall discussions and definitions of actions and recommendations

16:55-17:30 Session 7: Final discussion and formulation of actions; chair Astrid Bracher; rapporteur: Tiffany Moisan

16:55-17:15 Final discussion on open issues and whether the goals were met

17:15-17:30 Formulation of actions

Workshop Participant List

IOCCG workshop on "Phytoplankton Composition from Space: towards a validation strategy for satellite algorithms"

Chairs:

Astrid Bracher, Alfred-Wegener-Institute Helmholtz Center for Polar and Marine Research (AWI), Bremerhaven, and University Bremen, Germany

Nick Hardman-Mountford, CSIRO, Oceans and Atmosphere Flagship, Floreat, WA, Australia

Taka Hirata, Faculty of Environmental Earth Science, Hokkaido University (HU), Japan

Other participants:

Stewart Bernard, CSIR, South Africa

Emmanuel Boss, University of Maine, USA

Robert Brewin, Plymouth Marine Laboratory (PML), UK

Annick Bricaud, Laboratoire d'Océanographie de Villefranche-sur-Mer (LOV), France

Vanda Brotas, Universidade de Lisboa, Portugal

Alison Chase, University of Maine, USA

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Wonkook Kim, KIOST, Korea

Tihomir Kostadinov, University of Richmond Virginia, USA

Ewa Kwiatkowska, EUMETSAT, Germany

Samantha Lavender, Pixalytics, UK

Tiffany Moisan, NASA-GSFC, USA

Colleen Mouw, Michigan Tech, USA

Seunghyun Son, NOAA, USA

Heidi Sosik, WHOI, USA

Julia Uitz, LOV, France

Jeremy Werdell , NASA-GSFC, USA

Guangming Zheng, NOAA, USA

PFT workshop DAY 1, October 25, 2014

Session 1: Introduction

Chair: Astrid Bracher

The chairs of the workshop, Astrid Bracher, Nick Hardman-Mountford and Takafumi Hirata, welcomed the participants and explained the overall organization and scheduling of the workshop.

The workshop "Phytoplankton Composition from Space: towards a validation strategy for satellite algorithms" covered two full days starting with workshop breakfast on Saturday at 7:30 am and ending just before the ice breaker of the XXII Ocean Optics Conference 2014 on Sunday at 5:30pm. 25 scientists from 12 different countries with expertise on PFT algorithm development, ocean-color validation, in-situ measurements of PFT and representing space agencies attended the meeting. The workshop agenda included 15 talks (of about four and a half hours total), four hours for breakout sessions and five hours dedicated to open discussions. There was also time for informal discussions during breakfast, coffee breaks, lunch breaks and workshop dinner. At the opening of the workshop, participants briefly introduced themselves giving their expert background and affiliation.

Astrid then detailed the motivation, historical background and scope of the workshop to the participants. Since all participants have been well aware on the need of phytoplankton functional type (PFT) or size class (PSC) products from space, the introduction focused on giving an explanation on the objectives of the workshop. It was also explained why the workshop had been limited to invited participants. Past activities had brought together PFT/PSC algorithm developers, validation scientists, space agency representatives and user community without limitations but with different foci.

In 2006, the IOCCG founded the PFT working group (chaired first by Cyril Moulin until 2008 and subsequently by Shuba Sathyendranath), which released a final report in July 2014. Many scientists attending the workshop presented here contributed to the IOCCG report. The outcome of the report was briefly discussed at the beginning of Session 2.

A 1st PFT algorithm intercomparison with focus on the retrieval of PFT dominance took place between 2008 and 2010 and the results were published in Brewin et al. (2011). In 2011 a 2nd intercomparison round on global PFT algorithms chaired by Takafumi Hirata, Nick Hardman-Mountford and Robert (Bob) Brewin started to focus on the quantitative assessment of PFTs and PSCs. The status on this ongoing activity was presented in Session 2 as well.

In May 2013, during the IOCS (International Ocean Color Science) Meeting in Darmstadt, Germany, a splinter session "Phytoplankton community structure from ocean colour: methods, validation, intercomparison and application" was held, chaired by Astrid Bracher and Takafumi Hirata during one afternoon. In addition to presentations describing current global algorithms retrieving multiple PFT/PSC types and related validation and intercomparison activities, the well-attended session (60 participants in total) formulated recommendations to governmental agencies. Those recommendations were then presented the last day of the IOCS meeting to the general audience

and they were summarized in the IOCS meeting report. The following recommendations to and possible actions by space agencies were raised:

- Support *in-situ* measurements of HPLC, other means of quantifying PFT (i.e., size fractionation, flow cytometry) and optical data acquisition for current and upcoming missions (MODIS, VIIRS, OLCI)
- Support validation of PFT derived from HPLC with other datasets (e.g., taxonomy)
- Support PFT algorithm validation and intercomparison activities with funding
- Support activities to merge different techniques and multi-mission data sets
- Support development of PFT methods also by radiative transfer modeling of hyperspectral datasets, including satellite and *in-situ* (gliders, buoys, etc.) measurements.

Motivated by the positive and enthusiastic feedback of the participants at the splinter session, IOCCG asked the chairs to propose a follow-up workshop focusing on the development of a PFT validation strategy. IOCCG then accepted the proposal by Astrid Bracher, Nick Hardman-Mountford and Takafumi Hirata and agreed to fund the workshop.

In the past 10 years many different PFT or PSC algorithms have been developed at different spatial (local vs. regional vs. global) and temporal (selected satellite scenes vs. entire satellite mission) scales. The goal of this IOCCG workshop was to move towards a community strategy for validating PFT and PSC products in order to have PFT /PSC products available for operational applications (e.g. modeling and forecasts) in the near future as is now commonly done for satellite Chlorophyll *a* (Chl *a*) products. There is a need for (1) a consensus on validation strategies including validation data and analysis protocols, but also for (2) financial sources and collaborative community efforts, which have to be identified and specified. The specific goals and potential outcome of the workshop have been to:

1. Provide a summary of both:
   (a) the status of the activities of the 2nd PFT intercomparison working group (focus of Session 2)
   (b) PFT validation data sets and strategies, including also specific applications (focus of Sessions 2, 3, and 4).
2. Provide a PFT validation strategy considering different applications of the products: community consensus on datasets and analysis protocols (focus of Sessions 5 and 6).
3. Discuss possibilities for sustaining ongoing PFT algorithm validation and intercomparison activities (focus of Session 7), which includes a discussion how to improve liaison to PFT data users (modelers and other users).
4. Formulate actions (workshop report, more possible: proposals, publications; focus of Session 8).

Session 2: Report and intercomparison update

Chair: Taka Hirata, rapporteur: Colleen Mouw

The day 1 morning session aimed to provide (1) a summary assessment of global PFT/PSC algorithms and the products currently available and (2) a summary of on-going effort to collect *in*

situ data. Towards this end, 5 speakers gave the following presentations, followed by a group discussion.

Talk 1: IOCCG report 15 overview

The talk was presented by Robert Brewin (PML). Contents of the recent report published by the IOCCG were briefly introduced. Special attention was given to Chapter 6: "General Discussion and Conclusion" of the report: The report is (i) a review of what has been attempted so far, with the full realization and even optimism that future developments will outperform what has been achieved to date, (ii) a starting point for identifying gaps and highlighting areas where effort should be focused to move the field forward, (iii) a document to guide choices from among the various options available, so users may choose the appropriate algorithms or data products for their particular application. The report is available at http://www.ioccg.org/reports/IOCCG_Report_15_2014.pdf.

There was a question from participants as to whether retrieval code could be made available. There is no arrangement to share the code publically so far.

Talk 2: Introduction of Intercomparison Project

The talk was presented by Takafumi Hirata (HU). A brief history of the Satellite PSC Algorithm Intercomparison was explained. The first intercomparison effort was previously conducted (Brewin et al., RSE, 2011) to assess difference in "dominance of a specific PSC within the total phytoplankton community", derived from several PFT/PSC algorithms. Since then, a number of PFT/PSC algorithms have been developed and many of them are now able to estimate PFT/PSC quantitatively rather than with "dominance". Thus, there has been an increasing potential of PFT/PSC algorithms to be used to provide operational products from ocean color remote sensing. As a result, the second phase of the Satellite PFT Algorithm International Project was launched in 2011 (Project website: http://pft.ees.hokudai.ac.jp/satellite/index.shtml) by an international effort. The project accommodates four working groups (WG): (1) User Guide WG, (2) *In situ* Data WG, (3) Intercomparison WG, and (4) validation WG. (The updates from each WG followed this presentation). A special note was given in this presentation emphasizing that an HPLC *in situ* database can be accessed via the project's website although a password is required and can be obtained via a request to tahi@ees.hokudai.ac.jp. It was explained that communication among scientists is also possible via an email list and a password-protected wiki.

Talk 3: *In situ* database

The talk was presented by Lesley Clementson. A brief history and summary of the current status of the *in situ* database for PFT validation was reported. Efforts for constructing this in situ database started in 2011 during the Satellite PFT Algorithm Intercomparison Project, and the database was released in May 2014. This effort was built upon the AEsOP (Australian waters Earth Observation phytoplankton-type products) database, which is publically available (http://aesop.csiro.au): the database includes samples from 31 research cruises as well as other projects of Australian researchers, from the publicly available data bases such as PANGAEA, SeaBASS, GeP&Co, BioSOPE and NOAA, and from individual scientists David Antoine (LOV), Ray Barlow (BCRE), Astrid Bracher (AWI), Bob Brewin (PML), Susanne Craig (UDal), Toru Hirawake (HU), and Takeyoshi Nagai (CSIRO, AAD). All Australian data are now also available on SeaBASS. The dataset contains phytoplankton pigments from HPLC, the optical absorption coefficients (for particles, phytoplankton, detrital

materials and colored dissolved organic matter) at 22 wavelengths, pigments, and total suspended matter. Match-up with satellite data remains to be done.

