Structuring and Managing Biological Data

BIODIVERSITY.AQ

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museum
Operational Directorate Natural Environment
OD Nature | OD Natuur | DO Nature

The SCAR Antarctic Biodiversity Portal

Topical collection: “Antarctic and Southern Ocean biodiversity”

- Still open for submissions
- Type of papers
  - Data Paper (Biosciences)Methods
  - OMICS Data Paper
  - R Package
  - Software Description

Why publish data?

- In order to promote international cooperation in scientific investigation in Antarctica,.., the Contracting Parties agree that, to the greatest extent feasible and practicable:
  scientific observations and results from Antarctica shall be exchanged and made freely available.

- Open Science

What is Metadata?

"Data about data"

How, when, why

No (individual) measurements

E.g. license, institution, sampling method, …

FAIR principles

Findable

Accessible

Interoperable

Reusable

- Metadata
- Infrastructures
- Standardisation
- Machine readable
- Trusted repositories

MAKE YOUR DATA FAIR

Apply a suitable usage license

Provide end users with information on “intended use”

Make the data “as open as possible, as closed as necessary”

Ensure that metadata remain available even if the data cannot be accessed any more

FAIRness needs to be applied where it makes sense

As open as possible, as closed as needed

- Data
- (Partly) hide data
- Never hide metadata
- E.g. GDPR, Threatened species

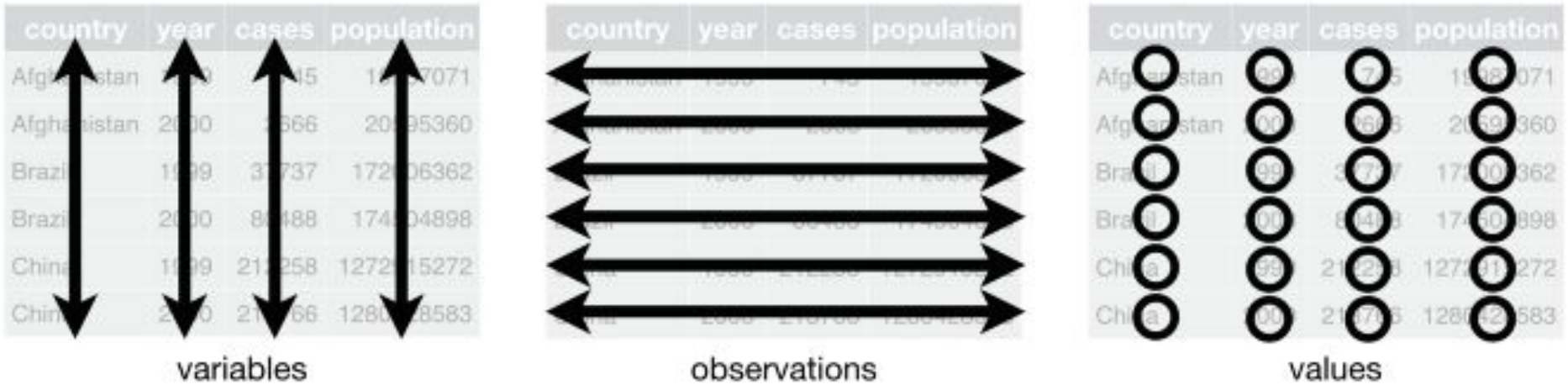
Standardised data

“Data Scientists spend up to 80% of the time on data cleaning and 20 percent of their time on actual data analysis” (*Dasu and Johnson 2003)*

The first person to benefit from clean structured data is future you

Tidy Data

- For downstream operations (QC)
- Necessary for repos
- Machine readability
- Human readability



R for Data Science 12.1

Tidy Data

Variable

Datapoint

catalogNumber	basisOfRecord	type	scientificName	kingdom	phylum	class	order	family	genus
MNA13174	PreservedSpecimen	PhysicalObject	Calanoides acutus (Giesbrecht, 1902)	Animalia	Arthropoda	Hexanauplia	Calanoida	Calanidae	Calanoides
MNA13175	PreservedSpecimen	PhysicalObject	Harpacticus furcifer (Edwards H., 1840)	Animalia	Arthropoda	Hexanauplia	Harpacticoida	Harpacticidae	Harpacticus
MNA13176	PreservedSpecimen	PhysicalObject	Metridia gerlachei (Giesbrecht, 1902)	Animalia	Arthropoda	Hexanauplia	Calanoida	Metridinidae	Metridia
MNA13177	PreservedSpecimen	PhysicalObject	Metridia gerlachei (Giesbrecht, 1902)	Animalia	Arthropoda	Hexanauplia	Calanoida	Metridinidae	Metridia
MNA13178	PreservedSpecimen	PhysicalObject	Tisbe gracilipes (Scott T., 1912)	Animalia	Arthropoda	Hexanauplia	Harpacticoida	Tisbidae	Tisbe

Cookiecutter project structure

```
├── README.md          <- The top-level README.
├── data
│   ├── external       <- Data from third party sources.
│   ├── interim        <- Intermediate data that has been transformed.
│   ├── processed      <- The final, canonical data sets for modeling.
│   └── raw            <- The original, immutable data dump.
│
├── references         <- Data dictionaries, manuals, and all other explanatory materials.
│
├── src                <- Source code for use in this project.
│   ├── data           <- Scripts to download or generate data.
│   │   └── make_dataset.R
│   │
│   ├── clean          <- Scripts to clean data.
│   │   └── clean_dataset.R
│   │
│   └── visualization  <- Scripts to create exploratory and results oriented visualizations
│       └── visualize.R
│
└── reports            <- Generated QC reports.
    └── figures        <- Generated graphics and figures to be used in reporting.
```

Give good names to your files

- Machine readable
- human readable
- orderable
- use of separators
- uniform style

```
~/Desktop/projects/01_cruise-reports ▷
2018-12-15_PS117_Cape-Town.pdf
2019-02-09_PS118_Punta-Arenas.pdf
2019-04-13_PS119_Punta-Arenas.pdf
2020-06-04_PS122-4_Arctic-Ocean.pdf
2020-08-12_PS122-5_Arctic-Ocean.pdf
```

OpenRefine

- 1. Explore Data
- 2. Clean and Transform Data
- 3. Reconcile and Match Data

This feature helps you find groups of different cell values that might be alternative representations of the same thing. For example, the two strings "New York" and "new york" are very likely to refer to the same concept and just have capitalization differences, and "Gödel" and "Godel" probably refer to the same person. Find out more ...

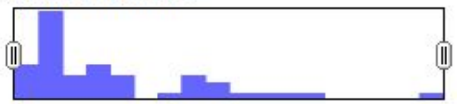
Method key collision ▼ Keying Function fingerprint ▼ **48** clusters found

Cluster Size	Row Count	Values in Cluster	Merge?	New Cell Value
3	63	• Pune Vidhyapeeth Gate (33 rows) • Pune Vidhyapeeth Gate (17 rows) • Pune Vidhyapeeth Gate (13 rows)	☐	Pune Vidhyapeeth Gate
3	101	• Hadapsar Gadital (83 rows) • Hadapsar Gadital (14 rows) • Hadapsar Gadital (4 rows)	☐	Hadapsar Gadital
3	12	• Devachi Uruli Phata (8 rows) • Devachi Uruli Phata (2 rows) • Uruli Devachi Phata (2 rows)	☐	Devachi Uruli Phata
2	2	• SRP Stadium (1 rows) • SRP Stadium (1 rows)	☐	SRP Stadium
2	8	• Khandoba Mandir Corner (6 rows) • Khandoba Mandir corner (2 rows)	☐	Khandoba Mandir Corner
2	7	• St Meera College (5 rows) • ST Meera College (2 rows)	☐	St Meera College
2	67	• Gunjan Corner (62 rows)	☐	Gunjan Corner

 # Choices in Cluster

2 — 3

 # Rows in Cluster

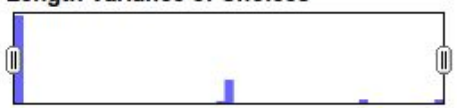


0 — 170

Average Length of Choices

3 — 31

Length Variance of Choices



0 — 1

Machine readability: Atomize columns

verbatimCoordinates	date	taxonomy
58°28'30''W,62°08'00''S	2022-08-05	Rhincalanus gigas, Brady (1883)
62°08'10''W,61°18'20''S	2022-08-09	Rhincalanus gigas, Brady (1883)
61°58'40''W,61°48'50''S	2022-08-10	Rhincalanus gigas, Brady (1883)

decimalLatitude	decimalLongitude	year	month	day	acceptedTaxonName	scientificNameAuthorship
-62.1333	-58.4750	2022	08	05	Rhincalanus gigas	Brady,1883
-61.3055	-62.1361	2022	08	09	Rhincalanus gigas	Brady,1883
-61.8139	-61.9778	2022	08	10	Rhincalanus gigas	Brady,1883

