



EuroGO-SHIP
Enhancing ocean observations

D3.1 Report on Best Practices and traceability, including gap analysis

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Summary

This deliverable describes key elements for a Best Practices and Standards (BP&S) strategy for a future EuroGO-SHIP research infrastructure (EGS-RI). The strategy considers generic elements of European RI rather than the specifics of a future EGS-RI, which are unknown at this stage. Two pillars addressed: the EGS-RI governance structure and technical aids. For the EGS-RI governance structure three elements are identified: an Person of Contact for all affairs related to Best Practices and Standards (BP&S-PoC), an EGS-RI Endorsement Panel, and EGS-RI topical Convergence Working groups. This structure will enable seamless workflow on all BP&S related issues in a future EGS-RI, it will enable overlooking an EGS-RI specific “endorsement process” to elevate Practices to be the recommended ones for trusted and fit-for-purpose operations in the future EGS-RI, and it will enable the dialogue needed with external expert groups of other hydrography practitioners (e.g., GO-SHIP), with Best Practices and standards initiatives (e.g., IOC-OBPS, EUMETNET), and with EGS-RI joint data/metadata management and knowledge transfer approaches. The EGS-RI Technical aids shall include an EGS-RI Best Practices repository, but not necessary maintained by the EGS-RI but eventually external (e.g., IOC-OBPS repository or a future EU BP repository). Given the design will very much depend on how the structure of a future EGS-RI is agreed on we here can only provide suggestions for an initial design and workflow within a future EGS-RI.

1. Introduction

Best Practices lay the foundation for a major strength of distributed Research Infrastructure (RI) – joint operations that become better and more complete, and thus generate added value for the individual members of the RI, when compared with operations without an RI. The need to work together in national, European and global groups of experts and practitioners has increased significantly in recent years. An important motivation for this development is that collaboration enables work processes to be optimized, which leads to improved results and lower costs at the same time. In order to enable heterogeneous groups (e.g., members of the EGS) to implement controlled and comprehensible workflows, jointly developed or approved documentation of procedures are required that are referred to as “Best Practices” (BP), “Standard Operating Procedures” (SOP), or “methodologies”. Sometimes these terms are seen as interchangeable or equivalent, but in the context of this document and also as an initial recommendation for a future EuroGO-SHIP Research Infrastructure (EGS-RI), the differences between the terms should be clarified and recognized, as it is precisely the differences that make it possible to document improved and also trustworthy processes of a group in contrast to single institutions or single research group approaches.

For this reason, we here will make use of the term “Best Practice” as defined in Pearlman et al. (2019): “A best practice is a methodology that has repeatedly produced superior results relative to other methodologies with the same objective. To be fully elevated to a best



practice, a promising method will have been adopted and employed by multiple organizations”. In particular, the second part of the sentence “...adopted and employed by several organizations” speaks directly to a distributed RI such as the future EGS-RI, where a number of experts from the member countries work together to enable research at a higher level than it would be possible for a single country or even institution or individual. This definition implies that all actors can and shall be involved in the BP creation process – either directly or indirectly to enable creation of “trusted practices” and which in turn the group supports and therefore feel committed to follow.

Best Practices may address areas like collection of observational data, quality control of data, standardization of data and metadata, but also include training and knowledge transfer activities. By following best practices, procedures are carried out in a controlled way and this in turn makes the underlying procedures traceable and transparent. Best practices promote, for example:

- Traceable and transparent uncertainty estimates for observational data points
- Global interoperability of observational data
- Efficiency of all processes (“don’t re-invent the wheel”)
- Transparency - Data traceability and reproducibility
- Seamless linkages between data, models and applications
- Training and capacity development

As mentioned, Best Practices are at the heart of operations within a RI. This is because in distributed RIs, such as it would be the case in a future EGS-RI, various actors, labs, sensors, analysis techniques, and skill-sets operate under one virtual umbrella but for common objectives. It therefore is mandatory to make the operations within the RI transparent, and traceable to enable production of data with *reproducible* quality. It has to be emphasized that the differences in labs, sensors, reference material, skill sets, circumstances (e.g., time constraints at sea) all will alter the uncertainty of a datapoint and eventually degrade it from the highest quality that is theoretically possible. Note that the term “uncertainty” not always characterizes a measure for the distance from a true value but other measures may apply for example heterogeneity might be a better descriptor for biological data. In any case, attributing uncertainties/heterogeneity to observational data is the key characteristic of the “Requirement Processes” within observing systems that aim for being “sustained” and that in turn is implicit under the framing of “quality specifications” in the concept of Essential Ocean Variables (EOVs; see Lindstroem et al. 2012). In other words – without traceable and reproducible uncertainties it is not possible to derive EOVs from observational data.

