

Planning the next GHRSSST Data Specification Document

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Summary



Collaborative editing and reviewing process

Planning evolutions and sharing the work

Editing the GDS - the old way

- GDS document became hardly manageable
 - big word document, not editable in libreoffice, gets mixed up through various word editors or human editors, losing content, images, ... hard to recover and clean
 - inserting ncdump or code examples is a nightmare - does not help for maintaining consistency
 - history of main changes and versions not properly tracked
 - not practicable for collaborative work => one people to maintain and fix it
 - need to engage GHRSST producers more during inter GHRSST periods
 - updates needs to happen online - we don't want to discuss this in GHRSST workshops
- from user perspective
 - not easy to navigate, difficult to quickly go to relevant examples and templates
 - usage does not fit “sequential” structure of document, lack of links and jumps to cross-references
 - many inconsistencies (between different sections, dead links, obsolete content, examples are not always updated,...)

The new way : jupyter book

adopting jupyter book
(consensus G25)

generation and publication of
document based on release
tags

possibility to revert to or
re-generate any older
(tracked) version

avoid formatting and cleaning
issues (fonts, ...)

sharing the document, full
traceability of changes

conversion for G26

<https://ghrsst.github.io/GDS/>

Skip to main content

 **GHRSST**
Group for High Resolution
Sea Surface Temperature

Search Ctrl + K

The Recommended GHRSST Data Specification (GDS) Version 2.2r0

- 1. Document Conventions
- 2. Overview of GHRSST and the GDS-2.2r0
- 3. Sea Surface Temperature
- 4. GDS Filenames and Supporting Conventions
- 5. GDS Data Product File Structure and attributes
- 6. Coordinate variables
- 7. Level 2 Pre-processed (L2P) Product Specification**
- 8. Level 3 (L3) Product Specification
- 9. Level 4 (L4) Product Specification

7.2.1. `sea_surface_temperature`

The variable `sea_surface_temperature` contains the native unmodified L2 SST of the input data file. L2 SST data are not adjusted in any manner and are identical to the input data set.

The `sea_surface_temperature` variable shall be included in a L2P product with the format requirements shown in table [Table 7.3](#).

Table 7.3 CDL example description of `sea_surface_temperature` variable

Storage type	Name	Description	Unit
short	<code>sea_surface_temperature</code>	Pixel sea surface temperature value	K (kelvin)

```
short sea_surface_temperature(time, nj, ni) ;
  sea_surface_temperature:_FillValue = -32768s ;
  sea_surface_temperature:long_name = "sea surface subskin temperature" ;
  sea_surface_temperature:standard_name = "sea_surface_subskin_temperature" ;
  sea_surface_temperature:units = "K" ;
  sea_surface_temperature:depth = "1 millimeter" ;
  sea_surface_temperature:source = "AVHRR_METOP_C" ;
  sea_surface_temperature:comment = "Temperature of the subskin of the ocean" ;
  sea_surface_temperature:coverage_content_type = "physicalMeasurement" ;
  sea_surface_temperature:coordinates = "lat lon" ;
  sea_surface_temperature:add_offset = 273.15 ;
  sea_surface_temperature:scale_factor = 0.01 ;
```

The standard_name attribute should be CF-1.7 or later compliant^[1] as described in table [Table 7.4](#):

Table 7.4 GHRSST short SST names and CF-1.7 standard names for `sea_surface_temperature`

GHRSST name	CF-1.7 standard name definitions
SSTint	<code>sea_surface_temperature</code>
SSTskin	<code>sea_surface_skin_temperature</code>
SSTsubskin	<code>sea_surface_subskin_temperature</code>

Contents

- 7.1. Overview description of the GHRSST L2P data product
- 7.2. L2P data record format specification**
 - 7.2.1. `sea_surface_temperature`**
 - 7.2.2. `sst_dtime`
 - 7.2.3. `sses_bias`
 - 7.2.4. `sses_standard_deviation`
 - 7.2.5. `dt_analysis`
 - 7.2.6. `wind_speed`
 - 7.2.7. `wind_speed_dtime_from_sst`
 - 7.2.8. `source_of_wind_speed`
 - 7.2.9. `sea_ice_fraction`
 - 7.2.10. `sea_ice_fraction_dtime_from_sst`
 - 7.2.11. `source_of_sea_ice_fraction`
 - 7.2.12. `aerosol_dynamic_indicator`
 - 7.2.13. `adi_dtime_from_sst`
 - 7.2.14. `source_of_adi`
 - 7.2.15. `l2p_flags`
 - 7.2.16. `quality_level`
 - 7.2.17. `satellite Zenith Angle`
 - 7.2.18. `solar Zenith Angle`
 - 7.2.19. `surface_solar_irradiance`
 - 7.2.20. `ssi_dtime_from_sst`
 - 7.2.21. `source_of_ssi`
 - 7.2.22. Optional experimental L2P variables included by data provider

