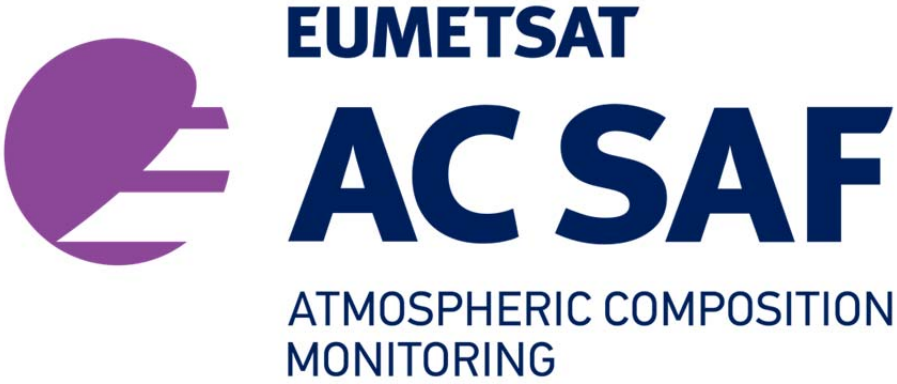

PRODUCT USER MANUAL

GOME-2 glyoxal columns

Data-records for GOME-2 on MetOp-A and -B

Prepared by: Pieter Valks German Aerospace Center

Deutsches Zentrum für Luft und Raumfahrt e.V. – DLR
Oberpfaffenhofen, Germany

Signatures

Action: Name	*Affiliation*	*Function*	*Date*	*Signature*
Prepared by: P. Valks	DLR-MF	AC SAF Project Scientist	15.02.2021	
Released by: P. Valks	DLR-MF	AC SAF Project Scientist	15.02.2021	

Distribution List

Function	*Organization*
GOME-2/AC SAF Team	DLR-MF, DLR-DFD
AC SAF Team	EUMETSAT, FMI, AUTH, BIRA, KNMI, various

Document Change Log

Issue	*Rev*	*Date*	*Section*	*Description of Change*
1/A	1	11.12.2020	all	initial version
1/A	2	15.02.2021	all	Update according to review

Table of Contents

EUMETSAT Satellite Application Facility on Atmospheric Composition Monitoring (AC SAF)

Background

The need for atmospheric chemistry monitoring was first realized when severe loss of stratospheric ozone was detected over the Polar Regions. At the same time, increased levels of ultraviolet radiation were observed.
Ultraviolet radiation is known to be dangerous to humans and animals (causing e.g. skin cancer, cataract, immune suppression) and having harmful effects on agriculture, forests and oceanic food chain. In addition, the global warming - besides affecting the atmospheric chemistry - also enhances the ozone depletion by cooling the stratosphere. Combined, these phenomena have immense effects on the whole planet. Therefore, monitoring the chemical composition of the atmosphere is a very important duty for EUMETSAT and the world-wide scientific community.

Objective

The main objectives of the AC SAF is to process, archive, validate and disseminate atmospheric composition products (O_3, NO_2, SO_2, BrO, HCHO, H_2O and OClO), aerosol products and surface ultraviolet radiation products utilising the satellites of EUMETSAT. The majority of the AC SAF products are based on data from the GOME-2 spectrometers onboard MetOp-A, MetOp-B and MetOp-C satellites.
Another important task of the AC SAF is the research and development in radiative transfer modelling and inversion methods for obtaining long-term, high-quality atmospheric composition products from the satellite measurements.

Product categories, timeliness and dissemination

Data products are divided in two categories depending on how quickly they are available to users:
Near real-time products are available in less than three hours after measurement. These products are disseminated via EUMETCast, WMO GTS or internet.

- Near real-time trace gas columns
  - O_3, NO_2, HCHO, SO_2
- Near real-time ozone profiles
  - coarse and high-resolution
- Near real-time absorbing aerosol indexes
  - from main science channels and polarization measurement detectors
- Near real-time UV indexes
  - clear-sky and cloud-corrected

Offline products are available in two weeks after measurement and disseminated via dedicated web services at EUMETSAT, FMI and DLR.

- Offline trace gas columns
  - O_3, NO_2, SO_2, BrO, HCHO, H_2O and OClO
- Offline ozone profiles
  - coarse and high-resolution
- Offline absorbing aerosol indexes
  - from main science channels and polarization measurement detectors
- Offline surface UV

Data record products are available for a fixed time range (e.g. 1.1.2007 to 30.6.2020). In contrast to the NRTI and OFFL products, the datasets are not automatically continued based on new observations. The respective data-sets are provided via dedicated web services at EUMETSAT, FMI and DLR.

Available data records are:

- GOME-2 tropospheric BrO columns
- GOME-2 glyoxal columns
- GOME-2 monthly gridded (Level-3) NO_2 an H_2O columns

More information about the AC SAF project, products and services:

http://acsaf.org/

AC SAF Helpdesk: helpdesk@acsaf.org

1 Introduction

1.1 Purpose and Scope

DLR produces on an operational basis a range of total column trace gases and cloud products for the GOME-2 instruments on MetOp-A, -B and -C in the framework of EUMETSAT's AC SAF.

DLR has a long experience in operational processing of GOME-2 data. This document is the user manual for the GOME-2/MetOp -A and -B glyoxal data records produced by DLR.

DLR provides near-real-time (NRT), off-line (OL), reprocessed and data-records products. The NRT products have the same granularity as the input GOME-2 data (i.e. downlink or PDU) and are made available and disseminated to the users within 2 hours 30 minutes of sensing. The OL products are consolidated orbits from ascending node crossing to ascending node crossing and are available and disseminated to the users within two weeks after sensing.

Additionally, DLR provides reprocessed and data record products for the complete GOME-2/MetOp-A data record starting in Jan. 2007, and the GOME-2/MetOp-B data record starting in Jan. 2013.

The network Common Data Format (netCDF version 4) has been selected as data format for the GOME-2 glyoxal data record product. NetCDF is a self-describing, machine-independent file formats commonly used for storage and transfer of scientific and meteorological data, it is based on the HDF5 (Hierarchical Data Format) which is also used frequently.

The present document is divided into the following sections:

- Overview of the GOME-2 instruments on MetOp-A, -B and -C including instrument modes
- Summary of the algorithm used for the retrieval of glyoxal columns
- Summary of the processing chain
- Product description including the used netCDF4 format

1.2 References

1.2.1 Applicable Documents

[A1] AC SAF Product Requirements Document, Issue 1.5, SAF/AC/FMI/RQ/PRD/001, Hovila et al., 2019.