In distributed RI the execution of experiments at sea or in labs always face challenges due to foreseeable or unforeseeable circumstances e.g., say a cruise takes place without having access to a salinometer or there is no pressure tank available in a lab for calibrating a pressure sensor on a CTD. BPs have to provide guidance for processing the data under various different conditions and thus have to have a modular structure ideally. The outcome of limitations could be a higher uncertainty for data sets that suffer certain procedures to be applied. Eventually secondary quality control procedures are required (e.g. see work in WP2/task 2.3).

Various factor have an impact on uncertainty of a data point and these can only be fully appreciated via respective uncertainty analysis (Figure 1). Several applications of an uncertainty analysis for ocean measurements exist (see e.g., JERICO D5.4 Guidelines for Uncertainty¹)

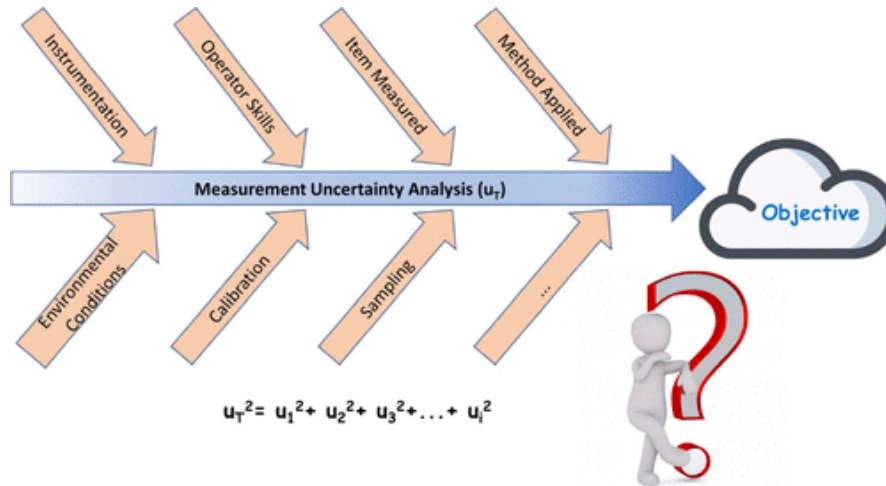


Figure 1: Schematic of factors to consider when doing a comprehensive measurement uncertainty analysis for a single data point (from Sanchez 2024). The outcome of such an analysis is answer the question if measurements can address the observational objectives.

This deliverable shall provide a base for a Best Practices strategy to be taken up by a future EGS-RI. The strategy includes the creation (also called “convergence”) and an initial set of characteristics of EuroGO-SHIP RI “endorsed” Best Practices, a governance model (with working groups and a central contact person) to ensure coordinated and transparent EGS-RI practices workflow and an EGS-RI practices document/media repository.

The International Standards Organization (ISO) defines standards as “documents of requirements, specifications, guidelines or characteristics that can be used consistently to ensure that materials, products, processes and services are fit for their purpose” (see Nair et al. 2023). Identifying needs and creating Standards is generally a top-down process with the intention to create something that serves as a mandatory, legislated instrument, such as the European INSPIRE legislation². At a national (and international) level standards following a framework that is embedded in metrology (“the science of measurements”) and that aims in accurately describing the process from a measurement result and a reference. In marine sciences, standards in a metrology sense, face various problems (e.g., Feistel et al, 2016; Pawlowicz et al. 2016).

