Consensus Field Protocols: Lessons Learned

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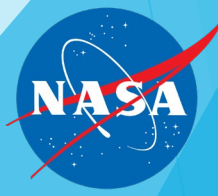
Ocean Ecology Laboratory
Field Support Group



Workshop on the Validation of Satellite-derived Optical and Water Quality Parameters for Coastal and Inland Waters 7-9 June 2022

NASA-Goddard Space Flight Center Field Support Group (FSG)

Technical lead:

Antonio Mannino

Core members:
Joaquin Chaves, Scott Freeman, Chris Kenemer, Chelsea Lopez, Aimee Neeley, Mike Novak, Harrison Smith & Crystal Thomas

Other contributors to FSG activities:
Andrea Andrew, Dirk Aurin, Ryan Vandermeulen

What we do:

- Our mission is to provide Field and Lab Measurement expertise, capability, and data to enable NASA to deliver the best quality ocean color data
- Develop consensus protocols for field and lab optical and biogeochemical measurements
- Provide HPLC pigment analysis and data to NASA PIs
- Perform SeaBASS data quality evaluation
- Conduct field instrument intercalibration and measurement uncertainty assessments
- Collect *in situ* optical and biogeochemical datasets for ocean color validation (SeaBASS) and algorithm development (NOMAD)
- Evaluate new instrument technologies and measurement approaches in collaboration with the US and international scientific community

Field equipment:
optical instruments
and other field gear

Labs in GSFC
for wet chemistry,
optics, etc.

Phytoplankton Pigment Analysis Lab

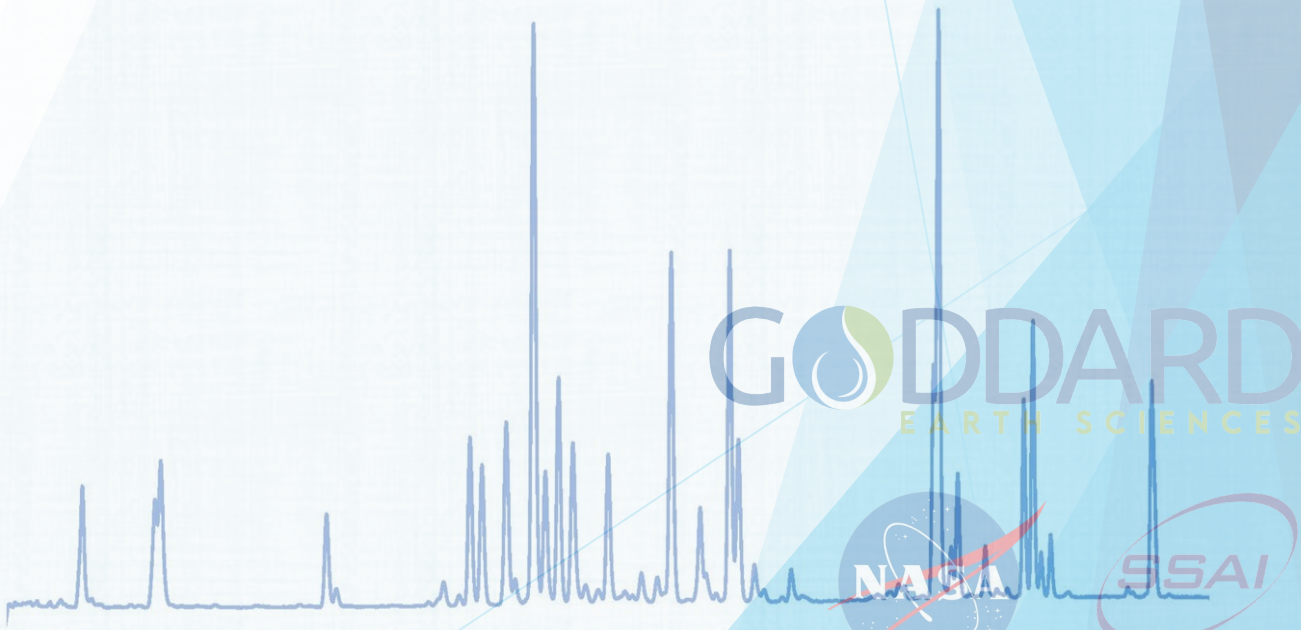

Chromatogram of pigments from
High-Performance Liquid Chromatography (HPLC)

Why?

- Pigments influence ocean color in much of the ocean and inform on phytoplankton community composition
- Chlorophyll-a relates to biomass and physiology
  - Used in Primary Productivity models
- Maintain NASA's long-term ocean color Climate Data Record since SeaWiFS in late 1997.
- Dedicated quality-assured lab necessary for validation and maintenance of chl-*a CDR*.

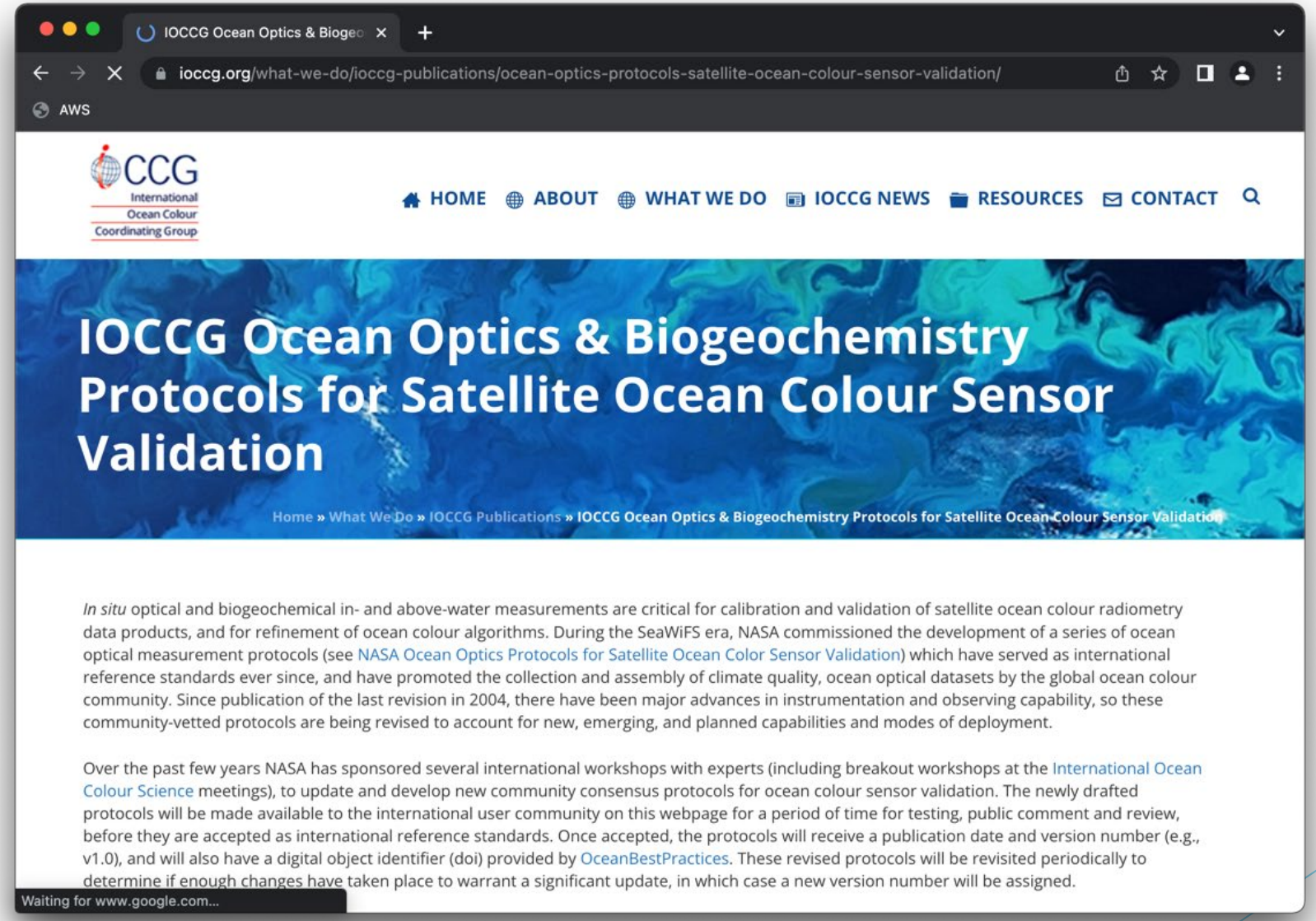
What?

