# Consensus Field Protocols: Lessons Learned

Joaquín Chaves SSAI, Inc. NASA GSFC Ocean Ecology Laboratory Field Support Group







# 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









Labs in GSFC for wet chemistry, optics, etc.



Field equipment optical instruments and other field gear



**Phytoplankton Pigment Analysis Lab** 

### 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.

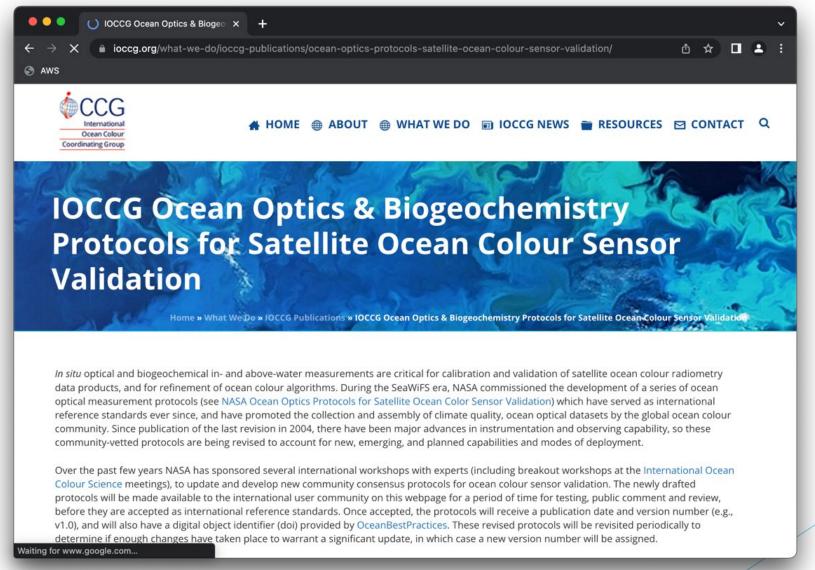
### What?

- 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





# **Protocols**, protocols...



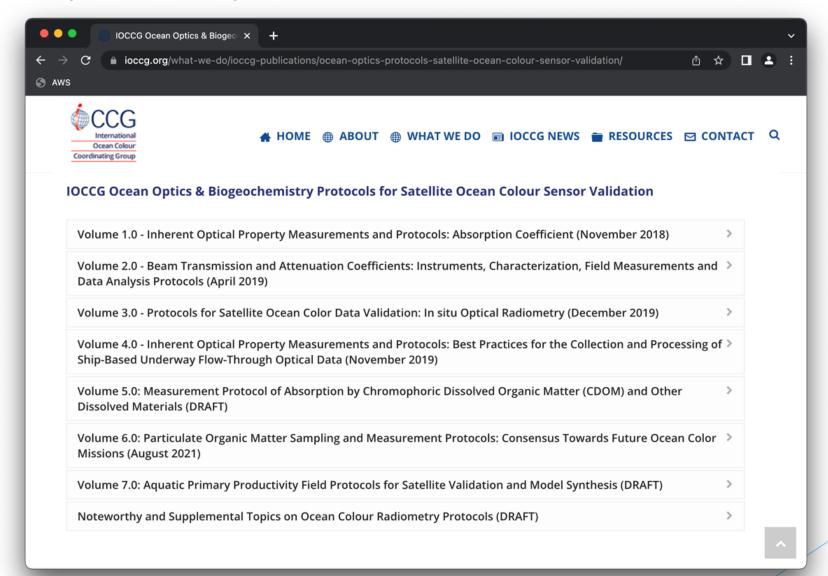






Workshop on the Validation of Satellite-derived Optical and Water Quality Parameters for Coastal and Inland Waters 7-9 June 2022