Best Practices should make use of standards whenever possible. However, very much in contrast to Standard is that Best Practices are intended to be changed whenever needed for improvement (e.g., new technologies, adding other approaches). Certain EU legislations and

¹ https://www.jerico-ri.eu/download/filebase/jerico_fp7/deliverables/D5.4_Guidelines-for-Uncertainty_v2.pdf

² <https://inspire.ec.europa.eu/inspire-legislation/26>



Regulation (EU) No 1025/2012³ take into consideration some European or international standards. In addition, EU bodies such as the working groups for the Marine Strategy Framework Directive have established and documented best practices⁴. Despite the clear mandate and multilateral efforts, there is no EU-competent body or procedure for suggesting, compiling, or agreeing on best practices. To improve effectiveness and efficiency, the EU has proposed the joint planning of observation activities and a framework for collaboration on a national and EU scale that will adhere to community-accepted standards and best practices⁵. These standards are not always easy to find or accessible. Recognizing that several external sources of best practices already exist (e.g. HELCOM monitoring Guidelines⁶, data management standards proposed by EU projects¹ or interest groups such as the Darwin Core⁷) a future EGS-RI should be tailored to is aware and also to address the needs of such groups.

2. Gaps, Convergence and endorsement

For the successful operation of an infrastructure, it is of central importance that harmonized processes exist, be it for data acquisition, training or the shared use of infrastructures. The fact that certain elements are missing can often be recognized by problems in the workflow. Gaps can open up here that need to be closed. Maybe the two most obvious gaps related to BP&S are (1) the non-existence of a Best Practice for a certain operation, and (2) gaps in existing Best Practices because certain circumstances when executing work are not covered e.g., handling of CTD salinities without salinometer reference data available.

To overcome these two types of gaps a key process is “convergence”, which is basically an assessment of existing knowledge and subsequently, if needed, creating a documentation that fills the the gap identified before. Creation and update of Best Practices is done by groups of experts. This process always shall include an open and inclusive review process by “the community” that eventually could not participate in the creation and update process. This way, existing knowledge is comprehensively considered. In addition, opening up documents for general audience review will create trust by the community in what is documented and in turn overcomes barriers for adaptation.

One such barrier is non-inclusiveness in the process, meaning if experts feel exclude from the convergence process the Best Practices created by a group are not trusted, and thus not used and its quality will degrade over time. Moreover, it also often is the case that practitioners are not aware of practices that may be superior to what they use. Another barrier is that BP

³ EUR-Lex - 32012R1025 - EN - EUR-Lex (europa.eu)

⁴ Marine Strategy Framework Directive - Competence Centre (europa.eu) and in particular MSFD Technical Group on Marine Litter (europa.eu)

⁵ https://cinea.ec.europa.eu/funding-opportunities/calls-tenders/standards-and-best-practices-ocean-observation_en

⁶ <https://helcom.fi/action-areas/monitoring-and-assessment/monitoring-guidelines/>

⁷ <https://dwc.tdwg.org/>

are too complex in formulation or that the BP is not modular, meaning that only very specialized procedures are considered and no alternative procedures are provided which again exclude certain groups for executing the Best Practice.

A proven approach for convergence has been summarized by Przeslawski et al. (2023; Figure 2). After identification of a need for a Best Practice from a certain operator group (e.g., a future EGS-RI) they will call for a working group of experts that are tasked to develop the content of the best practice. This development should make use of published methodologies on the subject under discussion (e.g., using the OBPS repository or the ODIS ocean info hub). In an iterative process the working group creates a first complete draft. This draft then will undergo review by the whole operator group (internal) as well as a review by external experts. After these reviews the document package is released and used for applications within the operational space of the group. Field testing will expose potential gaps that require further revision followed by another review. In addition, other external groups are invited for use. The experiences made by using the best practice is recorded (Assess uptake) and used for a further revision of the document which in turn is released as an updated version.