Discussion on free access to the data led to the suggestion to record it as a publication, so it will be publically available with a citing reference (as with the MAREDAT database by modelers). Coordination with MAREDAT may be desirable. However, the current database includes parameters such as absorption coefficients that are specific to remote sensing applications while MAREDAT does not, so differentiation between the two datasets is clear.

Some participants suggested retaining the full wavelength resolution for the absorption coefficient data, especially for future satellite missions that plan to have hyperspectral radiometric capability. Also it was suggested to include radiometric data such as remote sensing reflectance and the use of SeaBASS as a platform for these data since they now have a doi for given datasets, which could help with the issue of recognition of individual researchers.

The issue of uncertainty of *in situ* measurements was also raised. One participant highlighted the importance of establishing common ways to report uncertainty. Creation of a new working group about uncertainty may be the way forward, which will be discussed at the next IOCCG meeting. This group should focus on the phytoplankton composition uncertainty and leave other groups to deal with other measurements (such as radiometry).

Talk 4: PFT User's Guide

Colleen Mouw presented the talk. Even in light of the recent publication of IOCCG Report 15 (which was introduced earlier by Bob Brewin), participants felt that there was still a need for a document from the perspective of the user communities. Colleen presented an outline showing (i) a table linking inputs to outputs, (ii) a table indicating what was used for algorithm development vs. what is used for actual retrieval of PFTs, (iii) a summary of regions/missions for which the algorithms were developed (and their known limitations). It was felt that such would greatly help end-users to identify which algorithm would be most suitable for their application. The desire to move forward quickly with the manuscript to publish the current state of the science was expressed, as the literature is quickly expanding. Possible venues should be journals with a broad remote-sensing user and modeling audience (e.g., Biogeosciences). There were some comments from other participants on perhaps making materials available through alternative media as well, e.g. a web-based tutorial with example data sets and results. Also publishing the satellite data sets together with this guide paper would be advantageous (in ESSD and/or PANGAEA).

The document also may discuss scientific questions such as: how can we quantify the extent to which we are identifying something new (i.e. empirical vs. mechanistic)? For example, are we just mapping back statistics that are within the underlying *in situ* dataset utilized?

Talk 5: Algorithm Intercomparison

The talk was presented by Tihomir Kostadinov and Takafumi Hirata. The latest results of the intercomparison were presented. The intercomparison was based on temporal and spatial analysis by means of Discrete Fourier Transform (DFT). The temporal DFT analysis compared phenology of PFTs derived from satellite algorithms with phenology of carbon biomass from CMIP5 models. An improved future version should focus on specific PFTs from the CMIP5 models as well, where available. A spatial DFT analysis indicated there was no particular difference between optics-based and abundance-based approaches. An opinion was expressed that there is a need to point out the

limitations of the region for which an algorithm was parameterized in relation to how it is being applied (For example, an Arctic parameterization shouldn't be assumed to work well across the global ocean). To the extent possible, each algorithm needs to provide a map of locations of data used to develop it. Participants agreed that the intercomparison would be published as a group effort with all algorithm contributors as authors. For this process, it was suggested the intercomparison process should be shared with algorithm developers along the way to ensure all ideas are considered and to avoid the need to make changes after the analysis is mature.

Talk 6: Algorithm Validation

Bob Brewin presented the first steps of validating the global algorithms delivered for the intercomparison. Frequency distribution of the *in-situ* TChl *a* (total chlorophyll *a*) HPLC database compares well to the merged SeaWiFS-MODIS-MERIS OC-CCI TChl *a* database. Using the later datasets to produce PFT algorithms' output based on multispectral data will deliver probably three times as many match-ups to *in-situ* data compared to using SeaWiFS data only. There were several topics proposed to the participants in regards to establishing the validation strategy moving forward. For example, two possible options were introduced for validation:

1. Formulate common criteria to evaluate algorithms (as done in Brewin et al. RSE, 2011).
2. Perform independent validation of each algorithm in the same manner as they are calibrated.

From previous experience (Brewin et al., 2011), it was noted by the presenter that 2) is favored. On the other hand, there was an opinion from participants that it does not seem there is a single answer to choosing 1) or 2) since it depends on the user and the question pursued. Thus, research of user requirements (3-4 key requirements) may be necessary, assuming that the modeling community is setting the requirements. Meanwhile, many numerical models are adapting their outputs to comply with satellite observations of PFT, so it might be better that the requirements address underlying science questions. In addition, management agencies are starting to take note that PFTs are highly valuable/helpful for their operational needs. As a result, discussion led to an agreement that modelers are the most appropriate users from a global perspective while management agencies are more focused on regional and/or coastal applications.

Other questions to be considered should include (i) temporal/spatial scale of validation (spatial resolution of satellite data to be 1, 4 or 9 km? Temporal acceptance to be +/- a certain number of hours), (ii) what are the common validation parameters (e.g. should this be HPLC-based measurements?), (iii) if the validation should be focused regionally so that a sufficient number of matchups are available to characterize PFT composition, and its seasonality from *in situ* observations.

The need to compare algorithms was questioned given that we have a robust *in situ* dataset used to validate the algorithms. Answers to this were that users are able to decide which method might be best to use for their purpose (fit for purpose), and that algorithm developers can learn from each other as to robustness/weakness in their algorithms for further improvement.

A practical issue was raised that validation work requires an extensive amount of effort (i.e., time), such that it requires funding support.

Session 3: Validation strategies and moving beyond HPLC

Chair: Robert Brewin, rapporteur: Alison Chase

This session focused on techniques other than HPLC that may be useful to validate satellite PFT or PSC products, or to verify uncertainty in PFT and PSC estimates derived *in situ* using HPLC.

Talk 1 "Advances in optical methods for measuring phytoplankton size and functional type (from *in situ* IOPs)"

In the first talk by Annick Bricaud (LOV), the advantages and limitations of various optical methods for inferring size classes were explained. In-line systems (e.g. ac-s system) now give access to high-frequency measurements of IOPs (attenuation, absorption, backscattering), which are relatively easy and inexpensive to measure, whereas HPLC measurements are limited because they are from discrete water samples, rather than measured continuously. In addition, analysis by HPLC is expensive and time consuming. However, it was clearly stated that *in situ* IOP methods do not allow us to directly validate satellite PFT estimates (they include assumptions and uncertainties as with satellite methods), but they can help by separately validating the two steps existing in many satellite PFT methods (i.e., inverting IOPs from satellite reflectances, and deriving pigments/size/PFT from IOPs). IOP methods thus help to increase the number of match-ups between satellite and *in situ* data.

In the recent IOCCG PFT report many IOP related methods were presented. Therefore, the talk detailed only new studies not included in the PFT report and proposed by scientists from the PFT community. Three different IOP method types exist for PFT or PSC products:

1. These IOP methods focus on deriving pigments, pigment groups, or PSC from absorption spectra. Various methods have been developed in the past focusing on derivative analysis (Faust and Norris 1985, Bidigare et al. 1989), multiple linear regression analysis (Sathyendranath et al. 2005), neural networks (Chazottes et al. 2006, Bricaud et al. 2007, similarity algorithms (Millie et al. 1997, Kirkpatrick et al. 2000), inverse modeling (Moisan et al. 2011), decomposition into Gaussian bands (Hoepffner and Sathyendranath 1993, Lohrenz et al. 2003, Chase et al. 2013) and partial least square regression (PLS) analysis (Organelli et al. 2013).

The study by Chase et al. (2013) used inline ACS measurements from the TARA Oceans expedition and provided reliable predictions for concentrations of various pigments, including Chl *a*, Chl *b*, Chl *c*, and photosynthetic and photoprotective carotenoids. However, the pigments-absorption relationships are not univocal (e.g. photoacclimation, package effect) and pigments from different PFTs may have similar spectral signatures. In addition, there is no direct information on size or PFT if not all individual (taxonomic) pigment concentrations are retrieved.

Results from Organelli et al. (2013) using 4th derivative analysis of phytoplankton (a_{ph}) or particulate (a_p) absorption spectra coupled to a Partial Least Square (PLS) regression analysis showed that their method can predict diagnostic pigment concentrations associated with the three size classes of phytoplankton. The method was shown to be insensitive to non-algal particle (NAP) and CDOM absorption. However, hyperspectral information and a large data set for training are required for this method.

A study by Barlow et al. (unpublished results) on pigment data from the Mozambique Channel shows that relationships for PFTs derived from DPA (diagnostic pigment analysis) via Uitz et al. (2006), or from CHEMTAX can differ when trying to determine specific PFTs (>7 types). However, when grouping into only three size-related groups (diatoms, flagellates and prokaryotes), boundaries in absolute Chl *a* or a_{ph} used by some methods to partition dominance of the three groups (e.g. Hirata et al. 2008) agree reasonably well. The results suggests that we can use CHEMTAX to help tune satellite PFT models.

2. Here, IOP methods focus on deriving a PFT directly from absorption spectra (Subramanian et al. 1999, Sathyendranath et al. 2004), or alternatively cell size (Ciotti et al. 2002). These methods can also be applied to in-line measurements. The third method was found to be globally consistent with size estimates from diagnostic pigment concentrations (Bricaud et al., OOXXII poster). Limitations of this method are that the variable influence of nanophytoplankton is not explicitly taken into account, and that the shape of the absorption spectra is influenced by photoacclimation and not just size or PFT.