# Protocols, protocols...



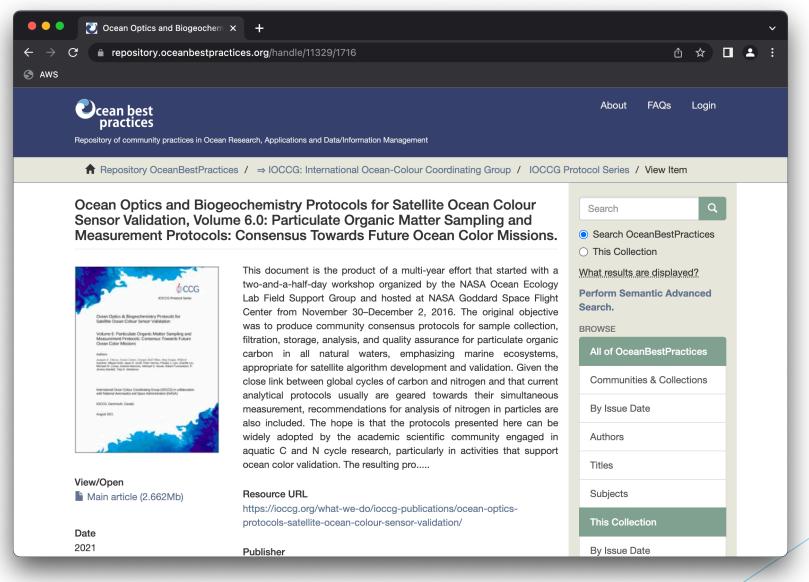






Workshop on the Validation of Satellite-derived Optical and Water Quality Parameters for Coastal and Inland Waters 7-9 June 2022

# **Protocols**, protocols...







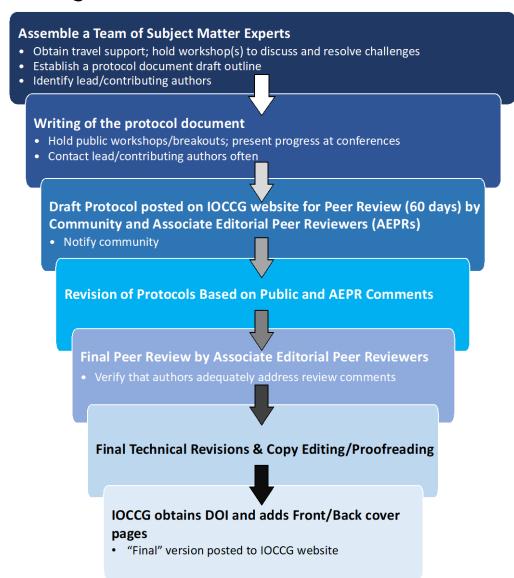


Workshop on the Validation of Satellite-derived Optical and Water Quality Parameters for Coastal and Inland Waters 7-9 June 2022

# Process for Development of Field Measurement Protocols

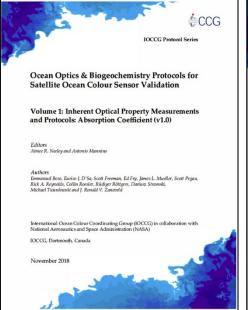
Under the auspices of the IOCCG

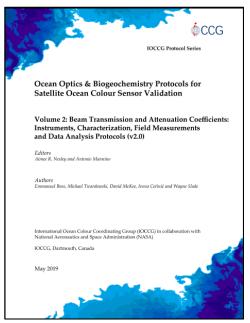
Systematic development, revision, testing, and dissemination of field data collection protocols in collaboration with experts in academia and other federal agencies.

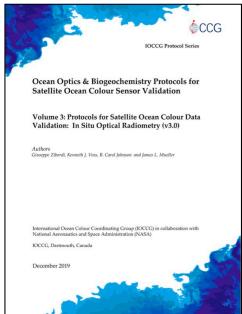




# Status of Protocols - Published











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-validation/



# Status of Protocols - CDOM Absorption



Ocean Optics & Biogeochemistry Protocols for Satellite Ocean Colour Sensor Validation

# Vol. 5.0 CDOM Absorption

### **Authors**

Antonio Mannino, Michael G. Novak, Norman B. Nelson, Mathias Belz, Jean-François Berthon, Neil V. Blough, Emmanuel Boss, Annick Bricaud, Joaquin Chaves, Carlos Del Castillo, Rossana Del Vecchio, Eurico J. D'Sa, Scott Freeman, Atsushi Matsuoka, Richard L. Miller, Aimee Neeley, Rüdiger Röttgers, Maria Tzortziou, Jeremy Werdell

