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Introduction to netCDF Files With CF Metadata Conventions

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Outline

- 1. About netCDF files:
 - a. History
 - b. Usage
- 2. Importance of metadata
- 3. CF Metadata Conventions:
 - a. History
 - b. Usage details:
 - i. Identifying physical quantities via their "standard_name" representation
 - ii. Representing different data geometries through "featureType"
 - iii. Suggested minimum list of metadata fields

NetCDF History

- "Network Common Data Format", concepts built on previous "Common Data Format" by NASA but not compatible with it
- UCAR ("University Corporation for Atmospheric Research"), a US-based nonprofit organization
- <u>https://www.unidata.ucar.edu/software/netcdf/</u>
- Software libraries to read/write (scientific) data files
- Original specifications released 1990 ("classic" netCDF format)
- Current versions have additional features, incl. compatibility with HDF5 format commonly used in astrophysics

NetCDF Usage

- Data are usually N-dimensional arrays (of numbers)
- Binary file format requires special software to read/write
- Metadata is included with data files are "self-explanatory"
- Can access subsets of data (for improved computer efficiency with large datasets)
- Widely used in meteorology and oceanography:
 - Numerical weather/climate models
 - Argo floats, OceanSITES moorings, satellite altimetry, ...



Importance of Metadata, or: "What's This?"

You find a file called "SriLanka_Data.dat" with the following lists of numbers.

What could they mean?

[23695.083 23695.167 23695.250 23695.333 ...]

[604.135	604.134	604.134	604.134]
[3889.274	3889.274	3889.273	3889.273]
[645.442	645.442	645.442	645.442]
Ē	4408.656	4408.656	4408.656	4408.655]

Importance of Metadata, or: "What's This?"

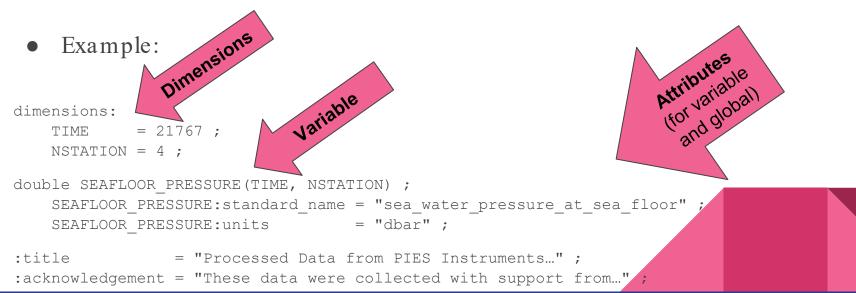
title	Processed Data from PIES Instruments (Pressure-Sensing Inverted Echo Sounders) Collected in the Sri Lankan Boundary Currents between 2014 and 2019					
summary	= 'In 2014/15, PIES instruments (Pressure-Sensing Inverted Echo Sounders) were deployed at four sites that span the boundary currents around Sri Lanka. Two sites are east, and two south of Sri Lanka. PIES are seafloor instruments that make observations of the water pressure and the travel time of a vertically transmitted acoustic signal. Data from these instruments are reported here, in a processed version that is on a common time grid with sensor drifts removed, and tidal signals separated out of the pressure records. The scientific rationale for collecting these data is to monitor the strengths of the boundary current flows.'					
<pre>publisher_name publisher_url contributor_name contributor_role time_coverage_start time_coverage_end</pre>	<pre>publisher_name = 'Matthias Lankhorst' publisher_url = 'https://orcid.org/0000-0002-4166-4044' contributor_name = 'Nilanthi Priyadarshani, Uwe Send' contributor_role = 'principal investigator, principal investigator' time_coverage_start = '2014-11-15T08:00:00Z'</pre>					
<pre>TIME [23695.083 23695.167 23695.250 23695.333] Size: 21767x1 Dimensions: TIME Datatype: double Attributes: units = 'days since 1950-01-01T00:00:00Z' standard_name = 'time' axis = 'T'</pre>						
SEAFLOOR PRESSURE Size: 4x2 Dimensions: NST Datatype: dou Attributes:	[604.135 604.134 604.134] 21767 [3889.274 3889.274 3889.273 3889.273] TATION,TIME [645.442 645.442 645.442] able [4408.656 4408.656 4408.656 4408.655]					
standard_name units comment	<pre>= 'sea_water_pressure_at_sea_floor' = 'dbar' = 'Sensor drift has been removed, and data have been low-pass filtered. Tides have been removed and are available in a separate variable.'</pre>					
ancillary_vari coordinates	Lables = 'SEAFLOOR PRESSURE TIDES' = 'LONGITUDE LATITUDE DEPTH TIME SITE_NAME'					

Take-Home Message:

Metadata are important. Without metadata, the data are only meaningless numbers.

