DEUTSCHE ALLIANZ MEERESFORSCHUNG

KüNO Workshop 'Data sharing in marine research

Data management workflows for experiment and model data

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HELMHOLTZ
RESEARCH FOR GRAND CHALLENGES

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Agenda

- Data management: who, when and how
- Components of data management workflow
- Examples:
  - Ocean modeling
  - Mesocosm experiments
  - Samples

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Data management: who, when and how

Who: scientists, data stewards, data manager

When: proposal, preparation of work, during expeditions/experiments/coding, exchange of results, publishing of results

How: agreement of group, set up of systems, using tools, monitoring and visibility

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Central data management workflow @ GEOMAR

1. Agreement on one **data policy or DMP** (expected data, responsible persons, timeframes)
2. Information system with metadata and linked data for exchange and monitoring deliverables (**OSIS**)
3. Accessibility and reuseability of research data based on **persistent identifiers** (DOI + handle)

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1. Data management plan (DMP)

- The **DMP** describes the expected data and how and when they will be handled, stored and made available
- The information system **keeps track** on the **deliverables** and sends reminder
- The result is an **overview on the outcome** of the project => data management record

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2. OSIS: Ocean Science Information System

- tool for search and share data for ongoing projects
- metadata are open access
- data can be login protected for project groups
- links to longterm repositories

→ Helps transparency (Open Science)

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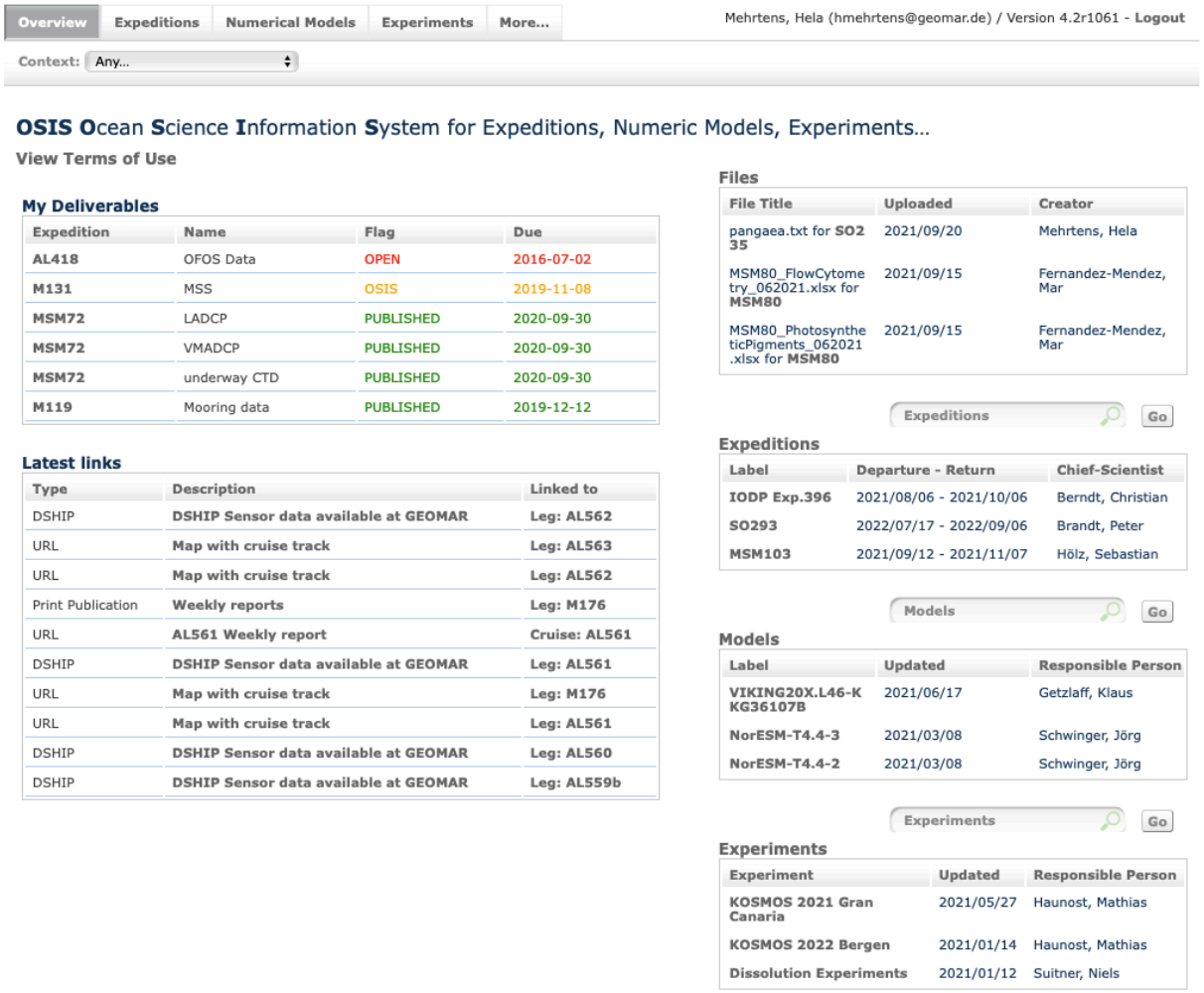
2. OSIS



Overview | Expeditions | Numerical Models | Experiments | More...

Mehrtens, Hela (hmehrtens@geomar.de) / Version 4.2r1061 - **Logout**

Context: Any...

OSIS Ocean Science Information System for Expeditions, Numeric Models, Experiments...

View Terms of Use

My Deliverables

Expedition	Name	Flag	Due
AL418	OFOS Data	OPEN	2016-07-02
M131	MSS	OSIS	2019-11-08
MSM72	LADCP	PUBLISHED	2020-09-30
MSM72	VMADCP	PUBLISHED	2020-09-30
MSM72	underway CTD	PUBLISHED	2020-09-30
M119	Mooring data	PUBLISHED	2019-12-12

Latest links

Type	Description	Linked to
DSHIP	DSHIP Sensor data available at GEOMAR	Leg: AL562
URL	Map with cruise track	Leg: AL563
URL	Map with cruise track	Leg: AL562
Print Publication	Weekly reports	Leg: M176
URL	AL561 Weekly report	Cruise: AL561
DSHIP	DSHIP Sensor data available at GEOMAR	Leg: AL561
URL	Map with cruise track	Leg: M176
URL	Map with cruise track	Leg: AL561
DSHIP	DSHIP Sensor data available at GEOMAR	Leg: AL560
DSHIP	DSHIP Sensor data available at GEOMAR	Leg: AL559b

Files

File Title	Uploaded	Creator
pangaea.txt for SO235	2021/09/20	Mehrtens, Hela
MSM80_FlowCytometry_062021.xlsx for MSM80	2021/09/15	Fernandez-Mendez, Mar
MSM80_PhotosyntheticPigments_062021.xlsx for MSM80	2021/09/15	Fernandez-Mendez, Mar

Expeditions Go

Expeditions

Label	Departure - Return	Chief-Scientist
IODP Exp.396	2021/08/06 - 2021/10/06	Berndt, Christian
SO293	2022/07/17 - 2022/09/06	Brandt, Peter
MSM103	2021/09/12 - 2021/11/07	Hölz, Sebastian

Models Go

Models

Label	Updated	Responsible Person
VIKING20X.L46-KKG36107B	2021/06/17	Getzlaff, Klaus
NorESM-T4.4-3	2021/03/08	Schwinger, Jörg
NorESM-T4.4-2	2021/03/08	Schwinger, Jörg

