NASA Science Mission Directorate
Research Opportunities in Space and Earth Sciences
NNH13ZDA001N - ROSES 2013
A.25 PACE Science Team

This program element of NASA's Research Opportunities in Space and Earth Sciences (ROSES) announcement (NNH13ZDA001N) formulated a Pre-Aerosol, Cloud, ocean Ecosystem (PACE) Science Team (ST) for a three-year period. PACE will be a polar-orbiting mission with an ocean color sensor and possibly an aerosol-cloud polarimeter. The mission will be capable of performing radiometric and possibly polarimetric ocean and atmosphere surveys, returning a range of geophysical data from which properties of the ocean and atmosphere can be produced to add to other critical climate and Earth system variables. As currently envisioned, the Pre-Aerosol, Clouds, and ocean Ecosystem (PACE) mission has multiple scientific goals, including making climate-quality global ocean color measurements that are essential for understanding the carbon cycle and global ocean ecology and determining how the ocean's role in global biogeochemical (carbon) cycling and ocean ecology both affects and is affected by climate change. NASA welcomed proposals from prospective Science Team members to pursue theoretical and analytical studies associated with one of two sets of measurements, Inherent Optical Properties (IOPs) and the Atmospheric Correction, in order to address research goals of the NASA's Earth Science Division. The focus of this solicitation was to do risk reduction and further clarify measurement requirements for future collaborative atmosphere and ocean science and applications for IOPs and the Atmospheric Correction on the PACE mission.

NASA's Earth Science Research aims to utilize global measurements to better understand the Earth system and interactions among its components as steps toward ultimate prediction of Earth system behavior. To achieve this goal, the selected ST is a diverse group of investigators who cumulatively bring end-to-end knowledge of different aspects of these two sets of measurements to the Science Team activities. End-to-end knowledge encompasses laboratory and field measurement protocols and quality assurance, radiative transfer modeling, remote sensing theory in the UV-to-SWIR spectral range, and ocean color, aerosol, and cloud algorithms. Proposers interested in focusing on aerosol and cloud retrievals in support of the PACE ocean color instrument or a possible PACE polarimeter proposed to the Atmospheric Correction group. Each "team" (IOPs and Atmospheric Correction) will collaboratively produce a final report that details recommended approaches for PACE for their respective measurement suite. The ultimate goal for each of the two measurement suite teams is to achieve *consensus* and develop community-endorsed paths forward for the PACE sensor(s) for the full spectrum of components within the measurement suite. The goal is to replace individual ST member recommendations for measurement, algorithm, and retrieval approaches (historically based on the individual expertise and interests of ST members) with consensus recommendations toward common goals. NASA welcomed proposals for a Principal Investigator who wishes to be the Science Team (ST) Leader. NASA selected one ST lead to oversee and coordinate activities for both measurement set groups. Prototypical algorithm or retrieval development activities using Hyperspectral Imager for the Coastal

Ocean (HICO) data were welcome. The HICO instrument is currently on orbit aboard the International Space Station (ISS).

The advertised budget of this program element was up to $3M/year for three years, for a total investment of up to $9M. Funds will come from the Earth Science Division. The outcome for the Pre-Aerosol, Cloud, ocean Ecosystem (PACE) Science Team Program is $3.0M for the first year, $3.0M in year two, and $3.0M in year three for a total of $9.0M/three years. Nineteen proposals were selected out of a total of 49 proposals submitted.

Steven Ackleson/Naval Research Lab
PACE Applications to Case II Waters: Quantifying the Uncertainty in Inherent Optical and Water Constituent Properties and the Impact On Remotely Sensed Ocean Color

In response to solicitation NNH13ZDA001N-PACEST, Pre-Aerosol, Clouds, and Ocean Ecosystem (PACE) Science Team, we propose to investigate uncertainties in Case II inherent optical properties (IOPs) and associated water constituent properties (e.g., concentration, composition, and morphology) and to examine the impact of uncertainties on recommended PACE data products for coastal ocean, estuarine, and inland waters. These objectives strongly address ocean color science needs articulated within the PACE Mission Science Definition Team Report (October 2012) pertaining to marine biogeochemical cycles associated with land-ocean interactions in response to climate change. As a collaborative member of the IOP working group (ST/IOP), we will utilize existing in situ and remotely sensed data sets as well as new observations to be collected during the period of performance through existing and planned field campaigns. Uncertainties will be estimated through direct comparisons of optical and water constituent properties measured or derived through independent means, comparisons of functional relationships between associated parameters with relationships that have been published and vetted by the research community, and through tests of optical closure. In addition to the proposed research and collaborations with other members of the ST/IOP, the PI, Dr. Steven Ackleson, proposes to be the overall PACE Science Team leader. Working closely with NASA-appointed representatives, Dr. Ackleson will be responsible for organizing, planning, and chairing team meetings, coordinating focused working groups, integrating results, building consensus on PACE science objectives and requirements, representing science team activities at professional meetings and symposia, and preparing progress reports and consensus statements as directed by NASA.

Emmanuel Boss/University Of Maine, Orono
A Global Database of High Horizontal Resolution IOPs for Validation of Remotely Sensed Ocean Color

The activity proposed here consists of 1. Creating a consortium of practitioners interested in standardizing collection and processing of high horizontal resolution data collected using flowthrough in-line systems, 2. Sharing associated codes, 3. Providing the community with a plan for deployment, processing and computation of estimated uncertainties associated with in-line data, and 4. Creating a uniformly processed dataset for Cal/Val activities and studies of inherent optical properties (IOP) distributions throughout the world's oceans.

Such a dataset will be unique in its global extent, being ideal for validation of remote sensing product and for algorithm development for a global mission such as PACE. Critical evaluation of the in-line IOP acquisition is necessary to assign realistic uncertainties to those IOPs.

Once processing methodology is agreed upon among the collaborators, UMaine will reprocess historical in-line data collected by the collaborators and provide them to SeaBASS with the processing algorithms and source codes for future use by the ocean color community. Efforts will be made such that data generated will have sufficient details so that alternative processing could be applied without the need to reprocess the raw data.

As part of this proposal we will use the data to answer the following SCIENCE question:

What are the characteristics of sub-satellite-pixel variability in IOPs in the ocean?

The utility of the in-line dataset goes well beyond the scope of this proposal and can be used to answer other science questions directly relevant to PACE (a global hyperspectral mission), such as:

What are the deviations of IOPs from published bio-optical relationships and how do they vary with variables such as temperature, salinity, date, distance from land and ocean depth?

What information is available in hyperspectral IOPs (and hence hyperspectral ocean color) in addition to that currently obtained with spectral sensors (e.g. added pigments in addition to chlorophyll a (e.g. Chase et al., 2014), size information etc.)?

