

A new paradigm for ocean color satellite calibration and validation: accurate measurements of hyperspectral water leaving radiance from autonomous profiling floats (HYPERNAV).

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Introduction: Maintaining sufficient accuracy over the lifetime of satellite-based ocean-viewing radiometry missions requires a robust vicarious calibration program that complements the onboard calibration devices and enables routine verification of the ocean color instrument calibration while on orbit (e.g. Clark et al., 1997, Del Castillo, 2012, McClain and Meister, 2012, Zibordi and Bailey, 2012). Vicarious calibration is the process of combining data from a satellite sensor with combinations of in situ measurements and models to determine the on-orbit calibration factor for the satellite sensor (Clark et al., 1997). Highly accurate in situ measurements of upwelling radiance near the sea-surface are used to estimate remote-sensing reflectance, or equivalently normalized water-leaving radiances, which provide the principal source of surface truth for the operational vicarious system calibration of ocean color satellite sensors.

The majority of vicarious calibration and validation activities have been carried out in areas of very uniform oceanic optical properties (Zibordi, et al, 2015), along with a simple, preferably clean, cloud-free atmosphere, namely the MOBY (Marine Optical BuoY) site (Brown et al., 2007) and the BOUSSOLE (BOUée pour l’acquiSition de Séries Optiques à Long termE; Antoine et al., 2008) site. While these sites provide excellent continuous in situ data, it is advantageous to collect data from additional clear ocean sites as well as covering regions with differing water masses, biogeochemical parameters and atmospheres that more fully envelop the satellite’s mission (see Voss et al., 2010). Our project addressed this need by increasing the areal and temporal extent of potential vicarious calibration match-ups using an autonomous profiling float equipped with high spectral resolution radiometric sensors to provide accurate in situ radiance measurements that meet the criteria needed for system vicarious calibration (SVC) of satellite borne radiometric sensors.

Specifically, we aimed to provide an accumulation of large numbers of vicarious calibration matchups on a global scale by reducing the statistical uncertainty in the estimation of the derived calibration factors. The desired standard error can only be achieved with a large number of matchups as the standard error follows the inverse of the square root of the number of pairs. Because the typical ocean color satellite radiance measurements are performed over varying

bandwidths, often with complicated spectral responses, it is useful to have many vicarious calibration sites across which the combination of a wide range of signals in the water-leaving radiance and atmospheric modulation provide a robust conditional data set (Franz, et. al, 2007). The observed and measured spectral variance within the collected data will illuminate problems due to out-of-band response, changes in the ocean BRDF and atmospheric correction issues, as well as contributing to data sets required for SVC.

The NASA Pre-Aerosol Clouds and ocean Ecosystem (PACE) mission builds on past ocean color remote sensing efforts to provide a global observational basis for understanding the living ocean and for improving skill in forecasts and projections of Earth System variability (Del Castillo, 2012). Envisioned significant advances include enhanced spatial resolution and a wider spectral range extending into the UV and near-infrared (350 to 900 nm) with hyperspectral resolution (5 nm). These enhancements flow down to drive the need to augment vicarious calibration capabilities, notably in regard to the extended spectral range into the UV, and especially with regard to the increased spectral resolution.

The goals of our project were to a) develop, fully characterize, and test a new hyper-spectral radiometric-based sensing system that meets requirements for system vicarious calibration of existing and future satellite ocean color radiometers; b) to integrate the radiometer with an autonomous profiling float (Navis) for long-duration untended observations; and c) to test and evaluate the system in the blue-water ocean in the context of meeting current and future requirements for vicarious calibration of ocean color satellite radiometric data. We call this system HyperNAV.

Approach: A set of high-level sensing capability requirements were identified to support NASA's PACE mission goals for in situ vicarious calibration. These capability requirements (Table 1) included radiometric spectral range, resolution, measurement uncertainty, and stability. As such, a significant proportion of our work focused on the radiometric sensor design and development to achieve the required sensing capabilities with measurement uncertainties < 4% in the blue to green portion, and < ~5% in the red to NIR regions. Additional capability requirements included that the system have full autonomous field operation with radiometric stability and operational maintenance requirements quantified.

