National Aeronautics and Space Administration
Goddard Earth Science Data Information and Services Center (GES DISC)

README Document for OMPS_NPP_NMSO2_PCA_L3_DAILY Product

Version 1.0

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Revision History

Revision Date	Changes	Author

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1.0 Introduction

This document provides basic information regarding the OMPS_NPP_NMSO2_PCA_L3_DAILY product (Version 1.0), which is the Suomi National Polar-orbiting Partnership (NPP) Ozone Mapping and Profiler Suite (OMPS) Nadir Mapper (NM) sulfur dioxide (SO_2) Principal Components Analysis (PCA) daily 0.25-degree by 0.25-degree Level 3 (L3) gridded product generated via the "best-pixel" approach.

The OMPS_NPP_NMSO2_PCA_L3_DAILY product is generated from the Version 2 OMPS_NPP_NMSO2_PCA_L2 Level 2 (L2) orbital swath product, which was publicly released in July 2020 (Li et al., 2020a). The Version 2 OMPS_NPP_NMSO2_PCA_L2 product makes use of a new anthropogenic SO_2 dataset consistent with the Version 2 Ozone Monitoring Instrument (OMI) Aura OMSO2 product (Li et al., 2020b; Li et al., 2020c). The Version 2 OMPS_NPP_NMSO2_PCA_L2 product is fundamentally based on the OMPS_NPP_NMEV_L1B Level 1B (L1B) orbital swath product (Jaross, 2017a). Also, the Version 2 OMPS_NPP_NMSO2_PCA_L2 product makes use of data from two other SNPP OMPS NM L2 orbital swath products: 1) the OMPS_NPP_NMTO3_L2 ozone product (Jaross, 2017b), and 2) the OMPS_NPP_NMCLDRR_L2 cloud product (Joiner, 2020).

The OMPS NM instrument aboard the NASA/NOAA Suomi NPP satellite, launched on 2011 October 28, began to produce science data needed for accurate OMPS_NPP_NMSO2_PCA_L2 retrievals starting on 2012 January 26. Thus, the OMPS_NPP_NMSO2_PCA_L3_DAILY product has been generated from 2012 January 26 onward.

There are no OMPS_NPP_NMSO2_PCA_L3_DAILY product files for the following dates (for which adequate OMPS_NPP_NMSO2_PCA_L2 input data are lacking): 2012 February 21, 2012 March 11, 2012 March 25, 2012 April 1, 2012 July 22, 2012 August 5, 2012 August 26, 2022 March 11 through 14, and 2022 July 27 through August 9.

1.1 Algorithm Description

Each OMPS_NPP_NMSO2_PCA_L3_DAILY product file is generated from a set of OMPS_NPP_NMSO2_PCA_L2 product files centered at noon UTC of the L3 day in question.

We make use of the Total Ozone Mapping Spectrometer (TOMS) definition of an L3 day (McPeters et al., 2000), which is defined as the ensemble of all L2 ground pixels with pixel centers that have the same local calendar date on the ground. The TOMS L3 day differs from 24 consecutive UTC hours of observations centered at noon UTC, which includes data from three consecutive local calendar dates on the ground, with temporal discontinuities (i.e., where adjacent data on the global map differ by almost 24 UTC hours) in the southwestern and northeastern parts of the map.

The calendar date of the L3 day is the calendar date at Greenwich midway through the L3 day. Note that some of the L2 observations at the beginning of an L3 day will correspond to the previous calendar date at Greenwich, and some of the L2 observations at the end of an L3 day will correspond to the next calendar date at Greenwich.

The adopted L3 grid is equirectangular in longitude and latitude with dimensions of size 1440 in longitude and 720 in latitude. The L3 grid cells are of size 0.25 degrees in longitude by 0.25 degrees in latitude. The center of the first grid cell is located at longitude -179.875 degrees east and latitude -89.875 degrees north. The center of the final grid cell is located at longitude 179.875 degrees east and latitude 89.875 degrees north. The center of the grid itself is located at longitude 0.0 degrees east and latitude 0.0 degrees north, which corresponds to the corners of four grid cells.

