Supporting *In situ* & Space Based Measurements Workshop

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BACKGROUND

In situ bio-optical global and coastal measurements have a critical function in the development of remote-sensing algorithms and statistical models that convert radiometric measurements (water leaving radiance or surface reflectance) to geophysical data products (chlorophyll *a* and others). The quality of these conversion algorithms cannot be better than that of the data sets of ocean properties used to create them. The applicability of these algorithms to different oceanic locations (clear ocean basins or turbid coastal waters) requires that the *in situ* data sets be representative of conditions in these locations. The continuity and consistency of the global and regional remote-sensing data sets are a direct reflection of the continuity and consistency of the *in situ* measurements used to calibrate and validate them.

All funded data collections are critical to advance NASA Ocean Biology and Biogeochemical research, as well as modeling efforts and advanced planning. Current challenges are as follows:

- Current submitted data are often not "complete datasets" of bio-optical and atmospheric measurements;
- Data collected often do not follow the NASA Ocean Optics Protocols for Satellite Ocean Color Sensor Validation (Mueller and Fargion, 2003). New measurements do not use agreed-upon community protocols and are not standardized;
- Collections of in situ data funded by NASA are required to be submitted to the official repository, but no delivery times are specified.

The NASA Ocean Optics Protocols for Satellite Ocean Color Sensor Validation were intended to provide standards, which if followed carefully and documented appropriately, would assure that any particular set of optical measurements would be acceptable for ocean color sensor validation and algorithm development. Close adherence to these protocols is the most straightforward way for an investigator to establish a measurement that is uncontaminated by artifacts and is accurate enough to meet the requirements of satellite ocean color product validation. Furthermore, these protocols identify a standard set of measurements that develop consistency across the variety of satellite ocean color missions either launched or scheduled for launch in the SeaWiFS and SIMBIOS era (1997-2003). It should be noted that some of the *in situ* instruments used are now considered to be obsolete, representing designs developed over 15 years ago. Today measurements such as pCO_2 don't have established or agreed-upon protocols. Many standard measurements do not yet have agreed-upon protocols (filter counts). NASA and the research community have recognized the need to update these protocols.

In addition, over the past ten years, synoptic ocean color research discoveries have raised new scientific questions and research challenges. From these scientific advancements NASA HQ has engaged the research community to develop comprehensive plans for current and future spaced-based missions. As a consequence of the 2005 NASA Ocean Color Research Team Meeting, a group of volunteers began discussions about what research needed to be done within the framework of the NASA Ocean Biology and Biogeochemistry research program during the next few decades, particularly utilizing satellite remote sensing. The goal of this group was to form two plans: an Advanced Plan for Research and a Calibration/Validation Plan, which would be integrated with the first plan. Emerging Scientific Questions addressed in the Advanced Plan for NASA OBB Program are:

1. How are ocean ecosystems and the biodiversity they support influenced by climate or environmental variability and change, and how will these changes occur over time (from “Earth’s Living Ocean”, page 11)?
2. How do carbon and other elements transition between ocean pools and pass through the Earth System, and how do these biogeochemical fluxes impact the ocean and Earth’s climate over time (from “Earth’s Living Ocean”, page 15)?
3. How (and why) is the diversity and geographical distribution of coastal marine habitats changing, and what are the implications for the well being of human society (from “Earth’s Living Ocean”, page 20)?
4. How do hazards and pollutants impact the hydrography and biology of the coastal zone? How do they affect us, and can we mitigate their effects (from “Earth’s Living Ocean”, page 25)?

WORKSHOP SUMMARY

The workshop was held in Montreal (Canada) before the Ocean Optics XVIII Conference from October 6 (afternoon) to October 7, 2006. The workshop agenda is presented in Table 1. There were a total of 18 participants representing the US and international science communities (Table 2).

While water leaving radiance accuracies are fundamental to future remote sensing observations, they are not enough. Classic ‘ocean color’ bands were not optimized for spectral matching algorithms and are not adequate for fully resolving the multitude of unique optical properties associated with specific in-water constituents. Enhanced measurement capabilities are necessary, both in spectral range and spectral resolution. Furthermore there are different scientific questions and research challenges. NASA would like a “new-revised” priority list of *in situ* parameters across the NASA OBB Program. The following important issues need to be assessed: (a) time frame within which we can hope to have "reliable" measurements (immediate, short- mid- long-term) for these parameters; (b) veracity of the measurement methods—i.e., how good are the instruments and protocols?—and (c) what are the instrumentation options and costs?

A majority of the workshop PIs suggested that the recommended *in situ* parameters should go beyond a purely calibration/validation satellite program. The participants discussed and considered:

1. That remote sensing science requirements and the related field validation program must be linked to the requirements of the modeling community and can be augmented to provide additional data for model parameterization.
2. The scientific questions addressed in the Advanced Plan for NASA OBB Program (2006); and
3. The utility of upcoming satellite missions like National Polar-orbiting Operational Environmental Satellite System (NPOESS) and the Ocean Carbon, Ecosystems, and Near-Shore (OCEaNS) not-yet-approved mission.

Several presentations were made on the first day of the workshop (see agenda and presentations in Appendix A) after which the group had an open discussion. A selection of notes of some of the more noteworthy material presented and discussed on the first day follows:

1) Modeling

The group felt that remote sensing science requirements and the related field validation program must be linked to requirements of the modeling community and could be augmented to provide additional data for model parameterization. However, different models have different requirements, and many, if not most, biological models do not take into account specific *in situ* bio-optical measurements. Spatial and temporal variability of the observations are required if the development of assimilation methods are desired. Very little research has been done on biological data assimilation. Physical models use assimilation methods based on statistical approaches.

Following, the group recognized a disconnect between what modelers want and what we produce. Dialog is needed, but it should be mutually cooperative (versus a scenario where modelers are dictating only the factors that they need). Clarification is needed about which modeling community (e.g., optical, biogeochemical, ecosystem, circulation modelers) will be interfacing with this group. However, modelers often desire datasets that simply can not be produced and their requirements are often unclear. Modelers often want differential measurements (rates), co-variances, coarse spatial scales, and consistent processing (as a lowest common denominator, they don't want to see change due to algorithm differences) and, models have reduced accuracy requirements in comparison to field validation studies.

Therefore, an open question is whether or not two climate datasets are needed: one for modelers and one for everyone else – that is, one for climate products and one for research studies.

It was generally agreed that the parameters used in physical-modeling are approaching maturity while the biological parameters (bio-optics) are still in their infancy. There is a risk that the mature overpowers the infant and works to its detriment. However, biological parameters tend to be very sensitive to some physical parameters (such as heat flux/mixing), and therefore they cannot be completely ignored.

The following questions were raised:

- What is the goal? The ability to accurately forecast (operational scenario) or to properly understand the processes?
- Are the Advance Planning questions supported by our science and the modeling community ? Are we on track to answer these questions? Which current or future missions support which questions?
- What are the modelers' impressions of our time-series? Answering this question helps build a foundation of support for new missions.
- Can there be give-and-take with the modeling community?

It was generally agreed that we need to start simple, with simple fusing of data products (e.g., overlay currents on color), before we move to full-blown bio-physical models. The group recommended a modeling (1 and 3D) workshop in the future.

2) Phytoplankton Functional Groups

There was a general discussion of a definition of PFTs and their importance. PFTs are groups of several phytoplankton species, which have in common a specific function:

- Biogeochemistry:
  - Pico-autotrophs [Chlorophytes, Prochlorococcus and Synechococcus]
  - N2-fixers [Trichodesmiums and N2-fixing unicellular prokaryotes]
  - Calcifiers [Coccolithophorids]
  - DMS-producers [Phaeocystis and small autotrophic Flagellates]
  - Mixed [autotrophic Dinoflagellates and Chrysophyceae]
  - Silicifiers [Diatoms]
- Primary production and export:
  - pico-phyto (< 2 μm) [Chlorophytes, Prochlorococcus and Synechococcus]
  - nano-phyto (2-20 μm) [Chromophytes, Nanoflagellates, Chryptophytes]
  - micro-phyto (> 20 μm) [Diatoms, Dinoflagellates]

PFTs have different impacts on climate (as they are a biological pump of CO_2, and a biogenic source of DMS) and they have different sensitivities to climate change (e.g., temperature, acidification). Knowledge of PTFs is very important at regional scales (e.g., HABs, higher trophic systems and fisheries).

Little is known about the relationship between PFTs and IOPs, PFT remote sensing is difficult because: (a) ocean color depends to the first order on the chlorophyll concentration; (b) current operational ocean color sensors have limited spectral resolution and atmospheric correction accuracy; and (c) *in situ* datasets are too sparse at global coverage for algorithm validation.

The question was raised as to whether or not PFTs can be identified from space. Purely empirical relationships are currently used, which are difficult to verify. Hyperspectral measurements may be needed, but subtle features may prevent identification even with perfect spectral resolution – that is, physical spectra may not contain sufficient information to separate functional groups. Further research is needed to ascertain whether or not this is possible.

3) SIMBIOS Lessons Learned and Future Funding

From SIMBIOS we have learned that *in situ* field programs must:

- accurately sample relevant measurements
- regularly review how well they can be measured
- make observations across a wide range of biological/biogeochemical provinces
- sample *in situ* observations according to agreed-upon protocols and relate observations to community measurement standards
- compare vicarious instrument calibration results with on-orbit methods

- drive the precision of the *in situ* measurements and the accuracy of the algorithms by the covariance of properties
- push advanced instrumentation development and ongoing instrument performance evaluations
- support calibration and data analysis round robins; and provide these data to a centralized data center

A question was raised as to whether or not the future integrated interdisciplinary measurements would be done via a team collection model or by individual PIs. The SIMBIOS team participated in the ACE-Asia and INDOEX interdisciplinary experiments, but was not a major player. SIMBIOS campaigns were add-ons (not among the original proposals), and therefore had limited funding, space, bunks and ship time. No workshops were held before or after on how to work-up the interdisciplinary data that was collected.

Regarding NASA the SeaWiFS Bio-optical Archive and Storage System (SeaBASS) data holdings (http://seabass.gsfc.nasa.gov/), the question was raised as to whether it is better to have global distributions with fewer parameters, or detailed measurements on localized scales? It was strongly felt that both approaches needed to be taken. However, as a first step, existing data needed to be analyzed and reviewed (e.g., temporally and spatially distribution), and then studies planned to fill in the data gaps (where data may be available, but not included yet in SeaBASS). Discussions followed on how to encourage and enforce delivery. A proposal was to provide assistance to investigators, (e.g., through the GSFC group) who do not have resources to process and deliver data. Another proposal was to establish workshops and funding to bring investigators together to compare data (e.g., IOP data).

Data reprocessing presents challenges for both PIs and data archives. It is difficult to maintain the quality of long-term datasets, because processing methods change over time, and additional time and funding is often needed to reprocess data with modern methods. Data processing is typically a much more involved and complex task than data collection, e.g., chlorophyll measurements. In addition, the science of processing methods is still evolving. PIs may discard and update data, but communication is required to facilitate updates of data in the archive.

4) Aerosol optical properties

It was generally agreed that atmospheric aerosol optical properties are a key to the success of atmospheric correction over the oceans. Aerosol optical parameters (measured, retrieved, and/or modeled) are crucial for atmospheric correction procedures. Current atmospheric aerosol models should be updated; available atmospheric aerosol optical data over the oceans (acquired through the AErosol RObotic NETwork (AERONET) and SIMBIOS programs) should be summarized and utilized in the atmospheric correction algorithms. New ship-based and island-based measurements are required in order to fill the gaps for particular geographic areas and for validation activities. AERONET information is available at http://aeronet.gsfc.nasa.gov/.

On the second day participants discussed several topics, such as whether to start from space-based capabilities and work down, or start from science goals and work up. Under general consideration was what new measurements needed to be supported in order to exploit the potential of new remote sensing systems (e.g., the hyperspectral Ocean Radiometer for Carbon Assessment (ORCA) instrument). In addition, is it more important to enhance existing capabilities (such as improve the utility of SeaWiFS) or support forthcoming technology (such as ORCA). The group agreed to the following approach: 1) define the question; 2) define the parameters needed; 3) determine priorities; 4) determine what can be measured with current or future sensors or *in situ* programs; and 5) determine what new measurements are needed.

The four scientific questions listed in the Advanced Plan for NASA OBB Program and carbon was identified as the link among them. The major science carbon themes are atmosphere-ocean CO_2 exchange; marine ecosystem-biogeochemical dynamics; and ocean carbon cycle and climate. Carbon missions considered by the group were:

- MODIS, SeaWiFS
- VIIRS
- Advanced/future missions
    - multi-spectral/hyperspectral LEO UV to SWIR
    - hyperspectral GEO, high spatial resolution
- LIDAR (particle abundance, mixed layer)

The group discussed and identified the following straw man parameter list:

- Chlorophyll, PP, POC, PIC, DOC, carbon export, TSM and TOM, T, S, oxygen, PAR, PFTs (phyto and non-algal) – diatoms, pico, cocco, tricho, dino. CDOM, pCO2 – DIC/alkalinity, beam-c particles, PSD and nutrients .

The group made the following overall recommendations:

- Collect a_cdom with all chlorophyll.
- Collect species counts with HPLC pigments.
- Collect radiometry (AOPs and IOPs) into the UV (300-800nm).
- Need full radiometric radiance distributions.
- Need volume-scattering functions.

In the afternoon the participants broke-up into three groups: (1) AOP and IOP measurements, (2) Primary Production and (3) characterizing standing stocks of seawater constituents including particle functional types. Each group discussed the feasibility/accuracy of the *in situ* measurement methods for each parameter; and the time frame within which we can hope to have "reliable" measurements (immediate, short- mid- long-term) for the parameters. Here we present, as given, some of the more noteworthy material discussed by the subgroups:

AOP AND IOP MEASUREMENTS BREAKOUT REPORT

Contributions from Arnone, Maritorena, McClain, Morel, Stramski, Voss and Zaneveld

It is recommended that several apparent and inherent optical properties be measured in support of current and future calibration/validation activities and algorithm development and validation. It is recommended that apparent and inherent optical properties be measured in the 300-900 nm range with the highest possible spectral resolution to take advantage of:

- the better separability of absorption components in the UV;
- the use of NIR in coastal waters; and
- to support advanced atmospheric correction schemes.

It is also recommended that vertical profiles are measured rather than just sub-surface measurements. Protocols for some of the AOP and IOP measurements need to be documented or updated. This mostly concerns acdm measurements with the new ultrapath capillary waveguide technique (Miller et al., 2002) and backscattering measurements. It is strongly suggested that a workshop to look into acdom measurement protocols (waveguide, spectrophotometry, and fluorescence) and associated issues (sensitivity in oligotrophic waters, derivation of slopes, etc) be organized in the near future. It is also timely to organize a workshop on backscattering instruments and measurement protocols. It would also be of major interest to look into VSF and PSD measurements during such a workshop. Operational definitions of the component absorption terms and backscattering should be revisited to take into account the fact that the filtering techniques involved in these determinations are not fully consistent (the ~0.7 to ~0.2 micron fraction is not accounted for).

Data submitted to SeaBASS must contain metadata that would allow reprocessing.

When possible, it is also important that the local spatial and temporal variability of a fixed station is assessed using gliders or by the tow-yo technique.

Recommended IOPs and AOPs to be measured are listed below. It is highly recommended that as many as possible of the properties listed below are measured together.

- AOPs

Lu, Ed, Es, Eu, Kd, KPAR. KPAR can be obtained with either a PAR sensor with a cosine collector or by integrating the Ed spectra if the spectral resolution of the measurements is sufficient. It is recommended that both approaches be employed simultaneously, so that one forms a check on the other.

The upward spectral radiance distribution is also required to address BRDF issues and to validate existing BRDF correction schemes (Morel et al., 2002). Because of the technical and instrumental difficulties associated with these measurements, it is acknowledged that at this point only a few investigators will be able to make these measurements. The investigators having the most complete expertise (e.g. Voss & Chapin, 2005) on the subject should continue their measurements and work toward validating a BRDF correction procedure that can be used by other investigators.

- IOPs

IOP	Instrument/method	Issues - comments
a total	AC-9 AC-S Spectrophotometry Integrating cavity	• Calibrations • Post-processing information (Salinity, temperature, corrections, volume filtered) must be in SeaBASS metadata • Vertical distribution (spectrophotometry covers the whole wavelength range from UV to NIR but samples at discrete depths. AC-9 like instruments do not cover the whole spectral range but make complete vertical profiles).
ap, aphy, ad	AC-9 (w/ filter) AC-S (w/ filter) Spectrophotometry Integrating cavity	• Methods for *ad*: Kishino et al., (1985), Tassan & Ferrari (1995) and spectral decomposition. • Beta value or correction scheme, filtered volume must be in SeaBASS metadata
acdom	Fluorometry Capillary waveguide Spectrophotometry AC-9 (w/ filter) AC-S (w/ filter) Integrating cavity	• Calibration. • Protocols. • Sensitivity in oligotrophic waters • Pure water • Slope calculation, zero value, how far in the UV.
b	AC-9 (w/ filter) AC-S (w/ filter) Transmissometer	• Calibrations • It is recommended that VSF and/or PSD is also measured with *b* or *bb*. • Pathlengths • Post-processing information (Salinity, temperature, corrections, volume filtered) must be in SeaBASS metadata
bb	Hydroscat ECoVSF VST (?) B. Balch's method LISST	• Method for *bb*: Balch et al. (2004) • Calibrations • It is recommended that VSF and/or PSD is also measured with *b* or *bb*. • Spectral characteristics, measurement angle(s) should be specified. • When reporting c-meter data one should always report the aperture of the instrument. For example the LISST and the c-star have very different apertures and will give different results.
c	AC-9 AC-S Transmissometer	• Calibrations • Path-lengths

PRIMARY PRODUCTION BREAKOUT REPORT

Contributions from Balch, Behrenfeld, Chavez, Letelier and Mitchell.