Use Persistent identifiers

Term	Example
scientificNameID	urn:lsid:ipni.org:names:37829-1:1.3
identifiedByID	https://orcid.org/0000-0002-1825-0097
taxonID	http://species.gbif.org/abies_alba_1753
materialSampleID	06809dc5-f143-459a-be1a-6f03e63fc083

Exchanging and publishing data

Darwin Core standard is a set of terms

Occurrence

occurrenceID | catalogNumber | recordNumber | recordedBy | recordedByID
individualCount | organismQuantity | organismQuantityType | sex | lifeStage
reproductiveCondition | behavior | establishmentMeans | degreeOfEstablishment
pathway | georeferenceVerificationStatus | occurrenceStatus | preparations
disposition | associatedMedia | associatedOccurrences | associatedReferences
associatedSequences | associatedTaxa | otherCatalogNumbers | occurrenceRemarks

Occurrence	Class
Identifier	http://rs.tdwg.org/dwc/terms/Occurrence
Definition	An existence of an Organism (sensu http://rs.tdwg.org/dwc/terms/Organism) at a particular place at a particular time.
Comments	
Examples	A wolf pack on the shore of Kluane Lake in 1988. A virus in a plant leaf in the New York Botanical Garden at 15:29 on 2014-10-23. A fungus in Central Park in the summer of 1929.

occurrenceID	Property
Identifier	http://rs.tdwg.org/dwc/terms/occurrenceID
Definition	An identifier for the Occurrence (as opposed to a particular digital record of the occurrence). In the absence of a persistent global unique identifier, construct one from a combination of identifiers in the record that will most closely make the occurrenceID globally unique.
Comments	Recommended best practice is to use a persistent, globally unique identifier.
Examples	`http://arctos.database.museum/guid/MSB:Mamm:233627`, `000866d2-c177-4648-a200-ead4007051b9`, `urn:catalog:UWBM:Bird:89776`

Record-level
Occurrence
Organism
MaterialSample
Event
Location
GeologicalContext
Identification
Taxon
MeasurementOrFact
ResourceRelationship
UseWithIRI

LivingSpecimen
PreservedSpecimen
FossilSpecimen
MaterialCitation
HumanObservation
MachineObservation

A data package is needed for data exchange

Occurrence

occurrenceID | catalogNumber | recordNumber | recordedBy | recordedByID
individualCount | organismQuantity | organismQuantityType | sex | lifeStage
reproductiveCondition | behavior | establishmentMeans | degreeOfEstablishment
pathway | georeferenceVerificationStatus | occurrenceStatus | preparations
disposition | associatedMedia | associatedOccurrences | associatedReferences
associatedSequences | associatedTaxa | otherCatalogNumbers | occurrenceRemarks

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Taxon
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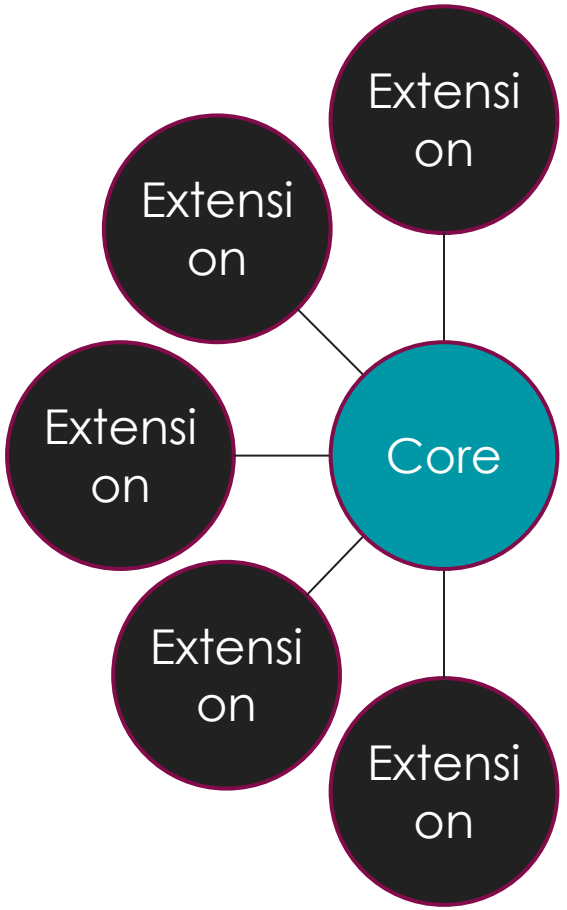
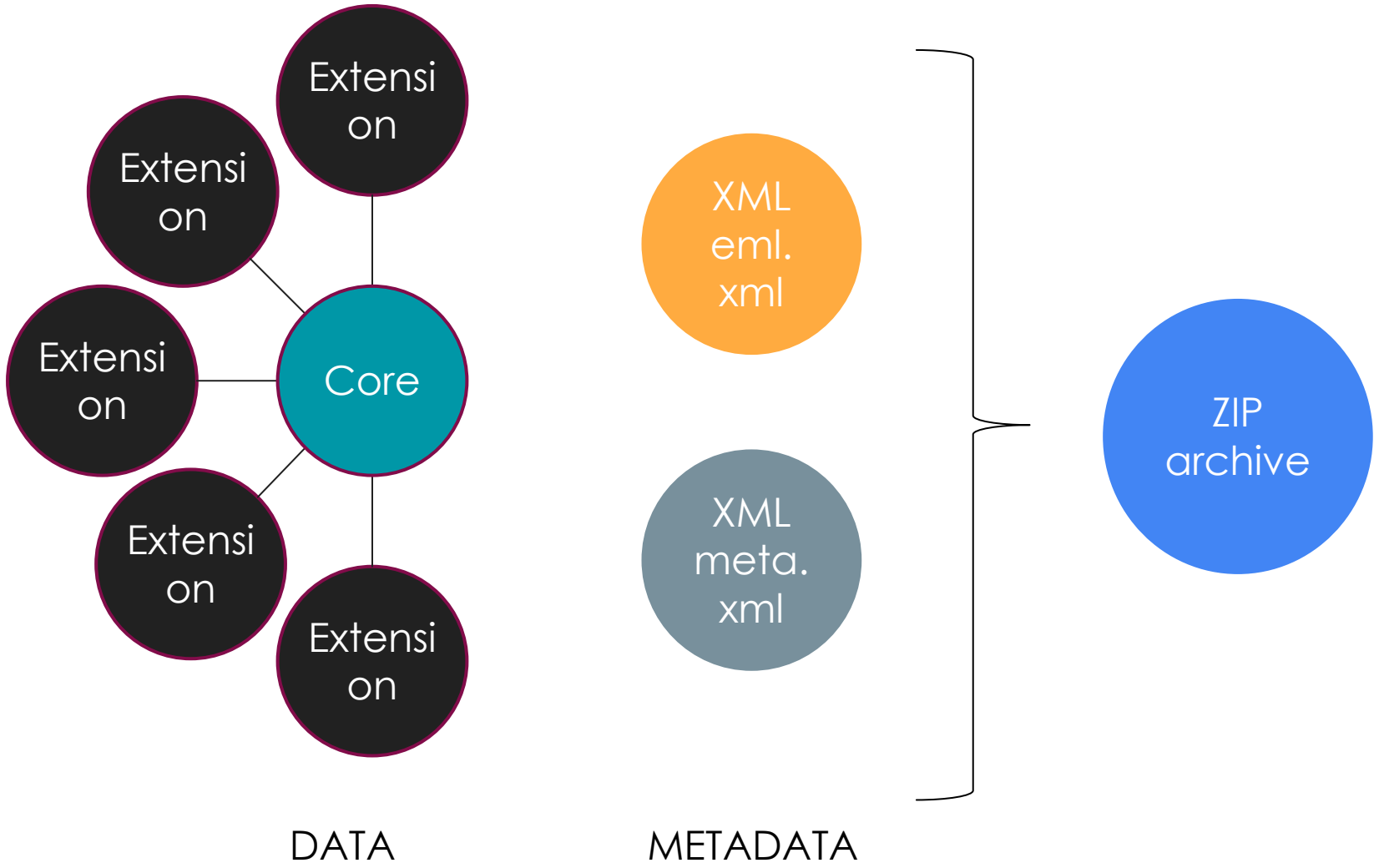
UseWithIRI