As part of this proposal we will use the data to answer the following METHODOLOGICAL questions:

1. What should we acquire as discrete samples to increase the utility of the in-line systems?
2. How do in-line data compare to in-water data collected with similar sensors at the same time (e.g. are there noticeable biases in in-line data?)?

Answering these methodological questions will improve in-line collection and our estimates of uncertainties for the data collected. Uncertainties are necessary to evaluate the degree of agreement between remote and in-situ estimates of IOPs as well as biogeochemical quantities.

PI Boss also proposes himself to be the IOP Science team lead

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Jacek Chowdhary/Columbia University
Atmospheric Correction for Retrieval of Ocean Spectra from Space (ACROSS)

The 2013 ROSES A.25 solicitation calls for studies on atmospheric correction in support of the PACE (Pre-Aerosol, Cloud, ocean Ecosystem) mission. To address this call, we will examine the capacity of PACE-like observations for atmospheric correction by (i) applying statistical methods to compute data information content, and (ii) inverting synthetic and real PACE-like observations into ocean spectra. In step (i), we will focus on the instrument options proposed in the PACE SDT (Science Definition Team) report. Specifically, we will consider the base instrument option OCI (Ocean Color Imager, which includes the 350, 865, 1240, 1640, and 2130 nm channels for atmospheric correction), and elements of instrument options OCI/OG (i.e. OCI base option augmented by a 820 nm band and an Oxygen A band), OCI/+ (i.e. OCI base option augmented by 940, 1378, and 2250 nm bands), OCI-3M (i.e. OCI base option plus a multi-angle multi-spectral multi-polarization, or 3M, imager), and OCI/A-3M (i.e. OCI/+ option plus a 3M imager). In step (ii), we will apply optimization techniques to extract ocean spectra from various data sets. Specifically, we will apply these techniques to synthetic data created for instrument options with a range of atmospheric-correction performances, as identified in step (i). In addition, we will apply these techniques to three existing measurement sets: the 2011 HOPE-COAST (Hands On Project Experience-Coastal and Ocean Airborne Science Testbed) and the 2013 OCEANIA/ACOCO (Ocean Color Ecosystem Assessments with Novel Instruments and Aircraft/Atmospheric Correction Over Coastal Oceans) measurements acquired in Monterey Bay (which include measurements of inherent optical properties and of chlorophyll), and coinciding HICO (Hyperspectral Imager for the Coastal Ocean) and CALIOP (Cloud-Aerosol Lidar with Orthogonal Polarization) measurements acquired across the globe. These measurement sets incorporate aspects of the instrument options proposed for PACE and contain data to validate atmospheric correction and/or ocean color spectra retrievals.

Using statistical methods to examine the information content and inversion of ocean color remote sensing observations is a complex undertaking that requires a multidisciplinary team. Dr. Chowdhary has worked on ocean and aerosol retrievals from observations by the RSP (Research Scanning Polarimeter) instrument, which is an airborne version of the Aerosol Polarimeter Sensor (APS) onboard the failed 2011 NASA/Glory mission. He wrote a radiative transfer program for polarized underwater light, was a member of the Glory ST (Science Team) and PACE SDT, and is PI of ACOCO. Dr. Alexandrov has written cloud inversion algorithms for RSP, and was also a member of the Glory ST. Dr. Knobelspiesse has worked on inverting coincident RSP and Lidar data, has done information content analyses for different satellite instrument options in support of Glory ST and PACE SDT reports, and was a member of the Glory ST. Dr. van Diedenhoven has expertise in simulating and analyzing hyper-spectral and polarimetry data and the Oxygen A-band, as well as in information content analyses. Dr. Cairns was a member of the Glory ST and the PACE SDT, and has developed techniques for the efficient implementation of inversion algorithms. Dr. Kudela has worked extensively on ocean color retrievals and modeling of underwater light field to describe biological-physical coupling in coastal waters. He is the PI of the coastal ocean project that collaborated with

OCEANIA. Dr. Guild has expertise in coastal ecosystem science, and was PI of HOPE-COAST and OCEANIA. She is now leading the HQ2O (High-Quality Optical Observations: Improving Atmospheric Correction and Remote Sensing of Water Quality in the Coastal Zone) project with Dr. Kudela. Dr. Palacios has expertise in discriminating phytoplankton types from ocean color, and is processing and analyzing coastal data from the HOPE-COAST and OCEANIA campaigns for the HQ2O project.

Susanne Craig/Dalhousie University
Derivation of Inherent Optical Properties from Satellite Top of Atmosphere Measurements in Optically Complex Waters

The inherent optical properties (IOPs) of a water body can serve as robust proxies for many important ecological and biogeochemical processes that are of fundamental importance to the Earth system. IOPs can be derived from measurements of satellite ocean color, and many successful derivation methods now exist, and provide a powerful means of synoptically monitoring these processes and their response to a changing climate. However, in waters such as the coastal ocean and inland water bodies, accurate retrieval of IOPs is often hampered by factors including difficulties in removing the contributions of the atmosphere from the satellite signal, and poor performance of standard ocean color algorithms due to the complex relationships amongst the water constituents.
The objective of this project, therefore, is to develop an approach to derive accurate estimates of IOPs from top of atmosphere (TOA) satellite radiance, thereby bypassing the difficulties often associated with atmospheric correction procedures. This is of particular relevance to coastal and inland water bodies where retrieval of robust ocean color products is notoriously challenging, and is frequently hampered by difficulties in achieving accurate atmospheric correction. The approach may be used for all waters, but most importantly, offers a means to accurately estimate IOPs from ocean color in scenarios where it may otherwise not be possible.

The proposed objectives will be achieved using an approach already proven for both in situ hyperspectral and satellite multispectral measurements. Using a combination of existing satellite and aircraft hyperspectral ocean color measurements and a custom generated TOA synthetic dataset, we will perform rigorous statistical model evaluation, sensitivity analyses to investigate variable oceanic and atmospheric effects on model skill, and finally, will develop operational implementation strategies. These activities will allow the model to be fully developed for hyperspectral TOA applications and a determination of the best model type “ regional, water type or global. The end product will be a set of methodologies to provide an accurate means of deriving hyperspectral IOPs in the most challenging scenarios and will represent a significant advance in our ability to fully exploit remote sensing of the planets most important and vulnerable water bodies.The proposed research directly addresses the requirements of the PACE mission to achieve accurate hyperspectral IOP estimates, and insight into the processes for which they are proxies, in critical coastal ocean and inland water bodies “ areas particularly susceptible to the impacts of climate change and anthropogenic perturbation. This is entirely in keeping with the broader NASA Earth Science Research Program to acquire new insights into the Earth system.