- Sample Collection and Filtration
- Reference Material
- Liquid Waveguide Spectroscopy
- Dual-Beam Spectrophotometry
- Data analysis and uncertainties
- Round Robin Results

- 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



IOCCG Protocol Series

Ocean Optics & Biogeochemistry Protocols for Satellite Ocean Colour Sensor Validation

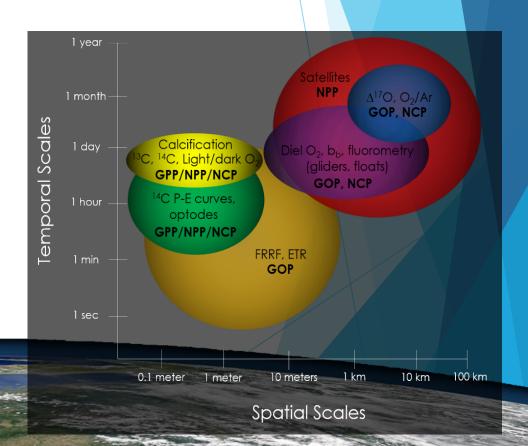
Vol. 7.0 Aquatic Primary Productivity

### Contributors

Balch, W.M., Carranza, M., Cetinic, I., Chaves, J.E., Duhamel, S., Erickson, Z., Fassbender, A., Fernandez-Carrera, A., Ferrón, S., García-Martín, E., Goes, J., Gomes, H., Gorbunov, M., Gundersen, K., Halsey, K., Hirawake, T., Isada, T., Juranek, L., Kulk, G., Langdon, C., Letelier, R., López-Sandoval, D., Mannino, A., Marra, J., Neale, P., Nicholson, D., Silsbe, G., Stanley, R., Vandermeulen, R.A. edited by R.A. Vandermeulen, J. E. Chaves

Coming out in late 2022

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, Joaquin Chaves. Other workshop participants (not pictured): Joe Salisbury, Susanne Craig, Jeremy Werdell, Paula Bontempi.

Screenshot







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- 1. Reconciling Estimates of Oceanic Primary Productivity from Cells to Satellite
- 2. The Metabolic Continuum of Primary Productivity
- 3. Carbon-Based Incubations
- 4. The H<sub>2</sub><sup>18</sup>O incubation method for the determination of gross oxygen production
- 5. Light and dark dissolved oxygen rate measurements using the Winkler method.
- 6. Calculating Net Community Production and Respiration from Continuous Optode Measurements
- 7. In Situ Gross Primary Production from Triple Oxygen Isotopes
- 8. In situ Net Community Production with dissolved  $O_2/Ar$
- 9. The use of variable fluorescence for assessment of phytoplankton photophysiology and rates of primary production
- 10. Autonomous Platforms









# Status of Protocols - Scattering Properties



Ocean Optics & Biogeochemistry Protocols for Satellite Ocean Colour Sensor Validation

Vol. 8 Volume Scattering Function, scattering, and backscattering coefficients

### Authors

Wayne Slade, Mike Twardowski, Emmanuel Boss, Xiaodong Zhang, Dariusz Stramski, James M. Sullivan, David Dana, David McKee, Giorgio Dall'Olmo, Deric Gray, Steve Ackleson, Barney Balch ...

- Instrumentation
- Measurement Process
- Deployment & Data Processing
- Current Topics

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









# Status of Protocols - more radiometry



Ocean Optics & Biogeochemistry Protocols for Satellite Ocean Colour Sensor Validation

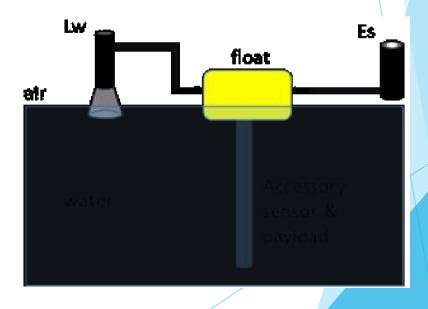
# Noteworthy & Supplemental Topics on Ocean Colour Radiometry

Leads:

