DAR DEUTSCHE ALLIANZ MEERESFORSCHUNG

KüNO Workshop 'Data sharing in marine research

Data management workflows for experiment and model data

Hela Mehrtens GEOMAR Helmholtz Centre for Ocean Research Kiel, Germany





INTRODUCTION



Agenda

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







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



INTRODUCTION

KüNO Workshop 'Data sharing in marine research', 29.9.2021 **HELMHOLTZ** RESEARCH FOR GRAND CHALLENGES



Central data management workflow @ GEOMAR

- 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)



INTRODUCTION



- 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







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)



KüNO Workshop 'Data sharing in marine research', 29.9.2021

HELMHOL

TOOLS



2. OSIS

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 Deliverable	s		
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

Files		
File Title	Uploaded	Creator
pangaea.txt for SO2 35	2021/09/20	Mehrtens, Hela
MSM80_FlowCytome try_062021.xlsx for MSM80	2021/09/15	Fernandez-Mendez, Mar
MSM80_Photosynthe ticPigments_062021 .xlsx for MSM80	2021/09/15	Fernandez-Mendez, Mar

Type Description Linked to DSHIP DSHIP Sensor data available at GEOMAR Leg: ALSI	
DSHIP DSHIP Sensor data available at GEOMAR Leg: AL5	
	52
URL Map with cruise track Leg: AL5	53
URL Map with cruise track Leg: AL5	52
Print Publication Weekly reports Leg: M17	6
URL AL561 Weekly report Cruise: A	L561
DSHIP DSHIP Sensor data available at GEOMAR Leg: ALS	51
URL Map with cruise track Leg: M17	6
URL Map with cruise track Leg: AL5	61
DSHIP DSHIP Sensor data available at GEOMAR Leg: ALS	60
DSHIP DSHIP Sensor data available at GEOMAR Leg: AL5:	59b

	Expeditions	Go
Expeditions		
Label	Departure - Return	Chief-Scientist
IODP Exp.396	2021/08/06 - 2021/10/06	Berndt, Christian
S0293	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-K KG36107B	2021/06/17	Getzlaff, Klaus
NorESM-T4.4-3	2021/03/08	Schwinger, Jörg
NorESM-T4.4-2	2021/03/08	Schwinger, Jörg

Exj	periments	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

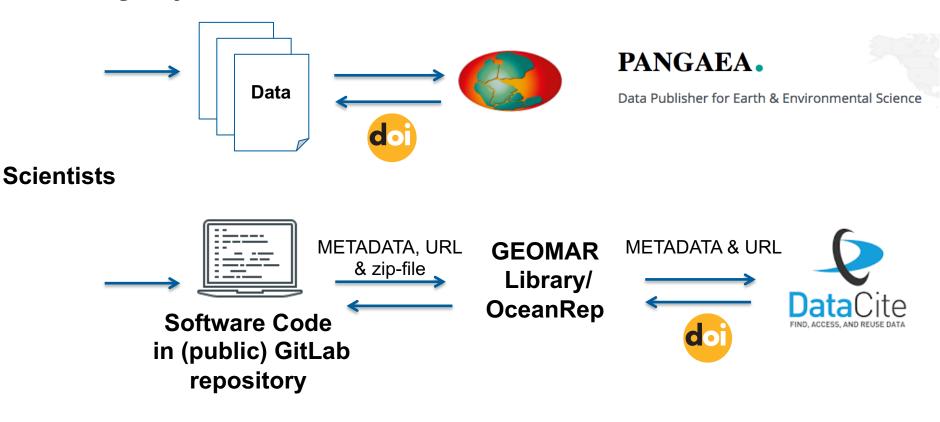






3. Persistent identifier

DOI-Registry at GEOMAR: Workflows



RESEARCH FOR GRAND CHALLENGES

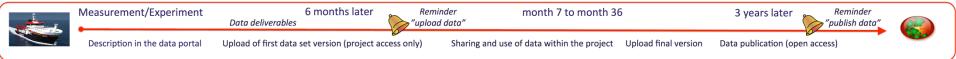
HELMHOLTZ





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







HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

Mesocosm experiments

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

Context: Any		\$						Go
15 Experimer	nt(s) match ter	m <i>kosmos</i>						
New Exp	eriment							
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	de 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.