1.2.2 Reference Documents

[R1] Algorithm Theoretical Basis Document for GOME-2 glyoxal column data records, SAF/AC/DLR/ATBD/GLY/01, Iss. 1/B, Valks, P., et al., 2020.

[R2] GOME-2 Level 1 Product Format Specification", EPS/MIS/SPE/97232, v9D, March 2012.

[R3] AC SAF Validation Report for CHOCHO Data Records from GOME-2, SAF/AC/IASB/VR/CHOCHO, Van Roozendael et al., November 2020.

[R4] NetCDF4 Format description https://www.unidata.ucar.edu/software/netcdf/

[R5] Eumetcast Dissemination Facility http://www.eumetsat.int/website/home/Data/DataDelivery/EUMETCast/index.html

[R6] Eoweb DLR Online User Service http://eoweb.dlr.de

[R7] Algorithm Theoretical Basis Document for GOME-2 surface LER product, SAF/AC/KNMI/ATBD/003, Iss 3.1, Tilstra et al. March 2019.

1.3 Abbreviations and Acronyms

A list of abbreviations and acronyms used throughout this document is given below:

AC SAF	SAF on Atmospheric Chemistry Monitoring
AMF	Air Mass Factor
BIRA-IASB	Belgian Institute for Space Aeronomy
CCSDS	Consultative Committee for Space Data Systems
DLR	Deutsches Zentrum für Luft- und Raumfahrt e.V. (German Aerospace Centre)
DOAS	Differential Optical Absorption Spectroscopy
D-PAF	German processing and archiving facility
DU	Dobson Unit
ERS-2	European Remote Sensing Satellite-2
ESA	European Space Agency
ESC	Effective Slant Column
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
GDP	GOME Data Processor
GOME	Global Ozone Monitoring Experiment
HDF	Hierarchical Data Format
IMF	Remote Sensing Technology Institute
MetOp	Operational Meteorological Satellite
netCDF	network Common Data Format
NRT	Near-Real-Time
NT	Nominal-Time
OL	Off-Line
OTO	Identifier used for off-line total column and cloud products
PDU	Product Dissemination Unit
PMD	Polarisation Measurement Device
RP	Postfix identifier user for reprocessed total column and cloud products
RMS	Root Mean Square
SAF	Satellite Application Facility
SCD	Slant Column Density
SZA	Solar Zenith Angle
TBD	To be Defined
TOA	Top of Atmosphere
UMARF	Unified Meteorological Archiving and Retrieval Facility
UV	Ultra Violet
UTC	Universal Time Coordinate
VCD	Vertical Column Density
VIS	Visible

2 GOME Instruments

2.1 Introduction

The Global Ozone Monitoring Experiment (GOME) and GOME-2 instruments are scanning spectrometers that captures light reflected from the Earth's surface and atmosphere. The spectrometer splits the light into its spectral components covering the UV/VIS region from 240 nm to 790 nm at a resolution of 0.2 nm to 0.5 nm.

The measured spectra are mainly used to derive ozone total column and vertical profile, nitrogen dioxide, formaldehyde, glyoxal, bromine oxide, water vapor, sulphur dioxide and other trace gases, as well as cloud properties and aerosols.

The next figure shows a schematic representation of GOME-2 optical layout. A scan mirror directs the light emitted from the Earth’s atmosphere or the Sun diffuser into the instrument. The spectrometer splits incoming light into four channels using a complex array of telescopes, prisms and gratings. Detectors at the end of each optical path collect information about the signal in each channel.

Figure 1: GOME-2 optical layout (courtesy of ESA)

2.2 GOME-2/MetOp

On 30 January 1998, the ESA Earth Observation Programme Board gave its final go-ahead for the MetOp Programme. The instruments on the MetOp satellites are designed to produce high-resolution images of the Earth's surface, vertical temperature and humidity profiles, and temperatures of the land and ocean surface on a global basis. In addition, there are instruments for monitoring trace gases and wind flow over the oceans. This instrument payload is of significant value to meteorologists and other scientists, particularly to those studying the global climate.

Given the need for global-scale routine monitoring of the abundance and distribution of ozone and associated trace gas species, a proposal was put forward for the inclusion of GOME-2 on the MetOp satellites. MetOp-A was launched on 19 October 2006 as part of the Initial Joint Polar System (IJPS) in co-operation with NOAA in the USA. A second polar-orbiting meteorological satellite in the series, Metop-B, was successfully launched on 17 September 2012. The third and last polar-orbiting satellite in the series, MetOp-C, was successfully launched on 7 November 2018.

The GOME-2/MetOp field of view of each step may be varied in size from 5 km x 40 km to 80 km x 40 km. The mode with the largest footprint (twenty four steps with a total coverage of 1920 km x 40 km) provides daily near global coverage at the equator [R2].

Based on the successfully work with the GOME Data Processors, the German Aerospace Centre (DLR) plays a major role in the design, implementation and operation of the GOME-2/MetOp ground segment for total column products. DLR is a partner in the Satellite Application Facility on Ozone and Atmospheric Chemistry Monitoring (AC SAF), which is part of the Eumetsat Polar System (EPS) ground segment, and is responsible in this project for the generation of total column amounts of the various trace gases and cloud properties (https://atmos.eoc.dlr.de/app/missions/gome2) which may be retrieved from GOME-2/MetOp level 1b products.

2.3 Measurement Scenarios, Timelines and Instrument Modes

GOME-2/MetOp has several operational scenarios, see:

http://gome.eumetsat.int

for more details.

- Earth Observation Mode

This mode includes nadir/narrow/static/north-polar/south-polar scanning measurements with various integration times depending on solar zenith angle. This is the default mode for the day side. Only the data acquired in this mode are used for geophysical retrievals.

- Calibration Modes

This mode includes Sun/Moon/dark/spectral-light/LED/white-light measurements. Most of these calibrations are performed on the night side.

