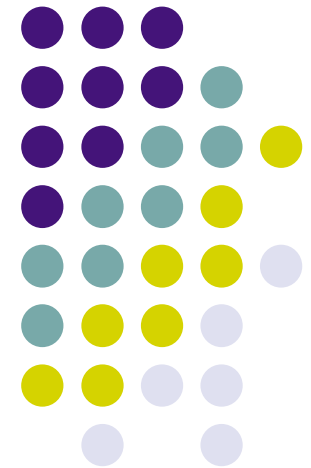


# Every bit counts

Data management and data publication in  
the earth sciences

Jens Klump *et al.*

International Data Exchange Workshop  
Kiel, 10 May 2007





# Autors

- Jens Klump<sup>1</sup>, Robert Huber<sup>2</sup>, Jan Brase<sup>3</sup>, Michael Diepenbroek<sup>2</sup>, Hannes Grobe<sup>4</sup>, Beate Hildenbrand<sup>5</sup>, Heinke Höck<sup>6</sup>, Michael Lautenschlager<sup>6</sup>, Uwe Schindler<sup>2</sup>, Irina Sens<sup>3</sup> and Joachim Wächter<sup>1</sup>



GFZ Potsdam (proposed WDC-TERRA)



WDC-MARE, Univ. Bremen



TIB Hannover (Nat. Lib. Sci. & Tech. Germany)



WDC-MARE, AWI Bremerhaven



WDC-RSAT, DLR-DFD Oberpfaffenhofen



WDC-Climate, MPI-MET Hamburg

# Data publication today



20 *B. Heim et al. / Global and Planetary Change 46 (2005) 9–27*

**Table 6**  
Overview on accuracies of chl-*a* algorithms (see also Table 4) applied on SeaWiFS data in July 2002 (07/20)

2002/07/20	HPLC	OC4	OC2	This study, July 2001+2002
<i>n</i> chl- <i>a</i> , all	22	17	17	17
<i>n</i> chl- <i>a</i> , case 1	17	17	17	17
Mean [µg l <sup>-1</sup> ]	1.6	1.35	1.3	0.85
Median [µg l <sup>-1</sup> ]	1.55	1.25	1.3	0.8
S.D. [µg l <sup>-1</sup> ]	0.8	0.5	0.4	0.25
Accuracy, all [µg l <sup>-1</sup> ]		±0.35	±0.3	±0.38
		±2.7%	±2.4%	±2.7%

2002/07/20	HPLC	Izar et al. (2003), years 1994–1996	Izar et al. (2003), year 1996	Gordon and Morel (1983), case 1
<i>n</i> chl- <i>a</i> , all	22	17	17	17
<i>n</i> chl- <i>a</i> , case 1	17	17	17	17
Mean [µg l <sup>-1</sup> ]	1.6	0.6	1	0.85
Median [µg l <sup>-1</sup> ]	1.55	0.6	0.94	0.8
S.D. [µg l <sup>-1</sup> ]	0.8	0.1	0.4	0.25
Accuracy, all [µg l <sup>-1</sup> ]		±0.6	±0.41	±0.45
		±54%	±27%	±27%

Chl-*a* algorithms are OC2 (A, Table 4) and OC4 (B, Table 4), empirical chl-*a* algorithm (D, Table 4) from ground truth data set of Lake Baikal in 2001 and 2002 (this study), chl-*a* algorithm from Izar et al. (2003); coefficient of studies from 1994 to 1996 (F, Table 4), coefficient of 1996 separately (G, Table 4), and case 1, Gordon and Morel (1983) (H, Table 4).

According to ground truth and SeaWiFS spectra for 2001–2002, the green peak of the highly transparent waters of Lake Baikal is commonly located at SeaWiFS band 4 (510 nm). However, the absorption and scattering optical activities in the presence of the terrigenous input shift the peak position towards SeaWiFS band 5 (555 nm). The waters in the observable cloud-free parts of the SeaWiFS acquisitions are not as turbid, so there does not occur a spectral shift in the peak position of the SeaWiFS spectra from SeaWiFS band 5 (555 nm) to band 6 (650 nm). This observed spectral behaviour of the peak shifting from 510 to 555 nm in the 2001–2002 SeaWiFS data sets of Lake Baikal can be simulated and reproduced using the bio-optical software ‘Water Colour Simulator’ (WASI) (Gege, 2004). This described spectral behaviour has been similarly shown from previous historical limnological studies. For example, Thomson and Jerome (1975) stated that clear waters of Lakes Ontario and Superior (USA) had a dominant wavelength of 490–530 nm, biologically more productive waters had a dominant wavelength of 550–560 nm, and waters with heavy sediment loadings had a dominant wavelength of >565 nm. This spectral shift is regarded as an indicator for the terrigenous input and can be used by applying a ‘mask of terrigenous input’ on the atmospherically corrected SeaWiFS data defined by reflectance ratio values of  $R_{RS510}/R_{RS555}$  below 0.9. This is in accordance to the SeaWiFS study done by Froidefond et al. (2002) in the Bay of Biscay, who observed chlorophyll overestimation (due to terrigenous input) in cases of  $R_{RS490}/R_{RS555}$  below 1. When calculating standard suspended matter products (Jorgensen, 2000; Blasing et al., 2003), the high organic fluvial input in Burgazinski Bay and local fluvial input into the South Basin shows inverse grading with lowest calculated SPM concentrations towards the river inlets. Field spectrometer measurements and ground truth data show that, for several bio-optical models, the assumption