Our design and development approach was driven by the need to achieve the lowest uncertainty radiometric measurements using an autonomous profiling platform. Protocols documenting the collection, processing and quality assurance of in situ radiometric measurements have been well described (Mueller et al., 2003a; Mueller et al, 2003b) and were used to generate a comprehensive radiometric uncertainty table (Table 2). This table served as a guide post for design decisions, as well as providing insight as to how design decisions impact the overall uncertainty budget. As shown in Table 2, the radiometric uncertainty matrix included uncertainties associated with the calibration sources, instrument characteristics, and in situ

measurement uncertainties. Throughout each stage of development, evaluations of the design solution and prototype system were completed to quantify these uncertainties.

The development approach generally followed three stages: 1) design and testing of a new in situ hyperspectral radiance sensor system and integration with the autonomous profiling float Navis; 2) completion of laboratory calibration and characterizations of the prototype radiance sensor; and 3) field testing of the HyperNAV system in a relevant ocean environment for use in satellite vicarious calibration.

Stage one focused on the development of a new radiance sensing system. Briefly, the final radiance sensor developed include the following optical characteristics: spectral range 350-900 nm, spectral resolution ~ 2.4 nm, spatial field of view 4.5° (half angle, half maximum), integration ranges from 11 to 1920 milliseconds, mechanical shutter for dark measurements, compact fore-optics fiber-coupled to separate electronics/spectrometer housing, and integrated tilt sensor in fore-optics. The system (Figure 1) was designed to be operated in either free-fall mode (without the float) or fully integrated with an autonomous profiling float, the Sea-Bird Scientific Navis float (HyperNAV). The design includes two independent upwelling radiance sensor systems, oriented 180 degrees apart, separating the fore-optics from the electronics and spectrometer. Advantages of this design included addressing issues of sensor stability and accuracy, potential self-shading, and providing a novel means to obtain radiance measurements within 20 cm of the water surface. In addition, a high resolution pressure sensor was integrated with HyperNAV system, as well as a combined chlorophyll fluorescence, CDOM fluorescence and backscattering sensor, and a four channel downwelling irradiance sensor. During the development phase, we chose not to focus on developing a spectral downwelling irradiance sensor as the upwelling radiance measurement is more directly relevant to SVC purposes, however, the radiometric design has potential to be adapted for irradiance measurements in the future.

This stage also included development of optimal mission operation modalities for the HyperNAV (Figure 2). The bandwidth requirements for transmittal of hyperspectral data are large and communication protocols from the float were optimized to enable transmission of the profile data from the HyperNAV. Software to process the transmitted HyperNAV data were developed, though more work is needed to automate processing and QA/QC processes.

The second stage focused on characterization of the radiometric sensors. These included characterizations for polarization sensitivity, thermal effects, integration time linearity, bandwidth effects, and immersion effects characterizations. Characterizations of counts linearity and stray light effects of HyperNAV's radiance measurement system were performed at National Institute of Standards and Technology. Finally, a series of radiometric calibrations were performed to quantify instrument to instrument uncertainty.

The final stage included a series of field experiments. Field testing results were used to quantify instrument performance as well as estimate uncertainties associated with the HyperNAV system in the field. A two-week deployment of the system was completed in late 2017 off Kona, Hawaii. A comprehensive presentation of the details of the radiometric sensor design, the HyperNAV integration, and the sensor characterizations are beyond the scope of this paper. This paper summarizes the results of the radiometric uncertainty matrix for the HyperNAV system and the field deployment of the system near the MOBY site.

Results: Table 2 shows the completed radiance uncertainty matrix for the HyperNAV system providing sections for the calibration, instrument and field for select wavelengths across the UV to red portion of the spectrum. The table also includes the method used to determine the uncertainty values for each source factor. Table 2 shows total uncertainties of $< 4\%$ in the blue-green spectral region and 5-6% for the HyperNAV system, which meet or exceed the requirements specified for the PACE mission.