LivingSpecimen
PreservedSpecimen
FossilSpecimen
MaterialCitation
HumanObservation
MachineObservation

subset of terms



Darwin Core archive is a data exchange format



Core: main observation

Occurrence Core

- Organisms at specific time and place
- Required terms: manual.obis.org/darwin_core.html
- E.g. Whales spotted

Event Core

- Sampling events
- Occurrence extension
- Required terms: manual.obis.org/darwin_core.html
- E.g. Trawls, sampling station

Extensions: other data

- 34 registered extensions https://rs.gbif.org/extensions.html
- Data not in Core
- Needs pointer to Core
- E.g. Temperature, Pictures, …

Ecological metadata Language (Eml.xml)

Automatically generated

- Basic Metadata
- Geographic Coverage
- Taxonomic Coverage
- Temporal Coverage
- Keywords
- Associated Parties
- Project Data
- Sampling Methods
- Citations
- Collection Data

meta.xml

RELATIONSHIP BETWEEN FILES

AUTOMATICALLY GENERATED

HUMAN AND MACHINE READABLE

Examples

eml.xml

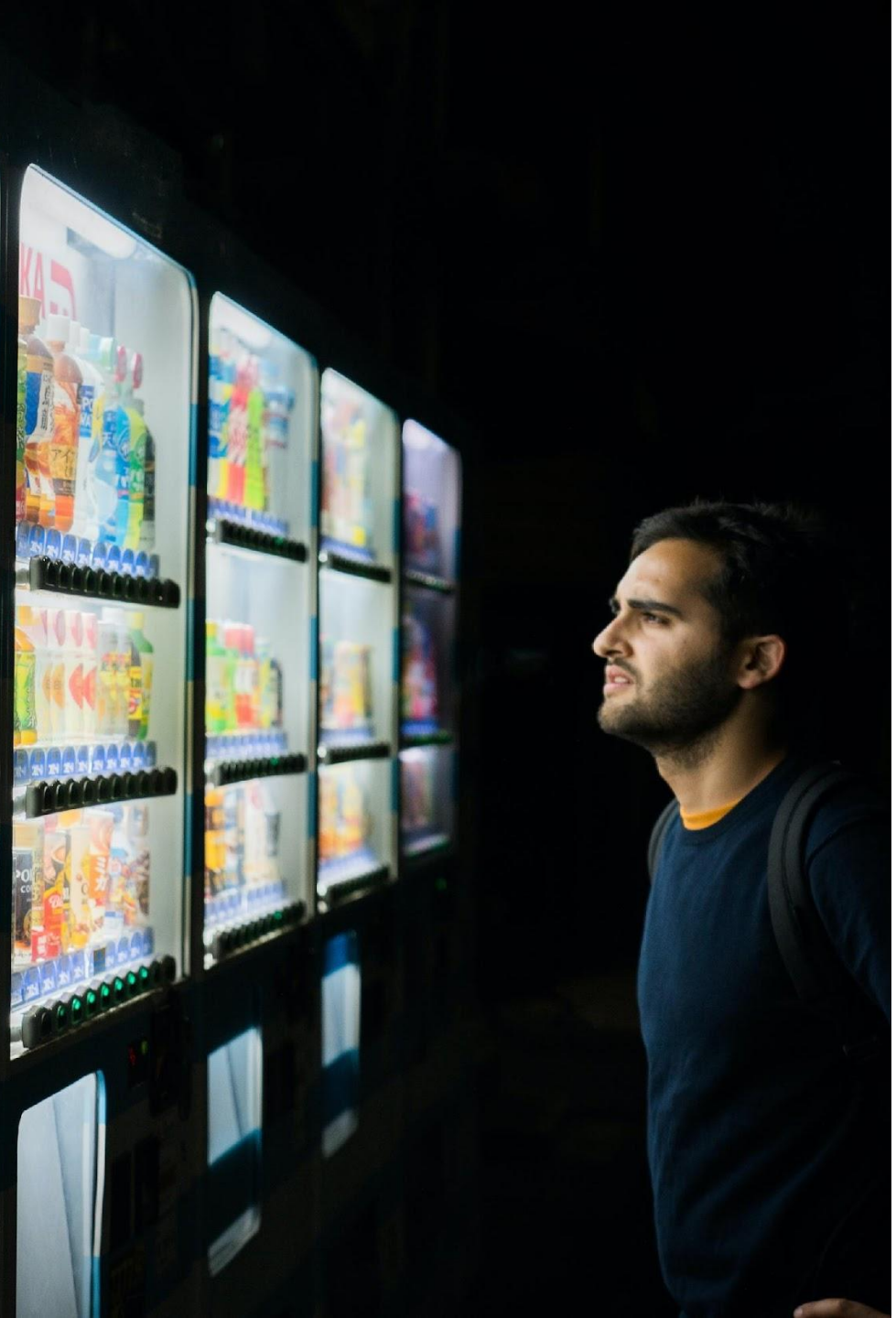
```
<?xml version="1.0"?>
<eml:eml
   packageId="eml.1.1" system="knb"
   xmlns:eml="eml://ecoinformatics.org/eml-2.1.1"
   xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
   xmlns:stmml="http://www.xml-cml.org/schema/stmml-1.1"
   xsi:schemaLocation="eml://ecoinformatics.org/eml-2.1.1
eml.xsd">


<dataset>
 <title>Data from Cedar Creek LTER on productivity and species
richness
 </title>
 <creator id="clarence.lehman">
   <individualName>
     <salutation>Mr.</salutation>
     <givenName>Clarence</givenName>
     <surName>Lehman</surName>
   </individualName>
 </creator>
 <contact>
   <references>clarence.lehman</references>
 </contact>
</dataset>
</eml:eml
```

metadata.xml

```
<archive xmlns="http://rs.tdwg.org/dwc/text/" metadata="eml.xml">

  <core encoding="UTF-8" fieldsTerminatedBy="\t" linesTerminatedBy="\n"
  fieldsEnclosedBy="" ignoreHeaderLines="1"
  rowType="http://rs.tdwg.org/dwc/terms/Occurrence">
    <files>
      <location>occurrence.txt</location>
    </files>
    <id index="0"/>
    <field index="1" term="http://purl.org/dc/terms/license"/>
    <field index="2" term="http://purl.org/dc/terms/bibliographicCitation"/>
    <field index="3" term="http://rs.tdwg.org/dwc/terms/institutionCode"/>
    <field index="4" term="http://rs.tdwg.org/dwc/terms/collectionCode"/>
    <field index="5" term="http://rs.tdwg.org/dwc/terms/basisOfRecord"/>
    <field index="6" term="http://rs.tdwg.org/dwc/terms/dynamicProperties"/>
    <field index="7" term="http://rs.tdwg.org/dwc/terms/occurrenceID"/>
    <field index="8" term="http://rs.tdwg.org/dwc/terms/eventDate"/>
    <field index="9" term="http://rs.tdwg.org/dwc/terms/country"/>
    <field index="10"
    term="http://rs.tdwg.org/dwc/terms/minimumDepthInMeters"/>
    <field index="11" term="http://rs.tdwg.org/dwc/terms/decimalLatitude"/>
    <field index="12" term="http://rs.tdwg.org/dwc/terms/decimalLongitude"/>
    <field index="13" term="http://rs.tdwg.org/dwc/terms/scientificNameID"/>
    <field index="14" term="http://rs.tdwg.org/dwc/terms/scientificName"/>
    <field index="15" term="http://rs.tdwg.org/dwc/terms/kingdom"/>
    <field index="16" term="http://rs.tdwg.org/dwc/terms/phylum"/>
    <field index="17" term="http://rs.tdwg.org/dwc/terms/class"/>
    <field index="18" term="http://rs.tdwg.org/dwc/terms/order"/>
    <field index="19" term="http://rs.tdwg.org/dwc/terms/family"/>
    <field index="20" term="http://rs.tdwg.org/dwc/terms/genus"/>
  </core>
</archive>
```



Darwin Core quick reference guide

- https://dwc.tdwg.org/terms/

Darwin Core extensions

- https://rs.gbif.org/extension/

Darwin core validator

- https://www.gbif.org/tools/data-validator/about

Darwin core instructions

- https://manual.obis.org/

MAKE YOUR DATA FAIR

Make a plan for the data before you start a project!