Each grid cell in the L3 product contains the data for the L2 observation for the L3 day in question that overlaps with the L3 grid cell and has the shortest geometric path length, which we define as

path length = 1/cos(solar zenith angle) + 1/cos(viewing zenith angle)

A ground-pixel mask with 0.01-degree by 0.01-degree resolution in longitude and latitude that has the approximate shape and size of the ground pixel is generated for each L2 observation.

The ground-pixel mask is used to determine whether a given L2 observation overlaps with a given L3 grid cell.

A single L2 observation can be mapped onto more than one L3 grid cell, if that L2 observation overlaps with and has the shortest path length for more than one L3 grid cell.

The L2 observations are not averaged or weighted in any way in the best-pixel L3 product.

Each L2 observation must survive several exclusion filters before the L2 observation can be considered as a best-pixel candidate for any L3 grid cell. These filters are listed here in the order in which they are applied:

1) An L2 observation is excluded if it has a vertical column amount SO_2 equal to the fill value.

2) As a rough first temporal cut, an L2 observation is excluded if the time of the L2 observation lies outside the 48-hour time interval centered at noon UTC of the L3 day.

3) An L2 observation is excluded if it has a local calendar date on the ground (calculated

from the time of the L2 observation and the longitude at the center of the L2 ground pixel) that corresponds to the day before the L3 day.

4) An L2 observation is excluded if it has a local calendar date on the ground (calculated from the time of the L2 observation and the longitude at the center of the L2 ground pixel) that corresponds to the day after the L3 day.

5) An L2 observation is excluded if it has a (1-based) scene number (cross-track position number) less than 2 or greater than 35.

6) An L2 observation is excluded if it has a cloud radiance fraction less than 0.0 or greater than 0.2.

7) An L2 observation is excluded if it has a solar zenith angle greater than 70.0 degrees.

8) An L2 observation is excluded if it has a calculated air mass factor less than 0.3. The air mass factor is calculated for each L2 observation from the scattering weight and an *a priori* profile based on the GEOS-5 model.

Finally, an empirical South Atlantic Anomaly (SAA) mask is applied to the results of the best-pixel selection process in the L3 grid.

1.2 Data Quality Issues

The main quality issue not addressed by the eight exclusion filters listed in Section 1.1 is the effect of the South Atlantic Anomaly (SAA) on the SO_2 retrievals. The empirical SAA mask that is applied (after the best-pixel selection process) is suggestive, and not definitive. The SAA can affect SO_2 retrievals beyond the empirical SAA mask. The SAA region at any given moment in time is poorly defined in both shape and extent. Also, the SAA region evolves with time. Therefore, noisy-looking vertical column amount SO_2 values just outside the SAA mask should be used with caution. An improved empirical SAA mask that is a function of time might be used to produce future versions of the OMPS_NPP_NMSO2_PCA_L3_DAILY product.