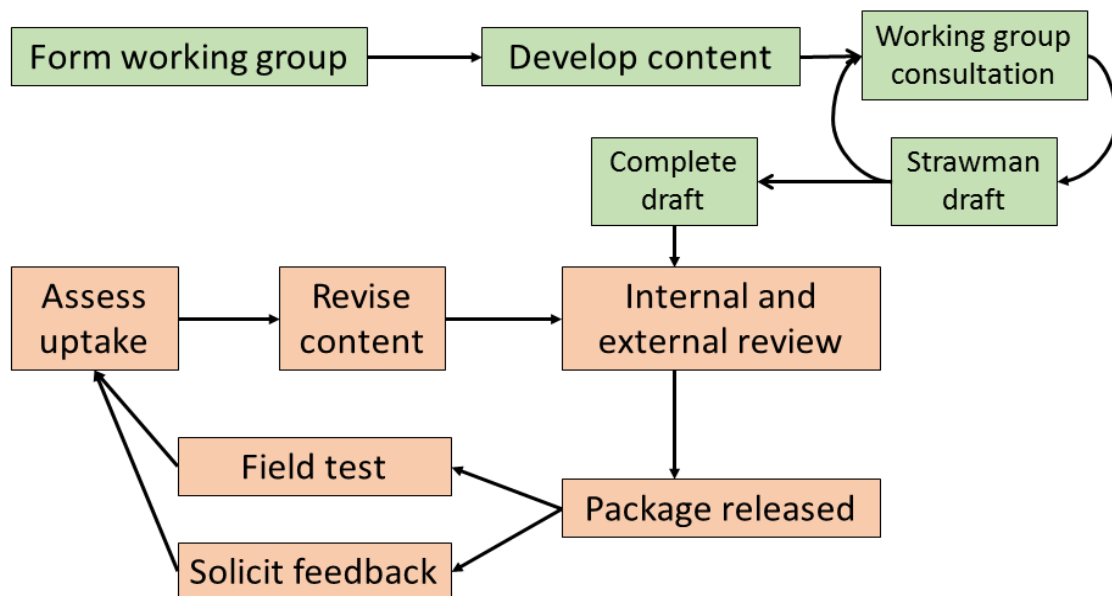


Figure 2: Workflow for creating a best practice (green part) and maintaining/updating a best practice (red part) from Przeslawski et al. (2023).

Considering that the whole workflow described above not always is fully completed a ‘Maturity Model’ for best practices has recently be proposed by Mantovani et al. (2024) were they differentiates five maturity levels (Figure 3). Level 1 is the formation of a document/practice and that is maybe realized only after Level 2 occurs – which is repeatability of a practice. If a working group summarizes, also considering other knowledge, what has been initiated in Level 1 and 2 a first release of the Practice can be done (level 3) and the document is labeled a “good practice” (the Levels 1 to 3 are covered by the green workflow in Figure 2). If the good practice has been released to the public and more and more groups make use of the practice the document transforms into what Mantovani et al. (2024) term “Better Practice” (Level 4). With increasing use and optimization of the content via regular

review the highest Level 5, similar to a Mature Best Practice is reached. One can discuss if this process is not a too complicated picture of the process – however, it illustrates that different levels of applicability and maturity of Practices exists based on the knowledge base they are created of. It also needs to be emphasized that with reaching the stage 5 (mature Best Practice) the evolution is not finished but a constant revision is required to maintain the mature stage. This point again stresses the need for a **Best Practices coordination person** in a future EGS-RI.

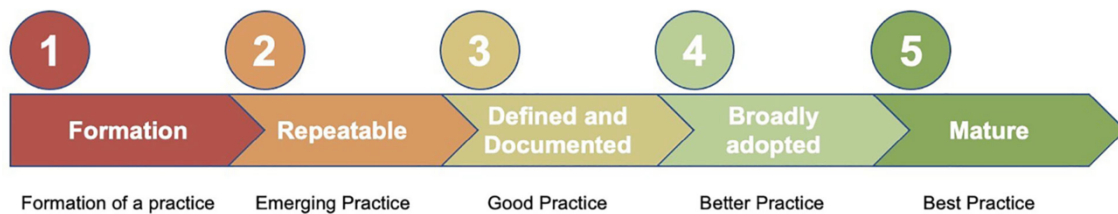


Figure 3: Maturity model for different stages of practices until the final and mature Best Practice (from Mantovani et. 2023).