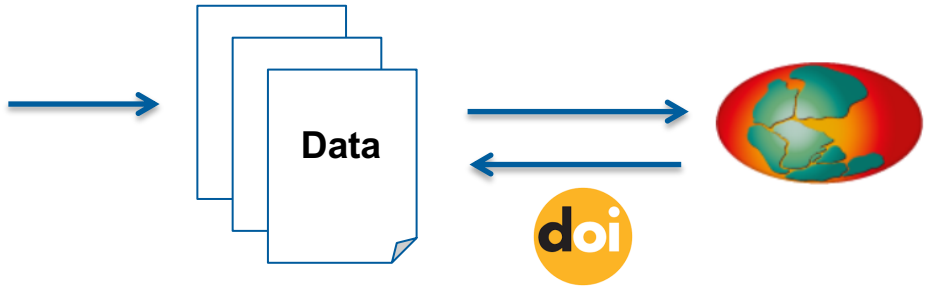
Experiments Go

Experiments

Experiment	Updated	Responsible Person
KOSMOS 2021 Gran Canaria	2021/05/27	Haunost, Mathias
KOSMOS 2022 Bergen	2021/01/14	Haunost, Mathias
Dissolution Experiments	2021/01/12	Suitner, Niels

3. Persistent identifier

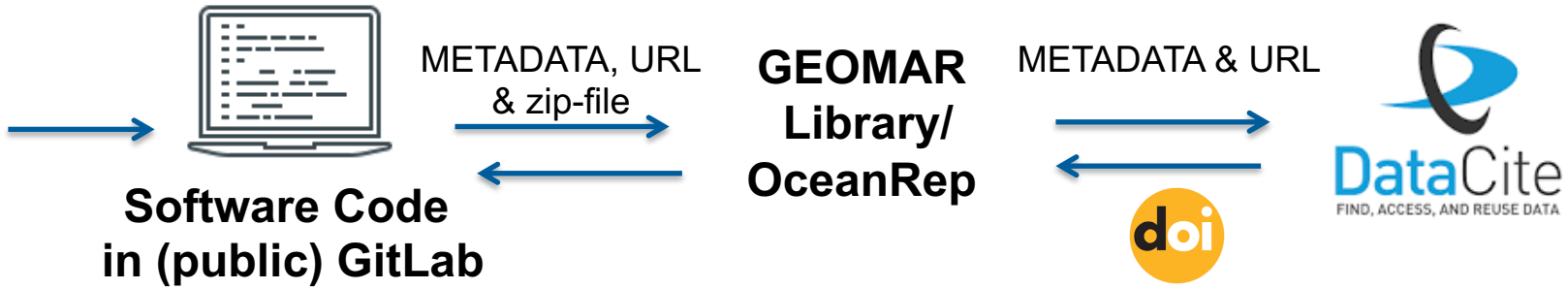
DOI-Registry at GEOMAR: Workflows



PANGAEA.

Data Publisher for Earth & Environmental Science

Scientists



Software Code in (public) GitLab repository

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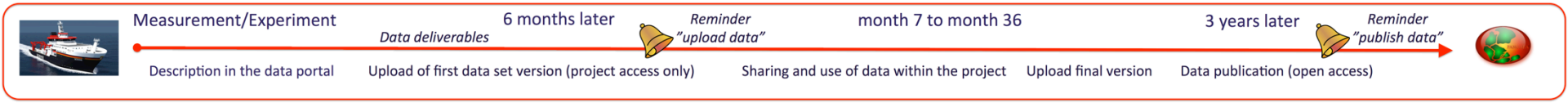
Example: Experiment workflow

Data curation process



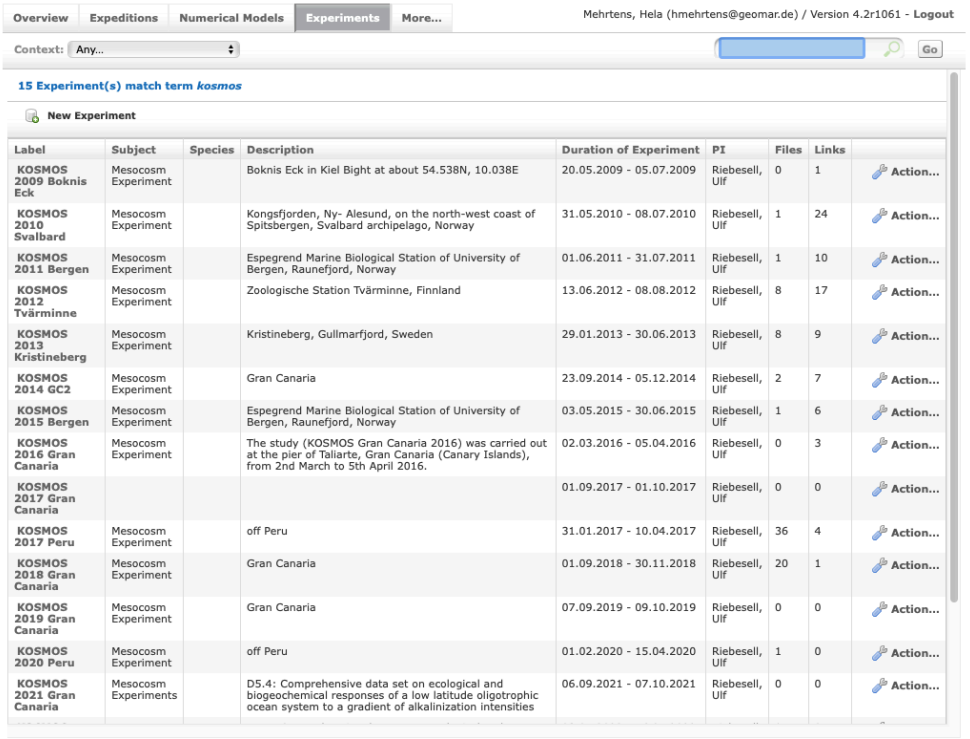
- Cruise planning involves DMP components
- Data reminder in OSIS used for several projects
- Deliverable done: data are openly available as data publications with DOI at PANGAEA

EXAMPLE I: Experiments

GEOMAR

Mesocosm experiments

- Information System used for 15 experiments (2009-2022)
- More than 130 data publications at PANGAEA



Overview | Expeditions | Numerical Models | Experiments | More...