Central points of the PP breakout group revolved around alternative approaches to modeling production and how these different approaches give rise to some common and some divergent observational requirements. The two fundamental approaches discussed involve the description of productivity as a function of (1) carbon and growth rate and (2) chlorophyll or absorbed light and light utilization efficiency. These relationships are:

PP = phytoplankton carbon biomass * growth rate. (1)

or

PP = absorbed light * light utilization efficiency (2)

In both cases, PP = standing stock * rate. Improvements in either approach will require information on, or observations of:

- Mixed layer light levels, which are a function of the physiological mixing depth, spectral downwelling sunlight, and spectral attenuation,
- Phytoplankton absorption,
- Temperature, and
- Nutricline depth, which is helpful for describing changes in photosynthetic efficiencies, subsurface structure of phytoplankton pigment and biomass, and export or ‘new’ production.

Field observations should aim to measure all of the above properties simultaneously and should obviously be accompanied by measurements of carbon fixation (^{14}C). It is also recommended that consideration/measurements should be given/made of the photosynthetic energy invested into calcium carbonate structures - which influence 14C measurements and are an important factor in carbon export from the photic zone to depth.

Solar simulated fluorescence or variable fluorescence measurements were also recommended in support of developing productivity algorithms and for understanding observed physiological variability. It is not recommended that such measurements be used in a quantitative manner to estimate photosynthetic performance, but rather as an index for identifying regional differences in nutrient constraints.

The traditional approach for estimating productivity is described above by (2) (e.g., Morel 1991, Longhurst et al. 1995, Balch et al. 1992, Behrenfeld & Falkowski 1997). The carbon-based approach (1) is a new alternative that will benefit from an expanded suite of observations for its development. The basis of this approach involves estimating phytoplankton carbon biomass from measures of light scatter and growth rates from carbon: chlorophyll ratios (Chl:C) (Behrenfeld et al. 2005). In the field, phytoplankton carbon is perhaps best related to particulate beam attenuation coefficients (c_p) and it is recommended that measurements of c_p following well-defined protocols be considered a standard component of field productivity studies and data bases. For satellite remote sensing, particulate backscatter coefficients (b_{bp}) will need to replace c_p as the index of phytoplankton carbon. Accordingly, b_{bp} measurements should also become a standard field measurement and integrated into productivity databases. Only recently have sensors for measuring b_{bp} become easily available. Protocols for collecting accurate b_{bp} data must be developed as soon as possible, particularly continuous measurements conducted on surface flow-through systems as such techniques are less well developed than protocols for vertical profile measurements.

The relationship between b_{bp} and phytoplankton carbon is not a universal constant and is influenced by the shape of the particle size distribution and the contribution of scattering components that do not covary with phytoplankton biomass. Thus, it is recommended that field productivity studies supporting satellite carbon-based algorithm development include measurements of particle size distributions and, to the degree possible, observations that help resolve the contribution of different light scattering constituents. Work is also needed on developing new approaches for measuring phytoplankton carbon biomass in the field. Such studies may be based on microscopic approaches, optical approaches, or other schemes. Routine measurements of phytoplankton carbon measurements have eluded biological oceanographers for decades and support should be given for developing innovate new approaches.

Additional supporting measurements for the carbon based approach should include 14C-based estimates of productivity and, when possible, measurements of chlorophyll per cell or fluorescence per cell for specific phytoplankton groups from flow cytometric systems.

The second component of the carbon based approach is the estimation of phytoplankton growth rates from phytoplankton Chl:C. Two of the primary factors influencing the relationship between Chl:C and growth rate are nutrient stress and photoacclimation. Accordingly, field campaigns should conduct measurements to assess these important terms. Nutrient stress is a difficult issue to resolve, but information on types of nutrient limitation (e.g., iron vs nitrogen vs other) will be beneficial, as well as broader proxies such as nutricline depth. Assessments of photoacclimation states will require accurate characterization of mixed layer light conditions, thus measurements of mixed layer depth, spectral attenuation, and incident irradiance. Clearly, measurements of phytoplankton growth rates in the field are also needed and technique development efforts are required. Approaches to assessing phytoplankton growth rates may include dilution experiments or estimates based on genetic approaches (e.g., fraction of population at different cell cycles states). Measurements of growth rates in the field will also be important for assessing maximum potential growth rates for natural phytoplankton assemblages, one of the important parameters in the carbon-based approach.

Finally, further analyses of historical laboratory study results and new laboratory studies are needed to improve our understanding of variability in phytoplankton Chl:C ratios and their link to growth rates and environmental forcing factors (e.g., nutrients, light, temperature). Such analyses should aim to understand how such relationships vary between taxonomic groups as well as within a given species.

PARAMETERS FOR CHARACTERIZING STANDING STOCKS OF SEAWATER CONSTITUENTS INCLUDING PARTICLE FUNCTIONAL TYPES

Contributions from Stramski and Moulin

Given the complexity and the large amount of parameters discussed, the authors discussed first the individual parameters, and then the status of measurement techniques and protocols. Below is presented, as given, the material discussed by the subgroup.

3.1. Standing Stock Parameters:

(1) Chlorophyll *a* and Other Pigments
(2) DOC (Dissolved Organic Carbon)
(3) POC (Particulate Organic Carbon)
(4) PIC (Particulate Inorganic Carbon)
(5) TSM (Total Suspended Matter)
(6) PIM (Particulate Inorganic Matter defined as a non-combustible fraction of TSM)
(7) POM (Particulate Organic Matter derived as a difference TSM-PIM)
(8) DIC (Dissolved Inorganic Carbon) and Alkalinity
(9) Nutrients
(10) PSD (Particle Size Distribution)
(11) PFTs (Particle Functional Types)

With regard to this list of parameters we have two explanatory notes.

Note #1: We recommend to broaden the concept of PFTs from Phytoplankton Functional Types to Particle Functional Types. The enhanced concept of Particle Functional Types includes not only the Phytoplankton Functional Types but also Non-Phytoplankton Particle Types (such as various kinds of non-living particle types, heterotrophic microorganisms, and viruses). The various particle types that belong to both living and non-living categories, play distinctively different roles in ocean biogeochemistry and optics, which includes distinctively different roles in carbon cycling and ocean color signal. This is the primary reason for why a new paradigm based on a more detailed description of seawater composition in terms of various Particle Functional Types (rather than the oversimplified traditional description in terms of a few broadly or vaguely defined particle categories) is needed to create advancements and long-term growth opportunities in ocean color science and applications.

Note #2: CDOM is not on our list of parameters because the current proxy for CDOM standing stock is the absorption coefficient $a_{\mathrm{CDOM}}(\lambda)$, which is part of the IOP list.

3.2. Status of Measurement Techniques and Protocols

Parameters 1 through 9

With regard to parameters (1) through (9), the measurement techniques are available and have been used for a number of years. The protocols for these parameters have been described and published in NASA Technical Reports, JGOFS publications, and/or journal articles. We recommend revisiting and updating these protocols, if warranted. We also point out that details of methodology for measuring these parameters can differ between labs and investigators. For example, the treatment of samples for TSM and PIM may be different and it is not necessarily obvious or known which treatment is best. These issues must be taken into account when preparing revised or new protocols for the purposes of the OBB program at NASA. Nevertheless we feel that a consensus on recommending the present state-of-the-art methodology for measuring the parameters (1) through (9) can be reached relatively easily. We should be aware, however, that the techniques for some, if not all of these parameters are still evolving and will likely improve with time, which will require revisiting and updating the protocols in the future.

Parameter 10 (PSD)

With regard to the Particle Size Distribution (PSD), the current status of measurement methodology appears to be much more complicated. There is no single method or single principle of measurement that would allow sizing of marine particles over the entire range of particle sizes that are biogeochemically and optically important, that is from the order of 10 nm to the order of 1 cm. Even if we consider a restricted range of particle sizes, for example from ~1 μm to ~100 μm, there exists a variety of measurement techniques and there is no well-established consensus amongst scientists in terms of which technique provides best results.

Under these circumstances our present recommendations with regard to PSD measurements must be naturally based on pragmatic and feasibility criteria. As a short-term goal (~3 - 5 years) we recommend to focus our efforts on developing consistent protocols for sizing particles with several types of instrumentation that are already available commercially and used by a number of labs within our research community. We also recommend a workshop to examine PSD measurements and methods with these different instruments in conjunction with the use of different instrumentation/methods for light scattering measurements. This recommendation is consistent with that provided by the IOP/AOP subgroup. We also suggest the development of guidelines for submitting the PSD data to the NASA database. Because the PSD data are scarce, we feel that it might be worth considering the possible submission and assembly of historical PSD data that are in possession of some investigators.

The instrumentation and methodology for particle sizing of particular interest at this stage of planning includes: (i) the Beckman-Coulter Particle Counter which is a bench-top instrument utilizing the electrical resistance of particles as a principle for sizing, (ii) the Sequoia LISST instrument which can be operated both *in situ* and as a bench-top instrument. The principle for sizing with LISST is based on the inversion of the optical scattering (forward diffraction pattern), and (iii) particle imaging and sizing with FlowCam instrument or with more traditional microscopy analysis. The particle size covered by these three techniques ranges from about 1 μm to hundreds of micrometers with significant overlap between the techniques. This size range includes a major portion of biogeochemically and optically important particles, but not all. A large portion of colloidal (submicron) particles (most abundant particles in the ocean with significant impact on biogeochemistry and optics) is not covered by the three techniques mentioned above. We also note that these three techniques are not particularly well suited for characterizing the largest suspended particles (flocs, aggregates, fecal pellets, marine snow particles from hundreds of micrometers to > 1 mm), which dominate sinking particulate matter (albeit there is a special version of LISST that extends the range of measurement to large flocs). In addition, we do *not* suggest that our near-term efforts on PSD measurements and development of protocols necessarily be limited to the use of the three instruments only, that is the Beckman-Coulter, LISST, and FlowCam. The important point of our recommendation is that these three types of instruments represent totally different principles for particle sizing; i.e., electronic sizing of individual particles with Coulter, inversion of optical diffraction produced by the bulk particulate assemblage with LISST, and camera-based imaging of individual particles for subsequent sizing analysis with FlowCam. We feel that it will be essential to combine these different methods of particle sizing to ensure the best possible results. We are also aware that there exist other instruments that use these three principles as well as other principles for particle sizing but they are less commonly used by oceanographic community at the present time.

A comment is in order on particle sizing with commercial flow cytometers. In our recommendation above, we have *not* included commercial flow cytometers as a core instrument/method for PSD measurements. This has been done by purpose because the principle of particle sizing with commercial flow cytometers is, in our opinion, *not* rigorous enough. The commercial flow cytometers should, however, play an important role in providing information on abundance of different particle (phytoplankton) functional types and their approximate particle sizes (see below). On the other hand, the custom-built flow cytometers may meet the criteria of scientific rigor for PSD measurement but this issue has been beyond the scope of our discussion.

In the mid- and long-term (>5-30 years), the most significant challenges in PSD measurements appear to exist on both ends of the particle size spectrum, that is within the submicrometer size range (colloids) and within the largest suspended particles being > hundreds of micrometers in size (particles such as large flocs, aggregates, fecal pellets, etc.). Very rare attempts of PSD measurements within the colloidal size range utilized electron microscopy technique. The studies of large particles have also been relatively rare and they typically rely on the use of large custom-built devices for *in situ* particle imaging. At present it would be premature to suggest including these types of measurements in the NASA list of required or recommended parameters. Nevertheless we strongly emphasize that the variability and the roles of these smallest and largest particles in the overall particle size distribution in the ocean are poorly documented and understood. The colloids and marine snow particles have implications to ocean optics, ocean color, and biogeochemical processes, so an increased basic research along with engineering efforts are needed to ensure a development of capabilities for characterizing these "elusive" groups of particles in the future.

Parameter 11 (i.e., the suite of yet undefined or poorly/incompletely defined parameters for characterizing PFTs)

The progress in measurements and characterization of Particle Functional Types (PFTs) including Phytoplankton Functional Types and Non-Phytoplankton Particle Functional Types has great potential for advancing the ocean color science and applications, especially in the mid- to long term (> 5-30 years). At present, our measurement capabilities are limited mostly to targeting the bulk properties of the entire particle assemblage, i.e., TSM, or the bulk properties of broadly-defined particle categories such as phytoplankton, organic particles, and inorganic particles, i.e., Chl *a*, POC, and PIM, respectively. The various PFTs that play specific roles in biogeochemistry and optics typically require tedious methods of analysis of seawater samples or are not amenable to direct measurements at all, so further advancements in measurement methodologies are needed. Also, the concepts and criteria for defining specific PFTs and specific parameters for quantifying the various PFTs require further research and discussion to achieve a broader consensus within the science community. We expect that the report that is now being prepared by the IOCCG Working Group on PFTs (led by C. Moulin) will provide a useful synthesis of concepts related to Phytoplankton Functional Types, measurement methods for characterizing or quantifying these types, and the present status of our capabilities for retrieving information about these types from ocean color. Non-phytoplankton particle types will *not* be addressed in the IOCCG report, however.

The PFTs will hopefully remain to be an active area of research in the years to come. With the growing basic knowledge of PFT properties, the range of information on PFTs and the methodology of retrieving this information from ocean color is expected to evolve. With regard to Phytoplankton Functional Types our present recommendation is to continue collecting data on the suite of pigments with HPLC method. These pigment data can serve as a basis for determining the presence or dominance of Phytoplankton Functional Types. At this time we do *not* suggest the submission of information about Phytoplankton Functional Types derived from HPLC pigments to the NASA database because there is no unified or unambiguous methodology for converting pigment data into PFTs. The access to HPLC data through the NASA database will simply make it possible for investigators to explore or use different methods for this purpose.

We also suggest considering data obtained with various instrumentation such as flow cytometer, FlowCam, or microscopes as an important source of information on PFTs, and possibly initiating the submission of these data to the NASA database. We point out that such data are not yet routinely collected during ocean color-related experiments. As an example, the flow cytometry data may include information on the abundance of prokaryotic picoplankton types and small eukaryotic phytoplankton types. The FlowCam data may include images of many types of individual particles present within the water sample, which can be used for taxonomic analysis of phytoplankton and microzooplankton, and possibly also for the estimation of non-living particles. This method can presently provide useful particle images in the size range above ~5 μm, so it covers the nano- and microplankton size ranges. The guidelines for preparing flow cytometry, FlowCam, or microscopy data sets for submission to databases and the question of whether the NASA database is appropriate for archiving these types of data deserve further discussion. Some of these data (such as microscopy-based phytoplankton taxonomy) may be available in limited amounts within other databases such as JGOFS. Nevertheless it seems worthwhile to consider creating a "new home" for such data sets and initiating their storage in some consistent pre-defined formats, especially that these data are scarce and do not appear to have been widely available to the science community at large.

With regard to non-phytoplankton particle functional types (i.e., heterotrophic plankton, various types of non-living particles such as organic colloids, clay or silt-sized minerals, organic detritus including small-sized particles as well as large flocs/aggregates, etc.), we believe that significant research efforts over many years to come are needed before we will be able to go beyond a few bulk parameters providing merely approximate information about these particles in a very general sense. For example, the bulk parameters TSM, POC, and PIM included in our list (see section 1) can provide approximate information about the contribution of organic and inorganic particles to the mass concentration of the total suspended particulate matter. We note that these bulk parameters are not even sufficient to allow partitioning of organic particulate matter into living and non-living fractions. At present no reasonable approach exists to allow such partitioning. Another example of a bulk proxy of non-phytoplankton particles is the absorption coefficient $a_d(\lambda)$ commonly referred to as the detrital absorption, which is now obtainable from measurements on particles upon bleaching treatment. The limitation of the operational definition of $a_d(\lambda)$ is that a great variety of particles can contribute to $a_d(\lambda)$, such as bacteria and other heterotrophic organisms, minerals, organic detritus, and even some cellular matter present within phytoplankton cells. In this particular example of $a_d(\lambda)$, the broad range of particle types contributing to $a_d(\lambda)$ but playing very different roles in biogeochemistry and optics is an obvious limitation for the use of $a_d(\lambda)$ in ocean color applications. We must realize, however, that in the near future we will have no choice but to accept the limitations and to use the combination of the bulk proxies (such as TSM, POC, PIC, a_d) as a source of approximate information on the composition of particulate matter.