With respect to the calibration section, uncertainty values were derived from calibration source and reflectance target certification sheets provided by the manufacturers. Geometric effects uncertainties were derived for the radiance sensor system of Hypernav using the work of Hooker et al. (2002) to map the plaque radiance for our system field of view. Reproducibility uncertainty values were derived based on existing uncertainty budgets for radiometric calibration reproducibility. We find that the overall uncertainty values for effects due to calibration to be lower than 2% across the UV to red spectrum.

The instrument uncertainties for the HyperNAV radiance system were derived primarily from laboratory measurements and correction functions derived based on the characterizations. In the case of Counts linearity and Stray light, values were derived based on characterizations performed by NIST on the Hypernav radiance system. The overall uncertainties for the HyperNAV radiance system are lower than 1.5% across the UV to red spectrum.

Field uncertainties were derived from a combination of modeling studies, literature and field data. In some cases, e.g. tilt effects, biofouling, wave focusing, the values provided represent a possible upper maximum as additional field deployments of HyperNAV are needed to fully validate these uncertainties.

A two week deployment of the HyperNAV system was conducted from 17 November to 4 December 2017. The location of the deployment was roughly 45 km WSW of Kona, Hawaii, located approximately 158 km from the MOBY mooring site. The HyperNAV was programmed to surface daily at noon (starting Nov 18), with a park depth at 700 m (Figure 2). The HyperNAV system subsequently completed 14 daily profiles following the trajectory shown in Figure 3. The solar zenith angle for the near-noon profiles varied from 39-42 degrees.

Radiance spectra obtained during a single profile ascent on November 18, 2017 collected in the upper 10 m for one of the HyperNAV heads on the Navis float is shown in Figure 4. We

selected November 18, 2017 as the best data to compare the HyperNAV radiance data to that obtained by the MOBY system, as satellite visible cloud cover imagery showed the two regions to be clear on that day. MOBY data was obtained from NOAA MOBY team.

The HyperNav data shown in Figure 4 was wavelength corrected, however, no corrections for self-shading or stray light have been applied. We converted the Hypernav upwelled radiance below the surface to water leaving radiance measurements using the equation from Quan and Fry (1995), assuming a temperature of 20° C and a salinity of 35, and a flat air-sea boundary.

The results of the comparison show good agreement in the UV to blue portions of the spectrum, with HyperNav values higher than MOBY in the green to red portions (Figure 4). Note that no stray light corrections have been applied to the data, which may be a cause for the deviation near 350 nm. Future comparisons between the MOBY radiance source and the HyperNav system are needed to understand the increased radiance values in the green to red regions in comparison to the MOBY in situ data. Our initial comparison results of the HyperNav system with the standard for ocean color satellite calibration radiance data (MOBY) are encouraging, and show promise towards implementing a new and novel method to obtain high quality radiance data to calibrate existing and future generations of ocean color satellites.

Discussion and conclusions: The significance of the successful completion of this effort is the availability of a new radiance sensing capability for accurate and precise in situ radiance measurement of the ocean at high spectral resolution (<3 nm) and spectral range (350-900 nm). Importantly with respect to in situ vicarious calibration, we demonstrate that the HyperNAV system can achieve radiometric uncertainties of < 4% in the blue-green spectral region and 5-6% in the red region as based on a detailed uncertainty budget completed for the system (Table 2). Initial comparisons of the field data collected by the HyperNAV system showed remarkable agreement across the UV to blue regions of the spectrum, particularly in lieu of the variety of radiometric uncertainties in the data from both the MOBY and the HyperNAV system. While future work is needed to validate the comparisons with respect to match-ups with Ocean color satellite, we believe that the HyperNAV system has great potential to provide high quality radiometric data for existing and future ocean color satellite sensing missions.

The novel aspect of the HyperNAV system is the ability to provide an autonomous method of collecting in situ various calibration data across a potential variety of spatial regions, thereby significantly augmenting SVC data provided from spatial consistent sites such as MOBY. This data can aid in illuminating satellite-borne ocean color sensor problems due to out-of-band response, changes in the ocean BRDF and atmospheric correction issues. Additionally, the data collected by a fleet of HyperNAV systems can also provide an expansive suite of vertical measurements of the ocean which contribute to other global observing efforts such as the BGC-Argo mission.