Fig. 2. The scattergram shows the relationship between concentrations of chl-*a* calculated from SeaWiFS OC2 and chl-*a* calculated determined from ground truth measurements during field expeditions in Lake Baikal during 2001 and 2002. Values of measured chlorophyll (HPLC) are the mean concentrations of each sampling point from 5 to 30 m depth. For the OC2 chl-*a* calculations, the most cloud-free acquisitions in 2001 (2001/07/19) and 2002 (2002/07/20) were chosen. Note the considerable chl-*a* overestimation caused by the influences of terrigenous input in case 2 waters. (Data available at: doi:10.1594/GFZ/ICDP/CONZ/004)

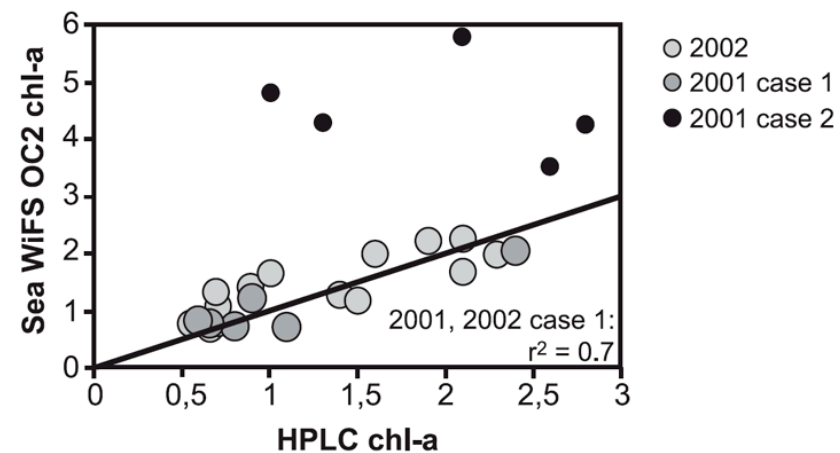


Fig. 2. The scattergram shows the relationship between concentrations of chl-*a* calculated from SeaWiFS OC2 and chl-*a* calculated determined from ground truth measurements during field expeditions in Lake Baikal during 2001 and 2002. Values of measured chlorophyll (HPLC) are the mean concentrations of each sampling point from 5 to 30 m depth. For the OC2 chl-*a* calculations, the most cloud-free acquisitions in 2001 (2001/07/19) and 2002 (2002/07/20) were chosen. Note the considerable chl-*a* overestimation caused by the influences of terrigenous input in case 2 waters.