in OSIS

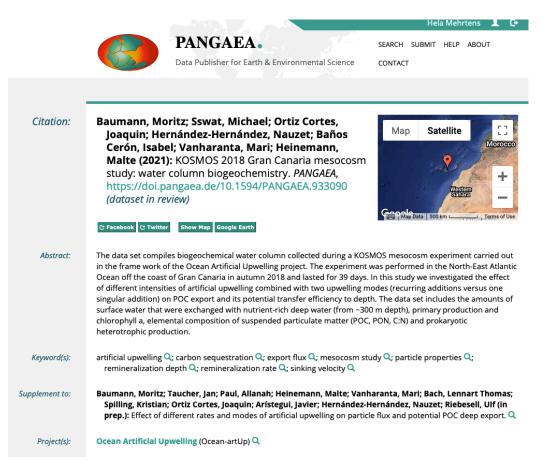
						Overview	Expeditions	Numerical Mode	els Experime	nts Mor	e	Mehrtens, Hela (hmehrte	ns@geomar.de) / Version 4	.2r1061 -	Logout
						Context:	Any	\$,				Filter experiments	0	Go
						Experime	nt Info Files ((36) Related Lir	nks (5)						
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											Subject:	Mesocosm Experiment			
										Orga	inisation:	Helmholtz Centre for Ocean Research k	liel		
										Experi	iment PI:	Riebesell, Ulf			
										St	art Date:	2017/01/31			
										E	nd Date:	2017/04/10			
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Co	ntext: Any	\$					Filt	ter experiments	Go	onsible	e Person:	Bach, Lennart T.			
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5												off Peru			
H	for this Ex	periment (5)									pothesis:				
	Create n	ew related link for Experiment H	COSMOS 2017 Peru.								omment:				
	Type of Lin	k Link Address (Path) / Des	cription					Date created		· · ·	Context:	[SFB754, SFB754-KOSMOS] Mehrtens, Hela / 2016-06-22 11:38			
	Open Data Repository	https://www.pangaea.de, Data archived in PANGAEA	/?q=event%3Alabel	%3AKO	SMOS_2017_Peru			2021-09-27 15:39	🤌 Action		Updated:				
	Print Publication	https://oceanrep.geomar. Overview of activities during		sm stud	y 2017 in the coastal u	upwelling syste	em off Peru	2019-09-10 13:07	🥜 Action						
	Print Publication	https://oceanrep.geomar. Temporal dynamics of surfa during the 2017 coastal El N	ce ocean carbonate ch	emistry i	in response to natural	and simulated	upwelling events	2021-05-12 11:04	🌽 Action						
	Print Publication	https://oceanrep.geomar. Nutrient cycling in the Peru		coastal E	I Ni~no conditions, a	mesocosm stu	dy	2018-07-03 12:42	🌽 Action						
	Print Publication	https://oceanrep.geomar. Influence of ocean acidificat plankton communities		s balance	s and particulate orga	nic matter stoi	ichiometry in natu	2018-02-16 ral 11:34	🎤 Action						







in PANGAEA







GEOMAR

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

	KOSMOS_2018_Mesocosm-M2 Q 06T00:00:00 * Date/Time End: 20 (KOSMOS Gran Canaria) Q * Met	18-12-14T00:00):00 * <i>Lo</i>	cation: Canarias Sea	Q * Campaig	
	KOSMOS_2018_Mesocosm-M3 Q 06T00:00:00 * Date/Time End: 20 (KOSMOS Gran Canaria) Q * Met	18-12-14T00:00):00 * <i>Lo</i>	<i>cation:</i> Canarias Sea	Q * Campaig	
Parameter(s):	show more	Short Name	Unit	Principal Investigator	Method/Device	Comment
r urumeter(s).	1 Event label Q	Event	onic	Baumann, Moritz Q	Wethou/Device	comment
	2 DATE/TIME Q	Date/Time		Baumann, Moritz Q		Geocode
	3 Experiment day Q	Exp day	day	Baumann, Moritz Q		debeude
	4 Mesocosm label Q	Meso label	,	Baumann, Moritz Q		
	5 Treatment Q	Treat		Baumann, Moritz Q		
	6 Treatment Q	Treat		Baumann, Moritz Q		
	7 Deep water exchange, total Q	Deep water exch	m ³	Sswat, Michael Q		
	8 DEPTH, water, experiment Q	Depth water exp	m	Baumann, Moritz Q		Geocode – top
	9 DEPTH, water, experiment Q	Depth water exp	m	Baumann, Moritz Q		Geocode - bott
	10 Primary production Q	PP	µmol/l/day	Ortiz Cortes, Joaquin Q		
	11 Primary production, cumulative Q	PP cum	µmol/l	Ortiz Cortes, Joaquin Q		
	12 Chlorophyll a Q	Chl a	μg/1	Ortiz Cortes, Joaquin Q		
	13 Carbon, organic, particulate Q	POC	µmol/l	Baumann, Moritz Q	Chl a [µg/l]	
	14 Nitrogen, organic, particulate Q	PON	µmol/l	Baumann, Moritz Q	Chi a [µg/i]	
	15 Carbon/Nitrogen ratio Q	C/N	mol/mol	Baumann, Moritz Q		
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EXAMPLE I: Experiments