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Tables & Figures:

Table 1 – High-level system requirements and capabilities to support ocean color satellite vicarious calibration and validation needs for existing and future missions.

REQUIREMENT	CAPABILITY
Spectral Range 350-900 nm	350 to >900 nm
Resolution < 3 nm	<=2.4 nm Channel spacing = <0.45 nm
Radiometric Uncertainty < 4% in blue-green	<p>< 4% in the blue-green. Uncertainty due to extrapolation from L(z) to L(0).</p> <p>High accuracy pressure and CT sensors for depth accurate to ~15cm. Further improvements complicated by wave-induced pressure changes.</p>
Radiometric Stability O(1%) per Deployment	System will park at 1000 m depth, inhibiting biofouling.
Autonomous Field Operation	<p>Excellent history of long-term float deployment. Float scheduling can be updated after deployment.</p>
Life Cycle - Sustainability and Field Maintenance	<p>Sustainability is achieved by deployment of new floats. Floats have been shown to operate reliably for long periods without maintenance.</p>

Table 2: Total uncertainty matrix of HyperNav radiance measurements. Note that an uncertainty value is provided for each of the Calibration, Instrument and Field sections. The total, k=1 uncertainty includes all sections highlighted in blue.

Source	380nm	412nm	443nm	490nm	510nm	550nm	665nm	Method
Calibration	1.88	1.87	1.80	1.74	1.68	1.68	1.71	
Irradiance Standard	0.55	0.51	0.48	0.44	0.42	0.4	0.34	Manufacturer certificate
Reflectance Target	1.1	1.1	1	0.9	0.8	0.8	0.9	Manufacturer certificate
Geometric Effects	1.4	1.4	1.4	1.4	1.4	1.4	1.4	Modeling based on Hooker et al (2020)
Reproducibility	0.23	0.23	0.23	0.23	0.23	0.23	0.23	Previous studies (see Orrico et al 2018)
Instrument	1.43	0.71	0.64	0.45	0.66	0.46	1.17	
Polarization	0.9	0.5	0.4	0.1	0.06	0.07	0.5	Laboratory measurements
Thermal	0.08	0.08	0.08	0.08	0.08	0.08	0.08	Laboratory measurements
Immersion	0.43	0.45	0.45	0.36	0.4	0.39	0.3	Laboratory measurements & Feinholz et al. (2017)
Integration Time Linearity	0.05	0.05	0.05	0.05	0.05	0.05	0.05	Laboratory measurements
Counts Linearity	0	0	0	0	0.01	0.03	1	Characterized by NIST
Stray Light	0.12	0.1	0.09	0.08	0.05	0.04	0.09	Characterized by NIST
Wavelength @ Cal	0.19	0.15	0.13	0.09	0.08	0.06	0.03	Laboratory measurements
Wavelength @ Field	1	0.1	0.1	0.2	0.5	0.2	0.1	Field data
Field	2.58	2.55	2.54	2.54	2.62	2.78	5.42	
Self-shading	0.3	0.26	0.22	0.24	0.32	0.56	2.7	Modeling using SimulO software
Tilt Effects	2.2	2.2	2.2	2.2	2.2	2.2	2.2	Field data and Kwiatkowska et al. (2017)
Biofouling	1	1	1	1	1	1	1	Brown et al. (2007)
Wave Focusing	0.5	0.5	0.5	0.5	0.5	0.5	0.5	Estimated from literature
Depth Uncertainty	0.7	0.56	0.54	0.54	0.82	1.14	4	Extrapolated from Voss et al. 2017 and field data
Surface Transmittance	0.1	0.1	0.1	0.1	0.1	0.1	0.1	Modeling based on Quan & Fry (1995)
Total, k=1	3.5	3.2	3.2	3.1	3.2	3.3	5.8	