# Use of Published Data

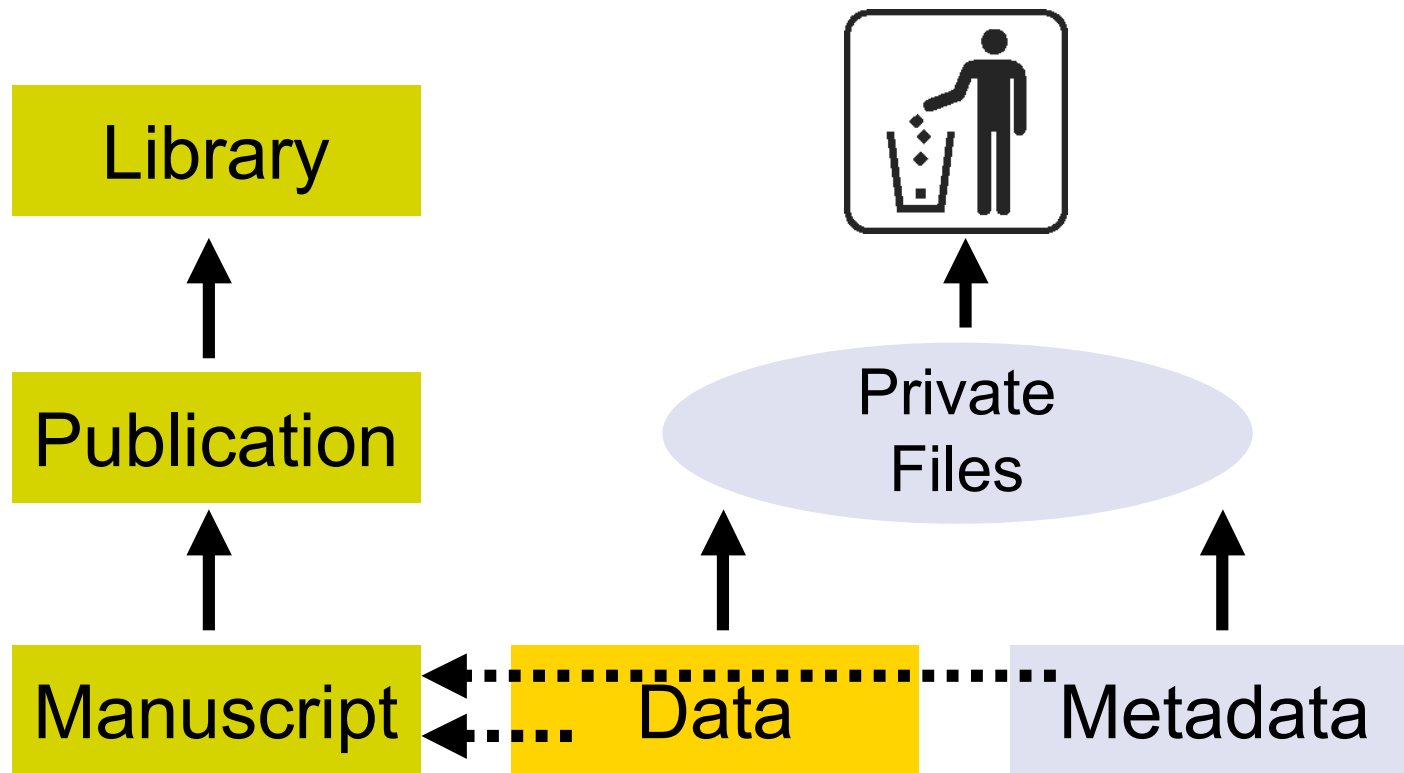


*Acknowledgements.* We thank H.-F. Tsai, T. Horinouchi, T. Nakamura, Y. Shibagaki for their fruitful discussions and comments on the manuscript. We also wish to thank GFZ (GeoForschungsZentrum), Potsdam for providing CHAMP/GPS RO data through the ISDC (INTEGRAL Science Data Centre ISDC) data center. One of the authors (MVR) wishes to thank JSPS (Japan Society for Promotion of Sciences) for providing fellowship to carry out this work. This work is also supported partially by MEXT (Japanese Ministry of Education, Culture, Sports, Science and Technology) using Grant-in-Aid for Scientific Research on Priority Areas (Grant number: (A03) 13136206; (A04) 13136203).

Topical Editor U.-P. Hoppe thanks two referees for their help in evaluating this paper.

- Often, the source of data is not acknowledged.
- No citation of the data source.
- The data source needs to be deduced from the paper. No Metadata.

# Data in the publication process today



After Helly *et al.* (2003)



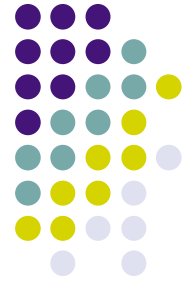
# The consequences

- Most data remain underutilised because they are not accessible.
  - Unnecessary duplication
- Research results cannot be verified.
  - Falsification of results.
- Calls to make data accessible and share data were welcomed but did not give any results.

# Why are data not made accessible?



- Data publication is hampered by structural barriers in the publication process:
  - Journals do not devote space to data tables due to economic constraints and have no interest in archiving data.
  - Authors do not receive professional recognition for publishing data because the datasets cannot be cited in a reliable way.
  - Data are not cited because their location (URL), in many cases, is transient.

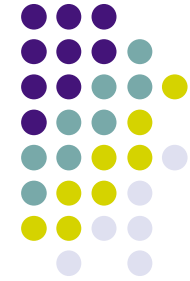


# Necessary steps

- Data need to be citeable to be “valuable”.
  - “Reputation” is the currency of science.
- Authors will only prepare data for publication if the effort is worthwhile.
  - Data publication is labour intensive.
- Data must be accessible to be re-used.
  - Access through persistent identifiers and long-term archives.
- Existence of data must be known.
  - Dissemination of metadata to catalogues and portals.
- Intellectual property rights need to be secured.
  - Authors need full control of their publications.



# Project “Publication and Citation of Scientific Primary Data”

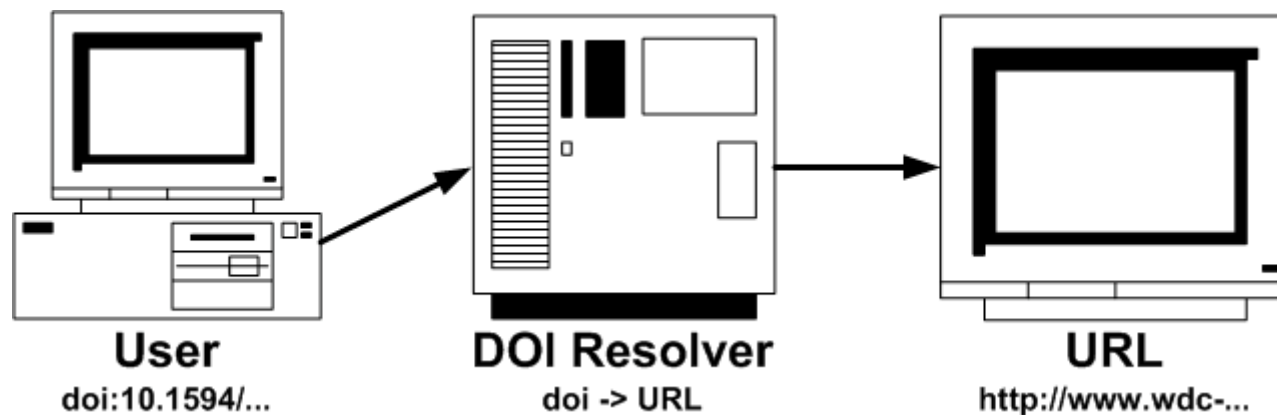


- Funded by the German Science Foundation.
- Project partners:
  - German Nat. Lib. Science and Technology (Hannover)
  - WDC-MARE (Bremen/Bremerhaven)
  - WDC Climate (Hamburg)
  - GFZ Potsdam (proposed WDC-TERRA)
  - WDC-RSAT (Oberpfaffenhofen)
- Implementation of services for the publication of data.
- DOI registration agency at German National Library for Science and Technology (TIB Hannover).
- To date 6 DOI registration agents. Inclusion of data publications into library catalogues.