Mehrtens, Hela (hmehrtens@geomar.de) / Version 4.2r1061 - Logout

Context: Any... Go

15 Experiment(s) match term *kosmos*

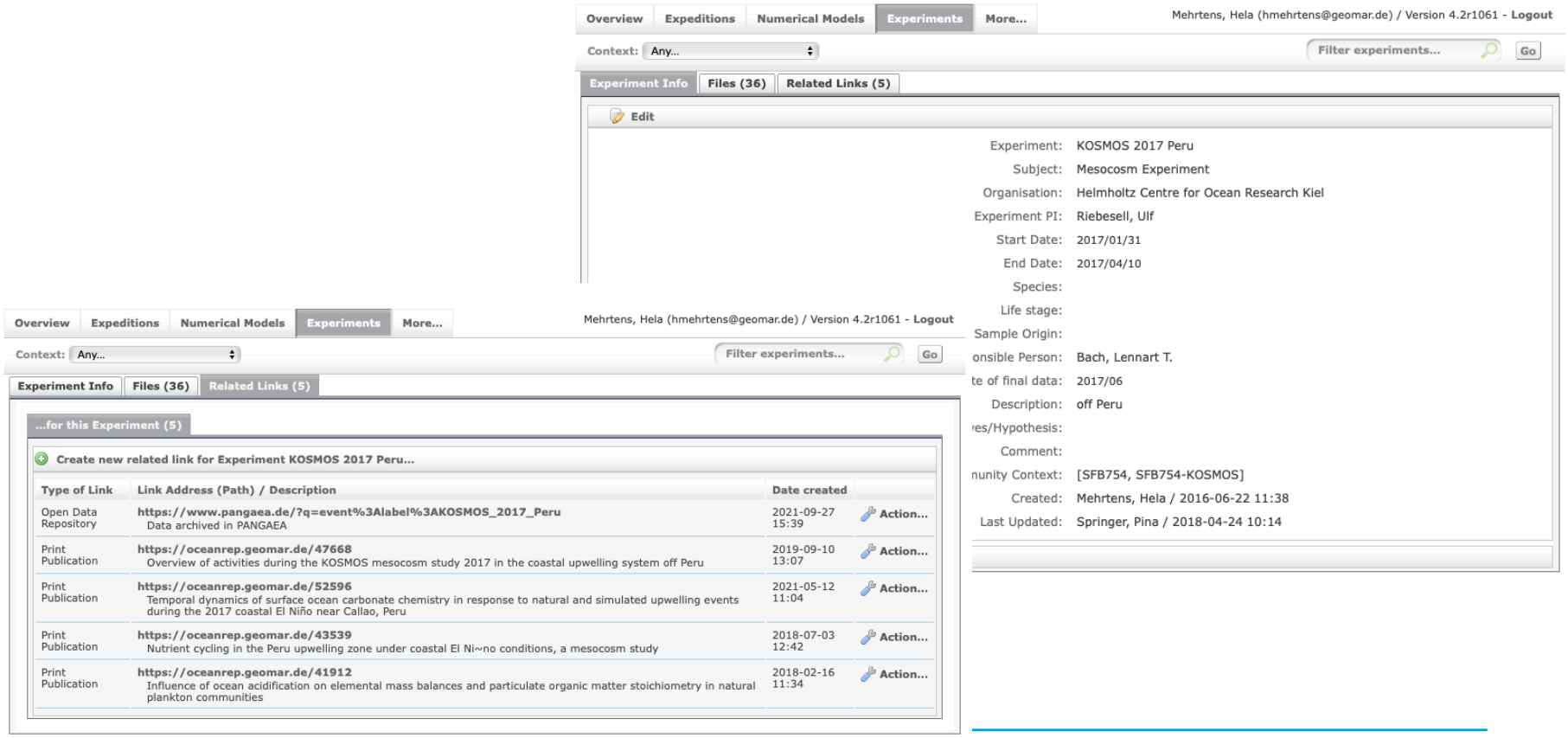
New Experiment

Label	Subject	Species	Description	Duration of Experiment	PI	Files	Links	
KOSMOS 2009 Boknis Eck	Mesocosm Experiment		Boknis Eck in Kiel Bight at about 54.538N, 10.038E	20.05.2009 - 05.07.2009	Riebesell, Ulf	0	1	Action...
KOSMOS 2010 Svalbard	Mesocosm Experiment		Kongsfjorden, Ny- Alesund, on the north-west coast of Spitsbergen, Svalbard archipelago, Norway	31.05.2010 - 08.07.2010	Riebesell, Ulf	1	24	Action...
KOSMOS 2011 Bergen	Mesocosm Experiment		Espegrend Marine Biological Station of University of Bergen, Raunefjord, Norway	01.06.2011 - 31.07.2011	Riebesell, Ulf	1	10	Action...
KOSMOS 2012 Tvärminne	Mesocosm Experiment		Zoologische Station Tvärminne, Finnland	13.06.2012 - 08.08.2012	Riebesell, Ulf	8	17	Action...
KOSMOS 2013 Kristineberg	Mesocosm Experiment		Kristineberg, Gullmarfjord, Sweden	29.01.2013 - 30.06.2013	Riebesell, Ulf	8	9	Action...
KOSMOS 2014 GC2	Mesocosm Experiment		Gran Canaria	23.09.2014 - 05.12.2014	Riebesell, Ulf	2	7	Action...
KOSMOS 2015 Bergen	Mesocosm Experiment		Espegrend Marine Biological Station of University of Bergen, Raunefjord, Norway	03.05.2015 - 30.06.2015	Riebesell, Ulf	1	6	Action...
KOSMOS 2016 Gran Canaria	Mesocosm Experiment		The study (KOSMOS Gran Canaria 2016) was carried out at the pier of Taliarte, Gran Canaria (Canary Islands), from 2nd March to 5th April 2016.	02.03.2016 - 05.04.2016	Riebesell, Ulf	0	3	Action...
KOSMOS 2017 Gran Canaria				01.09.2017 - 01.10.2017	Riebesell, Ulf	0	0	Action...
KOSMOS 2017 Peru	Mesocosm Experiment		off Peru	31.01.2017 - 10.04.2017	Riebesell, Ulf	36	4	Action...
KOSMOS 2018 Gran Canaria	Mesocosm Experiment		Gran Canaria	01.09.2018 - 30.11.2018	Riebesell, Ulf	20	1	Action...
KOSMOS 2019 Gran Canaria	Mesocosm Experiment		Gran Canaria	07.09.2019 - 09.10.2019	Riebesell, Ulf	0	0	Action...
KOSMOS 2020 Peru	Mesocosm Experiment		off Peru	01.02.2020 - 15.04.2020	Riebesell, Ulf	1	0	Action...
KOSMOS 2021 Gran Canaria	Mesocosm Experiments		D5.4: Comprehensive data set on ecological and biogeochemical responses of a low latitude oligotrophic ocean system to a gradient of alkalinization intensities	06.09.2021 - 07.10.2021	Riebesell, Ulf	0	0	Action...

EXAMPLE I: Experiments

GEOMAR

in OSIS



EXAMPLE I: Experiments

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in PANGAEA

Hela Mehrtens

PANGAEA.
Data Publisher for Earth & Environmental Science

SEARCH SUBMIT HELP ABOUT CONTACT

Citation:

Baumann, Moritz; Sswat, Michael; Ortiz Cortes, Joaquin; Hernández-Hernández, Nauzet; Baños Cerón, Isabel; Vanharanta, Mari; Heinemann, Malte (2021): KOSMOS 2018 Gran Canaria mesocosm study: water column biogeochemistry. *PANGAEA*, https://doi.pangaea.de/10.1594/PANGAEA.933090 *(dataset in review)*

Facebook Twitter Show Map Google Earth

Abstract:

The data set compiles biogeochemical water column collected during a KOSMOS mesocosm experiment carried out in the frame work of the Ocean Artificial Upwelling project. The experiment was performed in the North-East Atlantic Ocean off the coast of Gran Canaria in autumn 2018 and lasted for 39 days. In this study we investigated the effect of different intensities of artificial upwelling combined with two upwelling modes (recurring additions versus one singular addition) on POC export and its potential transfer efficiency to depth. The data set includes the amounts of surface water that were exchanged with nutrient-rich deep water (from ~300 m depth), primary production and chlorophyll a, elemental composition of suspended particulate matter (POC, PON, C:N) and prokaryotic heterotrophic production.

Keyword(s):

artificial upwelling; carbon sequestration; export flux; mesocosm study; particle properties; remineralization depth; remineralization rate; sinking velocity

Supplement to:

Baumann, Moritz; Taucher, Jan; Paul, Allanah; Heinemann, Malte; Vanharanta, Mari; Bach, Lennart Thomas; Spilling, Kristian; Ortiz Cortes, Joaquin; Arístegui, Javier; Hernández-Hernández, Nauzet; Riebesell, Ulf (in prep.): Effect of different rates and modes of artificial upwelling on particle flux and potential POC deep export.