Example I: Experiments



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Further Access: DAM Portal

DA.	DEUTSCHE ALLIANZ MEERESFORSCHUNG	HELMHOLTZ RESEARCH FOR GRAND CHAI				HOME	EXPEDITIONS	PLATFORMS	DATA	VIEWER
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Home	\$	МАР 🔨	ALL	DATASETS	PUBLICATIONS	REPORTS	MAPS	SORT BY:	RELEVANCE	DATE 🗸
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	PANGAEA (3406) IOW (614) ADC (612) NERC (555) CEDA (131) BSH (102) DKRZ (39)		Schulz, Kai Ge		2 mesocosm stu	dy: optical depth	ı (2016)			*





Example II: Model results



Example: Model results

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

Overview Expeditions	Numerical Models	Experiments More	Mehrtens, Hela (h	mehrtens@geom	ar.de) /	Version 4	.2r1061 - Logo
Context: Any	÷			Filter E	xperim	ents	Go
387 ModelExperiment(s) in t	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 stud		Bergman, Tommi	0	0	🌽 Action
ACCESS-ESM-T4.5-3		Scenario: alkalinization (case stud	iy 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/researc		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		Kjellsson, Joakim	0	0	🌽 Action
AMM7-EJK003	NEMO	AMM7 with coastal protection wall		Kjellsson, Joakim	0	0	🎤 Action
Arctic Tracer-Model		Example for a model experiment		Tanhua, Toste	1	0	🎤 Action





Example II: Model results



In OSIS

🌽 Edit			
Parent Model:	BSIOM		
ModelExperiment:	BSIOM-ERAinterim-WAVE-O2		
Description:	coupled Baltic Sea Ice-Ocean-waves simulation for the period 1979-2019 forced by ERA-Interim reanalysis; including simplified wave and oxygen consumption model	Storage: 《 Code: 《)
ModelGroup:	Regional model Baltic Sea	Forcing: (ERA-Interim 1979- 2019: yes
Resp. Person:	Lehmann, Andreas		runoff HELCOM
Start of run:		Restoring (SSS,SST): 🔇	
End of run:			
Status:	completed	Specification: (2
Comment:	Hind-cast 1979-2018 forced by ERA- Interim reanalysis; including simplified wave and oxygen consumption model		
Organisation:	Helmholtz-Zentrum für Ozeanforschung Kiel (GEOMAR), Germany		
Published:	\checkmark		
Community Context: (Add a community as context in which this ModelExperiment should be listed by default)	Add community \$ [UFO-TRINET]		
Created:	Springer, Pina / 2018-10-09 13:46		
Last Updated:	Getzlaff, Klaus / 2021-01-15 14:16		





Example II: Model results



+ + + + + + + +

In OSIS

Model Experiment Info Files (91) Related Links (2) for this Model Experiment (2) for this Model Experiment (2) Image: Create new related link for ModelExperiment BSIOM-ERAinterim-WAVE-02 Date created Type of Link Link Address (Path) / Description Date created Internal Data https://hdl.handle.net/20.500.12085/a3b523be-dc00-479a-8706-0b6b74c759d5 2020-10-09 hindcast simulation (1979-2019) using HRBSIOM configuration based on configuration described in https://doi.org/10.1016/j.jmarsys.2014.02.012 with ERA5 atmospheric forcing applied 2020-10-09	Index Provided Experiment Info Files (91) Related Links (2) Image: Second S	verview Expe	ditions Numerical Models	Experiments More	Mehrtens, Hela (hmehrtens@geomar.de) / Version 4.2r1061 - Logou
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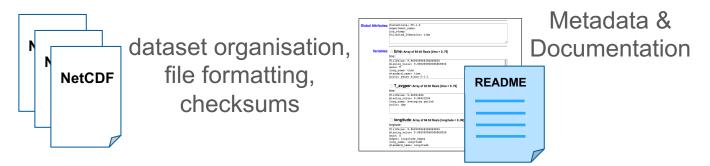




