

Report of Joint WP2-WP5 workshop: ASSIMILATING TECHNICAL BEST PRACTICE IMPROVEMENTS TO OPTIMIZE NETWORK DATA FLOW Date: 05 October 2017 Place: Bergen, Norway

> Grant Agreement n° 654410 <u>Project Acronym</u>: JERICO-NEXT <u>Project Title</u>: Joint European Research Infrastructure network for Coastal Observatory - Novel European eXpertise for coastal observaTories

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#### 1. Document description

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JERICO-NEXT

#### 2. Attendees

Family name	Name	Institution	Country
Anil	Akpinar	lfremer	France
Cardin	Vanessa	OGS	Italy
Carval	Thierry	lfremer	France
Charria	Guillaume	Ifremer	France
Cuevas	Antonio	Udec	Chile
Delauney	Laurent	Ifremer	France
Durand	Dominique	Covartec	Norway
Fernadez	Vicente	EuroGOOS	Belgium
Gorringe	Patrick	EuroGOOS	Belgium
Medeot	Nevio	OGS	Italy
Nair	Rajesh	OGS	Italy
Novellino	Antonio	ETT	Italy
Perivoliotis	Leonidas	HCMR	Greece
Petersen	Wilhelm	HZG	Germany
Petihakis	George	HCMR	Greece
Pfeil	Benjamin	BCDC/UiB	Norway
Pouliquen	Sylvie	Ifremer	France
Puillat	Ingrid	Ifremer	France
Ravangan	Elisa	IRIS	Norway
Seppala	Jukka	SYKE	Finland
Sorensen	Kai	NIVA	Norway
Collingridge	Kate	CEFAS	ик
Mader	Julien	AZTI	Spain
Delrio	Joaquin	UPC	Spain
Nolan	Glenn	EUROGOOS	Belgium
Turpin	Victor	CNRS	France



#### 3. Agenda

#### Thursday, October 05, 2017 (afternoon)

## Joint WP2-WP5 Workshop: Assimilating technical Best Practice Improvements to optimize network data flow

From - to	Title					
13:50-14:00	Overview of WP2 and WP5 of JERICO-NEXT (R. Nair, OGS/W.					
	Petersen, HZG, L. Perivoliotis HCMR)					
14:00-14:15	Biological observations using optics: the data manager's perspective					
	Veronique Creach, CEFAS					
14:15-14:30	Biological observations using optics: the data producer's perspective					
	Jukka Seppala, SYKE					
14:30-15:00	Discussion					
15:00-15:15	HF radar observations: the data producer's perspective.					
	Julian Mader, AZTI					
15:15-15:30	HF radar observations: the data manager's perspective					
	Antonio Novellino, ETT					
15:30-16:00	Discussion					
16:00-16:20	Coffee break					
16:20-16:35	Marine carbonate system observations: the data producer's					
	perspective Kai Sorenson, NIVA					
16:35-16:50	Marine carbonate system observations: the data manager's					
	perspective <b>Benjamin Pfeil, University of Bergen</b>					
16:50-17:20	Discussion					
17:20-17:35	Observations using AUVs: the data producer's perspective					
	John Allen, SOCIB (Rajesh Nair, OGS)					
17:35-17:50	Observations using AUVs: the data manager's perspective					
	Thierry Carval, Ifremer					
17:50-18:30	Discussion					



#### 4. Executive summary

In the JERICO-NEXT project, WP2 contains the initiatives planned to promote and facilitate the harmonization of the project's observing network from the technical standpoint principally through the promulgation of Best Practice as regards the technologies, methodologies and procedures underpinning actual measurement. On the other hand, WP5 contains the initiatives aimed at providing procedures and methodologies to enable data collected through the project to enter mainstream marine data conduits, complying with the international standards regarding their quality and metadata. The joint WP2-WP5 workshop was designed to examine the possibilities for closer collaboration between the above two WPs in order to better reconcile contrasts arising from differences in the way data are regarded by the project's observing and data management components.

During the workshop, the following kinds of data were targeted for attention: HF-radar data, data relating to biology based on optical measurements, data on the marine carbonate system, and data from AUVs (gliders). For each of the four data types, the perspectives of the data producer and the data manager were presented and discussed with a view towards proposing best practice strategies to mitigate current shortcomings in the way these data are being managed within the JERICO-NEXT network.



#### 5. Statement of decisions

Decision	WP	Content	Who	when

# Cast

#### 6. Main report

Leonidas Perivoliotis from HCMR, the WP5 leader, welcomed the participants of the workshop on behalf of its organizing committee (specifically, himself and the WP2 co-leaders, R. Nair from OGS and W. Petersen from HZG), and opened the event's proceedings with a short presentation of its main aims and topics. In the JERICO-NEXT project, WP2 contains the initiatives planned to promote and facilitate the harmonization of the project's observing network from the technical standpoint while WP5 contains the initiatives aimed at providing procedures and methodologies to facilitate the streaming of gathered data to European data infrastructures. The joint WP2-WP5 workshop was planned to gather the members of the two WP communities in order to try to:

- identify difficulties relative to current data-handling practices employed within the project
- provide clearer terms of reference for handling JERICO-NEXT data
- agree on more appropriate metadata requirements for JERICO-NEXT data, if needed

The following kinds of data were targeted for attention: HF-radar data, data relating to biology based on optical measurements, data on the marine carbonate system, and data from AUVs (gliders). For each of the four data types, the perspectives of the data producer and the data manager were to be presented and discussed with a view towards proposing best practice strategies to mitigate current shortcomings in the way these data are being managed within the JERICO-NEXT network.

## Biological observations analysing phytoplankton particles Data producer's perspective:

The collection and dissemination of biology-related data based on optical measurements was the first topic that was tackled. **Veronique Creach** (CEFAS) presented the data manager's perspective for phytoplankton observations using cytometry. She began by describing the different techniques in use and the relevant instrumentation (e.g. Imaging FlowCytobot, CytoSense, FlowCam, FASTCAM, Underwater Vision Profiler), and then reviewed the main tools utilized for processing the relative observations at the present time: manual clustering with CytoClus (CytoBuoy, The Netherlands), the RclusTool package (LISIC/ULCO, France), and EasyClus software (Thomas Rutten Projects, Middelburg, The Netherlands). She highlighted that results obtained from the processing step are very user- and machine-dependent, that the underlying technology tended to change quite quickly, and that there is a strong need for setting guidelines for equipment and sample handling, the processing of raw data, and quality assurance. She added that the processing and analysis procedures needed to be reassessed in the context of new coastal areas being covered in JERICO-NEXT. She also announced that from the 19<sup>th</sup> to 21<sup>st</sup> of March 2018, a JERICO-NEXT phytoplankton workshop was being organized in Marseille where a number of relevant standardization issues were to be discussed.

## Biological observations using optics Data producer's perspective:

**Jukka Seppala** (SYKE) continued with the topic by presenting the methodologies used for observing phytoplankton employing LED fluorometry, spectral fluorescence, spectral reflectance and spectral absorption for quantifying different algae pigments (e.g. chlorophyll-a concentrations) as well as measuring turbidity by light scattering. Furthermore, he presented methods of measuring the photophysiology of the phytoplankton cells by fluorescence induction. In addition to the talk of Veronique Creach he shortly described the kind of data derived from flow-cytometry by pulse shape recording and imaging. He said that it is important to define the raw data for each sensor type and to archive these data, since there are often many different ways of extracting the biological information



they represent. He added that there is a need to define best practices to ensure traceable primary calibrations of sensors used in making these kinds of measurements, and to find ways to adequately capture the relative details in the metadata information to improve data inter-comparability. On a closing note, the fact that it is often the manufacturers of instrumentation who establish data formats and processing methods for many such measurements was underlined, and a case was made for greater engagement with this community to enhance the comparability of measurements made with sensors of differing origins.

#### HF Radar observations Data producer's perspective:

The second topic to be addressed was HF radar data. **Julien Mader** (AZTI) presented the data producer's view. He began by describing the underlying technologies and the basic steps that should be followed during the planning and installation phases of the equipment, together with the theory behind HF radar measurements. Then, he focused on known issues in the operation of HR radars, such as, for example, problems arising from environmental changes around installations that modify the electromagnetic field in the vicinity of the antennas, often invalidating antenna patterns and calibration parameters.

#### Data manager's perspective:

The presentation of the data manager's perspective on HF radar data was prepared by **Antonio Novellino** (ETT), but the actual talk was again given by **Julien Mader**. In the talk, the following key areas requiring action to achieve the necessary level of consensus to set up a roadmap for the creation of a European HF radar network were analyzed: data formats, metadata structures, and QC tests and flagging schemes for both the radial and the combined data. The concepts of "data production", "node" and "distribution unit", and their interconnectedness and final link to the major European Data Infrastructures was elaborated. It was suggested that the corresponding radial measurements should accompany the standard measurements coming from HF-radar systems, and that the waverecording component should also start to be developed.