We believe that a strong need for basic research on PFTs (including both phytoplankton and non-phytoplankton particle functional types) should be recognized at NASA and the community at large as a vital component and prerequisite for long-term (>10-30 years) advancements of ocean color science and applications. It is obvious that the performance of any algorithm based on ocean color signal depends on natural variations in the detailed composition of optically significant seawater constituents. There is already enough scientific evidence in our databases to say that surpassing the present limits of accuracy of ocean color (in-water) algorithms or creating reasonably accurate algorithms for new data products is unlikely, if not impossible, unless basic research picks up a pace along a new paradigm in which seawater consists not just of a few broadly-defined constituent categories but of a larger number (perhaps 10-20) of cleverly-defined constituents, each of which plays distinctive and different role in seawater optics, biogeochemistry, and ocean color. To support this statement, we can give just one example related to our discussion of particle functional types. The present-day models, algorithms, and methods of data interpretation in the areas of optics and ocean color treat normally *all particles*, or *all phytoplankton specie*s, or *all non-phytoplankton particles* as a *single particulate component*. This is a big problem because such single particulate component consist in reality of a great variety of particle types. As an example, the non-phytoplankton particulate component includes different particle types such as viruses, bacteria, clay minerals, larger-sized minerals, and organic detritus of various sizes from tiny colloids to large flocs and aggregates. These different particle types have not only different function in biogeochemistry including carbon cycling but, importantly, they also differ dramatically in terms of their optical properties and their contributions to ocean color signal (e.g., the optical cross-sections of particles differ by many orders of magnitude among these particle types). Therefore, even relatively small variations in the detailed composition of particulate matter (i.e., variations in the proportion of the abundance of various particle types) can produce sizable variations in the IOPs of seawater and ocean color signal. This obviously has implications to ocean color algorithms and their performance.

In conclusion, we think that undertaking a dialogue between the various funding agencies (from the US and abroad) and the representatives of science community with a purpose of creating specific initiatives and incentives for basic research and development of new measurements in these areas with high potential for breakthrough advancements in ocean color science in the long-term (~20-30 years) is highly desirable. One important objective of these new research initiatives would be to bring back a balance between: (i) applied-oriented efforts, (ii) basic research focused on short-term benefits, and (iii) basic research focused on producing major or breakthrough advancements in the long term. Whereas the applied-oriented and near-term basic research activities are, at present, supported and emphasized comparatively strongly, the long-term oriented basic research is largely neglected and undermined, especially in the US. This does not seem like a "healthy" condition for the ocean color science in the long run, and this is why we have focused some of our considerations on this issue in this report.

Phytoplankton Carbon

Phytoplankton carbon is an important parameter that is not currently observable or easily derivable. At the meeting in Montreal there was a discussion that emphasized a need to make progress in this area, indicating a few possible avenues for this progress. W. Balch pointed out that there exists a traditional method of converting the phytoplankton cell size (more specifically, cell volume) to cellular carbon content. This method has been proposed in 1960s and has been used by oceanographers since then, although not often. In this method the cell size is typically determined from microscopic analysis of samples and then the cellular carbon is calculated using a cell volume-to-carbon conversion factors. The traditional microscopic analysis is tedious because it requires identifying and sizing of many individual cells. The newer techniques of particle imaging and analysis (for example, FlowCam) could improve this situation.

Nevertheless, this traditional method has a major weakness because of significant interspecies and intraspecies variability in the cell volume-to-carbon conversion factors (Mullin et al. 1966; Strathmann 1967; Moal et al. 1987; Nagata and Watanabe 1990; Verity et al. 1992; Montagnes et al. 1994; Stramski 1999). The intraspecies variability is associated with changes in physiological status of cells in response to varying environmental conditions (such as light, nutrients, temperature). In practice, the values of the conversion factors must be determined in advance in laboratory studies with cultures, but then in field applications we actually never know whether these factors are applicable to cells from a given seawater sample. The main consequence is that the natural variability in the cell volume-to-carbon conversion factors can produce large errors in the final estimates of phytoplankton carbon obtained with this method. In our opinion, this traditional method cannot be recommended as a reliable method supporting ocean color programs.

An alternative methodology for determining phytoplankton carbon was indicated by D. Stramski. The basic principle of this methodology relies on the relationship between the refractive index of biological cells and the intracellular carbon concentration. This relationship has solid basis, is relatively robust, and is expected to show only weak sensitivity to interspecies and intraspecies variability. The proof-of-concept study with two phytoplankton species was described in Stramski (1999) and further support was provided by a study of several species in DuRand et al. (2002). Whereas this method was demonstrated so far in lab experiments using instrumentation such as spectrophotometer, particle counter, and flow cytometer, the development of a similar capability for field applications seems feasible. The main requirement of this method is to be able to measure simultaneously the particle size and light scattering pattern (possibly also absorption) on individual particles. In principle, the information from these measurements can then be used to determine the cellular carbon content (as well as the cellular chlorophyll *a* content) on a per particle basis, and consequently to determine the phytoplankton carbon pool as well as the distribution of carbon among different particle types/phytoplankton groups. This concept represents an example of novel research area that can lead to breakthrough advancements with large impact on ocean color science and applications. We also note that the third possible approach for estimating phytoplankton carbon was indicated by M. Behrenfeld, which is addressed in the section of the report prepared by the Primary Production subgroup. In conclusion, we recommend a continuation of this discussion of the methodologies for estimating phytoplankton carbon and investment of resources to explore more full innovative approaches to this fundamental problem in the ocean biology and biogeochemistry sciences. This could possibly involve creating a working group of investigators to focus on this issue and to coordinate relevant discussion.

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Table 1: Participant List
Supporting *In situ* & Space Based Measurements Workshop

Robert Arnone Naval Research Laboratory, Stennis Space Center, MS 39248 E-mail: arnone@nrlssc.navy.mil	William M. Balch Bigelow Laboratory for Ocean Sciences 180 McKown Point Road W. Boothbay Harbor, ME 04575 U.S.A. E-mail: bbalch@bigelow.org
Michael J. Behrenfeld Dept. Botany Plant Pathology Oregon State University Cordley Hall 2082 Corvallis, OR 97331 E-mail:mjb@science.oregonstate.edu	Paula Bontempi NASA Headquarters 300 E St., SW Washington, DC 20546 E-mail: paula.s.bontempi@nasa.gov
Francisco Chavez, MBARI 7700 Sandholdt Rd Moss Landing, CA 95039 E-mail: chfr@mbari.org,	Giulietta S. Fargion CHORS, San Diego State University, 6505 Alvarado Rd., Suite 206 San Diego, CA 92120 E-mail: gfargion@chors.sdsu.edu
Bryan A. Franz, SAIC, Ocean Biology Processing Group Earth Sciences Division Greenbelt, MD 20771, USA E-mail: bryan.franz@gsfc.nasa.gov	Ricardo M Letelier COAS - Oregon State University 104 COAS Admin Bldg Oregon State University Corvallis, OR 97331-5503 E-mail:letelier@coas.oregonstate.edu
Stéphane Maritorena ICESS 6841 Ellison Hall UCSB Santa Barbara, CA 93106 E-mail: stephane @icess.ucsb.edu	Charles R. McClain GSFC, NASA Ocean Biology Processing Group Earth Sciences Division Mail Code 614.8 Greenbelt, MD 20771, USA E-mail: Charles.R.McClain@nasa.gov
B. Greg Mitchell Scripps Institution of Oceanography, UCSD 9500 Gilman Drive La Jolla CA, 92093-0218 E-mail: mitchell@spg.ucsd.edu	Andre Morel Observatoire Océanologique de Villefranche Laboratoire d'Océanographie de Villefranche B.P. 08, 06238 Villefranche-sur-mer FRANCE E-mail: morel@obs-vlfr.fr
Cyril MOULIN Laboratoire des Sciences du Climat et de l'Environnement CEA Saclay - bat.712 91191 France E-mail: cyril.moulin@cea.fr	Alexander Smirnov Goddard Earth Sciences & Technology Center, UMBC code 614.4, Greenbelt, MD 20771 E-mail: asmirnov@aeronet.gsfc.nasa.gov
Dariusz Stramski Marine Physical Laboratory Scripps Institution of Oceanography University of California at San Diego La Jolla, CA 92093-0238 E-mail: dstramski@ucsd.edu	Kenneth J. Voss Physics Department University of Miami Coral Gables, Fl. 33124 E-mail: voss@physics.miami.edu
P. Jeremy Werdell Science Systems & Applications, Inc. Ocean Biology Processing Group Earth Sciences Division Greenbelt, MD 20771, USA E-mail: jeremy.werdell@gsfc.nasa.gov	J. Ronald V. Zaneveld WetLabs 620 Applegate St. Philomath, OR 97370 E-mail: ron@wetlabs.com

Table 2: Agenda

Supporting In Situ & Space Based Measurements Workshop
Delta Centre-Ville
777 University Street, Montréal, Quebec
October 6, 2006

14:10 Welcome. P. Bontempi
14:20 Opening Remarks and Goals. G. Fargion
14:40 AERONET & Upcoming Measurements Over the Oceans. A. Smirnov
14:45 Phytoplankton Functional Types. C. Moulin
15:05 Road Map for Integrating Ocean Color into Models. B. Arnone
15:25 European Ocean Color Climate Data Sets. A. Morel
15:50 Open discussion focusing on scientific questions, observational requirements, satellite missions and other)
18:30 Adjourn

October 7, 2006

7:30-on Breakfast (Victoria Room - on level C)
8:15 Open discussion focusing on which *in situ* parameters, possible ranking as required, recommended,
10:30 Break
13:30 Lunch at the Hotel restaurant
14:30 Break out group discussion (focusing on feasibility/accuracy of the *in situ* measurement methods for each parameter; the time frame within which we can hope to have "reliable" measurements (immediate, short- mid- long-term) for the parameters.)
16:00 Group reporting & discussion
16:30 Closing comments. P. Bontempi
17:25 Adjournment

APPENDIX A

1. “Supporting in Situ & Space Based Measurements” NASA Workshop: G. S. Fargion
2. AERONET and Upcoming Measurements over the Oceans”: A. Smirnov
3. “PFT from Ocean Color Measurements”: C. Moulin
4. “Ocean Color Climate, a Merging Project: Globcolour”: A. Morel
5. “Modeling Review”: B. Arnone

"SUPPORTING *IN SITU* & SPACE BASED MEASUREMENTS"
NASA Workshop

Giulietta S. Fargion

***CHORS*, San Diego State University**

Montreal
October 6, 2006

All funded data are critical to advance NASA Ocean Biology and Biogeochemical research, as well as modeling efforts and advanced planning

Presently we have some issues:

- Current submitted data are often not a "complete dataset" of bio-optical and atmospheric measurements;
- Data collected often do not follow the old NASA protocols. New measurements do not use agreed community protocols and are not standardized;
- Measurements are not coordinated;
- Collections of *in situ* data funded by NASA are required to be submitted to the official repository, but no delivery times are specified;

Outline

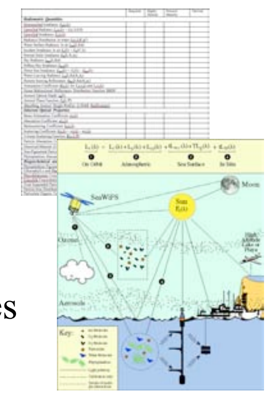
- Background
- Why this Workshop ?
- Lessons learned from SeaWiFS/SIMBIOS
- Highlights of PI contributions
- What we would like
- Agenda and logistics

Scientific Questions

Observational Requirements

Observational Strategies

Satellite Missions

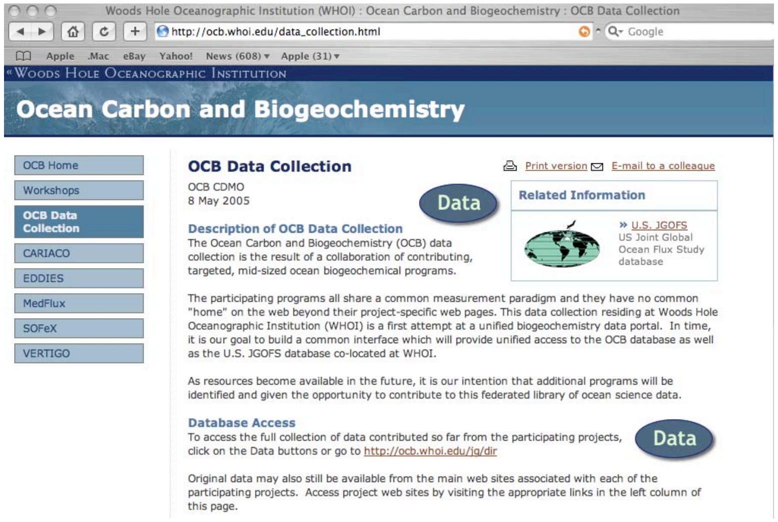


Over the past ten years, synoptic ocean color research discoveries have raised new scientific questions and research challenges.

Why this workshop ?

- We now have different scientific questions and research challenges.
- These recommended *in situ* parameters will go beyond a purely calibration/validation satellite program
- NASA would like a "new-revised" priority list of *in situ* parameters across the NASA OBB Program. We should identify a time frame within which we can hope to have "reliable" measurements (immediate, short- mid- long-term) for these parameters.
- Veracity of the measurement methods needs to be discussed (how good are the instruments and protocols?)
- What are the instrumentation options and costs?

⇨ Will these integrated interdisciplinary measurements be done via a team collection model or by individual PIs ?



SeaBASS ⇔ OCB

Not every parameter !

- When discussing the variables we need to be careful not to reinvent the wheel, and to take advantage of existing efforts. The Ocean Carbon & Biogeochemistry (OCB) Program will be building on the JGOFS and GLOBEC legacies.
- If a federated system between different agencies is envisioned, the an OpenDAP (DODS) server for SeaBASS may be desirable. JGOFS already uses such a mechanism for distributing their data.

Lessons Learned from SeaWiFS & SIMBIOS Programs

Will interdisciplinary measurements be done via a team collection model or by individual PIs ?

- SIMBIOS team participated in the ACE-Asia and INDOEX experiments
- *Lessons learned:*
  - not a major player - we piggy-backed
  - campaigns were add-ons (not in original proposals), and therefore had limited funding
  - limited space, bunks and ship time
  - no workshops before or after on how to work up the interdisciplinary data collected

→ This interdisciplinary data has not yet been fully utilized

In situ field program must:

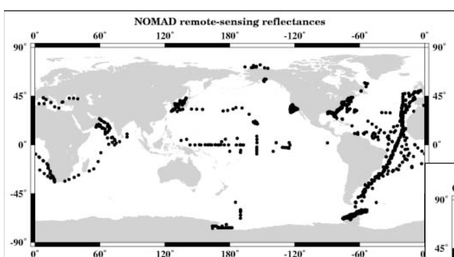
1. Accurately sample relevant measurements;
2. Regularly review how well they can be measured;
3. Make observations across wide range of biological/biogeochemical provinces;
4. Sample *in situ* observations according to agreed protocols and relate observations to community measurement standards;
5. Compare vicarious instrument calibration results with on-orbit methods; The precision of the *in situ* measurements and the accuracy of the algorithms should be driven by the covariance of properties;
6. Push advanced instrumentation development & ongoing instrument performance evaluations;
7. Support calibration and data analysis round robins; and
8. Provide these data to a centralized data center.

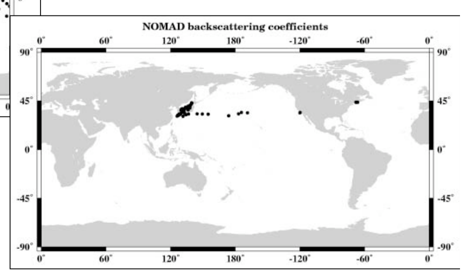
Under SeaWiFS/SIMBIOS, we were following recommended protocols and sampling parameters … some of which were defined more than 10yrs ago

2) We need to re-define a <u>minimum set</u> of parameters

What we have learned…

1) <u>High quality data</u> are needed for both vicarious calibration and product validation. These data must follow sampling, analysis, QC and protocol methods approved by the community.





Impact on Algorithm Development

Majority of PIs suggested that the recommended *in situ* parameters should go beyond a purely calibration/validation satellite program

We need to consider:

1. That remote sensing science requirements and related field validation program must be linked to requirements of the modeling community and can be augmented to provide additional data for model parameterization.

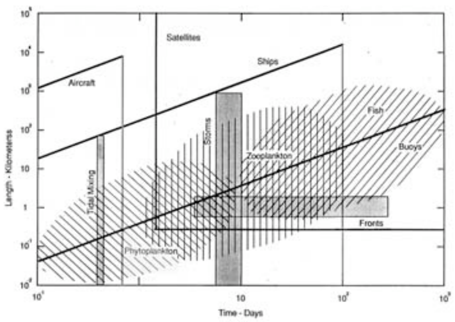
   …. but which modeling community (optical, biogeochemical, ecosystem, circulation) ???

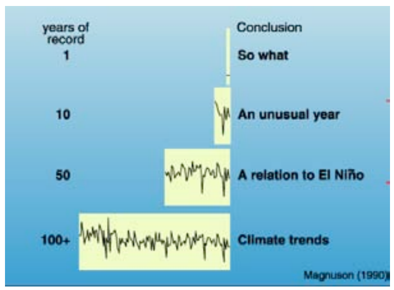
2. The scientific questions addressed in the Advanced Plan for NASA OBB Program (2006);
3. The upcoming satellite missions: OCEaNS, ORCA, NPOESS…

Scientific Questions

Observational Requirements & Strategies :

- What measurements do we need?
- What kind of spatial and temporal resolution do we need in order to “measure” it?
- What observational strategy?
- What do we need to develop?





Not many modelers in the room

- Field validation folks should be talking to the modelers, but it should not be a one-way street where modelers are dictating only the factors that they need.
- Modeling (1 and 3D) workshop in the future to discuss and agree on:
    - » Parameterization of which parameters ?
    - » Evaluation of which parameters ?
    - » Gridded data and available tools
    - » Other

What are the modeling parameters that are required ?

Bob Arnone proposed some requirements for integration and assimilation of the ocean color data into models:

- 1-5 years: Monitoring and assessing present ocean color products (extension of where we are now in algorithms and push into optics). Thrust in atm. correction and vertical bio-optics. This requires *in situ* data for algorithm calibration and validation.
- 5-10 years: *In situ* data for monitoring spatial and temporal variability (i.e., coastal observing systems)
- 10+ years: Assimilation of data streams from satellites into models. Evaluation and validation of models, metrics for model validation and evaluation.

more in Bob’s talk ….