3. These methods refer to use of spectral attenuation or backscattering by particles (not just phytoplankton) to infer size distributions, as the slope of the c_p or b_{bp} spectrum increases when the average size of the particulate pool decreases (Boss et al. 2001 (c_p), 2004 (b_{bp}); Loisel et al. 2006 (b_{bp}); Kostadinov et al. 2009, 2010 (b_{bp})). They have a sound theoretical background, and b_{bp} and c_p are measured in-line already, as well as by profiling floats and gliders. However, the particle size distribution is not necessarily well related to that of phytoplankton, as shown by comparisons between S_f and the slope of c_p (Bricaud et al., OOXXII poster). Cetinic et al. (2014) suggest that an "optical community index" for phytoplankton could be derived from the ratio between Chl fluorescence and b_{bp}. For the open ocean (Atlantic Ocean) Martinez–Vicente et al. (2013) showed that b_{bp} is well correlated with the phytoplankton carbon concentration for cells less than 20 µm, so that estimates of pico- and nanophytoplankton carbon biomass from b_{bp} could be derived. However, regional and temporal variations in these relationships have to be verified.

The following discussion confirmed the conclusions of the talk that optical methods are applicable to *in situ* IOPs and can help in validating the two-step satellite methods by increasing the number of match-ups. However, many of these "new" methods have still to be fully validated themselves.

Talk 2 "Size-fractionation techniques"

Vanda Brotas (Universidade de Lisboa) discussed the use of information on size fractionated data for validating PSC satellite algorithms. She explained the origin of the concept from Reynolds (2006) and why and how competition, stress and disturbance tolerance of phytoplankton are linked to cell size. A group of species that exploit the same class of environment resource in a similar way are called a *guild* whereas a *functional trait* is a well-defined and measurable property of the organism (for more details see McGill et al. 2006). Functional traits can be used to identify functional groups and types and can be related to cell size. The amount of Chl *a* per cell, but also the content per cell of carbon, nitrogen, and protein are well related to the size of phytoplankton (Montagnes et al. 1994). The rate of resource utilization is the main factor controlling phytoplankton size structure in the ocean. So, there is a strong connection between PFT, PSC and ecological requirements.

The method of size-fractionated filtration enables to study the phytoplankton community based on size classes, but it also suffers from unknown uncertainties resulting from filter clogging, cell breakage, elongate cells passing through pores, etc. This can be seen by comparison to total filtration (generally characterized by $\Sigma Chla_{\_sizefraction} = 0.91\ Chla_{\_total} - 0.03$; Del Amo et al. 1997).

In a study by Brewin et al. (2014), size fractionated chlorophyll data were compared with PSC derived from HPLC pigments. Results showed that the HPLC method underestimates picoplankton and overestimates nanoplankton while TChl *a* agrees with total pigment concentration. It was also pointed out that HPLC techniques have evolved a lot within the past 20 years (now 72 instead of 42 phytoplankton pigments can be detected, 25 classes are identified as opposed to 12), and hopefully better knowledge about groups, for example picoeukaryotes can be expected.

Marañon et al. (2012) looked at the relationship between size structure and climatic regions defined using temperature. They found that the partitioning of biomass between different size classes is independent of temperature, but depends strongly on the rate of resource use as is reflected in the rate of primary production. Picoplankton are not well detected using just HPLC. Another technique to detect size fraction of phytoplankton is flow cytometry (limited to nano- and picoplankton) which also helps to assess picoplankton much more quantitatively. Flow cytometry data can clearly reveal that DCM (deep Chl max.) picoplankton are different from those at the surface. However, phytoplankton cells larger than 10 or 20 μm (depending on instrument settings) are difficult to enumerate by this method (the method is further discussed in the following talk).

The study by Brotas et al. (2014) re-parameterized the phytoplankton size-class model of Brewin et al. (2010) in the Eastern Atlantic using HPLC and compared it with cell counts derived from cell flow cytometry and by microscope. The Chl/cell for each size class was determined for this data and cell abundance of pico-, nano-, and microplankton was estimated from TChl *a* obtained in a MODIS image. Results indicated a background population of picoplankton, while in more productive areas the microplankton increase.

Taylor et al. (2011) showed that size classes derived from CHEMTAX and from diagnostic pigments analysis (DPA, according to Vidussi et al. 2001, modified by Uitz et al. 2006), had a similar outcome, but the microplankton fraction was generally lower in CHEMTAX due to the interference of fucoxanthin in DPA. This pigment is representative of diatoms but also found in haptophytes or chrysophytes. Barlow et al. (in prep.) showed for size-fractionated particle absorption data from the Mozambique channel that the size fraction-related pigment CHEMTAX information indicates a lower diatom and a greater dinoflagellate proportion than that derived by the Uitz et al. (2006) approach. This may be due to the fact that most dinoflagellates were heterotrophic (confirmed by microscopy) and Peridinin was either not detected or in low concentration. CHEMTAX can distinguish *Synechococcus* and *Prochlorococcus* and in addition indicates a greater pelagophyte proportion at the DCM than Uitz et al. (2006), and also greater proportion of prokaryotes (*Prochlorococcus*). Noted that the higher proportion of *Synechococcus* than *Prochlorococcus* is also at the surface for CHEMTAX analysis.

Vanda Brotas also pointed out that the validation database of the Ocean Color Climate Change Initiative (led under her responsibility) does not only contain HPLC but also data from other methods which can be exploited. In the future, efforts should focus on assessing uncertainties in size fractionated filtration data (both HPLC and SFF), extending the sparse global *in situ* database and standardizing among methods in order to produce a valid data set with which to compare algorithms.

Talk 3 "PFTs from microscopy, flow cytometry and genetic analyses"

Heidi Sosik (WHOI) discussed measurement principles, and strengths and weaknesses of each method.

Light microscopy has been shown to be effective for microplankton, while epifluorescence microscopy is effective for picoplankton. Techniques like continuous plankton recorder (CPR) and electron microscopy (EM) always mean a trade-off between costs and time spent and abundance of data analyzed. CPR data is often obtained for whole cruise tracks but only can count cells >10 μm. EM methods have, so far, not produced a substantial data set and can only be used for verification of certain PFTs in a sample. Light microscopy achieves high taxonomic details, but is limited to microplankton (or cells >5 μm), is time consuming, requires a high level of expertise for taxon specification and errors can arise with sampling/preserving methods.

Flow cytometry is used to measure light scattering and fluorescence from single cells. These measurements are then used to identify pico- (prokaryotic and eukaryotic) and nanophytoplankton and are automatic, rapid, precise and quantitative. Some taxonomic detail for selected groups (*Prochlorococcus*, *Synechococcus*) is obtained and the optical cell size can be estimated. Problems arise with larger cells. The improvement of this method for microplankton uses laser-triggered image collection (e.g., Imaging FlowCytobot). But, especially for pico- and nanoplankton many taxa are not separated by any flow cytometry method, and measurements are fairly costly and require expertise and specialized instruments. There is a note of caution: some of the cheaper current flow cytometers (often also *in situ* instrument) do not have enough sensitivity to detect signals from some small-celled groups (e.g., *Prochlorococcus*), where instrument noise interferes.

Genetic analyses include a wide range of methods which are changing fast. Some are of interest to PFT validation: clone libraries, PCR-based assays, and microarrays for selected specific sequences make it possible to detect presence/absence/relative abundance of phytoplankton taxa or functional types. Further, high throughput sequencing and ribosomal marker surveys make it possible to derive relative abundances of phytoplankton taxa without *a priori* knowledge of target species. The metagenomics, or other '–omics' allow sequencing of everything, potentially for functional information; however, these approaches remain more challenging to apply for eukaryotes (vs. prokaryotes). With genetic analyses, taxa can be targeted with a high degree of specificity and *in situ* tools are emerging, but these approaches contain no direct cell size information and require complex interpretation and underlying sequence databases. Depending on the gene sequenced, the results could be very different regarding detection of different phytoplankton groups.

Cross-cutting challenges for these data sets:

a) Space/time mismatch with satellite observations
b) Abundances are obtained, which then have to be converted into biomass based on common parameterizations
c) Biomass metrics are at first biovolume and then carbon (C) biomass which is different from HPLC outputs (pigment or Chl concentration). From microscopic observations the cell dimensions are determined and the cell volume (biovolume) is estimated, and from that the cell C is derived which relies on standard shape assumptions and literature-based C to volume relationships. Similarly this is done for flow cytometric results, but more automated with a higher throughput of data. Here, for pico- and nanoplankton, the cell volume is determined through the light scattering relationship, which must be calibrated with phytoplankton and not beads, and relationships are instrument specific.

For nano- and microplankton, the Imaging FlowCytobot (Olson and Sosik 2007) is now being used for taxon-specific volume calculations (Sosik and Olson 2007, Moberg and Sosik 2012), while laser-based light scattering can be used for pico- and nanoplankton (Olson et al. 2003). Cell carbon calculated from cell biovolume (e.g., Menden-Deuer and Lessard 2000) can be used to estimate populations of cyanobacteria, diatoms, etc. and size classes changing through time (e.g. over one year). For instance, results from a coastal US study do not show a constant background of picoplankton. Very different slopes are seen in comparison of carbon and Chl *a* biomass (derived from HPLC and CHEMTAX) for different taxonomic groups, implying very different C:Chl ratios for different phytoplankton types. This also impacts use of size fractions to characterize the assemblage. The fraction of microplankton is different when using HPLC pigment-based size classes vs. carbon estimated from the single cell approaches. Challenges of biomass estimation arise when different metrics are compared: for instance, in this study the total phytoplankton carbon is fairly constant with changing seasons, but the C:Chl ratio changes noticeably throughout the year, probably due to different types of phytoplankton.

The following questions were posed by the speaker and discussed at the end of this day in the general discussion:

Which metrics will best serve which questions?