3 Algorithm Description

3.1 CHOCHO retrieval

The glyoxal (CHOCHO) retrieval is based on the GOME-2 CHOCHO slant columns retrieved from the Level-1 data. The retrieval uses a DOAS fit to retrieve slant column densities (SCD) of several trace gases from the measured spectra. The CHOCHO SCD fit is performed in a fitting window between 435 and 460 nm. During a calibration prefit the GOME-2 slit function is optimized, the cross-sections of CHOCHO, NO_2, H_2O, O_2-O_2 and O_3 are convoluted online using the optimized slit funtion. The DOAS slant column retrieval is followed by the Air Mass Factor (AMF) conversions to generate vertical column densities. Cloud information used in the trace gas retrieval and in calculation of the CHOCHO column is obtained with the OCRA and ROCINN algorithms. A detailed description of the CHOCHO algorithm is given in [R1].

Table 1 GOME-2 glyoxal data records from MetOp-A and –B provided by the AC SAF

Data record	*AC SAF identifier*	*Wavelength region (nm)*	*Period for GOME-2A*	*Period for GOME-2B*
CHOCHO Column	O3M-120	435.0-460.0	23. Jan 2007 – 31. Dec. 2017	23. Dec 2012 – 28. June 2020

3.2 GOME-2/MetOp processing chain

DLR has developed the operational processing chain for GOME-2/MetOp total column products. The level 1b products are generated at the EPS ground segment in EUMETSAT [R2] and received at DLR via EUMETCast ([R5]). DLR generates GOME-2/MetOp level 2 total column and cloud products using level-1-to-2 (DOAS-type) processors.

There are different modules for quality control and monitoring, production control, archiving and order handling. The level 2 products generated at DLR are validated on a regular basis by the AC-SAF partner institutes AUTH, BIRA, and FMI. The GOME-2/MetOp level 2 NRT products are disseminated primary with EUMETCast and internet. The off-line products and data records are disseminated via Internet. The ordering of products can be done via dedicated user services.

The GOME-2/MetOp level 1 products are delivered in NRT (approx. 1:45 hours after sensing) in so called PDU files (product dissemination unit) containing 3 minutes of measurements via EUMETCast. The ground-segment at DLR needs less than 15 minutes for acquiring the input data, retrieving the trace gas total columns and disseminating the resulting level 2 products (Figure 2), that means the GOME-2/MetOp total column products are available to the users in less than 2 hours after sensing.

The GOME-2/MetOp operational processing is performed in a high availability virtualized environment on a blade center farm.

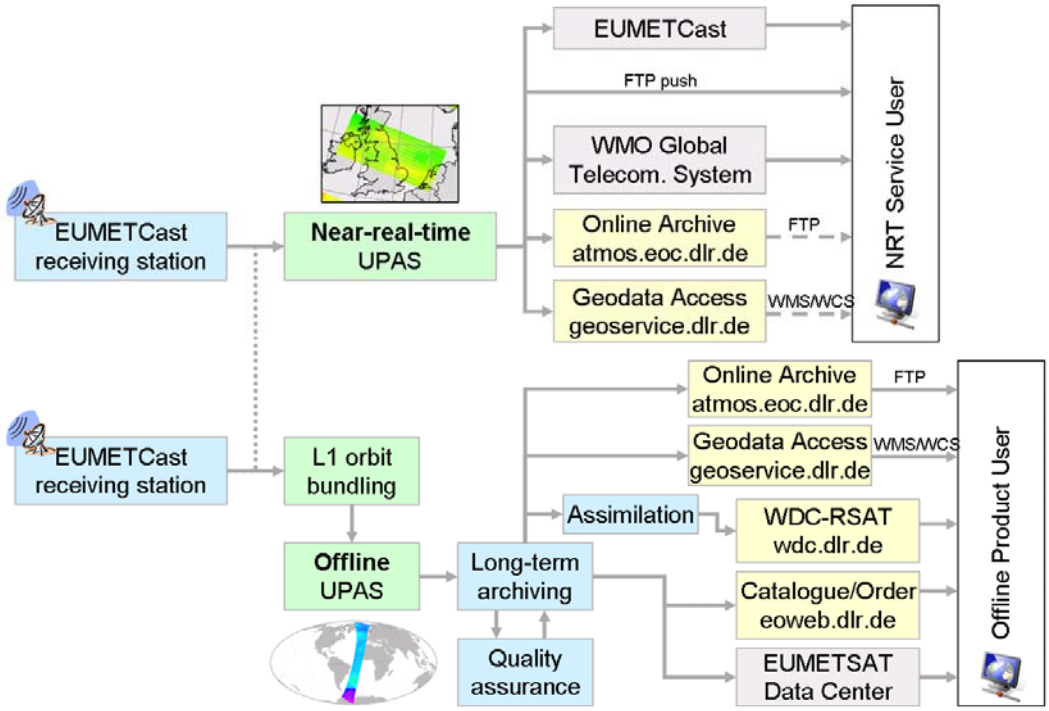

Figure 2: GOME-2/MetOp processing chain

3.3 Data Management

The processing of GOME-2/MetOp data is embedded in DLR's multi-mission facility ensuring high availability and sustainability. The German National Remote Sensing Data Library stores the data for the long-term enabling monitoring of global change and data reprocessing based on enhanced methodology.

Information and data of AC-SAF products generated at DLR are disseminated through different channels: via a dedicated AC SAF FTP-server, through the EUMETCast broadcast system for near-real-time users, through the EUMETSAT user services (Figure 2 and [R5]).

3.4 Quality Control and Monitoring

The quality of the off-line products and data records is controlled before they are archived and disseminated to the users. A dedicated quality control tool integrated into DLR's data management system displays a set of parameters generated automatically for each processed orbit. The quality control tool performs limit checks and computes some statistics to show the confidence levels of the product and its evolution within time.

3.5 Geophysical Validation

The geophysical validation of the official GOME products is performed by an independent partner organizations: BIRA. The validation is accomplished using ground-based measurements from the MAX-DOAS networks and other satellite data. The validation results [R3] are publicly available on the Internet, see Sect. 4.9.

3.6 User Services

Information about data and services are accessible through the websites given at the end of this section. The central point of access to this GOME-2 L2 trace gas column data is the AC SAF web-portal at FMI:
http://acsaf.org.