- Process ~3000 HPLC pigment samples per year
- On-going efforts to maintain and improve data quality and analytical efficiency:
- cross-calibration with Horn Point Lab (UMD), international round robins, analysis on sources of uncertainty
- Methods development for phycobilin pigments
- Methods development for uHPLC and uHPLC-LC-MS

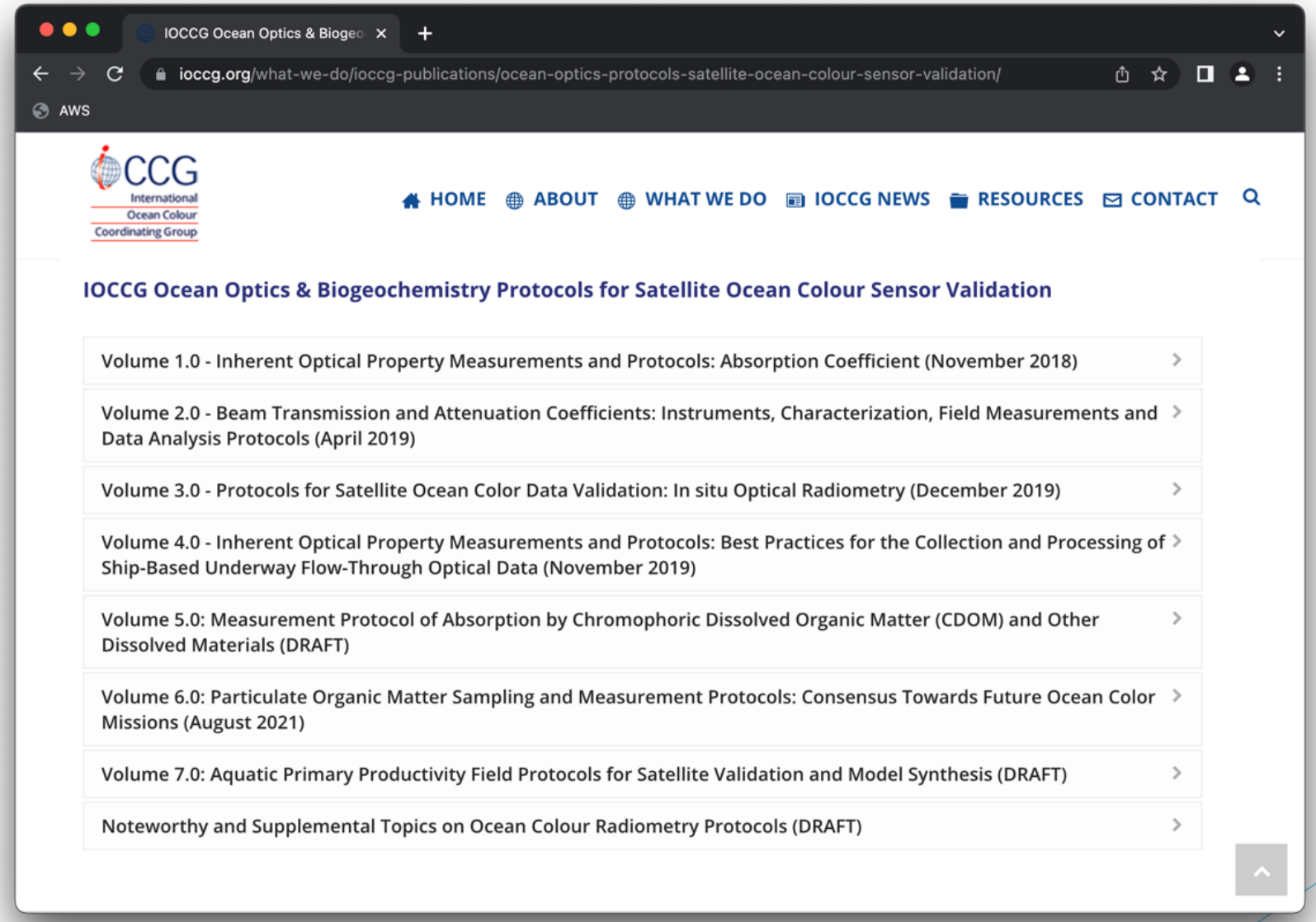


Technical lead contact: crystal.s.thomas@nasa.gov

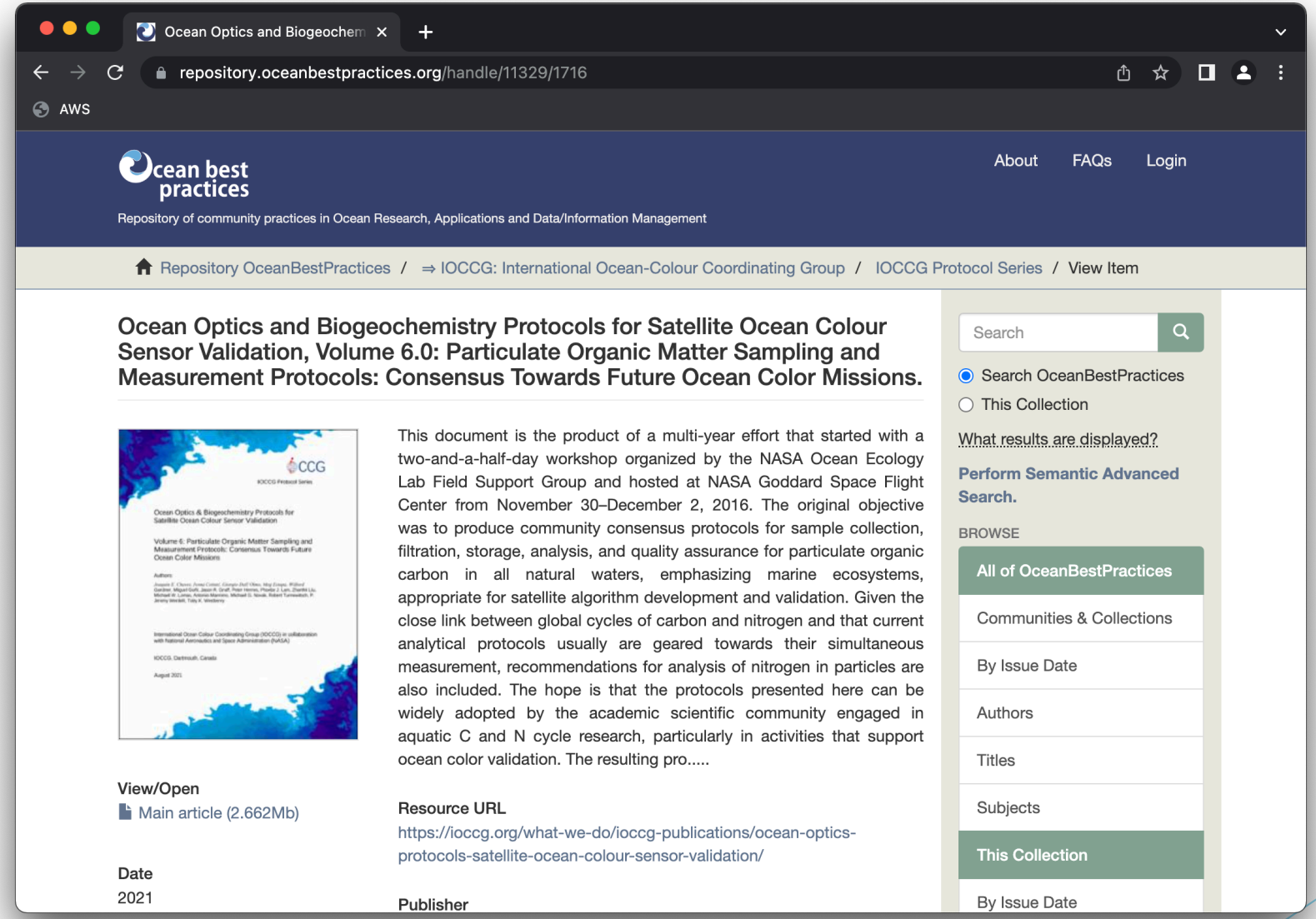
Protocols, protocols, protocols…



Protocols, protocols, protocols…