Collect detailed descriptive information (= metadata) throughout

Use standards and formats common to your discipline

Store the data in a trusted & sustainable repository or data center

See to that the data gets persistent identifiers (DOIs)

Recording and publishing data

Which variables? TDWG Vocabulary

Some Required by repo:

Occurrence Core	Event Core
occurrenceID	eventID
basisOfRecord	
scientificName	
scientificNameID	
occurrenceStatus	
decimalLongitude	
decimalLatitude	
eventDate	eventDate

Many more optional or recommended

Occurrence Core	Event Core
occurrenceStatus	parentEventID
recordedBy	minimumDepthInMeters
taxonRank	
kingdom	
coordinateUncertaintyInMeters	
individualCount	

Useful Links

- https://manual.obis.org/index.html
- https://dwc.tdwg.org/terms/

Consistency

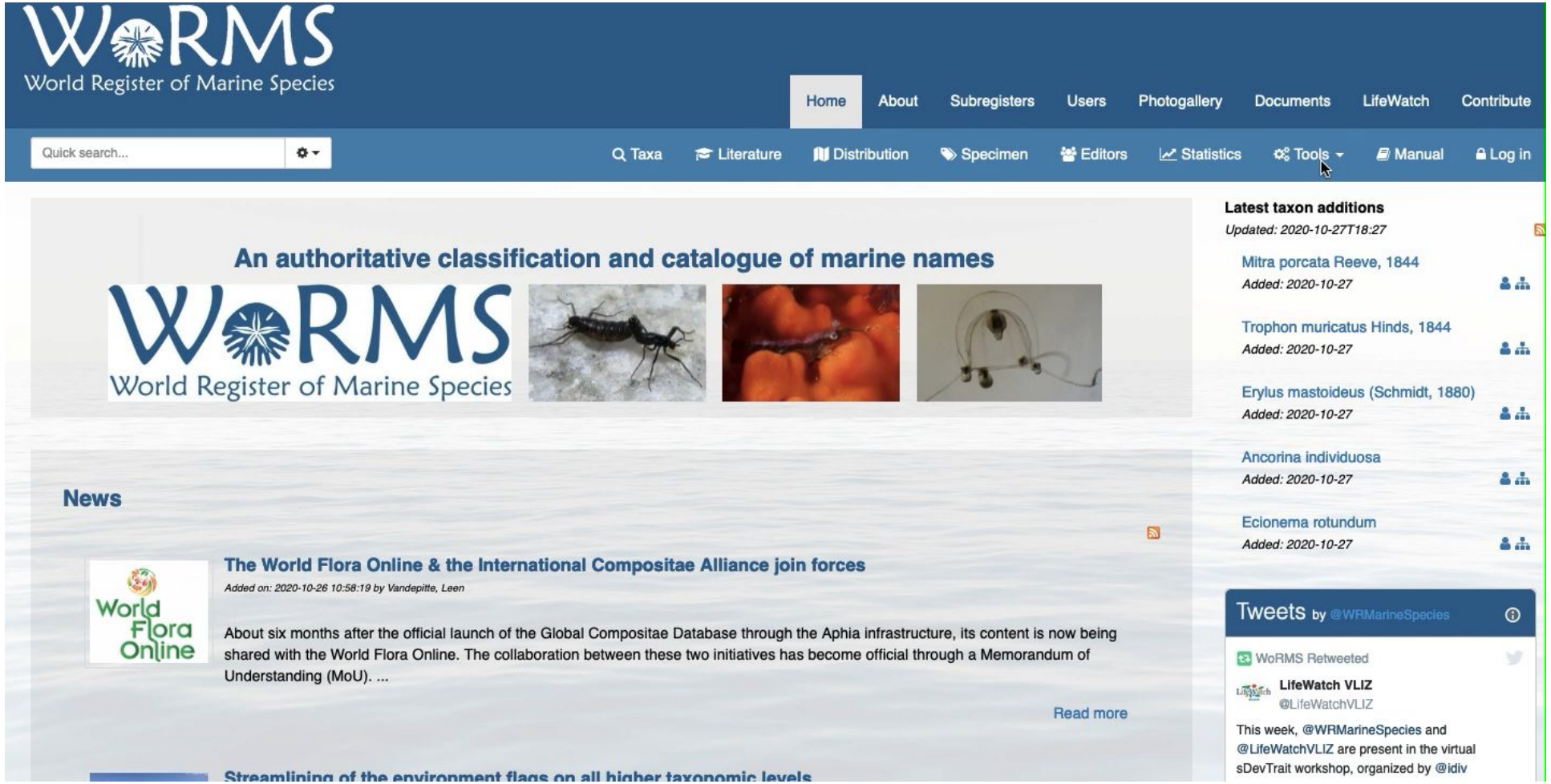
Geographic coordinates

- Type of decimal point
- Order of longitude, latitude
- Degree minute second vs degree decimal minute
- Padding with 0

verbatimCoordinates
58°28'30''W, 62°7'0,10''S
58°28'42,00''W, 62°7'15,00''S
62°08.0958'S, 058°24,1625'W
62°10.4680'S, 058°25.2137'W
62°09.7174'S, 058°21,5886'W
62°11.2075'S, 058°18,9951W
62°11.9764'S, 058°22.5800W
62°12.1942'S, 058°23.4483'W
62°53.6407'S, 58°26.8232'W

Taxonomy

Match scientific name to taxon using WoRMS taxon match service



Taxonomy

Keep original scientific name
Use persistent identifier to refer to the taxon in a checklist

Do not change to accepted scientific name

scientificName	scientificNameAuthorship	scientificNameID	taxonomicStatus	taxonRank
Akanthophoreus antarcticus	(Vanhöffen, 1914)	urn:lsid:marinespecies.org:taxname:448316	unaccepted	species
Akanthophoreus multiserratus	(Hansen, 1913)	urn:lsid:marinespecies.org:taxname:136343	unaccepted	species