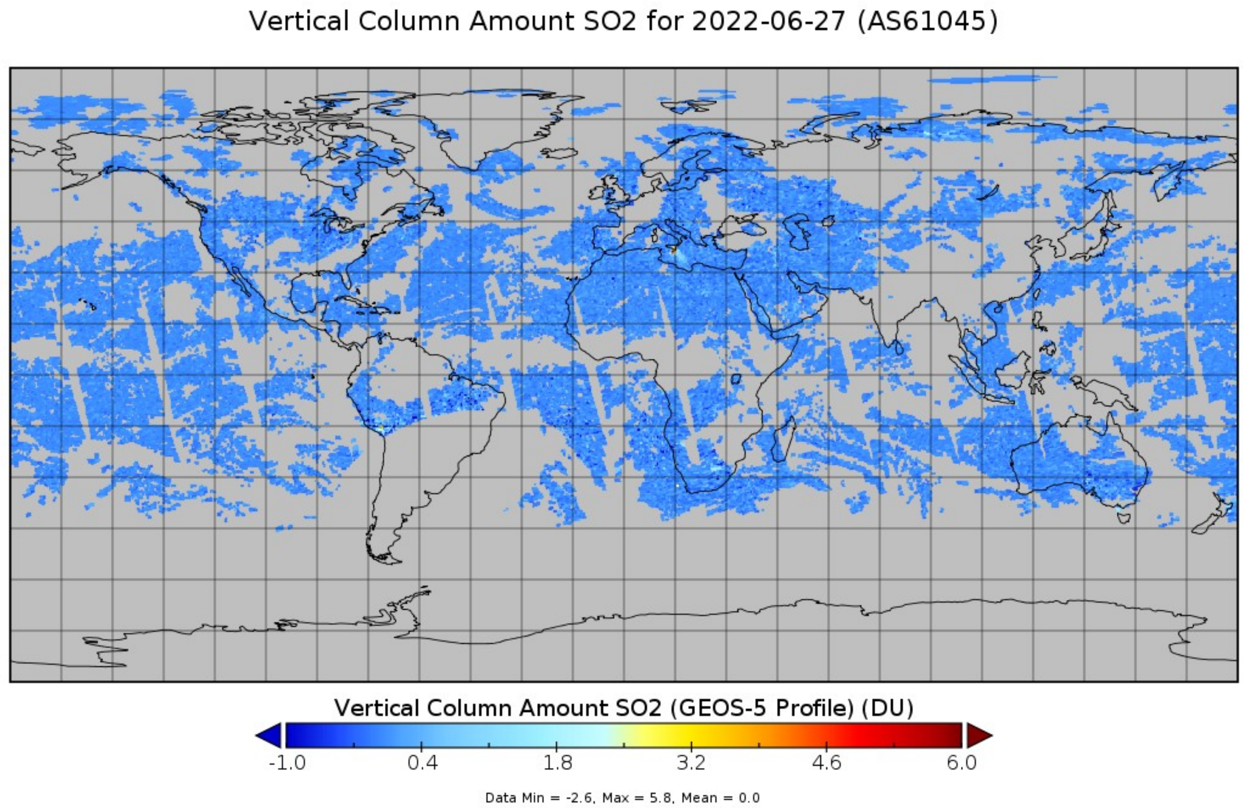

Figure 1. A global map of the vertical column amount SO_2 generated via the Panoply tool from the OMPS_NPP_NMSO2_PCA_L3_DAILY product file for 2022-06-27. Enhanced SO_2 can be seen in the Norilsk region of Russia, from an eruption of Mount Etna, and from power plants in South Africa. The empirical South Atlantic Anomaly (SAA) mask can be seen over southern South America and over part of the South Atlantic Ocean. The SO_2 enhancement visible on the west coast of South America just north of the empirical SAA mask is likely due to the Ilo copper smelter and/or the nearby Sabancaya volcano, while the noisy-looking enhancements along the rest of the northern edge of the SAA mask are likely artifacts.

1.3 Data Citation and Acknowledgment

The OMPS_NPP_NMSO2_PCA_L3_DAILY product should be acknowledged by citing the product in publication reference sections as follows:

Can Li, Nickolay A. Krotkov, Peter J. T. Leonard (2023), OMPS/NPP L3 NM PCA Sulfur Dioxide (SO2) Total Column Daily Best Pixel Global Gridded 0.25 degree x 0.25 degree V1, Greenbelt, MD, USA, Goddard Earth Sciences Data and Information Services Center (GES DISC), Accessed: [Data Access Date], 10.5067/OMPS/OMPS_NPP_NMSO2_PCA_L3_DAILY.1

2.0 Data Organization

Each OMPS_NPP_NMSO2_PCA_L3_DAILY product file contains data based on the SO_2 retrievals for a single calendar date on the ground. These data are presented on an equirectangular grid in longitude and latitude with dimensions of size 1440 in longitude and 720 in latitude. Also, each file includes a time dimension of size one to aid in the production of space-time "data cubes" from a set of consecutive L3 files.