What methods are required for those metrics?

Recommendations for observations?

Session 4: PFT validation activities with specific applications

Chair: Astrid Bracher, rapporteur Emmanuel Devred

This session focused on validation tasks of PFT/PSC where it becomes especially challenging.

Talk 1 "Validation of phytoplankton functional type algorithms in coastal water, with a focus on harmful algal blooms analyses"

Stewart Bernard (CSIR) outlined the importance of validation of PFTs in coastal waters, with a focus on harmful algal bloom (HAB) proxies, considering the difficultly of detecting biological properties (such as Chl *a*) from ocean color in these regions. These two main reasons for such difficulties are 1) the hydrodynamics are an important driver of the biophysical interactions and ii) the waters are optically complex. One of the main issues that remains unsolved in ocean color remote sensing in coastal systems is the atmospheric correction, even if tremendous efforts have been made. Secondly, one way to go is the use of coupled phytoplankton population-radiative transfer models, which account for chlorophyll-specific phytoplankton type spectra (i.e. Robertson-Lain et al 2014). The ability to detect phytoplankton types from reflectance is directly related to the phytoplankton community's influence on the remote sensing reflectance (R_{rs}) signal. In case 2 waters with lots of non-algal scattering, the signal reduces significantly and contribution of phytoplankton assemblage to total R_{rs} signal in low biomass waters is very small and probably undetectable. It probably becomes impossible to retrieve PFTs or PSCs directly from the optical signal as seen for the St. Lawrence River Estuary or in the Gulf of Oman, especially as certain HABs are already harmful at low concentrations. Using ocean color as one component of a multi-parameter ecosystem classification - effectively using Margalef's Mandala to create an earth observation based metric - will potentially allow the detection of some other bloom types as shown for the two above mentioned studies. For case 1 water HABs detection, one specific detection algorithm proves often to work (as shown for the Benguela upwelling; Bernard et al. 2007)

In high Chl *a* concentration waters, rapid change in hydrodynamic conditions (e.g. tides) at the coast leads to high uncertainties in the retrieval of Chl *a*. In addition, errors with atmospheric correction make retrievals challenging. So, we need to account for the specific IOPs in inversion schemes and the contribution of each phytoplankton group to the total signal has to be assessed. This involves a good knowledge of the particle size distributions, and also fluorescence should not be ignored when modeling the range of R_{rs} for various cell size or different PFT assemblages (shown in Evers-King et al. 2014). It was stated that the higher the biomass, the lower the variability is with change in size, and the size error decreases as Chl increases.

Since radiometry is a second order measurement, uncertainties on *in situ* data are needed for validation measurements. Also, more details (e.g. flow cytometry, genetics) on phytoplankton community structure are required since HPLC only contains a given amount of information on the phytoplankton community (but gives a first assessment). HPLC pigments are also linked to

photophysiology as well as PFTs. The accessory pigment to Chl *a* pigment ratios may represent very different phytoplankton populations.

The following recommendations are given.

Measurements

- New bio-optical sampling and processing protocols are needed to reduce and quantify errors in validation/algorithm development data and subsequent algorithm products
- Need for better, more widespread & commonly adopted phytoplankton community structure observations to reduce regional biases and uncertainties in PFT classification
- Better characterization and modeling of diversity, abundance, succession etc. – ideally through a common quantitative bio-physical parameterization

Bio-Optical/Radiative Transfer Models

- More effective use of bio-optical modeling capabilities to offer signal analysis over a wide range of optical complexity and phytoplankton communities and the use of hyperspectral information; and more effective algorithm development and validation. Currently this is constrained by input data so the question arises how to appropriately simulate phytoplankton community variability from a bio-physical perspective.

Algorithm Frameworks & Products

- Approaches that offer dynamic and scalable means of characterization, algorithm optimization and error quantification for both empirical, statistical and bio-physical approaches are needed.
- Need for routine error determination and analysis, preferably across the processing chain i.e. L1 onwards

Networks & Communities

- IOCCG INSITU-OCR can assist in taking forward common protocols & community building
- Global networks of regional ocean color/observation sites: interact with other communities such as GEO and GEOHAB, who have proposed a network of global sites acquiring routine, detailed community structure & other data

Talk 2 "PFT validation activities with special applications: *Trichodesmium*"

Cecile Dupouy (M.I.O.) gave an overview on the challenges in validating *Trichodesmium* satellite retrievals, which are of high relevance especially for global nitrogen budget calculations (Westberry et al. 2005; Dupouy et al. 2011). *Trichodesmium* live near the surface (0-20 m), are filamentous, form colonies, and are extremely unevenly distributed. If the sea is calm they can accumulate but they can also disappear rapidly (i.e. within a few hours). Chlorophyll concentration can change by a factor of 7 within a few meters from the surface to depth (Tenorio 2006), and within a few hours (Hu and Feng 2014). Satellite overpasses around noon local time may introduce a bias into biomass estimates. Therefore validating *Trichodesmium* algorithms is challenging because of this high variability. In addition it is difficult to choose the right *in situ* method to correctly assess their biomass. *Trichodesmium* is often mixed with picoplankton and large cells and then TChl *a* does not determine the total biomass (Tenorio 2006; Neveux et al. 2006). They also vary in colony size, and are difficult to filter or to catch with nets. The relationship between abundance and phycocyanin and phycoerythrin pigments is useful (Neveux et al. 2006) and their IOPs show clearly distinct

spectra due to absorption of phycobiliproteins as opposed to other PFTs, distinct CDOM peaks, and high specific backscattering efficiencies (Subramaniam et al. 1999; 2002; Dupouy et al. 2008). Since *Trichodesmium* blooms are extremely patchy and also have different colors (Shanmungan et al. pers. comm., Desa et al. 2005), it is extremely difficult to detect them using R_{rs} spectra (McKinna et al. 2012), as colonies are unevenly distributed at and under the sea interface. Hyperspectral sensors are needed to measure *Trichodesmium* by satellite (Dupouy et al. 2008). Another issue is the inhomogeneity of the spatial distribution within an ocean color pixel (currently 1km at best). For the validation of *Trichodesmium* satellite algorithms the following recommendations were given in order to improve their in situ biomass assessment:

- Encourage the science community to routinely sample (<10μm and >10μm fractions to avoid confusion with *Synechococcus*) accessory phycobilin pigments and use spectrofluorometry to determine PE and PC (high correlation with counts if same 8L water sample is used)
- Phycoerythrin algorithms will need higher spectral resolution than current sensors provide
- Determine all biomass parameters in at least an 8L volume
- Recognize that nets do not provide quantitative measurements
- New sampling platforms present interesting potential (Desa, pers. comm.), as AUVs can measure properties under *Trichodesmium* patches and gliders could also have potential to provide detailed measurements in space and time of *Trichodesmium* blooms

Talk 3 "Validation of diagnostic pigment analysis in polar waters and first results from using PFT satellite data in fish habitat modeling"

Toru Hirawake (Hokkaido University) discussed the validity of the DPA (diagnostic pigment analysis) for polar waters. Many algorithms are based on DPA and applied to global datasets. Only a small number have been developed for the polar seas (Montes-Hugo 2008; Fujiwara et al. 2011; Soppa et al. 2014). Soppa et al. (2014) showed that for the Antarctic Ocean the global relationships between diagnostic pigments and TChl *a* do not hold and have to be regionally tuned. Soppa et al. (2014) showed that a substantial improvement of diatom abundance retrieval can be obtained when the DPA is adapted to the Southern Ocean, and a regional model is applied. HPLC and size fractionated Chl *a* fluorescence data from the Chukchi and Bering Seas were successfully compared to microplankton Chl *a*; however, picoplankton does not compare well because they do not contain or contain very little zeaxanthin pigment which is a marker for picoplankton. When Chl *b* is included as a diagnostic pigment for picoplankton, there is a better relationship. Also, it appears that in the Arctic small diatoms (~10μm) are frequent, and as a result the DPA is overestimating microplankton (represented by fucoxanthin) compared to the size fractionated TChl *a* analysis. It was recommended that Chl *b* in the DPA should be associated with picoplankton, as in Uitz et al. (2006) rather than Hirata et al. (2011). One has to consider that diatoms in the Arctic are often smaller, and more water volume needs to be filtered to detect the pigments associated with picoplankton. Flow cytometry could help to solve that problem.

First results from a possible practical application of PFT/PSC information to fisheries, where the median size of phytoplankton is related to upper trophic levels by habitat modeling, were presented. The study focused on the Pacific saury, a delicious and popular fish, population. There was no significant difference in outputs of presence or absence of the Pacific saury among using Chl *a*, microplankton Chl *a*, or diatom Chl *a* in the habitat models.

General discussion towards Goal 2

At the end of the last session of the first day we initiated the general discussion towards Goal 2 of the workshop, which is to develop a community consensus on which data sets for validation are optimal and which measurement and analysis protocols should be followed to support the sustained validation of PFT products considering different applications. This discussion was continued the next morning after the talk by Jeremy Werdell (NASA).

First the physical limits to what we can detect from satellite remote sensing (shown previously in radiative transfer model studies by Evers-King et al. (2014) and Roberston-Lain (2014)) were discussed. It was made clear that in low biomass case 2 waters the optical signature of PFT or PSC will be small compared to other optical signals, and therefore in the future very difficult to retrieve using a spectral-based approach.