Project(s):

Ocean Artificial Upwelling (Ocean-artUp)

EXAMPLE I: Experiments

GEOMAR

Event(s):

KOSMOS_2018_Mesocosm-M1 * *Latitude:* 27.927880 * *Longitude:* -15.364330 * *Date/Time Start:* 2018-11-06T00:00:00 * *Date/Time End:* 2018-12-14T00:00:00 * *Location:* Canarias Sea * *Campaign:* KOSMOS_2018 (KOSMOS Gran Canaria) * *Method/Device:* Mesocosm experiment (MESO)

KOSMOS_2018_Mesocosm-M2 * *Latitude:* 27.927880 * *Longitude:* -15.364330 * *Date/Time Start:* 2018-11-06T00:00:00 * *Date/Time End:* 2018-12-14T00:00:00 * *Location:* Canarias Sea * *Campaign:* KOSMOS_2018 (KOSMOS Gran Canaria) * *Method/Device:* Mesocosm experiment (MESO)

KOSMOS_2018_Mesocosm-M3 * *Latitude:* 27.927880 * *Longitude:* -15.364330 * *Date/Time Start:* 2018-11-06T00:00:00 * *Date/Time End:* 2018-12-14T00:00:00 * *Location:* Canarias Sea * *Campaign:* KOSMOS_2018 (KOSMOS Gran Canaria) * *Method/Device:* Mesocosm experiment (MESO)

Show more...

Parameter(s):

#	Name	Short Name	Unit	Principal Investigator	Method/Device	Comment
1	Event label	Event		Baumann, Moritz		
2	DATE/TIME	Date/Time		Baumann, Moritz		Geocode
3	Experiment day	Exp day	day	Baumann, Moritz		
4	Mesocosm label	Meso label		Baumann, Moritz		
5	Treatment	Treat		Baumann, Moritz		
6	Treatment	Treat		Baumann, Moritz		
7	Deep water exchange, total	Deep water exch	m^3	Sswat, Michael		
8	DEPTH, water, experiment	Depth water exp	m	Baumann, Moritz		Geocode – top
9	DEPTH, water, experiment	Depth water exp	m	Baumann, Moritz		Geocode – bottom
10	Primary production	PP	µmol/l/day	Ortiz Cortes, Joaquin		
11	Primary production, cumulative	PP cum	µmol/l	Ortiz Cortes, Joaquin		
12	Chlorophyll a	Chl a	µg/l	Ortiz Cortes, Joaquin		
13	Carbon, organic, particulate	POC	µmol/l	Baumann, Moritz		
14	Nitrogen, organic, particulate	PON	µmol/l	Baumann, Moritz		
15	Carbon/Nitrogen ratio	C/N	mol/mol	Baumann, Moritz		
16	Prokaryotic heterotrophic production	P het prod	µmol/l/day	Baños Cerón, Isabel		

Chl a [µg/l]

Status: *Curation Level:* Enhanced curation (CurationLevelC)

Size: 2094 data points

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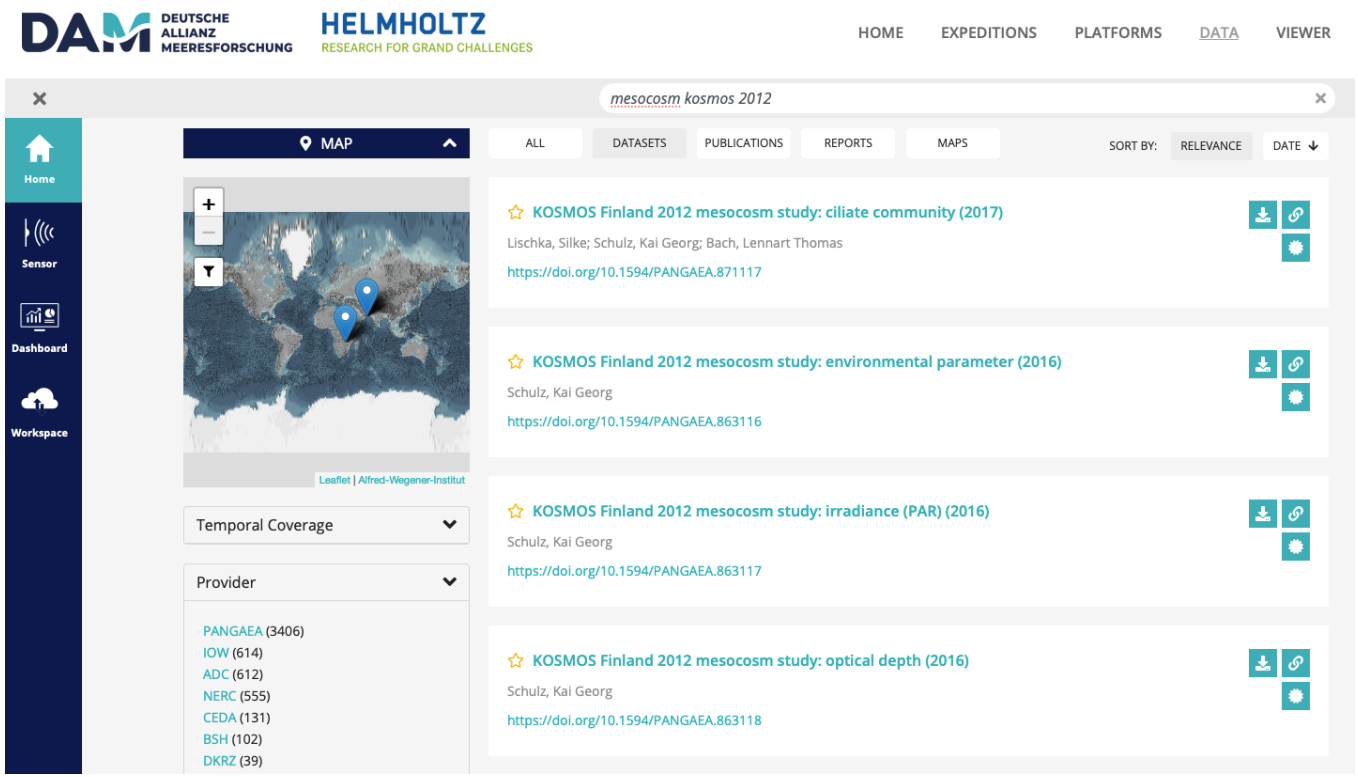
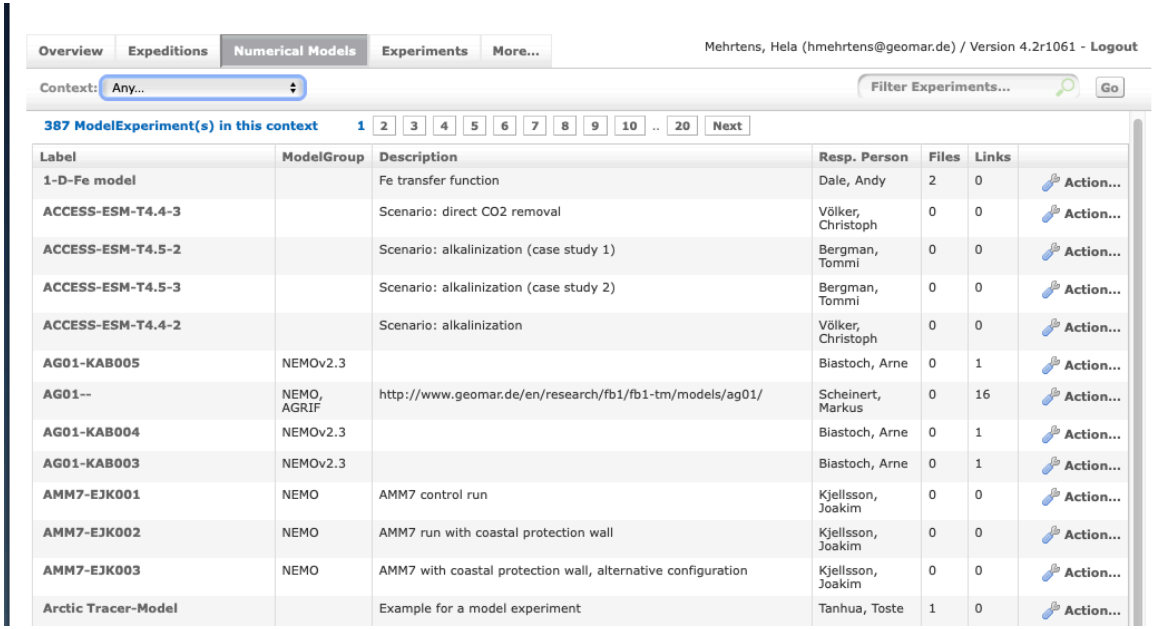
Further Access: DAM Portal



