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AUTHORS/ CONTRIBUTORS LIST

Name	Function	Organization
Stein Vidar Hagfors Haugan	sWP 2.2.5 leader	Universitetet i Oslo (UiO)
Mats Carlsson	WP10 lead	UiO

SCIENTIFIC APPROVAL CONTROL FROM SUB-WP & WP LEAD

Control	Name	Organization	Function	Date
Prepared	Stein Vidar Hagfors Haugan	UiO	sWP 2.2.5 leader	July 5th, 2020
Revised	Stein Vidar Hagfors Haugan	UiO	sWP 2.2.5 leader	July 6th, 2020
Approved	Dan Kiselman	Stockholms universitet (SU)	WP 2 lead	July 6th, 2020
Authorized	Dan Kiselman	SU	WP 2 lead	July 9th, 2020

ADMINISTRATIVE APPROVAL CONTROL FROM PROJECT OFFICE

Control	Name	Organization	Function	Date
Approved	Tirtha Som	Leibniz-Institute for Solar Physics (KIS)	Project Manager	July 9th, 2020
Approved	Rolf Schlichenmaier	KIS	Project Coordinator	July 23rd, 2020
Authorized	Markus Roth	KIS	Project Scientist	July 23rd, 2020

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Leibniz-Institut für Sonnenphysik (KIS)
Schöneckstr. 6, 79104 Freiburg im Breisgau, Germany
Tel.: +49-761-3198-224; Email: SOLARNET-office@leibniz-kis.de

Preface

Until now, sharing of simulated data within the Solar Physics community has been mostly on a "private communication" basis, with the description of the data format and content conveyed in an *ad hoc* manner. However, funding bodies are more and more likely to require simulation data to be made publicly available and usable by other research groups. This requires a standard for how the data is represented and described, and this document aims to establish and describe such standards and recommendations.

Within observational Solar physics, the most common file format is Flexible Image Transport Format (FITS – see FITS Standard 4.0). It is also the file format used to share BIFROST simulations and derived products (e.g. synthesised observables) through the Hinode archive at ITA/UiO. Additionally, most visualization software within Solar physics use FITS files as input. Therefore, these metadata recommendations are expressed here through FITS keywords. *However, this does not preclude the use of other file formats expressing the same metadata in different forms*.

In this document, "simulated observations" refers to any "observation-like" data product derived from the simulations themselves, defined over a two-dimensional footprint of a simulation). Typically, simulated observations are normal observables such as synthetic spectra or images, but they may also represent e.g. the height at which τ=1. Any three-dimensional derived products should normally be treated on par with actual simulation data.
In order to facilitate reuse of analysis and visualization software written for true Solar observations, simulated observations should mimic true observations to a high degree.
For that reason, *almost all of deliverable D2.18 SOLARNET Metadata Recommendations (D2.18 hereafter) applies to simulated observations*, thus for these we will here only mention some of the applicable deviations and additions, give some clarifying remarks, and reiterate a few important points. The notation used is the same as in deliverable D2.18 (e.g. FITS keyword names and values are in bold monospace font).

The latest version of this document can be found at http://sdc.uio.no/open/solarnet/. For any questions, contact s.v.h.haugan@astro.uio.no.

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Part A. Simulated observations

1. General considerations

As for true observations, HDUs containing simulated observations must have **SOLARNET=0.5** or **1**, **OBS_HDU=1**, and may use the keyword **SOLNETEX** to exclude certain keywords from being interpreted within the **SOLARNET** metadata framework. All Obs-HDUs must have a unique **EXTNAME.**
Any HDU with a nonzero value of **SOLARNET** may use the mechanisms described in the Appendices of D2.18 (e.g. variable keywords, pixel lists and meta-HDUs).