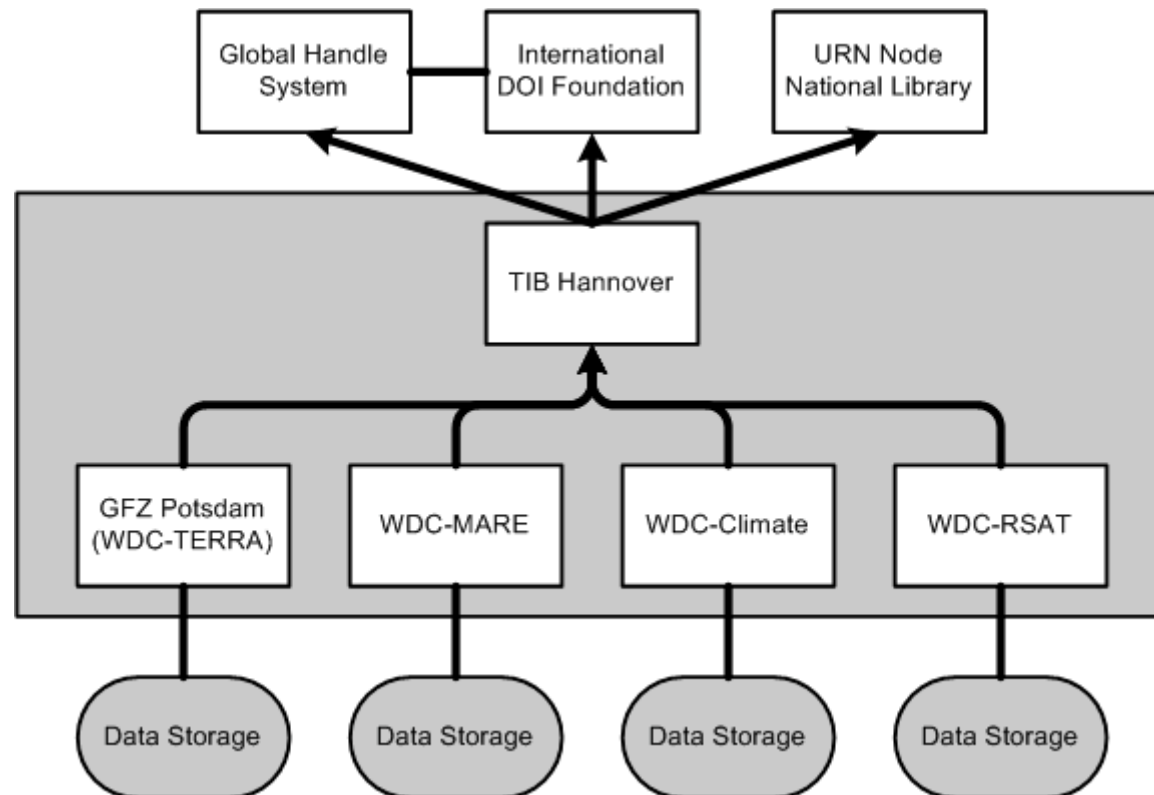


# What is a DOI?

- DOI = Digital Object Identifier, a persistent, digital identifier of an object.
- DOI = Name of object, URL = Location of object.
- The location may change, the name persists, irrespective of the location of the object.



# STD-DOI System Architecture



# Example Data Publication

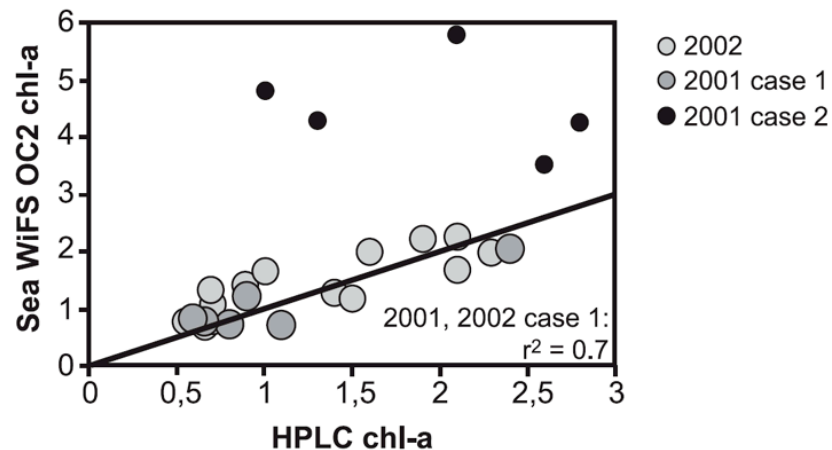
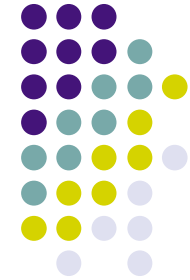


Fig. 2. The scattergram shows the relationship between concentrations of chl-*a* calculated from SeaWiFS OC2 and chl-*a* calculated determined from ground truth measurements during field expeditions in Lake Baikal during 2001 and 2002. Values of measured chlorophyll (HPLC) are the mean concentrations of each sampling point from 5 to 30 m depth. For the OC2 chl-*a* calculations, the most cloud-free acquisitions in 2001 (2001/07/19) and 2002 (2002/07/20) were chosen. Note the considerable chl-*a* overestimation caused by the influences of terrigenous input in case 2 waters.