The marine science and operators community is very large and operates at different levels and with maybe different intentions. To create trust and provide guidance to defined groups and consortia a certain labeling of best practices can be proposed that is summarized under “endorsement”. One example has been documented for the Global Ocean Observing System (GOOS) (Hermes 2020). Endorsement is based on defined content and expectations on Best Practices being formulated by the endorsing body (e.g., the EuroGO-SHIP RI). To elevate the endorsement to a larger level, the endorsing body can enter the dialogue with the IOC-OBPS and seek their guidance on mandatory content but also on formatting etc. that is required to serve the endorsed documents via the global repository systems (OBPS repository).

3. Best Practices process in the EuroGO-SHIP project

The key role of Best Practices in RI has been outlined already in section 1 and these objectives are directly applicable to the EuroGO-SHIP RI design. The EuroGO-SHIP project has executed demonstrator activities that address parts of the Best Practices creation workflow, specifically on maturity (Mantovani et. 2023) and convergence (Przeslawski et al. 2023). More specifically, the demonstrator activities addressed improvements of procedures for estimating salinity, nutrients, carbon system parameters, velocity, and oxygen data (incl. use of reference material), data delivery for a more sustained workflow (real-time CTD data), and work on training. This work on the Best Practices workflow was embedded in WP2 (Shared facilities) and WP3 (Concept demonstration).

Key for the success of the demonstrator activities was embedding them into the field work executed within the EuroGO-SHIP project. In WP3 we could execute best practice demonstrators on salinity measurements (D3.3), on nutrient sample storage (D3.5), on carbonate system analysis (D3.4), and also training activities have been executed (D3.2).



The **salinity demonstrator** investigated the effect of different salinometer models, and sampling and analysis methodology. The demonstrator took advantage of at least five cruises where replicate samples were taken considering commonly-used types of sampling bottles (OSIL plastic insert and generic swing-top), the analysis was performed in different labs (both shipboard and on-shore, including a calibration standard laboratory), and also by making use of different models of salinometers (Portasal and Autosal). Out of the execution of the demonstrator to generic (not only salinity related) lessons were drawn:

- **Importance of field experiments:** For determining current practices, comparing written procedures may miss differences in how those procedures are applied in practice
- **Sufficient lead time:** Planning and executing dedicated intercomparison experiments across labs to distinguish the important factors (e.g., sampling versus analysis methods versus storage time versus analysis environmental conditions) require a sufficient lead time

The **Nutrient demonstrator** was primarily concerned with the impact of long-term storage of seawater on the estimation of dissolved nutrients. sampled at sea but analyzed in institutional labs. The sampling exercises considered high (deep water) and very low (surface water) samples and preservation by freezing (-20°C) and by a pasteurization process (samples were heat treated at 80°C for 2 hours followed by storage at room temperature). Assessment was based on successive lab analysis over a period of 12 month in comparison with on-board analysis.

The **Carbonate system analysis demonstrator** focused on the production of a reference material (RM) for the carbonate system. Thus, it touches on the realm of Standards that are used within Best Practices for creating truly interoperable data that also carries reproducible and transparent uncertainty estimates. The process was documented in the deliverable (D3.4). More specifically, a batch of North Atlantic seawater was prepared to be used as RM. More than 100 bottles (250 mL each) were filled with this RM and measured to assign reference values. In addition, the experiment also looks at the impact of the canisters being used and therefore 5L plastic bags were filled with the same water to test the stability with respect to the CO₂ content.

The **Data flow demonstrator** assessed the current practices on how the EGS countries organize the pathway of data from PI level into respective data and metadata repositories and in turn see if the practices enable FAIR data access, incl. ingestion into the European and global data systems. The results are summarized in deliverable D2.3 (Data curation recommendation).

Further activities that are to be considered in a BP&S workflow in a future EGS-RI include:

- **Training & Knowledge transfer:** Various training and knowledge transfer activities have been conducted during the pilot cruises. Introducing students and young scientists into observational techniques on ships are activities that sometimes are

linked to universities circular. In the future Training & Knowledge transfer will benefit from EGS-RI endorsed BP&S documents. Furthermore, will these activities provide a benchmark for the applicability of BP&S documents, an important part of the Convergence workflow (See red blocks in Figure 2)