editing jupyter books

```

  _config.yml
  conventions.md
  coordinates.md
  generators
    l2p.py
    l3s.py
    l4.py
    nonregular_grid_coords.py
    regular_grid_coords.py
  images
    ghrsst-logo.png
    regridding1.png
    regridding2.png
    rgts1.png
    rgts2.png
    sst-definition.gif
  intro.md
  l2p.md
  l3.md
  l4.md
  logo.png
  naming.md
  overview.md
  README
  references.bib
  requirements.txt
  sea_surface_temperature.md
  structure.md
  _toc.yml

```

Éditeur de texte

sea_surface_temperature.md

Sea Surface Temperature

SST is a challenging parameter to define precisely as the upper ocean (~10 m) has a complex and variable vertical temperature structure that is related to ocean turbulence and air-sea fluxes of heat, moisture and momentum. A theoretical framework is therefore required to understand the information content and relationships between measurements of SST made by different satellites and in situ instruments, especially if these are to be merged together. The definitions of SST developed by the GHRSSST SST Science Team (agreed at the 2nd and 3rd workshops) achieve the closest possible coincidence between what is defined and what can be measured, taking into account current scientific knowledge and understanding of the near-surface thermal structure of the ocean.

The definitions of SST defined by GHRSSST are currently being refined by the Science Team. Once approved, the GHRSSST SST definitions will be iterated with the Climate and Forecast (CF) metadata convention definitions of SST to ensure they are in agreement.

The figure below presents a schematic diagram that summarises the definition of SST in the upper 10 m of the ocean and provides a framework to understand the differences between complementary SST measurements. It encapsulates the effects of dominant heat transport processes and time scales of variability associated with distinct vertical and volume regimes of the upper ocean water column (horizontal and temporal variability is implicitly assumed).

```

```{figure} images/sst-definition.gif
name: sst_definition
Overview of SST measurement types used within GHRSSST
```


CF Definition:



sea_surface_temperature is usually abbreviated as "SST". It is the temperature of sea water near the surface (including the part under sea-ice, if any), and not the interface temperature, whose standard name is surface_temperature. For the temperature of sea water at a particular depth or layer, a data variable of sea_water_temperature with a vertical coordinate axis should be used.