- [TIBORDER](#) catalogue of the German National Library of Science and Technology.
- [doi:10.1594/GFZ.SDDB.1043](https://doi.org/10.1594/GFZ.SDDB.1043) at the ICDP Scientific Drilling Database.

# TIBORDER / GBV Catalogue



Catalogue of the TIB - results/titledata - Mozilla Firefox

http://tiborder.gbv.de/psi/DB=2.63/SET=2/TTL=1/SHW?FRST=1

Basic search | Advanced search | **Results** | My shelf | Search history | Help

TIBORDER Katalog

search [and] all words sort by year of publication

Heim Birgit search

User id: [logout](#)

Title list | **title data**

■ **results** search [and] (all words) Heim Birgit 1 of 4

**Title:** The [relationship between concentrations](#) of [chl-a calculated](#) from [SeaWiFS OC2](#) and [chl-a calculated determined](#) from [ground truth measurements during field expeditions in Lake Baikal during 2001 and 2002](#) / Geoforschungszentrum Potsdam (GFZ) , Potsdam, Germany .**Birgit@Heim**

**Collaborator:** [Birgit Heim](#) ; [Hedi Oberh??nsli](#) ; [Susanne Fietz](#) ; [Hermann Kaufmann](#)

**Corporate body:** [Geoforschungszentrum Potsdam \(GFZ\)](#)

**Published:** 2006-09-15

**Extent:** Online-Ressource (54 Datapoints).

**Note:** Mode: Abstract  
StructuralType: Digital  
CreationDate: 2006-03-08

**Abstract:** Values of measured chlorophyll (HPLC=High Performance Liquid Chromatography) are the mean concentrations of each sampling point from 5 to 30 m depth. For the OC2 chl-a calculations, the most cloud-free acquisitions in 2001 (2001/07/19) and 2002 (2002/07/20) were chosen. Note the considerable chl-a overestimation caused by the influences of terrigenous input in case 2 waters.

**Techn. data:** Format: text/tab-separated-values

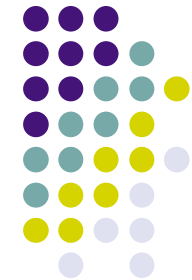
**Links:** doi: [10.1594/GFZ.SDDB.1043](#)  
URN: [urn:nbn:de:tib-10.1594/GFZ.SDDB.10432](#)

**Holding:** [Display free access!](#)  
Note: Primaerdaten

1 of 4

Fertig

# ICDP Scientific Drilling Database



## Scientific Drilling Database

Data from Deep Earth Sampling and Monitoring

Citation:

Heim, Birgit; Oberhänsli, Hedi; Fietz, Susanne; Kaufmann, Hermann; (2006): The relationship between concentrations of chl-a calculated from SeaWiFS OC2 and chl-a calculated determined from ground truth measurements during field expeditions in Lake Baikal during 2001 and 2002, *Scientific Drilling Database*, 10.1594/GFZ.SDDB.1043

[Download Citation \(EndNote\)](#)

+ Sampling Gear  
+ Parameters  
+ Admin



**Title:** The relationship between concentrations of chl-a calculated from SeaWiFS OC2 and chl-a calculated determined from ground truth measurements during field expeditions in Lake Baikal during 2001 and 2002

**Abstract:** Values of measured chlorophyll (HPLC=High Pressure Liquid Chromatography) are the mean concentrations of each sampling point from 5 to 30 m depth. For the OC2 chl-a calculations, the least clouded acquisitions in 2001 (2001/07/19) and 2002 (2002/07/20) were chosen. Note the considerable chl-a overestimation caused by the influences of terrigenous input in case 2 waters.

[Show in Google Earth](#)

**Related Identifier:**

- Heim, B., Oberhänsli, H., Fietz, S. and Kaufmann, H. (2005). Variation in Lake Baikal phytoplankton distribution and fluvial input assessed by SeaWiFS satellite data. *Global and Planetary Change* 46 (1-4), 9-27. doi:10.1016/j.gloplacha.2004.11.011

**Activities:**

<b>CON01-501-1</b>
Latitude: 52.6667
Longitude: 107
Elevation: -1250
Date/Time: 2001-07-16 00:52:00
Program: High-resolution CONTINENTAL paleoclimate record in Lake Baikal
Expedition: CON01-5
Platform: R/V Vereshchagin
Gear: Water sample

<b>CON01-502-1</b>
Latitude: 52.9561

# Data Syndication



- Many available data remain underutilised because their existence is not known.
- Metadata can be harvested and indexed by data portals using OAI-PMH or RSS.
- Both OAI-PMH and RSS can be used to carry discipline specific metadata.
- Examples:
  - PANGAEA Data Portals (OAI-PMH)
  - Open Geospatial Consortium GeoRSS
- Portals can provide specific views on existing data.