NetCDF File Contents

- Variables: the structures that hold the "numbers"
- **Dimensions**: the "sizes" of the variables
- Attributes : metadata fields
 - Can be associated with a single variable, or
 - with the entire file ("global" attribute)



Take-Home Message:

What do netCDF files contain?

Variables, dimensions, and attributes.

CF Metadata Conventions

- "Climate and Forecast", <u>http://cfconventions.org/</u>
- Additional reference: Hassell et al., 2017. <u>doi:10.5194/gmd-10-4619-2017</u>
- History:
 - Builds on COARDS conventions (1990s, Cooperative Ocean/Atmosphere Research Data Service, a collaboration between US NOAA and universities)
 - Governed by a panel and committees, typically professionals volunteering some of their time to this service, "community-driven"
 - CF Version 1.0 released in 2003
- Assumes (but does not strictly require) netCDF files
- Principles: self-describing files, metadata readable by people and software, ...
- Intended use: climate science (meteorology, oceanography, ..)

CF Metadata Conventions

Side note: ACDD

- Attribute Convention for Data Discovery
- <u>https://wiki.esipfed.org/Attribute_Convention_for_Data_Discovery</u>
- Provides additional standards for basic metadata information (title, authorship, ..)
- Compatible with CF
- Many applications in oceanography use both CF and ACDD



CF Metadata Conventions

- Global attributes :
 - Long list of metadata fields to describe file content, authors, institutions, acknowledgments, use restrictions, etc.
 - Fields for overall time and space extent covered by the data (time, lat/lon, depth ranges)
- Assumption that data are located in space/time
 - "Coordinate variables" contain time, latitude, longitude, depth/height (or pressure)
 - Regular data variables are linked to their coordinates (several methods exist)
- Physical quantity inside a variable is defined via (a variable-level) attribute called "**standard_name**" (i.e. not the name of the variable itself)
 - List of names, their definitions and canonical units: <u>http://cfconventions.org/Data/cf-standard-names/current/build/cf-standard-name-table.html</u>
- Units for a variable are defined via an attribute called "units"
 - Use only those that the software "UDUNITS" understands, cf.: <u>https://docs.unidata.ucar.edu/udunits/current/</u>

Practice: What are the "global attributes" on this page?

title	Processed Data from PIES Instruments (Pressure-Sensing Inverted Echo Sounders) Collected in the Sri Lankan Boundary Currents between 2014 and 2019'
summary	= 'In 2014/15, PIES instruments (Pressure-Sensing Inverted Echo Sounders) were deployed at four sites that span the boundary currents around Sri Lanka. Two sites are east, and two south of Sri Lanka. PIES are seafloor instruments that make observations of the water pressure and the travel time of a vertically transmitted acoustic signal. Data from these instruments are reported here, in a processed version that is on a common time grid with sensor drifts removed, and tidal signals separated out of the pressure records. The scientific rationale for collecting these data is to monitor the strengths of the boundary current flows.'
publisher_name publisher_url contributor_name contributor_role time_coverage_start time_coverage_end	<pre>= 'Matthias Lankhorst' = 'https://orcid.org/0000-0002-4166-4044' = 'Nilanthi Priyadarshani, Uwe Send' = 'principal investigator, principal investigator' = '2014-11-15T08:00:00Z' = '2019-11-03T04:00:00Z'</pre>

[23695.083 23695.167 23695.250 23695.333 ...]