Emerging Scientific Questions for NASA OBB Program

How are ocean ecosystems and the biodiversity they support influenced by climate or environmental variability and change, and how will these changes occur over time?

How do carbon and other elements transition between ocean pools and pass through the Earth System, and how do these biogeochemical fluxes impact the ocean and Earth’s climate over time?

How (and why) is the diversity and geographical distribution of coastal marine habitats changing, and what are the implications for the well-being of human society?

How do hazards and pollutants impact the hydrography and biology of the coastal zone? How do they affect us, and can we mitigate their effects?

What we need to assess for each measurement:

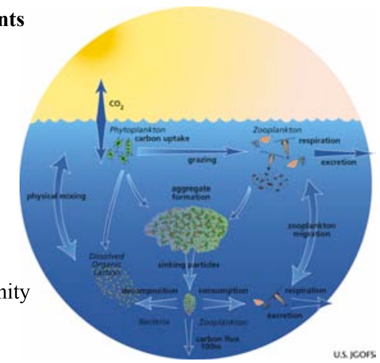
- Veracity of the measurement methods, i.e., how good are the instruments and protocols?
- What space & time sampling strategies apply to each product, i.e., what depths are really required?
- What is the cost for processing a sample?
- What are the instrumentation options and costs?

If we include sporadic phenomena like HABS, how do we get enough data to develop and validate an algorithm?

Ecosystems & diversity, **Carbon & Biogeochemistry,** Habitats & Hazards

Observational requirements:

- **Accurate assessment of ocean BGC constituents**
  - Accurate detection of long-term changes
    - Atmospheric correction…
    - Calibration / validation...
  - Separate optically active components
    - CDOM from Chl…
  - Measure particle biomass
- **Assess ocean productivity & carbon fluxes**
  - Net primary production
  - New & secondary production
  - Physiological status of phytoplankton community
- **Integrate with biogeochemical models**
  - Air-sea CO_2 fluxes
  - Carbon export by both sinking & physical pumps
  - Shelf carbon exchanges



Ecosystems & Diversity, Carbon & Biogeochemistry, Habitats & Hazards

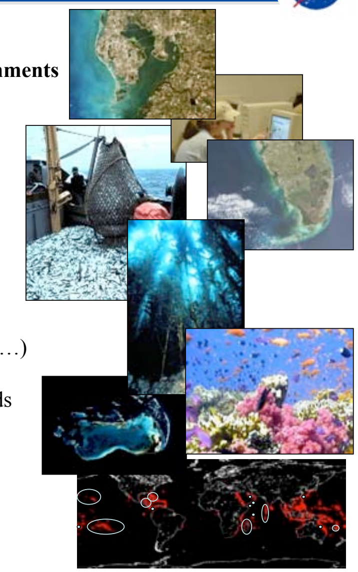
Observational requirements:

- **Accurately determine ecosystem biomass**
  - Accurate detection of long-term changes
    - Atmospheric correction…
    - Calibration / validation…
  - Separate optically active components
    - CDOM from Chl…
  - Global coverage sampling all biomes
- **Assess biodiversity**
  - Phytoplankton functional groups
  - Special phytoplankton species
  - Particle size spectrum
- **Measure ocean productivity**
  - NPP rate determinations
  - Physiological status of phytoplankton community
  - Grazing & secondary production
- **Understand the oceanographic setting**
  - MLD, incident and in situ light levels, SST, SSS, sea level, vector winds, …

Ecosystems & diversity, Carbon & Biogeochemistry, **Habitats** & Hazards

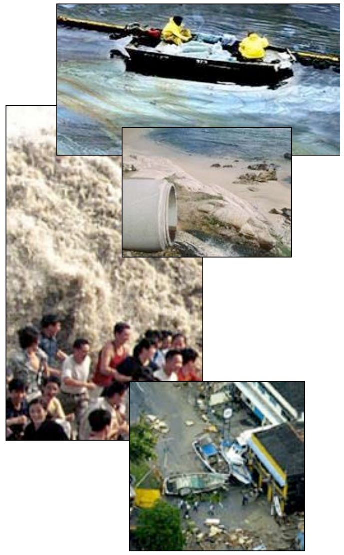
Observational requirements:

- **Assess in-water constituents in coastal environments**
  - Accurate detection of long-term changes
    - Atmospheric correction…
    - Calibration/sensor characterization...
  - Separate optically active components
    - CDOM from Chl…
  - Develop capabilities for all biomes – globally
- **High temporal resolution**
  - Within a day revisit time – tidal phenomena
- **High spatial / spectral resolution**
  - Use existing/upcoming technologies (LDCM, …)
  - New high resolution ocean color capability
    - 10 m – 100 km swath - 20 ocean color bands
- **Understand the coastal ocean setting**
  - Land-ocean interactions – river outflows
  - Tidal & coastal fronts
- **Couple with in situ observations**
  - Ocean observatories
  - Sub-orbital AUV vehicles



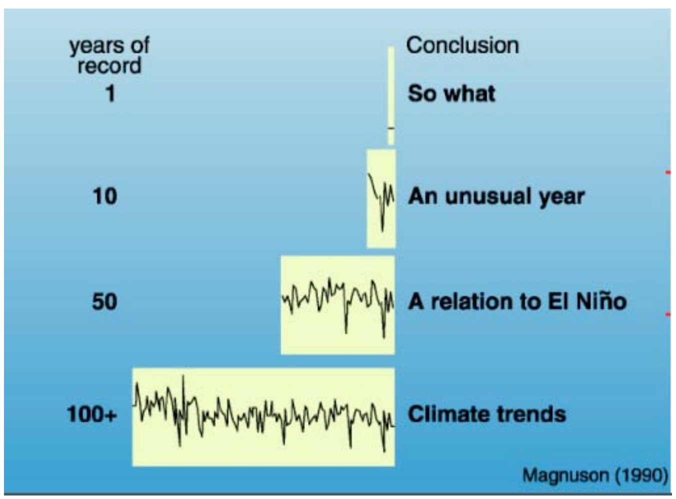
Ecosystems & diversity, Carbon & Biogeochemistry, Habitats & **Hazards**

- **Observational requirements:**
  - **Respond to acute hazards**
    - Instantaneous data dissemination
    - Rapid revisit cycle
    - All weather capabilities –> SAR/UAV's
  - **Assess chronic hazards**
    - Accurately measure ecosystem parameters
      - Atmospheric correction…
      - Calibration/sensor characterization...
    - Separate optically active components
      - CDOM from Chl…
  - **High temporal resolution**
    - Rapid revisit cycle – follow events
    - Use temporary platforms (sub-orbital assets)
  - **High spatial resolutions**
    - Use existing/upcoming technologies (LDCM, …)
    - New high resolution ocean color capability
      - 10 m – 100 km swath



Morel suggestions:

- AOPs
  - Classical [Lu,Eu, Es, Ed (z)] and derived (Rrs,R,K_d,$K_u$$Q_{nadir}$)
  - Upward radiance distribution (BRFD, Q)
  - Surface PAR and K_d (PAR); PAR (z) profiles, euphotic depth Z_{eu}
- IOPs
  - In situ a, b, c (AC-type, preferably hyperspectral), b_b (VSF would be nice)
  - $A_{dissolved}$ (dissolved= CDOM), a_{phyto} and a_{det}
  - Derived quantities: the Chl-specific coefficients such as a^*_p, a^*_{ph}, a^*_{det} and a^*_{CDOM} possibly carbon-specific coefficients
  - Mass specific absorption and scattering coefficient
- Bio-optical parameters (biochemical parameters related to IOPs)
  - Particle size and composition, SPM, POM (combustible fraction)
  - POC, PIC, DOC, PIC (calcite) scattering (Barney's technique)
- Bio-geochemical parameters: all those listed at the OCRT meeting are relevant. Few comments:
  - Better to associate in situ PP meas. with in vitro determination of the physiological parameters (P vs E experiments to provide alpha,P^b_{max}, E_k)
  - Determination of iron concentration, total Fe, and dissolved Fe, Fe-speciation (I or II organic bound or mineral)



Straw man list of *in situ* parameters:

Stramski suggestions:

- SPM (or TSM) - the mass concentration of suspended particulate matter;
- POM - the mass concentration of particulate organic matter; as well as PIM - the mass concentration of particulate inorganic matter obtained as a difference between SPM and POM.
- COC - colloidal organic carbon
- Some elements are present in particulate matter which may be diagnostic of the presence of mineral matter (Al, Si Fe)
- For the future we should move towards PARTICULATE FUNCTIONAL GROUPS, not just phytoplankton functional groups:
  - small colloids (non-living but possibly including viruses), < 0.2 micron in size;
  - coarse (non-living) colloids; ~ 0.2 - 1 micron;
  - heterotrophic bacteria;
  - Microzooplankton
  - several groups of inorganic (mineral) particles -
  - organic detritus - also divided in subgroups covering different size ranges, at least a few size ranges (for example, less than 5-10 um fraction, intermediate fraction perhaps up to ~100 um, and finally larger aggregates).
- Today all these particles are pooled together into one category referred to as detritus. This is a big problem and this is one of the major reasons for why we cannot understand well enough the sources of optical (including ocean color) variability.

Arnone suggestions:

Additions from the OCRT list:

- Density stratification (intensity of MLD)
- Surface and subsurface light field
- Vertical structure of the bio-optical properties
- Spectral absorption (total, CDOM, detritus, phytoplankton)
- Spectral bb
- Particle size and composition
- f/Q for all waters (coastal and open)

Balch suggestions:

On the OCRT list, assign “required ” and “recommended” fields and add the following:

- Absorption/attenuation
- Aerosol optical depth
- Mineralogy

…. **more suggestions are available in the emailed comments**

OCRT list:

- Volume scattering function (“backscattering”) and particle size distribution
- Upwelling radiance
- Phytoplankton functional groups (what about physiological parameters ?) Biovolumes of functional groups are most useful in relation to carbon biomass
- Carbon data set measurements: dissolved inorganic carbon (DIC), dissolved organic matter (DOM), particulate organic carbon (POC), particulate inorganic carbon (PIC), biogenic silica concentration (BSi), calcite, alkalinity, T, S, O2, and related tracers such as CFC’s, 14C, pC02, etc.
- Sediment trap data (if export production is a future product)
- Primary production (GPP, NPP), and PAR, mixed layer depth
- Sea surface temperature (SST), Nutrients

What we would like :

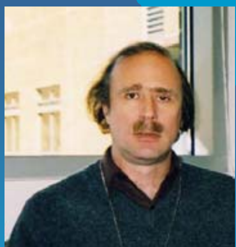
A revised straw man list of parameter group by time (1-5, 5-10 and 10+ years). The list should be a matrix that should include:

- the targeted goal;
- the parameters needed to develop/validate algorithms or models for that goal;
- the feasibility/accuracy of the in situ measurement methods for each parameter;
- the time frame within which we can hope to have "reliable" measurements (immediate, short- mid- long-term) for the parameters.

If there are measurement issues (protocol, accuracy, instrument maturity, etc.), then we should not be out collecting data until they are addressed. This will help prioritize what measurements get funded early and which will need to be deferred to later.

AERONET and Upcoming Measurements Over the Oceans

A.Smirnov, B.Holben, C.McClain, K.Knobelspiesse



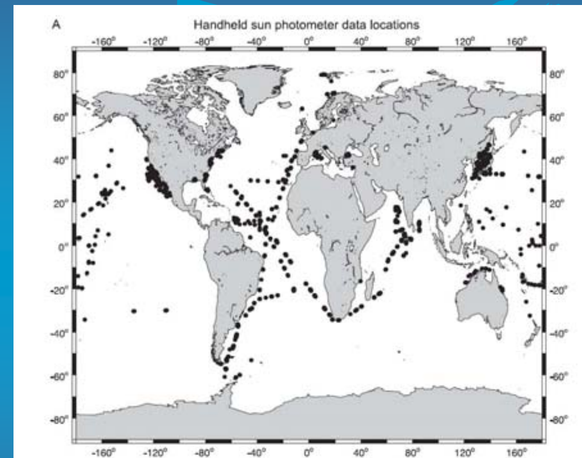
Alexander Smirnov – presenter

Alexander = Sasha

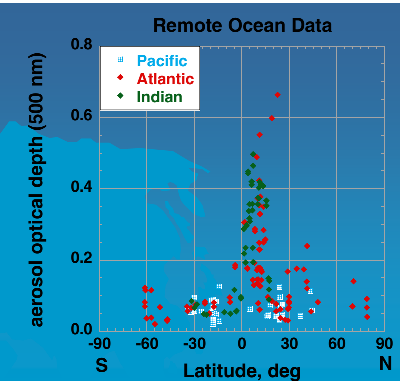
NASA Workshop, Montreal, Quebec, Canada

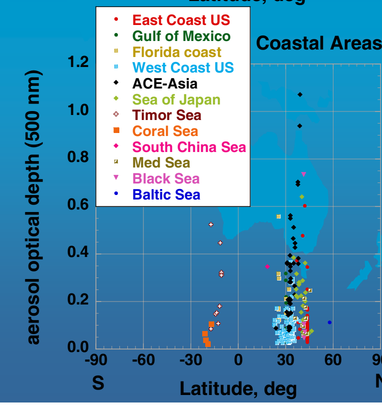
6-7 October 2006

SIMBIOS

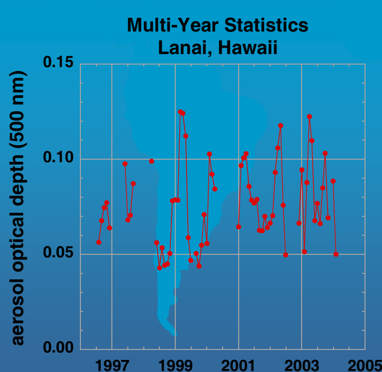


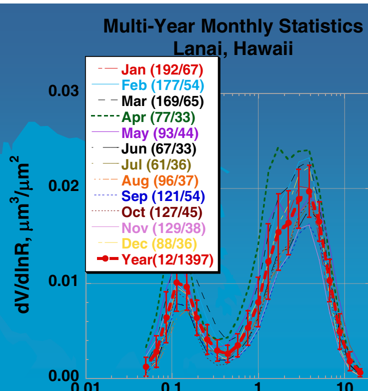
1997-2003, 458 measurement days

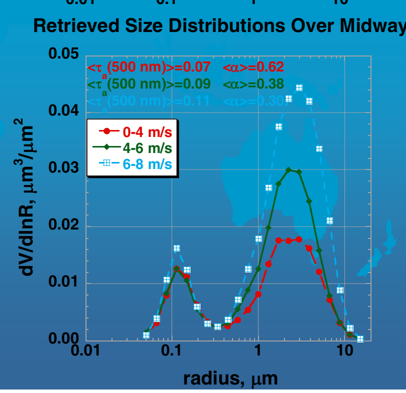




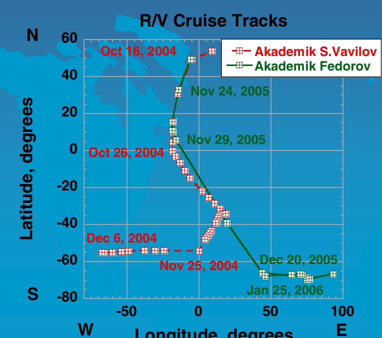
AERONET

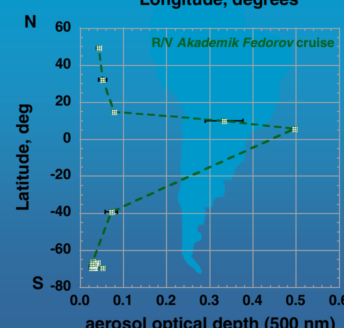


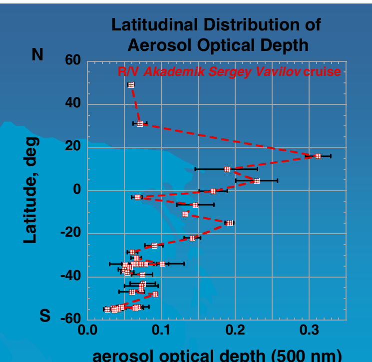


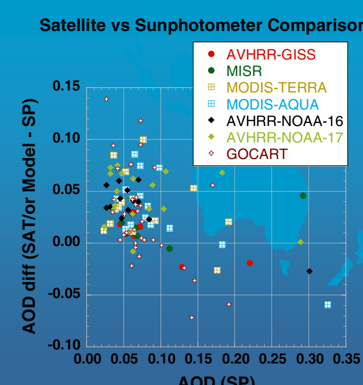


New Results









AERONET - OC

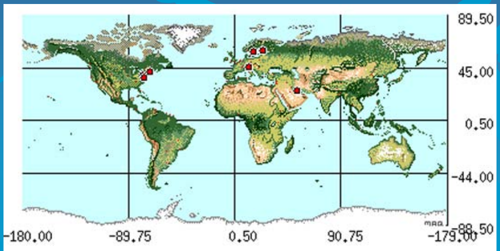


Fig. 1. Picture of the Gustaf Dalén Lighthouse Tower (GDLT) in the northern Baltic Proper off the Swedish coast. The inset displays a picture of the SeaPRISM above-water autonomous radiometer installed on the tower.