The data are provided via a dedicated AC SAF FTP-server and can be directly downloaded via: ftp://acsaf.eoc.dlr.de

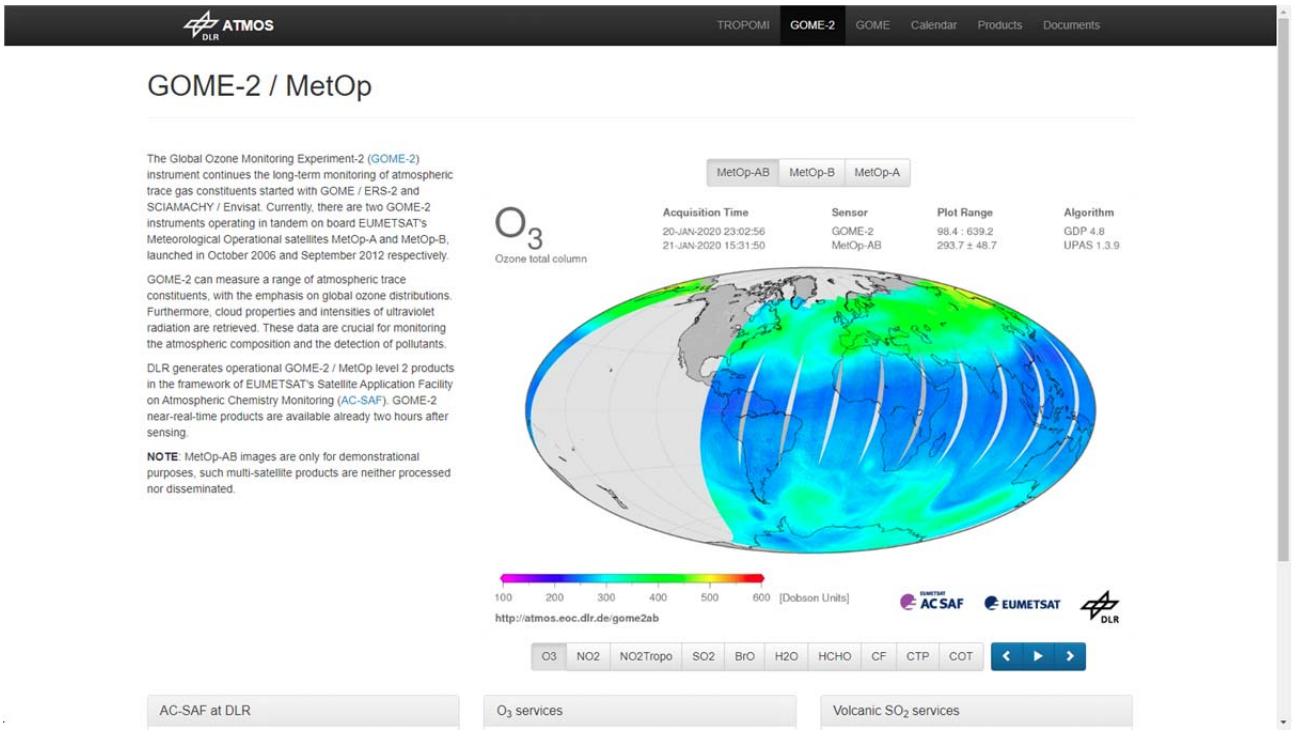

Figure 2: GOME-2/MetOp web page at DLR

4 Total Column Trace Gases and Cloud Products

The GOME-2 level 2 column products contain retrieved trace gas vertical columns and cloud properties, as well as other geophysical parameters; corresponding errors on these quantities, and a number of additional diagnostics, quality flags and intermediate results.

4.1 Units

Dataset	Units
Total ozone column	[DU] and [molecules/cm^2]
Other trace gas column amounts	[molecules/cm^2]
Cloud fraction and cloud-top albedo (optical thickness)	(unitless) [1]
Height	[km]
Pressure	[hPa]
Angles are given at satellite and at Top-of-Atmosphere (TOA) (70 km)	[0 to 360 degrees]
Geographical Coordinates	longitude [-180 to +180 degrees] latitude [–90 to +90 degrees]
Errors	absolute values [molecules/cm^2] or [DU]

4.2 Geographical Coverage and Granularity

GOME-2/MetOp has a daily near global coverage at the equator. Depending on the scanning mode used, the measured ground pattern may be different.

The NRT, off-line and reprocessed/data-record products have by default a global coverage. The coverage of trace gases available only under special conditions may be reduced.

The NRT products have the same granularity as the downlink or PDU. The off-line and reprocessed/data-record products are consolidated orbits from ascending node to ascending node.

4.3 Spatial Resolution

GOME-2/MetOp has 24 forward-scan pixels with a nominal resolution of 40 km x 80 km. In the tandem mode, GOME-2/MetOp-A operates on a reduced swath width of 960 km with an increased spatial resolution (approx. 40 km x 40 km), while GOME-2/MetOp-B and -C operate on a nominal wide swath at 1920 km. This implementation increases both the daily coverage and the spatial resolution of GOME-2 measurements. GOME-2 tandem operations started on 15 July 2013. Only forward scan pixels are processed and written to the glyoxal products.

4.4 Delivery Time

DLR generates near-real-time (NRT), off-line (OL), and reprocessed (data-record) products (RP). The NRT products are available for distribution in less than 15 minutes after the reception of the GOME-2 level 1 product.
Assuming that the input data is received at DLR 1:45 hours after sensing, then the GOME-2 total column products will be disseminated to the users in less than 2 hours after sensing.
The GOME-2/MetOp OL products are available within two weeks after sensing.
Reprocessed GOME-2/MetOp level 2 products (data-records) are generated on a regular basis.

4.5 Expected Accuracy

Detailed estimates of the uncertainties in each of the GOME-2 trace gas column products are provided in the ATBD [R2].

4.6 Product Formats

The format of the product file is netCDF4. A detailed description of the product format is given in Chap. 5.

4.7 File Name

The file name of a product already contains important information about the dataset including trace gases and sensing time. It is built according to the following structure:

SENSOR_GAS_LV_YYYYMMDDhhmmss_ddd_MISSION_#####_PRO_RV.TYPE

- *SENSOR* denotes the instrument, i.e. GOME
- *GAS* is a “-” separated list of trace gases included in the product. The acronyms from the above table are used, e.g. “CHOCHO" is a product containing glyoxal columns
- *LV* is the product level, i.e. L2
- *YYYYMMDD* are the year, month and day of the first processed ground pixel
- *hhmmss* are the hours, minutes and seconds of the UTC time stamp of the first processed ground pixel
- *ddd* is the three digit duration of the product in minutes
- MISSION denotes the mission: METOPA, METOPB
- ##### is the five digit orbit number
- *PRO* is the processing center, i.e. DLR
- *RV* is the two digit product revision
- *TYPE* denotes the product format used: netCDF4

The following example is a typical name for a GOME-2/MetOp-A product:

GOME_CHOCHO_L2_20070302111155_047_METOPA_ 01900_DLR_05.nc

4.8 Product Dissemination

The GOME-2/MetOp data set products are available at the DLR AC SAF FTP–server (anonymous login):

ftp://acsaf.eoc.dlr.de/

The products are organized in directories *YYYY/MM/DD* where *YYYY* is the year, *MM* the month, *DD* the day.