#### Marine Carbonate System Data producer's perspective:

The next topic dealt with was marine carbonate system data. **Kai Sørensen** (NIVA) provided the data producer's perspective on these data. He divided marine carbonate data into two categories: the data gathered by sensors and those obtained from the analysis of discrete samples. Regarding the  $pCO_2$  and pH data generated by sensors, he talked about the basic principles of the measurements themselves, the calibration procedures, the continuing necessity of in-situ data for correcting and converting to final reported values. Other associated variables like total dissolved inorganic carbon and total alkalinity were also discussed. Furthermore, the fact that both automatic and manual measurements, and any computations involving them, needed corrections to account for the difference between in-situ and measurement temperatures was emphasized.

#### Data manager's perspective:

The data manager's perspective on marine carbonate system data was presented by **Benjamin Pfeil** (University of Bergen) who spoke about the ways these data are being handled at the European and international levels. He said that the data are currently being collected and managed through multiple



initiatives that include data repositories, data brokers, integrated networks, research infrastructures and research products. The European Research Infrastructure, ICOS (Integrated Carbon Observation System), the GOOS (Global Ocean Observing System) Biogeochemistry panel, the IOCCP (International Ocean Carbon Coordination Project), EMODNET Chemistry, BiogeoChemical Argo and I3 relevant initiatives were specifically mentioned. The poor inclusion of coastal stations and FerryBox systems in many of the databases was explicitly acknowledged. The need for complementary efforts, more interaction between research infrastructures and networks, and greater interoperability between systems was also stressed. He mentioned that the requirements of quality in terms of precision and accuracy depend on the purpose of the data. To measure the impact of climate changes (e.g. ocean acidification) requires more precise carbon data than monitoring the carbon dynamic in highly biologically active coastal areas.

#### Glider Observations Data producer's perspective:

The last topic of the workshop concerned data coming from gliders. **John Allen** (SOCIB), who had prepared the presentation on the data producer's perspective for this kind of data, was unable to come to Bergen due to last minute engagements, and his talk was given by **Rajesh Nair** (OGS). After a short introduction on the current capabilities of the technology itself, the presentation focused on the SOCIB toolbox for processing glider observations that generated data on three different quality levels. Then, the current procedures employed at SOCIB for correcting glider data based on field data from other platforms (mainly CTD casts), work that is being implemented in task 5.7 of WP5, was illustrated. It was shown that the corrected data files were accompanied by some new additions to the associated metadata containing information on the applied corrections, and suggestions for a number of other global attributes that could be further included were put forward. The standardization and semi-automation of depth-averaged velocity calculations, combining navigation data, flight models, and compass correction data files, was mentioned as one of the challenges of the moment.

#### Data manager's perspective:

**Thierry Carval** (Ifremer) presented the data manager's perspective on glider data, portraying the EGO ("Everyone's Gliding Observatories") data management system, a product of the consensus, networking and support of the many groups actively participating in that international initiative. He explained that the netcdf CF format had been selected by EGO contributors as the common data format to use for sharing glider observations with specific metadata information included, and that this choice was successively endorsed by Copernicus, SeaDataNet and AtlantOS. Furthermore, all data were being subjected to 14 quality control steps derived from Argo real-time QC protocols, while there were no standard procedures for delayed mode QC in place as yet. An EGO data processing tool (based on Matlab routines) and a netcdf file format checker were also being made freely available to the glider community.

#### 7. Conclusions

The outcomes of the discussions that took place during the workshop are briefly summarized below.

- The maturity levels as concerns data collection and data processing are different for the four data types that were addressed at the workshop.
- The procedures for the HF Radar and glider data are well implemented and their connections to data infrastructures at the European level are well-established.
- The glider community is by far the most advanced: the parameter naming conventions and QC procedures endorsed by them are in use by other RIs and major research projects, and they also provide detailed guidelines and tools for uploading data to CMEMS and SDN.
- HF radar data are currently linked directly to EMODNET Physics, and there is a drive towards standardization of the relative QC procedures within the community.
- The collection and dissemination of biological data obtained from optical measurements is currently in the very early stages of the long process of standardization from all points of view. Much of the data collected (especially those based on imaging) are very user- and machinedependent. This imposes serious problems in data comparability, especially between similar measurements collected in different regions by different institutions. There is also still a lot of work that needs to be done as regards appropriate metadata.
- The JERICO NEXT biological data integration plan is based on the data delivery to the EMODNET Biology infrastructure. The processed biological data that matches the EMODNET Biology's data scheme will be fully integrated in this data bank and will be discoverable and accessible though the standard EMODNET Biology tools. However, since a significant part of the JERICO NEXT flow-cytometry data cannot fit this existing scheme, a dedicated to the project data catalogue has been created (<u>http://www.emodnet-biology.eu/datacatalog?module=dataset&show=search&spcolid=910</u>), where detailed metadata information for each data set will be available together with direct links to raw and/or processed data.
- Marine carbonate system data are currently available through a variety of initiatives such as RIs, data infrastructures, integrated networks and research projects. However, the quality of the information on offer can vary, and there is a need for closer collaboration between the different initiatives to avoid duplication of efforts.

8. Annexes and references

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JOINT WP2-WP5 WORKSHOP

**Assimilating Technical Best Practice** 

**Improvements to Optimize Network** 

**Data Flow** 

Rajesh Nair, OGS

Wilhelm Petersen, HZG

Leonidas Perivoliotis, HCMR



#### WP2 : Harmonization of technologies and methodologies - technical strategy

WP2 of JERICO-NEXT contains the initiatives planned to promote and facilitate the harmonization of the project's observing network from the technical standpoint, principally through the promulgation of Best Practice as regards the technologies, methodologies and procedures underpinning actual measurements.

#### WP5: Data Management

WP5 of JERICO-NEXT contains the initiatives aimed at providing procedures and methodologies to enable data collected through the project to enter mainstream marine data conduits, complying with the international standards regarding their quality and metadata.

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This workshop has been planned to gather the members of the WP2 and WP5 communities of JERICO-NEXT to try to:

- identify difficulties relative to current data-handling practices employed within the project;
- provide clearer terms of reference for handling JERICO-NEXT data;
   agree on more appropriate metadata requirements for JERICO-NEXT
- data, if needed

#### Possible areas of cooperation that will be discussed in this workshop

- HF-radar data
- · data relating to biology based on optical measurements
- data on marine carbonate system variables
- · data from AUVs (gliders)

#### 

#### OUTLINE (the data producer's perspective)

- Description of sensors/systems for the specific variable under consideration (measuring technique, type of technology, Technology Readiness Level ...).
- Known requirements for proper deployment and common operating configurations for the described sensors/systems.
- Calibration and operational issues affecting data quality (e.g. limitations of calibration procedures, sampling modes, fouling, pressure effects, ...).
- "Meaning" of data acquired (measurement interferences, influences of seasonality and other environmental effects, sensibility to maintenance practices, descriptors used to express the quality of measurements, ...).
- Availability and sources of useful documentation in relation to the above topics.

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#### OUTLINE (the data manager's perspective)

- Currently applied protocols (including metadata requirements) for handling data relating to the specific parameter under consideration within JERICO-NEXT.
- Known limitations of the described protocols, and their level of compatibility with other EU and global data management initiatives.
- Issues affecting data dissemination (e.g. scales, units and conversions, processed vs. unprocessed data, data reduction practices, further metadata needs ...).
- Proposals/suggestions for improving the JERICO-NEXT terms of reference for handling data relating to the specific parameter under consideration.
- Suggestions for better and more efficient connection with major European Data infrastructures

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	Kai Sorenson, NIVA
16:35-16:50	Marine carbonate system observations: the data manager's perspective
	Benjamin Pfeil, University of Bergen
10.00 17.00	Discusion
16:50-17:20	Discussion
17:20-17:35	Observations using AUVs: the data producer's perspective
	John Allen, SOCIB (Rajesh Nair, OGS)
17:35-17:50	Observations using AUVs: the data manager's perspective
	Thierry Carval, Ifremer
17.50.40.20	Disputing
17:50-18:30	Discussion





#### Biological observations: the data producer's perspectives for phytoplankton

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ASSIMILATING TECHNICAL BEST PRACTICE IMPROVEMENTS TO OPTIMIZE NETWORK DATA FLOW, Bergen, 5 of October 2018









# JERIC® Biological observations: tool for processing the data

Manual clustering with CytoClus© (CytoBuoy, The Netherlands):

Long, need knowledge of the community in the area of interest and experience

#### RclusTool package (LISIC/ULCO, France)

The RClusTool is a toolbox based on machine learning, the tool designs automatically clusters of the phytoplankton functional types, with eventually the possibility of correcting the results.