Heidi Dierssen/University of Connecticut, Storrs
Atmospheric Correction Over Bright Water Targets with Non-Negligible Radiances in the Near Infrared

Many scientists working with ocean color satellite imagery are required to conduct independent or partial atmospheric correction due to high backscattering in the Near Infrared (NIR). The standard atmospheric correction algorithms typically interpret the enhanced NIR from whitecaps, coccolithophores, cyanobacteria, floating vegetation, suspended sediments, and the benthos as enhanced scattering by aerosols. This creates both omission and commission errors such that the derived water-leaving reflectance and backscattering products are decreased and the aerosol products are increased in magnitude. If the PACE mission aims to derive climate quality aerosol concentrations and ocean biogeochemistry metrics, then better methods must be developed for dealing with water with non-negligible NIR and partitioning top of the atmosphere reflectance into the appropriate streams (aerosol, whitecap, glint). Having published on a variety of bright water targets over the last 15 years, I propose to be considered for the PACE Atmospheric Correction Science Team to bridge the gap between the atmospheric and water column approaches. I currently serve on the International Ocean Colour Coordinating Group and have served on a standing committee of the Space Studies Board, as well as several strategic working groups and satellite project teams. As part of this effort, I also propose to conduct targeted field measurements to provide better estimates of elevated reflectance due to whitecaps, foam and bubbles. Modeling enhanced reflectance due to whitecaps and bubbles requires a more complex treatment than a single windspeed parameterization, which cannot capture the orders of magnitude variability between the parameters. Here, we propose to conduct local measurements of the enhancement in reflectance due to whitecaps from the ultraviolet through the short wave infrared (SWIR). Coincident measurements of bubble entrainment will be conducted, as well as host of physical and bio-optical parameters. These data will be combined with available satellite imagery to evaluate partitioning whitecaps and bubbles from various atmospheric correction schemes. Correctly estimating whitecaps could also be an important climate relevant science parameter for those studying air-sea gas exchange, generation of sea spray aerosols and potentially applicable for estimating mixed layer depth for primary productivity models. Data collected in conjunction with this field effort, and other relevant project we and others have gathered on regions prone to elevated non-negligible NIR will be compiled in an archive of coincident satellite top of the atmosphere reflectance and high quality field measurements of water leaving reflectance. Such a database can be used to evaluate approaches across a variety of challenging bright water targets where common algorithms fail.

Robert Frouin/University Of California, San Diego
Bayesian Methodology for Atmospheric Correction of PACE Ocean-Color Imagery

The PACE mission will carry into space a spectrometer measuring at 5 nm resolution in the UV to NIR and at lower resolution in spectral bands in the NIR and SWIR and, eventually, a multispectral, multi-angle polarimeter measuring in the UV to SWIR. These instruments have great potential for improving estimates of marine reflectance in the post-EOS era. In view of this, the proposal objectives are as follows. The first objective is to evaluate, using the Bayesian approach to inverse problems, the gain in marine reflectance accuracy expected by 1) including observations in the UV and SWIR and 2) further including polarimetric and directional observations in selected spectral bands. This for the PACE threshold aggregate bands with respect to the standard MODIS set of bands used to generate ocean color products. The second objective is to assess, also in a Bayesian context, the utility of hyper-spectral information for improving atmospheric correction in the aggregate bands, and to quantify the accuracy of the atmospheric correction at 5 nm resolution for separating ocean constituents and characterizing phytoplankton communities.

To achieve these objectives, the TOA signal measured by the PACE spectrometer and the eventual polarimeter will be simulated for a variety of realistic atmospheric and oceanic conditions. Typical prior distributions for the aerosol, water reflectance, and surface parameters, suitable for utilization at a global scale, will be used, as well as noise distributions. The noise will encapsulate all the sources of uncertainties in the radiative transfer (RT) modeling and include sensor noise. The inverse models will be constructed based on several considerations, i.e., computational cost, convenience to approximate the conditional covariance (a second order quantity), and detection of abnormal values (due to limitations of the forward model). Ways to improve performance by specifying prior distributions from independent information about regional and temporal variability (e.g., from output of numerical transport models) will be investigated, and practical implementation of the Bayesian methodology will be outlined for routine application.

The investigation will provide a Bayesian methodology for atmospheric correction of the PACE spectrometer data. The methodology makes it possible to incorporate known constraints of the marine reflectance (i.e., correlation between components) and to account for the varied sources of uncertainty (i.e., measurement noise, RT modeling errors). Importantly, it allows the construction of reliable multi-dimensional confidence domains of the retrieved marine reflectance. Specifically, the mean and covariance of the posterior distribution are computed. These quantities provide, for each pixel, an estimate of the marine reflectance and a measure of its uncertainty. Situations for which observation and forward model are incompatible are also identified. Thus the methodology will offer the means to analyze and interpret PACE ocean-color imagery in view of confidence limits and model adequacy, on a pixel-by-pixel basis.

By evaluating via theoretical studies the accuracy of the atmospheric correction of PACE ocean-color radiometry and the expected improvements with respect to current ocean-color sensors, by identifying optimum sets of spectral bands, and by providing an inverse methodology adapted to the problem, which can be viewed as a generalization of the standard algorithm, the investigation responds directly to the PACE Science Team Announcement of Opportunity, which seeks methods and approaches that will maximize the new capabilities of the PACE mission for understanding global ocean ecology in a changing climate.

Bo-Cai Gao/Naval Research Lab
Hyperspectral and Multispectral Atmospheric Correction Algorithms for Supporting the NASA PACE Mission