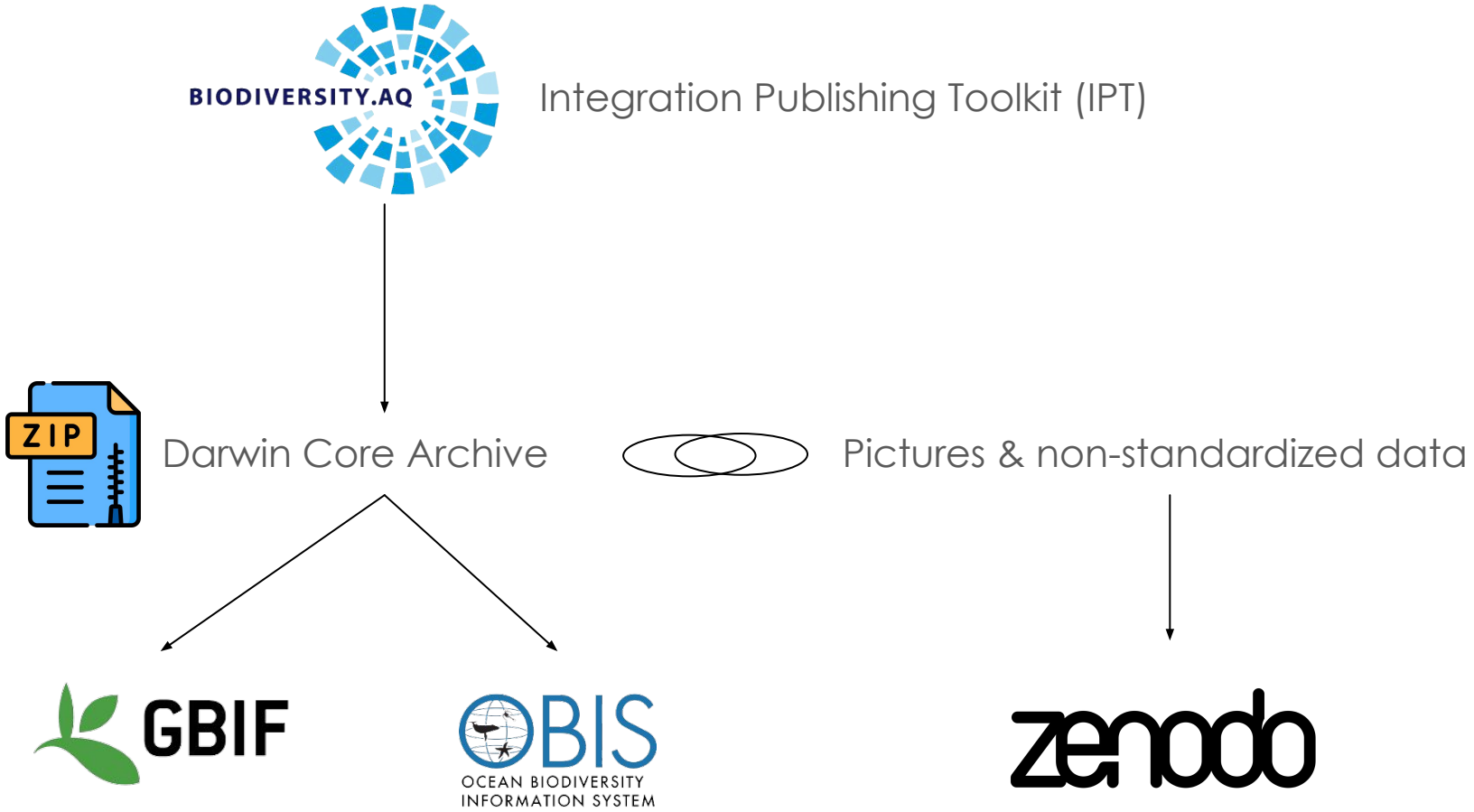
Persistent identifiers

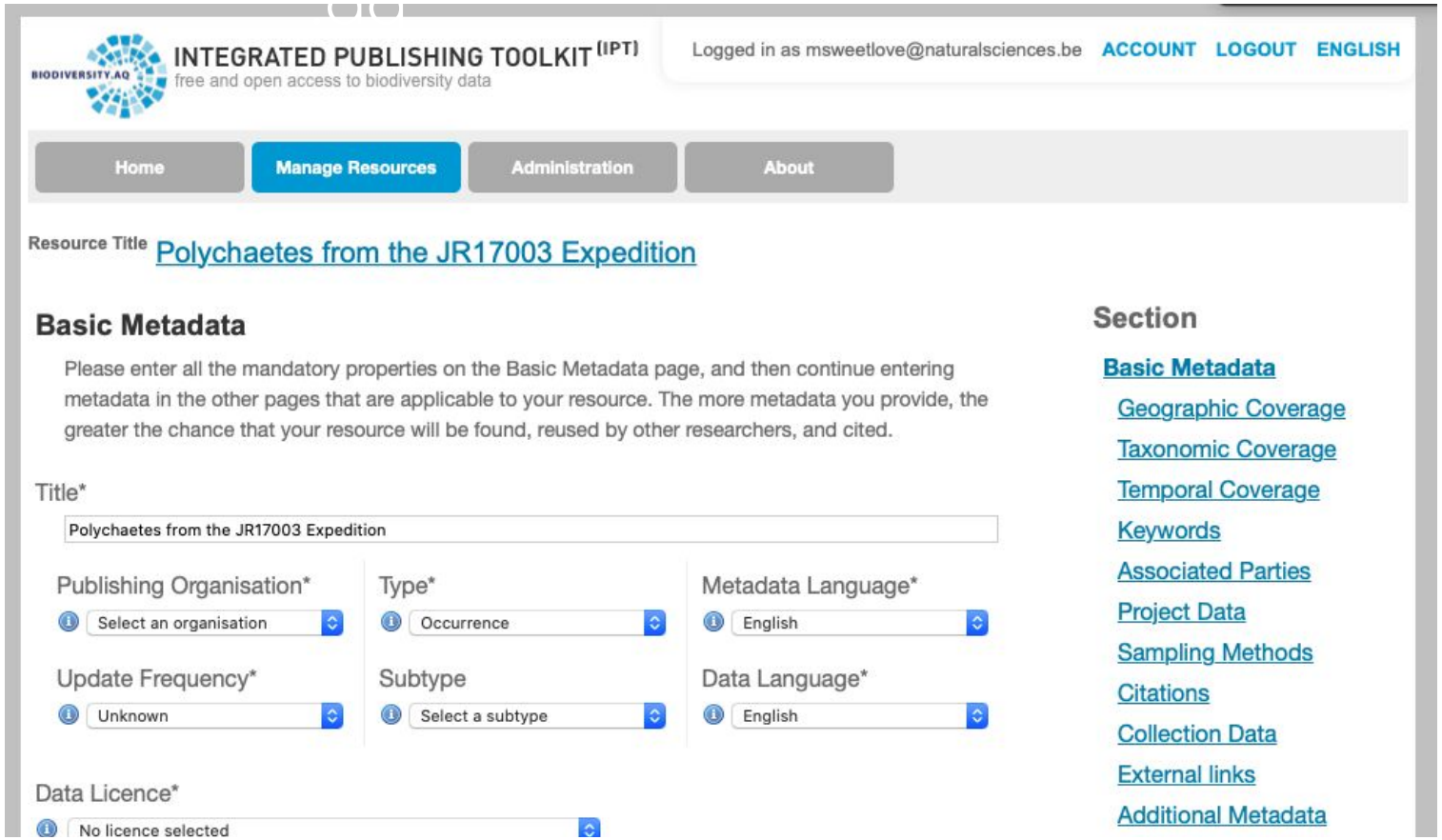
Useful links

- https://dwc.tdwg.org/terms/
- https://www.marinespecies.org/
- https://www.doi.org/

Uploading to repository

Biodiversity repositories




INTEGRATED PUBLISHING TOOLKIT (IPT)
free and open access to biodiversity data
Logged in as msweetlove@naturalsciences.be ACCOUNT LOGOUT ENGLISH
Home
Manage Resources
Administration
About
Resource Title Polychaetes from the JR17003 Expedition
Basic Metadata
Please enter all the mandatory properties on the Basic Metadata page, and then continue entering metadata in the other pages that are applicable to your resource. The more metadata you provide, the greater the chance that your resource will be found, reused by other researchers, and cited.
Title*
Polychaetes from the JR17003 Expedition
Publishing Organisation*
Select an organisation
Type*
Occurrence
Metadata Language*
English
Update Frequency*
Unknown
Subtype
Select a subtype
Data Language*
English
Data Licence*
No licence selected
Section
Basic Metadata
Geographic Coverage
Taxonomic Coverage
Temporal Coverage
Keywords
Associated Parties
Project Data
Sampling Methods
Citations
Collection Data
External links
Additional Metadata

Darwin Core Archive Dataset metadata is very similar to Pensoft Data Paper

not in Darwin Core Archive dataset metadata

Screenshot from ARPHA Writing Tool

Links

https://GBIF.org

https://OBIS.org

www.biodiversity.aq

https://ipt.biodiversity.aq/

https://zenodo.org/

Are your data FAIR?

- ANDS FAIR self-assessment tool

https://ardc.edu.au/resources/working-with-data/fair-data/fair-self-assessment-tool/

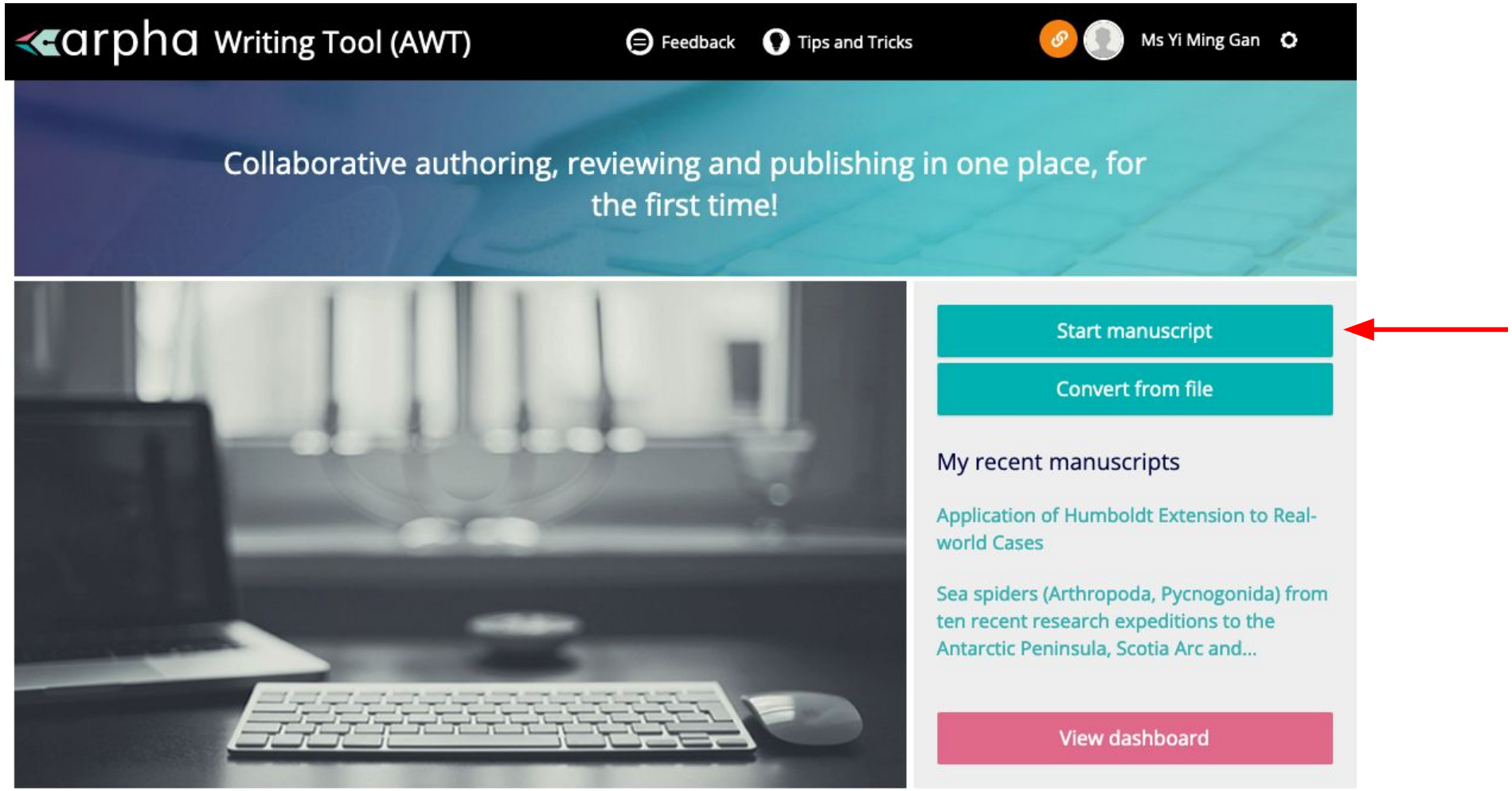
- FAIRDAT assessment tool (prototype)