Fast but not yet optimised and need more intercomparison with manual clustering

#### EasyClus® software (Thomas Rutten Projects, Middelburg, The Netherlands)

The EasyClus<sup>©</sup> software proposes many tools to organize, cluster and handle flow cytometric data (of many types of instruments) and uses the Matlab<sup>®</sup> environment.

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# Biological observations: Standardisation



Best practices: Intercalibration workshop (Gothenburg, September 2016) Sharing

ciuises.								
			C10	PIPCM (C)	PINCM (R)	inaging spins	127	Therma- calinometer
	"La Cardhage" CNRD 4000			ж		Cylatence	x	
			ж	×		2 Cytatienses	х	
	n.		х	х	х	Cytobence	х	
	Tangeound Observationy	2006	х		х	PCB+ PartCam		
	"Le Carthage"			х			х	
	"Endeavour" Nephris Tir harvey Celas		×	×		Cyllifience	×	
	"Ende accur" Pelagicitică Cefas		х	х		Cyllifence	х	
	"Endnavour" Cefas		х	х			х	
	"Cille i de la Maeshe" PoliCO CNIES LOS		х	х	х	Cytobence	×	
	"Linux Bruix" VLZ		х	х	х	1 Cytateoses	х	
	"Drived" RMS		х	х	х	2 Cytatienses	ж	
	"Aranda" SYRE/SM04	305.7	x	×	×	Cylatence + FilowCam + UNPS	×	
	"Sepiral" HUMO CNRI 600		х	x		Cytobence		×
	"Cites de la Mandie" ETOLE PERMIN(CNR)		х	x	x	Cyllifience		×

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The technology changes very quickly and new coastal areas have been added during JERICO-NEXT, analytical procedures need to be reassessed. · the flow cytometer analysis is user and machine dependant setting a control quality procedures for equipment, sample and result analysis under guidelines

**Biological observations** 

#### Equipment:

- some parameters related to instrument and the analysis are crucial to report such as the specifications and configuration of the instrument
- Each FCM needs to be calibrated during each analysis day with beads (fluorescence, size) and algae (from time to time)
- Performance indicators should be listed in an instrument dependent specification can could be provided by the manufacturer during the maintenance operation

#### JERIC@ Biological observations: listed in the metadatabase

#### analysis :

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ERIC®

- follow a procedure according to the specifications of the machine and phytoplankton community
- mandatory paramaters: volume, trigger level, time of analysis
- results : Mandatory information:
- . Total number of phytoplankton particles per ml
- Contribution of the phytoplankton particles to the total particles (%)
- Total number of particles by functional types: picoeukaryotes and Synechococcus, nano- and microphytoplankton per ml per sample recognized microalgae (pictures) .

Median size of the phytoplanktonic community

- Contribution relative of the main category to total red fluorescence (%)
- Optional information:
- Total red fluorescence standardised to total chlorophyll a for each sample
- Number of sub-groups in each main 4 categories and number of phytoplankton particles in the sub-groups)

Biologio	al obser	vation				
Comparisor	of results b	etween expe	erts (manual	clustering)		
	CNRS LC	IG / ULCO	chito counts	S MIO	CEFA	S Scontrib fir
Smp2	43298 (94.4%)		41278 (90.0%)		41484 (90.75%)	
- Synechococcus	1773	0,1	945	0.1	1728	0,1
- Picoeukaryotes	2361	0,5	1332	0.4	832	0,3
	38842	91,5	37332	45.1	37718	89.6
- Microeukaryotes	322	8,0	1669	54.4	1206	10,0
Smp3	15357 (89.22%)		12557 (72.9%)	0.90	13621 (79.14%)	
- Synechococcus	3964	0,2	2478 40	0.1	3899	0,2
- Picoeukaryotes	4622	0,7	3939 60 -	0.2	4038	1,6
Nanoeukaryotes	5506	40,6	19.	23.1	3933	39,5
- Microeukaryotes	1265	58.5F10''	1921	76.6	1751	58,7
Smp4	6073 (34.09%)		6086 (34.2%)		5589 (23.88%)	
- Synechococcus	3030	0,3	2303	0.1	2805	0,3
- Picoeukaryotes	1344	0,6	1018	0.1	915	0,3
Nanoeukaryotes	1270	7,6	2326	7.0	1365	5,9
- Microeukarvotes	429	91.4	439	97.8		





# **Biological observations**



Improving the visibility of ocean data from new technologies: a case study of high frequency flow cytometry. (Euromarine workshop if funded)

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Session 1: How to harmonise flow cytometry data: from individual scientist to

pan-European research network. Session 2: Use of flow cytometry information by users from different fields Session 3: Integrating of new types of phytoplankton data in Europe's ocean

Session 4: practical workshop on clustering and identification of phytoplankton functional types.





#### Biological observations using optics: the data producer's perspective

Jukka Seppälä Finnish Environment Institute, SYKE Jukka.seppala@ymparisto.fi

A lot of information/figures reused from JERICO-NEXT D2.2 & D3.1, thanks to those who contributed!!

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#### **LED Fluorometry**

- By selecting appropriate LEDs and filters, excitation and emission wavebands may be matched with the fluorescence properties of different compounds; like Chlorophyll a, phycoerythrin, phycocyanin, CDOM.
- Small size sensors (100 g->, diam. 3-10 cm), relatively low price (1000-5000€), suitable for all oceanographic platforms.
- Well established technology, TRL 8-9, but lack of harmonization.
- Instruments from different manufacturers have different optical setups & different calibration practices by users -> challenging the consistency of data.



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**LED Fluorometry** 

Primary calibration of LED fluorimeters has not been agreed and the results are

most often in relative units (or in µg/L but without any traceability of calibration)

Fluorescence typically considered as a semi-quantitative proxy of concentrations

Validation with field samples is an important step in analysing fluorescence data

when the changes in the phytoplankton physiology are "larger" than changes in biomass (example day-night shifts in non-photochemical quenching).

Most common validation method is linear regression, but this tend to fail, e.g.

Alternative methods for validation are (and will be more) available, but no

guidelines/decision-tree what to use (user/event/location specific validation).

#### 

#### **LED Fluorometry**

- Key issues related to the long or short term stability of the instruments, due to biofouling, condensation of water inside or deteriorating of the optics. As the LED fluorimeters are single channel instruments, resolving blanks, biofouling, drift or other interferences requires discrete sampling, additional measures or good knowledge of the system.
- Fluorometers are most often providing accurate description of fluorescence intensity, but the interpretation of this signal as concentration of pigments or cell numbers is not straightforward due to photobiological processes in living cells affecting the fluorescence yield.

#### $F = [Chla] \cdot R$

R varies 2-4 fold for single species, and up to 50-fold between different species.



#### **GERICONEXT** Spectral fluorescence

- Phytoplankton fluorescence excitation spectra shows the spectral shape of the light absorption by accessory pigments.
- Consistent differences between spectra of different taxonomic pigment groups: green algae (Chlorophyta); brown algae (e.g. Dinophyta and Bacillariophyta) cryptomonads (Cryptophyta), Cyanobacteria (Cyanophyta)
- Two major brands Multiexciter (JFE Advantech Co, Ltd, Japan), FluoroProbe & AlgaeOnlineAnalyzer (bbe Moldaenke GmbH, Germany)
- Weight 1.6 6.4 kg, price 20k€-> . May be used in "Logging" or "Online" modes; profiling & flow-through.
- High TLR (8-9), but the agreed traceable calibration is lacking decreasing the value of instruments



50.0

50'9

JERICO-NEXT

#### **Spectral fluorescence**

- Primary data is (uncalibrated) fluorescence intensity at different wavebands.
- Secondary instrument output is Chlorophyll a concentration in different taxonomic groups, based on 1) linear unmixing and 2) laboratory measured norm-spectra (fingerprints).
- Several reasons the method above is biased: selection of correct spectral groups, no co-varying spectral groups allowed, diversity of spectral properties within taxonomic group, variability in fluorescence quantum yield. -> Chlorophyll a concentrations largely biased by selection of fingerprints.
- · Other data analysis methods available, but they are rather unstandardized





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#### **GERICONNY** Fluorescence induction

- Fluorescence induction measurements result in several parameters describing the state of photophysiology of the phytoplankton cells
- Two main techniques in measuring variable fluorescence: single turnover technique like Fast Repetition Rate Fluorometry (FRRF) and multiple turnover technique like Pulse Amplitude Modulation (PAM) fluorometry.
- In Jerico-Next: FastOcean (Chelsea Technologies Group Ltd, UK) FRRF sensor with accessories can be used as profiler, as bench top model and in flow-through system & PhytoPAM (Heinz Walz GmbH, Germany) PAM sensor is bench top model.
- Sensors are relatively large and expensive (20k€->), limiting their use.