Violeta San Juan and Susanne Craig

- Instrumentation
- SBA Method
- Radiometry under sub-optimal conditions
- "Recipe" for collection and processing of aquatic radiometric measurements
- Processing software tool
- Current topics

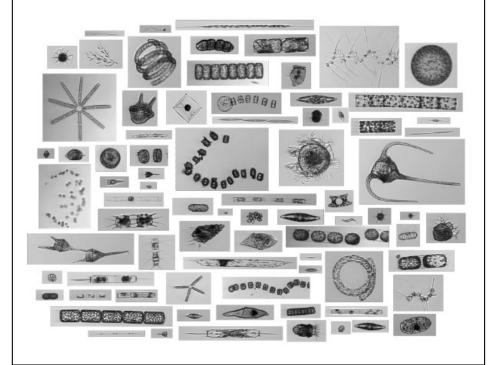
- Document is in planning stages
- A chapter describing the "on-water" skylight-blocked approach (SBA) by Lee et al. is posted on the IOCCG website



# Reporting Data from Particle Images

Standards and practices for reporting plankton and other particle observations from images

Technical Manual



# **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









# 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





# tatus of Protocols - POC



Ocean Optics & Biogeochemistry Protocols for Satellite Ocean Colour Sensor Validation

# Vol. 6.0 Particulate Organic Carbon

### **AUTHORS**

Joaquín E. Chaves, Ivona Cetinić, Giorgio Dall'Olmo, Meg Estapa, Wilford Gardner, Miguel Goñi, Jason R. Graff, Peter Hernes, Phoebe J. Lam, Zhanfei Liu, Michael W. Lomas, Antonio Mannino, Michael G. Novak, Robert Turnewitsch, P. Jeremy Werdell, Toby K. Westberry

- Sample Collection and Filtration
- DOC Adsorption

**Authors** 

- Sample Processing
  - Removal of Inorganic Carbon
- Elemental Analysis
- Data analysis and uncertainties

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







# 66 99

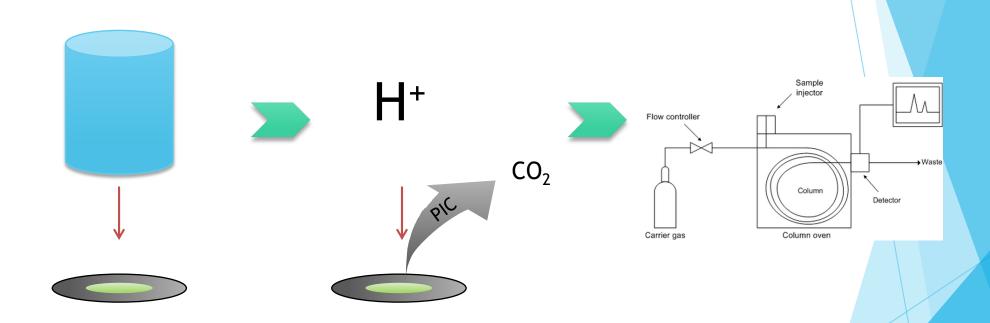
- ✓ "Since carbon is the "coin of the realm" for [...] future programs seeking to understand biogeochemical processes, it is imperative that we come to closure on the methods used to measure particulate carbon". Gardner, 2003
- ✓ "As present <u>procedures do not exist to correct</u> for all possible biasing effects due to artificial particle formation and/or miss/loss of filterable material, <u>uncertainties</u> of filtration-based estimates of POC concentrations need further testing". Turnewitsch et al. 2007
- ✓ "the mechanisms leading to such a <u>large POC difference are still</u>
  <u>unclear</u> and need to be <u>further investigated</u>". Liu et al. 2009







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  $\mu g$  C/kg) and particulate nitrogen (0.5 - 100.0  $\mu g$  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  $\mbox{POC}$  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

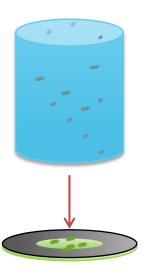






Knap, A. H., A. Michaels, A. R. Close, H. Ducklow & A. G. Dickson, 1994. Protocols for the Joint Global Ocean Flux Study (JGOFS) Core Measurements JGOFS Report. UNESCO, 170.