GEOMAR

Example: Model results

- Information System contains >300 descriptions
- Links to articles and storage



Overview | Expeditions | Numerical Models | Experiments | More... — Mehrtens, Hela (hmehrtens@geomar.de) / Version 4.2r1061 - Logout

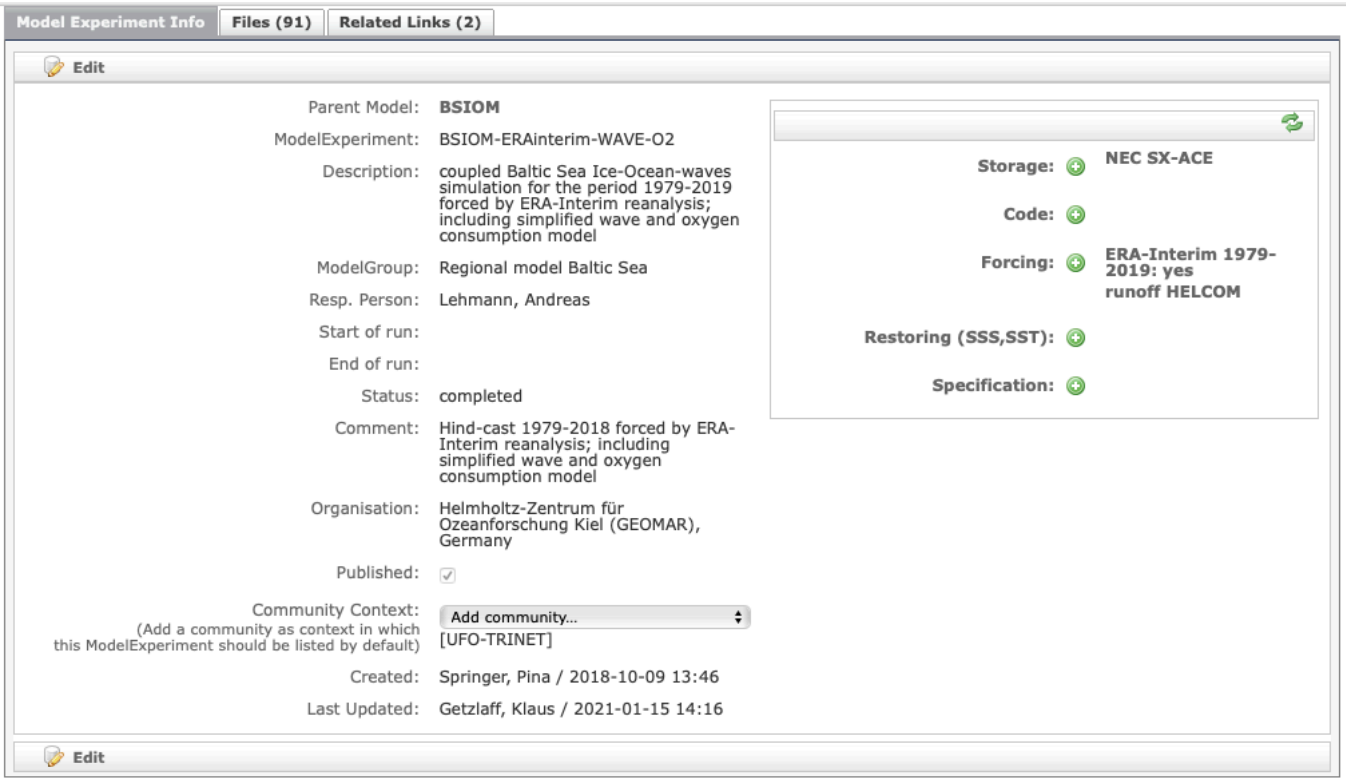
Context: Any... — Filter Experiments... — Go

387 ModelExperiment(s) in this context — 1 2 3 4 5 6 7 8 9 10 .. 20 Next

Label	ModelGroup	Description	Resp. Person	Files	Links	
1-D-Fe model		Fe transfer function	Dale, Andy	2	0	Action...
ACCESS-ESM-T4.4-3		Scenario: direct CO2 removal	Völker, Christoph	0	0	Action...
ACCESS-ESM-T4.5-2		Scenario: alkalinization (case study 1)	Bergman, Tommi	0	0	Action...
ACCESS-ESM-T4.5-3		Scenario: alkalinization (case study 2)	Bergman, Tommi	0	0	Action...
ACCESS-ESM-T4.4-2		Scenario: alkalinization	Völker, Christoph	0	0	Action...
AG01-KAB005	NEMOv2.3		Biastoch, Arne	0	1	Action...
AG01--	NEMO, AGRIF	http://www.geomar.de/en/research/fb1/fb1-tm/models/ag01/	Scheinert, Markus	0	16	Action...
AG01-KAB004	NEMOv2.3		Biastoch, Arne	0	1	Action...
AG01-KAB003	NEMOv2.3		Biastoch, Arne	0	1	Action...
AMM7-EJK001	NEMO	AMM7 control run	Kjellsson, Joakim	0	0	Action...
AMM7-EJK002	NEMO	AMM7 run with coastal protection wall	Kjellsson, Joakim	0	0	Action...
AMM7-EJK003	NEMO	AMM7 with coastal protection wall, alternative configuration	Kjellsson, Joakim	0	0	Action...
Arctic Tracer-Model		Example for a model experiment	Tanhua, Toste	1	0	Action...