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#### **Spectral absorption**

- HyAbs (Nexos development) & Oscar (Trios Gmbh, Germany): integrating cavity, which allows sensitive measurements due to a long optical path length and eliminates errors introduced by light scattering by particles.
- Light transmission difference between the sample (seawater) and the reference (purified water) can be measured and used together with reflectivity, temperature, salinity and calibration factors to calculate the spectal absorption coefficient of the water constituents in units [m<sup>-1</sup>].
- Absorption coefficient may be decomposed mathematically into different components (phytoplankton, inorganic particles, organic particles, CDOM)
- TRL level 5-6, price 20k€+, for flow-through systems / profiling.
- Needs extensive cleaning procedure (which need to be automated for commercial sensor)



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Spectral radiance and irradiance sensors used to estimate light reflectance above water , e.g. to validate satellite products.

Spectral reflectance

- irradiance sensor towards zenith providing the total downwelling light Ed
- radiance sensor providing upwelling light from the sea and sea surface, Lt
- radiance sensor providing sky contributions from the upwelling component, Ls Established technology, measurements in physical units (µmolq m² s¹ nm²) , may
- be used in stationary or moving platforms
- Traceable calibration of sensors available
- Challenges to achieve ideal conditions, such as weather and sea conditions, sensor angles relative to sun, and selection of the Fresnel Coefficient, and subsequent data flagging.



#### 

#### **Fluorescence induction**

- Complex data flow when most advanced systems used
- $-\,$  Fluorescence induction curves  $\mu s$  scale, some hundreds of raw data points per curve + model output
  - Fluorescence induction curves carried out in different light steps
     Modelled data summarizing the light curves
- Meaning of all parameters not well described (e.g. additional wavebands)
- Between model (FRRF vs. PAM) comparison difficult.
- Calibration protocol established (may need revisit?)
- Fluorescence induction methods provide estimates on electron transport rate, and with some assumptions this may be converted to rates of oxygen evolution or carbon fixation, but still there are large uncertainties in this conversion



#### 

- In principle, data in physical units, comparable to other techniques.
- For reliable measurements, the reflectivity of the integrating cavity has to be determined by a calibration measurement (OSCAR - Nigrosin, HyAbs – solid standard)

Spectral absorption

- Primary data absorption coefficient spectra in the range of the visible light (400-710 nm)
- 1<sup>st</sup> Secondary data: absorption spectra of different in-water constituents
- 2<sup>nd</sup> Secondary data: [Chla], [TSM], [DOC], algal pigment classes



#### **CERIFORMENT** Turbidity and scattering

- For turbidity, measure of light scattering, the standard is a Nephelometric laboratory method based on a 90° (+/-2.5°) scattering at 860 nm (+/- 10-15 nm) wavelength detection.
- Turbidity is a proxy for the total suspended material.
- Other techniques: 1) total beam attenuation (c) at different wavelength and resolving total scattering (b) and absorption (a) at 9 wavelengths and 2) backscattering coefficient (bb) at different wavelengths with fixed angles.
- Calibration traceable but interpretation of data sometimes challenging due to different measuring geometries, wavelengths etc. data from different instruments not directly comparable
- Metadata information of the sensor specifications of e.g. wavelength and scattering angles are important to report since this influence the optical signal (turbidity) from different particles types



#### **CERCONER** Pulse shape-recording flow cytometry

- · Three interoperating systems: Optical, Fluidics and Electronics.
- PSR FCM from the Cytobuoy<sup>®</sup>: automatically recording the optical pulse shape of every particle passing through a laser beam.
- Benchtop, continuous (e.g. ferrybox) and submersible (e.g. buoy)
- Use of calibration beads for laser alignment, size calibration and fluorescence calibration.
- Different setups (lasers, power) -> intercomparison of machines required
- Raw data need to be retained. One issue with the data reliability is the significance
   of abundance estimation for rare species/particles
- Manual/automated/semi clustering & classification methods -> affect interpretation of data (user dependent)



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#### For further discussion

- Defining raw data for each sensor type

   Storing raw data is very important especially in the cases when there exist
  many different ways of calculating biological information
- Defining best practices for traceable primary calibration and it's inclusion in metedata
  - raw data is relatively useless if there is no traceability of data!! Without
- traceability raw data from different sources/instruments cannot be compared!
  Often the "data" issue is driven by manufacturers with a major market within non
  - scientific monitoring activity. – As scientific community we call for traceability and correct measuring practices, while bulk selling point is to provide instruments which replace lab-
  - based measurements; i.e. why should fluorometer manufacturer sell an instrument measuring at relative scale to please us, while majority of customers like the (biased) µg/L scale.
  - -> collaboration with manufacturers
  - -> providing demonstrations of the added value of traceability & best practices i.e. showing examples of consistent and comparable multisensor data-sets

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#### Imaging flow cytometry

- Imaging FlowCytoBot (McLane Research Laboratories), FlowCAM (Fluid Imaging Technologies), FastCAM prototype (IFREMER - LDCM), Underwater Vision Profiler UVPS (Hydroptic)
- Images are the main product for all instruments but due to instrument-specific differences in optical and fluidic characteristics, various results in terms of image resolution (magnification/size of particles analysed) and measurements (features). Specific training sets are built for each instrument.
- Standardization of analytical and data processing as well as data management need more development
- Classification based on training sets involving taxonomic expertise.
- Importance of keeping raw data, images



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#### HF radar observations: the data producer's perspective.

Julien Mader, AZTI, <u>imader@azti.es</u> Carlo Mantovini, CNR, Italy Jochen Horstmann, HZG, Germany

#### 

#### OUTLINE (the data producer's perspective)

- Description of sensors/systems for the specific variable under consideration (measuring technique, type of technology, Technology Readiness Level ...).
- Known requirements for proper deployment and common operating configurations for the described sensors/systems.
- Calibration and operational issues affecting data quality (e.g. limitations of calibration procedures, sampling modes, fouling, pressure effects, ...).
- "Meaning" of data acquired (measurement interferences, influences of seasonality and other environmental effects, sensibility to maintenance practices, descriptors used to express the quality of measurements, ...).
  - Availability and sources of useful documentation in relation to the above topics.

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#### OUTLINE (the data producer's perspective)

 Description of sensors/systems for the specific variable under consideration (measuring technique, type of technology, Technology Readiness Level ...).

#### Hardware overview

- · Land based remote sensing instrument
- HF = High Frequency (from 3 to 30 MHz)
- One receiving and one transmi@ng staAon (plus electronics)
- different antennas configurations (depending on frequency and signal processing technique)

#### 

#### OUTLINE (the data producer's perspective)

Description of sensors/systems for the specific variable under consideration (measuring technique, type of technology, Technology Readiness Level ...).

#### Hardware overview



4-element square array received

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#### OUTLINE (the data producer's perspective)

Description of sensors/systems for the specific variable under consideration (measuring technique, type of technology, Technology Readiness Level ...).

#### Hardware overview



16-element linear array receiver

#### OUTLINE (the data producer's perspective)

Description of sensors/systems for the specific variable under consideration (measuring technique, type of technology, Technology Readiness Level ...).

#### Hardware overview



Compact transmitting and 3-element receiving antenna

#### OUTLINE (the data producer's perspective)

 Description of sensors/systems for the specific variable under consideration (measuring technique, type of technology, Technology Readiness Level ...).

#### Hardware overview



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#### OUTLINE (the data producer's perspective)

Description of sensors/systems for the specific variable under consideration (measuring technique, type of technology, Technology Readiness Level ...).

#### What HF Radars can measure

Ocean surface\* currents velocity over wide areas (thousands of square Km) with high temporal and spatial resolution



#### OUTLINE (the data producer's perspective) Description of sensors/systems for the specific variable under consideration (measuring technique, type of technology, Technology Readiness Level ...). Theory of operation



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#### OUTLINE (the data producer's perspective)

Description of sensors/systems for the specific variable under consideration (measuring technique, type of technology, Technology Readiness Level ...).

#### Theory of operation



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#### OUTLINE (the data producer's perspective)

Description of sensors/systems for the specific variable under consideration (measuring technique, type of technology, Technology Readiness Level ...).



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#### OUTLINE (the data producer's perspective)

Description of sensors/systems for the specific variable under consideration (measuring technique, type of technology, Technology Readiness Level ...).

#### Theory of operation



Two or more radial maps overlapping are combined to provide total velocity map.

#### OUTLINE (the data producer's perspective)

Description of sensors/systems for the specific variable under consideration (measuring technique, type of technology, Technology Readiness Level ...).

#### Theory of operation

Radar Frequency (MHz)	Radar Wavelength (m)	Ocean Wavelength (m)	Ocean Wave Period (s)	Depth of Current <sup>1</sup> (m)	Typical Range <sup>2</sup> (km)	Typical Resolution (km)	Typical Bandwidth (kHz)	Upper H <sub>t/</sub> Limit <sup>4</sup> (m)
5	60	30	4.5	2	175-220	6-12	15-30	25
	25	12.5	2.5	1-1.5	60-75	2-5	25-100	13
	12.5	6	2	.5-1	35-50	1-3	50-300	7
	6	3	1.5	<.5	15-20	.25-1	150-600	3

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#### OUTLINE (the data producer's perspective)

Description of sensors/systems for the specific variable under consideration (measuring technique, type of technology, Technology Readiness Level ...).