Then the discussion went back to Heidi Sosik's presentation. Here she had shown that PFT estimated from different *in situ* techniques (HPLC, flow cytometry) cannot directly be compared due to variable carbon to Chl *a* ratio (HPLC is based on pigments; flow cytometry is converted to carbon). It was agreed that flow cytometry and imaging are useful to characterize the phytoplankton community further. The parameters of interest by a given scientist should be defined according to the scientific question to address and serve for algorithm development. Flow cytometric and microscopic data are valid to provide the radiative transfer model and algorithm developers with detailed PFT information. The correct calculation of IOPs, e.g. a more precise assessment of the phytoplankton scattering and backscattering, might be missing for the use of radiative transfer modeling (RTM). With the help of RTM, HPLC and flow cytometry or imaging data can be much better related to each other.

A possible opportunity to enlarge tremendously the database of pico- and nanoplankton cell counts and carbon estimates could be realized through comparing and standardizing flow cytometry and microscopic data. In this way, different flow or imaging data sets can be put together with assessed uncertainties which would make that type of data more useful but also more accessible, in particular providing information about the smaller phytoplankton. Also, flow cytometry data may be of use for RTM but needs further investigation as to how these data could be interpreted within the RTM.

It was also mentioned that it has to be ensured that data used for algorithm development should not be used in their validation. This will be a significant challenge with partitioning the HPLC data set in various ways. Algorithms developers need to identify their development data subsets.

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Session 5: Community consensus on data sets for validation and analysis protocols

Chair: Lesley Clementson, rapporteur: Sam Lavender

This session started with a talk summarizing the lessons learned from Chl *a*, IOPs and reflectance validation strategies and protocols and then continued with discussion from the end of session 4 towards developing a strategy for a community consensus on validation data sets and methods to be used for verifying satellite PFT products.

Talk "NASA strategies for & challenges with PFT algorithm validation"

The talk by Jeremy Werdell (NASA) summarized NASA's advanced planning for potential future hyperspectral missions that will have relevance to PFT detection: PACE (2021-ish launch), GEO-CAPE (under study, 2025+), HyspIRI (under study, 2025+). For details of the missions refer to the slides. For PACE, three of the science questions it is designed to address rely on being able to study phytoplankton composition from space, so this will be a metric for mission success. The first PACE science teams, focused on atmospheric correction and IOPs, were announced in Sep 2014 and these will operate over the period 2014-2017. Emmanuel Boss is the lead for the IOPs team. Other science teams will be competed post 2017. NASA-GSFC has begun preparing for PACE in terms of SeaBASS support for *in situ* measurements relevant to PFT/PSC algorithm development and validation.

Challenges and lessons learned from previous validation activities: Validating PFTs is different from validating radiances, and more challenging. Key challenges include:

(1) the (increased) degrees of separation between the satellite and *in situ* measurements

(2) the (increased) number of satellite methods to model PFTs/PSCs

(3) the (increased) number of *in situ* methods to infer PFTs/PSCs

When considered in relation to previous validation exercises, there are some common limitations:

(i) the quality of the *in situ* data is highly variable & difficult to assess;
(ii) *in situ* data coverage is limited, both geographically & temporally;
(iii) availability of *in situ* data in future is unknown;
(iv) highly localized measurements at the meter scale compared with satellite pixels (>km scale);
(v) satellite-to-*in situ* comparisons require expertise to prepare & evaluate;
(vi) validation results are generally useful only for assessing static biases in final products.

Additional anticipated challenges for validating PFTs include:

(1) Data collection with appropriate horizontal, temporal, vertical resolution. This may require working with daily L2 products to avoid losing resolution of features due to binning. Resolution experiments show sharp features become temporally/spatially blurred with compositing, spectral distortion can occur due to varying wavelength penetration with depth.
(2) Data archival and preparation. Consensus protocols will need to be agreed for measurements and databases will need to be standardized between organisations. A level of post-processing will be required on *in situ* data for match-up analysis.
(3) Satellite algorithms. Algorithm intercomparisons and targeted development, sensitivity analysis and validation at each stage of the processing chain given the degrees of separation between the in water and satellite measurements. Availability of global datasets and reliance on HPLC.

NASA Ocean Biology Processing Group are proposing to host a follow-on workshop on these issues in mid-2015, possibly as part of the IOCS meeting.

Finally Jeremy presented results from a survey of the meeting participants on their challenges. The points raised were:

- availability of global datasets for algorithm development & satellite validation; need to rely on HPLC (thus, DPA & CHEMTAX); limitations of HPLC as a proxy (5 responses);
- mismatch between spatial & temporal scales of satellite & *in situ* measurements (2 responses);

- satellite uncertainties & sensitivities to algorithm inputs (1 response);
- satellite limits of PFT detectability (1 response);
- *in situ* methods & their differences & uncertainties (1 response);
- differences in algorithm outputs (size, taxonomic groups or species, fraction of Chl vs fraction of absorption, etc.) (1 response);
- PSC definitions (1 response).

Plenary discussion "Status of different validation databases and measurement protocols for different PFT applications"

There was considerable discussion around selecting appropriate units for phytoplankton type products from the various algorithms. While it is accepted that different types of products (and different PFT definitions) may need to have different units, choosing these units requires care. The types of products could be organized according to an agreed 'taxonomy'. Products retrieved in biophysical units have a quantitative advantage when it comes to validation and acceptance. Products should not stray too far from optical causality, e.g. size measurements have a causal link back to an optical signature, whereas a specific HAB species may not have an optical signature. However, while size affects the ratio of blue to red light, this ratio is influenced by acclimation and backscattering so it is also important to understand the relationships mechanistically. Bio-physical units will assist in making this traceable. Consideration needs to be given to whether optically defined products (e.g. bb/a) are more or less useful than converting optical proxies to biogeochemical measures (e.g. carbon or chlorophyll). Determination of appropriate products and units should be undertaken in consultation with the user community, particularly the ocean modeling community. It may be of benefit to establish a reference user group. However, we recognize that we may not be able to provide everything modelers initially want, rather we can find a meeting point between what is feasible from the algorithms that relates to properties of models.

Regarding the validation strategy, with limited resources there will always be a trade-off between the spatial extent over which observations can be made and the intensity of the measurement campaign that can be undertaken. Jeremy's point regarding the need to validate at each stage of the analytical chain agrees with the discussion from Day 1. However, within the validation strategy we should assume radiometric and IOP validation will be happening anyway (this will be the first stage of PACE validation). There are outstanding questions regarding the relationships between different optical and biogeochemical quantities, particularly backscattering versus carbon from flow cytometry versus HPLC. This will require the full suite of IOPs, including the bbp fractions. Work on cultures by Emmanuel Boss and others (e.g. Latimer in the 1960s) suggests the bbp from phytoplankton cells is larger than Mie theory would suggest. PACE may also have a polarimeter allowing derivation of the bb ratio, hence an estimate of beam attenuation. In-line and in situ absorption sensors suffer from drift and require scattering correction (although a new instrument from Turner should avoid the need for scattering correction). In-line systems allow for measurements of sub-pixel variability and can be used on ships of opportunity. Three years of ap data have been collected from the Tara Oceans voyage and is available in SeaBASS.

Flow cytometer data also has potential use for validation of smaller cells (including bacteria which affect backscattering) and there are various archives that could be incorporated into our in situ

database (e.g. AMT, Tara), although the volume of water sampled is a fraction of the volume filtered for traditional water samples exacerbating scaling-up issues between in situ and satellite observations. Knowing which limited metrics we will require from flow cytometry for comparison with PFT algorithms needs consideration, particularly with advanced instruments like the Imaging FlowCytobot where millions of images are generated alongside the flow cytometer measurements (Note, FlowCytobot can also be installed for in-line sampling). An alternative approach may be to generate metrics from the full database on the fly depending on individual requirements. Knowing the cell volume alongside HPLC would assist with estimating the chlorophyll to cell volume ratio. Determining these metrics will probably require its own workshop. New '–omics' approaches may also provide useful metrics, again this requires a further workshop to investigate. Moving to more up-to-date methods from microscopy will require running both methods in parallel to allow comparison of historical data with modern techniques. Pictures should be taken rather than preserving samples so they can be re-analysed later.

Session 6: Break-out Groups

Chair: Nick-Hardman-Mountford, Samantha Lavender

Two breakout sessions were defined, Break-out session 1 focused on "Validation of current algorithms" and Break-out session 2 on "Work plan to prepare for validation of future missions". A third theme for a break-out session "Involving users' needs for defining PFT satellite products validation strategy" was decided to be discussed briefly in the plenary after discussing the outcome of the other two break-out sessions.

Breakout group 1: Validation of current algorithms

Chair: Samantha Lavender; rapporteurs: Bob Brewin and Lesley Clementson. Participants: Emmanuel Boss, Annick Bricaud, Vanda Brotas, Jong-Kuk Choi, Nick Hardman-Mountford, Toru Hirawake, Wonkook Kim, Tihomir Kostadinov, Seunghyun Son, Julia Uitz, Jeremy Werdell.

The group started off discussing the current validation approach, using OC-CCI Level 3 data and then Level 2 SeaWiFS match-ups. The OC-CCI data is merged based on the SeaWiFS bands and so we 'lose' the MERIS and MODIS bands that do not match SeaWiFS. Would this represent a significant loss of useful information for some algorithms? Bob Brewin then explained the approach going forward. For abundance based approaches the algorithm is first calibrated and then applied to satellite data. Limitations include using pigments to infer size and the number of groups that can be separated. For Tiho Kostadinov's backscattering approach, it would be important to include PSD data (LISST and coulter counter) in the database.

It was agreed by the group that the ideal approach would be to validate the individual steps (i.e. Reflectance > IOPs and IOPs > Chl *a*, if they occur) as well as the final step where PFTs are derived. This would benefit from both an open code and data (*in situ* and satellite product) policy. It will be useful to partition results into open ocean, polar and coastal waters or provinces / biomes.