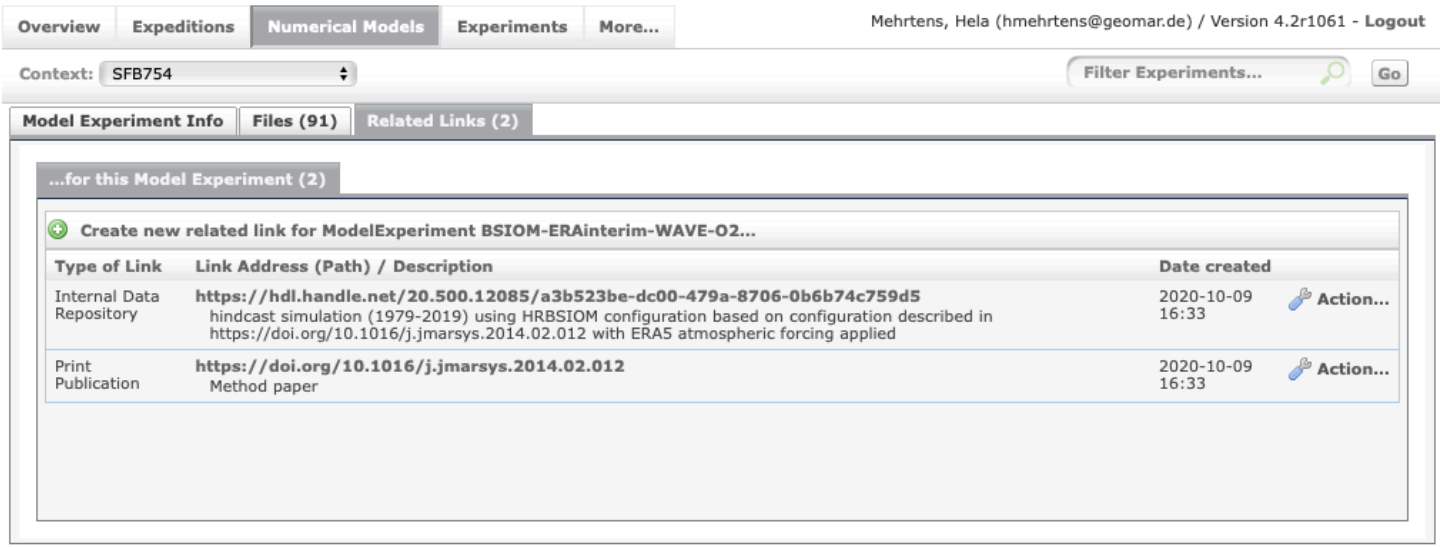
Example II: Model results

In OSIS



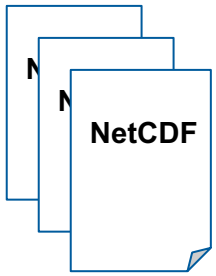
Example II: Model results

In OSIS

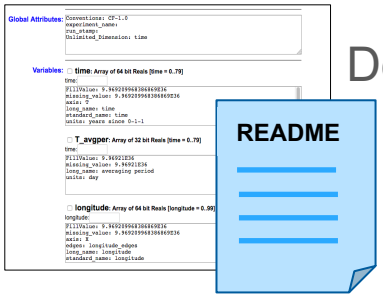


Example II: Workflow

1. Preparation of model data for publication by data owner



dataset organisation,
file formatting,
checksums



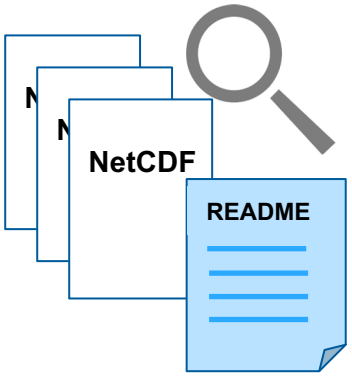
Metadata &
Documentation

2. Dataset submission to the data management team

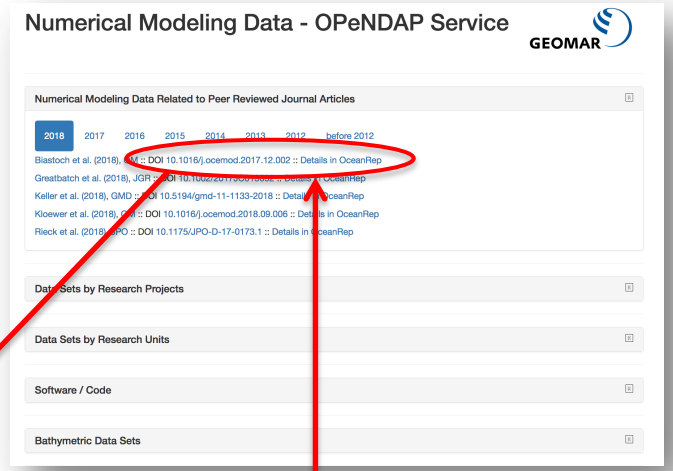
data transfer via
GEOMAR cloud or
(S)FTP server
&
data submission
information to DM
via web form

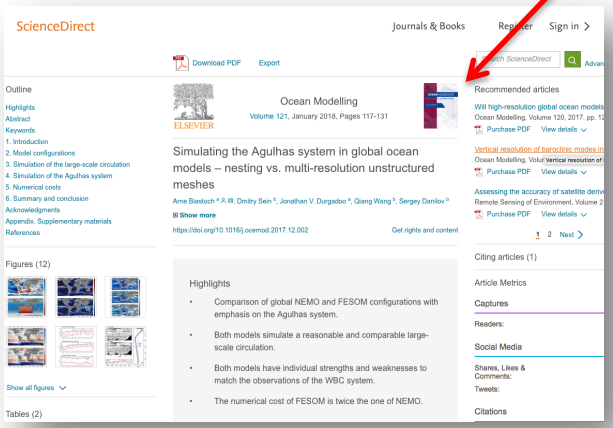
Example II: Workflow

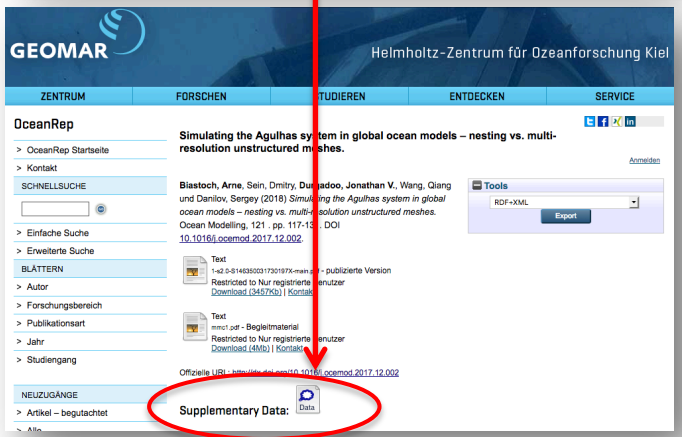
3. Data publication on data.geomar.de (OPeNDAP Service)