#### Conclusions

#### Some advantages:

- □ Land based -> low maintenance cost
- Continuous monitoring of the sea state in automated way
- Wide area covered

#### Some limitations:

- Radio frequency bands are busy -> radio interferences
- $\hfill\square$  Possible gaps in space and time due to bad S/N ratio
- Only surface measurements

#### 

#### OUTLINE (the data producer's perspective)

Known requirements for proper deployment and common operating configurations for the described sensors/systems.

#### Planning and installation phase

- Selection of the desired resolution, range and coverage of the HF-radar
   Selection of the major parameter of interest (in the majority of today's setups,
- these are ocean surface currents)
  Depending on these criteria, the operating frequency as well as the number of systems and their relative locations can be defined.
- systems and uterative relative locations can be eximited. To identify potential installation sites, taking into account: relative location (of the sites to each other), available space (depending on the type of system), infrastructure availability and status (power supply, accessibility), and sources of possible interaction (e.g. other nearby antennas, metal fences, etc.).
- Possible sites should be chosen to satisfy logistical prerequisites first, before going on to fulfill the specific requirements in relation to the particular application, the coverage and the resolution.
- It is recommended to monitor the HF-spectrum at the selected sites in order to identify any interference issues and to plan appropriate countermeasures, e.g. selecting the most suitable frequencies

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#### OUTLINE (the data producer's perspective)

Calibration and operational issues affecting data quality (e.g. limitations of calibration procedures, sampling modes, fouling, pressure effects, ...).

#### Main Operational Issues

- Various factors affect the radar performance directly, and therefore the accuracy of the measurements, or lead to an interruption of the data flow
- Generally, data coverage is not regular for a number of reasons. Spatial and temporal data gaps may occur at the outer edge, as well as inside the measurement domain.
- This can be due to several environmental and/or electromagnetic causes: the lack of Bragg scattering ocean waves or severe ocean wave conditions, low salinity environments, and the occurrence of radio interference.
- The most frequent problems arise from environmental changes, which lead to changes of the electromagnetic field in the vicinity of the antennas and therefore to invalid antenna patterns and calibration parameters.
- Changes of antenna patterns are more significant for direction-finding systems than for phased array systems.

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#### OUTLINE (the data producer's perspective)

Calibration and operational issues affecting data quality (e.g. limitations of calibration procedures, sampling modes, fouling, pressure effects, ...).

#### Main Operational Issues

- Another problem is the quality loss or failure of antennas due to the environment. This happens more frequently to phased array systems as significantly more antennas are involved. For phased array systems, the performance is strongly affected if the Tx array and/or antennas close to the center of the Rx array are compromised in some way. Usually, these problems arise from damaged or broken cables, connectors or radials caused by wildlife or vandalism.
- A breakdown of the internet connection can lead to measurement gaps in the longterm record. The stability of the power supply, particularly at very remote sites, can also be a problem. These can lead to permanent data gaps but typically do not occur very often, and can be mitigated by using UPSs.
- Further dangers to operational integrity include malfunctions or downtime arising from air-conditioning failures, electromagnetic interferences, lightning strikes, accidental fires, coastal erosion and inherent system weaknesses

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#### OUTLINE (the data producer's perspective)

"Meaning" of data acquired (measurement interferences, influences of seasonality and other environmental effects, sensibility to maintenance practices, descriptors used to express the quality of measurements, ...).

Quality assessment is being discussed in WP2

Many associated variables are included in the mandatory ones for enable QA/QC

#### OUTLINE (the data producer's perspective)

Availability and sources of useful documentation in relation to the above topics.

- Best practices in Deployment and Operation: Capacity Building, Lucy R Wyatt, ACORN, Australia
   DEPLOYMENT & MAINTENANCE of a High-Frequency Radar for Ocean Surface Current Mapping: BEST PRACTICES. Feb 2008. Radiowave Operators Working Group
   Guidelines for Assessing HF Radar Capabilities and Performance, George Voulgaris, 2011. University of South Carolina
   CODDB Second on AGC Departs Maniharing Checklist

- CODAR SeaSonde QA/QC Remote Monitoring Checklist
   CODAR SeaSonde QA/QC Setup and Diagnostics

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#### HF Radar observation: the data manager's perspective

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- Data format

- QC tests

Currently applied protocols (including metadata requirements) for handling data relating to the specific parameter under consideration within JERICO-NEXT.

#### Analysis of four key points for achieving a commo

and set up a road

cilleving a common conse	ilisus		
nd set up a roadmap:		Final scheme of	f processing levels for HFR
Data format	Processing Level		Products
Metadata structure QC flagging scheme	LEVEL O	Reconstructed, unprocessed instrument/payload data at full resolution; any and all communications artifacts, e.g. synchronization frames, communications headers, duplicate data removed.	Signal received by the antenna before the processing stage. (No access to these data in Codar systems)
QC tests	LEVEL JA	Reconstructed, unprocessed instrument data at full resolution, time-referenced and annotated with ancillary information, including radiometric and geometric calibration coefficients and georeferencing.	Spectra by antenna channel
	LEVEL 18	Level 1A data that have been processed to sensor units for next processing steps. Not all instruments will have data equivalent to Level 1B.	Spectra by beam direction
	LEVEL 2A	Derived geophysical variables at the same resolution and locations as the Level 1 source data.	Radial velocity data
	LEVEL 28	Level 24 data that have been processed with a minimum set of $\ensuremath{QC}$ .	Radial velocity data
	LEVEL 3A	Variables mapped on uniform space-time grid scales, usually with some completeness and consistency	HFR total velocity data
	LEVEL 38	Level 3A data that have been processed with a minimum set of $\ensuremath{QC}$ .	HFR total velocity data
	LEVEL 4	Model output or results from analyses of lower level data, e.g.	Energy density maps, residence

#### JERICO-NEXT

#### Currently applied protocols (including metadata requirements) for handling data relating to the specific parameter under consideration within JERICO-NEXT.

	Basic products: da	ta format and QA/QC	
data format	metadata structure	QC flagging scheme	QC tests
netCDF-4 data, and netCDF-4 3.6.1     CMEMS IN-SITU TAC archiving strategy and folder structure, CMEMS IN-SITU TAC naming convention. Data var names: SeaDataNet P09*	Mondetory Attr. and OceanSITES conventions. Recommended Attr. to comply with INSPIRE and Unidata Dataset Discovery conventions. Suggetted Attr. • relevant in describing the data, whether it is part of the standard or not.	CMEMS IN-SITU TAC – OceanSITES: 0. unknown, no QC 1. good, all GC passed 2. probably good, 3. Probably correctable, data used without scientific correction/calibration correction/calibration correction/calibration correction/calibration reported 9. Interpolated value 1. Mominal value, data not observed but reported 8. Interpolated value	<ul> <li>chosen among the ones listed in the QARDD manual.</li> <li>are manufacturer- independent, i.e. they do not rely on particular variables or information provided only by a specific device.</li> <li>defined for both radial and total velocity data required for idabiling the data as i.evel 28 (for tradial velocity) and Leve 38 (for total velocity) data.</li> </ul>
		9 Missing value	

#### JERICO-NEXT

Currently applied protocols (including metadata requirements) for handling data relating to the specific parameter under consideration within JERICO-NEXT.

QC tests define	ests defined for radial data QC tests defined for total data				
QC test	Meaning	QC variabl type	e QC test	Meaning	QC variab type
Syntax	Test ensuring the proper formatting and the existence of fields within the radial netCDF file.	scalar	Data Density Threshold	Test checking if the minimum number of radial velocity is present for the	gridded
Over-water Test labeling vectors that lie on land. gridded		gridded		combination into the total velocity	ay
Velocity Threshold	Test labeling velocity vectors beyond a maximum velocity threshold	gridded	_	vector.	
Variance Threshold	Test labeling velocity vectors beyond a maximum variance threshold.	gridded	Balance of contributing radials	Test checking if the number of radials coming from the different contributing sites are balanced for	gridded
Median Filter	For each source vector, the median of all velocities within radius of <rclim> and whose vector bearing</rclim>	gridded		the combination into the total velocity vector.	
	(angle of arrival at site) is also within <anglim- degrees from the source vector's bearing is evaluated. If the difference between the vector's</anglim- 		Velocity Threshold	Test labeling velocity vectors beyond a maximum velocity threshold.	gridded
	velocity and the median velocity is greater than a threshold, then the median velocity is used		Variance Threshold	Test labeling velocity vectors beyond a maximum variance threshold.	gridded
Average Radial Bearing	Test determining that the average radial bearing is close to shore normal and does not fluctuate from each hourly measurement.	scalar	GDOP Threshold	Test labeling velocity vectors beyond a maximum GDOP threshold.	gridded

#### 

data dissemination (e.g. scales, units and conversions, processed vs. unprocessed data, data reduction practices, further metadata needs ...).