Size: 2 Dimensions: T Datatype: d Attributes: units standard_na axis	IME louble me =	'days since 1 'time' 'T'	1950-01-01T00:	00:002'			-
SEAFLOOR_PRESSUR Size: Dimensions: Datatype: Attributes:	4x21767 NSTATION,		[604.135 [3889.274 [645.442 [4408.656	3889.274 645.442	645.442	3889.273 645.442]
standard_na units comment	:	= 'dbar' = 'Sensor drif	pressure_at_se ift has been re removed and ar	moved, and			ss filtered. Tides Le.'
ancillary variables = 'SEAFLOOR PRESSURE TIDES' coordinates = 'LONGITUDE LATITUDE DEPTH TIME SITE_NAME'							

TIME

Practice: What defines physical quantities on this page?

title	= 'Processed Data from PIES Instruments (Pressure-Sensing Inverted Echo Sounders)					
<pre>Summary Collected in the Sri Lankan Boundary Currents between 2014 and 2019' = 'In 2014/15, PIES instruments (Pressure-Sensing Inverted Echo Sounders) were deployed at four sites that span the boundary currents around Sri Lanka. Two sites are east, and two south of Sri Lanka. PIES are seafloor instruments that make observations of the water pressure and the travel time of a vertically transmitted acoustic signal. Data from these instruments are reported here, in a processed version that is on a common time grid with sensor drifts removed, and tidal signals separated out of the pressure records. The scientific rationale for collecting these data is to present the astronometer of the boundary current for the pressure to be present for the pressure to be pressure to be present for the pressure to be pressure</pre>						
<pre>publisher_name publisher_url contributor_name contributor_role time_coverage_star time_coverage_end</pre>	<pre>publisher_url = 'https://orcid.org/0000-0002-4166-4044' contributor_name = 'Nilanthi Priyadarshani, Uwe Send' contributor_role = 'principal investigator, principal investigator' time_coverage_start = '2014-11-15T08:00:00Z'</pre>					
TIME Size: 217 Dimensions: TIM Datatype: dou Attributes: units standard_name						
Dimensions: NS Datatype: do Attributes:	uble [4408.656 4408.656 4408.656 4408.655]					
standard_name	= 'sea_water_pressure_at_sea_floor'					
comment	= 'Sensor drift has been removed, and data have been low-pass filtered. Tides have been removed and are available in a separate variable.'					
ancillary_variables = 'SEAFLOOR PRESSURE TIDES' coordinates = 'LONGITUDE LATITUDE DEPTH TIME SITE_NAME'						

CF: More on Coordinate Variables

Different options to provide a **variable** that is From previous example: a **coordinate variable**:

- 1. Its dimension has the same name as the variable itself.
- It has a "standard_name" attribute that is known to be geospatial information, such as "latitude", "longitude", "time", "depth", "height", "pressure".
- 3. It has an attribute called "axis", with content "X", "Y", "Z", or "T".

```
TIME

Size: 21767x1

Dimensions: TIME

Datatype: double

Attributes:

units = 'days since 1950-01-01T00:002'

standard_name= 'time'

axis = 'T'
```

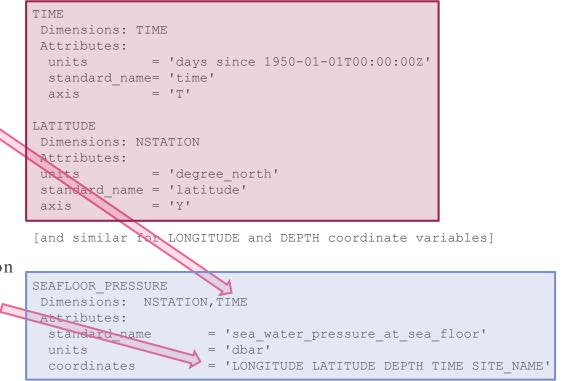
(Note: Not all of these options need to be present!)

CF: Even More on Coordinate Variables

Data (in regular variables) are linked to the coordinate variables (spatiotemporal) by any of the following:

- A dimension that is also the name of both a coordinate variable and its dimension,
- 2. An attribute called "coordinates" that lists names of coordinate variables (example on right has no lat/lon coordinates for option 1. because they do not vary independently).

From previous example:



Take-Home Message:

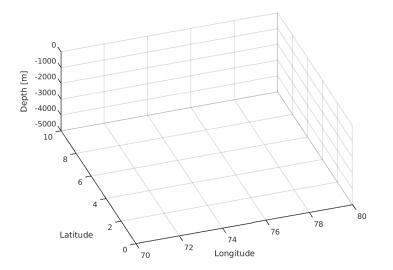
Coordinate variables locate data in X, Y, Z, T.