At the core of the PACE mission is an advanced optical instrument, the Ocean Color Imager (OCI), designed to provide hyperspectral ultra violet (UV), to visible (VIS) and near-infrared (NIR) and multi-spectral short-wave infrared (SWIR 1.0 - 2.5 micron) observations of the earth ecosystems. We propose to join the PACE Atmospheric Correction team, to work together with other team members in developing hyperspectral and multispectral atmospheric correction algorithms to retrieve water leaving reflectances from OCI radiance measurements. We have extensive experience developing atmospheric correction algorithms. In early 1990s, we developed the first model-based land version of hyperspectral atmospheric correction algorithm (nicknamed ATREM) (Gao et al., RSE, 1993) to support the NASA HIRIS (High Resolution Imaging Spectrometer) Project. In late 1990s, we developed an ocean version of hyperspectral atmospheric correction algorithm for the Navy (Gao et al., Applied Optics, 2000), which was based on Robert Fraser's formulation (Fraser et al., JGR, 1997). In early 2000s, with funding support from the NASA SIMBIOS Project, we modified the ocean version of the hyperspectral atmospheric correction algorithm, and developed a MODIS version of multi-channel algorithm for remote sensing of water leaving reflectances over turbid coastal waters (Gao et al., IEEE TGRS, 2007) from a combination of MODIS land and ocean channels. A SWIR spectrum-matching technique using MODIS channels centered at 1.24, 1.64, and 2.13 micron was used to estimate aerosol models and optical depths. More recently we developed a VIIRS version of coastal water atmospheric correction algorithm. The VIIRS channels centered at 1.24, 1.61, and 2.25 micron with proper modeling of atmospheric CO_2 and CH_4 absorption effects and a SWIR spectrum-matching technique were used for atmospheric corrections. Over the past 6 years, we have supported the HICO (Hyperspectral Imager for Coastal Ocean) Project. We developed the L1B software for converting raw digital numbers to L1B radiances with proper consideration for instrument artifacts, such as spectral smear and second order light. We developed spectrum-matching algorithms for refining HICO wavelength calibrations and for monitoring the stability of the HICO instrument with time. We developed a functional version of atmospheric correction algorithm for processing HICO data. Here we propose to use our experience in hyperspectral and multi-channel algorithm development and in analysis of AVIRIS, MODIS, VIIRS, and HICO data, to help the development of atmospheric correction algorithms for processing PACE OCI data, and support the spectral and radiometric calibrations of the hyperspectral portion of the OCI instrument. We would work together with other PACE atmospheric correction team members for the design and implementation of a consensus OCI atmospheric correction algorithm.

Olga Kalashnikova/Jet Propulsion Laboratory
Evaluation of UV Atmospheric Correction in the Presence of Absorbing Aerosols, and Quantification of Enhancements Provided by Multiangle, Polarimetric and Oxygen A-Band Observations

Satellite remote sensing of ocean color is an invaluable tool for assessing the productivity of marine ecosystems and monitoring changes resulting from climatic or environmental influences. Yet water-leaving radiance comprises less than 10% of the signal measured from space, making correction for absorption and scattering by the intervening atmosphere imperative. Traditional ocean color algorithms are based on a standard set of aerosol models and the assumption of negligible water-leaving radiance in the near-infrared. Modern improvements have been developed to handle absorbing aerosols such as urban particulates in coastal areas and transported desert dust over the open ocean, where ocean fertilization can impact biological productivity at the base of the marine food chain. Even so, imperfect knowledge of the absorbing aerosol optical properties or height distribution results in well-documented sources of error. At short wavelengths, where PACE spectrometry intends to improve the separation of chlorophyll from CDOM as well as quantify different phytosynthetic pigments contributing to light absorption spectra, these problems are amplified due to the increased Rayleigh and aerosol optical depth, especially at off-nadir view angles. This proposal is to the Atmospheric Correction category of the PACE Science Team. Through sensitivity studies and simulated retrievals employing both Mie and nonspherical particle scattering codes in conjunction with a vector Markov Chain radiative transfer code, we will quantitatively evaluate the relative merits of various measurement modalities for meeting the PACE Science Definition Team uncertainty requirements of max (5%, 0.001) in water-leaving reflectance in the visible and max (10%, 0.002) in the near-UV. In particular we will quantify water leaving radiance measurement uncertainty in the presence of absorbing aerosols from ultraviolet observations at single view angles representative for the PACE ocean color spectrometer. Then we investigate the added value of observations from (a) multiangle UV radiometry, (b) multiangle visible photopolarimetry, and (c) oxygen A-band for simultaneous characterization of absorbing aerosol microphysical properties, effective altitude, and non-zero water-leaving radiance. Bio-optical models will be used to characterize surface bidirectional reflectances. Theoretical sensitivities will be then evaluated against AirMSPI observations at AERONET-OC UC SeaPrism site collected during PODEX, SEAC4RS, and HyspIRI campaigns. Measurements by TOMS, OMI, and JPL's airborne sensor AirMSPI demonstrate the importance of UV observations for detecting absorbing aerosols. Theoretically, multiangle UV radiometry, blue wavelength polarimetry, and narrowband (~5 nm) oxygen A-band measurements have the potential to estimate aerosol height. Our experience with MISR demonstrates the ability of multiangular radiances to distinguish dust from other airborne particles, and shows the value of such observations for separating aerosol and surface scattering over non-black ocean waters. Polarimetry offers additional constraints on aerosol size distribution and real refractive index. Drawing upon our expertise in aerosol remote sensing instrumentation and associated aerosol and surface retrieval algorithm development for MISR, AirMSPI, and AirMSPI-2, we will refine the requirements for a PACE imager with multiangular, UV-shortwave infrared, A-band, and polarimetric sensing capability (the polarimeter), assess the practicality of the required observations, and quantify the added value of imaging polarimeter to the PACE ocean color spectrometer in compensating for the effects of absorbing aerosols.

ZhongPing Lee/University Of Massachusetts, Boston
Development of Datasets and Algorithms for Hyperspectral IOP Products from the PACE Ocean Color Measurements

Inherent optical properties (IOPs) play a key role in modulating the color of oceanic and coastal waters, and provide the critical link to infer the concentrations of constituents in the upper water column. In the recent decade, various algorithms, both empirical and semi-analytical, have been developed for the retrieval of IOPs from ocean color, which is measured by the spectrum of remote-sensing reflectance (Rrs, sr-1). These algorithms, in particular the algebraic algorithm (QAA) and the spectral optimization algorithms (e.g., GSM, GIOP), have been implemented to retrieve various IOPs from Rrs measured by SeaWiFS and MODIS, thus providing prototype IOP products at a few bands for the global oceans. The quality of these products, however, depends on the validity of the spectral shapes of the IOPs (SSIOP) used in these semi-analytical algorithms, but the determination of the SSIOP from remote sensing is far from mature. More importantly, the PACE mission will provide hyperspectral Rrs of the global oceans, thus the derivation of hyperspectral IOP products will demand accurate estimation of hyperspectral SSIOP. The improvement of the SSIOP estimation and the determination of hyperspectral IOP algorithms for PACE will depend critically on a robust hyperspectral Rrs-IOPs dataset, but there is no such a dataset yet for the community to use. To fill this void, with an ultimate goal to maximize the IOP products from the PACE hyperspectral measurements, we propose to 1) compile a hyperspectral Rrs-IOPs dataset from field measurements; 2) improve the estimation of SSIOP from ocean color; 3) revise the QAA and HOPE (a hyperspectral optimization algorithm) to take advantage of the hyperspectral and UV measurements offered by PACE, with a goal to expand the current IOP products to include information beyond chlorophyll-a (e.g., the absorption coefficients of chlorophyll-b,-c, and phycocyanin); and 4) test and evaluate these semi-analytical algorithms with HICO measurements.
Outcomes from this effort will be fourfold: 1) a hyperspectral Rrs-IOPs dataset with closure for the community to use, 2) improved estimation of SSIOP from ocean color to benefit all semi-analytical algorithms, 3) revised QAA and HOPE to derive hyperspectral IOP products, and 4) experience with HICO in processing and storing hyperspectral image products. These results will provide desired tools and knowledge for processing hyperspectral measurements by PACE, and contribute to "consensus and community-endorsed paths forward for the PACE sensor(s)".