2.1 File Naming Convention

The OMPS_NPP_NMSO2_PCA_L3_DAILY product files are named as in this example:

OMPS-NPP_NMSO2-PCA-L3-DAILY_v1.0_2022m0627_2022m1228t180556.nc

The components of this filename pattern are as follows:

1. The instrument name (OMPS).
2. The spacecraft name (Suomi NPP).
3. An abbreviated product name (NMSO2-PCA-L3-DAILY).
4. The product version (1.0).
5. The L3 observation date (2022 June 27 UTC in this case).
6. The production date-time of the file (2022 December 28 at 18:05:56 UTC in this case).

2.2 Data Format and File Format

The OMPS_NPP_NMSO2_PCA_L3_DAILY product files have been produced in netCDF-4 (https://www.unidata.ucar.edu/software/netcdf/) and are CF-compliant (https://cfconventions.org/).

Each OMPS_NPP_NMSO2_PCA_L3_DAILY product file contains file-level attributes, dimensions, geolocation and science variables, and their associated attributes (see Figure 2). These things are described in detail in Section 3.

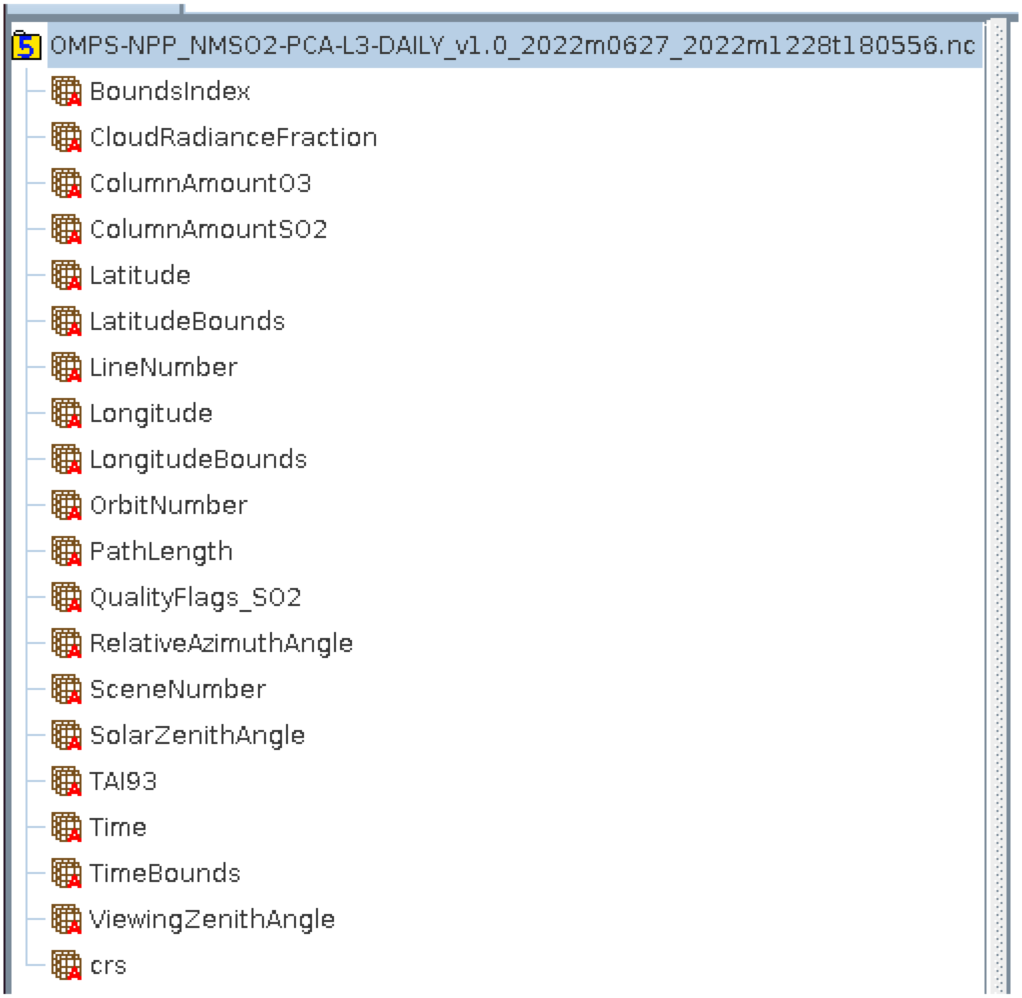

Figure 2. A screen shot from HDFView that displays the overall file structure of the OMPS_NPP_NMSO2_PCA_L3_DAILY product.

2.3 Key Science Data Variable

The key science data variable in the OMPS_NPP_NMSO2_PCA_L3_DAILY product is ColumnAmountSO2, which contains the vertical column amount SO2 (based on the GEOS-5 *a priori* profile) in DU for the L2 observation with the shortest path length.

3.0 Data Contents

This section describes, in detail, the file format of OMPS_NPP_NMSO2_PCA_L3_DAILY product, including the file-level attributes, dimensions, groups, variable-level attributes, fill values, geolocation variables, bounds variables, and science variables.

3.1 File-Level Attributes

The following table describes the 51 file-level attributes that appear at root level in the OMPS_NPP_NMSO2_PCA_L3_DAILY product.

Attribute Name	Description	Data Type
AuthorAffiliation	The institutional affiliation of the author(s) (same as institution).	String
AuthorName	The names of the author(s).	String
Conventions	The conventions plus version numbers used in the product.	String
DataSetQuality	An assessment of the quality of the data in the product.	String
DayNightFlag	The flag indicating whether the observations were made on the day or night side of Earth.	String
EasternmostLongitude	The longitude of the easternmost data in the granule.	32-bit floating-point
EndOrbit	The orbit number of the final orbit used to construct the granule.	32-bit integer