4.9 Product Ordering

The GOME-2/MetOp total column products are generated at DLR in the framework of EUMETSAT's AC SAF

EUMETSAT AC SAF ATMOSPHERIC COMPOSITION MONITORING

For information and access to all AC SAF products, please refer to the AC SAF web page and help desk:

AC SAF Web page

http://acsaf.org

AC SAF Helpdesk
helpdesk@acsaf.org

Additional information can be found in EUMETSAT's product Navigator accessible through the following link:

http://navigator.eumetsat.int

Current and historical quick look images of other trace gas products as well as value added products generated by DLR are available at:

http://atmos.eoc.dlr.de/gome2

5 NetCDF4 Product Format Description

The NetCDF4 file structure of the GOME-2 glyoxal column data is explained below. The DATA GROUPS are written in CAPITAL letters, the variables are written in small letters. The variables related to the GOME-2 measurements are stored in a 2D format (Groundpixel x Scanlines). Groundpixel 0 is in the east and groundpixel 23 in the western part of the scanline. All data are geo-referenced.

On the top level the file is divided in META_DATA and PRODUCT groups. The META_DATA contains relevant metadata, like orbit number or start time.

The PRODUCT group contains the main results total glyoxal column, as well as latitude and longitude of the pixel centre coordinates and the subgroup SUPPORT_DATA. In the subgroup additional information is provided depending on whether it is part of the analysis process eg. DOAS results or position data eg. viewing geometry or additional information that is provided by external sources eg. surface albedo the data are stored in the DETAILED_RESULTS, GEOLOCATION, or INPUT_DATA respectively.

The product content comprises the following groups:

- *META_DATA*
  - AC_SAF_METADATA

    see section 5.1
- *PRODUCT*

  see section 5.2
  - *SUPPORT_DATA*
    - *DETAILED_RESULTS*

      see section 5.3
    - *GEOLOCATIONS*

      see section 5.4
    - *INPUT_DATA*

      see section 5.5

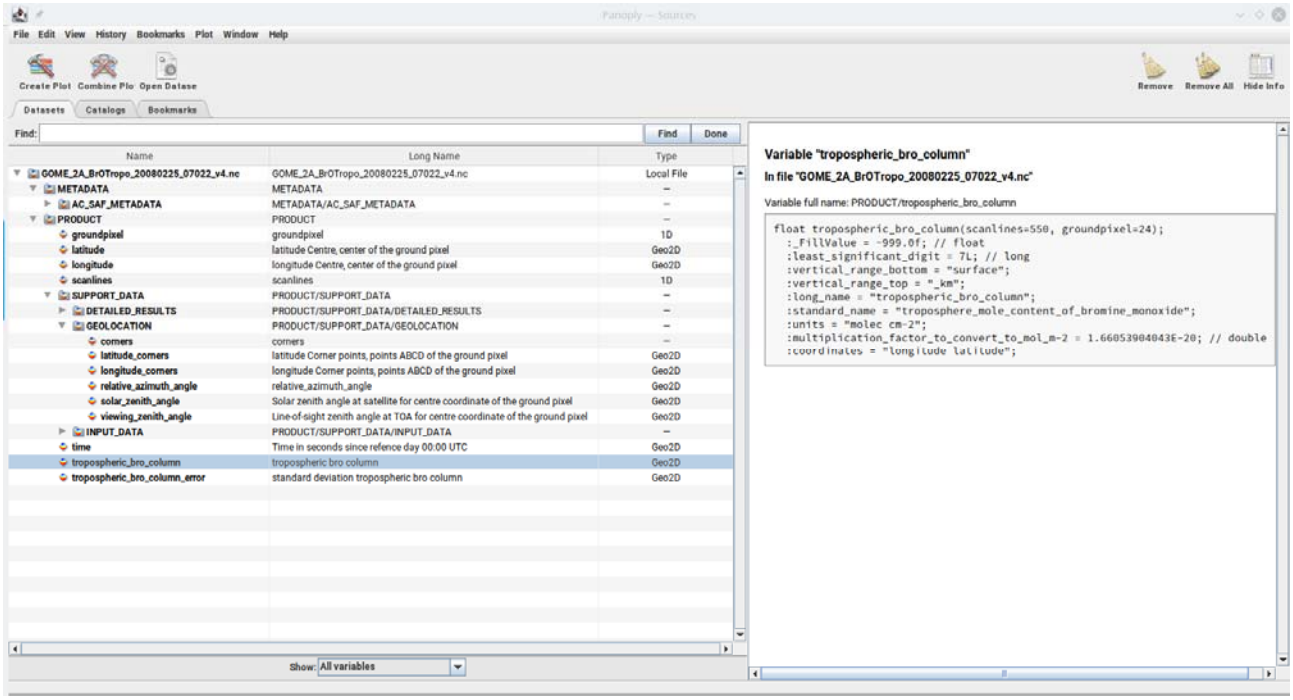

Figure 3: Screenshot of a GOME-2 L2 NetCDF-4 file opened with Panoply

5.1 *META_DATA* Group

The content of the *META_DATA* group is shown in the following table. Allowed values specified in italics indicate any value of the given type.