Stephane Maritorena/University Of California, Santa Barbara
How Useful Will the PACE UV Bands be for IOP Retrievals and Atmospheric Correction?

Several prospective ocean color sensors such as PACE will have spectral bands in the UV in addition to those in the visible and those designed for atmospheric correction in the NIR and SWIR regions. The expected usefulness of the UV bands for ocean color sensors is two-fold: 1) they should allow a better discrimination between phytoplankton and CDOM -through their inherent optical properties, IOPS-in the ocean and 2) they can help in the atmospheric correction when absorbing aerosols are present. They PACE UV bands are expected to help mostly in coastal and turbid waters where both high amounts of CDOM and the presence of absorbing aerosols are frequent. Because both CDOM and absorbing aerosol show increased absorption toward short wavelengths, confounding effects may limit the ability of the UV bands to discern the role of CDOM and aerosols in the remote sensing signal.

Here, we propose to test the use of the PACE UV bands for both IOP retrievals and atmospheric correction. We will test the performance of a semi-analytic ocean color algorithm (an upgraded version of the GSM model) for the retrieval of IOPs using available in situ data that cover the UV and visible domains. Using simulated data, we will also test how perturbations in the NIR and SWIR atmospheric bands affect the spectral IOP retrievals (from UV to the green wavelengths). Last, we will test if the UV bands can be used to better constrain the aerosol path radiance and improve atmospheric correction. Some of these analyses will also be considered with the HICO data.

Brian Mitchell/University of California, San Diego
Improved Satellite Ocean Color Retrievals of Ocean Inherent Optical Properties and Biogeochemical Properties Utilizing the Capabilities of PACE

To support algorithm development for PACE, we propose to use a globally diverse and detailed optical and biogeochemical data set to develop new parameterizations of absorption and scattering, to advance our understanding of the scattering phase function, and to assess closure of forward and inverse model predictions compared to measured optical and biogeochemical variables. Our data spans the range of spectral relevance for PACE for ocean retrievals (350-750 nm) and includes inherent and apparent optical properties (IOP, AOP) and the most fundamental biogeochemical parameters of interest for remote sensing of ocean ecology. Contemporary satellite retrievals of several IOP variables (phytoplankton absorption, the sum of detrital and correlated spectral channels on orbit. These limitations restrict retrievals of IOPs at few wavelengths and limit our ability to accurately estimate chlorophyll a, particulate organic carbon, and adg, defined as the sum of soluble absorption and detrital particle absorption (CHLA, POC and adg). Using our global data set, we evaluate in this proposal the performance of current empirical and inverse algorithms demonstrating important limitations that can be greatly improved by the work we propose.   Combining our uniquely detailed and global data set with UV-Vis numerical modeling in Hydrolight we propose to develop new parameterizations of relationships between the most important ecological variables that govern upper ocean IOP and AOP over the extended spectral range of PACE (350-750 nm). Due to the improved spectral range and resolution of PACE, we envision an ability to broaden the number of biogeochemical constituents to also include UV-absorbing mycosporine amino acids (MAA), phycobiliproteins (PBP) and particle size distribution (PSD) that are needed to specify phytoplankton functional groups and plankton ecosystem structure. PSD data will be based on our global observations of Coulter Counter size distributions and flow cytometer (FCYT) analysis. FCYT data will provide important details of phytoplankton functional groups and size distributions , 2 Âµm. We will analyze our liquid nitrogen archived samples for FCYT, MAA and PBP collected over the past 15 years and integrate these new analytical results to our uniquely detailed and global data base to allow us to pursue our proposed goals. Our goal will be to develop forward models of IOP and AOP as governed by CHLA, POC, adg, MAA, PBP and PSD. We will implement a system of optimization combining Hydrolight code extended to the UV, and our large, detailed and globally distributed measurements, to develop forward radiative transfer models dependent on the expanded set of biogeochemical variables. We will use our optimized data to create synthesized ocean spectral reflectance 350-750 nm that will be combined with our expanded set of biogeochemical observations to develop novel inverse algorithms for PACE (MAA, PBP, Nd), spectral values of IOPs, and more robust algorithms for the heritage retrievals (CHLA, POC, adg). We will also utilize our hyperspectral global ocean phytoplankton absorption, HPLC pigments, MAA, PBP and Nd data to develop improved estimates of phytoplankton functional groups. As we did for SeaWiFS (SeaBAM; O'Reilly et al. 1998), as participants in the PACE Science Team we will evaluate our data, models and satellite algorithms in a collaborative way to contribute to the community goal of robust consensus algorithms for a dramatically expanded set of biogeochemical variables that will be enabled by the capabilities of PACE.

Steven Platnick/Goddard Space Flight Center
Retrieval Studies In Support of Cloud Property Products from the PACE Ocean Color Imager

Obtaining cloud climate data records from the current generation of global imagers (MODIS, VIIRS) is challenging due to the need for exacting reflectance stability over multiple decades. Imager stability requirements for ocean color applications have been demonstrated to the sub-percent level for SeaWiFS using lunar observations; similar capabilities for the PACE Ocean Color Instrument (OCI) are defined in the PACE Science Definition Team (SDT) report, in addition to stringent requirements in other radiometric/spectral specifications that are essential for the establishing climate records. Understanding the extent to which the PACE imager can be used to produce relevant and stable cloud products is of strategic importance. We propose to support PACE ocean color imager instrument requirements related to cloud property retrievals as part of the Atmospheric Correction measurement suite. Initial studies on the use of OCI for initiating cloud records were studied by the SDT for instrument options that included three additional spectral channels (OCI+) in addition to higher spatial resolution in selected channels (OCI/A). The team will participate in instrument specification, trade studies, and mission/instrument development laboratory studies as they pertain to cloud retrievals and information content from OCI+/A. Studies will include use of the instrument for cloud detection, thermodynamic phase detection, optical/microphysical retrievals, and cloud-top information from the O2 A-band and water vapor bands. More broadly, the team will study the retrieval capability of an OCI+/A instrument relative to MODIS and VIIRS cloud data records, with the goal of understanding the ability of a PACE imager to continue and/or compliment the existing imager products using a combination of theoretical and empirical retrieval studies. The SDT report has already provided nominal retrieval capabilities and associated science for a 3M polarimeter. Though our team has theoretical and practical experience with polarimetric cloud retrievals, we have not explicitly budgeted for additional studies due to continued uncertainty in a PACE polarimeter. The PACE SDT report provided details on imager options, measurement specifications, and derived science. However, as acknowledged in the solicitation, the PACE mission instrument suite and measurement requirements have yet to be determined, especially with regard to cloud retrieval capabilities. Further, the team is being solicited before the scope of an Announcement of Opportunity (AO) for the PACE instrument(s) is known. Therefore, it is critically important to have comprehensive cloud retrieval expertise on the PACE Science Team. The proposed multi-institution team collectively provides broad research, observational, and measurement experience in cloud remote sensing, and is well-suited for carrying out retrieval studies as PACE mission instruments and objectives evolve. Several team members contributed to the PACE SDT report and associated Instrument and Mission Design Lab studies.