EndUTC	The UTC at the end of the granule.	String
Format	The data format used for the product (e.g., netCDF-4).	String
GranuleDay	The day of the month at the beginning of the granule.	32-bit integer
GranuleDayOfYear	The day of the year at the beginning of the granule.	32-bit integer
GranuleID	The full name of the granule (same as LocalGranuleID).	String
GranuleMonth	The month of the year at the beginning of the granule.	32-bit integer
GranuleYear	The year at the beginning of the granule.	32-bit integer
IdentifierProductDOI	The Digital Object Identifier (DOI) of the product.	String
IdentifierProductDOIAuthority	The URL of the relevant DOI authority.	String
InputPointer	A list of the input file(s) used to produce the granule.	String
InstrumentShortName	The short name of the instrument.	String

LatitudeResolution	The resolution in latitude of the grid in the granule.	32-bit floating-point
LocalGranuleID	The full name of the granule (same as GranuleID).	String
LocalityValue	The flag indicating the locality of the granule.	String
LongName	The long name of the product (same as title).	String
LongitudeResolution	The resolution in longitude of the grid in the granule.	32-bit floating-point
NorthernmostLatitude	The latitude of the northernmost data in the granule.	32-bit floating-point
PGEName	The name of the software that produced the granule.	String
PGEVersion	The version of the software that produced the granule.	String
ParameterName	The name of the geophysical parameter contained in the product.	String
PlatformShortName	The short name of the platform carrying the instrument.	String
ProcessingCenter	The data processing facility that produced the granule.	String
ProcessingLevel	The processing level of the granule.	String
ProductType	The type of product.	String
ProductionDateTime	The production date-time of the granule.	String
RangeBeginningDate	The date at the beginning of the granule.	String
RangeBeginningTime	The time at the beginning of the granule.	String
RangeEndingDate	The date at the end of the granule.	String
RangeEndingTime	The time at the end of the granule.	String
SensorShortName	The short name of the sensor.	String
ShortName	The short name of the product.	String
SouthernmostLatitude	The latitude of the southernmost data in the granule.	32-bit floating-point
StartOrbit	The orbit number of the first orbit used to construct the granule.	32-bit integer