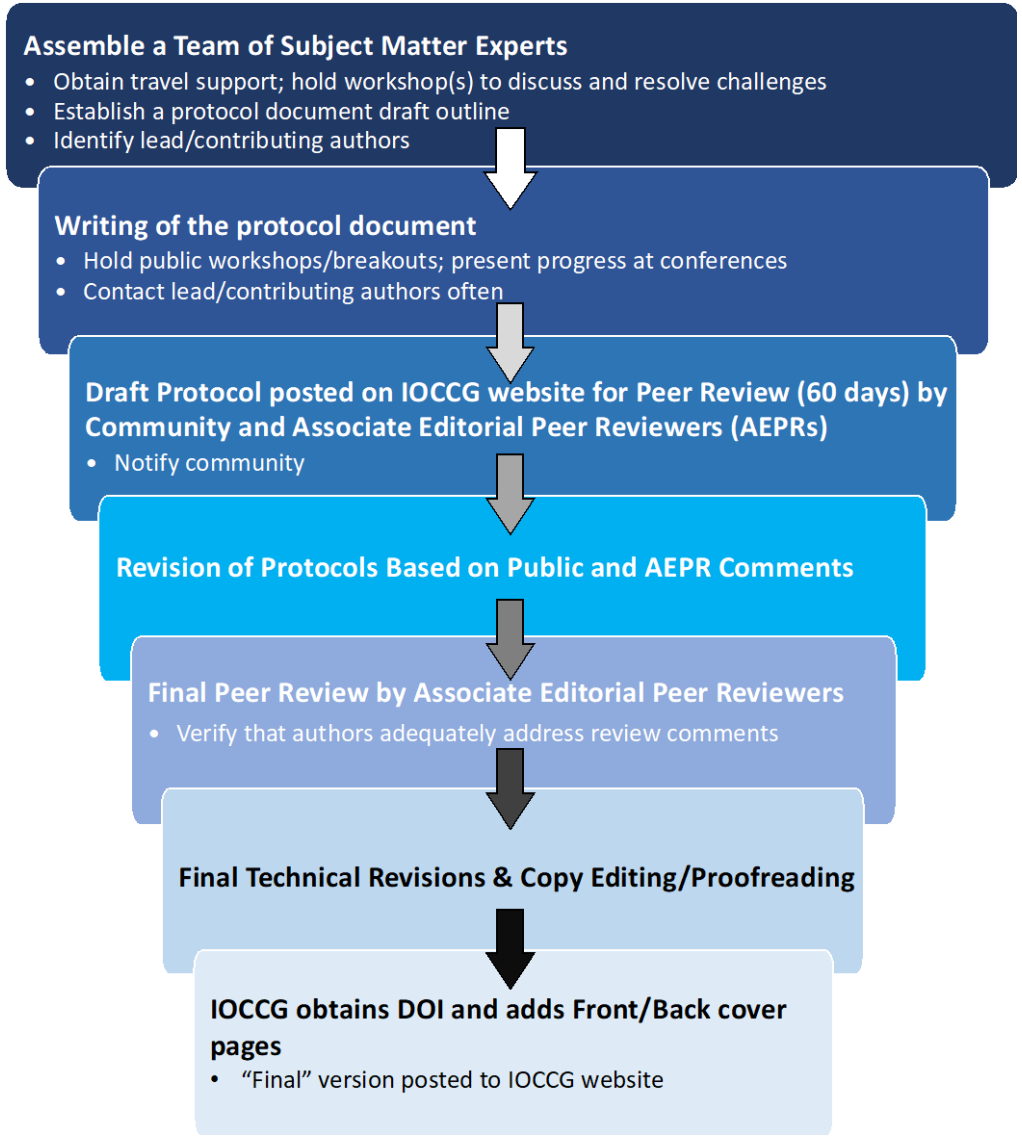
Protocols, protocols, protocols…



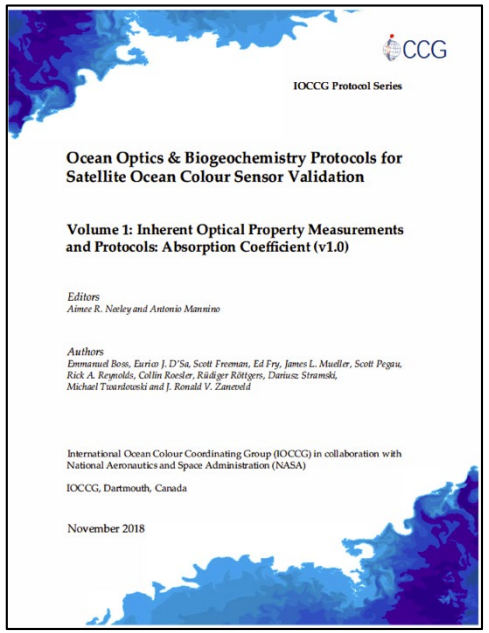
Process for Development of Field Measurement Protocols

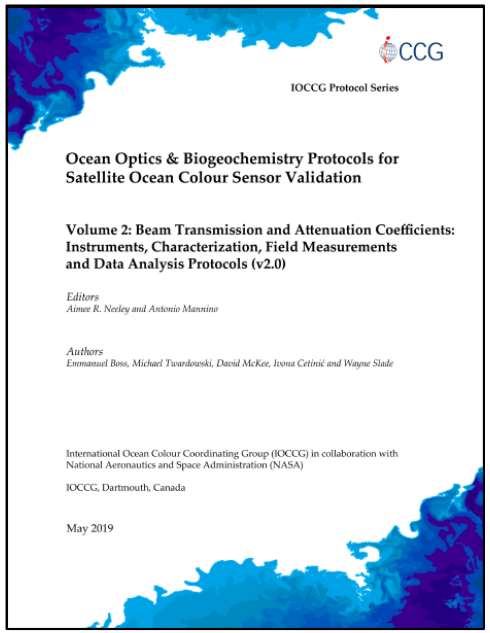
Under the auspices of the IOCCG

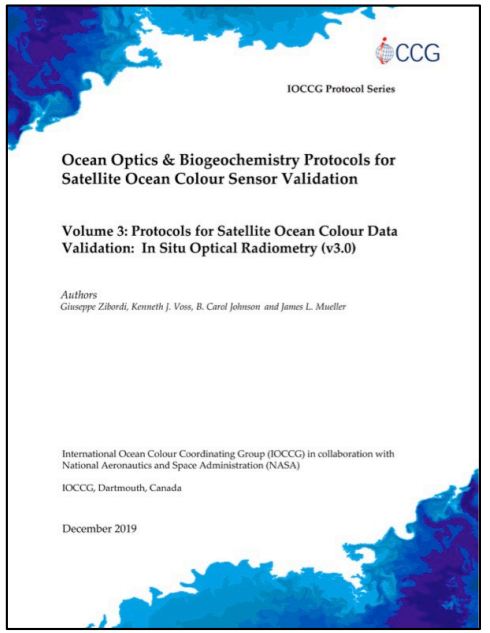
Systematic development, revision, testing, and dissemination of field data collection protocols in collaboration with experts in academia and other federal agencies.

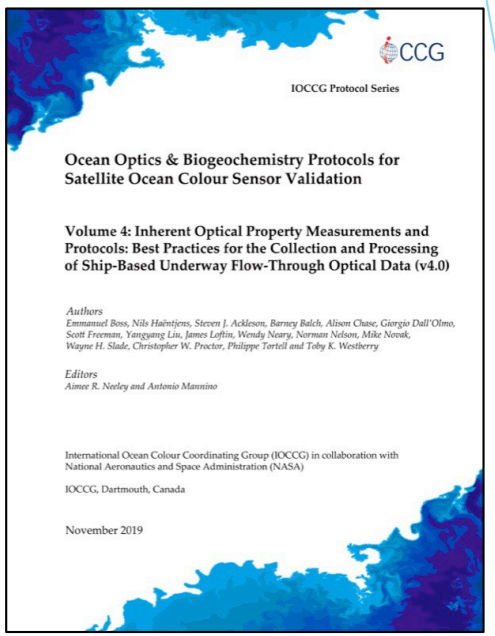


Status of Protocols - Published









Vol. 1.0 Absorption (particles)