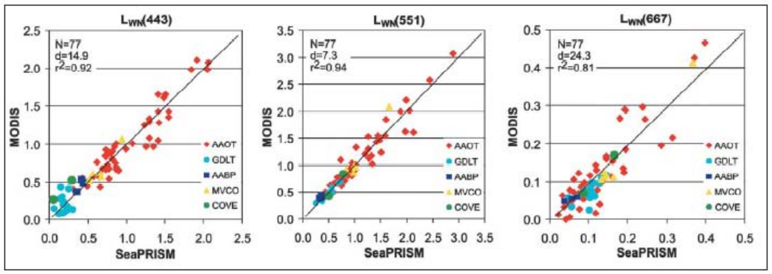


Fig. 3. Scatterplots of satellite-derived (MODIS-AQUA) versus in situ L_{WN} in units of mW cm^{-2} μm^{-1} sr^{-1} at the 443-, 551-, and 667-nanometer MODIS center wavelengths, for the AERONET-OC test sites (N is the number of matchups, d is the median of the absolute percent differences, and r^2 is the determination coefficient). MODIS data were processed using the SeaWiFS Data Analysis System (SeaDAS), release 4.8. The matchups are 50 for AAOT, 16 for GDLT, three for AABP, six for MVCO, and two for COVE.

What is to be done?

- Reestablish NASA's ship-based optical depth measurement network
- Develop an archival system, similar to the AERONET browser, but specifically designed for "moving" objects – ships
- Develop a calibration protocol
- Develop stand alone processing, utilizing AERONET's Version 2 algorithm
- Develop centralized archiving and distribution - public domain web-based access

PFT from Ocean Color Measurements

- The IOCCG WG on PFT:

  J. Aiken, A. Ciotti, H. Claustre, L. Clementson, S. Craig, S. Sathyendranath, C. Le Quéré, C. Moulin, C. Roesler, H. Sosik, D. Stramski

What are PFTs and why are they important?

- PFTs have different <u>impacts on climate</u> (biological pump of CO_2, biogenic source of DMS,…)

- they have different <u>sensitivities to climate change</u> (temperature, acidification,…)

- they are also very important at <u>regional scales</u> (HABs, higher trophic systems and fisheries)

First meeting in July 2006 (CNES, Paris)

- try to agree on PFT definition
- summarize the different algorithms
- PFT and IOP
- structure of the future report

What are PFTs and why are they important?

PFTs are groups of <u>several phytoplankton species</u>, which have in common a specific function:

- Biogeochemistry:
  - Pico-autotrophs [Chlorophytes, Prochlorococcus and Synechococcus]
  - N2-fixers [Trichodesmiums and N2-fixing unicellular prokaryotes]
  - Calcifiers [Coccolithophorids]
  - DMS-producers [Phaeocystis and small autotrophic Flagellates]
  - Mixed [autotrophic Dinoflagellates and Chrysophyceae]
  - Silicifiers [Diatoms]

- Primary production and export:
  - pico-phyto (< 2 µm) [Chlorophytes, Prochlorococcus and Synechococcus]
  - nano-phyto (2-20 µm) [Chromophytes, Nanoflagellates, Chryptophytes]
  - micro-phyto (> 20 µm) [Diatoms, Dinoflagellates]

What are PFTs and why are they important?

« By chance », most phytoplankton species belong only to one PFT (diatoms are micro-phyto and silicifiers,…).

However some groups are not associated to a function (prochlorococcus and synechococcus are pico-phyto but does not have a specific biogeochemical impact)

There is thus a sort of « confusion » between phtoplankton groups (based on pigment composition) and functional types.

This is something we are going to try to clarify in the **first chapter** of our report.

Remote Sensing: Existing PFT algorithm

In addition to the fact that we don’t know much about relationships between PFTs and IOPs, PFT remote sensing is difficult because:

- ocean color depends to the first order on the Chlorophyll concentration
- current operational ocean color sensors have limited spectral resolution and atm. corr. accuracy.
- in situ datasets are too sparse (global coverage,…) for algo validation

PFTs and IOPs

This « confusion » is reinforced by the fact that phytoplankton IOPs, which make the remote sensing of PFTs possible, are controlled by both the species (specific absorption of pigments) and the size (package effect, backscattering).

Chapter 2 of our report will be dedicated to the relationships between PFTs and IOPs, in the perspective of PFT remote sensing.

Remote Sensing: Existing PFT algorithm

Two types of algorithms have been developped:

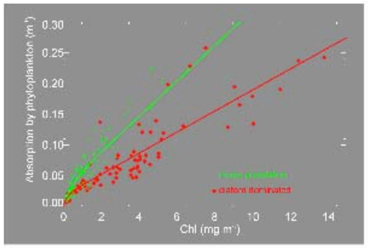
- **Analytical algo** based on a <u>more or less complex inversion of the Rrs spectrum</u>. They are usually validated for a given region/PFT and their applicability to the global ocean is “touchy”.
  e.g., Roesler et al. (2005), Ciotti and Bricaud (2006), Sathyendranath et al. (2004), Westberry et al. (2005)

- **Empirical algo** based on statistical analysis of various datasets related to the PFT and to the environmental conditions. They are usually global but their accuracy is difficult to assess.
  e.g., Uitz et al. (2006), Aiken et al. (2006), Alvain et al.,(2005)

Chapters 3 and 4 of the report will summarize these algorithms.

An example of a “simple” analytical algorithm

Sathyendranath et al. 2004 : use of specific optical properties of diatoms to distinguish them from other PFTs in the North West Atlantic.

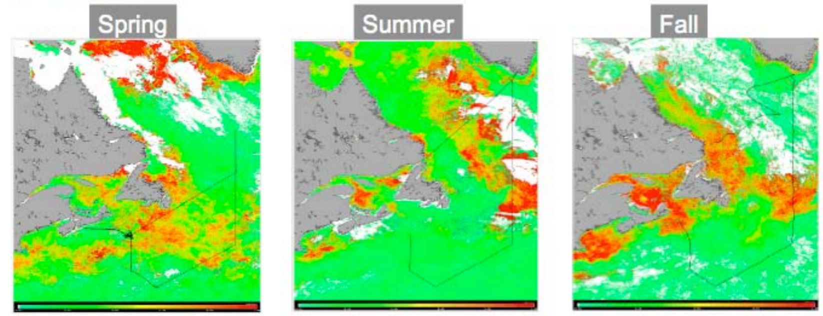


222 data collected between 1996 and 1998.

Cells classification using HPLC:
-Fuco/chl-a > 0.4 ⇒ Diatoms
-Chl-c_3/chl-a < 0.02

An example of a “simple” analytical algorithm

At the end, diatoms are identified by selecting the closer ratio, as shown on these probability maps of diatom occurrence.



⇒ Results allowed to distinguish between diatoms and others in the majority of cases studied in the North West Atlantic.

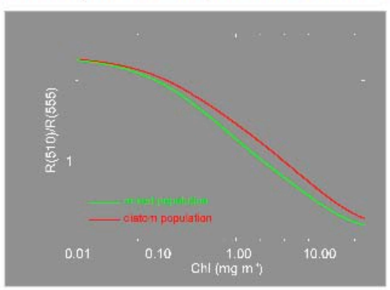
An example of a “simple” analytical algorithm

Refl. α bb (λ, chl a) / [a(λ, chl a, ‘group’ + bb (λ, chl a)]

a: absorption coefficient

bb: backscattering coefficient

It is thus possible to calculate theoretical reflectance ratio as a function of chl a for diatoms and others.



A more “complex” analytical algorithm

Roesler et al., 2005 : Inversion of a reflectance model based on a dataset of simulations in case of red tides.

1. *Determine specific absorption spectra for some PFTs*
2. *Generate a dataset of reflectance spectra for varying Concentrations, composition and size distribution*
3. *Invert these spectra to retrieve the relative contribution of each PFT.*

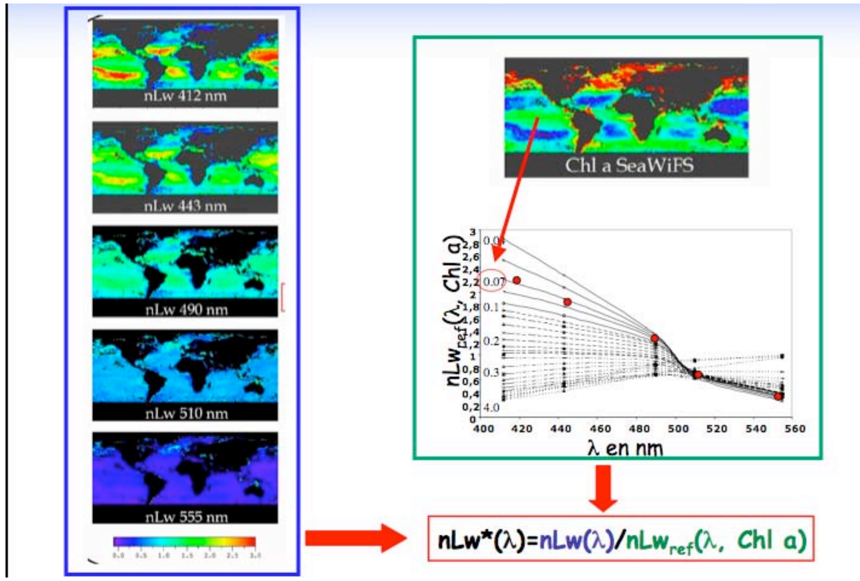
A more "complex" analytical algorithm

Five PFTs have been identified by their specific absorption spectra : Dinoflagellate, Diatoms, Dinophysis, Mesodinium and chlorophytes.

A test of this method have been made during an expensive red tide bloom near the west coast of South Africa.

⇒Results are quite <u>successful</u> in the <u>study area</u> but <u>in case of red tides and with hyperspectral data.</u>

A semi-empirical global algorithm

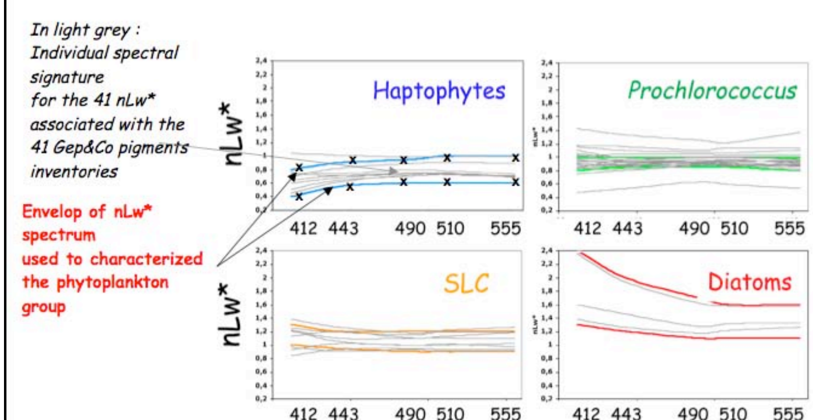


A semi-empirical global algorithm

Alvain et al, 2005 :

Empirical relationships between dominant phytoplankton groups (pigments criteria determined) and ocean color measurements, after having removed the first order chl a effect.

A semi-empirical global algorithm



A semi-empirical global algorithm

nLw$_{obs}$ and Chl-a SeaWiFS pixel

↓

Selection criteria
(optical depth, case 1 water)

↓

$nLw^* = nLw_{obs} / nLw_{ref}(Chl\text{-}a)$

↓

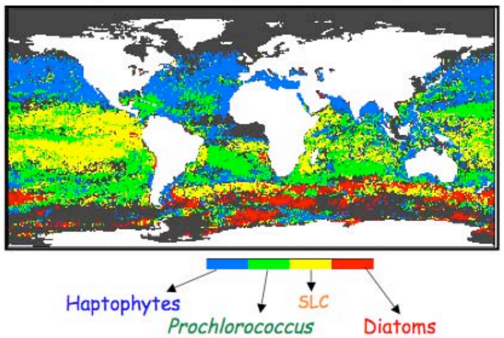
Dominant group for the pixel

↓

Most frequent dominant
group for a month on a
1x1 degree grid

PHYSAT

Example : Dominant species for January 2001



A purely empirical algorithm

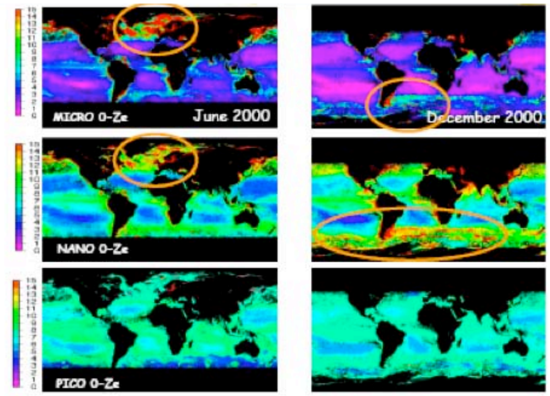


Figure from the Uitz et al. (phytoplancton functional groups climatology)

⇒Results allowed to quantify the phytoplankton biomass
Associated with **each size class at the global scale.**

A purely empirical global algorithm

Uitz et al., 2006 : relationships between surface chl a and the size distribution (micro-, nano-, and picoplankton) from a large in-situ database.

Comparison of existing PFT algorithm

In **Chapter 5** of the report, we are going to try to compare some of these algorithms, when possible (regional vs. global,…).

Future improvements and Recommendations

The difficulty of PFT remote sensing comes from the fact that measured Rrs spectra depend simultaneously on the species (pigment composition), on the cell's size and on the bulk ecosystem composition (CDOM, detritus,…) associated with a given PFT.

In **Chapter 6** of the report, we'll try to provide recommendations for future algorithm developments, sensor characteristics, and in situ measurements for validation.

Note that we haven't really work on this yet within the WG, but this field requires coincident Rrs, HPLC, particle's size and IOP measurements in contrasted environment…

2nd meeting on Sunday (Oct. 8th, Montreal)

- brief presentation of the structure of each chapter by the lead author.
- define methods for algo comparison (apply to in situ database and/or to seawifs data,…)
- start thinking about recommendations in general.

OCEAN COLOR CLIMATE,

A MERGING PROJECT: globcolour

ESA DUE (data user element)

NASA Workshop, October 6, 2006

André Morel

CONSORTIUM

ACRI-ST (France)	Prime contractor / management specifications / products design Processor development
University of Plymouth (UK)	User requirements follow up/ design justification
NIVA (Norway)	validation (DDS)
DLR & Brockman Consult (Germany)	cross characterization tools development / Web server:
ICESS (USA) & LOV(France)	scientific support

- ESA DUE project i.e. driven by end users:
- **IOCCG, IOCCP,UK-MetOffice**

Objectives

- Satisfy emerging demand for validated merged ocean colour derived information (cf. SIMBIOS)
- Demonstrate the current state of the art in merging together data streams from different ocean-colour sensors:
  - MERIS, SeaWiFS, MODIS-AQUA, (POLDER-Parasol)
- Provide a long time-series (10 years) of ocean-colour information
- Put in place the capacity to continue production of this time series in the future
- Demonstrate a global NRT ocean-colour service based on merged satellite data

GlobCOLOUR expected outputs

Global ocean colour (Level 3) data set covering 1997-2006
daily, weekly, monthly products:

- Chlorophyll-a concentration
  Diffuse attenuation coefficient
  Fully normalised water leaving radiances (available bands)

- Total suspended matter (or bbp)
- Coloured organic matter (dissolved and particulate)

- Aerosol optical thickness

- Data quality flags
- Cloud fraction
- Departure from radiance range at ~ 560 nm (turbidity index)

- Error estimates per pixel for each layer   OTHER PRODUCTS ?

LIST OF PARAMETERS and MERGING METHODS (tbc)

Parameter	Description	L3 merging method	M
CHL_1	chlorophyll-a concentration (mg/m^3) for case 1 water	averaging methods + GSM model	
CHL_2	chlorophyll-a concentration (mg/m^3) for case 2 water	averaging methods	✪
CHL_m	chlorophyll-a concentration (mg/m^3) for merged case 1 and case 2	averaging methods	✪
YSBPA	yellow substance and bleached particle absorption (m^{-1})	averaging methods	✪
CDOM	coloured dissolved organic matter (m^{-1})	GSM model	
TSM	total suspended matter concentration (g/m^3)	averaging methods + GSM model	✪
Kd(490)	diffuse attenuation coefficient at 490 nm (m^{-1})	analytical from merged CHL_1	
Lxxx	fully normalised water leaving radiances at xxx nm ($mW/cm^2/\mu m/sr$)	averaging methods	
L555	inter-calibrated fully normalised water leaving radiances at 555 nm ($mW/cm^2/\mu m/sr$)	averaging methods (1)	
EL560	relative excess of radiance at 560 nm, actually 555 nm (%)	analytical from merged L555 & CHL_1	
PAR	daily photosynthetic available radiation ($\mu Ein/m^2$)	averaging methods	
T865	aerosol optical thickness over water (-)	averaging methods	
CF	cloud fraction (%)	classification & statistical methods	

(1): spectral inter-calibration is applied prior to the merging.
✪: averaged data is only available from MERIS data

Optical and Bio-optical properties merging

Simple or weighed averaging
e.g. average of log (Chl a) or (Chl a) , of nLW …

GSM01 method
Both (averaging and GSM) fast and easy methods;require unbiased data sources, account for error bars

---

Subjective analysis
requires quantitative quality information on sensors (W)
computationally demanding; information questionable

Blended analysis
needs to have a reference (« truth field »), used as internal boundary condition
Proven method for in situ - satellite data merging, but not qualified for satelite-satellite merging

Optimal interpolation
Purely statistical approach (correlations); would provide only Chlorophyll product.