StartUTC	The UTC at the start of the granule.	String
TAI93At0zOfGranule	The TAI93 time at UTC midnight for the day of the granule.	64-bit floating-point
VersionID	The product version.	String
WesternmostLongitude	The longitude of the westernmost data in the granule.	32-bit floating-point
_NCProperties	A netCDF-4 attribute that lists the versions of netCDF-4 and HDF5 used.	String
comment	An overall comment regarding the product.	String
history	The history of the granule.	String
institution	The institutional affiliation of the authors (same as AuthorAffiliation).	String
references	A list of references for the product.	String
source	The instrument and platform that gathered the observations for the product.	String
title	The title of the product (same as LongName).	String

3.2 Dimensions

The following table describes the four dimensions in the OMPS_NPP_NMSO2_PCA_L3_DAILY product.

Dimension Name	Description	Dimension Size
BoundsIndex	The dimension representing the index for the bounds variables.	2
Latitude	The dimension representing terrestrial latitude (in degrees) at the center of the grid cell.	720
Longitude	The dimension representing terrestrial longitude (in degrees) at the center of the grid cell.	1440
Time	The dimension representing time (in continuous days since 1972-01-01 00:00:00 UTC) for the observations in the grid file. This dimension of size one facilitates the concatenation of data from several consecutive grid files.	1

3.3 Groups

There are no groups in the OMPS_NPP_NMSO2_PCA_L3_DAILY product – all variables appear at root level.

3.4 Variable-Level Attributes

The following table describes the attributes attached to the variables in the OMPS_NPP_NMSO2_PCA_L3_DAILY product. Not all of the listed attributes are attached to every variable.

Attribute Name	Description	Data Type
_FillValue	The fill value used for the variable.	Same as for variable
axis	The axis for the (applies to the Latitude, Longitude and Time variables only).	String
bounds	The path to the relevant bounds variable (applies to the Latitude, Longitude and Time variables only).	String
calendar	The calendar used (applies to the Time variable only).	String
coordinates	The paths to the relevant coordinate variables (if applicable).	String
description	A detailed description of the variable.	String
grid_mapping	The mapping used in the grid.	String
grid_mapping_name	An attribute for the Coordinate Reference System (crs) dummy variable.	String
inverse_flattening	An attribute for the crs dummy variable.	32-bit floating-point
long_name	The name for the variable that can be used in plots.	String
longitude_of_prime_meridian	An attribute for the crs dummy variable.	32-bit floating-point
semi_major_axis	An attribute for the crs dummy variable.	32-bit floating-point
standard_name	The standard name for the variable (if applicable).	String
units	The units for the variable.	String
valid_max	The maximum valid value for the variable.	Same as for variable
valid_min	The minimum valid value for the variable.	Same as for variable

3.5 Fill Values

The following table summarizes the fill values used in the OMPS_NPP_NMSO2_PCA_L3_DAILY product.

Variable Data Type	Fill Value
32-bit integer	-2147483648
32-bit floating-point	-1.2676506E30
64-bit floating-point	-1.2676506002282294E30

3.6 Geolocation Variables

The following table describes the nine geolocation variables in the OMPS_NPP_NMSO2_PCA_L3_DAILY product. The dimensions of these variables are Longitude, Latitude and Time, except for the Coordinate Reference System (crs) dummy variable, which has no dimensions.