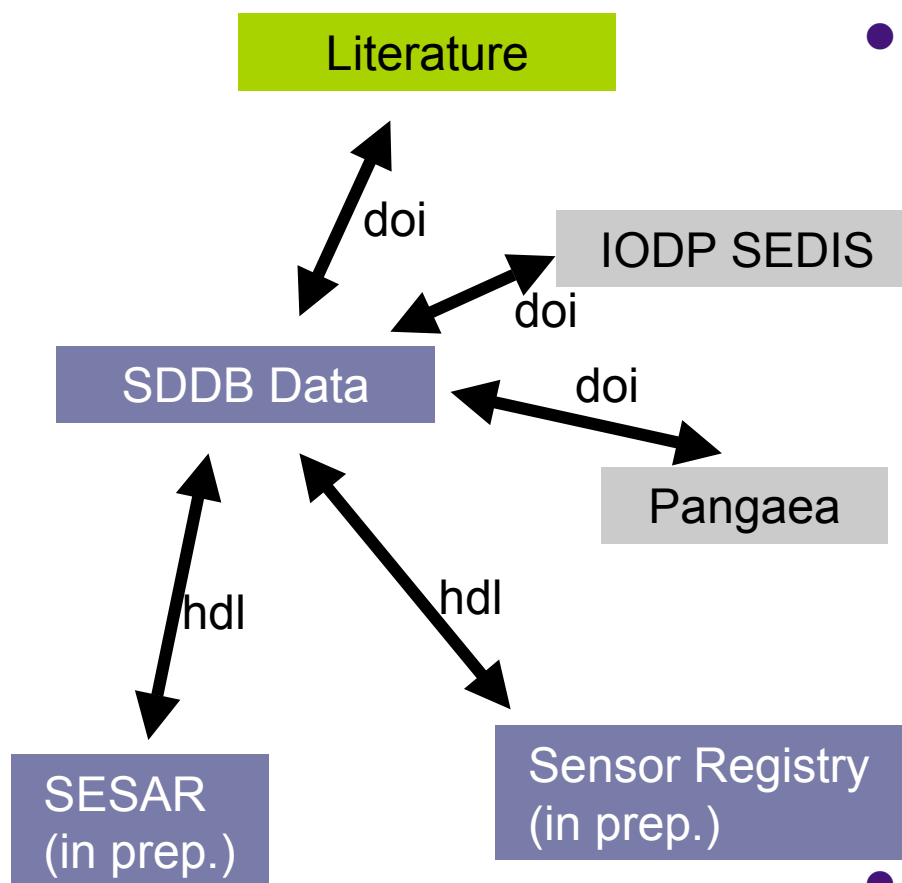
## DOI metadata

- The STD-DOI metadata are mainly Dublin Core elements, plus system specific elements.
- The metadata transmitted to the National Library via web service (HTTP/SOAP) and incorporated into the library catalogue.
- The metadata may contain references to other objects.
  - Element <RelatedIdentifier>
  - isCitedBy, isDuplicateOf, isAlsoPublishedAs, ...



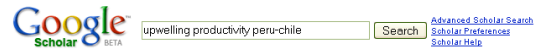
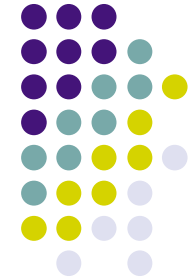


# External Semantics



- The element `<RelatedIdentifier>` can be used to point to other electronic objects:
  - Point to the literature where the data set is interpreted.
  - Point to samples, from which the data were derived.
  - Point to other datasets that belong to the same collection of datasets.
- Improve data discovery.

# Information Discovery



- Scholar**
- ... sediment distribution along the Chilean continental slope
  - D Hebbeln, M Marchant, T Freudenthal, G Wefer - Marine Geology, ... coastal upwelling system of the Peru-Chile Current belongs ... productivity known from ... about varying influences of upwelling ... Cited by 17 - Web Search
  - Evolution and biological effects of the 1997-98 El Niño in O Ulloa, R Escribano, S Homazabal, RA Quinones, ... - GEOPHY ... The rich biological productivity of the Peru-Chile marine ecosystem-driven coastal upwelling, which brings colder, nutrient-rich, surface sediments below the Peru-Chile Current: controlling mechanisms with productivity ... water production: coastal upwelling off northern Peru - Cited by 5 - View as HTML - Web Search
  - High and low latitude climate control on the position of the Peru-Chile Current (PCC ... km) and an exceptionally high productivity ... Cited by 13 - View as HTML - Web Search - BL Direct
  - Peru Upwelling Region Sediments Near 15°S. 2. Dissolved trace metals and ... The Peru upwelling region is of special interest ... part to variability in the ... in sulphide biota under Peru-Chile subsurface ... Cited by 21 - Web Search - SFZ Telegramfenberg
  - Seasonal variations of the particle flux in the Peru-Chile Current - Cited by 14 - Web Search
  - Peru Upwelling Region Sediments Near 15°S. 1. Remotely sensed ... SM Heinrichs, JW Farrington - Limnology and Oceanography, 1984

Link to publication

20 B. Heim et al. / Global and Planetary Change 46 (2005) 9–27

Table 6  
Overview on accuracy of chl-a algorithms (see also Table 4) applied on SeaWiFS data in July 2002 (07/20)

	2002/07/20	HPLC	OC4	OC2	This study July 2001+2002
n chl-a, all case 1	22	17	17	17	17
Mean [µg l <sup>-1</sup> ]	1.6	1.35	1.3	0.85	
Median [µg l <sup>-1</sup> ]	1.55	1.25	1.3	0.8	
S.D. [µg l <sup>-1</sup> ]	0.8	0.5	0.4	0.25	
Accuracy, all [µg l <sup>-1</sup> ]		±0.35 ±27%	±0.3 ±24%	±0.38 ±27%	