Duration 3 years (Dec 2005-Dec. 2008)

First phase: demonstration of feasibility, one year, ending with User Consultation Workshop (Villefranche Dec. 2006)

This phase includes

- Pre-merger sensor characterization

- Diagnostic data set
  (basis for characterization and merging methods intercomparison)

- Production of a «Preliminary Product Set » (4 months)

- First Merging algorithm intercomparison
  (mainly simple or weighed averaging, and GSM01 methods)

Some Issues…

Case 1 & 2 waters?

Case 2 water processing still subject for research
Only MERIS has an “official” case 2 waters processing (validation…)
Case 2 algorithms exist for MODIS and SeaWifs, but are not used within nominal processing chains

Fully normalised water leaving radiance?

MODIS, SeaWiFS,and MERIS fully normalized according to IOCCG recommendations. F/Q tables valid for Case 1 waters (and validated)

BUT, fully normalized water leaving radiance in case 2 waters ?

Sensor cross-characterization

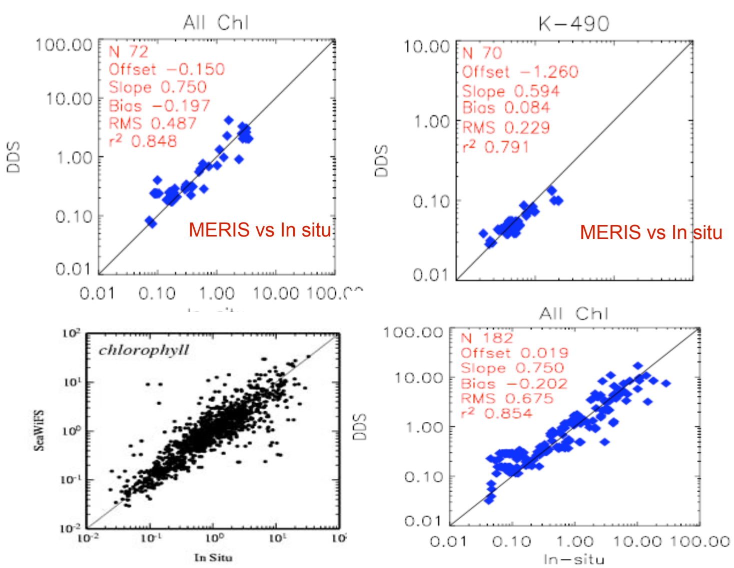
Sensors characterization review based on published literature
Comparison of normalized radiances (in-situ, overlapping time periods)
Comparison of derived products (Chl, Kd…)

First results of the characterization (NOMAD, NILU, Boussole)

	MERIS from globCOLOUR	MODISA from McClain, 2005	SeaWiFS from McClain, 2005
L412	29.3	30.9	24.1
L442	21.5	n/a	n/a
L443	n/a	18.8	17.5
L488	n/a	14.6	n/a
L490	18.4	n/a	15.1
L510	21.5	n/a	13.7
L531	n/a	15.0 ? ✣	n/a
L551	n/a	12.3	n/a
L555	n/a	n/a	16.9
L560	26.4	n/a	n/a
L620	36.2	n/a	n/a
L667	n/a	36.4	n/a
L670	37.7	n/a	45.7
Chl (all)	31.0	40.4	33.1
K_d(490)	20.0	19.1	15.0
T865	50 ?	56.7	43.4

Error bars are expressed in %
✣: insufficient data points
n/a: the parameter is not available for the instrument

Instances of inter-sensor characterizations



SeaWiFS OBPG

DDS-Globcolour

Merging the [Chl] products

- Not the same algorithms
- Not the same band settings
- Problems or coherency ?

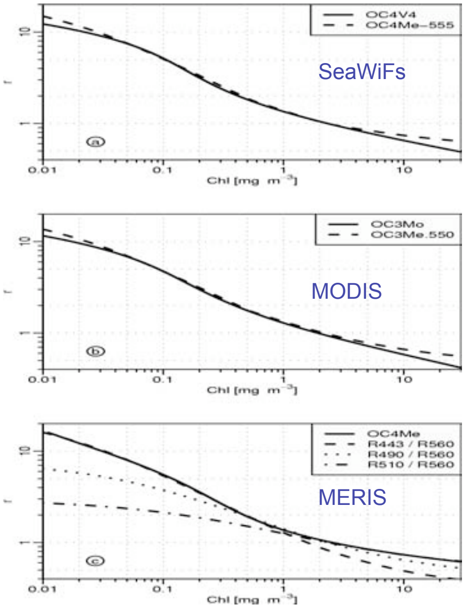
Differing Algorithms for [Chl]

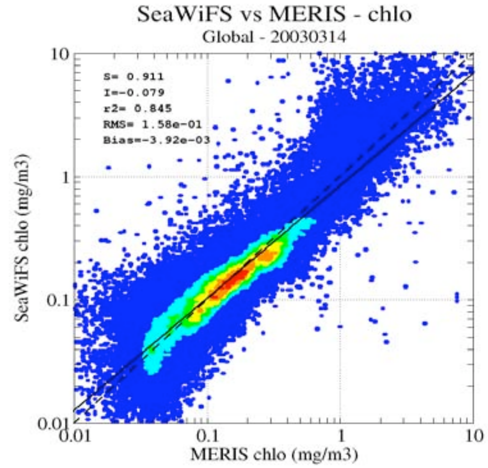
° OC4v4 and OC3Mo empirical

° OC4Me semi-analytical
(based on a hyperspectral model
for Case 1 waters)

The same hyperspectral
model allows the
Derivation of MERIS-type algo.
spectrally tuned
for the other sensors,

Such as
OC4Me555 -> OC4v4
OC3Me550 -> OC3Mo





Example of
comparison

Chl products

Daily L3

Same Reflectance
ratios (Ri/Rj)
Introduced into

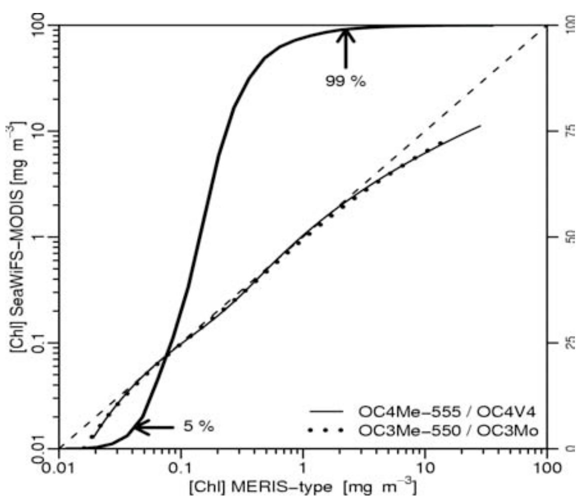
OC4v4 and its MERIS-type
Counterpart (OC4Me555)
and
OC3Mo and OC3Me550

THEN

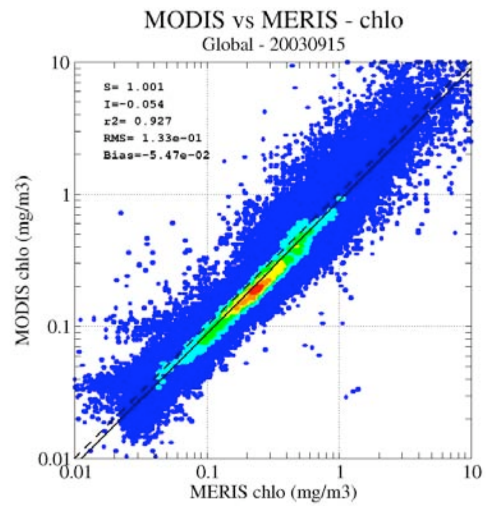
Compare the [Chl] returns

Conclusion:

- Small discrepancies
When [Chl] < 0.04
And [Chl] > 2 mg/m3
- Agreement for 94% of the whole ocean



Transfer functions (convertibility) available

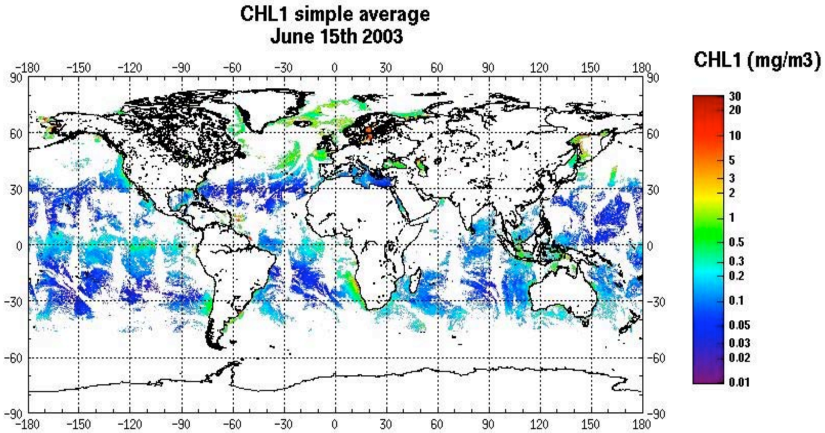


Example of
comparison

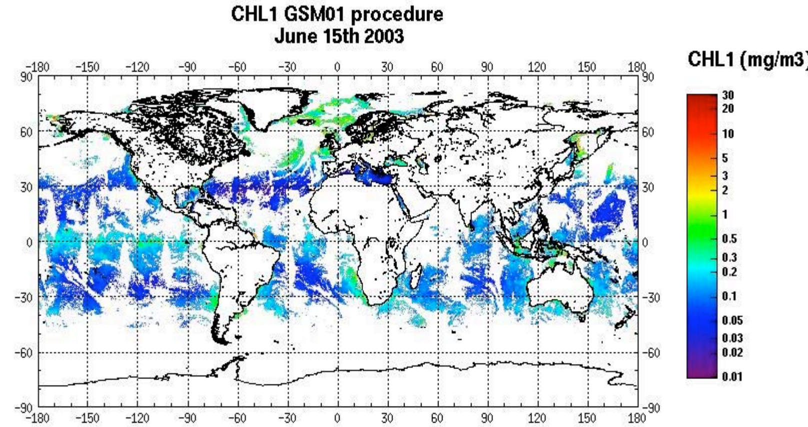
Chl products

Daily L3

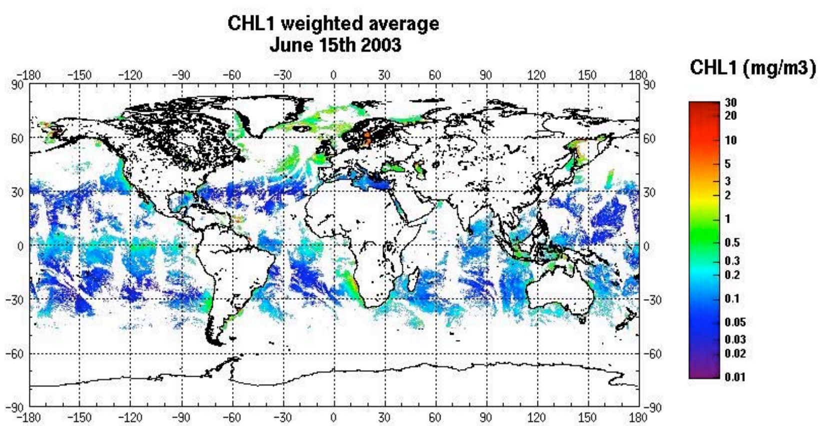
Examples of Merged [chl] (daily L3, June 15, 2003)



Examples of Merged [chl] (daily L3, June 15, 2003)

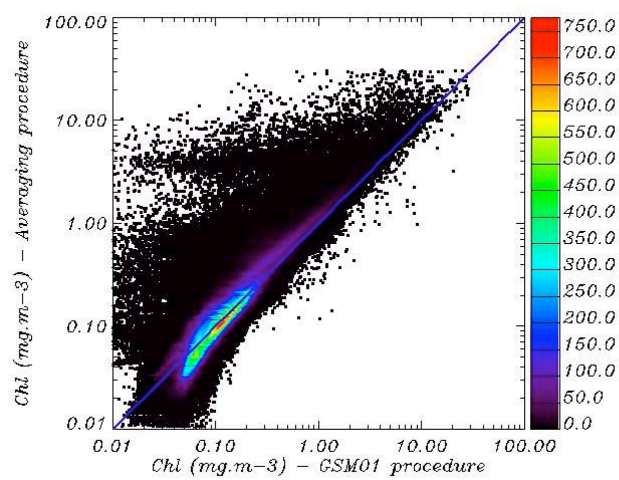


Examples of Merged [chl] (daily L3, June 15, 2003)



[CHL]

Average
Versus
GSM



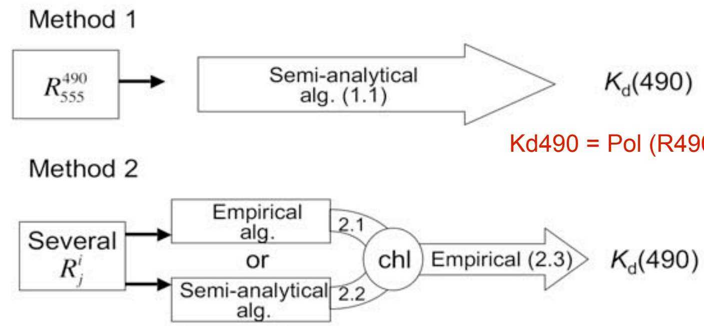
Y = 1.088 X + 0.103 r2 = 0.899

MERGING the Kd(490) products

- Presently, Kd(490) is not a product for MERIS
  (→ Need for an algorithm)

- Algorithms for MODIS and SeaWiFs
  (Initially Mueller, 2000 → now Werdell, 2005)
  Problem: lack of curvature in this algorithm
  (can be modified -> Method 1)

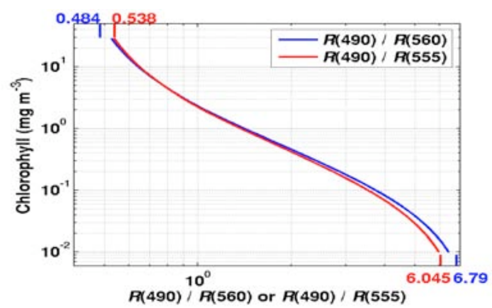
Possible unified solution: use [Chl] as an intermediate tool
(-> Method 2)



Kd490 = Pol (R490/R555)

1.1 OC2Kd

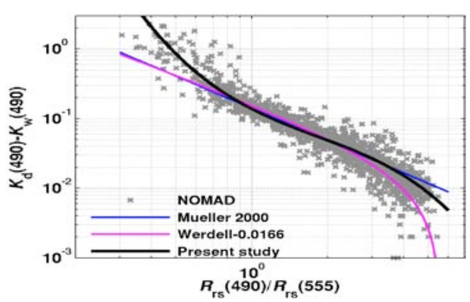
2.1 OC4V4, OC3M
2.2 OC4Me
2.3 Equation 8



(Newport Workshop)

Curvature (sigmoidal shape)
In the relationships between
Ri/Rj and [Chl]

Must be present in



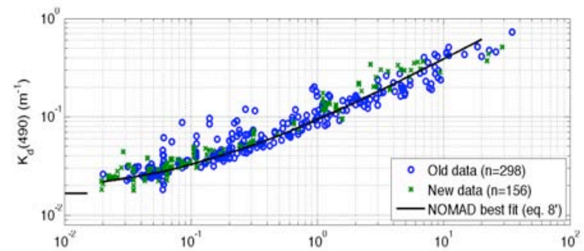
The relationship between
Ri/Rj and Kd

Analytically derived relationship
(black curve) + NOMAD data

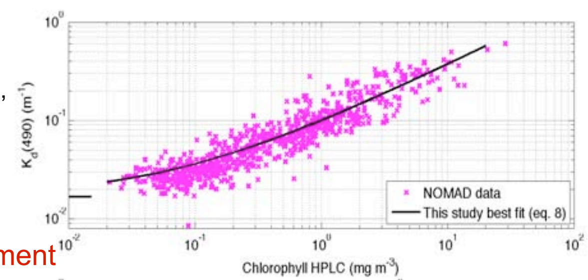
This relationship can be used
as algorithm (METHOD 1)

Kd(490) and [Chl] relationships (Case 1 waters only)

LOV data
NOMAD best fit



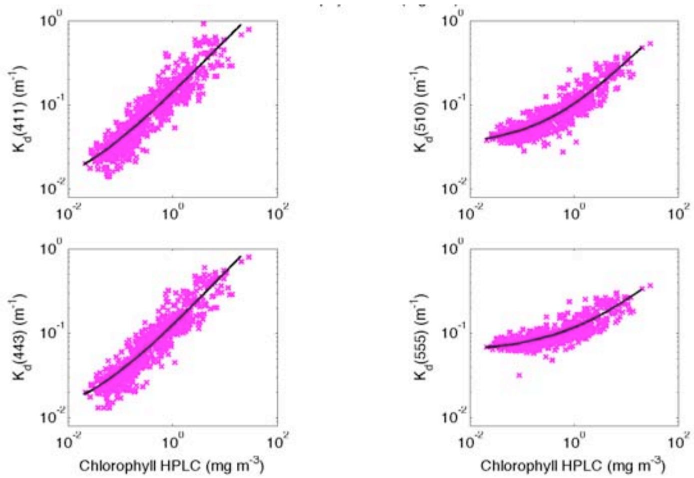
NOMAD data
LOV best fit
(Morel-Maritorena, 2001)