2. The World Coordinate System (WCS) and related keywords

Simulations are normally not meant to represent an actual Solar region. As a result, the location in time and space is traditionally not specified at all for neither simulations nor the simulated observer. However, assigning some definite time and location to a simulation makes it possible to represent the temporal and spatial relationship between a simulated observation and its simulation by specifying the time and location of the observer. Thus, a single simulation may be "observed" from multiple vantage points in a consistent way that may be recognised by generic software, allowing correlation of image positions between both multiple vantage points and the simulation itself. This can be achieved in FITS files using the World Coordinate System (WCS), see Paper I.

The most common situation is that a simulation is viewed from directly above when creating a simulated observation. This can be represented by fixating the positions of both observer and simulator at Stonyhurst heliographic longitude and latitude zero, i.e. directly above the Solar Equator, on the same meridian as Earth. Using WCS to represent this simple case, the following keyword values should be used *for both the simulation and the observation*:

```
HGLN_OBS=        0.0 / [deg] Sim/obs at same Longitude as Earth
HGLT_OBS=        0.0 / [deg] Sim/obs directly above Solar Equator
DSUN_OBS= 1.4960E+11 / [m]  Sim/obs is at 1AU from Sun Centre
DSUN_AU =        1.0 / [AU] Sim/obs is at 1AU from Sun Centre
```

The **DSUN_AU** keyword is merely for convenience, it is the **DSUN_OBS** value that applies in WCS.

For real Solar observations, the "spatial" coordinates are normally sky coordinates, not physical coordinates, and unfortunately some analysis and visualization software may have hardcoded in that "the *X* axis is the one labelled with **HPLN** and the *Y* axis is labelled with **HPLT**". We therefore propose that simulated observations masquerade as true observations in this respect, representing their *primary* spatial coordinates in terms of Helioprojective Cartesian coordinates (see Paper VI). Also, for guaranteed compatibility with the CRISPEX visualization software, the simulated observation data cube should have 5 dimensions (any dimension may be singular), in the order (*X*, *Y*, *wavelength*, *Stokes*, *time*). The *Stokes* dimension is used to represent Stokes *IQUV* parameters, see Paper I. Some reduced-dimensionality cases can be handled by CRISPEX, see the documentation.

For most simulated observations, the use of WCS should be extremely simple, as they represent data from a "perfect instrument" with no distortions etc. This may be different, of course, if the synthesis is meant to represent data from an actual instrument – in which case the WCS treatment will be identical or at least very similar to that of the represented instrument. Also, in some cases, mechanisms such as tabulated coordinates may be useful in order to represent uneven resolution/sampling in some direction, whether to emulate a specific instrument or to save storage space.

Leibniz-Institut für Sonnenphysik (KIS)
Schöneckstr. 6, 79104 Freiburg im Breisgau, Germany
Tel.: +49-761-3198-224; Email: SOLARNET-office@leibniz-kis.de

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In the simple case discussed so far, for a 1024x1024 pixel simulated observation movie with 1s cadence, located at Sun centre, with spatial resolution 10km and with no spectral or polarization information, the corresponding *coordinates* may be specified like this:

```
CTYPE1  = 'HPLN-TAN'          / Coordinate 1 is Helioprojective Longitude
CDELT1  =             0.01379 / [arcsec] 10km resolution (1.379 arcsec/Mm)
CUNIT1  = 'arcsec'            / Units for coordinate 1
CRPIX1  =               512.5 / Reference pixel (HPLT = 0.0 arcsec)

CTYPE2  = 'HPLN-TAN'          / Coordinate 2 is Helioprojective Latitude
CDELT2  =             0.01379 / [arcsec] 10km resolution (1.379 arcsec/Mm)
CUNIT2  = 'arcsec'            / Units for coordinate 2
CRPIX2  =               512.5 / Reference pixel (HPLN = 0.0 arcsec)

CTYPE3  = 'WAVE'              / Singular coord. 3 is wavelength

CTYPE4  = 'STOKES'            / Singular coord. 4 is Stokes parameter(I)

CTYPE5  = 'UTC'               / Coord. 5 is time
CDELT5  =                 1.0 / [s] Time resolution 1 second
CUNIT5  = 's'                 / Unit for axis 1
CRPIX5  =                   1 / Reference pixel (time = 0s after DATEREF)
```