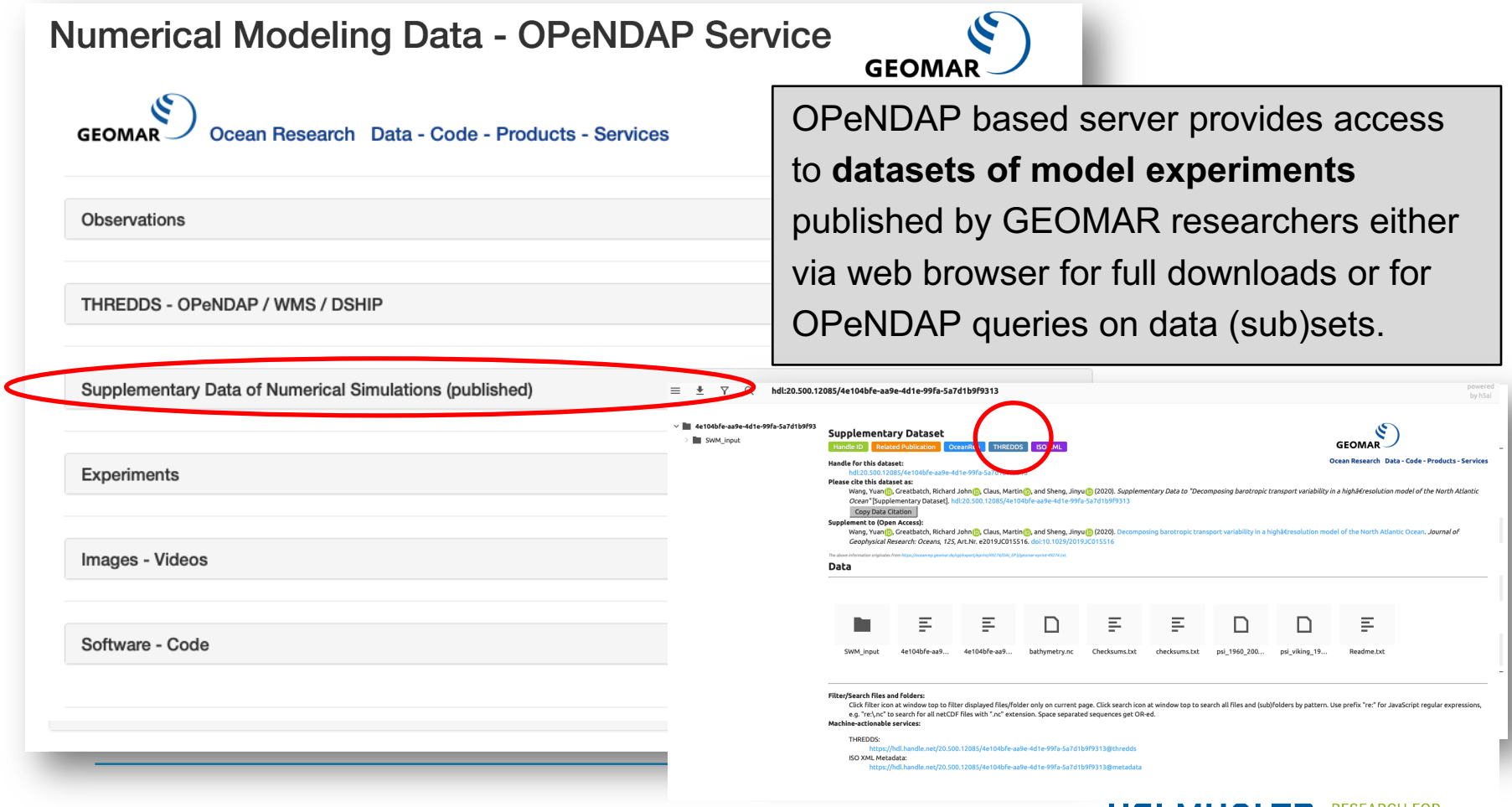
data integrity check
&
data dissemination
via THREDDS-Server
by data manager







Example II: Access



OPeNDAP based server provides access to **datasets of model experiments** published by GEOMAR researchers either via web browser for full downloads or for OPeNDAP queries on data (sub)sets.

Example II: Access

GEOMAR

GEOMAR THREDDS Server

THREDDS Data Server

Catalog https://data.geomar.de/thredds/20.500.12085/4e104bfe-aa9e-4d1e-99fa-5a7d1b9f9313/catalog.html

Dataset: Supplementary Data to "Decomposing barotropic transport variability in a model of the North Atlantic Ocean" (hdl:20.500.12085/4e104bfe-aa9e-4d1e-99fa-5a7d1b9f9313)/psi_viking_1960_2009.nc

- *Data format:* netCDF
- *Data size:* 252.5 Mbytes
- *Data type:* GRID
- *Naming Authority:* de.geomar
- *ID:* 20.500.12085/4e104bfe-aa9e-4d1e-99fa-5a7d1b9f9313/psi_viking_1960_2009.nc

Documentation:

- Decomposing barotropic transport variability in a highâresolution model of the North Atlantic Ocean (doi:10.1029/2019JC015516)
- Decomposing barotropic transport variability in a highâresolution model of the North Atlantic Ocean (http://oceanrep.geomar.de/49274)
- **rights:** cc_by_4.0
- **summary:** A method using a linear shallow water model is presented for decomposing the temporal variability of the barotropic streamfunction in a high based in the verticallyâaveraged momentum equations and is applied to the time series of annual mean streamfunction from the model configuration V An important result is the role played by the nonlinear advection terms in VIKING20 for driving transport. The method is illustrated by examining how th recirculation region responds to the winter North Atlantic Oscillation (NAO). While no statistically significant response is found in the year overlapping w tendency for the Gulf Stream transport to increase as the NAO becomes more positive. This becomes significant in lead years 1 and 2 when the mean momentum flux (EMF) contributions, associated with nonlinear momentum advection, dominate. Only after 2 years, does the potential energy (PE) tern play a role and it is only after 5 years that the transport dependence on the NAO ceases to be significant. It is also shown that the PE contribution to th memory of up to 5 years in the Labrador and Irminger Seas. However, it is only around the northern rim of these seas that VIKING20 and the transport This is due to masking by the MFA and EMF contributions.

Access:

1. **OPENDAP:** /thredds/dodsC/20.500.12085/4e104bfe-aa9e-4d1e-99fa-5a7d1b9f9313/psi_viking_1960_2009.nc
2. **HTTPServer:** /thredds/fileServer/20.500.12085/4e104bfe-aa9e-4d1e-99fa-5a7d1b9f9313/psi_viking_1960_2009.nc
3. **WCS:** /thredds/wcs/20.500.12085/4e104bfe-aa9e-4d1e-99fa-5a7d1b9f9313/psi_viking_1960_2009.nc
4. **WMS:** /thredds/wms/20.500.12085/4e104bfe-aa9e-4d1e-99fa-5a7d1b9f9313/psi_viking_1960_2009.nc
5. **NetcdfSubset:** /thredds/ncss/20.500.12085/4e104bfe-aa9e-4d1e-99fa-5a7d1b9f9313/psi_viking_1960_2009.nc
6. **NCML:** /thredds/ncml/20.500.12085/4e104bfe-aa9e-4d1e-99fa-5a7d1b9f9313/psi_viking_1960_2009.nc
7. **UDDC:** /thredds/uddc/20.500.12085/4e104bfe-aa9e-4d1e-99fa-5a7d1b9f9313/psi_viking_1960_2009.nc
8. **ISO:** /thredds/iso/20.500.12085/4e104bfe-aa9e-4d1e-99fa-5a7d1b9f9313/psi_viking_1960_2009.nc

Keywords:

- north atlantic
- transport variability
- high resolution model

NetCDF Attribute Convention for Dataset Discovery Report

The Unidata Attribute Convention for Data Discovery provides recommendations for netCDF attributes that can be added to netCDF files to facilitate discovery of those files using standard metadata searches. This tool tests conformance with those recommendations using this stylesheet. More Information on Convention and Tool.