Attribute Name	*Data Type*	*Description*	*Allowed Values*
ArchiveFacility	string	Centre where the data is archived.	DLR
SatelliteID	string	Platform identifier (mission and spacecraft).	M*nn*
Satellites	string	Platform name	MetOp
StartOrbitNumber	integer	Orbit number at the start of sensing, i.e. at the beginning of a dump.	*integer*
InstrumentID	string	Instrument which acquired the product	GOME_2
InstrumentMode	VIEW_MODES structure	Specifies how many ground pixels were observed in the corresp. view modes.	*VIEW_MODES structure*
SensingStartTime	CCSDS_ASCII	UTC date and time at sensing start.	*Date in CCSDS format (ASCII)*
SensingEndTime	CCSDS_ASCII	UTC date and time at sensing end.	*Date in CCSDS format (ASCII)*
ProcessingCentre	string	Centre that generated the data.	O3DLR
ProcessingMode	string	Processing mode applied for generation of the product.	N (nominal), B (backlogged), R (reprocessed), V (validation) T (near-real-time)

Revision	string	Global product revision, required e.g. for reprocessing, part of logical product identifier.	*string*
ProductType	string	Description of the product type	AC GLY
ProcessingLevel	string	Processing level applied for generation of the product.	02
ProcessingTime	CCSDS_ASCII	UTC date and time at processing finish.	CCSDS Date
BaseProductAlgorithmVersion	string	Version of the algorithm used to generate the L1B parent product upon which the L2 product is based.	string
BaseProductsName	string	Name of the Level1 spectra file	string
L2BaseProductsName	string	Name of the Level2 data file for GOME-2 cloud information	string
FIleName	string	Name of the glyoxal data file	string
ProductAlgorithmVersion	string	Version of the algorithm that produced the product.	string
InternalProcessorRevision	string	Version of the processor used to generate this product.	string
ProductFormatType	string	Data format of the product.	netCDF
ProductFormatVersion	string	Version number of the product format.	int
DOI	string	Digital Object Identifier (DOI)	*string*
ProductContents	string	Trace gase included in the product	*CHOCHO*
SolarSpectraDate	CCSDS_ASCII, string	Date and time of the DOAS reference spectra	CCSDS Date, *earthshine*
NumberGroundPixels	integer	Number of ground pixels per scanline	int (*24*)
NumberScanlines	integer	Number of scanlines in the file	int
NumberOfTotalPixels	integer	NumberGroundPixel x NumberScanlines	
SubsettingRegion	string	Description of the sub setting region. “full” means: no subsisting was applied.	string
SubSatellitePointStartLat	float	Latitude of the sub-satellite point at start of acquisition. (For EPS products: either the first measurement or first complete scan start point (tbd), at start of dataset.)	-90... 90
SubSatellitePointStartLon	float	Long. of the sub-satellite point at start of acquisition.	0... 360
SubSatellitePointEndLat	float	Latitude of the sub-satellite point at end of acquisition.	-90... 90
SubSatellitePointEndLon	float	Long. of the sub-satellite point at end of acquisition.	0... 360
SatellitePosition	POS_VEC	Position vectors (X,Y,Z) in km	Vector in POS_VEC
SatelliteVelocity	POS_VEC	Velocity vector (dx/dt, dy/dt, dz/dt) in km/s	Vector in POS_VEC
OrbitSemiMajorAxis	float	Semi-major axis (km)	float
OrbitExcentricity	float	Excentricity	float
OrbitInclination	float	Inclination (deg)	float
OrbitRightAscOfAscNode	float	Right asc. of asc. node (deg)	float
OrbitArgumentOfPerigee	float	Argument of perigee (deg)	float
OrbitMeanAnomaly	float	Orbit mean anomaly (deg)	float
OrbitUTCDaysSince2000	integer	UTC days since 1.1.1950	int
OrbitMsSinceMidnight	integer	UTC ms since midnight	int
OrbitAscendingNodeCrossingDateTime	CCSDS_ASCII	Ascending node crossing UTC date and time	CCSDS Date
OrbitAscendingNodeLongitude	float	Ascending node longitude	-180... 180
OrbitActualDuration	integer	Orbit duration in minutes, only counting valid pixels	0...~60

5.2 *PRODUCT Group*

The glyoxal (CHOCHO) columns are stored in the PRODUCT group together with some essential additional variables. Additional results are given in the respective subgroups of PRODUCT/SUPPORT_DATA. The following table contains the variables in the PRODUCT group.

Dataset Name	*Data Type*	*Dimensions*	*Unit*	*Description*
glyoxal_tropospheric_column	float	scanlines x groundpixel	molecules/cm^2	tropospheric vertical column of glyoxal
glyoxal_tropospheric _column_error	float	scanlines x groundpixel	molecules/cm^2	total error in tropospheric vertical column of glyoxal
latitude	float	scanlines x groundpixel	° North	latitude of the Pixel Centre (point F in figure 3) (-90° to 90°)
longitude	float	scanlines x groundpixel	° East	longitude of the Pixel Centre (point F in figure 3) (-180° to 180°)
delta_time	integer	scanlines x groundpixel	milliseconds	milliseconds since midnight of the reference day reference day is given as attribute
time	integer	scanlines x groundpixel	seconds	To reference day since midnight 2000-01-01
scanlines	integer	scanlines	1	dimension variable counting the scans from North to South
groundpixel	integer	groundpixel	1	dimension variable counting the groundpixel fom East to West

The measurement time is given in the delta_time variable, as milliseconds since midnight of the reference day. The reference day is given in three different variables or attributes. First it is given as attribute to the delta_time variable in the “YYYY-MM-DD” format. It is also given in days since 2000-01-01 in the global file attributes (OrbitUTCDaysSince2000), or it is given in the time variable in seconds since 2000-01-01. The global attribute and the time variable therefore differ by the constant factor 24*3600.

5.3 *DETAILED_RESULTS Group*

The *DETAILED_RESULTS* group encompasses additional results that are related to the glyoxal column. The following table gives an overview of all the data in the subgroup.

Dataset Name	*Data Type*	*Dimension*	*Unit*	*Description*
air_mass_factor	float	scanline x groundpixel x	1	air mass factor (clear sky)
air_mass_factor_error_sys	float	scanline x groundpixel	1	air mass factor systematic error
glyoxal_tropospheric_column_error_sys	float	scanlines x groundpixel	molecules/cm^2	systematic error in tropospheric vertical column of glyoxal
glyoxal_slant_column	float	scanline x groundpixel	molecules/cm^2	glyoxal slant column uncorrected
glyoxal_slant_column_corrected	float	scanline x groundpixel	molecules/cm^2	glyoxal slant column corrected
glyoxal_slant_column_error	float	scanline x groundpixel	molecules/cm^2	glyoxal slant column error
fit_results	float	scanline x groundpixel x fits	molecules/cm^2	slant columns of the other absorbers in the DOAS fit
cross_sections	string	fits	--	Cross section names of the other absorbers: O3, O2-O2, H2O, NO2_220K, NO2_296K, liquid water, Ring
fitted_root_mean_square_residuals	float	scanline x groundpixel	1	root mean squared of DOAS fit
pressure_levels	float	levels	hPa	centre of the pressure grid
averaging_kernel	float	scanline x groundpixel x levels	1	averaging kernel (AK)
apriori_glyoxal_profile	float	scanline x groundpixel x levels	vmr	A priori profile of glyoxal for the AMF and AK calculation
processing_quality_flag	integer	scanline x groundpixel	1	quality indicator 0 is good data see section 5.6.4 for flag description

5.4 *GEOLOCATION* Group

The *GEOLOCATION* group contains information for the four corner points for the ground pixel, denoted by letters A to D in Figure 5. As well as the viewing geometry for the central point F.