	2002/07/20	HPLC	Daz et al. (2001) years 1994–1996	Daz et al. (2003) year 1996 case 1	Cloeren and Morel (1993)
n chl-a, all case 1	22	17	17	17	17
Mean [µg l <sup>-1</sup> ]	1.6	0.6	1	0.85	
Median [µg l <sup>-1</sup> ]	1.55	0.6	0.94	0.8	
S.D. [µg l <sup>-1</sup> ]	0.8	0.1	0.4	0.25	
Accuracy, all [µg l <sup>-1</sup> ]		±0.6 ±54%	±0.41 ±27%	±0.45 ±27%	

Chl-a algorithms are OC2 (A, Table 4) and OC4 (B, Table 4) empirical chl-a algorithms (D, Table 4) from ground truth data set Lake Baikal in 2001 and 2002 (this study), chl-a algorithms from Daz et al. (2003); coefficient of studies from 1994 to 1996 (F, Table 4); coefficient of 1996 separately (G, Table 4), and case 1, Cloeren and Morel (1993) (H, Table 4).

According to ground truth and SeaWiFS spectra: 2001–2002, the green peak of the highly transparent waters of Lake Baikal is commonly located SeaWiFS band 4 (510 nm). However, the absorption optical activities in the presence of the signal at the peak position (wavelength) are not the same for all the stations. The absorption optical activities in the presence of the signal at the peak position of the SeaWiFS band 4 (510 nm) are not the same for all the stations. The absorption optical activities in the presence of the signal at the peak position of the SeaWiFS band 4 (510 nm) are not the same for all the stations.

## Scientific Drilling Database

Data from Deep Earth Sampling and Monitoring

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- + Authors
- + Dataset
- + Research Programs
- + Sampling Gear
- + Parameters
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### Dataset Description

Citation: Heim, Birgit; Oberhänsli, Hedi; Fietz, Susanne; Kaufmann, Hermann; (2005) The relationship between concentrations of chl-a calculated from SeaWiFS OC2 and chl-a from ground truth measurements during field expeditions in Lake Baikal during 2001 and 2002. *Scientific Drilling Database*. doi:10.1594/GFZ.SDDB.1043

[Download Citation \(EndNote\)](#)

DOI: 10.1594/GFZ.SDDB.1043

Title: The relationship between concentrations of chl-a calculated from SeaWiFS OC2 and chl-a from ground truth measurements during field expeditions in Lake Baikal during 2001 and 2002

Abstract: Values of measured chlorophyll (HPLC=High Pressure Liquid Chromatography) and chl-a concentrations of each sampling point from 5 to 30 m depth. For the OC2 least clouded acquisitions in 2001 (2001/07/19) and 2002 (2002/07/20) we observed a considerable chl-a overestimation caused by the influences of terrigenous particles.

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Activities: **COND1-501-1**

Latitude: 52.6667  
Longitude: 107  
Elevation: -1250  
Date/Time: 2001-07-16 00:52:00  
Program: High-resolution CONTINENTAL paleoclimate record in Lake Baikal  
Expedition: COND1-5  
Platform: R/V Vereshchagin  
Gear: Water sampler

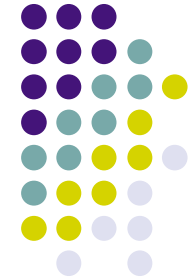
**COND1-502-1**

Latitude: 52.9561  
Longitude: 107.5926

IGSN points to sample

- Glossary
- Catalogue

# SDDDB Metadata Management



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  - + Edit Data
  - + Edit Category
  - + File Upload
  - + Example File Upload
  - + Edit Dataset
  - + Dokumentation
  - + Publish Data
  - + Update Publication

**GFZ** **icdp**  
POTSDAM

### File Upload

Title: Gas mass spectrometry of gas samples from the KTB Main Hole HB1  
Description: The main objective of this drilling fluid analysis was the detection of inflows of formation fluids. Therefore different gases dissolved in the drilling mud were measured continuously and automatically at drill site with three different methods (Fig.: KTB-Report 92-2 page C13). The operation principles of the mass spectrometer and the gaschromatograph have been explained by STROH et al. (1988) and FIGGEMEIER et al. (1991). The principle of radon determination is published by ERZINGER et al. (1992). In the complete KTB-VB and in in the KTB-HB down to a depth of 3003 m the gas phase was released and collected by twirl degassers attached in front of the mud shakers. This open system led to gas losses as well as air contamination. Therefore results obtained down to this depth have only qualitative character. After casing the KTB-HB to a depth of 3003 m a bypass system was installed at the BOP (blow-out preventer) 50 cm below the flow line.