```{admonition} Additional details


The interface temperature (SSTint) is a theoretical temperature at the precise air-sea interface. It represents the hypothetical temperature of the topmost layer of the ocean water and could be thought of as an even mix of water and air molecules. SSTint is of no practical use because it cannot be measured using current technology. It is important to note that it is the SSTint that interacts with the atmosphere. Within GHRSSST, most variables containing SST are named "sea_surface_temperature" to simplify the development of client applications wishing to read these variables. The variable attribute "standard_name" indicates the precise form of the SST, using the following definitions. More detail is given in the Level 2P (Section 9), Level 3 (Section 10), and Level 4 (Section 11) specification.


```

\*\*\*sst sea\_surface\_temperature SUBJECT SECTION TUTORIAL CCTB101\*\*\*

Markdown Largeur des tabulations : 4 Lig 11, Col 7 INS

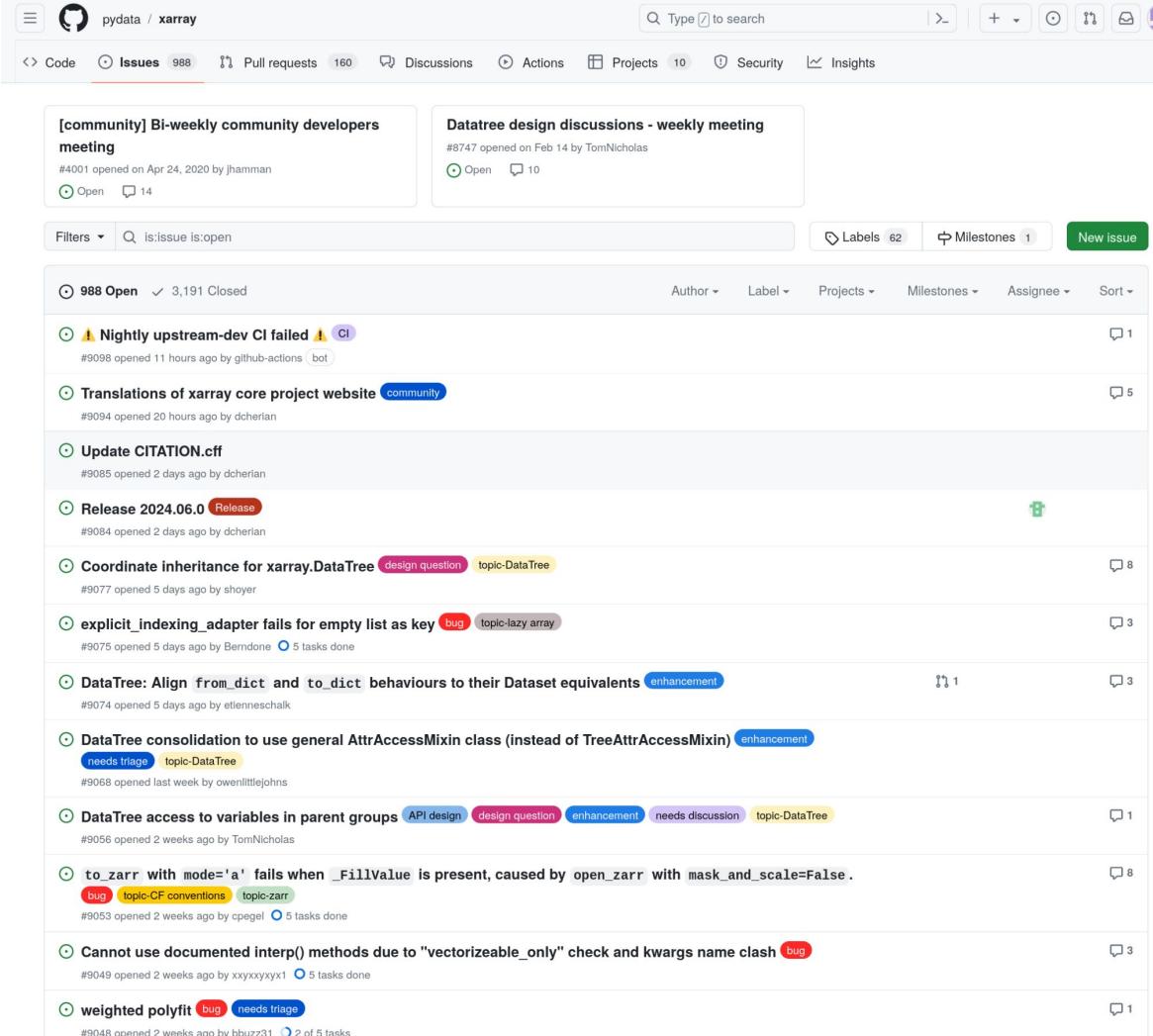
# Proposed new editing process

manage changes and revisions “as a open-source software” under github :  
<https://github.com/GHSST/GDS>

**github issue tracking** to discuss the main changes, assigning sections/updates to editors - can be related to GDS change commits

use **branches** to implement specific new feature or section (e.g. IST, uncertainties,...)

pull request to merge implemented feature



The screenshot shows the GitHub repository 'pydata/xarray'. The repository has 988 open issues. The issues list includes:

- [community] Bi-weekly community developers meeting
- Datatree design discussions - weekly meeting
- 988 Open ✓ 3,191 Closed
- Nightly upstream-dev CI failed (CI)
- Translations of xarray core project website (community)
- Update CITATION.cff
- Release 2024.06.0 (Release)
- Coordinate inheritance for xarray.DataTree (design question, topic-DataTree)
- explicit\_indexing\_adapter fails for empty list as key (bug, topic-lazy array)
- DataTree: Align from\_dict and to\_dict behaviours to their Dataset equivalents (enhancement)
- DataTree consolidation to use general AttrAccessMixin class (instead of TreeAttrAccessMixin) (enhancement, needs triage, topic-DataTree)
- DataTree access to variables in parent groups (API design, design question, enhancement, needs discussion, topic-DataTree)
- to\_zarr with mode='a' fails when \_FillValue is present, caused by open\_zarr with mask\_and\_scale=False. (bug, topic-CF conventions, topic-zarr)
- Cannot use documented interp() methods due to "vectorizable\_only" check and kwargs name clash (bug)
- weighted polyfit (bug, needs triage)



# organization of collaborative editing

open to anyone (producer or user) interested (not only ST member) - leverage on Task Teams

get a github account

get permissions and status (contributor, reviewer,...) from GPO (?)

create an issue per new feature - main leader

create new branch for documentation update

exchange through issue tracking system, telecon,...

interact, commit, update, ...

pull request when consensus

review from book captain(s) merge into master document (GDS v3)

update github pages

review created pages

fix, iterate,...

summary of changes

Clean the different GPO contact emails in GDS examples #1

[Open](#)

**jfpiolle** opened on Jun 13, 2024

Page 56, publisher\_email = "[gpo@ghrsst.org](mailto:gpo@ghrsst.org)";  
 Page 146, publisher\_email = "[gpc@ghrsst.org](mailto:gpc@ghrsst.org)";  