Nov. 2018

Vol. 2.0 Beam Attenuation

April 2019

Vol. 3.0 Radiometry for Validation

Dec. 2019

Vol. 4.0 Inline Flow-Through IOPs

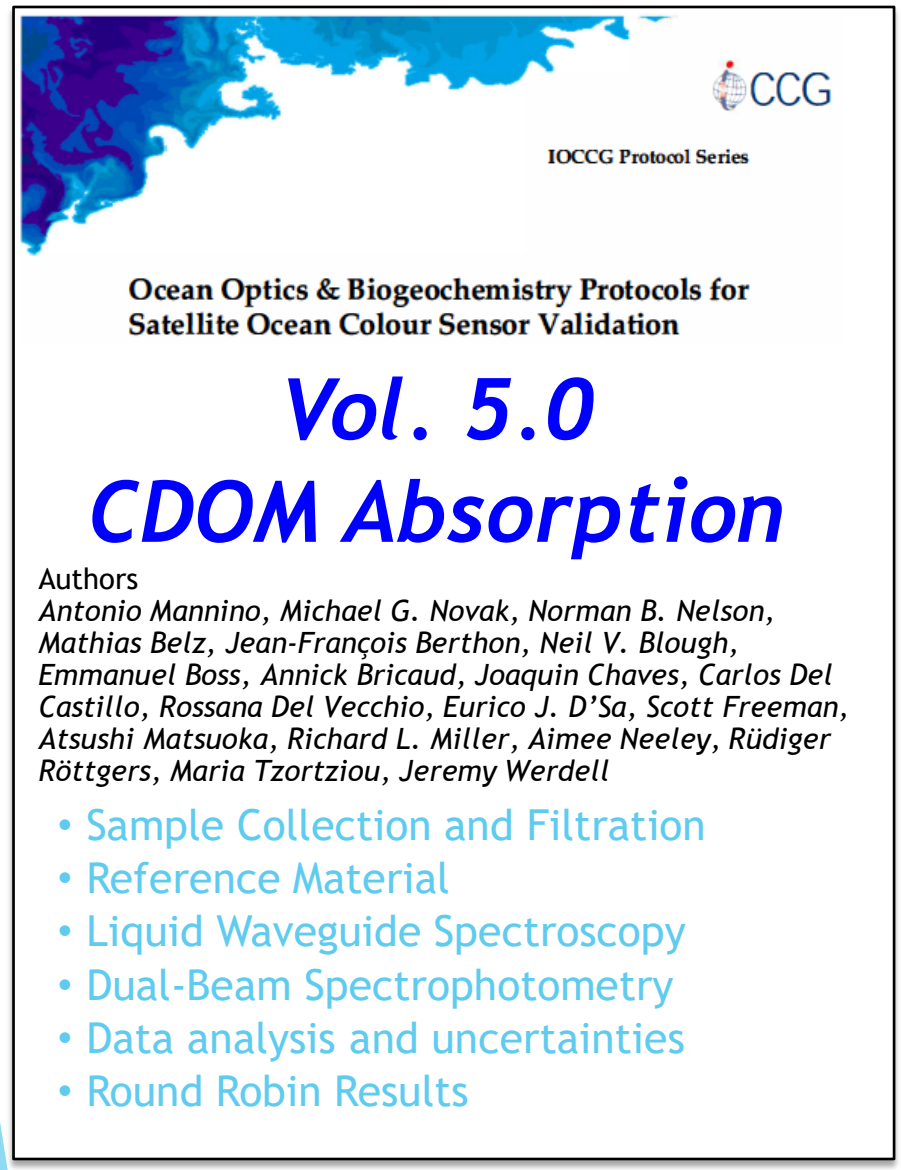
Nov. 2019

Vol. 6.0 Particulate Organic Carbon

August 2021

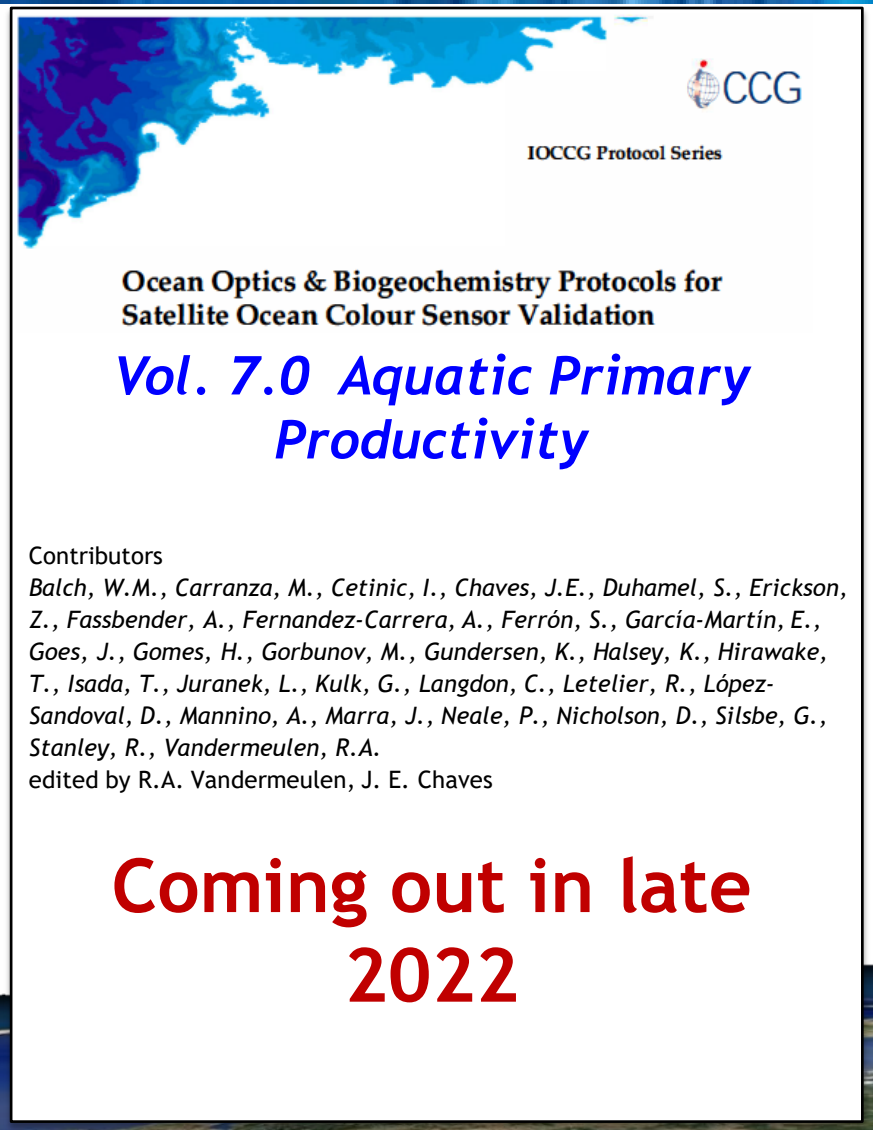
https://ioccg.org/what-we-do/ioccg-publications/ocean-optics-protocols-satellite-ocean-colour-sensor-validation/

Status of Protocols – CDOM Absorption

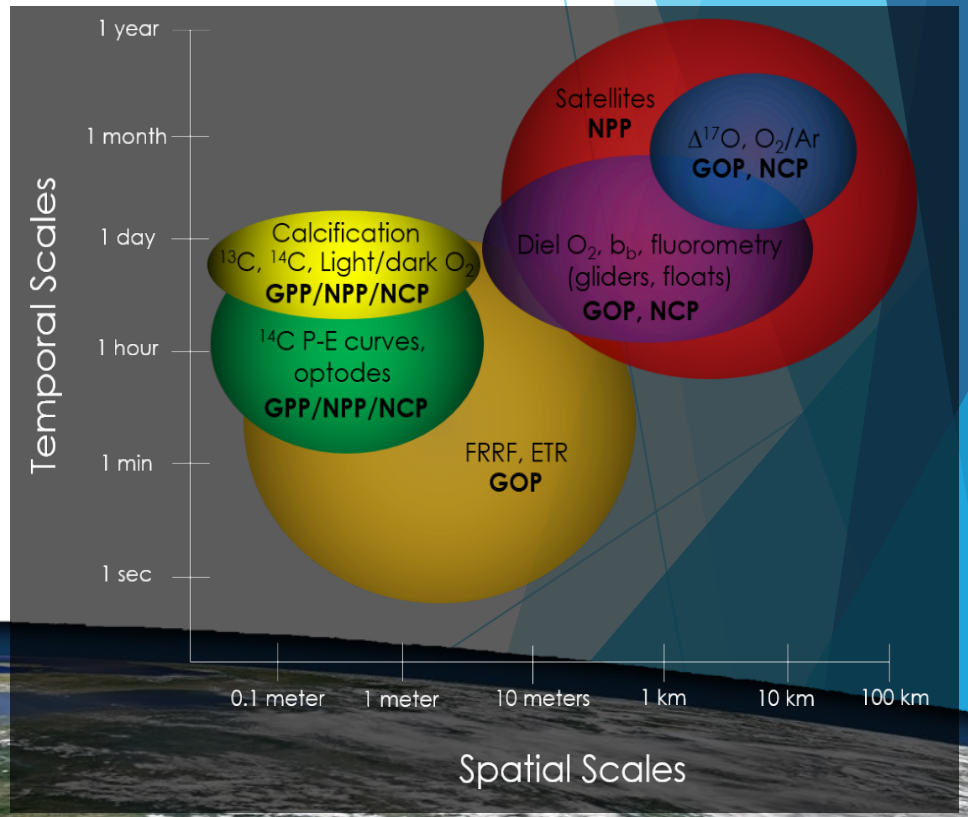


- Protocol has undergone review by AEPRs & Community
- Currently being revised per those comments
  - Updating CDOM reference material to SRFA-III
  - Merging of LWCC UV-Vis and spectrophotometer UV
- Back to AEPRs *circa* Dec. 2021
- Final version in 2022

Status of Protocols – Primary Productivity



- Protocol posted for community & AEPR review in August 2021



Top row, left to right: Solange Duhamel, Mary Jane Perry, Helga Gomes, Maxim Gorbunov, Gemma Kulk, Greg Silsbe, Roo Nicholson, Rachel Stanley, Patrick Neale, John Marra, Mark Brzezinski, Barney Balch, Tomonori Isada, Laurie Juranek, SeungHyun Son, Toru Hirawake; Bottom row, left to right: Joaquim Goes, Ana Fernandez Carrera, Antonio Mannino, Ryan Vandermeulen, Ricardo Letelier, Kimberly Halsey, Priscila Kienteca Lange, Joaquín Chaves. Other workshop participants (not pictured): Joe Salisbury, Susanne Craig, Jeremy Werdell, Paula Bontempi.