Attributes "standard_name" and "units" define physical quantity and units of measure.

Use case: Output from a numerical ocean model on a 4-d (X-Y-Z-T) grid

Variable **LATITUDE** (Dimensions: ???)

...other coordinate variables ???



Variable **SALINITY** (Dimensions: ???)

Use case: Output from a numerical ocean model on a 4-d (X-Y-Z-T) grid

Variable **LATITUDE** (Dimensions: LATITUDE)

Variable LONGITUDE (Dimensions: LONGITUDE)

Variable **DEPTH** (Dimensions: DEPTH)

Variable **TIME** (Dimensions: TIME)

Variable **SALINITY** (Dimensions: LATITUDE x LONGITUDE x DEPTH x TIME)

Use case: Output from a glider that travels along a path through space

Variable **LATITUDE** (Dimensions: ???)

...other coordinate variables ???

Variable **SALINITY** (Dimensions: ???)



Use case: Output from a glider that travels along a path through space

Variable **LATITUDE** (Dimensions: TIME)

Variable LONGITUDE (Dimensions: TIME)

Variable **DEPTH** (Dimensions: TIME)

Variable **TIME** (Dimensions: TIME)

Variable **SALINITY** (Dimensions: TIME) SALINITY:coordinates = "LATITUDE LONGITUDE DEPTH TIME"

CF: featureType

Current versions of CF have (optional!) specifications for discrete sampling geometries that describe the "logic" in dimensionality and coordinates for different situations.

- Global attribute "featureType" defines what the sampling geometry is.
- Proper use of the "coordinates" attribute for variables links each variable to its spatiotemporal coordinates
- If there are multiple instances of a feature (e.g. multiple glider trajectories) in one file, there should be a coordinate variable that is designated as the ID for each instance, through the attribute "cf_role"
- Representation via ragged (compressed) arrays exist
- Current definitions: point, timeSeries, trajectory, profile, timeSeries Profile, trajectoryProfile

CF: featureType "trajectory"

Example: data from an underwater glider

All data collected along a trajectory in 3d-space, with the vehicle traveling along that trajectory as time progresses.

Dimensions: TIME

Coordinate variables and their dimensions:

TIME(TIME), DEPTH(TIME), LATITUDE(TIME), LONGITUDE(TIME)

Data variables and their dimensions:

DATA(TIME)



CF: featureType "timeSeries"

Example: seafloor pressure data from a PIES instrument

All data collected at the same location in space as a time series.

Dimensions: TIME

Coordinate variables and their dimensions:

TIME(TIME), DEPTH(1), LATITUDE(1), LONGITUDE(1)

Data variables and their dimensions:

DATA(TIME)



CF: featureType "profile"

Example: a CTD cast or an Argo float profile

All data collected at the same time and horizontal location, but as a function of depth.

Dimensions: DEPTH

Coordinate variables and their dimensions:

TIME(1), DEPTH(DEPTH), LATITUDE(1), LONGITUDE(1)

Data variables and their dimensions:

DATA(DEPTH)



CF: featureType "timeSeriesProfile"

Example: repeat CTD casts at the same station, or a mooring with multiple sensors in the water column

Multiple profiles collected after one another at the same location.

Dimensions: TIME, DEP TH

Coordinate variables and their dimensions:

TIME(TIME), DEP TH(DEP TH), LATITUDE(1), LONGITUDE(1)

Data variables and their dimensions:

DATA(TIME, DEPTH)



Take-Home Message:

"featureType" describes discrete sampling geometries and the corresponding linkage/dimensionality of variables and their coordinates.

Practice: What Metadata is Useful?

(Students suggest metadata to address questions about a dataset)

What?	Who?	Why?	How?	Where?	When?

Take-Home Messages:

- Need metadata to understand the data!
- NetCDF files contain variables, dimensions, and attributes.
- Coordinate variables for X, Y, Z, T
- Attributes "standard_name" and "units" define physical quantity in a variable, and its units
- Attribute "featureType" to describe sampling geometries (profiles, time series) with different coordinate "logic"

Practice: Inspect Contents of a netCDF File

(Read metadata and data of an example file)