https://www.surveymonkey.com/r/fairdat

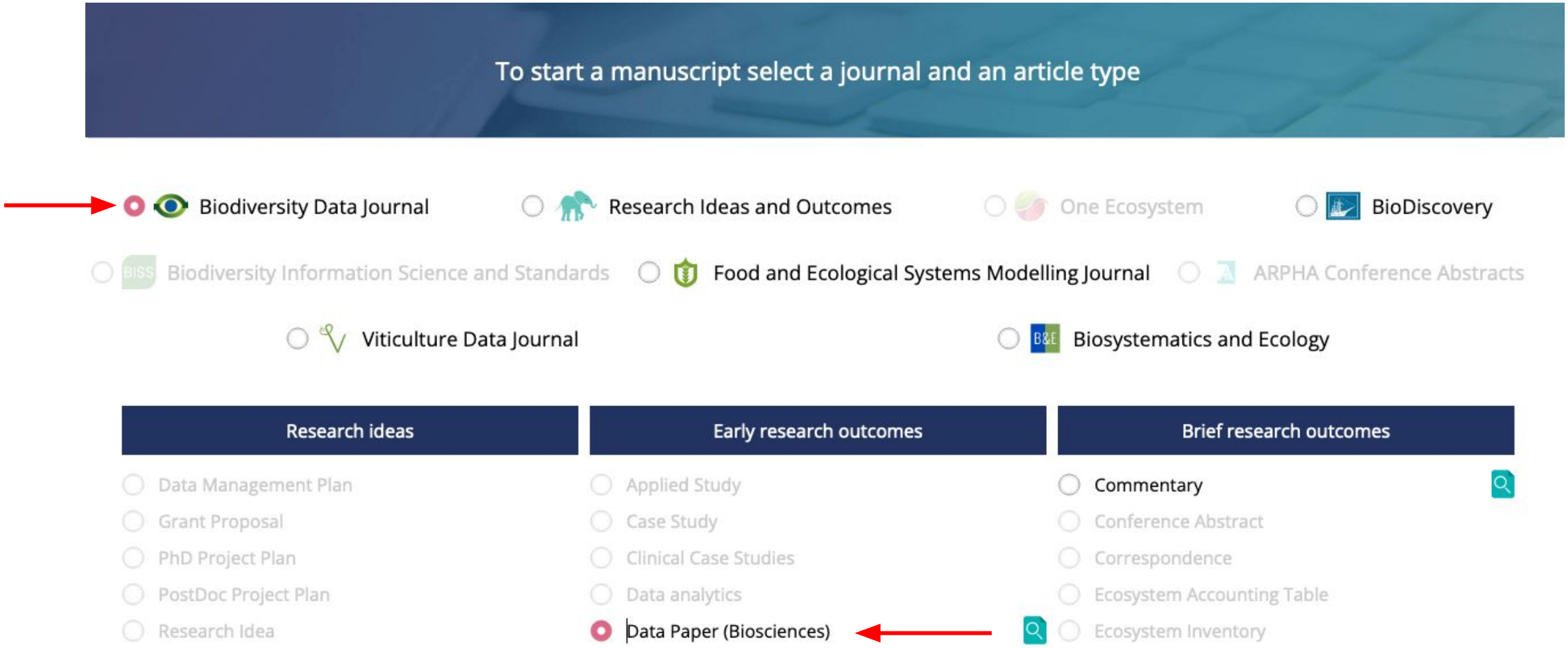
- How FAIR is your data?

https://forms.gle/eBagszpWKVz5NKpp7

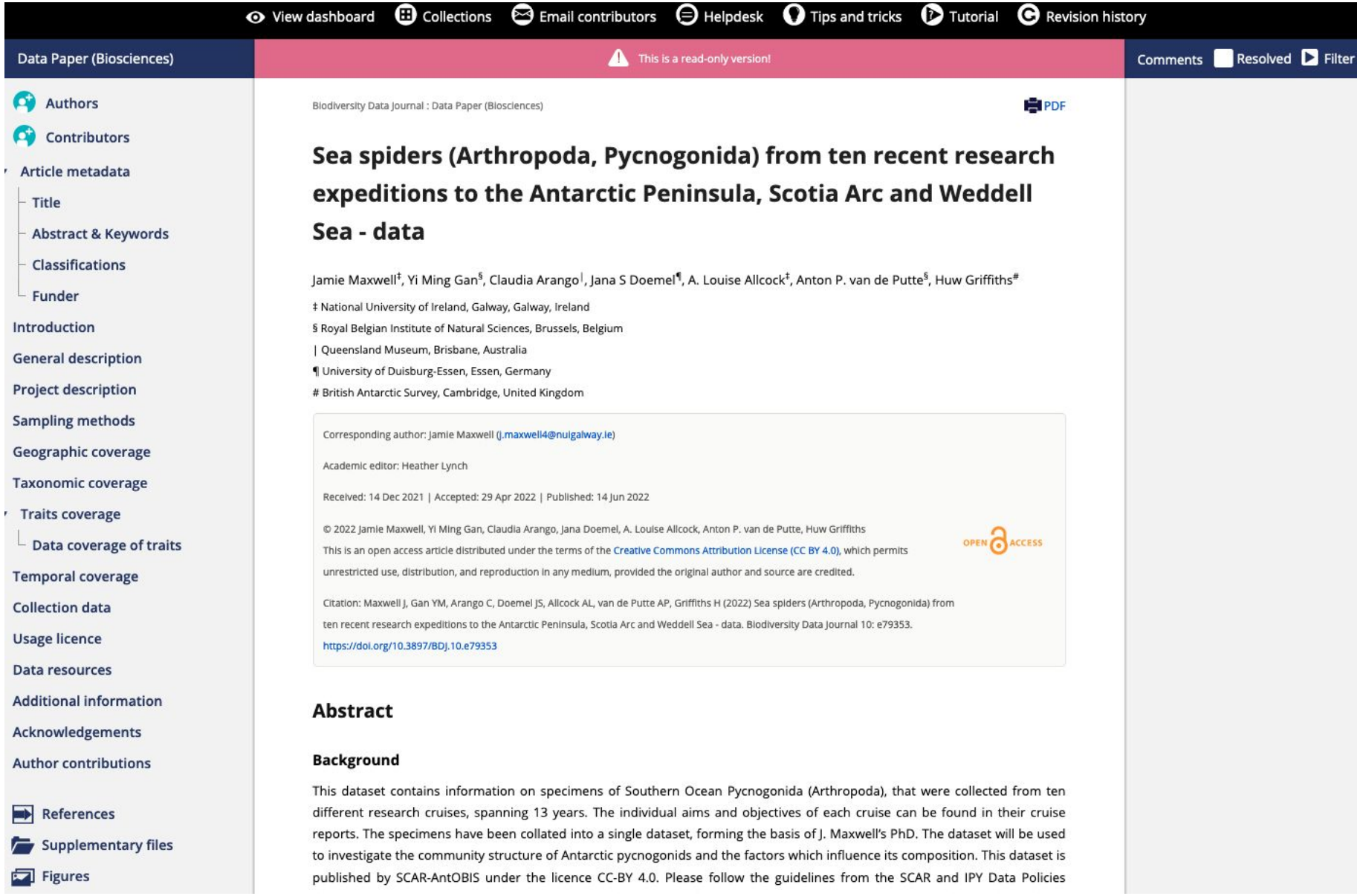
How to use ARPHA writing tool



Select BDJ & Data Paper (Biosciences) article type



ARPHA writing tool interface



Example data paper: https://bit.ly/3JyNfl4

FAQ

Kudos to everyone who sent in the example dataset

What is expected for this topical collection?