Lorraine Remer/University of Maryland Baltimore County
Aerosol Absorption Retrievals from Base-Line OCI Observations:
Risk Reduction for Atmospheric Correction of the PACE Mission

Aerosol absorption is a key aerosol parameter required for quantification of direct aerosol radiative forcing and has been linked to changes in atmospheric circulations and large-scale precipitation patterns and to cloud macrophysical properties over large regions. Thus, a satellite aerosol product that quantifies absorbing aerosols will make a significant contribution to climate science. Absorbing aerosols also confuse atmospheric correction over oceans and interfere with determination of ocean water-leaving radiances, even at low aerosol loading. Thus, both the atmospheric and oceanic communities are united by their need to identify and quantify absorbing aerosols over the global oceans.

The Pre-Aerosols-Clouds-Ecosystem (PACE) mission will attempt to push oceanographic science a full step forward by defining the Ocean Color Instrument (OCI) with hyperspectral capability from the ultraviolet (UV) to the near-infrared (NIR), and with additional wavelengths in the shortwave infrared (SWIR). We propose here that the basic PACE OCI instrument, with no enhancement, will also make a significant improved contribution to aerosol science.

OCI is an exciting instrument for aerosol scientists because it will be the first truly broad spectrum U.S. instrument, effectively combining the aerosol-retrieval capabilities of MODIS and OMI, but on the same instrument, at the same spatial resolution. Sensitivity tests tell us that we should be able to retrieve 3 pieces of aerosol information from this configuration: nominally loading, absorption and either particle size or layer height. These published sensitivity tests are far from complete and they do not cover the wide range of circumstances that are required to identify optimal wavelength configurations and retrieval assumptions necessary to prepare for producing an aerosol product from OCI.

Here we propose a series of theoretical studies to determine the uncertainties involved in 1) identifying absorbing aerosol at low aerosol optical depth (AOD) for the purposes of atmospheric correction, and 2) retrieving aerosol information including AOD and absorption at moderate to high AOD. Our focus is on the over ocean retrievals, where the new broad spectrum OCI offers enhanced possibilities, but this will be overlaid on a global (ocean and land) product that would represent adapting existing OMI and MODIS algorithms to OCI radiances.

We are offering a perspective towards atmospheric correction that is aerosol-centered, proposed by investigators who are undisputed experts in aerosol retrieval from an OCI-type of sensor. This work represents the major theoretical exploration and defining of uncertainties necessary for producing an operational product from satellite data.

In addition, the PI (Remer) is volunteering to serve in a leadership capacity on the PACE Science Team.

Collin Roesler/Bowdoin College
Quantifying Uncertainties in Phytoplankton Absorption Coefficients forAccurate Validation of the PACE Ocean Color Sensor: Moving Towards Satellite Retrieved Phytoplankton Functional Types (PFTs)

NASA’s fleet of ocean color satellites have provided an enduring times series of phytoplankton chlorophyll concentration of a quality sufficient for a climate data record. Following on from SeaWiFS and MODIS missions, the Pre-Aerosol, Cloud, ocean Ecosystem (PACE) mission is designed to fulfill the climate continuity requirements, with a launch readiness in the time frame of 7 years. Beyond the estimation of phytoplankton chlorophyll concentration, the goals of PACE are to provide climate-quality global ocean color measurements that are essential for understanding the carbon cycle and global ocean ecology and determining how the ocean’s role in global biogeochemical (carbon) cycling and ocean ecology both affects and is affected by climate change. Among the improvements for the ocean color specifications are increased spectral and spatial resolution.

One of the specific objectives of the PACE mission is the retrieval of the inherent optical properties (IOPs), absorption and backscattering, via ocean color inversion algorithms. The capability for retrieving spectral phytoplankton absorption coefficients is key to addressing questions of carbon cycling and ocean ecology as these coefficients provide not only an estimate of algal concentration (that can be linked by proxy to algal carbon) but also to algal composition via pigment-based taxonomic discrimination. Pigment-based taxonomic composition provides a key approach to defining phytoplankton functional types (PFTs) as many of the pigment-based lineages coincide with biogeochemical niches, calcifiers, silicifiers, nitrogen fixers, etc. One challenge for the PACE mission is to define robust protocols with quantified uncertainty terms for constructing validation data sets for phytoplankton absorption. While in situ optical technologies exist to measure hyperspectral absorption on the spatial and temporal scales approaching those required for satellite validation, extracting the signature associated solely with phytoplankton cannot currently be performed analytically and thus we rely on model estimates.

Measuring phytoplankton absorption requires collection of discrete water samples, collecting the particles on glass fiber filters to remove the optical contribution by colored dissolved organic matter (CDOM), and measuring the absorption spectrophotometrically before and after pigment extraction. The absorption by the phytoplankton pigments in vivo is calculated by difference. However, the filter pad contaminates the signal due to its strong scattering properties and additionally amplifies the optical pathlength of transmitted photons in the spectrophotometer. These two error sources are inadvertently combined into a single correction factor, beta, called the pathlength amplification factor. Many researchers over the years have investigated this factor using a variety of strategies and technologies and yet it remains the largest source of uncertainty in the quantification of phytoplankton absorption. Unfortunately, models for extracting the phytoplankton absorption from in situ observations of whole water or particulate absorption are based upon laboratory investigations in which beta was poorly constrained at worst, or at best for which the uncertainties were not quantified. Thus in order to address the need for ocean color validation of phytoplankton absorption coefficients, a unified approach linking the quantitative filter pad technique to continuous in situ absorption observations is required and is the primary focus of this proposal. The secondary focus of this proposal is to investigate whether multispectral chlorophyll fluorescence can provide a quantitative proxy for phytoplankton absorption at the excitation wavelengths. This approach would expand the opportunities for in situ phytoplankton absorption validation by making use of a simple, economical, easily deployed technology that does not require the same level of optical expertise as absorption technologies.