#### HFR Data Production:

\*) to be updated with HFR related variable

Data Production: run HFR site or assemble HFR data
 Quality control: apply automatic quality controls that have been agreed

#### HFR Node:

quire Data: gather available HF Radar data though collaboration with regional and national

- action of the data provider can set up the data flow according the defined standards, the regional coordinator only has to link and include the new catalogue and data stream
  If the data provider cannot setup the data flow (because of lack of experience, technical
- capacity etc), the regional coordinator has to work on harvestign the data from the provider, harmonize and format these data and make them available from the regional catalogue
   Data format and naming harmonization
- validation/Assessment: Assess the consistency of the data over a period of time and an area to detect data that are not coherent with their neighbors but could not be detected by automatic QC.

#### HFR Distribution Unit:

Distribution Unit: assemble data into an integrated dataset and uniform catalogue, make the data available in NRT within the European infrastructures and to the external users.



data dissemination (e.g. scales, units and conversions, processed vs. unprocessed data, data reduction practices, further metadata needs ...).

#### Data infrastructure:

Data infrastructure:

- THREDDS data server + INSTAC naming conv
   Last day- RR\_LATEST\_ZZ.XX\_CODE\_YYYYMMDD.nc
   Lasts: RR\_LATEST\_ZZ.XX\_CODE.nc
   Monthly- RR\_YYYYMLXZ\_XX\_CODE.nc
   History- RR\_YYYYZ\_ZX\_XCODE.nc
   (e.g. IR\_2016\_TL\_HR\_BasqueHRR.nc )
- - RR = regional bigram ZZ = type of prod. (TL/RD) XX = HF CODE = system name



data dissemination (e.g. scales, units and conversions, processed vs. unprocessed scaled at a reduction practices, further metadata needs ...).

#### Details of the THREDDS catalogue for a given platform - last 60 days

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Implification
 Add to COMMUNICATION INFORMATION
 Add to COMMUNICATION INFORMATION
 Add to COMMUNICATION INFORMATION

data dissemination (e.g. scales, units and conversions, processed vs. unprocessed data, data reduction practices, further metadata needs ...).



#### 

Proposals/suggestions for improving the JERICO-NEXT terms of reference for handling data relating to the specific parameter under consideration.

- Make Radials available
- Start working on waves

Suggestions for better and more efficient connection with major European Data infrastructures

- Use of EDMO
- Mapping of HFR metadata vs. SDN CDIs
- Need for ragistry of systems
- Unique identifier for HFR → easier integration into GOOS

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Suggestions for better and more efficient connection with major European Data infrastructures

Data gap filling and refined grid products	Short term prediction	Lagrangian products
Needed for key applications (using a Lagrangian Particle- Tracking Model (LPTM) Gap filling by Open Mode Analysis (OMA) <sup>1</sup> from radials or Variational Analysis <sup>1</sup> to provide accuracy estimations also on the gap- filled products Product to come together with total current field without dat gap-filling	<ul> <li>Simple approaches e.g. empirical models to forecast future currents based on a short time history of past observations Products of interest for Marine Services - SAR and oil spill apps methods to be tuned up on the geographical areas of application («predictable» patterns).</li> </ul>	trajectory predictions using currents derived from HFR Lagrangian particle transport model  Not for CMEMS catalogue but as downstream application

1) Lekien et al., 2004, Kaplan and Lekien, 2007 2) Yaremchuk and Sentchev, 2009



#### Marine carbonate system observations: the data producer's perspective

Andrew King and Kai Sørensen Marine Biogeochemistry and Oceanography Norwegian Institute for Water Research (NIVA)



#### Basic principle

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- Equilibration of CO<sub>2</sub> with air space
- Either showerhead or membrane CO<sub>2</sub> in air is typically dried
- CO2 measured by detector (mostly
- NDIR, e.g., LICOR)

#### **Calibration**

- Most systems only calibrate the detector (i.e., equilibration system assumed to be constant)
- Air:CO<sub>2</sub> mixtures are humidified and sent to drying system + detector
- Best calibration gases are from NOAA Earth System Research Lab (<0.1 ppm uncertainty)



#### What you are measuring and how to get to in

- <u>situ</u> xCO<sub>2</sub> (dry) is being measured at chamber T and P, need P to convert to pCO<sub>2</sub> Measured pCO2 is dry, need P to convert to
- 100% humidity Measured pCO<sub>2</sub> of seawater is at the
- chamber T during equilibration; need in situ T to correct for warming
- Most labs will also correct for non-ideality of CO<sub>2</sub> and calculate fCO<sub>2</sub> using salinity, in situ T and chamber T

#### What is reported

fCO<sub>2</sub> (µatm) at in situ temperature Could useful to report fCO2 at chamber T, chamber T, and in situ T?



#### What type of data do we produce?

Sensor observations pCO<sub>2</sub> pН





Discrete samples Total alkalinity Total dissolved inorganic carbon pH (Total scale and NBS)

-JERIC@





#### Sensor observations: pH

#### **Basic principle**

- Seawater is pumped into a cell that has light sources and light detectors
- (spectrophotometry)
- pH sensitive indicator dye is added
- (e.g., thymol blue)
- Absorption at different wavelengths are measured and the ratio of these
- wavelengths are used to calculate pH

#### Calibration

- Indicator dyes need to be fully characterized to determine extinction coefficients
- Indicator dye addition can change sample pH standard addition of dye
- should be carried out
- Can be calibrated using CO2 CRMs or

Tris buffer



#### What you are measuring and how to get to in situ

- pH (total scale) of seawater sample at cuvette T and perturbated by dye addition
- Need to correct for dye addition perturbation by making standard additions
- Need to correct from cuvette T to in situ T using empirical pH-T relationship

#### What is reported

pH (total scale) at in situ temperature Again, could useful to report pH at

#### cuvette T. cuvette T. and in situ T?

#### Discrete samples: CT (total dissolved inorganic C)

#### Basic principle

Seawater is warmed up in a closed bottle to 25 deg C and pumped into

#### stripping cell

- Phosphoric acid is added to convert
- all DIC into  $CO_2$  $CO_2$  is dried in a Peltier cooler and
- carried to coulometric detector by an
- N<sub>2</sub> gas stream

#### Calibration

- Pipette (~20 ml) for measuring out seawater sample needs to be checked for volume
- Sample S and T are important to calculate sample density which is combined with volume to calculate
- mass Na<sub>2</sub>CO<sub>2</sub> standards can be used Also CO2 CRMs should be used on a \*
- regular basis



#### What you are measuring and how to get to in

- Total DIC (μmol kg<sup>-1</sup>)
- Total DIC in a sample is independent of T as long as the bottle is gas tight
- The fraction of total DIC that is CO32-, HCO3-,
- and CO<sub>2</sub> is dependent on in situ T DIC speciation can be calculated using CO2SYS as long as you have CT, AT or pH or fCO<sub>2</sub>, S, and
- T: phosphate and silicate are needed if you are using AT and nutrients are high

#### What is reported

- Total DIC (µmol kg<sup>-1</sup>), and in situ S and T Normally it is also reported with total alkalinity next slide
- Data analyzers are free to choose which constants to use in CO2SYS for further work

#### Discrete samples: AT (total alkalinity) **Basic principle**

- Seawater is warmed up in a closed bottle to 25 deg C and pumped into
- stripping cell 0.1 M HCl is added in small aliquots
- to titrate total alkalinity components
- Sample pH during the titration and the volume of titrant added are used
- to compute total alkalinity

#### Calibration

- Pipette (~100 ml) for measuring out seawater sample needs to be checked . for volume
- Sample S and T are important to
- calculate sample density which is
- combined with volume to calculate mass
- 0.1 M HCl titrant and dosimat need to
- be carefully checked =.
- Na<sub>2</sub>CO<sub>3</sub> standards can be used
- Also CO, CRMs should be used on a
- regular basis



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- Total alkalinity (umol kg<sup>-1</sup>) Total alkalinity is independent of T as long as
- the bottle is gas tight AT is used in CO2SYS along with CT or pH or fCO2, S, T, and phosphate and silicate if nutrients are high to calculate the rest of the carbonate system
- If you are in coastal waters (high humic content) or in very productive waters, there can be substantial non-carbonate alkalinity component - this is not characterized in CO2SYS

#### What is reported

<u>situ</u>

- Total alkalinty (µmol kg<sup>-1</sup>), and in situ S and T Normally it is also reported with CT Data analyzers are free to choose which
- constants to use in CO2SYS for further work

#### Discrete samples: pH

#### **Basic principle**

- Spectrophotometric method is the same as the pH sensor, except samples should be warmed to a fixed temperature (typically 25 deg C)
- Potentiometric pH measurements are made using an electrode that
  - measures electromotive force

- Calibration Spectrophotometric method: same as for pH sensor
- Potentiometric pH electrode needs to be calibrated using NBS buffers, but
- better to calibrate using seawater Tris buffers to reduce shock of going between low/high ionic strength Ξ

#### JERICO

Sensor observations

• Both need to be corrected for in

characterization of pH indicator

situ T and measurement T

 $\mathsf{pCO}_2$  is calibrated using calibration gases

pH is based on standard

pH (total scale)

dve

#### What you are measuring and how to get

- to in situ Spectrophotometric method: pH (total scale) of seawater sample at cuvette T and perturbated by dye addition
- . Potentiometric method: If using seawater Tris buffers. pH (total scale): if using NBS buffers, pH (NBS scale)
- Both require knowledge of measurement T and in situ T
- Any sample warming/cooling must be done with closed gas tight bottle

#### What is reported

- pH (total scale or NBS scale) at in situ temperature .
- Could useful to report pH at measurement T, measurement T, and in situ T?