Excellent agreement
-> METHOD 2

Excellent agreement… for other _ (412, 443, 510, 555 nm)

(→ Possibility of spectral extension, other Kd, Kpar)

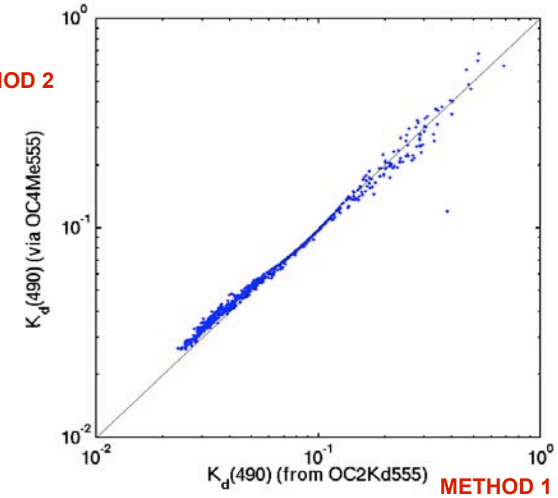


NOMAD Data and LOV best fit

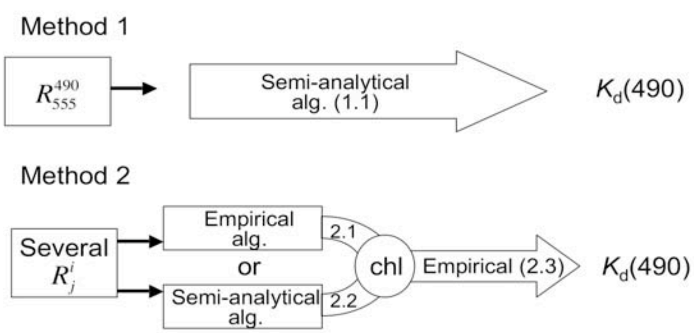
INTER-COMPARISON

NOMAD
N = 1751

METHOD 2



METHOD 1



1.1 OC2Kd

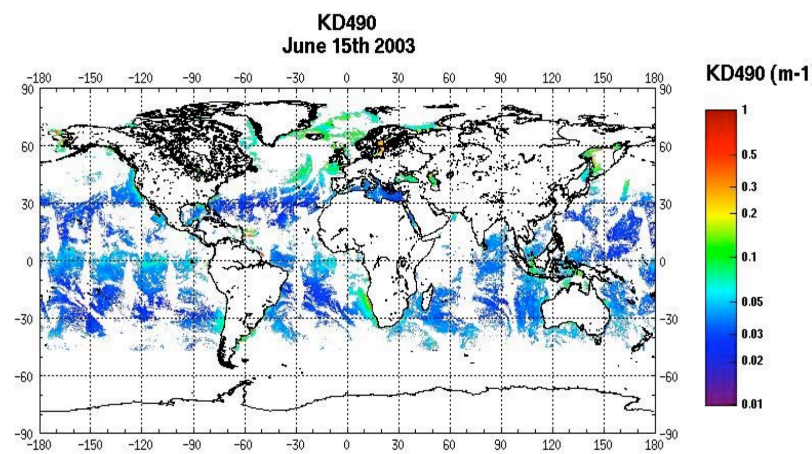
2.1 OC4V4, OC3M
2.2 OC4Me
2.3 Equation 8 (Kd490 = 0.0166 + 0.0835[Chl]^0.633

Methods 1 and 2-2 provide exactly the same results
(both are semi-analytical and resting on the same hyperspectral bio-optical model)

Methods 1 and 2-1 slightly diverge (empirical vs semi-analytical for Chl retrieval)

Example of unified Kd(490) from merged [Chl]

(daily L3, June 15, 2003)



SOME PRELIMINARY CONCLUSIONS

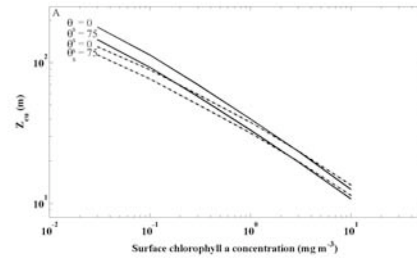
In situ Characterization seems satisfactory (error bars are determined for each sensor, they are rather similar)

Merging Tools and Protocols will be ready for approval (in Dec 06)

Probably, merging procedures limited to averaging, weighed averaging, and GSM

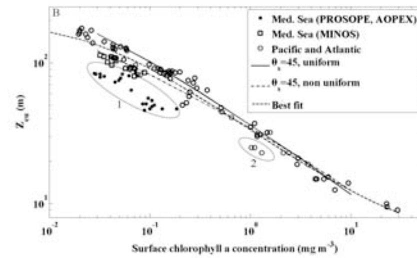
Additional products, simply derivable from Chl in Case 1 waters, could be proposed, (as thickness of the heated layer through Kpar, depth of the euphotic zone, Secchi disk depth,..). Can be produced separately by each sensor, or as well from the mergeg information.

Thanks to Globcolour people (particularly to oha, am, gb, sam, sm, da….) and to NOMAD, SeaBASS, NILU people.



Zeu (?)

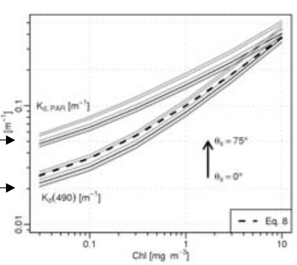
RTE computation with MM01 as IOP input



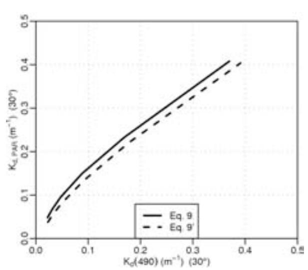
Recent data

Kd(PAR)

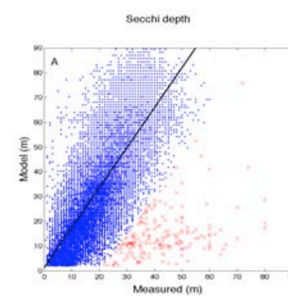
Kd(490)



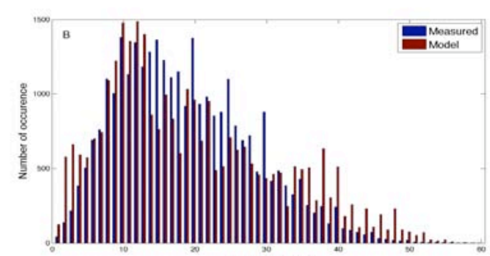
KdPAR ?



Relationship between Kd(PAR) And Kd(490) for the upper layer (2/Kd(490) thick)



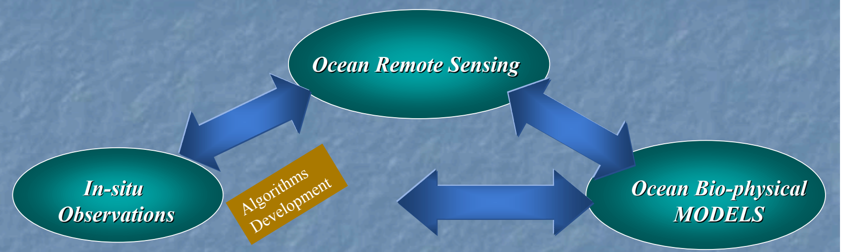
Zsd ?



MODIS
Summer 2003
vs
NODC 1900-1990
Summer

(N= 66009 data)

Ocean Sciences



-Basic Ocean measurements
-Bio-optical measurements
-Measurement Protocols

-Image Processing
-Algorithms implementation
-Sensor Calibration

-Extend obs in time and space
-Comparison with obs
-Validation
-Assimilation
-

R. Arnone
NASA Workshop
Oct 6,2006
Montreal,CA

What is limiting our capabilities today for understanding bio-geo physical ocean processes?

Understand spatial and temporal variability .

- Limitations Observations --
- Field programs
- Satellites (Remote Sensing)

- Limits in coupling observations with models.
Data Fusion
Assimilation etc

Both address the need for measurement covariances.
Evoles from / through assimilation of physical measurements

MODAS – Module Ocean Data Assimilation System
Altimetry and synthetic BT etc

Thrusts for Remote Sensing / Satellite program
Bio-physical Models

-

Algorithms → Beyond chlorophyll
-Bio-optical algorithms
-Bio-optical physical algorithms
-Role of Hyperspectral sensing

Looking below the surface
-Lasers
-Coupling Physics and Bio-optics

Improving the Spatial and temporal coverage
- Frequency of Coverage
- Spatial resolution
- Coastal applications

Geostationary programs –
Higher Spatial ad temporal coverage

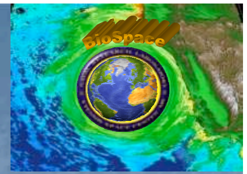
Nowcasting, Forecasting , Hindcasting ocean conditions
- Coastal monitoring and prediction
- Evolution of ocean weather
-Coupling remote sensing with models → data assimilation.

Modeling Roadmap "Spiral" development.
20 year program

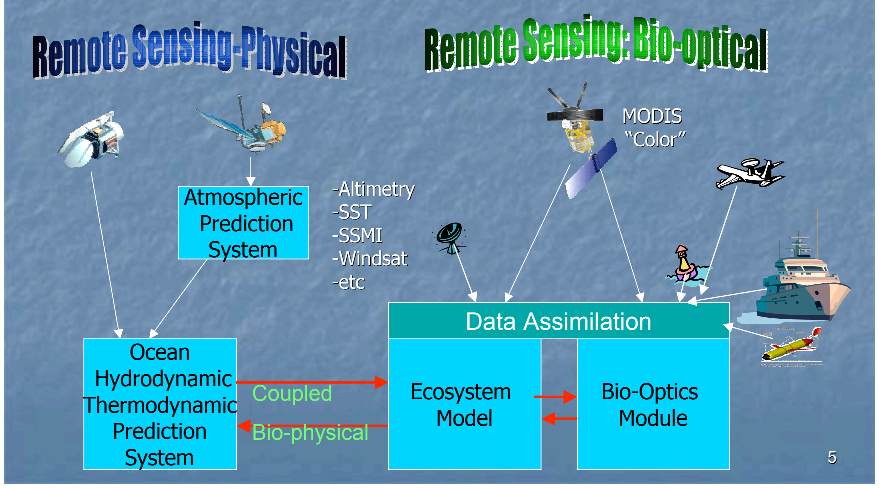
Merging of Observations with models -"Start simple"

1) Fusing of Data
satellites and models
new observations with satellites with models
- physical and bio-optical linkages.
- surface and subsurface conditions
- comparison of models and observations (remote sensing)
2) Empirical - simple data links
Advection of particles
Advection of processes
Defining the "importance of processes"
Physical vs biological
biological vs coastal
3) Bio-optical ocean models
- Full physics, basic growth and decay models – extremely complex
- Biological models, sediment transport models etc
- Assimilation of both physical AND bio-optical data into models
How do we couple and link with observations?

West Coast – Bio-Optical Models



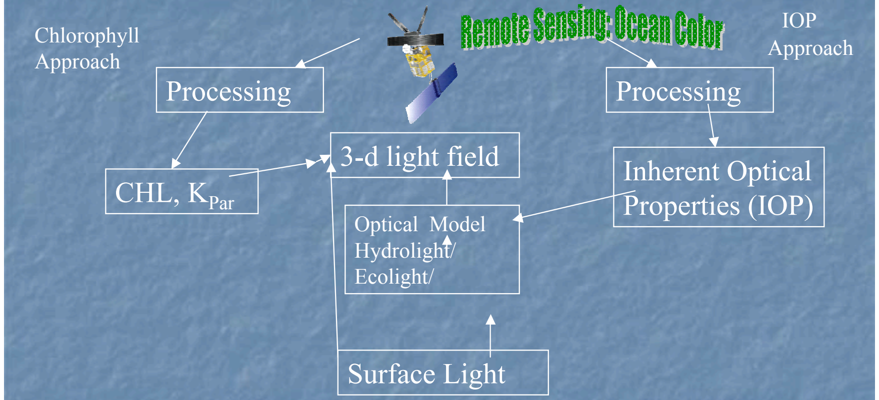
Goal: Coupled Ocean Prediction Systems



Research Questions

- What are the dominant space-time characteristics of variability in bio-optical properties of the coastal ocean?
- What is relative importance of physical versus biological processes governing variability on 1-5 ?? day time scales(TS)
- How complex a biological-optical model is required to represent biological forcing of variability of optical properties on 1-5 TS?
- How important is the feedback between biological and physical processes in the coastal ocean on 1-5 day TS?
- What is relative importance of local vs remote forcing to variability?
- How do we best deploy autonomous assets in sampling variability of optical properties in coastal ocean? Gliders? AUV's? Remote Sensing requirements?
- How predictable are the bio-optical properties in coastal ocean on TS of 1-5 days? Better than persistence? Under what conditions?

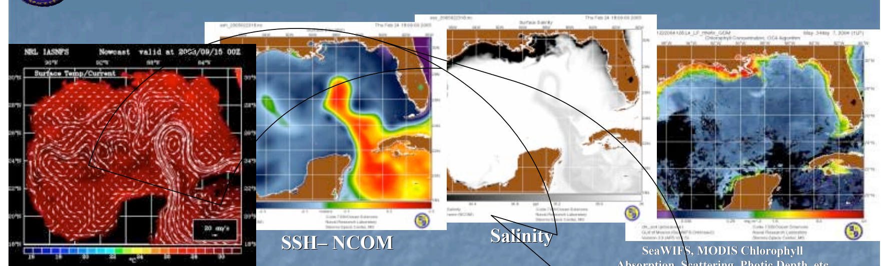
Satellite Derived Light Field



K_{Par} = Attenuation Coef.

$$PAR(z) = PAR(0)\, e^{-K_{PAR}\, z}$$

Fusing the Satellite Optical Products and Physical Models



Currents – NCOM "Intra Americas Seas"

SSH– NCOM

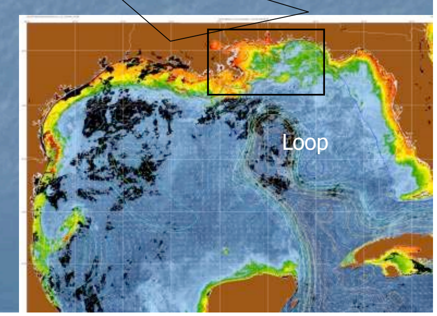
Salinity

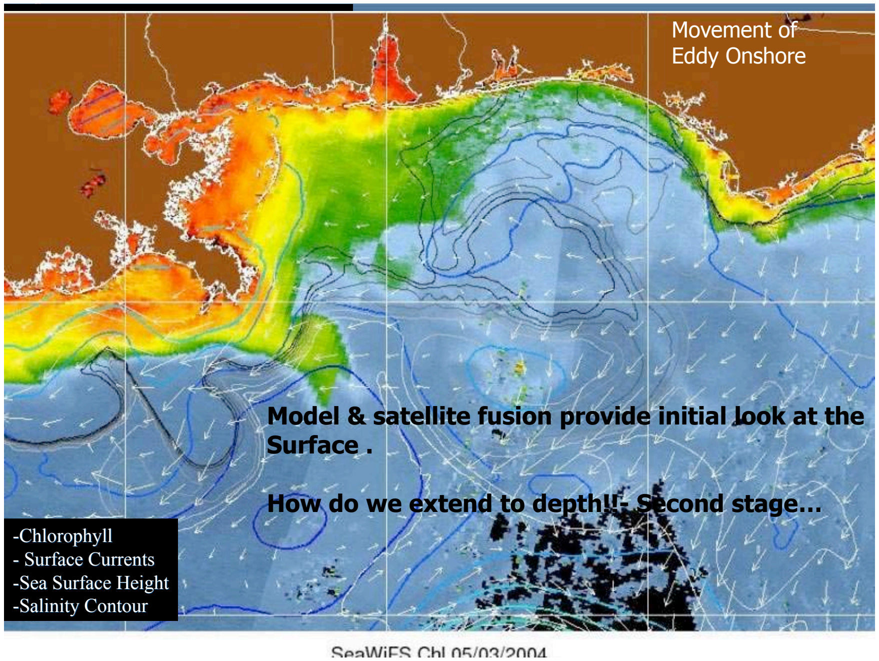
SeaWIFS, MODIS Chlorophyll Absorption, Scattering, Photic Depth etc

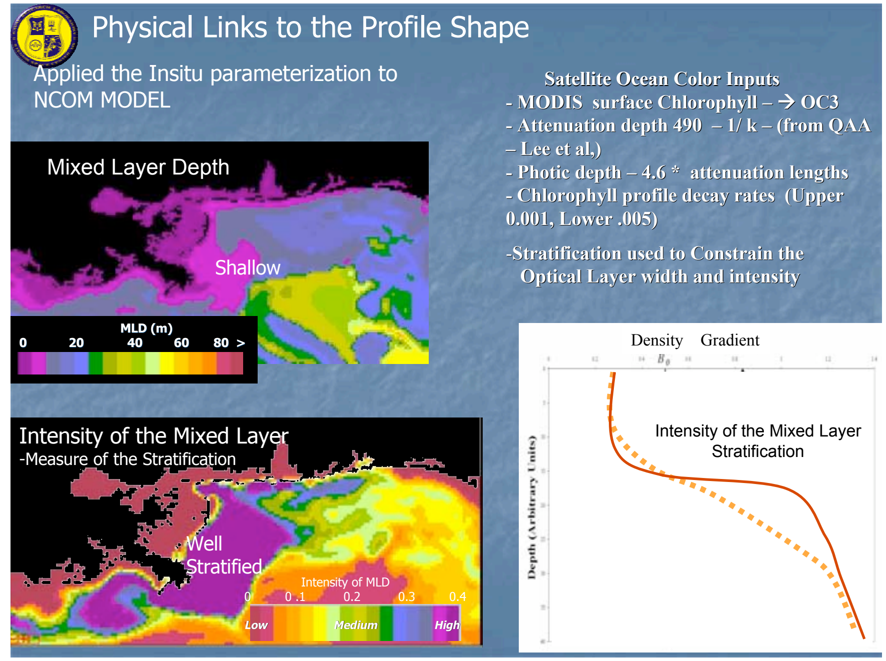
-Naval Coastal Ocean Model (NCOM)
-41 Vertical layers,
-Wind Forcing (CAMPS)
-Assimilation of Altimetry and SST (MODIS)
- River inputs → Climatology