Variable Name	Description	Data Type
LineNumber	The line number of the L2 observation with the shortest path length.	32-bit integer
OrbitNumber	The orbit number of the L2 observation with the shortest path length.	32-bit integer
PathLength	The path length, 1/cos(solar zenith angle) + 1/cos(viewing zenith angle), of the L2 observation selected for the L3 grid cell.	32-bit floating-point
RelativeAzimuthAngle	The relative (solar + 180 - viewing) azimuth angle (in degrees) of the L2 observation with the shortest path length.	32-bit floating-point
SceneNumber	The scene number of the L2 observation with the shortest path length.	32-bit integer
SolarZenithAngle	The solar zenith angle (in degrees) of the L2 observation with the shortest path length.	32-bit integer
TAI93	The TAI93 of the L2 observation with the shortest path length.	64-bit floating-point
ViewingZenithAngle	The viewing zenith angle (in degrees) of the L2 observation with the shortest path length.	32-bit floating-point
crs	A dummy variable with attributes that specify the Coordinate Reference System used for the grid.	32-bit integer

3.7 Science Variables

The following table describes the four science variables in the

OMPS_NPP_NMSO2_PCA_L3_DAILY product. The dimensions of these variables are Longitude, Latitude and Time.

Variable Name	Description	Data Type
CloudRadianceFraction	The cloud radiance fraction (derived with the help of data from the OMPS_NPP_NMCLDRR_L2 product) at 313 nm of the L2 observation with the shortest path length.	32-bit floating-point
ColumnAmountSO2	The vertical column amount SO_2 (based on the GEOS-5 *a priori* profile) in DU of the L2 observation with the shortest path length.	32-bit floating-point
ColumnAmountO3	The best total ozone solution (from the OMPS_NPP_NMTO3_L2 product, with a correction made for cases with large volcanic SO_2 column amounts) in DU of the L2 observation with the shortest path length.	32-bit floating-point
QualityFlags_SO2	The SO_2 quality flags for the L2 observation with the shortest path length (0 = good best-pixel result, 1 = no best-pixel result, 2 = lies within the empirical South Atlantic Anomaly region).	32-bit integer

4.0 Options for Reading the Data

4.1 Command Line and Other Utilities

4.1.1 ncdump

The ncdump tool can be used as a simple browser for HDF data files, to display the dimension names and sizes; variable names, types, and shapes; attribute names and values; and optionally, the values of data for all variables or selected variables in a netCDF file. The most common use of ncdump is with the -h option, in which only the header information is displayed.

ncdump [-c|-h] [-v ...] [[-b|-f] [c|f]] [-l len] [-n name] [-d n[,n]] filename.nc

Options/Arguments:
[-c] Coordinate variable data and header information
[-h] Header information only, no data
[-v var1[,...]] Data for variable(s) <var1>,... only data
[-f [c|f]] Full annotations for C or Fortran indices in data
[-l len] Line length maximum in data section (default 80)
[-n name] Name for dumped netCDF dataset (default derived from file name)

[-d n[,n]] Approximate floating-point values with less precision
filename.nc File name of input netCDF file

(https://www.unidata.ucar.edu/software/netcdf/workshops/2011/utilities/Ncdump.html)

4.1.2 HDFView

HDFView is a Java-based graphical user interface created by the HDF Group which can be used to browse HDF files. The utility allows users to view all objects in an HDF file hierarchy which is represented as a tree structure. Additional information about HDFView can be found at https://support.hdfgroup.org/products/java/hdfview/ and for HDF at https://portal.hdfgroup.org/display/support

4.1.3 Panoply

The Panoply tool (https://www.giss.nasa.gov/tools/panoply/), developed at the Goddard Institute for Space Studies (GISS), can be used to generate geo-referenced plots from the data in OMPS_NPP_NMSO2_PCA_L3_DAILY product files (e.g., Figure 1).