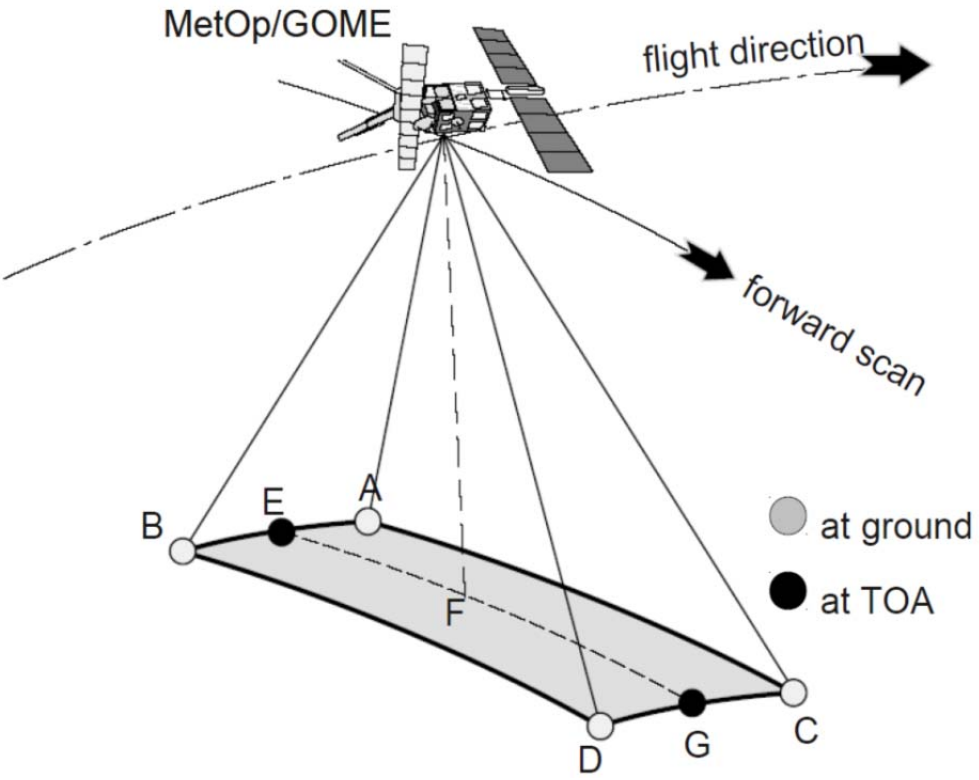

Figure 3: Ground Pixel Geometry

The data sets in the *GEOLOCATION* group are given in the following table:

Dataset Name	Data Type	Dimension	Unit	Description
corners	string	4	--	dimension variable, order of the corner points
latitude_corners	float	scanline x groundpixel x corners	° North	Latitude of the corner points
longitude_corners	float	scanline x groundpixel x corners	° East	Longitude of the corner points
solar_zenith_ angle	float	scanline x groundpixel	degrees	Solar zenith angle at TOA (Point F)
viewing_zenith_ angle	float	scanline x groundpixel	degrees	Line-of-sight zenith angle at TOA (Point F)
relative_azimuth_angle	float	scanline x groundpixel	degrees	Relative azimuth at TOA (Point F)

5.5 *INPUT_DATA* Group

During the data retrieval additional data are read and stored together with the product. The data are necessary for the processing and partly for the interpretation of the glyoxal columns. An overview of the data is given in the following table:

Dataset Name	Data Type	Dimension	Unit	Description
cloud_fraction	float	scanline x groundpixel	1	Cloud fraction
cloud_top_albedo	float	scanline x groundpixel	1	Cloud top reflectance
cloud_top_pressure	float	scanline x groundpixel	hPa	Cloud pressure
intensity_weighted_cloud_fraction	float	scanline x groundpixel	1	Intensity weighted cloud fraction
surface_altitude	float	scanline x groundpixel	km	surface altitude
surface_pressure	float	scanline x groundpixel	hPa	surface pressure
surface_albedo	float	scanline x groundpixel	1	Derived from AC-SAF GOME-2 DLER data set [R7]
surface_condition_flag	int	scanline x groundpixel	1	land-water-snow/ice flag (see Table 5.6.2)

5.6 Detailed Flag Description

This section gives an overview of all flag datasets. In Sect. 5.6.4, a detailed description on how the flag data can be interpreted can be found.

5.6.1 SwathMode and ViewMode

The SwathMode dataset provides the information about the Swath or Scanning mode of the instrument at the time of acquisition. The information is stored as integer values (see *InstrumentMode* in Sect. 5.1 for how many ground pixels were observed in the corresponding scanning mode of the instrument view).

Value	*Description*
0	Nominal
1	Narrow
2	Static
3	SouthPolar
4	NorthPolar

The ViewMode dataset combines the information about the Swath or Scanning mode of the instrument at the time of acquisition (bits 0-7), and the information about the orbital mode (i.e. acquisition during ascending or descending node)

Bit(s)	*Value*	*Description*
0-7	0-4	0=Nominal, 1=Narrow, 2=Static Nadir, 3=SouthPolar, 4=NorthPolar
8	256	DescendingFlag Set when ground pixel is in descending part of orbit

5.6.2 surface_condition flag

These flags give additional information about the surface state during the retrieval. See Sect. 5.6.4. for an example how to use this flag.

Bit	*Value*	*Description*
0	0	**Land** Set when at least 40% of the ground pixel's area is classified as "land"
0	1	**Sea** Set when at least 60% of the ground pixel's area is classified as "sea"
1	2	**Sun glint** Set when at least one of the PMD subpixels is affected by sunglint
2	4	**Snow/Ice**

5.6.3 processing_quality_flag

The QualityFlag dataset provides flags if the measured data is valid. These flags give additional

information about the quality of the total column retrieval. If for example the fitting of the slant column does not succeed flag is set to 1 indicate this condition. If the flag is set to 1 to 8 a fill value is written to the results file.