Screenshot

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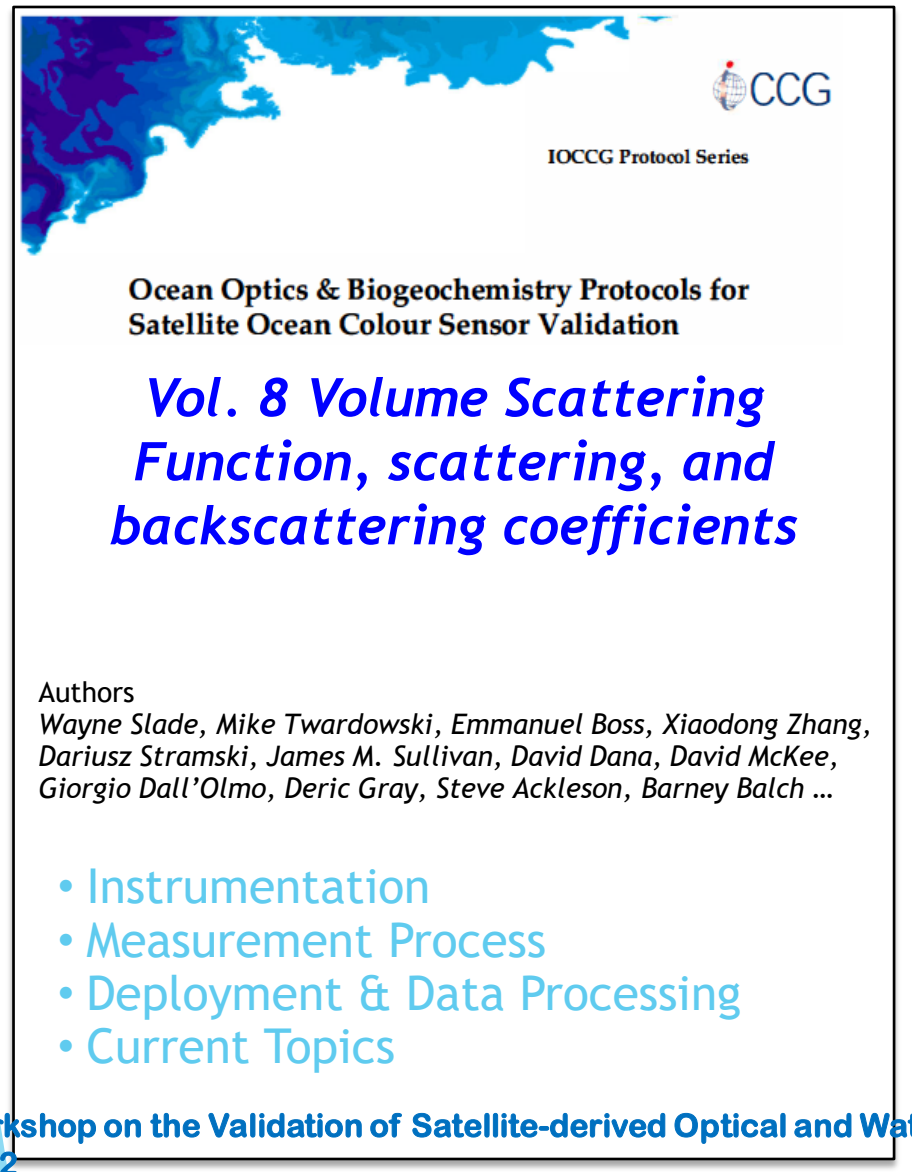
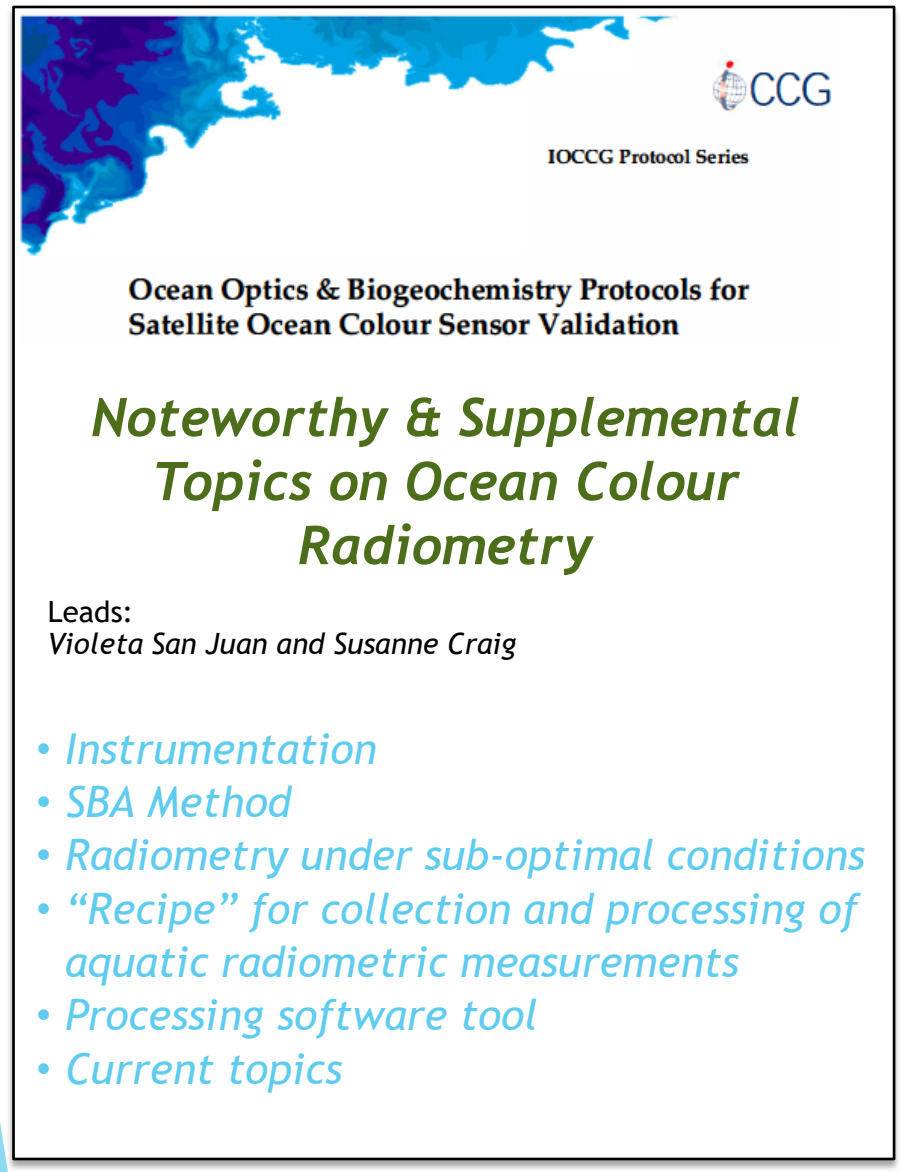
Status of Protocols - Scattering Properties

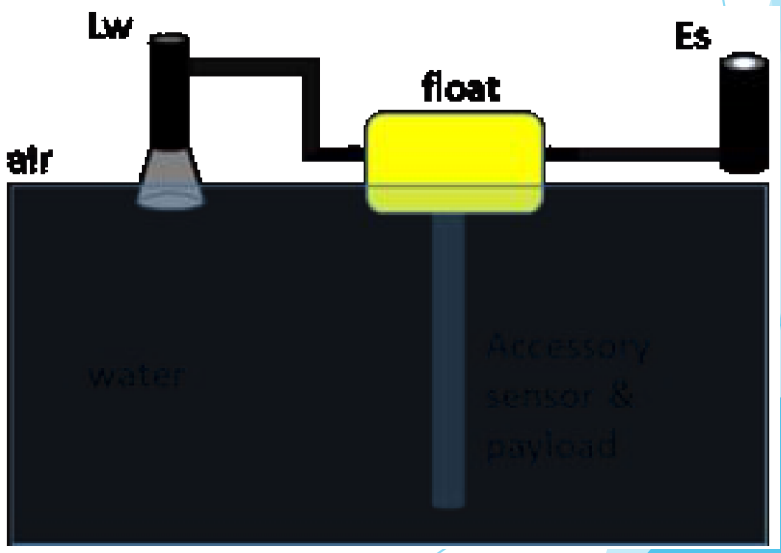


- Draft protocol in preparation
- Post protocol for community & AEPR review by end of 2021/early 2022.

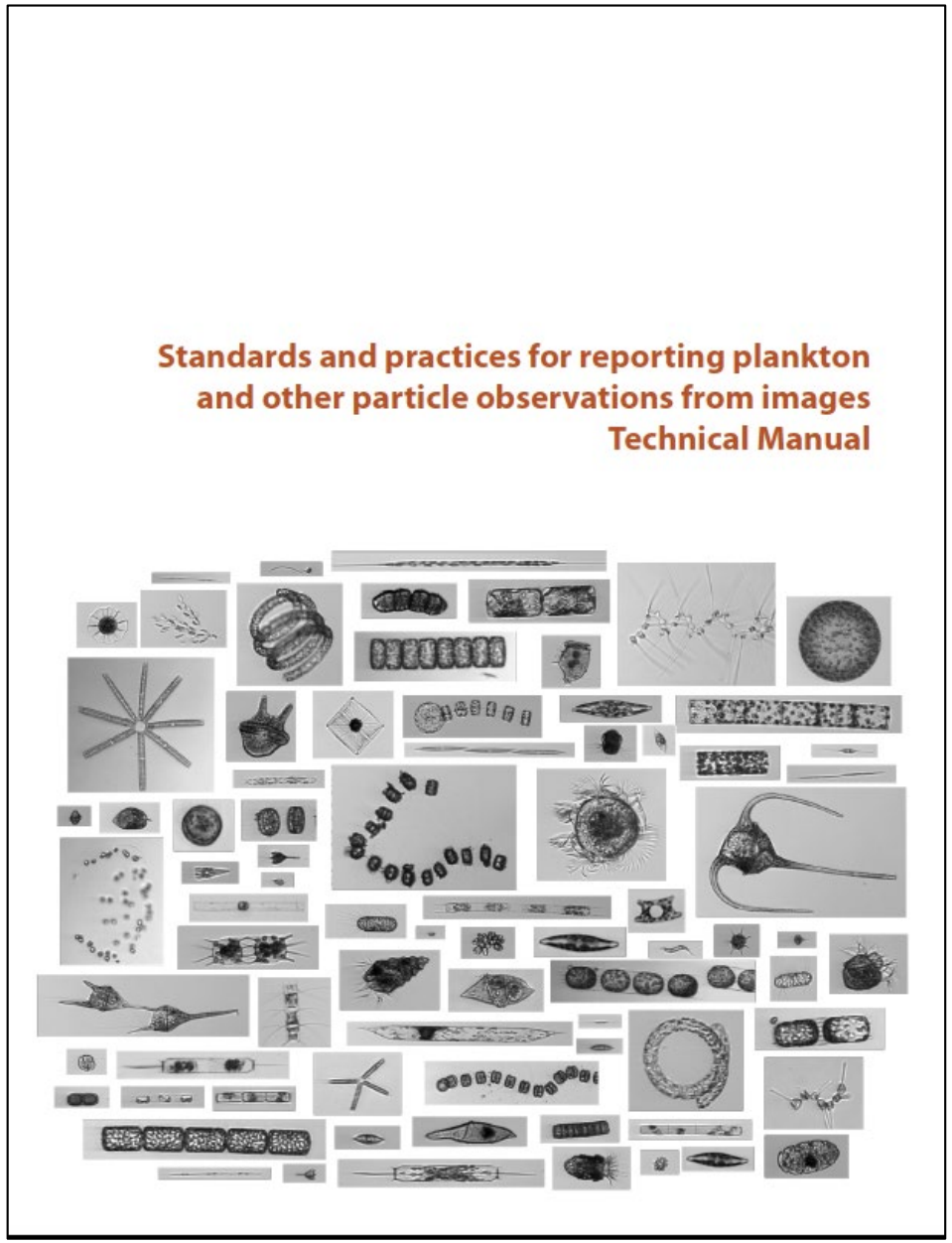
Status of Protocols – more radiometry



- Document is in planning stages
- A chapter describing the "on-water" skylight-blocked approach (SBA) by Lee et al. is posted on the IOCCG website