The mandatory keyword **DATE-BEG** should be set to the value of **DATE-BEG** in the *simulation* plus any simulated (Solar) time elapsed *in the simulation* prior to the starting point for the *observation*. Likewise, **DATE-END** should be set to **DATE-BEG** plus the simulated elapsed time covered by the observation. **DATEREF** – the reference time at which the time coordinate is zero – should be set to the same value as in the simulation (the wall time at which the simulation was started), and the time coordinate (**UTC**) must be set to ensure that the time coordinates of the simulation and the simulated observation match up (see Paper IV and D2.18). This, together with a matching of the spatial coordinates will allow generic software to browse both simulation and observation data together.
In WCS it is possible to specify more than one coordinate system. Thus, a physical coordinate system may be specified in addition to the primary system, using one of the coordinate systems mentioned in Paper VI. See the discussion about WCS coordinates for actual simulations in Part B, Section 11.

In general, care must be taken so that the coordinates of the observation (both Helioprojective and physical) match up with the physical coordinates of the simulation.

3. Description of data contents

A description of the actual data contents is important for the interpretation of a simulated observation. Such a description is also important for finding relevant observations in an SVO. The **BTYPE** and **BUNIT** keywords should be used for this purpose - we refer to the corresponding Section in D2.18 for details but recognize that simulated observations may represent other/additional types of data, which will require further study and discussions.

Much of the contents in the corresponding Section in D2.18 is not relevant for simulations, such as exposure times and binning (unless simulating an actual observation with a specific instrument), but we would like to highlight some of the keywords that *are* relevant: **CADENCE**, **WAVEMIN**/**WAVEMAX**, **WAVELNTH**, **WAVEBAND**, **POLCCONV**, and **DATAMIN**/-**MAX**/-**MEAN**. Note that in case of variable time steps, the **CADENCE** keyword may be represented as a variable keyword plus a scalar average.
ELAPSED should be used to indicate the number of seconds of simulated time has passed since the start of the simulation.

Leibniz-Institut für Sonnenphysik (KIS)
Schöneckstr. 6, 79104 Freiburg im Breisgau, Germany
Tel.: +49-761-3198-224; Email: SOLARNET-office@leibniz-kis.de

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4. Metadata about affiliation, origin, acquisition, etc.

Much of the metadata mentioned in the corresponding section of D2.18 is not applicable to simulated observations. However, some should/may still be used for searchability purposes – though perhaps in an analogous rather than strict interpretation of the description in D2.18. Although the keyword names are not a 100% match heuristically speaking, using the same keywords as those defined in D2.18 will greatly simplify the adaptation of regular SVOs to include simulated observations. In particular: **OBSRVTRY** (the institution at/by which the code was run), **PROJECT**, **INSTRUME** (the name of the code used), **OBS_MODE** (if the "observation" program has discrete modes of operation), **SETTINGS** (similar to **OBS_MODE** but more for fine-tuning than overall operation mode), **OBSERVER** (the one actually running the simulation), **PLANNER, AUTHOR** (of the software – comma-separated list or a reference to a group)**, DATATAGS** and **INFO_URL**. Although the definition of these keywords (and others mentioned in D2.18) are difficult to express precisely, what is most important is that they are interpreted and populated in a consistent manner within each project. We also define a new keyword, **SMLATION**, which should be set to a unique identifier referring to the actual simulation data being "observed", identical to the value of the same keyword in the simulation data. The keyword **PAPERS** may be used for a comma-separated list of relevant papers regarding the code and/or methodology used.

SNAPSHOT should be set to the snapshot number(s) of the simulation used to generate the observation. If the observation is derived from a series of snapshots, the numbers should be given through the variable-keyword mechanism, with the scalar value of the keyword set to a comma-separated list containing the same numbers.