Cecile Rousseaux/Universities Space Research Association, Columbia
Phytoplankton Composition Algorithms for PACE

We propose to develop an algorithm to derive phytoplankton composition using a radiation model that provides hyperspectral data similar to what we expect from the PACE mission. Because there has not been any previous global mission with similar capabilities, there is a need for assessing the best approaches and anticipate potential problems if we are to get the most information out of this mission. Here we propose to use the Ocean-Atmosphere Spectral Irradiance Model (OASIM) to derive the total water-leaving radiance of single and mixed phytoplankton functional groups. We will then use an extensive dataset to develop an algorithm or algorithms to derive phytoplankton composition from these hyperspectral data. We will test this algorithm against in situ data that were withheld from the algorithm development. Finally we will apply this algorithm to a state-of-the-art biogeochemical model (NASA Ocean Biogeochemical Model) that has been shown to represent reasonably well the global distribution of phytoplankton composition. Using this model, we will assess how well this newly developed algorithm does in representing the natural global distribution of phytoplankton groups. Comprehensive quantitative error and uncertainty analysis will be integral in each of the stages of the proposal. Additionally, we propose simulations to test different configurations of the sensor to understand the capabilities and limitations associated with engineering options. Although we acknowledge that there may be formidable challenges throughout these steps, we believe that we can learn some valuable information from these challenges.

Dariusz Stramski/University of California, San Diego
Quantifying the Spectral Absorption Coefficients of Phytoplankton and Non-Phytoplankton Components of Seawater from in Situ and Remote-Sensing Measurements

As members of the PACE Science Team we propose to pursue analytical and theoretical studies as part of the measurement suite area "Inherent Optical Properties (IOPs) of the Ocean". Our goal is to improve field measurements of particulate absorption coefficients and remote sensing estimates of absorption coefficients of phytoplankton and non-phytoplankton components and particulate carbon pools associated with these components. The main objectives are to: (1) Develop a protocol and quantify the uncertainties of a new filter-pad approach and the existing filter-pad methods to measuring the particulate absorption coefficient; (2) Develop a model to partition the absorption coefficient of seawater into phytoplankton, nonalgal particulate (NAP), and colored dissolved organic matter (CDOM) components with a key novel aspect of separating NAP from CDOM; and (3) Conduct a pilot study of the relationship between NAP absorption and NAP organic carbon to enable a capability for remote sensing of carbon pools associated with separate phytoplankton and non-phytoplankton components. The overall approach to address these objectives will be based primarily on the analysis of existing laboratory and field data, but will also encompass a combination of limited number of laboratory and field measurements to collect new data, and the application of remote sensing data from high spectral resolution sensor HICO. With regard to Objective 1 we will examine the filter-pad methods for determining the absorption coefficient of particles with high spectral resolution(~ 1 nm) over a broad spectral range from UV through NIR; specifically the traditional transmittance (T) and transmittance-reflectance (T-R) methods as well as the inside-sphere (IS) method which is the most recent refinement with the filter placed inside an integrating sphere. The IS method offers several advantages over the T and T-R methods, leading to improved accuracy and precision of absorption measurements. We will determine complete protocols including new optimal correction algorithms for pathlength amplification factor (which is the main source of uncertainty) and will quantify uncertainties for all three methods, benefiting the interpretation of historical data and acquisition of future data of particulate absorption. We anticipate that the IS approach will serve as the new recommended (preferable) method for measurements of particle absorption. With regard to Objective 2 we will develop a model to provide for the first time a capability for estimating the three major absorption components separately (phytoplankton, NAP, and CDOM) from the total absorption coefficient of seawater, which is derivable from remote sensing. In this development, we will use the existing quality-verified field data of absorption coefficients from various regions of the world's ocean and will expand the approach that has been successful for partitioning the absorption coefficient into phytoplankton and non-phytoplankton (NAP+CDOM combined) components (Zheng and Stramski 2013). The significance of the proposed partitioning model is associated with relationships between the component absorption coefficients and biogeochemical stocks, such as DOC, particulate nonalgal and phytoplankton carbon, chlorophyll-a, as well as phytoplankton community structure and primary productivity. As a prototyping activity (Objective 3) we will examine one such unexplored link, specifically the relationship between the NAP absorption and NAP organic carbon, which will provide a basis for estimating separate pools of phytoplankton and nonalgal organic carbon from remote sensing. This project will create new and advance existing algorithms for deriving ocean color data products, in particular IOPs and carbon stocks associated with separate phytoplankton and non-phytoplankton components, which will contribute to scientific goals of PACE mission to understand ocean carbon cycling and ecology.

James Sullivan/Western Environmental Technology Laboratories, Inc.
Improving IOP Measurement Uncertainties for PACE Ocean Color Remote Sensing Applications

A goal of the PACE Science Team is to achieve consensus and develop community-endorsed paths for measurement suites required for the PACE mission. This proposed work will specifically address the inherent optical properties of absorption and backscattering, better quantifying uncertainties using current and emerging methods, and improving uncertainties in both reprocessed historical data and future data collections for the PACE mission. Accurate values of absorption and backscattering, and estimates of their uncertainties, are critical for remote sensing validation and development/refinement of retrieval algorithms. However, one aspect of each property stands out as an enduring source of uncertainty. For absorption measurements in particle fields, this aspect is the scattering error associated with reflective tube absorption technologies (as in the widely used WET Labs ac devices). Recent testing in our labs has shown that the different schemes used to correct this error in virtually all of the ac device data submitted to SeaBASS over the last 20 years has significant errors (10% or >). At this time, these errors are acknowledged (e.g. Leymarie et al. 2010; McKee et al. 2013), but there is no consensus on a recommended protocol for correcting scattering errors with the best accuracy possible. For backscattering, the largest area of uncertainty in clear ocean waters is the backscattering contribution from the pure seawater itself, which can comprise 80-90% of total backscattering for great swaths of the ocean. Recently, Zhang et al. (2009) revised the theory to describe pure seawater scattering as a function of the physical properties of water (i.e., temperature, salinity, pressure), but a single critical physical constant of pure water used in these calculations remains poorly known: the depolarization ratio, which is the ratio of horizontally polarized light to vertically polarized light in the scattered beam at 90Â°. The value the in situ optics community is currently using comes from a single study conducted nearly 40 years ago (Farinato & Rowell 1976). In that work, 3 experimental values were actually derived: 0.051, 0.045, and 0.039, each with different viewing optics. Currently, the lowest one measured, 0.039 is usually recommended because of the difficulties with stray light contamination possibly elevating their other experimental values. For decades, the remote sensing community has typically used the pure seawater scattering values of Morel (1974), which followed a different theoretical approach, with a recommended depolarization value of 0.09 (more than 100% higher than our current best guess), based on the state of knowledge at the time. Thus, one is left with virtually no confidence in the accuracy of this parameter, only a gut feeling that we are in the ballpark. We should note here that even relatively modest uncertainties in the depolarization ratio (e.g. 10%) could translate to large uncertainties in open ocean particulate backscattering retrievals (e.g. 40%), due to the fact that the subtracted pure seawater component can be 80-90% of the entire water-leaving signal.