Reporting Data from Particle Images



Published August 2021

Neeley, Aimee, Beaulieu, Stace E., Proctor, Chris, Cetinić, Ivona, Futrelle, Joe, Soto Ramos, Inia, Sosik, Heidi M., Devred, Emmanuel, Karp-Boss, Lee, Picheral, Marc, Poulton, Nicole, Roesler, Collin S., Shepherd, Adam, "Standards and practices for reporting plankton and other particle observations from images", 2021-07-26, DOI:10.1575/1912/27377, https://hdl.handle.net/1912/27377

NSF

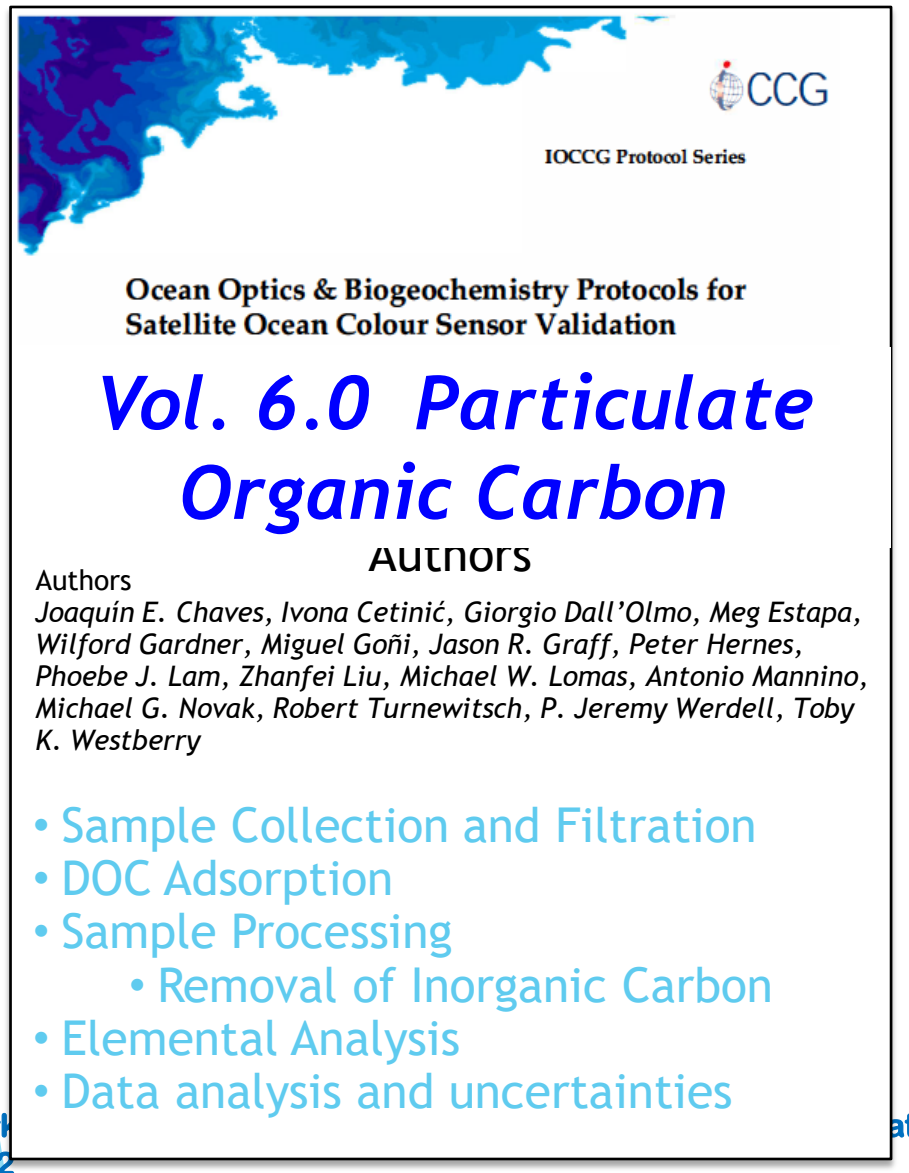
NASA

OCB
Ocean Carbon & Biogeochemistry

Planned Protocol Activities

- Future Protocols
  - Phytoplankton community composition & biovolume – kicking off soon
  - Phytoplankton Carbon – kicking off soon
  - HPLC Pigments update – in-house activity underway
  - Suspended Particulate Matter (in house literature review)
  - Dissolved Organic Carbon (in house)
  - Phycobilin Pigments – in-house activity underway
  - Optical and Biogeochemical Properties in Very Turbid Waters
  - Particle Size Distribution (with PCC ?)
  - Particulate Inorganic Carbon
  - Fluorescence properties
  - Review ship-based atmospheric aerosol and trace gas measurement protocols
- Updates to current IOCCG protocols as required

Status of Protocols - POC



- Workshop at GSFC in Nov 2016
- Published in Aug 2021

“ ”

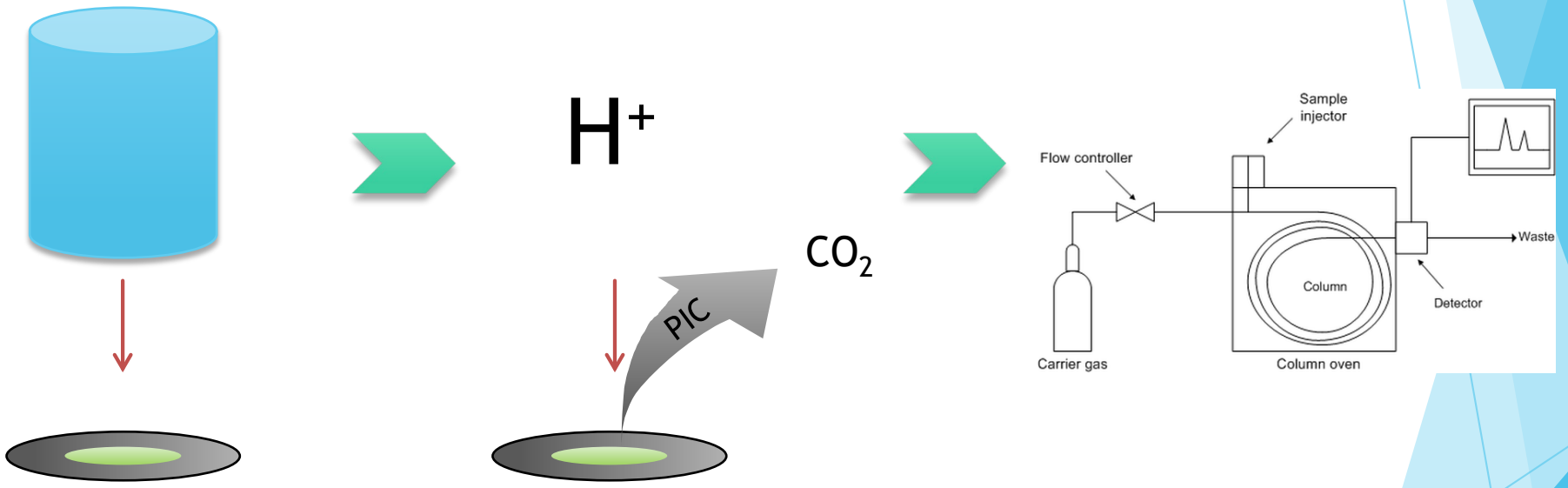
- ✓ “Since carbon is the “coin of the realm” for […] future programs seeking to understand biogeochemical processes, it is imperative that we come to closure on the methods used to measure particulate carbon”. ***Gardner, 2003***

- ✓ “As present procedures do not exist to correct for all possible biasing effects due to artificial particle formation and/or miss/loss of filterable material, uncertainties of filtration-based estimates of POC concentrations need further testing”. **Turnewitsch et al. 2007**

- ✓ “the mechanisms leading to such a large POC difference are still unclear and need to be further investigated”. **Liu et al. 2009**