#### What type of data do we produce?

#### Discrete samples pCO<sub>2</sub> (ppm pCO<sub>2</sub> or µatm fCO<sub>2</sub>)

Total alkalinity (µmol kg-1) Total DIC (µmol kg<sup>-1</sup>) pH (total or NBS scale)

> AT, CT, pH all are measured at a fixed T (e.g. 25 deg C) and need CO2SYS software to calculate other carbonate system variables at in situ T dependent on with constants you . choose

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- AT and CT both use carbonate standards AND CRMs
- Electrode pH can be on total or NBS scale depending on the kind of calibration solutions used









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#### Marine carbonate system observations: the data manager's perspective

Benjamin Pfeil Bierknes Climate Data Centre RI ICOS Ocean Thematic Centre University of Bergen benjamin.pfeil@uib.no



#### Marine inorganic carbon observations: marine biogeochemistry community's perspective

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Driven by requirements, negotiated with feasibility

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#### OUTLINE

- · Purpose why do we measure: climate vs environmental monitoring
- · Quality vs coverage
- · Global vs regional
- Research infrastructures vs networks, projects
- Data availability
- NRT data
- Collaboration



- · We cannot measure everything, nor do we need to
- Basis for including new elements of the system, for expressing requirements at a high level Driven by
- requirements, negotiated with feasibility
- Allows for innovation in the observing system over time

#### **Essential Ocean Variables according to GOOS**

EOV Information	Inorganic Carbon
Sub-Variables	Dissolved Inorganic Carbon (DIC), Total Alkalinity (TA), Partial pressure of carbon dioxide (pCO2) and pH. [At least two of the four Sub-Variables are needed.]
Derived Products	Saturation state (aragonite, calcite), Dissolved carbonate ion concentration, Air-sea flux of CO2, Anthropogenic carbon, Change in total carbon
Supporting Variables	<b>Temperature, Salinity,</b> wind speed, Atmospheric CO2 (xCO2), Barometric pressure, Oxygen, Calcium concentration, Transient tracers, Oxygen to argon ratio (O2/Ar)

#### 

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#### Landscape for EOV Inorganic Carbon Data Management



#### Data availability

- · Data repositories, observing and community networks
- · Data products (e.g. SOCAT, GLODAP)
- Data brokers (e.g. IODE, GCMD, SeaDataCloud, GEO)
- · Integrated networks (EMODnet, JERICO-Next)
- · Research infrastructures (IOOS, ICOS; ARGO, EMSO)
- · Research projects



#### ICOS Coceau Them Centr Software for automated data reduction and QC **ICOS Ocean Thematic Centre** · Enables integration, interoperability and Mission: highest possible guality! ICOS 🚟 Dr. Steve D. Jones QuinCe The suggested network of Developing an online tool for data reduction and quality control of surface ocean fCO<sub>2</sub> data stations for the ocean-network: 18 SOOP/VOS lines 22 fixed time series stations ٠ 7 repeat hydrographic sections Currently the official OTC network is around 50% ICOS Framework for Ocean Observing **IOCCP Mission and Field of Expertize** IOCCP SSG Approved governance structure Chair Toste Tanhua (Germany) The IOCCP promotes the development of a global network Underway pCO<sub>2</sub>: Rik Wanninkhof (USA) **GOOS Steering Committee** of observations for marine biogeochemistry through technical coordination and communication services, international agreements on standards and methods, and Surface CO<sub>2</sub> Data: m Currie (New Zealand) Repeat Hydrography: Masao Ishii (Japan) advocacy and links to the global ocean observing system. In each of the fields of our interest (left) IOCCP follows the following scheme: Ocean Interior Data: Are Olsen (Norway) Time Series Networks: Laura Lorenzoni (US) **GOOS** Panels 11.00 Todd Martz (US) Data Management: Benjamin Pfeil (Norway) nd GCOS on glo Nutrients Michio Aoyama (Japan) Ocean Acidification Richard Feely (USA) SOLAS/IMBER: Andrew Lenton (Australia) Niki Gruber (Switzerland) Project Director: Maciej Telszewski (Poland) CP). The B a. Biolog w. 2013 nks to the Three different Panels

try Panel (IOCCP)

(Observing technologies and networks, Variable focus: data and products, synthesis, link to models)

(....



![](_page_29_Picture_1.jpeg)

glodapv2

![](_page_29_Picture_2.jpeg)

![](_page_29_Picture_3.jpeg)

![](_page_29_Picture_4.jpeg)

C02

Is the global community (under GOOS) in perfect shape?

- No
- Severe lacks in data availability (time series stations, coastal data)
- EOV Inorganic Carbon data often not covered entirely (e.g. SOCAT)
- 'New' sensors (e.g. AUVs)
- · Certain systems are not included (FerryBox)
- NRT data availability

#### (.....

![](_page_30_Picture_10.jpeg)

#### 

#### Issues - Data availability

- Duplicates
- Lack of documentation for metadata and quality control
- · Varying quality control
- Movement towards *Big Data* but limited integration and access to long-tail data from individual researchers

![](_page_30_Figure_17.jpeg)

#### 

#### Data access and user friendliness

- · Difficult to access data across data sources
- · Reproducibility and citation
- · Uncertainties (lack of QC, metadata)
- NRT data availability
- Lack of integration, interoperability and consistency (vocabulary, flags, data, metadata)
- · Data products exist but just for certain data
- · EOV Inorganic Carbon not covered entirely

#### 

![](_page_30_Figure_28.jpeg)

#### 

![](_page_30_Figure_30.jpeg)

#### We can not do everything!

- Insufficient funding for data management activities
- Need for complimentary efforts
- More interaction between RIs, networks -> room for each other activities
- Need for modernisation
- Focus on expertise (let the experts do the QC for the various EOVs)
- Interoperable systems (QC feedback)

#### **Collaboration instead of competition!**

#### 

#### Demands from funding agencies and society

- Data availability across networks (GEO, SDC)
- FAIR (Findable, Accessible, Interoperable, Re-usable)

![](_page_31_Picture_13.jpeg)

<image><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><text><text><text><text><text>

1895

Community effort ensures stability

Global Data Assembly Centre for

![](_page_31_Figure_18.jpeg)

![](_page_32_Picture_0.jpeg)

![](_page_32_Picture_1.jpeg)

![](_page_32_Picture_2.jpeg)

Gliders are now a mature robotic ocean observing platform

-, pursony, gauces carry an instrument payload that includes a pumped CTD, an oxygen sensor and one or more biogeochemical sensors such as a fluorometer, an optical backscatter sensor and/or a PAR sensor.

· Additional payloads have included passive acoustic hydrophones, high frequency ADCPs, a nitrate sensor and a micro-structure/turbulence sensor

 Data are typically available in three modes,
 Real Time – a reduced dataset sent each time the glider surfaces for communications Near Real Time – a complete dataset downloaded after each glider mission recovery Delayed Mode – a complete dataset that has been 'field' corrected to historic datasets

 Automatic and semi-automatic data QC criterion continue to be developed and refined for the first two of these modes. Data from the RT and NRT modes are then suitable for rapid environmental assessment, and model constraint and assimilation

 Delayed mode, 'field' correction is being adopted and adapted for glider data from historical experiences with towed and lowered observational platforms. At SOCIB we are beginning to look at how this can be applied in a more semi-automatic manner – this is the subject of deliverable D 5.15, and, to a large extent, this presentation.

#### 

#### OBJECTIVES

Respond to scientific and societal challenges by maintaining and enabling world class quality control of glider data at high temporal and spatial resolutions.

Develop methods and tools to apply well-established procedures before, during, and after every mission.

- · Incorporate routine multi-platform calibration and inter-calibration procedures in the validation and correction process.
- Monitor and record information concerning the calibration, validation and correction in the metadata file
- Quantify and clearly describe the achieved accuracy and therefore residual error in the final delayed mode product.
- Guarantee traceability in the data calibration, validation and correction chain.