- Shared Facilities will have a specific demand in respect to BP&S. On the one-side the operations may require very specific operations instructions, tailored to respective facilities. However, EGS-RI will have to speak out recommendations on protocols and standards (e.g., reference material, metadata and data reporting) that comply with the requirements for EGS-RI endorsement. With the sharing of equipment via an European Marine Equipment Pool (EMEP) the BP&S endorsed by the future EGS-RI will be shared as well. It is expected that users of the EMEP follow the EGS-RI endorsed practices and this way generating data that is of known quality and with reproducible quality control applied. This will also provide an important branding to the EGS-RI design elements within the EMEP.
- While EuroGO-SHIP has put its focus on the applied side of hydrographic observations and executed via pilot missions there also was exchange with parallel projects and activities related to Metrology. Specifically, the H2020 MINKE (Metrology for Integrated Marine Management and Knowledge-Transfer Network) infrastructure project that is looking at the traceability side of measurements in ocean science has provided important thought-provoking impulses. By merging what has been done in the *metrology realm* (e.g., MINKE, EUMETNET) with the practitioner experience from EuroGO-SHIP, an improved and optimized workflow can be defined that ensures optimal (under given circumstances) quality and including reproducible uncertainty.

4. Best Practices workflow in a future EGS-RI

The exact design of the future EGS-RI has not been defined yet. The synthesis workshop for the statement of requirements for the future EGS-RI is scheduled for December 12, 2024. The draft agenda for the workshop includes all elements to be addressed in the strategy for a future RI (data curation, shared facilities, quality control, data acquisition, training).

However, for formulating recommendations for a Best Practices workflow for a future EGS-RI we make use of the RI definition by the European Commission⁸. In brief, RIs are facilities that provide resources and services for research communities to conduct research and foster innovation. They can be used beyond research e.g., for education or public services and they may be single-sited, distributed, or virtual. They include:

- major scientific equipment or sets of instruments

⁸ https://research-and-innovation.ec.europa.eu/strategy/strategy-2020-2024/our-digital-future/european-research-infrastructures_en



- collections, archives or scientific data
- computing systems and communication networks
- any other research and innovation infrastructure of a unique nature which is open to external users

Producing and making available research data of known and traceable quality is a major product of RIs. It shall be stressed that a future EGS-RI shall put specific care into the complete uncertainty estimates (Figure 1) as being a central attribute of any endorsement. Here the collaboration with national metrology office, with potential EU-wide metrology infrastructure (e.g., what now is MINKE) or/and metrology initiatives (e.g., EMETNET) is recommended.

Based on the experience from the EuroGO-SHIP project the following groups and design elements are proposed for a future EGS-RI:

1. Person of Contact for all affairs related to Best Practices and Standards (BP-PoC)
2. EGS-RI Endorsement Panel
3. EGS-RI topical Convergence Working groups
4. EGS-RI Best Practices repository

Further details on the needs and expectations are provided in the following. These are only suggestions for the initial design and workflow within a future EGS-RI.

Person of Contact for all affairs related to Best Practices and Standards (BP-PoC)

- Function:
 - Oversees and coordinate Best Practices general workflows
 - Contact for all groups intern to EGS-RI that deal with BP&S matters, specifically the EGS-RI Endorsement panel and the EGS-RI topical Convergence Working groups
 - Contact for external groups and initiatives that are of relevance for EGS-RI BP&S matters (e.g., GO-SHIP, EUMETNET for metrology, GOOS OCG, EOOS)
 - Reports to the Steering/Executive group of the future EGS-RI on BP&S matters
 - Be the person to contact if a potential BP&S gaps are identified
 - Overlook the process for initiating BP&S related actions (e.g., instalment of an EGS-RI topical convergence working group)
- Position in a future EGS-RI
 - Employed via base RI budget
 - Should be part of a future EGS-RI secretariat (if that will exist)

EGS-RI Endorsement Panel

- Function:
 - Define new and review existing key elements that qualify documents to be “EGS-RI endorsed” (e.g., document must include an uncertainty estimate)



- Maintain the dialogue with and is PoC for other endorsement bodies (e.g., GOOS endorsement)
- Position in a future EGS-RI:
 - Representatives of structural elements of a future EGS-RI (e.g., training and knowledge transfer, data and metadata, infrastructure sharing, international collaboration) and PB-PoC