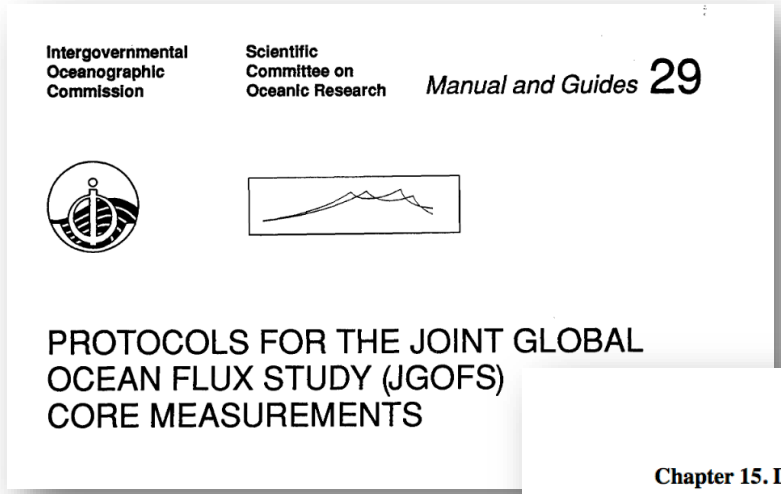
POC Methods: Persistent uncertainties

Basic POC Method:



Filtration Processing Analysis

Legacy POC Methods:

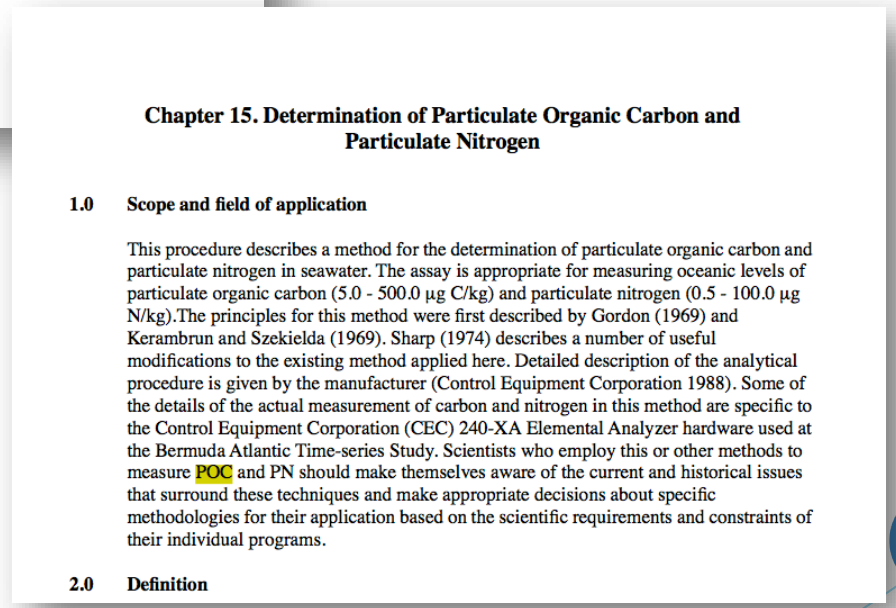


Intergovernmental Oceanographic Commission

Scientific Committee on Oceanic Research

Manual and Guides 29

PROTOCOLS FOR THE JOINT GLOBAL OCEAN FLUX STUDY (JGOFS) CORE MEASUREMENTS



Chapter 15. Determination of Particulate Organic Carbon and Particulate Nitrogen

1.0 Scope and field of application

This procedure describes a method for the determination of particulate organic carbon and particulate nitrogen in seawater. The assay is appropriate for measuring oceanic levels of particulate organic carbon (5.0 - 500.0 µg C/kg) and particulate nitrogen (0.5 - 100.0 µg N/kg).The principles for this method were first described by Gordon (1969) and Kerambrun and Szekielda (1969). Sharp (1974) describes a number of useful modifications to the existing method applied here. Detailed description of the analytical procedure is given by the manufacturer (Control Equipment Corporation 1988). Some of the details of the actual measurement of carbon and nitrogen in this method are specific to the Control Equipment Corporation (CEC) 240-XA Elemental Analyzer hardware used at the Bermuda Atlantic Time-series Study. Scientists who employ this or other methods to measure POC and PN should make themselves aware of the current and historical issues that surround these techniques and make appropriate decisions about specific methodologies for their application based on the scientific requirements and constraints of their individual programs.

2.0 Definition

U.S. JGOFS
U.S. Joint Global Ocean Flux Study

DDARD
EARTH SCIENCES

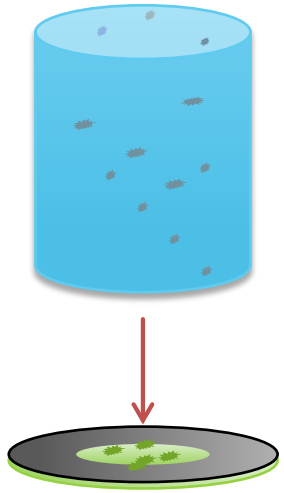
Knap, A. H., A. Michaels, A. R. Close, H. Ducklow & A. G. Dickson, 1994. Protocols for the Joint Global Ocean Flux Study (JGOFS) Core Measurements JGOFS Report. UNESCO, 170.

NASA

SSAI

POC Methods: Persistent uncertainties

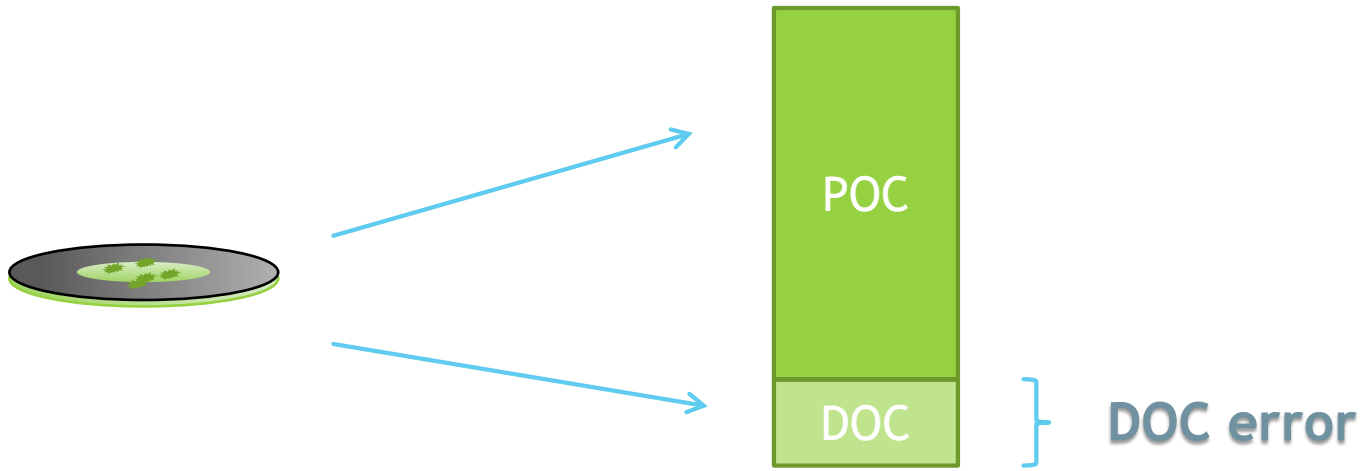
Dissolved Organic Carbon Artifact
(colloidal fraction ?)