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#### **SOCIB Glider Toolbox**

- · A set of MATLAB/Octave scripts and functions the toolbox
- · Supports Slocum, Seaglider and recently added SeaExplorer platforms
- Provides
  - Tools to generate standard netCDF files and figures from raw glider data
  - Advanced processing features, e.g. thermal lag correction
  - . Standard RT and NRT quality control tests (range, spikes)
  - Covers main initial steps of the glider data management process
- · Modular structure and user configurable output, for addition of new sensors, etc.
- · Built for an operational facility, also useful for scientist users as standalone

User-friendly, real-time/delayed mode, processing toolkit for glider data Delivers data ready for science and operations - available at https://github.com/socib/glider toolbox

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![](_page_32_Picture_35.jpeg)

- Flow diagram the best guide information processing levels, scripts, inputs and outputs, user configurable components
- Essentially 4 processing steps and 3 levels of output: L0, L1 and L2

![](_page_32_Picture_38.jpeg)

dider data pr C. Troupin<sup>4,4</sup>, J.P. Beltran<sup>4</sup>, E. Heslop<sup>4</sup>, M. Torner<sup>4</sup>, B. Gara J. Allen<sup>4</sup>, S. Ruiz<sup>6</sup>, J. Tintoré<sup>4,6</sup>

#### 

#### **Delayed Mode – Field Correction**

Focusing on CTD data, develop methods and software tools to make routine inter-calibrations between gliders and other platforms. Following international leading procedures and standards where they exist and taking an international lead in promoting new standards where they do not.

e.g. "virtual bottle stops" points of T/S comparison with CTDs or maximising "white space" in T/S diagrams (Allen, Gardiner and Heslop, in prep.)

conductivity = A \* (measured conductivity)

#### $conductivity = A + B^*(measured conductivity)$

 $conductivity = A + B^* (measured conductivity) + C^* (measured conductivity)^2$ 

![](_page_33_Figure_0.jpeg)

![](_page_33_Figure_1.jpeg)

![](_page_33_Figure_2.jpeg)

#### Metadata ....

To gu	arantee the traceability, the netCDF file should have an updated header, containing all the
inform	ation necessary to understand how and when the calibration was performed.
We pr	opose the following global attributes to be added:
correc	tion_date = "2015-05-26T10-33-35+00.00";
correc	tion_datter = "J, Alen"
correc	tion_datter = "J, Alen"
correc	tion_detter = Casas-square literar regression"
correc	tion_detter = 0.9887554
If all th	ne variables are calibrated using the same instrument (e.g., the R/V CTD), then two more
lines c	an be added:
comed comed "http:// 011_9 or corred	tion_instrument = "SeaBilitSCTD" Ion_datuat = thmodes.socb.net#redds/doct/research_vessel/idd/acdb_rv-scb_sbe9002/L12015/dept orb-rv_scb-be9002L1_2015-65-91 nc" orb-rv_scb-be9002L1_2015-65-91 nc"
If som	e variables are calibrated against different instruments or data set, then this information
shouk	the reflected in the variable attributes, not the global attributes.
double	sambly_constant(sime) is an end of the second secon

#### 

#### Task 5.7: Deliverable D5.15 - Draft

![](_page_33_Figure_8.jpeg)

int WP2-WP5 Workshop: assimilating technical Best Practice improvements to optimize network data flow Bergen, Norway, 05 October 2017

#### 

#### Potential and collaborations with other WPs

![](_page_33_Figure_12.jpeg)

![](_page_33_Picture_13.jpeg)

#### **Challenging Topics**

 Delayed Mode scientific correction Metadata close to full implementation at SOCIB now for physical parameters – Biogeochemical data will be a bigger challenge as parameters such as community structure will have a large part to play, as will multi-instrument diagnoses, e.g. using a combination of optical backscatter and fluorescence to determine DCMs, surface quenching, and auto versus mixo – trophic communities.

 Automating the QC and correction, where possible, of bad data resulting from bio-fouling of the conductivity sensor is still problematic and more work needs to be done. Nonetheless significant progress has been made in this direction.

 Standardise and semi-automate Depth Averaged Velocity calculations, combining navigation data, flight models, and compass correction data files. This is now well understood throughout the community, but generally follows a very manual and non-routine process.

![](_page_34_Picture_0.jpeg)

#### **Observations using AUVs** The glider data manager's perspective

Thierry Carval Ifremer Thierry.Carval@Ifremer.fr

FIFRICO-NEXT

#### The data manager's perspective

- Currently applied protocols (including metadata requirements) for handling data relating to the specific parameter under consideration within JERICO-NEXT.
- Known limitations of the described protocols, and their level of compatibility with other EU and global data management initiatives.
- Issues affecting data dissemination (e.g. scales, units and conversions, processed vs. unprocessed data, data reduction practices, further metadata needs ...).
- Proposals/suggestions for improving the JERICO-NEXT terms of reference for handling data relating to the specific parameter under consideration.
- Suggestions for better and more efficient connection with major European Data infrastructures

#### EGO data management

EGO contributors agree on a common NetCDF-CF file format to manage glider metadata and observations, organized by deployment

- EGO gliders NetCDF format reference manual version 1.2. <u>http://doi.org/10.13155/34980</u>
- EGO gliders Quality Control on time series and profiles data <u>http://doi.org/10.13155/51485</u>
- EGO gliders data processing chain <u>http://doi.org/10.17882/45402</u>
- EGO gliders NetCDF file format checker <u>http://doi.org/10.17882/45538</u> CHERICO NEXT

#### EGO NetCDF-CF implementation for gliders

EGO gliders NetCDF format reference manual http://doi.org/10.13155/34980

- One file per glider deployment
  - Metadata : a list of NetCDF global attributes
  - Observations : a timeseries of parameters (each observation has a time stamp)
- EGO & Argo share the same list of CF parameters <u>http://www.argodatamgt.org/Documentation</u> Coreand
  - Endorsed by AtlantOS, Copernicus Marine, SeaDataNet

#### Quality control procedures

EGO gliders QC on time series and profiles data <u>http://doi.org/10.13155/51485</u>

- Real-time quality control
  - 14 quality controls derived from Argo real-time QC
- Delayed mode quality control
  - A long work underway
    - Physical parameters
    - BGC parameters

#### EGO data processing chain

#### EGO gliders data processing chain <a href="http://doi.org/10.17882/45402">http://doi.org/10.17882/45402</a>

- A matlab data processing chain, freely available under CC-BY-4.0 license
- The EGO data processing chain decodes, processes, formats glider data Slocum, SeaGlider, SeaExplorer
- The decoder also performs the additional actions
  - Apply Real Time Quality Control (RTQC) tests on EGO file time series,
  - Estimate Slocum subsurface currents and store them into the EGO file,
     Generate NetCDF profile files from EGO file data and apply specific RTQC tests to them.

#### EGO data processing chain

- The data processing chain works with
  - The deployment data files sent from the glider
  - A JSON collection of metadata
    - One deployment metadata JSON file
    - One JSON file for each sensor
    - Example

ftp://ftp.ifremer.fr/ifremer/glider/v2/ifm12/ifm12\_20170403/

![](_page_35_Figure_8.jpeg)

#### EGO ftp data server

- The EGO GDAC (Global Data Assembly Centre) is available at:
  - http://www.ifremer.fr/co/ego/ego/v2
  - ftp://ftp.ifremer.fr/ifremer/glider/v2
- A directory per glider, a sub-directory per deployment
- Each deployment contains
  - The EGO NetCDF data and metadata file
  - The deployment JSON file (used for data processing)
  - A directory of all vertical profiles
     One NetCDF file per profile (Argo NetCDF format)
    - Extracted from EGO data file (descending and ascending phases)

#### EGO file format checker

### NetCDF file format checker for EGO gliders <u>http://doi.org/10.17882/45538</u>

- Useful to check glider NetCDF files format from various providers
  - EGO data processing chain is not mandatory IMR and SOCIB use their own tools

#### Data citation

- Work underway with AtlantOS funding
  - Assign a DOI for each deployment
  - Manage DOIs of DOIs to group a series of deployment
    - Network level
    - Science process
  - Use ORCID to give credit to PIs and contributors

#### Examples

- Tintin in Greenland <u>http://doi.org/10.17882/51473</u>
- Tintin & Moose <u>http://doi.org/10.17882/51472</u>

![](_page_35_Picture_35.jpeg)

Data management System
EGO NetCDF formating

![](_page_35_Figure_37.jpeg)

Back up / operational piloting service

RTQC DOI on demand Distribution to Data integrators .GTS .EGO website .Copernicus Marine .EMODNET .SeaDataNet .OccanGilders

#### The last 30 days of observations

![](_page_35_Picture_40.jpeg)