It was discussed that adding more *in situ* data to the current AEsOP PFT database could help, e.g. SeaHARRE HPLC plus HOT & BATS as time-series data, if not already present. However, it is also

important to find out from algorithm developers how much of the *in situ* database has been used for algorithm calibration, to understand the level of independence.

Discussion then focused on several non-abundance-based algorithms to understand what the above discussions meant in practice:

- Ciotti & Bricaud (size index): Currently the size parameter, S_f, is correlated to contributions of size classes to algal biomass to understand its behaviour, but could calculating an *in situ* Sf also validate it? Use pigments converted to size index?
- Alvain (PhySat): Calibration is using pigments.
- Bracher (SCIAMACHY algorithms): Compare PFT Chl *a* (from HPLC), comparison to hyperspectral IOPs not really possible (because only differential, not absolute, phytoplankton absorption is derived)
- Kostadinov (backscattering approach): can validate against HPLC, but b_{bp} is better, however there is a lack of *in situ* b_{bp} slope data globally. Validating b_{bp} or its slopes would be validation of Loisel's algorithm, not the Kostadinov (KSM2009) algorithm per se. Validation at the preliminary steps before PSCs of the KSM2009 algorithm requires PSD data, which is even scarcer.

Finally, the idea of a future hyperspectral intercomparison exercise was discussed.

Actions from breakout group 1

1. Update of database: Lesley Clementson will add further HPLC and phytoplankton absorption data to the international AEsOP database from new sources (e.g. LOV, Tara Oceans, non-duplicated data from MAREDAT) and time series data from BATS and HOT. Lesley to follow-up with dataset holders following the meeting, data to be included by Dec 2014.
2. Bob Brewin to send out an invitation via the IOCCG list to new algorithm developers to participate in the intercomparison by Dec 2014.
3. (a) SeaWiFS L2 and OC-CCI L3 match-ups will be extracted. Initially validation on L2 will be compared with L3 to see if there is a major difference in results and then a decision will be made on whether to use L2 or L3 going forward. Bob Brewin, SeungHyun Son and Jeremy Werdell to generate and evaluate match-ups by Jan 2015. Matchup satellite data extraction should include the solar zenith angle (SZA) and region/province as ancillary information to help further analysis.
   (b) SCIAMACHY match-ups to be generated by Astrid Bracher by Jan 2015.
   (c) Bob/Seunghyun/Jeremy to provide match-ups to PFT algorithm developers for algorithms to be applied (including radiance/reflectance data plus derived satellite IOPs) by Jan 2015.
4. Output received from algorithm developers, including output for each processing stage that requires validation (e.g. AOPs/IOPs, pigments, PFTs) by April 2015 in order to provide something in time for the IOCS meeting.
5. First results from algorithm validation against match-ups, organized by region/province, output type (e.g. fraction, concentration, dominance) for each type that can be validated

against HPLC, including both the global spatial analysis and a time-series analysis. To be produced by Sam Lavender and Bob Brewin by the IOCS meeting (June 2015).

6. Show preliminary results at IOCS in an intercomparison project side meeting (Astrid Bracher: write email to Venetia Stuart for room by Nov 2014; Bob Brewin and Samantha Lavender to organize, Astrid Bracher, Nick Hardman-Mountford and Taka Hirata can help).

Breakout group 2: Work plan to prepare for validation of future missions

Chair: Aurea Maria Ciotti; rapporteur: Alison Chase. Participants: Heidi Sosik, Astrid Bracher, Stewart Bernard, Colleen Mouw, Taka Hirata, Tiffany Moisan, Ewa Kwiatkowska, Emmanuel Devred, Cecile Dupouy, Jeremy Werdell, Guangming Zheng.

Locations

The group discussed the need for collecting *in situ* data on PFTs from all types of measurements, providing well-resolved information about the phytoplankton community, biologically and optically. It was suggested that a number of locations could be selected for both local time series sites and larger areas that are repeatedly visited. Consideration was given to the dynamic range of phytoplankton community in different regions in relation to the sensitivity of different approaches of satellite retrieval on PFT information as different sets will be usefully retrieved from deep-water versus coastal locations. Some algorithms are global and some regional. What are needed are proof-of-concept locations to provide *in situ* data to validate regional algorithms. Arctic and coastal regions are likely to have strong location specific characteristics, so a global algorithm is unlikely to be as useful as regional approaches for these locations. The Arctic will be challenging for retrieving satellite match-ups due to cloud cover and will be different between coastal and deep water Arctic locations. Proximity to ice (high albedo, adjacency issues?) is also a consideration of polar sites. While coastal sites are easier to access and maintain, not all time series sites should be coastal, restricting deep-water work to repeat transects. Nonetheless, having high resolution and high-quality data in coastal sites should be useful for improving and developing new retrieval methods, as well as informing broader spatial data sets. Locations will likely need to leverage existing time series sites and also repeat transects and ships-of-opportunity – together these will provide both spatial and temporal variability. The following existing sites that could provide the basis for PFT validation locations were listed:

- In deeper water, established locations such as HOT and BATS (and other OceanSites) could be leveraged to add more measurement types.
- An Arctic observatory is planned by the AWI group (gliders and stationary platforms).
- The Martha's Vineyard Coastal Observatory site is relatively coastal but not always case 2. It has high resolution data on phytoplankton, both in time and automated taxonomic identification, from the Imaging FlowCytobot. This is supplemented by basic fluorometry,

hydrography, other physical parameters and multiband radiometry; a HyperSAS may be added in future. HPLC is measured ~once-twice per month. It is lacking in high temporal resolution IOPs.

- [The Western Channel Observatory (WCO) operated by PML in the UK and the Australian Integrated Marine Observing System (IMOS) may also provide useful sites]

Choice of locations will also need to be informed by the benefit they provide with regard to user needs and reducing uncertainties. It is important to note the need for taxonomists to attend all the sites. Choices for high latitude and coastal locations need further discussions.

There would need to be some level of standardization between sites with regard to measurement protocols but also in post-processing, calculation of uncertainties and QA/QC procedures.

Requirements

Different definitions of functional types will have different user requirements and different validation requirements. Users include modelers and direct users of products in operational agencies as well as researchers. The justification for the products and hence the *in situ* measurements needs to be based on addressing these requirements in a focused way. Funding justification for long term measurements is always difficult so this justification is critical.

Core products will need to include measures of carbon, size (classes, fraction, particle distribution), Chl *a* and other pigments and some level of taxonomic composition. Not all parameters required by users will be directly measurable so consideration should be given on how to make conversions between quantities to derive e.g. carbon estimates of different size classes.

Phytoplankton size classes are not necessarily well defined, for example some researchers consider the nano-phytoplankton low-end cut-off at 2μm as less than ideal. As well as the three main size classes that are resolved by PFT algorithms (micro, nano, pico), there may be user requirements for an intermediate size class between nano and pico: the ultraplankton. Is it possible to derive this size class from satellite? Measures of the particle size distribution (PSD) would provide better resolution of the size structure, but it is more difficult to measure. If the slope of the PSD is obtained, the size structure can be separated as required. However, determining one slope is difficult; a Junge slope does not work well with phytoplankton, only total particles.

Although the current three-size class approach proposed by Sieburth et al. (1978) does not fully capture the phytoplankton size structure, it has pragmatic value so is considered to be worth retaining currently. The new data sets to be constructed must allow for an eventual re-definition of number and size limit of these classes. Comparison of size-fractionated HPLC and absorption data can also be helpful as long as the physical separation of phytoplankton communities followed the same protocol, including not only pore filter sizes but also types of filters. Hyperspectral data may be of benefit in providing greater taxonomic resolution however, this requires further investigation, because the optimal spectral resolution needed for detecting PFTs is presently unknown. Generally, further discussion and protocol work is needed.

Measurements

Consideration of the measurements required for validating PFT algorithms produced the following list.

- Size-fractionated measurements of both HPLC pigments and particulate light absorption.
- Measurements of phycobilin concentrations, equally in size fractions, to the suite of pigments (for *Synechococcus*, cryptophytes, *Trichodesmium*)
- FlowCytobot/FlowCAM/flow cytometry (both traditional and imaging)
- Radiometry, both above water and in-water, hyperspectral
- Inherent optical properties (absorption, backscattering, VSF)
- Particle size distribution (PSD, e.g. via LISST)
- Size-fractionated measurements
- Genetics/-omics

All these measurements need to be connected back to what is observable from remote sensing, as there are many things to measure in the field that we cannot hope to sense with satellites. Again, this underlines the importance of knowing the user requirements.

Substantial effort will be required not just to collect data but also to analyze and interpret it. Comparison of the distinct approaches such as FlowCytobot, FlowCAM, pigments and particle imaging will be required to understand uncertainties derived by each kind of measurement.

Data Management

The large amount of data generated by particle imaging technologies (FlowCytobot, FlowCAM) requires a consideration for the optimum database format. A workshop focused on how best to use this type of data (e.g. share codes, data uses, etc.) would be useful, perhaps as part of the IOCS protocols follow-on activity. It was recommended that a series of workshops based on different aspects of phytoplankton observation were organised in conjunction with the IOCS protocols activities. The most urgent need was thought to be for a particle characterization workshop.

Taxonomy data needs particular consideration to archive and curate (e.g. Tree of Life). Aggregation of taxonomic data into higher level groups (e.g. all diatoms) will be important for algorithm validation, but the best choice for ideal groups are unknown. The hierarchical organization and grouping of data can be built into the annotation/metadata scheme, and a number of participants stressed the need for giving some flexibility to the data sets and eventual groups that will be used as metrics for PFT characterization. Data storage potential at existing repositories and standardized formats/protocols for archiving are also considerations.