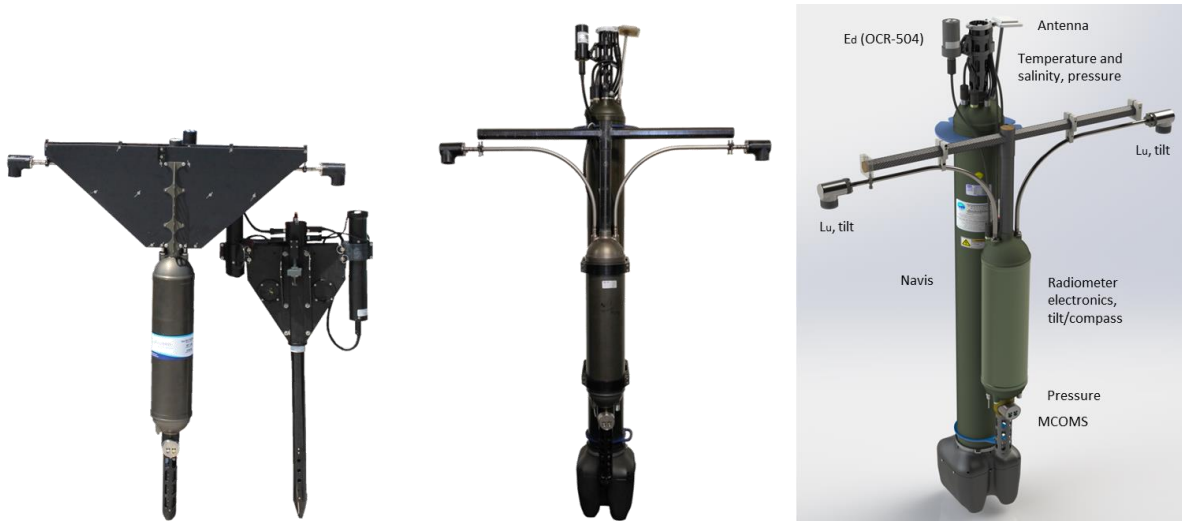


Figure 1: Left to right: The freefall (without Navis float) HyperNAV configuration shown next to a Sea-Bird Scientific HyperPro II series; HyperNAV configuration (mounted on a Sea-Bird Scientific Navis float); Rendering of the HyperNav system showing associated instrument locations.

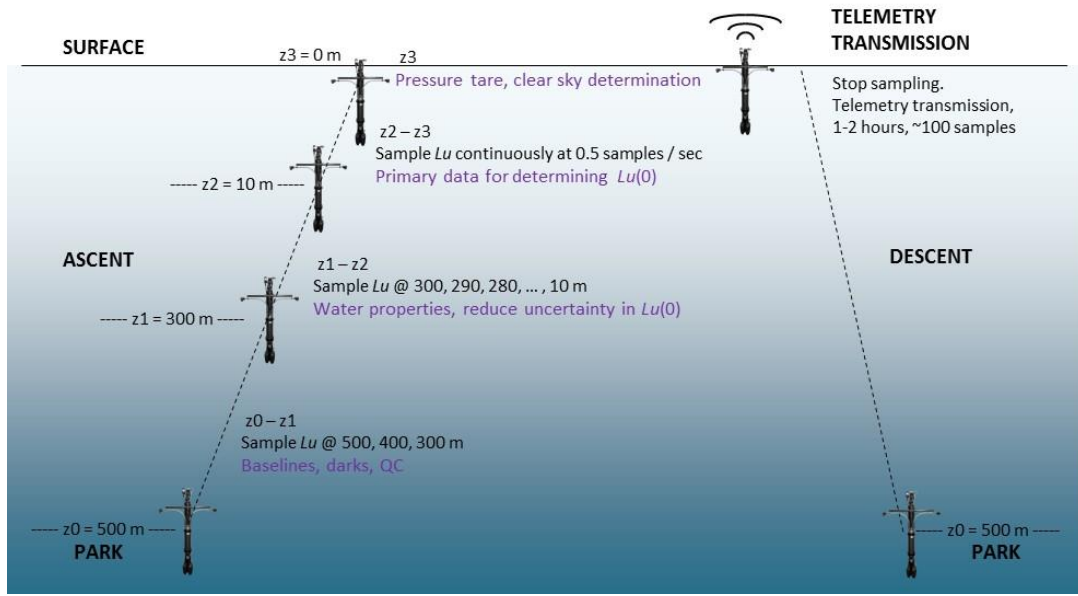


Figure 2: Idealized HyperNav profile mission sequence.