4.2 Tools/Programming

The product files can be read and queried using the netCDF-4 library and tools maintained by Unidata (http://www.unidata.ucar.edu/software/netcdf/). Support for reading netCDF is offered in many programming languages, including Python, Matlab, IDL, C/C++ and Fortran. NetCDF-4 files are legal HDF5 files with additional bookkeeping information managed by the netCDF-4 library. It is therefore possible to inspect and copy data out of the netCDF-4 files by using the HDF5 utilities and libraries maintained by the HDF Group (https://www.hdfgroup.org/products/hdf5_tools/index.html) or by using the HDF5 interface in your favorite programming language. However, the two libraries should not be considered fully interchangeable.

Matlab users should note that the Matlab netCDF-4 interface is currently (as of version R2017a) not able to read attributes that are string arrays, and it will throw an exception if that is attempted.

4.2.1 Python

The following code snippet is a generic example showing how to read the variable lat, lon, and nh3_vmr from a hypothetical data file with the name “filename”. Also shown is some basic information about the size of the variable arrays. Changes to the code snippet below are necessary to read OMPS_NPP_NMSO2_PCA_L3_DAILY product with Python.

```
import netCDF4
```

```
from netCDF4 import Dataset

nc_fid = netCDF4.Dataset( filename ,mode='r',format='NETCDF4')

#read in the variables
lat = nc_fid.variables['lat'][:]
lon = nc_fid.variables['lon'][:]
nh3 = nc_fid.variables['nh3_vmr'][:]

# print out the minimum, maximum, and dimensions for the three variables
print("-- lat  Min/Max values", lat[:].min(), lat[:].max())
print("lat.shape:", lat.shape)
print("-- lon Min/Max values:", lon[:].min(), lon[:].max())
print("lon.shape:", lon.shape)
print("-- nh3 Min/Max values:", nh3[:].min(), nh3[:].max())
print("nh3.shape:", nh3.shape)
```

5.0 GES DISC Data Services

If you need assistance or wish to report a problem:

Email: gsfc-dl-help-disc@mail.nasa.gov
Voice: 301-614-5224
Fax: 301-614-5268
Address:
Goddard Earth Sciences Data and Information Services Center, NASA Goddard Space Flight Center, Code 619, Greenbelt, MD 20771 USA

5.1 "How To" Articles

The GES DISC web site contains many informative articles under the "How To Section", "FAQ" (frequently asked questions), "News", "Glossary", and "Help". A sample of these articles includes:

Earthdata Login for Data Access

How to Download Data Files from HTTPS Service with wget

How to Obtain Data in NetCDF Format via OpeNDAP

Quick View Data with Panoply

How to Read Data in NetCDF Format with R

[How to Read Data in HDF-5 or netCDF Format with GrADS](#)

[How to read and plot NetCDF MERRA-2 data in Python](#)

[How to Subset Level-2 Data](#)

[How to use the Level 3 and 4 Subsetter and Regridder](#)

6.0 Product Contacts

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7.0 Acknowledgments

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8.0 References

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Can Li, Nickolay A. Krotkov, Peter Leonard, and Joanna Joiner (2020b), OMI/Aura Sulphur Dioxide (SO2) Total Column 1-orbit L2 Swath 13x24 km V003, Greenbelt, MD, USA, Goddard Earth Sciences Data and Information Services Center (GES DISC), 10.5067/Aura/OMI/DATA2022

Li, Can, Krotkov, Nickolay A., Leonard, Peter J. T., Carn, Simon, Joiner, Joanna, Spurr, Robert J. D., Vasilkov, Alexander. 2020c. Version 2 Ozone Monitoring Instrument SO2 product (OMSO2 V2): new anthropogenic SO2 vertical column density dataset. Vol. 13, No. 11, pp. 6175-6191. DOI: 10.5194/amt-13-6175-2020 ISSN: 1867-1381

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Joanna Joiner (2020), OMPS-NPP L2 NM Cloud Pressure and Fraction swath orbital V2, Greenbelt, MD, USA, Goddard Earth Sciences Data and Information Services Center (GES DISC), 10.5067/CJAALTQUCLO2

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