2 publications are expected, but they are almost identical

BIODIVERSITY.AQ

What is expected after you submitted your manuscript to BDJ?

Someone will audit your data before your data paper can go to review

Data audit based on:
https://zookeys.pensoft.net/about#DataQualityChecklistandRecommendations

eventDate that conforms to ISO8601 standard

https://en.wikipedia.org/wiki/ISO_8601

Adapted from: https://www.instagram.com/punhubinsta/

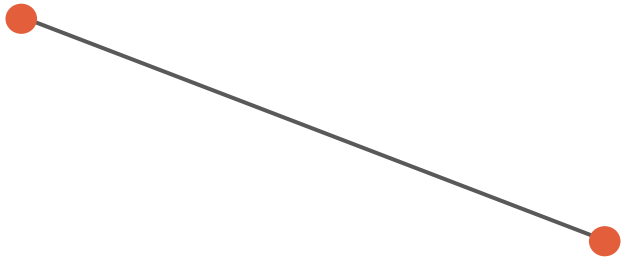
Uncertain temporal scope

All these are ok:

eventDate		year	month	day	
2022-08		2022	08		day unknown
2022		2022			month & day unknown
2020/2022					if year unknown, provide known year range

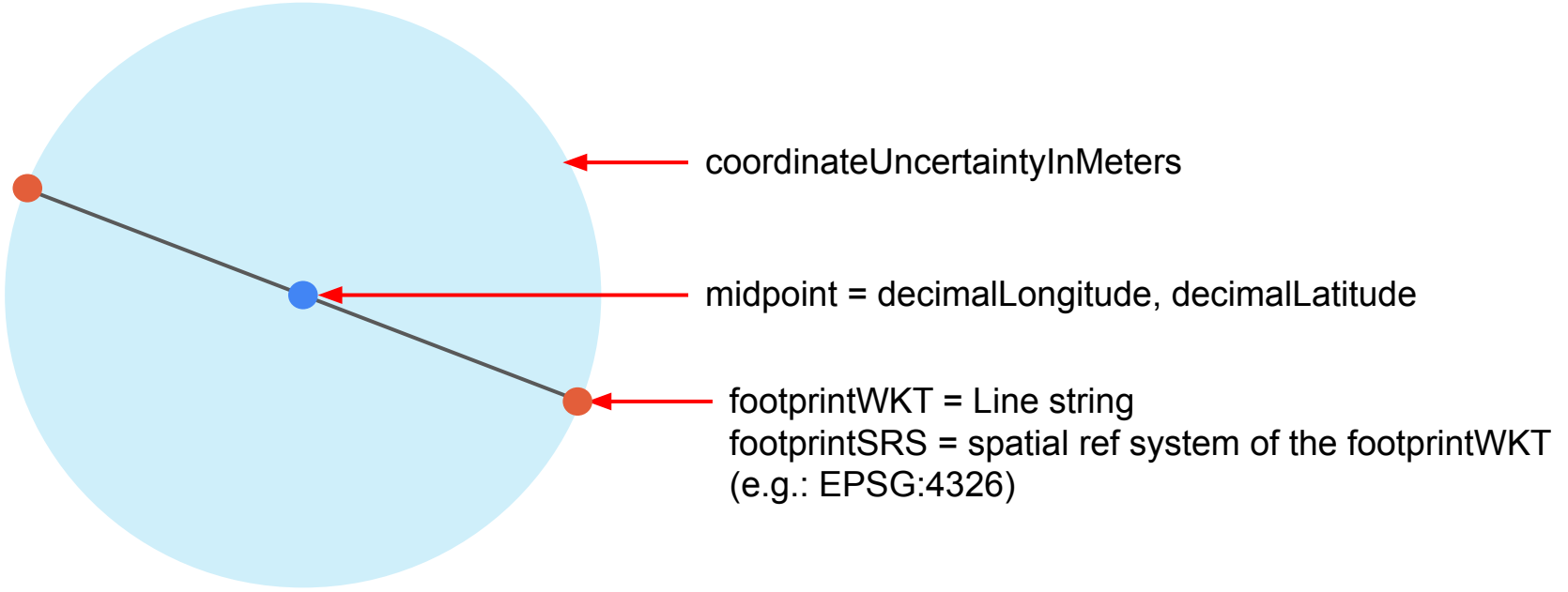
eventDate still conforms to ISO8601 standard

What if my sampling location is not a point? (e.g. trawl)



start point & end point

What if my sampling location is not a point? (e.g. trawl)



footprintWKT	footprintSRS	decimalLongitude	decimalLatitude	coordinateUncertaintyInMeters
LINESTRING (-29.42462 -74.67411, -29.43436 -74.67504)	EPSG:4326	-29.4295	-74.6746	153

coordinateUncertaintyInMeters is strongly recommended in GBIF & OBIS, please provide it regardless

Precision of decimalLongitude & decimalLatitude

decimalLongitude	decimalLatitude	geodeticDatum	coordinatePrecision	coordinateUncertaintyInMeters
-29.42	-74.67	EPSG:4326	0.01	1155
-29.4200	-74.6700	EPSG:4326	0.0001	12

Excel conversion may lead to coordinates with more decimal places than it should be

“sp.” “cf.” in identificationQualifier

scientificName	identificationQualifier	scientificNameID	genus	taxonRank
Caprella	sp.	urn:lsid:marinespecies.org:taxname:101430	Caprella	genus

Keep the most confident identification in scientificName column

Some fields are paired

organismQuantity	Property
Identifier	http://rs.tdwg.org/dwc/terms/organismQuantity
Definition	A number or enumeration value for the quantity of organisms.
Comments	An organismQuantity must have a corresponding organismQuantityType.
Examples	`27` (organismQuantity) with `individuals` (organismQuantityType). `12.5` (organismQuantity) with `% biomass` (organismQuantityType). `r` (organismQuantity) with `Braun Blanquet Scale` (organismQuantityType). `many` (organismQuantity) with `individuals` (organismQuantityType).

organismQuantityType	Property
Identifier	http://rs.tdwg.org/dwc/terms/organismQuantityType
Definition	The type of quantification system used for the quantity of organisms.
Comments	A dwc:organismQuantityType must have a corresponding dwc:organismQuantity.
Examples	`27` (organismQuantity) with `individuals` (organismQuantityType). `12.5` (organismQuantity) with `%biomass` (organismQuantityType). `r` (organismQuantity) with `BraunBlanquetScale` (organismQuantityType).

No vocabulary suits my data

lifeStage	
Identifier	http://rs.tdwg.org/dwc/terms/lifeStage
Definition	The age class or life stage of the Organism(s) at the time the Occurrence was recorded.
Comments	Recommended best practice is to use a controlled vocabulary.
Examples	`zygote` , `larva` , `juvenile` , `adult` , `seedling` , `flowering` , `fruiting`

- Use commonly used term
- include remarks in relevant ____Remarks field: organismRemarks, eventRemarks, occurrenceRemarks etc…