EGS-RI topical Convergence Working groups

- Function:
 - Review requests on creation of new or revision of existing that have been received by the BP&S PoC
 - If needed, create new and review existing BP&S documentation
 - Seek to apply the “Guide to the expression of uncertainty in measurement” (GUM 2008) principles for uncertainty estimates outlined in the BP&S documentation.
- Composition:
 - Experts for the EGS-RI member countries that are interested to work on synthesizing present knowledge on emerging topics in the realm of the EGS-RI structural elements (e.g., training and knowledge transfer, data and metadata, infrastructure sharing, international collaboration)
 - Representatives of relevant external bodies (e.g., metrology offices, international GO-SHIP)
 - Should have a chair that reports on progress during regular (monthly?) EGS-RI steering group meetings

EGS-RI Best Practices repository

- Function:
 - Provide open and free access to documents that are of importance for BP&S in a future EGS-RI
 - Should highlight “EGS-RI endorsed” documentation
 - Should provide Persistent Identifies (e.g., DOI) for documents & media created with the future EGS-RI
- Instalment:
 - External, with a preference to make use of the IOC-OBPS repository or a future European BP repository, to ensure the interoperability with these systems
 - EGS-RI internal if eventually a data base is also planned for other coordination activities within the EGS-RI (e.g., expert data base)

5. KPI addressed in this deliverable

KPI-1.4	Made a statement of system requirements for the new RI
	This deliverable introduces design elements to be considered for a Best Practices workflow within a future EGS-RI
KPI-1.6	Made a description of the scope of the new RI and proposals for its architecture, governance and financing structures that supports long term sustainability
	This deliverable introduces the design elements to be considered for a Best Practices workflow for a future EGS-RI
KPI-2.1	<p>Determined the requirement, cost and possible supply models for new user facilities including:</p> <ol style="list-style-type: none"> 1. Specialist analytical capabilities to measure key parameters, such as transient tracers and low concentration nutrient analyses 2. Certified reference materials (CRMs) for nutrients and inorganic carbon 3. Training in at sea operations, data processing and interpretation 4. Development and maintenance of shared best practices 5. A European Marine Equipment Pool (EMEP) that shares scientific equipment across Europe
	<p>Re 1. This deliverable introduces how practices that are applied in shared facilities of a future EGS-RI can be shared and eventually improved via a Best Practices working group as one governance element in a future EGS-RI.</p> <p>Re. 2. As 1. But for all kind of reference material.</p> <p>Re. 3. The Best Practices workflow of a future EGS-RI is considering application of the practices also for training of various kinds (at sea, data processing, data interpretation)</p> <p>Re. 4. One element of the Best Practices workflow will be choosing an EGS-RI trusted repository for making accessible documents and media.</p> <p>Re. 5. With the sharing of equipment via an EMEP the respective Best Practices that have been endorsed by the future EGS-RI will be shared as well. It is expected that users of the EMEP follow the EGS-RI endorsed practices and this way generating data that is of known quality and with reproducible quality control applied. This will also provide an important branding to the EGS-RI design elements.</p>

KPI-4.3	Evaluated the requirement for regional nutrient reference materials reflecting variability in water chemistry in European Seas.
	The work on nutrient reference materials was an important pilot case for assessment of requirements that shall be addressed by a future EGS-RI Best Practices workflow.
KPI-5.3	Developed and trialed a method to add uncertainty to observations that will open up data usage to non-specialists
	The estimation of uncertainties is identified one mandatory element in all EGS-RI endorsed Best Practices. Ideally the process to estimate uncertainties should follow the “Guide to the expression of uncertainty in measurement (GUM 2008)”



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Appendix: Acronyms

BP:	Best Practice
BP&S:	Best Practice and Standards
EOV:	Essential Ocean Variable
EGS:	EuroGO-SHIP
EGS-RI:	EuroGO-SHIP Research Infrastructure
GOOS:	Global Ocean Observing System
GO-SHIP:	International research vessel observations coordination group
IEEE:	Institute of Electrical and Electronics Engineer
RI:	Research Infrastructure
RM:	Reference Material
SOP:	Standard Operation Procedures