Author 1: Kamm,H  
Author 2: Machon,L  
Author 3: Donner,S  
File: KTB-HB GC.txt  
Activities: KTB-HB

Parameter:	N2
77.64	Method: gas chromatography
77.59	Material: gas from drilling mud
77.63	Investigator: Kamm,H
77.62	Laboratory: KTB Field Lab
77.6	Remarks:

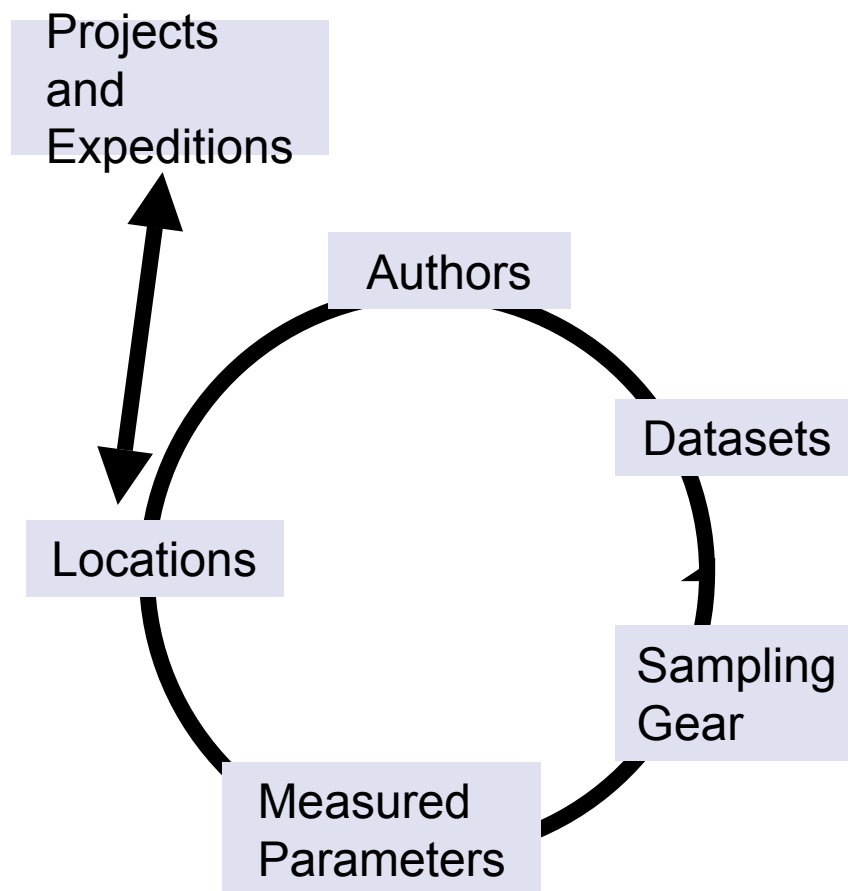
  

Parameter:	O2
20.25	Method: gas chromatography
20.26	Material: gas from drilling mud
20.25	Investigator: Kamm,H
20.22	Laboratory: KTB Field Lab
20.1	

- Management of Metadata is kept simple by offering a data upload assistant.
- Data upload process is styled in analogy to eBay sales upload assistant.
- Most metadata are in the system already.

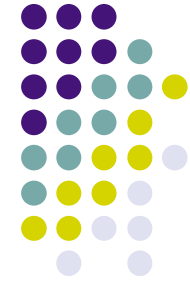


# Internal Semantics



- SDDB metadata are held in a fully normalised relational database.
- SDDB metadata are fully browseable to allow iterative search.
- SDDB has (so far) no full-text search.

# Putting data into context



Scientific Drilling Database - Mozilla Firefox

Datei Bearbeiten Ansicht Chronik Lesezeichen Extras Hilfe

http://www.icdp-online.de/contento/lakedb/frc

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- + Admin

> parameter > age models > radiocarbon

"radiocarbon" contains the following parameters:

- ◆  $\delta^{13}\text{C}$  [‰]
- ◆  $\delta^{13}\text{C}$  error [‰]
- ◆ age (C-14 years) [yr]
- ◆ age (calibrated C-14 years) [yr]
- ◆ age error (C-14 years) [yr]
- ◆ carbon yield [%]
- ◆ estimated purity [%]
- ◆ reservoir effect [a]
- ◆ target weight [mg C]

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GFZ icdp | POTSDAM

Last Modification: 2006-08-04 | Some rights reserved by Daten- und Rechenzentrum, GeoForschungsZentrum

Fertig

- Parameters are organised in a tree-structure.
- Homonyms are allowed – the parameter tree is ordered according to scientific context.

# The spatial dimension



Will soon be supplemented by  
OGC Web Services.

Google Earth interface showing a map of Irkutsk with numerous location markers labeled with alphanumeric codes (e.g., CON01-501-1, CON02-814-2, CON02-817-3, CON02-818-2, CON02-811-6, CON02-840-3, CON01-505-1, CON01-507-2, CON02-833-5, CON02-829-1, CON02-827-1, CON02-830-2, CON02-831-3, CON01-503-1, CON01-502-2, CON01-502-1, CON01-501-1, CON01-522-2, CON01-521-2, CON02-854-1, CON02-806-6, CON02-809-2). The interface includes a search bar, a 'Places' list, and a 'Layers' panel.

Pointer: 53°00'57.24" N 106°58'05.33" E elev. 475 m  
Streaming 100%  
Eye alt: 448.14 km



## **SDDB Plans for 2007/2008**

- Integration of GSI components (deegree2).
- Introduction of links to IGSNs.
- Migration of web frontend from PHP to Java/JSP/JSR168.
- Introduction of Fedora Repository as middleware to integrate data, publications and services.

# More Information

- Project “Publication and Citation of Scientific Primary Data”

<http://www.std-doi.de>

- ICDP Scientific Drilling Database

<http://www.scientificdrilling.org>

Thank you!



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