We propose to conduct comprehensive historical data analyses to fully characterize uncertainties in the scattering error for reflective tube absorption meters, and to determine and validate optimal scattering correction methods through minor lab experimentation for different deployment configurations and suites of ancillary measurements. The impacts of using different depolarization ratio values for the determination of pure water backscattering on uncertainties in ocean color retrieval algorithms will also be investigated. We further propose to use modern, specialized, bench top volume scattering function equipment and water purification methods in our lab to determine and validate with rigorous uncertainty the precise value of the depolarization ratio to improve the accuracy of retrievals for historical data and the future PACE mission.

Michael Twardowski/Western Environmental Technology Laboratories, Inc.
Improving Retrieval of IOPs from Ocean Color Remote Sensing Through Explicit Consideration of the Volume Scattering Function

Radiative transfer (RT) approximations form the basis of semi-analytical (SA) inversion algorithms formulated to derive IOPs and subsequently biogeochemical parameters from ocean color remote sensing. Leading SA inversion algorithms, however, have not been rigorously assessed with respect to particulate volume scattering function (VSF) variability in the ocean, as, up until very recently, the comprehensive VSF data sets required for such an assessment have not been available. It is generally recognized by the community that there is likely no larger source of uncertainty in current SA algorithms to derive IOPs than the uncertainty associated with variability in VSF shapes, as the other important parameters in the inversions have been rigorously assessed (Loisel et al. 2001; Morel et al. 2002; Gordon 2002). Through field work since 2005 supported by NASA and other sources, we now have extensive in situ IOP data sets from 18 locations that contain fully resolved VSFs in a wide range of Case I and Case II waters throughout the world (Sullivan and Twardowski 2009; Czerski et al. 2011; You et al. 2011; Twardowski et al. 2012; Gilerson et al. 2013; Randolph et al., in press). Included in these data sets are NASA ocean color validation experiments with concurrently collected IOP (including VSF) and radiometric measurements, where the technological assets employed, scope of the measurements, and attention to accuracy make these data sets special and unique. Not only are they some of the few nominally complete data sets from an RT closure perspective that we are aware of (as they include full VSFs and full radiance distributions), but the data quality is the highest possible that can be achieved at this time. With such measurements in hand, we have an exciting opportunity to evaluate the effects of varying VSF shape on retrieval uncertainties for the leading SA inversions, and to assess performance for a variety of specific environmental conditions. There is also the opportunity to reevaluate RT approximations such as a Zaneveld (1995) model that explicitly includes VSF shape information, as these models have generally been avoided due to the historical lack of representative VSF data.

The specific goals of this work are to 1) assess the full range of variability in VSF shapes in the ocean using an extensive data base of custom VSF measurements collected by our lab, 2) evaluate uncertainties in leading SA inversion approaches associated with this natural VSF variability through RT modeling, and 3) to resuscitate, rework, and evaluate uncertainties in native, analytical RT approximations developed by Zaneveld (1995) and Jerlov (1976) that have received little attention to date specifically because of the fact that they included explicit VSF formulations that could not be practically applied in the past. Our approach will first involve computing remote sensing reflectances from our extensive data sets using the Hydrolight RT solution. Reflectances will then be validated using concurrently measured radiometry data to assess convolved errors in the measurements (separate from uncertainties related to inversion approximations), and to ensure the data sets are sound from a theoretical standpoint. The SA inversion algorithms will then be applied, with the retrieved absorption and backscattering compared to the original measurements to quantify uncertainties. Our overall goal is to quantify and minimize errors in inversion results when applied to a representative range of observed VSFs in the ocean, leading to recommendations in SA algorithm applications for the future PACE mission.

Xiaodong Zhang/University Of North Dakota, Grand Forks
Understanding Natural Variability of VSFs and Its Impact on Biogeochemical Retrieval from Ocean Color

A key challenge in applying ocean color remote sensing for assessing biogeochemical stocks in the ocean is to link the signal seen by satellite or airborne sensors with the optically active water constituents and their biogeochemical origin. The linkage between ocean color and biogeochemical stocks is established via the inherent optical properties of water, most importantly the volume scattering function (Î², m-1 sr-1) and the total absorption coefficient (a, m-1). While our ability to understand and separate the various components of absorption has improved over the last decades, the major challenge remains in the understanding of the sources of variability in the volume scattering function, and particularly the backscattering that are directly relevant to ocean color observation. This has hindered our ability to derive IOPs accurately and to interpret their variability biogeochemically.
Of IOPs, the VSF is most difficult to measure with only few data available. The scarcity of data has led to unrealistic assumptions, such as that the phase function of particles can be represented by the average of Petzold’s data. This in turn has led to uncertainties in understanding the roles played by particles of different type in generating remote sensing reflectance and the color of the ocean. Recent technological and theoretical advances have allowed us 1) to measure the full angular scattering over a diverse aquatic environments and 2) to interpret the measurements in terms of particle size distribution and composition. We have greatly improved our understanding of natural variability of the VSF and the biogeochemical origin of the variability. However, these improved knowledge has yet to applied to ocean color. The objective of this study is to understand the natural variability of the VSF and its impact on biogeochemical interpretation of ocean color. The answers to this question will help to constrain two major uncertainties

affecting both the current and future PACE ocean color missions: bidirectional effect and sources of backscattering.

Our approach is centered on in-depth analysis of the field measurements of complete sets of IOPs (including full range VSFs) and biogeochemical stocks covering various aquatic environments through both forward and inverse modeling. The information of biogeochemical stocks is also contained in the detailed angular pattern of the VSF and can be retrieved by VSF-inversion. Applying forward modeling to simulate spectral backscattering from the inversion results will tell what biogeochemical information about particles (such as the size or the type) is retained in, and hence can be possibly retrieved from, the backscattering coefficient derived from ocean color. Comparisons of the modeled and measured biogeochemical stocks and comparisons of the modeled and measured spectral backscattering will aid in the interpretation of the modeling results and will also provide a basis for validating, and possibly refining, the overall modeling approach.

The proposed study addresses a fundamental, yet poorly known, linkage between the optical scattering and biogeochemical properties of natural waters. The potential outcome of the study can not only advance our understanding of the VSF as an key IOP parameter but also improve the performance of existing ocean color algorithms by further constraining the uncertainty associated with angular scattering as well as to guide the development of new approaches for ocean color algorithms.