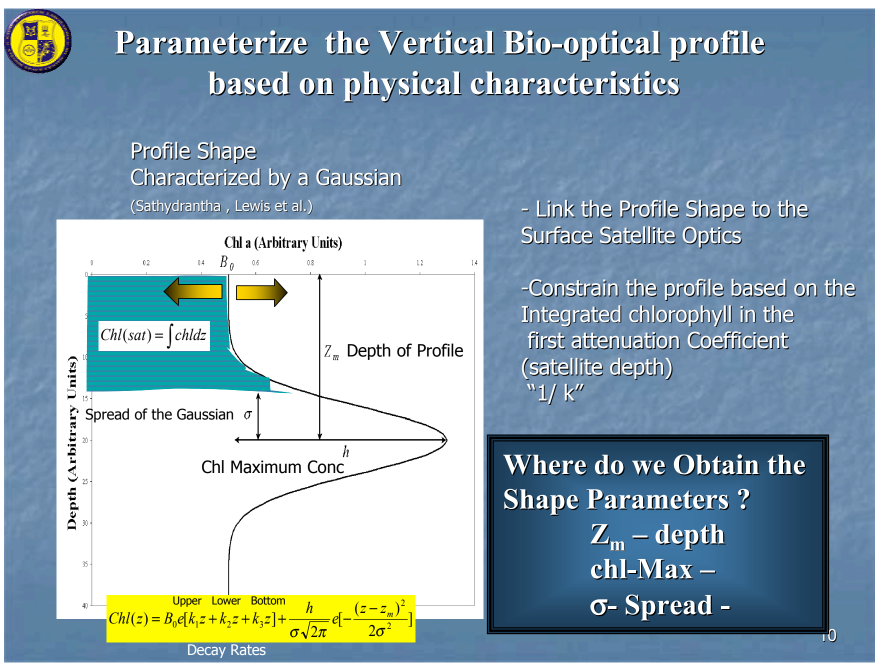
-How are "color" and physics linked ?

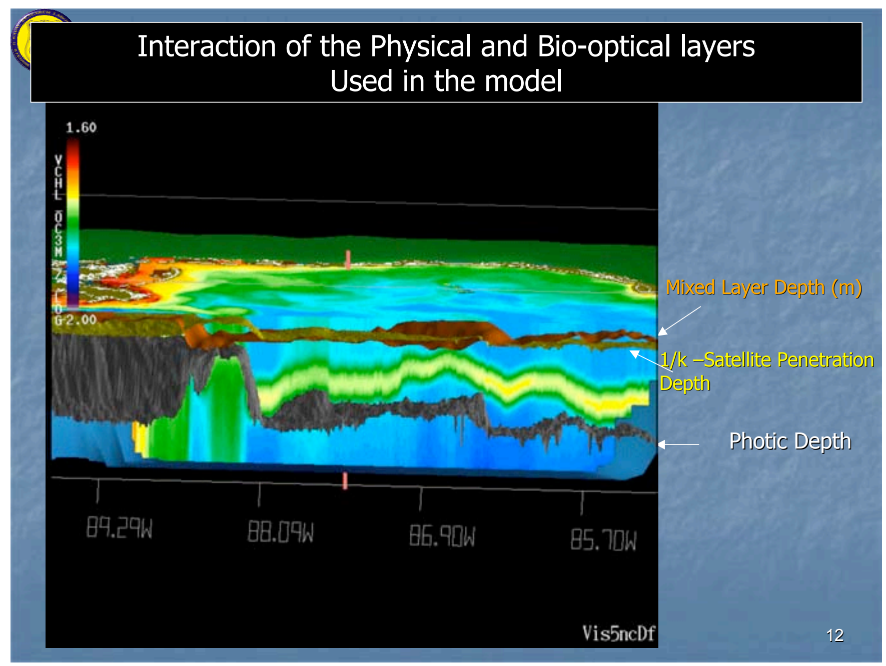
--Extending ocean color observations to physics.

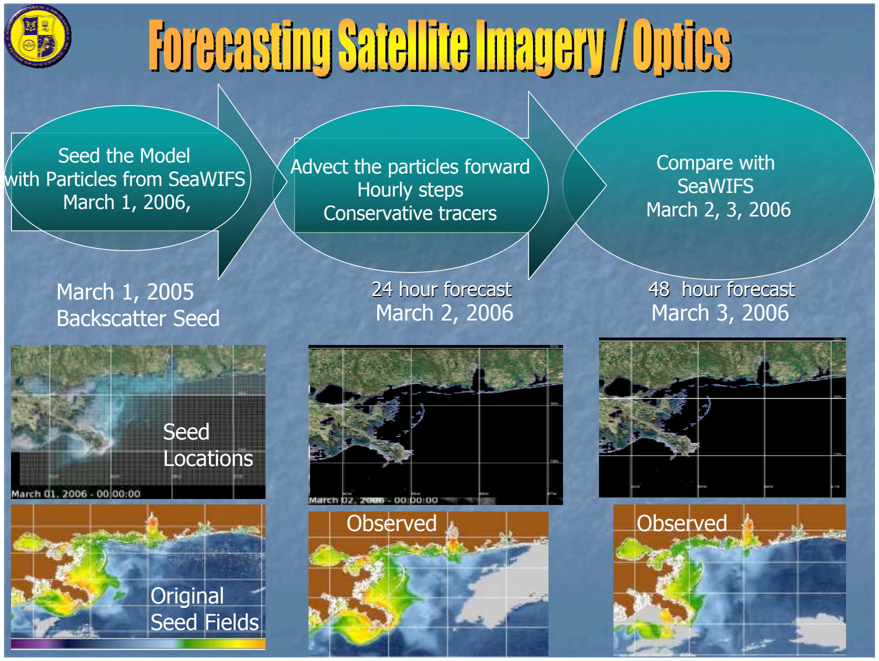


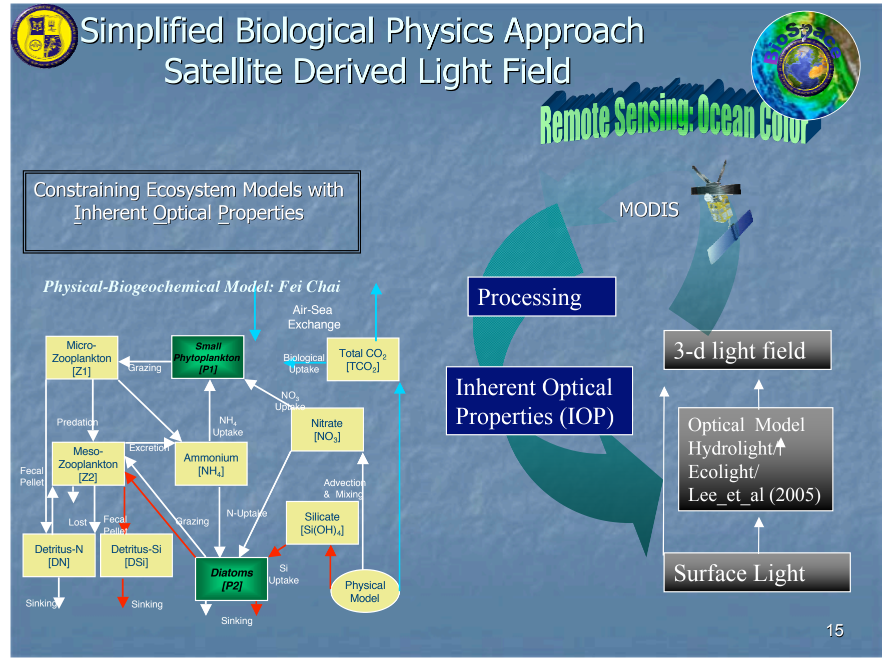

Movement of
Eddy Onshore
Model & satellite fusion provide initial look at the Surface .
How do we extend to depth!! Second stage…
-Chlorophyll
- Surface Currents
-Sea Surface Height
-Salinity Contour
SeaWiFS Chl 05/03/2004

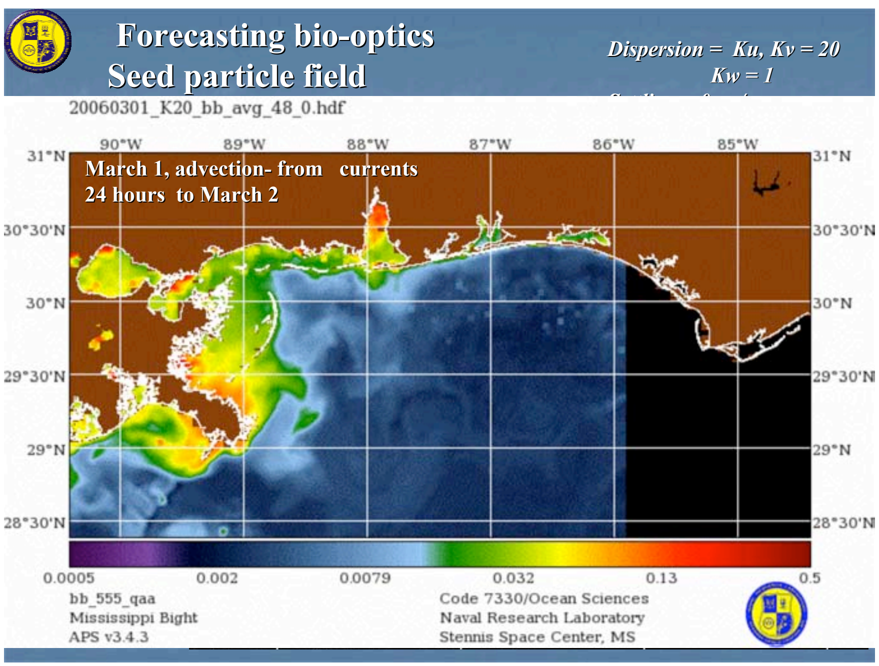

Physical Links to the Profile Shape
Applied the Insitu parameterization to
NCOM MODEL
Satellite Ocean Color Inputs
- MODIS surface Chlorophyll – → OC3
- Attenuation depth 490 – 1/ k – (from QAA – Lee et al.)
- Photic depth – 4.6 * attenuation lengths
- Chlorophyll profile decay rates (Upper 0.001, Lower .005)
-Stratification used to Constrain the Optical Layer width and intensity
Mixed Layer Depth
Shallow
MLD (m)
0 20 40 60 80 >
Intensity of the Mixed Layer
-Measure of the Stratification
Well
Stratified
Intensity of MLD
0 0.1 0.2 0.3 0.4
Low Medium High
Density Gradient
Intensity of the Mixed Layer
Stratification
Depth (Arbitrary Units)

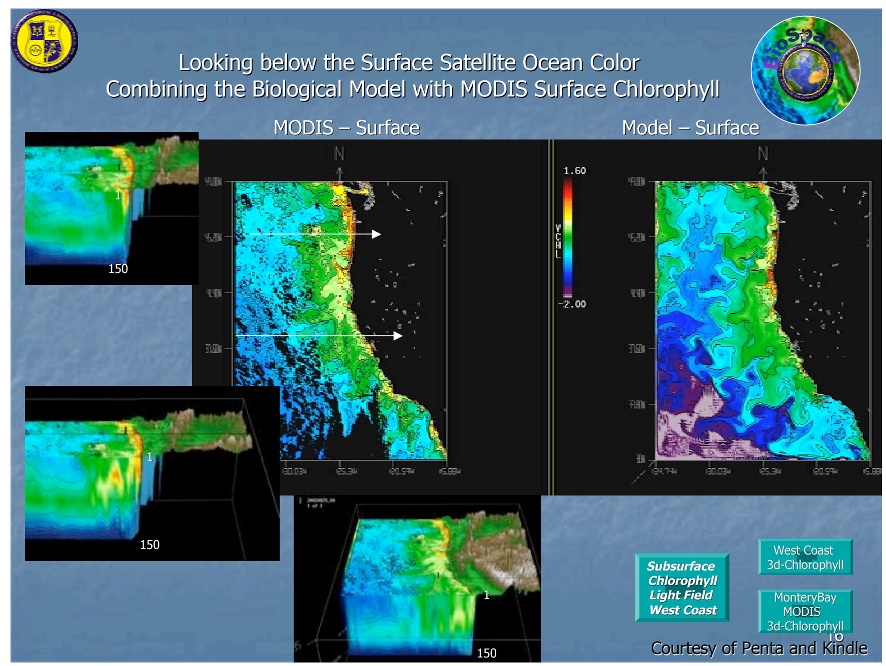

Parameterize the Vertical Bio-optical profile
based on physical characteristics
Profile Shape
Characterized by a Gaussian
(Sathydrantha , Lewis et al.)
Chl a (Arbitrary Units)
B_0
$Chl(sat) = \int chldz$
Z_m Depth of Profile
Spread of the Gaussian σ
h
Chl Maximum Conc
Depth (Arbitrary Units)
Upper Lower Bottom
$Chl(z) = B_0 e[k_1 z + k_2 z + k_3 z] + \frac{h}{\sigma\sqrt{2\pi}} e[-\frac{(z-z_m)^2}{2\sigma^2}]$
Decay Rates
- Link the Profile Shape to the Surface Satellite Optics
-Constrain the profile based on the Integrated chlorophyll in the first attenuation Coefficient (satellite depth)
"1/ k"
Where do we Obtain the Shape Parameters ?
Z_m – depth
chl-Max –
σ- Spread -
10


Interaction of the Physical and Bio-optical layers
Used in the model
1.60
VCHL OC3M
2.00
Mixed Layer Depth (m)
1/k –Satellite Penetration Depth
Photic Depth
89.29W
88.09W
86.90W
85.70W
Vis5ncDf
12


Forecasting Satellite Imagery / Optics
Seed the Model with Particles from SeaWIFS March 1, 2006,
Advect the particles forward Hourly steps Conservative tracers
Compare with SeaWIFS March 2, 3, 2006
March 1, 2005 Backscatter Seed
24 hour forecast March 2, 2006
48 hour forecast March 3, 2006
Seed Locations
March 01, 2006 - 00:00:00
March 02, 2006 - 00:00:00
Original Seed Fields
Observed
Observed


Simplified Biological Physics Approach
Satellite Derived Light Field
Remote Sensing: Ocean Color
Constraining Ecosystem Models with Inherent Optical Properties
MODIS
Processing
3-d light field
Inherent Optical Properties (IOP)
Optical Model Hydrolight/ Ecolight/ Lee_et_al (2005)
Surface Light
Physical-Biogeochemical Model: Fei Chai
Air-Sea Exchange
Micro-Zooplankton [Z1]
Small Phytoplankton [P1]
Biological Uptake
Total CO2 [TCO2]
Grazing
Predation
NH4 Uptake
NO3 Uptake
Nitrate [NO3]
Meso-Zooplankton [Z2]
Excretion
Ammonium [NH4]
Fecal Pellet
Advection & Mixing
Lost
Fecal Pellet
Grazing
N-Uptake
Silicate [Si(OH)4]
Detritus-N [DN]
Detritus-Si [DSi]
Diatoms [P2]
Si Uptake
Physical Model
Sinking
Sinking
Sinking
15


Forecasting bio-optics
Seed particle field
Dispersion = Ku, Kv = 20
Kw = 1
20060301_K20_bb_avg_48_0.hdf
90°W 89°W 88°W 87°W 86°W 85°W
31°N
30°30'N
30°N
29°30'N
29°N
28°30'N
March 1, advection- from currents
24 hours to March 2
0.0005 0.002 0.0079 0.032 0.13 0.5
bb_555_qaa
Mississippi Bight
APS v3.4.3
Code 7330/Ocean Sciences
Naval Research Laboratory
Stennis Space Center, MS


Looking below the Surface Satellite Ocean Color
Combining the Biological Model with MODIS Surface Chlorophyll
MODIS – Surface
Model – Surface
150
150
150
Subsurface Chlorophyll Light Field West Coast
West Coast 3d-Chlorophyll
MonteryBay MODIS 3d-Chlorophyll
Courtesy of Penta and Kindle
16

Summary

- **Full- bio-physics model long term goal**
  - **Biology is very sensitive to physics**
  - **Assimilation required !! Both – Physics and biology**
  - **High temporal and short time scales more difficult.**
  - **Satellite products provide enormous data stream for assimilation..**

What properties and how do we assimilate??

Summary Continued..

-Different models require different approach's for assimilation

-Don't make the Models too complex.
  -65 state variables models may be necessary but present "systems" can't address them.

Spiral development of MODELS → simple to complex.

What products are required for models?

How subsurface properties are linked with the surface ?
Both physical properties and the Bio-optics properties.
Subsurface Light levels – important → IOP
Degradation rates, CDOM, detritus etc.
others….