 on GHRSSST web site: [gpa@ghrsst.org](mailto:gpa@ghrsst.org)

Create sub-issue

**jfpiolle** self-assigned this on Jun 13, 2024

Add a comment

Write Preview

Use Markdown to format your comment

Paste, drop, or click to add files

[Close Issue](#) [Comment](#)

**Assignees**  
 jfpiolle

**Labels**  
 No labels

**Type**  
 No type

**Projects**  
 No projects

**Milestone**  
 No milestone

**Relationships**  
 None yet

**Development**  
[Code with Copilot Agent Mode](#)

[Create a branch](#) for this issue or link a pull request.

**Notifications**  
[Unsubscribe](#)

You're receiving notifications because you're subscribed to this thread.

# New GDS features



Danish Meteorological Institute



# 1. Ice Surface temperature (IST)



More datasets provide both IST and SST

Existing draft specification by EUMETSAT, OSI SAF

**Lead:** High Latitude TT

## 2. Spatial and temporal coordinates



Splitting **time** in two variables (*time*+*sst\_dtime*) is not really needed for L2P (possibly for L3 to stack data into a cube) => one unique full precision *time* variable ?

better describes projection for gridded datasets (CRS,...)

cell bounds and cell method attribute for averaged pixels (L3, L4)

### **Coordinates for ultra high resolution :**

should we still store full lat/lon matrix ? already optional for reprojected data.

Include specification on GCP/Tie points?

<https://cfconventions.org/cf-conventions/cf-conventions.html#compression-by-coordinate-subsampling>

Documenting better what lat/lon refer to exactly, what is the accuracy ? what is the accuracy

Lead: TT Coastal SST ? engage agencies (TRISHNA, LSTM,...)



# 3. Data scaling and quantization

NetCDF quantization (**scale\_factor** and **add\_offset**) is confusing for users and source of problems;

- clipping or overflow for saturated values (beyond the possible range, positive values becoming negative,...)
- decoding errors / some people implementing hard coding of unscaling preventing from changing the scale
- was used to reduce file size (float variables)
- NetCDF4 now provides internal compression and number of significant digits
- Cons: number of significant digits result in non “round” numbers

free data storage types for integers (and floats? or not ?)

Removing NetCDF scaling of variables and using true data type (e.g. float instead of integer)

**Lead:** R/G TS TT

# 4. Additional fields

## **ancillary variables:**

- total water vapour content
- aerosols : not often provided... need better requirement ?

## **additional free fields** : lift off limits on extra variables

## **more traceability ?**

- processors and processing steps and settings
- used inputs (for instance in L3S/L4)
- **Lead** : L4 TT ?

# 5. Groups

NetCDF4 introduced **groups of variables**, e.g. in a single file:

- gather related variables in different groups (**Core** : SST + quality + uncertainties, **ancillary** or **experimental** fields, ....)
- several core groups possible, per **sensor view** (e.g. nadir / oblique) or **SST type** (e.g. skin, depth,...) with their own quality\_level, uncertainties, etc...
- issue: seamless usage of SST in applications and tools (we need a **primary SST field with consistent naming**)
- gather into different groups variables with **different coordinate systems**, e.g. multi-resolution L3S :
  - separate microwave ( $0.25^\circ$ ), geostationary ( $0.05^\circ$ ) and polar orbiting ( $0.02^\circ$ ) and combined ( $0.02^\circ$ ) multi-mission grids