5. Grouping

*See D2.18. A*lthough simulated observations typically do not have a notion of "pointing", if there are multiple files that belong together as one "observation" or "observation series", they should have a common **POINT_ID** value, and files that do *not* belong together should have a *different* **POINT_ID**.

6. Pipeline processing applied to the data

Although the term "data pipeline" is not regularly used in the context of simulated observations, they are in fact the result of a pipeline consisting of *at least* one step – conversion from the simulation to the simulated observation. As such, the PRxxxxna mechanism mentioned in the corresponding section of D2.18 may be used to specify details about the processing.

7. Integrity and administrative information

See the corresponding section (section 11) in deliverable D2.18 of this project.

8. Reporting of events

See the corresponding section (section 12) in deliverable D2.18 of this project, and note that for simulated observations, features and events detected inside the simulation can be pinpointed using the pixel list mechanism.

Leibniz-Institut für Sonnenphysik (KIS)
Schöneckstr. 6, 79104 Freiburg im Breisgau, Germany
Tel.: +49-761-3198-224; Email: SOLARNET-office@leibniz-kis.de

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Part B. Simulation data

1. Introduction

Actual simulation data are fundamentally different from simulated observations – they are typically 3-dimensional rather than 2-dimensional and may represent a wide range of physical parameters.
Also, actual simulation data volumes are usually orders of magnitude larger than both real and simulated observations, and the data are often defined on a nonrectangular and nonuniform grid (staggered mesh, varying spatial resolution with height, etc).
With respect to the data volume, it will often be necessary to publish down-sampled versions of the simulation data rather than the raw simulation data.

2. General considerations

HDUs containing simulation data (Sim-HDUs) must have **SOLARNET=0.5** or **1**. and may use the keyword **SOLNETEX** to exclude certain keywords from being interpreted within the **SOLARNET** metadata framework. But it should *not* have **OBS_HDU=1**, but rather **SIM_HDU=1**. All Sim-HDUs must have a unique **EXTNAME.**
Any HDU with a nonzero value of **SOLARNET** may use the mechanisms described in the Appendices of D2.18 (e.g. variable keywords, pixel lists and meta-HDUs).

3. WCS and related keywords for simulation data

Of course, simulations have no true “observer position”, but an observer position must be given in order to be able to specify the simulation position/coordinates in a simple manner. *See Section 2 for a straight-forward explanation of how the observer position can be given.*

For simulation data, the most appropriate coordinate system might be to use Heliocentric Cartesian coordinates, **SOLX**, **SOLY**, **SOLZ**. However, the **SOLZ** coordinate is defined as the distance towards the observer measured from the **SOLX**/**SOLY** plane going through the Sun centre, which might give rise to precision problems. Additionally, visualizing data with an axis that varies between 150.7 Gm and 150.8 Gm for a 100Mm high simulation is not very useful. Instead, we propose to use the **HECH** coordinate, defined by Paper VI as the radial distance (height) from the Solar surface. In that case, **RSUN_REF** *must* be set to the radius of the Sun used to define the Solar surface – or rather as *the distance from the center of the Sun at which the* **HECH** *coordinate is zero*. When feasible, it is recommended that the zero point of the **HECH** coordinate matches the coordinates used internally by the simulation software.

Beware that the **HECH** coordinate is a radial coordinate, whereas the **SOLX**/**SOLY/SOLZ** coordinates are Cartesian. For most cases, the spatial footprint of a simulation is small enough that this is not an issue, but it may have to be taken into account for large simulations in the future.

A varying vertical resolution with height can be fairly easily dealt with by using lookup coordinates (see Paper III). However, it may often be the case that the simulation data must be interpolated onto a more regular grid than what has actually been used by the simulation software – but as mentioned before, interpolation may be needed anyway in order to reduce file sizes.

Most simulation data are stored one snapshot at a time, but all snapshots need to have an accurate time coordinate that is common and consistent between them and can be referenced in simulated observations. The **DATEREF** keyword defines the zero point for the time coordinate and should be set to the (wall) starting time of the simulation program.