Darwin Core Quick Reference Guide: https://dwc.tdwg.org/terms/

No vocabulary suits my data

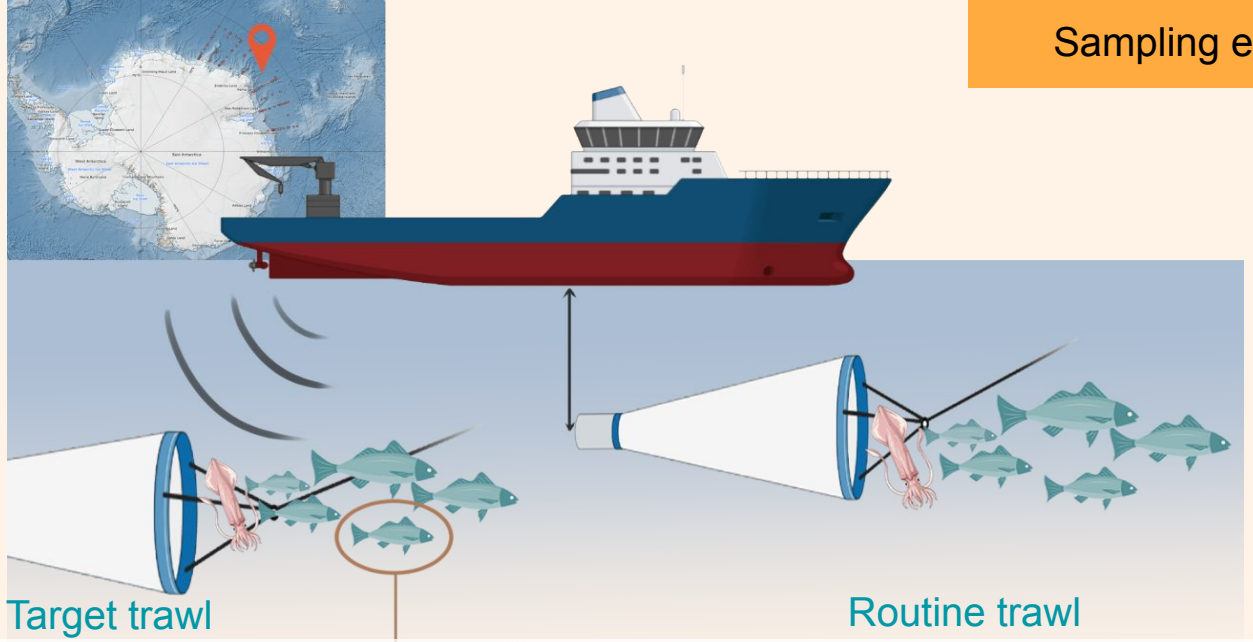
lifeStage	organismRemarks
chicks	chicks are age 0 juveniles but older than newborns

Use full name & full link in recordedBy(ID), identifiedBy(ID)

recordedBy	recordedByID	
Yi-Ming Gan	https://orcid.org/0000-0001-7087-2646	Recommended
YM Gan	0000-0001-7087-2646	common name without recordedByID is confusing, ORCID is implicit here

Sampling event core

An **action** that occurs at some **location** during some **time**.



Station grid 2006-01-17/2006-03-03
POLYGON(30 -69, 30 -32,147 -32, 147 -69)

- Sampling station with target trawl
- Sampling station with routine trawl

Identification

Preservation method

Body length

Gut content for calorimetry

Occurrence extension

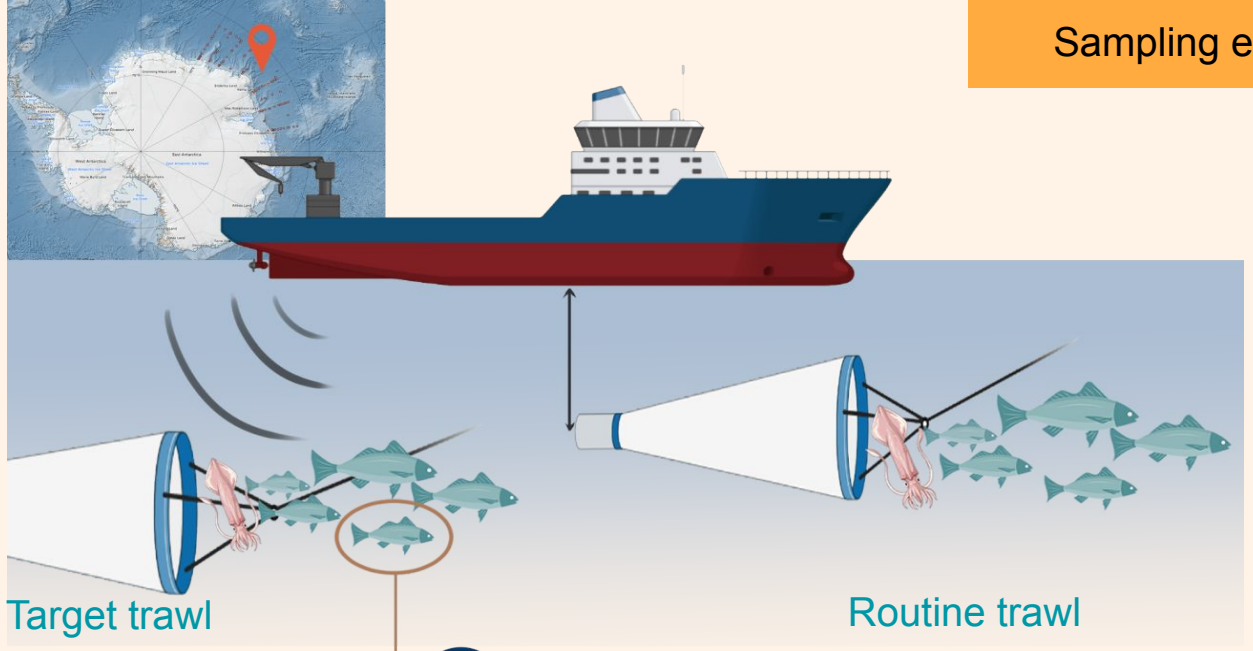
scientificName	occurrence Status	preparations
Notolepis coatsi	Present	Formalin

eMOF extension

measurementType	measurement Value	measurement Unit
Sample volume	30320	m^3
Body length	67	mm
Energy content dry weight	25.88	KJ/g

Sampling event core

An **action** that occurs at some **location** during some **time**.



Station grid 2006-01-17/2006-03-03
POLYGON(30 -69, 30 -32,147 -32, 147 -69)

- Sampling station with target trawl
- Sampling station with routine trawl

Identification

Preservation method

Occurrence extension

An existence of an **Organism** at a particular **place** at a particular **time** (sampling event)

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Notolepis coatsi	Present	Formalin

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Energy content dry weight	25.88	KJ/g

Body length

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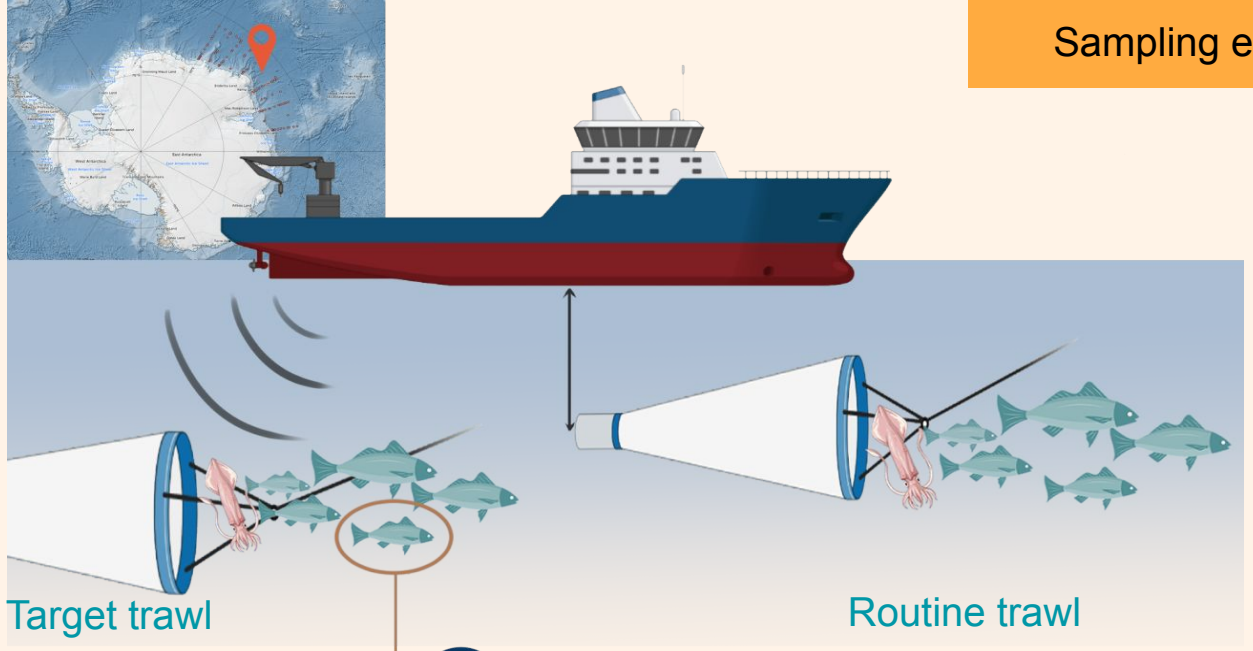

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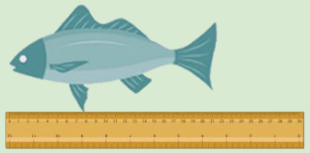

Body length

Gut content for calorimetry