# 6. Uncertainties

- replacing SSES\_bias and SSES\_standard\_deviation
- simple unique uncertainty (**total**) vs separation of random and systematic uncertainty components
- metrological approach ? can it be implemented ?
- specific uncertainties to be defined per processing level (L2P, L3, L4)
- agree first on terms and content (variables) before actual how to ?

Lead ? L4 TT for L4?

## 7. Regridding

**regridding rules** - is it followed by all producers ? Is it a “specification” ? is a consensus reachable ?

Several presentations / posters on this topic

Attached uncertainties

**Lead:** ?

# 8. Format

New formats used by cloud providers or agencies

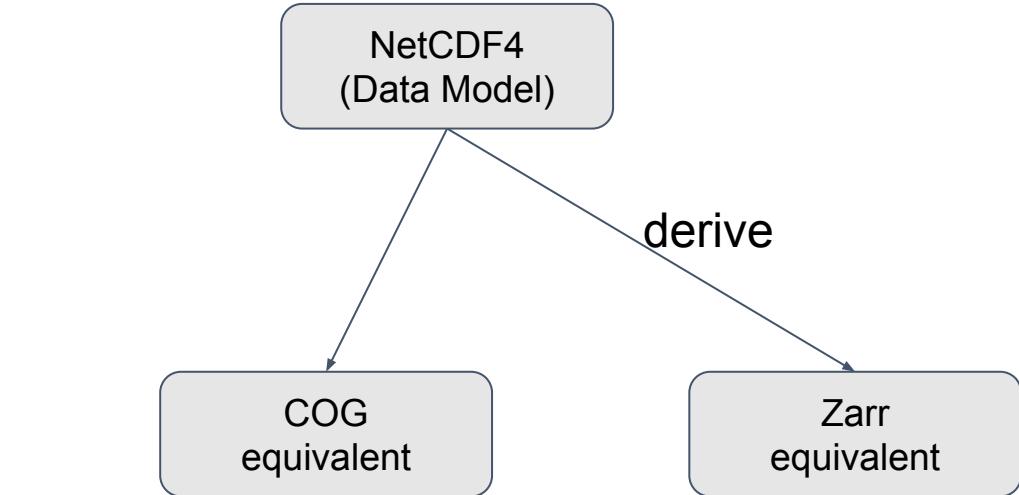
How to ensure GHRSSST specification model heritage through new ways of data distribution

keep NetCDF4, change reference format or define equivalencies, conversion rules (and accept different formats)

NetCDF data model is applicable to other formats and could remain the reference description

Unsure about benefit of COG/Zarr over NetCDF for L2P, Zarr emulation is an alternative for gridded data

Lead : R/G TS TT



# 9. Cloud optimization

Improving NetCDF formatting rules

[https://docs.google.com/presentation/d/1CT0pT0UJkUNUkyf2TyW8Mvu  
xe6962zkj/edit?usp=sharing&ouid=103571070828337788870&rtpof=true  
&sd=true](https://docs.google.com/presentation/d/1CT0pT0UJkUNUkyf2TyW8Mvu xe6962zkj/edit?usp=sharing&ouid=103571070828337788870&rtpof=true&sd=true)

# 10. Fixing GDS issues - Filenaming

Currently:

**<Indicative Date><Indicative Time>-<RDAC>-<Processing Level>\_GHSST-<SST Type>-<Product String>-<Additional Segregator>-v<GDS Version>-fv<File Version>.<File Type>**

- **<SST Type>** = SSTfnd, SSTskin, SSTsubskin, SSTdepth
  - missing IST, ISST
  - accounting for multiple SST type fields (e.g. skin + depth)
- **<Product String>** = **<platform code>\_<sensor code>(\_<additional text if needed>)**
- relax requirement on using CEOS mission names, e.g. allow usage of both operational and early mission names (MTG-I1 <> Meteosat-12, Metop-SG-A1 <> Metop-D), or abbreviated names (build reference table?)

# 11. file\_quality attribute

A code value:

0 = *unknown quality*

1 = *extremely suspect (frequent problems, e.g. with known satellite problems)*

2 = *suspect (occasional problems, e.g. after launch)*

3 = *excellent (no known problems)*

do many producers care about this attribute and is it used ? usually been filled with 3, except for some producer on the first months of a new satellite (2).

**rationale for setting this information should be clarified**

is this necessarily over a long stable period (manually) or can it be automatically calculated (for example downgraded to 2, from the L1 over\_all\_quality\_flag) ?

If the file quality is automated, should file quality also be lowered if one PDU is missing ?

Maybe better to replace with a percent\_missing\_data or similar field if this field can be dynamically calculated by the data producer

# R/G TS Evolutions



- Data access services
  - file aggregation / subsetting time series : future of THREDDS? replacing with “NetCDF (or whatever) on the cloud”
- STAC in complement / replacement to OpenSearch for file inventory / selection

# way forward

- finalize editing process and guidelines (GPO with R/G TS)
- list of issues
- enlist contributors
- aim at v3 draft to be reviewed at next GHRSSST meeting