Title: Supplementary Data to "Decomposing barotropic transport variability in a highâ€resolution model of the North Atlantic Ocean"

Total Score: 31/46

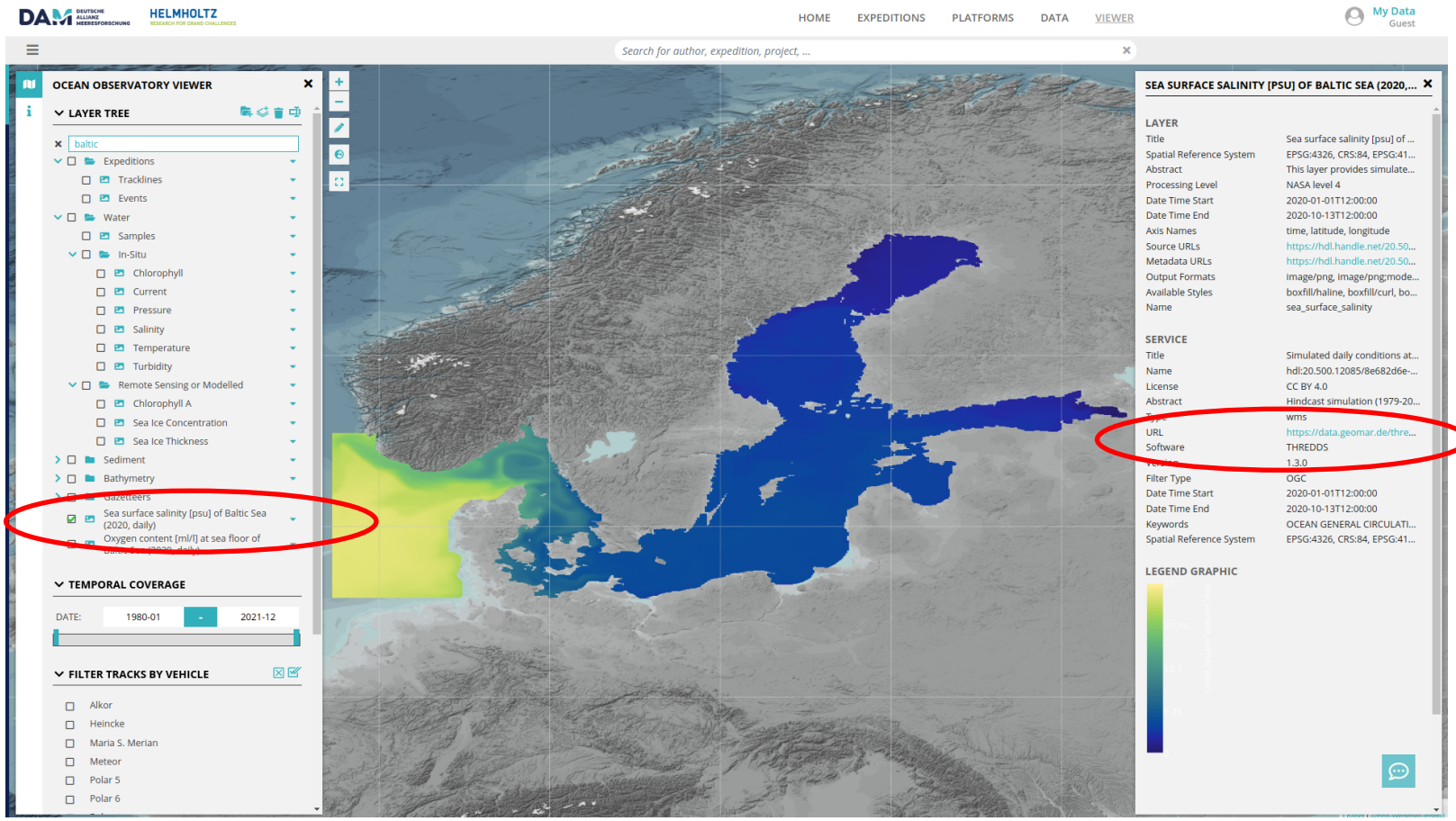
General File Characteristics

Number of Global Attributes	19
Number of Variables	5
Number of Variable Attributes	12
Number of Standard Names	0
Number of Services	4

Spiral	None	1-33%	34-66%	67-99%	All
Total				X	
Identification					X
Text Search				X	
Extent Search			X		
Other Extent Information			X		
Creator Search				X	
Contributor Search					X
Publisher Search					X
Other Attributes				X	

Identification | Text Search | Extent Search | Other Extent Information | Creator Search | Contributor Search | Publisher Search | Other Attributes

Example II: Further Access



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Samples (in progress)

- Sample management systems for geosamples and biosamples
- Connection to OSIS for field samples as sediment cores and biological measurements and experiments
- Connection to Nagoya Protocol information necessary
- Metadata export for DAM Viewer

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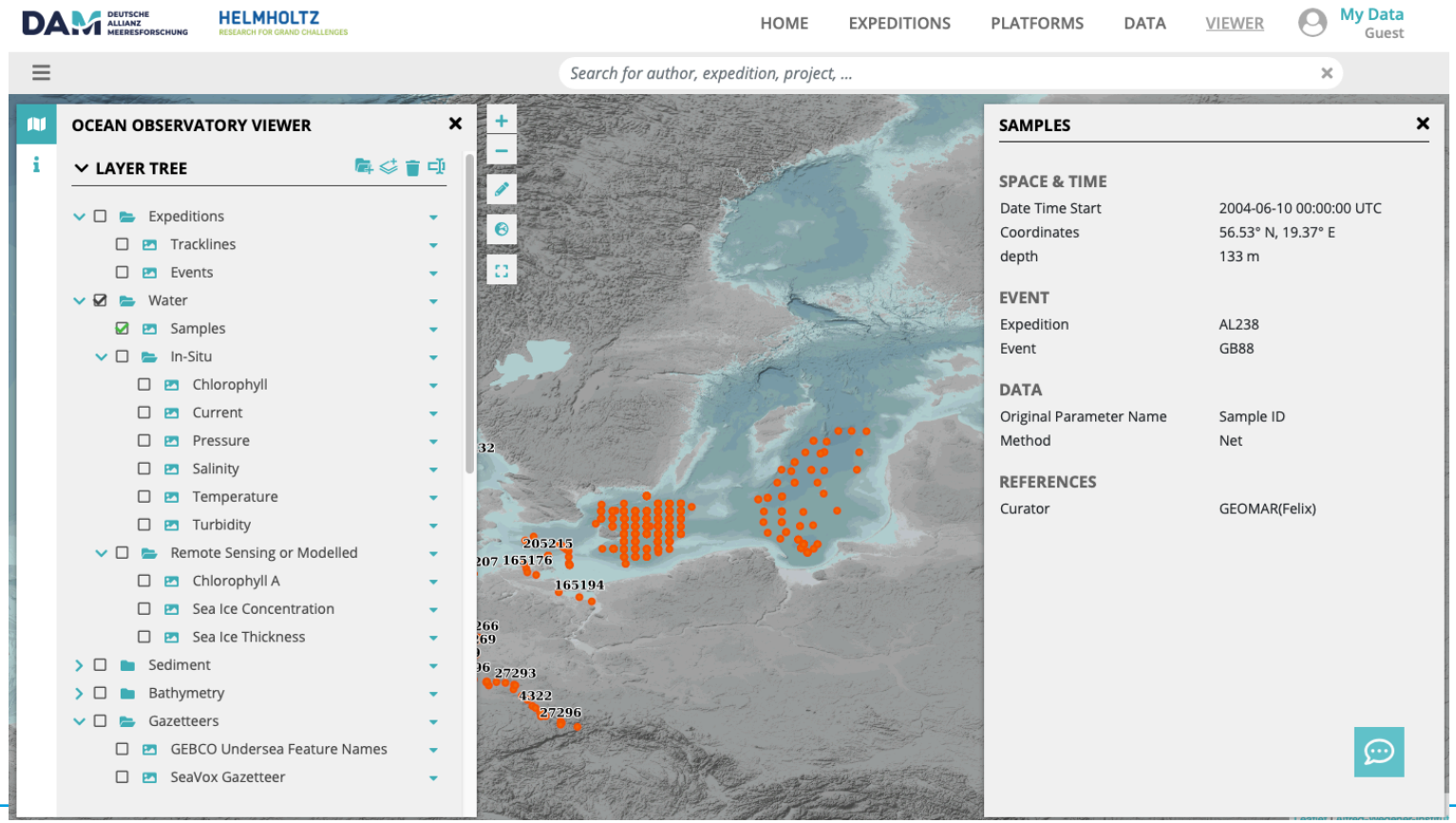
Access: DAM Portal



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Questions and comments?

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