Filtration

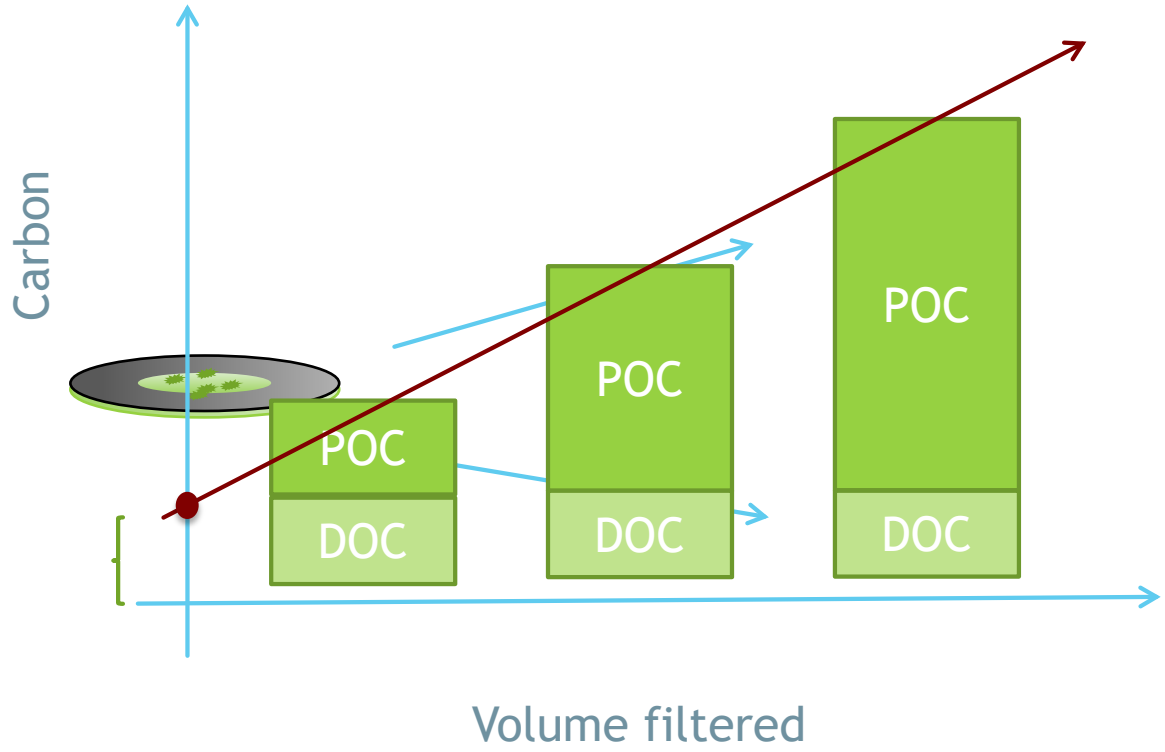
POC Methods: Persistent uncertainties

Dissolved Organic Carbon Artifact



POC Methods: Persistent uncertainties

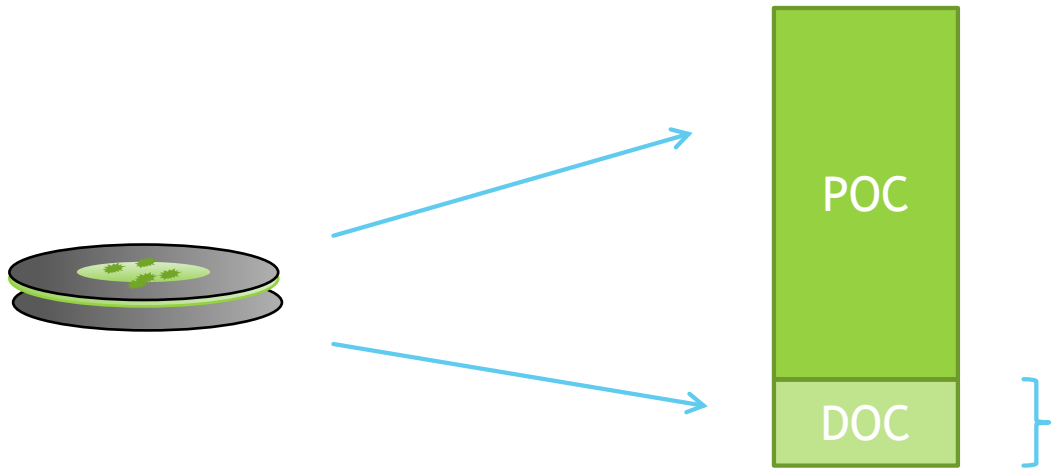
Dissolved Organic Carbon Artifact



Different volume replicates

POC Methods: Persistent uncertainties

Dissolved Organic Carbon Artifact



In-line double filters

Basic measures of uncertainty and performance metrics for POC/PN

et al. (2019) can provide further guidance.

6.4.1 *Uncertainty Budget*

For a quantity derived from addition or subtraction of independent variables a and b, $y=a+b$ or $y=a-b$, the combined uncertainty in y, u_y, is given by

$$u_y = \sqrt{u_a^2 + u_b^2}, \tag{16}$$

which is the sum in quadrature of the uncertainties u_a and u_b for the quantities a and b used to calculate y. For quantities, q, derived from a product or quotients of measured magnitudes $a,\ldots,f$

$$q = \frac{a \times \cdots \times c}{d \times \cdots \times f}, \tag{17}$$

the fractional or relative uncertainty of q, provided that the uncertainties in $a,\ldots,f$ are independent and random, is given by the sum in quadrature of their respective fractional uncertainties

$$\frac{u_q}{|q|} = \sqrt{\left(\frac{u_a}{a}\right)^2 + \cdots + \left(\frac{u_c}{c}\right)^2 + \left(\frac{u_d}{d}\right)^2 + \cdots + \left(\frac{u_f}{f}\right)^2}. \tag{18}$$

Given that in (9), the mass of C as POC, $M^{\mathrm{C}}_{\mathrm{POC}}$, is derived from the total uncorrected mass of C, $M^{\mathrm{C}^*}_{\mathrm{T}}$, measured on sample filters, by subtracting the blank signals described in 6.3.2. from (16) it follows that the propagated uncertainty for $M^{\mathrm{C}}_{\mathrm{POC}}$ is given by

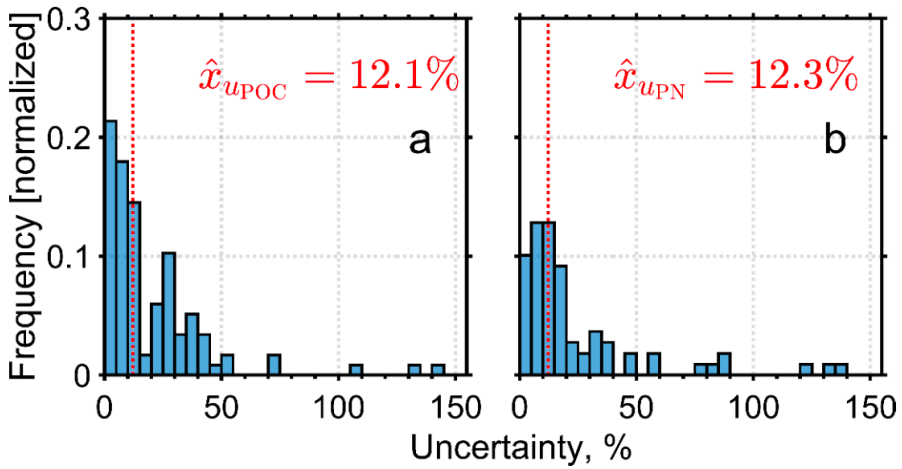


Figure 14. Histograms of fractional uncertainty as percentages for (a) POC and (b) PN for samples collected during the GO-SHIP P06 Leg 2 2017 campaign. Vertical red lines depict the median fractional uncertainties in each case.

Screenshot

Uncertainty budgets for a POC/PN dataset

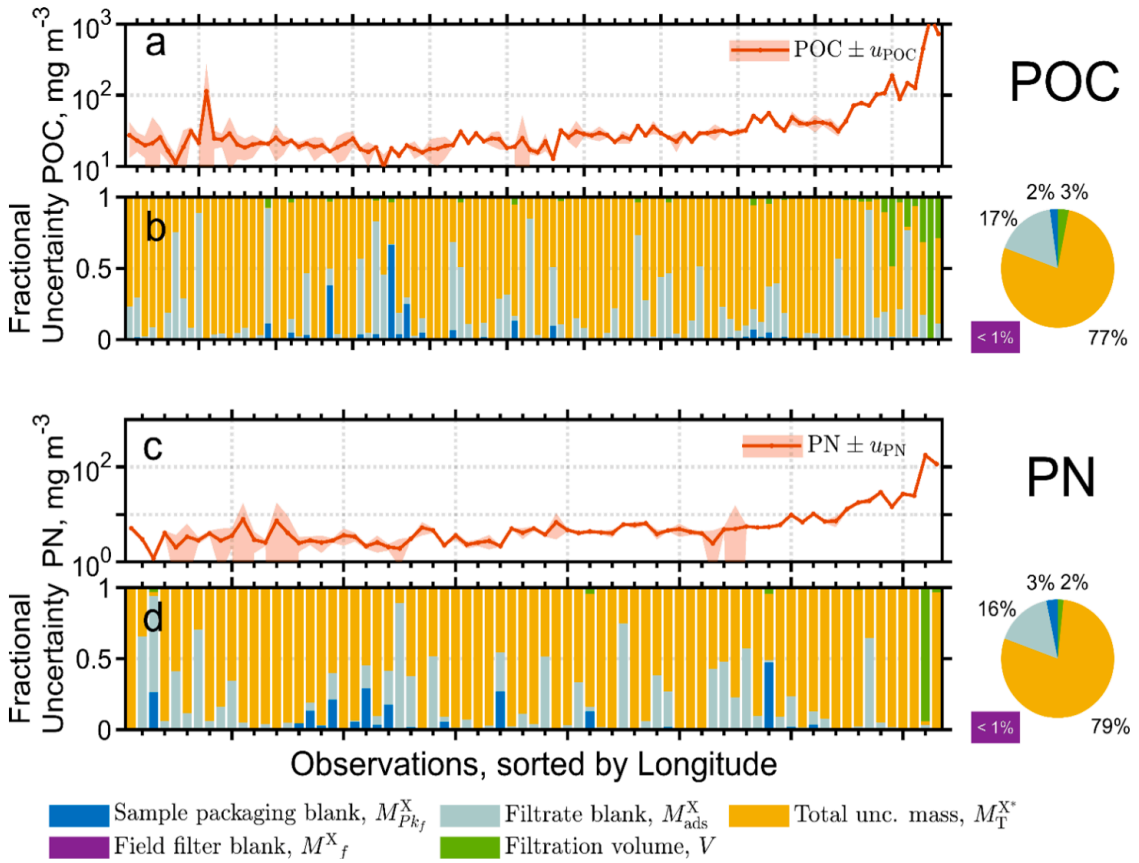


Figure 15. (a, c) Concentration of POC, PN during the GO-SHIP P06 Leg 2 2017 sorted in ascending order by station longitude along sampling transect in the South Pacific Ocean across the Gyre to the Peru-Chile upwelling region. Shaded regions depict the best estimate of concentration ± the propagated uncertainty. (b, d) Bar plots depict the contribution to measurement uncertainty (i.e., uncertainty budget) for each of the values in panels a and c by the variables in equations 17, 18. The respective mean uncertainty budgets for POC and PN are depicted in the pie charts to the right on panels b and d.

Questions?