Dissolved Organic Carbon Artifact (colloidal fraction?)



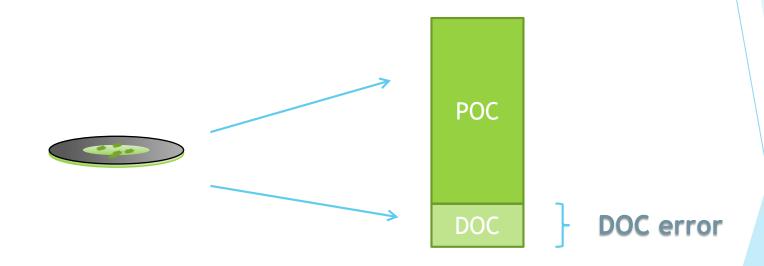
**Filtration** 



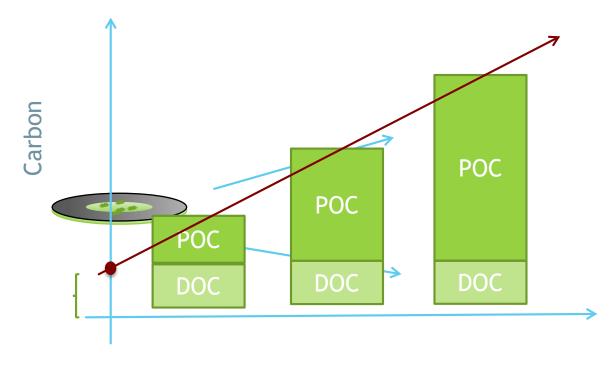




Dissolved Organic Carbon Artifact



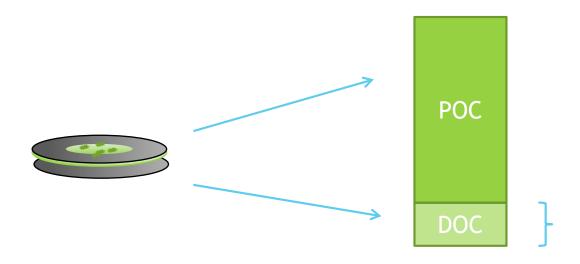
# Dissolved Organic Carbon Artifact



Volume filtered

Different volume replicates

Dissolved Organic Carbon Artifact



In-line double filters

# 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

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

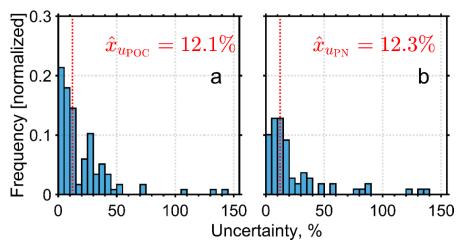
which is the sum in quadrature of the uncertainties  $u_a$  and  $u_b$  for the quantities a and b used to calculate y. For quantities, q, derived from a product or quotients of measured magnitudes a, ..., f

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

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

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

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

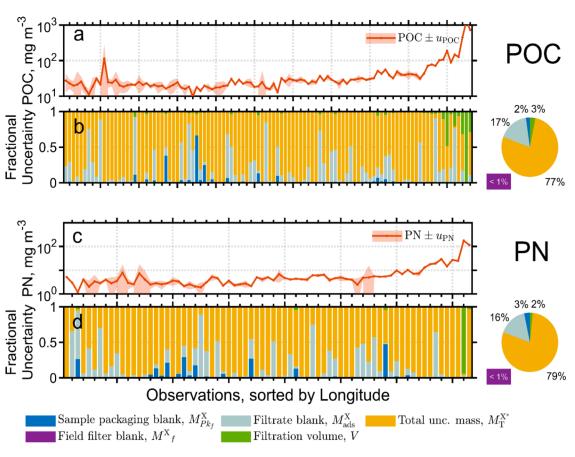


Figure 15. (a, c) Concentration of POC, PN during the GO-SHIP P06 Leg 2 2017 sorted in ascending order by station longitude along sampling transect in the South Pacific Ocean across the Gyre to the Peru-Chile upwelling region. Shaded regions depict the best estimate of concentration ± the propagated 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?**