Leibniz-Institut für Sonnenphysik (KIS)
Schöneckstr. 6, 79104 Freiburg im Breisgau, Germany
Tel.: +49-761-3198-224; Email: SOLARNET-office@leibniz-kis.de

One exception may apply: if a simulation attempts to model the physics underlying *one specific actual* observation or event, the **DATEREF** keyword should be set to a time that is appropriate for this purpose, such as the starting time of the observation or event to be modeled. If the simulation starts earlier, the time coordinate may be negative for the period leading up to **DATEREF**.

Assigning a time coordinate to a snapshot (with no intrinsic time coordinate) may be achieved through the fact that a FITS HDU may have more coordinates than data cube dimensions. E.g. if a simulation data cube has three dimensions, setting **WCSAXES** to **4** while leaving **NAXES=3** allows the description fourth coordinate, setting **CTYPE4="UTC"**, **CRPIX4=1**, and **CRVAL4** equal to the time coordinate (relative to **DATEREF**) that applies to the snapshot.

The mandatory FITS keyword **DATE-BEG** can be set to the same time as the "phantom" time coordinate for the snapshot, and **DATE-END** may be set to the same time. However, in particular when dealing with uneven time steps, it may be prudent to set **DATE-BEG** to represent the mid-way point from the previous snapshot, and **DATE-END** to represent the mid-way point to the next snapshot.

4. Description of the simulation and the data contents

There are, of course, many pieces of metadata that can be associated with a simulation and its data contents other than WCS and related information. However, unlike for observational data, there is very little tradition to build on, and only a limited set of metadata concepts valid for observational data are applicable to simulation data.
However, we suggest that some effort is made to make connections between observational metadata and simulation metadata, reusing keywords used for observational data when making a reasonable (though not necessarily perfect) connection or analogy is possible. This will make it somewhat easier to reuse SVO designs for simulation archives.
First of all, the keywords **BTYPE**/**BUNIT** should be used to describe the nature of and units for the data represented in the keywords. For the units, combinations of SI units can be used. For **BTYPE**, it needs to be discussed what format and what descriptors should be used – one alternative is to use LaTeX notation according to the simulation community standard. Another alternative is to use some simplified syntax. One benefit of using a simplified syntax is that the **BTYPE** value can then be reflected in the file name.
DATAMIN/-MAX/-MEAN/-MEDN should be used to specify the min, max, mean and median values of the data cube, likewise the DATAPnn may be used to specify the percentiles of the data cube values.
Of course, a single snapshot does not have an actual cadence, but the keyword **CADENCE** should be set to the "local" cadence to indicate the time between snapshots, perhaps the average of the time difference to the previous and subsequent snapshots. **SNAPSHOT** should be set to the snapshot number. **ELAPSED** should be used to indicate the number of seconds of simulated time has passed since the start of the simulation.

5. Metadata about affiliation, origin, acquisition, etc.

See Section 4, Part A of this report.

6. Grouping

For one-off simulations, **POINT_ID** can be identical to the **SMLATION** keyword, but for simulations that are part of an overarching series of simulations, **POINT_ID** should be set to an identifier of that overarching series, so it can be separated from other series.

7. Pipeline processing applied to the data

See Section 6, Part A of this report.

8. Integrity and administrative information

See Section 7, Part A of this report.

9. Reporting of events

See corresponding section (section 12) in D2.18 and note that features and events detected inside the simulation can be pinpointed using the pixel list mechanism.