Recommendations:

1. Locations. While some locations have been suggested, no specific locations are recommended so far as more work is needed to define requirements. Currently several locations are estimated as being required. This may be an issue to take forward as a splinter session at IOCS-2015.

2. Measurements. The following measurements were identified as required for PFT validation:

- Standard HPLC protocols plus protocols for phycobilin measurements
- Flow cytometry and FlowCytobot / FlowCAM
- Inherent optical properties (e.g. absorption, backscattering, VSF)
- Hyperspectral radiometry (both above and in-water)
- Particle size distribution (PSD, e.g. via LISST)
- Size-fractionated measurements of HPLC and phycobilin pigments and absorption
- Genetic / -omics data

An intercomparison of methods / instruments over several years at a few sites would be important to understand our capabilities to fully characterize the phytoplankton community. In these events, a more detailed sampling, including a number of suggested size-fractionation of the different variables, would be performed.

3. Workshops and person effort are required, particularly in the following areas:

- Techniques for particle analyses, characterization and classification
- Engagement with modellers and understanding end-user requirements
- Data storage and management, standards for data contributors, data challenges

Action:

An IOCS splinter session on future directions for PFT remote sensing (including a link to genetics / -omics) that engages the users community is needed (Colleen Mouw, Astrid Bracher, Nick Hardman-Mountford will propose a splinter session).

Session 7: Possibilities for sustaining ongoing PFT algorithm validation and intercomparison activities

Chair: Nick Hardman-Mountford, rapporteur: Tiffany Moisan

This session focused on the presentation of the agencies requirements for PFT validation and discussion of the possibilities for sustaining ongoing PFT algorithm validation and intercomparison activities" (Goal 3 of the workshop).

Talk 1: ESA-EUMETSAT

The talk was presented by Ewa Kwiatkowska. ESA has delivered ocean color data obtained by the MERIS instrument which was onboard ENVISAT (2002-2012), and plans to launch its next ocean color sensor, the OLCI instrument, onboard Sentinel-3 in 2015.

There is no PFT activity using MERIS. The latest processing (3rd processing) of MERIS was completed in 2011 and another processing (4th) in 2016 is under preparation. The core products include: water leaving radiance, algal pigment indices, total suspended matter, colored detrital and dissolved material absorption and photosynthetically active radiation (PAR). Document available http://earth.esa.int/handbooks. MERIS validation team has a match-up dataset for these products: http://hermes.acri.fr/mermaid/home/home.php.

OLCI/Sentinel3 launch is planned for September 2015, and EUMESAT operates the Marine Branch. There is no core activity on PFT. OLCI is similar to MERIS and the ocean colour products include: water leaving reflectance, algal pigment indices, total suspended matter, the absorption of coloured dissolved material (CDOM) and PAR. More details available at https://earth.esa.int/web/sentinel.

Nonetheless, ESA has a project on PFT starting in December 2014, led by Astrid Bracher. The contract is to develop synergistic OC products around PFT classes using SCIAMACHY and MERIS and eventually OLCI and TROPOMI.

Routine validation for ESA ocean color products is performed with operational platforms such as BOUSSOLE, AERONET-OC, bio-Argo etc. The Sentinel-3 Validation Team has been formed by a rolling call which is continuously open, but no funding is provided from ESA or EUMESAT. Currently 90 teams contribute from Europe and around the globe, in which 40 are ocean color teams. Validation Team activities include: measurement round robins, SI traceability, standardization and education as well as calibration of field instruments.

EUMESAT/EC data service development requires (1) definition of requirements, (2) service specification and (3) technical requirements. Now the EC is going through these processes for later Copernicus satellites. ESA/EUMESAT requires the definition of user requirements, algorithm development, product definition and validation.

Talk 2: JAXA

The talk was presented by Takafumi Hirata on behalf of Hiroshi Murakami. JAXA plans a launch of the SGLI instrument onboard GCOM-C1 satellite in 2016, otherwise early 2017, under the Global Change Observation Mission – Climate (GCOM-C) mission. The SGLI 10 bands are in near-ultraviolet to visible wavelengths. In the GCOM-C mission, there are 14 ocean products. The products are classified into 2 groups, namely standard products and research products. The standard products are defined as products required to achieve mission goals and suitable for operational data distribution. The research products are defined as products still in research phase and not necessarily ready for operational data distribution (i.e. “evaluation products”). PFT dominance (including occurrence of “red tides”) is one of the research products in the GCOM-C mission. Validation of the satellite products is planned using HPLC pigment analysis for defining in situ PFTs. A proposal for a field campaign was submitted for post-launch validation of PFTs derived from SGLI/GCOM-C1. JAXA’s requirements are (1) PFTs must be defined by means of routinely measurable quantities, (2) the definition must have been documented or published, (3) PFTs must be validated globally with a sufficient number of in situ data, (4) PFT algorithm is expected to return a sufficient number of outputs, (5) uncertainty of the PFTs is expected to be known.

Talk 3: KIOST

The talk was presented by Jong-Kuk Choi. There is an activity to develop PFT algorithms for GOCI, using both abundance-based and optics-based approaches. In an abundance-based approach, HPLC pigment data with Diagnostic Pigment Analysis (DPA) is used to define PFTs. A correction scheme for the DPA is under development. For the optics-based approach, the spectral absorption coefficients for 3 size fractions are under investigation. HPLC pigments as well as size-fractionated Chl a and the spectral absorption coefficient has been obtained from seven field campaigns around Korea. It is unclear at this time whether GOCI is going to have PFT development as a mainstream project.

Talk 4: NOAA

The talk was presented by Paul DiGiacomo. NOAA has a strong focus on Integrated Ecosystem Assessments and Ecosystem-Based Approach to Management, with an increasing emphasis on developing ecological forecasting services. In this context, accurate, timely, consistent and fit-for-purpose PFT and PSC data/products will support NOAA and related users for ongoing coastal, ocean and inland water application, especially fisheries and marine resource management. These applications include documenting, monitoring and forecasting the response of marine ecosystems to environmental variability and climate change, assessing biodiversity and examining variations in PFT abundance and distribution patterns temporally & spatially, vis-à-vis biogeochemical cycles and food quality, food-web structure and secondary/tertiary production.

Currently, PFTs/PSCs in the northeast are under investigation using phytoplankton pigments derived from ocean color measurements. The activity also uses in situ HPLC pigments and taxonomy data to determine the best way to use these data. In particular, PSC information is being used to investigate fisheries production potential in models.

NESDIS Center for Satellite Applications and Research (STAR) will be working with users to develop PFT and PSC products. VIIRS Cal/Val cruises led by NESDIS, starting in November 2014 on the R/V Nancy Foster, will provide valuable opportunities to collect suitable validation data. Additional periodic NESDIS sampling in Chesapeake Bay and other regions, as well as cruises led by OAR working with NMFS on ocean acidification impacts, will afford additional validation opportunities.

Talk 5: NASA

This talk was given by Jeremy Werdell. NASA is supporting more innovative optical techniques to identify phytoplankton functional types by increasing spectral resolution of their satellite sensors and changing the temporal resolution of observation of ecological events. Satellite sensors will be able to give unprecedented coverage of harmful algal blooms and carbon cycle events such as bloom conditions of different PFTs. A parallel program is ongoing to observe and analyze methods of detection of changes in the magnitude and spectral changes for backscatter and absorption. While each of the mission concepts are unique in nature, satellite coverage will provide new and innovative approaches to observing PFTs.

A hyperspectral (~5 nm) imager, with greater spatial resolution than prior ocean color missions, is the planned ocean color sensor for the Pre-Aerosol, Clouds, and ocean Ecosystem (PACE) Mission that is expected to launch no later than 2023. The PACE mission will collect global ocean color measurements on global ocean ecology and biogeochemistry (e.g. carbon cycle) along with possible polarimetry measurements to obtain coherent observations on clouds and aerosols. Expanding our understanding of the impacts and feedbacks of the Earth system to climate are of critical importance for this mission. Another sensor to be proposed is the Geostationary Coastal and Air Pollution Events (Geo-CAPE; http://geo-cape.larc.nasa.gov/). The Geo-CAPE mission was recommended by the NRC's Earth Science Decadal Survey to measure tropospheric trace gases and aerosols and coastal ocean phytoplankton, water quality and biogeochemistry from geostationary orbit while providing multiple daily observations. Multiple observations per day are required to explore the physical, chemical, and dynamical processes that determine tropospheric composition and air quality over spatial scales ranging from urban to continental, and over temporal scales ranging from diurnal to seasonal. The Hyperspectral InfraRed Imager (HyspIRI) mission will study the world's ecosystems and provide critical information on natural disasters such as volcanoes, wildfires and drought. HyspIRI will be able to identify the type of vegetation that is present and whether the vegetation is healthy. The mission will provide a benchmark on the state of the world's ecosystems against which future changes can be assessed. The mission will also assess the pre-eruptive behavior of volcanoes and the likelihood of future eruptions as well as the carbon and other gases released from wildfires.

Session 8: Final discussion and formulation of actions

Chair: Astrid Bracher, rapporteur: Tiffany Moisan

During the final discussion we went through the goals set for the workshop and discussed if we have moved forward. It was decided that within the first morning Goal 1 (Provide a summary assessment of currently available global PFT / PSC products, based on outputs of the 2nd PFT intercomparison WG and PFT validation data sets and strategies also including specific applications) was met. To move towards Goal 2 (Provide a PFT validation strategy considering different applications of the products: community consensus on data sets and analysis protocols) the first two break-out sessions defined clear near future actions. For Goal 3 (Discuss possibilities for sustaining ongoing PFT algorithm validation and intercomparison activities) it became clear that, to some extent, the agencies will support the activities by way of the meetings / workshops recommended by the two breakout groups.