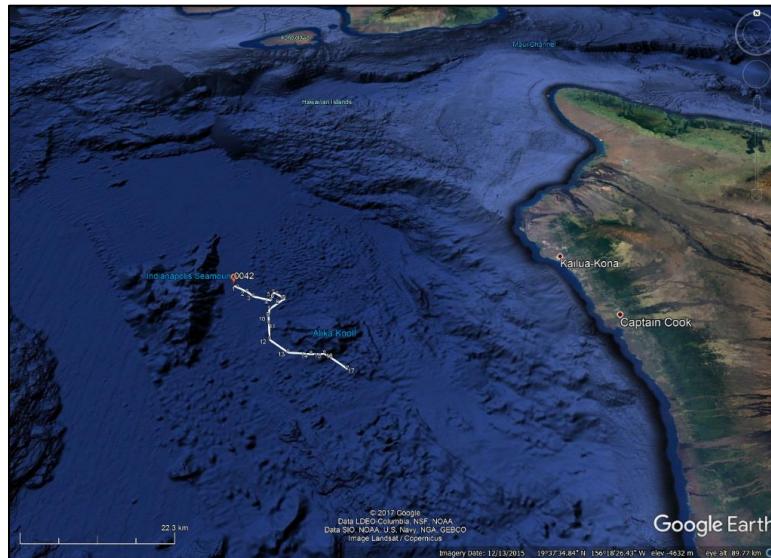


Figure 3: Path of the HyperNav profiling float over two weeks, near Hawaii Nov/Dec 2017.

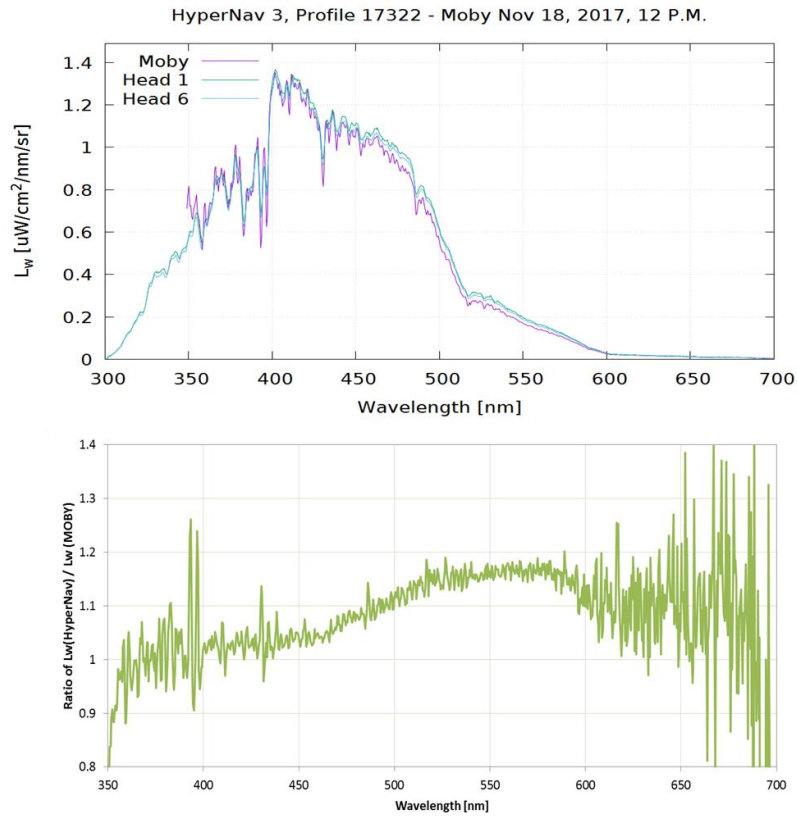


Figure 4: Top: Comparison between derived water leaving radiance spectra of HyperNAV and MOBY for data collected on 18 November 2017 HyperNAV deployment WSW of Kona, Hawaii (~158 km from MOBY site). Bottom: Ratio of HyperNAV derived water leaving radiance to MOBY. Note that HyperNAV data are not corrected for stray light or self-shading.