10. References

- The FITS Standard, version 3.0 (Pence et al, 2010, A&A, **524**, A42, 40 pp., https://www.aanda.org/articles/aa/pdf/2010/16/aa15362-10.pdf)
- Paper I: Representations of World Coordinates in FITS (Greisen & Calabretta, 2002, A&A, **395**, 1061-1075, http://www.aanda.org/articles/aa/pdf/2002/45/aah3859.pdf)
- Paper II: Representations of celestial coordinates in FITS (Calabretta & Greisen, 2002, A&A, **395**, 1077-1122, http://www.aanda.org/articles/aa/pdf/2002/45/aah3860.pdf)
- Paper III: Representations of spectral coordinates in FITS (Greisen, Calabretta, Valdes & Allen, 2006, A&A, **446**, 747-771, http://www.aanda.org/articles/aa/pdf/2006/05/aa3818-05.pdf)
  - Authors' web sites, supplemental background: Eric Greisen, Mark Calabretta, http://www.atnf.csiro.au/people/mcalabre/WCS/index.html
  - An unofficial errata for Papers I, II, and III (Calabretta & Greisen, http://fits.gsfc.nasa.gov/wcs/errata_20071222.pdf)
- Paper IV: Representations of Time Coordinates in FITS (Rots, 2015, A&A, **574**, A36, https://www.aanda.org/articles/aa/pdf/2015/02/aa24653-14.pdf)
- Paper V: Representations of distortions in FITS world coordinate systems (Calabretta, Valdes, Greisen, Allen, ADASS, 2004, **314**, http://fits.gsfc.nasa.gov/wcs/dcs_20040422.pdf)
- Coordinate systems for solar image data (Thompson, 2006, A&A, **449**. 791-803, http://www.aanda.org/articles/aa/pdf/2006/14/aa4262-05.pdf)
- FITS: A Flexible Image Trasport System (Wells et al, 1981, A&AS, **44**, 363)
- Precision effects for solar image coordinates within the FITS world coordinate system (Thompson, 2010, A&A, **515**, A59, http://www.aanda.org/articles/aa/pdf/2010/07/aa10357-08.pdf).
- The SolarSoft WCS Routines: A Tutorial (Thompson, http://hesperia.gsfc.nasa.gov/ssw/gen/idl/wcs/wcs_tutorial.pdf)
- Binary table extension to FITS (Cotton et al., 1995, A&AS, **113**, 159-166, http://adsabs.harvard.edu/abs/1995A%26AS..113..159C).
- Checksum Keyword Convention (http://fits.gsfc.nasa.gov/registry/checksum.html)
- The FITS Header Inheritance Convention (https://fits.gsfc.nasa.gov/registry/inherit/fits_inheritance.txt
- The CONTINUE Long String Keyword Convention (https://fits.gsfc.nasa.gov/registry/continue_keyword.html)

Leibniz-Institut für Sonnenphysik (KIS)
Schöneckstr. 6, 79104 Freiburg im Breisgau, Germany
Tel.: +49-761-3198-224; Email: SOLARNET-office@leibniz-kis.de

- Space Physics Archive Search and Extract (SPASE) instrument types (http://www.spase-group.org/data/reference/spase-2_2_8/spase-2_2_8_xsd.htm - InstrumentType and http://www.spase-group.org/docs/dictionary/spase-2_2_8.pdf)
- Recommendations for Data & Software Citation in Solar Physics (2012AAS...22020127H)
- Best Practices for FITS Headers (2012AAS...22020128H, http://sdac.virtualsolar.org/docs/SPD2012/2012_SPD_FITS_headers.pdf)
- VSO Checklists, http://virtualsolar.org/checklists
- VSO Minimum Information for Solar Observations, http://docs.virtualsolar.org/wiki/MinimumInformation
- The Unified Content Descriptors, Version 1+ (UCD1+) http://www.ivoa.net/documents/latest/UCDlist.html

Other sources of keywords with established use:

- Solar Orbiter FITS keyword definitions (in preparation, contact s.v.h.haugan@astro.uio.no for latest version)
- STEREO Standard FITS keywords (http://jsoc.stanford.edu/doc/keywords/STEREO/STEREO_site_standard_fits_keywords.txt)
- SDO/AIA FITS keyword definitions (https://www.lmsal.com/sdodocs/doc?cmd=dcur&proj_num=SDOD0019&file_type=pdf)
- IRIS FITS keyword definitions (http://www.lmsal.com/iris_science/irisfitskeywords.pdf)

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