Bit	*Value*	*Description*
0	0	**Valid data**
0	1	**Invalid column** (retrieval failed) e.g. the DOAS retrieval failed glyoxal_tropospheric_column contains fill-values
1	2	**Measurement with large solar zenith angle** SZA > 70° glyoxal_tropospheric_column contains fill-values
2	4	**Unfulfilled external dependencies** GOME-2 input (cloud) data had a fill value/not available glyoxal_tropospheric_column contains fill-values
3	8	**Cloudy conditions** Cloud fraction larger than 0.2 glyoxal_tropospheric_column contains fill-values
4	16	**WARNING Large error in slant column** Set if the slant column error exceeds the specific threshold glyoxal_tropospheric_column contains data.

Note that if the flag is 16 the data are still valid but the retrieval error is large and the user have to be cautious about the results,

5.6.4 Flag usage

The flag datasets in the L2 product are stored as binary flags in order to combine different flags in a single dataset. In this way adding further flags in one dataset at a later stage does not affect the dataset itself, so users can still use their routines to read the flag datasets even if new information was added. In the tables above the integer value of a flag as well as the bit of the flag is given. The integer value can be calculated from $\sum 2^{\text{bit}}$.Here we give an extensive example for the SurfaceConditionFlag dataset (Sect. 5.6.2) in order to explain how to read and interpret these datasets.

In the SurfaceConditionFlag several scenarios can appear: Land/Sea and Sun glint. In principle for a single pixel several scenarios can occur e.g. a pixel over the sea which is subject to sun glint. Represented in binary form it would look like:

0 | 0 | Value 1 | 0 | Bit Integer value: 0 (no bit set)	No flag set, i.e. pixel over land, no sun glint
0 | 1 | Value 1 | 0 | Bit Integer value: 1 (2^0, first bit set)	Pixel over sea (Land/Sea flag set), no sun glint
1 | 0 | Value 1 | 0 | Bit Integer value: 2 (2^1, second bit set)	Pixel over land, sun glint (sun glint flag set)

1	1	Value
1	0	Bit

Integer value: 3 (2^1+2^0, first and second bit set)

Pixel over sea, sun glint (both flags set)

In order for a user to check if one of the flags is set the bitwise AND operator has to be used. E.g. in order to check if the sunglint flag bit is set the user has to do the operation 1^{bit} AND SurfaceConditionFlag(Pixel). The snow/ice flag is stored in the 1^{nd} bit, hence the operation would be 1^2 AND SurfaceConditionFlag(Pixel).

As a second example we describe how to use the ViewMode dataset (Sect.5.6.1). This dataset combines two flags within one dataset – first the swath mode of the instrument is stored in the first 8 bits (bits 0-7) and second the information whether it was taken on the ascending or descending node is stored in the 9^{th} bit (bit 8).

In order to filter for a specific swath mode x (x=0: nominal, x=1: narrow, etc), the first seven bits have to be checked for it i.e. ($2^0+2^1+2^2+2^3+2^4+2^5+2^6+2^7$) AND ViewMode = x or 255 AND ViewMode = x
To select all pixels from the descending node the user has to check whether bit 8 has been set, i.e. according to our previous example the condition 2^8 AND ViewMode > 0 must be fulfilled. For the pixels on the ascending node the condition 2^8 AND ViewMode = 0 applies

Here we give some examples:
Nominal swath, ascending orbit: (255 AND ViewMode) = 0 & (256 AND ViewMode) =0
Nominal swath, descending orbit: (255 AND ViewMode) = 0 & (256 AND ViewMode) >0
Narrow swath, ascending orbit: (255 AND ViewMode) = 1 & (256 AND ViewMode) =0
Narrow swath, descending orbit: (255 AND ViewMode) = 1 & (256 AND ViewMode) >0

Of course the user can also directly check for the integer value of the ViewMode dataset (in the examples above the integer values would be 0; 256; 1; 266, respectively), but if at a later stage the ViewMode dataset it expanded and more information is stored, then this would affect how the data is filter out by the user's algorithm (e.g. if the user uses all data with ViewMode > 256)

6 Using the Products

This chapter contains practical information on using the GOME-2 glyoxal product.

The data are stored in a 2D array with 24 ground pixels of the instrument's forward-scan and the scan lines along the track.

6.1 Confidence Flags and Ancillary Fields

The users should check the quality flags associated with the product. Detailed information is given in the corresponding tables.

6.2 Averaging Kernels

For the glyoxal columns, averaging kernels are provided together with the error budget for each individual GOME-2 pixel. The column averaging kernels A_l are calculated for optically thin absorbers (such as NO_2, HCHO and glyoxal) as follows:

$$A_l = \frac{m_l}{M_t}$$

where m_l is the altitude-dependent air mass factors for layer l and M_t the tropospheric air mass factor. The tropospheric air mass factor depends on the a priori profile **v** via:

$$M_t = \frac{\sum v_l \cdot m_l}{\sum v_l},$$

with v_l being the vertical sub columns of the a priori profile.

Column averaging kernels are essential information on the measurement vertical sensitivity and are particularly useful when comparing measured columns with e.g. model simulations, because they allow removing the effect of the a priori profile shape information used in the retrieval and is required for comparison with other types of data.

The averaging kernels are provided for the model layers of the tropospheric a priori profiles as used in the retrieval (altitude at layer centre). The a priori glyoxal profiles profiles (in molec/cm^3) are also provided in the GOME-2 product. Combining the information given it is possible to calculate the tropospheric AMF M_t for any given glyoxal profile **v**' (e.g. retrieved from MaxDOAS observations).

First the tropospheric AMF M_t' is calculated:

$$M'_t = \frac{M_t \cdot \sum A_l \cdot v'_l}{\sum v'_l}$$

Then the new tropospheric vertical column V'_t is given by:

$$V'_t = V_t \cdot \frac{M_t}{M'_t}$$

6.3 Software and Tools for reading the products

The netCDF products can be read using the standard netCDF4 software and tools available at:

https://unidata.github.io/netcdf4-python/netCDF4/index.html

NASA offers the netcdf data viewer panoply for download at:

https://www.giss.nasa.gov/tools/panoply/