The PFT workshop ended with a desire to define the user community and engage them in another workshop to transition algorithms into agency-supportable products. Understanding the requirements of operational models, forward thinking models (e.g. Follows et al. approaches), coastal models, and their relationship to radiative transfer models was identified as a priority. Generically, the group decided that it required input on requirements from an operational model which serves an agency and several research-type models with defined goals. Gaining this knowledge will require an engagement with fisheries agencies, ecosystem modelers, and people working within the Harmful Algal Bloom community in order to learn user requirements before

development of the PFT products. The applications for PFT development using satellite remote sensing would serve both the HAB and water quality communities. Major initiatives are going on now in several governmental agencies such as NASA, NOAA, ESA, JAXA and KIOST. Currently, there is much discussion on how to move forward on ecosystem-based management. The PFT community expects user requirements to evolve over time and will be in a continuous process to reach a consensus approach. In addition, the community needs to give an action to agencies for formal assessment. For larger funding concerning validation and intercomparison activities, the link to the PFT/PSC satellite product user community must be clarified and emphasized as a first step. It was stated that the detailed user requirements will evolve over time and will be a continuous process and we need a consensus approach. There is a need to give an action to agencies for formal assessment which then will result in evidence of the user need for PFT/PSC products.

Finally, the following actions were stated and responsible persons were selected regarding recommendations from the specific break-out groups and plenary discussions.

Action items regarding outcome of break-out group 1

(Break-out group 1: Validation of current global PFT algorithms - restated from Session 6)

1. Update of database: Lesley Clementson will add further HPLC and phytoplankton absorption data to the international AEsOP database from new sources (e.g. LOV, Tara Oceans, non-duplicated data from MAREDAT) and time series data from BATS and HOT. Lesley to follow-up with dataset holders following the meeting, data to be included by Dec 2014.
2. Bob Brewin to send out an invitation via the IOCCG list to new algorithm developers to participate in the intercomparison by Dec 2014.
3. (a) SeaWiFS L2 and OC-CCI L3 match-ups will be extracted. Initially validation on L2 will be compared with L3 to see if there is a major difference in results and then a decision will be made on whether to use L2 or L3 going forward. Bob Brewin, SeungHyun Son and Jeremy Werdell to generate and evaluate match-ups by Jan 2015. Matchup satellite data extraction should include the solar zenith angle (SZA) and region/province as ancillary information to help further analysis.
   (b) SCIAMACHY match-ups to be generated by Astrid Bracher by Jan 2015.
   (c) Bob/Seunghyun/Jeremy to provide match-ups to PFT algorithm developers for algorithms to be applied (including radiance/reflectance data plus derived satellite IOPs) by Jan 2015.
4. Output received from algorithm developers, including output for each processing stage that requires validation (e.g. AOPs/IOPs, pigments, PFTs) by April 2015 in order to provide something in time for the IOCS meeting.
5. First results from algorithm validation against match-ups, organized by region/province, output type (e.g. fraction, concentration, dominance) for each type that can be validated against HPLC, including both the global spatial analysis and a time-series analysis. To be produced by Sam Lavender and Bob Brewin by the IOCS meeting (June 2015).
6. Show preliminary results at IOCS in an intercomparison project side meeting (Astrid Bracher: write email to Venetia Stuart for room by Nov 2014; Bob Brewin and Samantha Lavender to organize, Astrid Bracher, Nick Hardman-Mountford and Taka Hirata can help).

Action items regarding outcome of break-out group 2

(Breakout group 2: Prepare for validation of future missions, new expertise (methods and people))

1. Propose (by 31 Dec 2014) IOCS splinter session on PFT future directions (link to genetics, users); Colleen Mouw, Astrid Bracher (help: Nick Hardman-Mountford)
2. For the 1st recommendations concerning the implementation of ~10 ocean observatory locations with capability for the full suite of measurements required for PFT and PSC validation (as defined in the recommendations) a workshop will be organized. As a first step, the IOCS II PFT splinter session on PFTs should discuss which locations are possible, what efforts have to be taken to achieve this goal and how method standardization (e.g. round-robins) among sites can be implemented.
    1. For the 2nd recommendation to hold workshops on techniques and human effort for advancing and standardizing other PSC/PFT, focusing on:
        (a) Techniques for particle characterization, classification
        (b) Modeling and end user requirements
        (c) Data storage and management, standards for data contributors, data challenges

        → as a first step, it should be investigated if/how agencies can support these workshops and funding be obtained as part of a collaborative effort.

    The following people will approach the agencies within the next few months:
    Tiffany Moisan and Jeremy Werdell with NASA
    Paul DiGiacomo with NOAA
    Stewart Bernard with IOCCG
    Taka Hirata with JAXA
    Jong Kuk Choi with KIOST
    Astrid Bracher with ESA/EUMETSAT)
    Aurea Maria Ciotti with FAPESP/Brazil (only after IOCS meeting)

    All will discuss at IOCS PFT splinter meeting collaborative funded possibilities.

Other Action items

1. Access for all to IOCCG PFT WS Dropbox; lead Astrid (closed 27 Oct 2014)
2. Report to ESA/EUMETSAT user link / need for PFT products incl. PFT specification on 3. Dec 2014; see above: Astrid Bracher
3. Intercomparison activities finalized and linked to data producers (lead: Tiho, Taka; finalized Nov 2014) – then peer-review Paper send to all data products contributors (Dec/Jan), submission April 2015. After that the code for all participating algorithms should be published in one unified place, with documentation – data on which we are now basing intercomparison should be published in PANGAEA or something similar, so that all authors are always properly cited.
1. Guide may take form of ESSD paper WITH the data & possibly code there.
2. Participant list with email address by 30 Oct; Astrid (closed)
3. Reference User group (Stewart, Nick will work on it) by beginning Nov
4. Write and publish report as NASA technical memo (if IOCCG agrees)

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List of Acronyms

AERONET-OC	Aerosol Robotic Network – Ocean Color
AEsOP	Australian waters Earth Observation Phytoplankton-type products
AMT	Atlantic Meridional Transect
AOP	Apparent Optical Properties
AWI	Alfred-Wegener-Institute Helmholtz Center for Polar and Marine Research
BATS	Bermuda Atlantic Time-series Study
BCRE	Bayworld Centre for Research & Education
BioSOPE	Biogeochemistry and Optics South Pacific Experiment
BOUSSOLE	BOUée pour l'acquiSition d'une Série Optique à Long termE ("buoy for the acquisition of a long-term optical series")
CDOM	Colored dissolved organic matter
Chl *a*	Chlorophyll *a*
Chl *b*	Chlorophyll *b*
Chl *c*	Chlorophyll *c*

CMIP5	Coupled Model Intercomparison Project Phase 5
CPR	Continuous Plankton Recorder
CSIR	Council for Scientific and Industrial Research
CSIRO	Commonwealth Scientific and Industrial Research Organisation
DFT	Discrete Fourier Transform
EM	Electron Microscopy
ENVISAT	Environmental Satellite
ESA	European Space Agency
ESSD	Earth System Science Data
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
GCOM-C	Global Change Observation Mission - Climate
GEO	Global Earth Observation
GEOHAB	Global Ecology and oceanography of Harmful Algal Blooms
Geo-CAPE	GEOstationary Coastal and Air Pollution Events
GeP&Co	Geochemistry, Phytoplankton, and Color of the Ocean
GSFC	Goddard Space Flight Center
HAB	Harmful Algal bloom
HOT	Hawaii Ocean Time-series
HPLC	High Performance Liquid Chromatography
HU	Hokkaido University
HyspIRI	Hyperspectral Infrared Imager
IOCCG	International Ocean Color Coordinating Group
IOCS	International Ocean Color Science
IOP	Inherent Optical Properties
IRD	Institute of Research for Development
JAXA	Japan Aerospace Exploration Agency
KIOST	Korea Institute of Ocean Science and Technology
LISST	Laser In-Situ Scattering and Transmissometry
LOV	Laboratoire d'Océanographie de Villefranche-sur-Mer
MAREDAT	MARine Ecosystem DATa
MERIS	MEdium Resolution Imaging Spectrometer
M.I.O.	Mediterranean Institute of Oceanology
MODIS	Moderate Resolution Imaging Spectrometer
NAP	Non-algal particles

NASA	National Aeronautics and Space Administration
NESDIS	National Environmental Satellite, Data, and Information Service
NMFS	National Marine Fisheries Service
NOAA	National Oceanic and Atmospheric Administration
NRC	National Research Council
OAR	Oceanic and Atmospheric Research
OLCI	Ocean Land Colour Instrument
PACE	Pre-Aerosol, Clouds, and ocean Ecosystem
PC	Phycocyanin
PE	Phycoerythrin
PFT	Phytoplankton Functional Type
PML	Plymouth Marine Laboratory
PSC	Phytoplankton Size Class
SCIAMACHY	SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY
SeaBASS	SeaWiFS Bio-optical Archive and Storage System
SEAHARRE	SeaWiFS HPLC Analysis Round-Robin Experiment
SeaWiFS	Sea-Viewing Wide Field-of-View Sensor
S_f	size factor
SFF	Size fractionated filtration
SGLI	Second generation GLobal Imager
TChl *a*	Total Chlorophyll *a*
TROPOMI	TROPOspheric Monitoring Instrument
UDal	Dalhousie University
VIIRS	Visible Infrared Imaging Radiometer Suite
WHOI	Woods Hole Oceanographic Institute
a	total absorption
a_p	particulate absorption
a_g	dissolved matter absorption
a_{ph}	phytoplankton absorption
b_p	particulate scattering
b_{bp}	particulate backscattering
c_p	particulate beam attenuation