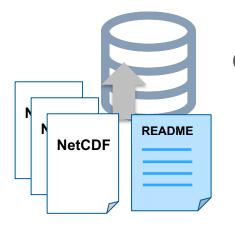


Example II: Workflow

1. Preparation of model data for publication by data owner



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

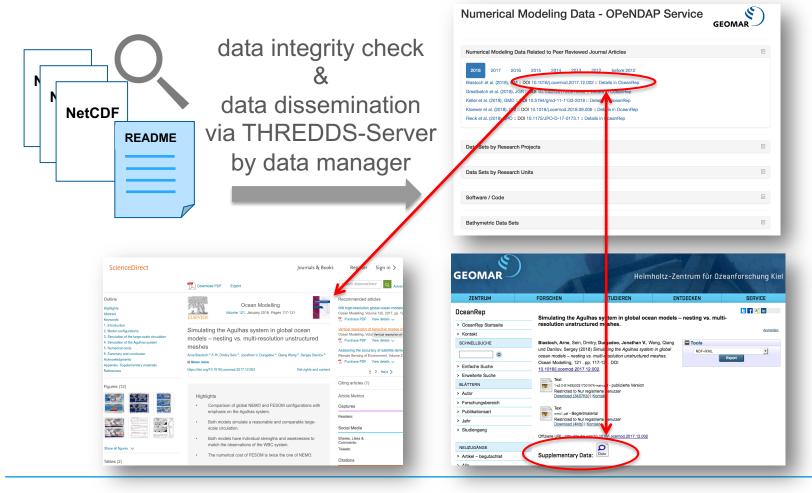
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ec -	RESEARCH DATA	TUTORIALS	SIGN UP	PROJECTS	READ MORE	CONTACT US		_
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HELMHOLTZ RESEARCH FOR GRAND CHALLENGES



Example II: Workflow

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

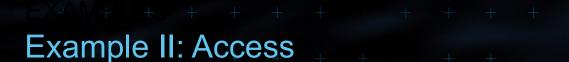






Example II: Access + + + + +

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Images - Videos		The above information originates Data	'ren https://oceanep.geamar.de/	gifexport/eprint/19274/CM_EP3/g	peanar-eprixe-49274.txt.						
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Software - Code		SWM_input	4e104bfe-aa9	4e104bfe-aa9	bathymetry.nc	Checksums.txt	checksums.txt	psi_1960_200	psi_viking_19	Readme.txt	
		Filter/Search files a Click filter icor e.g. "re:\nc" to Machine-actionable	at window top to fill search for all netCD	er displayed files/fold Files with ".nc" exten	ler only on current p ision. Space separate	age. Click search icor ed sequences get OR	at window top to s ed.	earch all files and (su	b)folders by pattern.	Use prefix "re:" for JavaScript reg	gular expressions,
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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 Mbvtes
- 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 higharesolution 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 verticallyaaveraged momentum equations and is applied to the time series of annual mean streamfunction from the model configuration VI An important result is the role played by the nonlinear advection terms in VIKING20 for driving transport. The method is illustrated by examining how the 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) term 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 the 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
- WCS: /thredds/wcs/20.500.12085/4e104bfe-aa9e-4d1e-99fa-5a7d1b9f9313/psi_viking_1960_2009.nc
 WMS: /thredds/wms/20.500.12085/4e104bfe-aa9e-4d1e-99fa-5a7d1b9f9313/psi_viking_1960_2009.nc
- 5. NetcdfSubset: /thredds/ness/20_500_420054
- 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

GEOMAR

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 Number of Variable Attributes 12 Number of Standard Names 0 Number of Services

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

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



Example II: Further Access

		Search for author, expedition, project,		×		
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HELMHOLTZ RESEARCH FOR GRAND CHALLENGES



Samples (in progress)

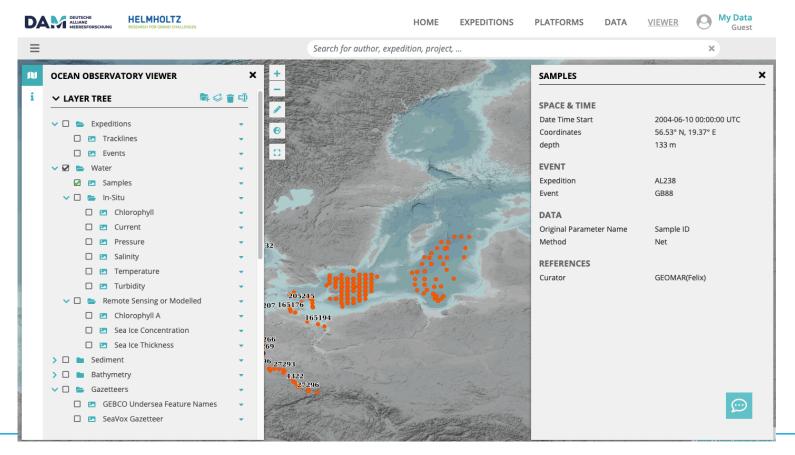
- Sample management systems for geosamples and biosamples
- Connection to OSIS for field samples as sediment cores and biological measurements and experiments
- Connection to Nagoya Protocol information necessary
- Metadata export for DAM Viewer



Example III: Samples



Access: DAM Portal



DAM

KüNO Workshop 'Data sharing in marine research', 29.9.2021

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Questions and comments?

Data Management Team @GEOMAR

datamanagement@geomar.de



