



# **Cosmic-Ray neutron Sensor PYthon tool (crspy): An open-source tool** for the processing of cosmic-ray neutron and soil moisture data

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# Abstract.

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Understanding soil moisture dynamics at the sub-kilometre scale is increasingly important especially with continuous development of hyper-resolution land-surface and hydrological models. Cosmic Ray Neutron Sensors (CRNS) are able to provide estimates of soil moisture at this elusive scale and networks of these sensors have been expanding across the world over the previous decade. However, each network currently implements its own protocol when processing raw data into soil moisture estimates. As a consequence, this lack of a harmonized global dataset can ultimately lead to limitations in the global assessment of the CRNS technology from multiple networks. Here we present crspy, an open-source python tool that is

- 15 designed to facilitate the processing of raw CRNS data into soil moisture estimates in an easy and harmonized way. We outline the basic structure of this tool discussing the correction methods used as well as discussing the metadata that crspy can create about each site. Metadata can add value to global scale studies of field scale soil moisture estimates by providing additional routes to understanding catchment similarities and differences. We demonstrate that current differences in processing methodologies can lead to misinterpretations when comparing sites from different networks and having a tool to provide a
- 20 harmonized dataset can help to mitigate these issues. By being open source, crspy can also serve as a development and testing tool for new understanding of the CRNS technology as well as being used as a teaching tool for the community.

# 1 Context and Background

Soil moisture exerts a large influence on hydrological (Van Loon et al., 2015), biogeochemical (Schlesinger et al., 2015), and climatic processes (Dobriyal et al., 2012; Koster et al., 2004), agricultural systems (Fontanet et al., 2018; Dutta et al., 2014),

- 25 landslide modelling (Zhuo et al., 2019) and earth system sciences (Fang and Lakshmi, 2014; Bonan, 2008). Its accurate measurement is important to advance our understanding of these areas of research. In-situ point scale soil moisture estimates, such as Time Domain Reflectometry (TDR), can provide higher temporal resolution; however spatial resolution is still limited, on the order of centimetres. Soil heterogeneity can lead to uncertainties when upscaling to the field scale (Western et al., 1999), which would be required for regional or larger scale hydrological modelling. Alternatively, satellite remote sensing products
- 30 such as Soil Moisture Active Passive (SMAP) and Soil Moisture and Ocean Salinity (SMOS) can provide global estimates of soil moisture at a coarser spatial (~40km resolution) and temporal (~3 days) scale, and at much shallower depths (~5cm)





(Entekhabi et al., 2010; Kerr et al., 2001). It is accepted that we will require a finer spatial resolution than currently achievable through remote sensing estimates for tasks such as increasing our understanding of sub-kilometre land-atmosphere interactions, or towards the improvements of farming practices (such as through the process of irrigation scheduling), and so there is a need for additional processing of ancillary data for the despendence of these products (Partal et al., 2020). Alemahammed et al.

- for additional processing of ancillary data for the downscaling of these products (Portal et al., 2020; Alemohammad et al., 2018). In addition, the recent push for hyper resolution global modelling means we require measurements at a finer spatial resolution, on the order of sub-kilometer scales (Wood et al., 2011). Bierkens et al., (2015) discussed the implications of moving from a more standard resolution ~50km model to a hyper-resolution model that is sub-kilometre. The study further discussed the need to move from sub-grid paradigms, that represent a conceptualized form of earth system dynamics from within the standard 50km resolution model, to explicit dynamics of earth system processes at scales < 50km. This requires a</p>
- greater understanding of environmental functions at sub-kilometre, spatial scales, which in turn requires accurate measurements of environment states at the same scales.
- Cosmic-Ray Neutron Sensors (CRNS) is a relatively new technology that allows estimates of soil moisture at the field scale (~600m diameter) at hourly temporal resolution. Zreda et al., (2008) demonstrated that fast neutrons are mainly moderated by hydrogen atoms, which allows us to infer changes in water content in the soil profile. A tube attached to the sensor, filled with a gas such as helium or boron trifluoride, is able to detect fast neutrons that pass through it by inducing a voltage difference. Desilets et al., (2010) introduced an equation used to convert neutron counting rates into gravimetric soil moisture which has been further improved upon by Dong et al., (2014) and Hawdon et al., (2014) (equation 1). This equation forms the core to using cosmic-ray neutron sensors for, now, volumetric soil moisture estimates in the field:

$$\theta_{vol} = \left[\frac{a_0}{\frac{Nraw \cdot f_p \cdot f_l \cdot f_h \cdot f_v}{N_0} - a_1} - a_2 - LW - WSOM\right] \rho_{bd} \tag{1}$$

where  $\theta_{vol}$  is volumetric soil moisture (cm<sup>3</sup>/cm<sup>3</sup>);  $a_0, a_1, and a_2$  are coefficients obtained from neutron particle physics 55 modelling (Zreda et al., 2008; Desilets et al., 2010) and assumed to be constants; *LW* is the lattice (chemically-bounded mineral) water (%), *WSOM* is the water equivalent of soil organic carbon (g/cm<sup>3</sup>), and  $\rho_{bd}$  is the bulk density of the dry soil (g/cm<sup>3</sup>).  $N_{raw}$  is the measured raw, uncorrected, neutron count identified over the given integration time, usually set to one hour.  $f_p$ ,  $f_i$ ,  $f_h$ , and  $f_v$  represent correction factors applied to  $N_{raw}$  to account for additional influences on the neutron signal other than soil moisture; they are correctios for air pressure, incoming neutron intensity, atmospheric water vapour and above

60 ground biomass, respectively.  $N_0$  is the theoretical neutron count found in absolutely dry conditions (i.e., the maximum number of neutrons that can be found at the site without the direct presence of hydrogen). This term is unique to each site and is found through the calibration process, explained in detail in Section 2.2.





The detection of background neutrons in the atmosphere, as a method to infer estimates of field scale soil moisture, was first 65 described in Zreda et al., (2008). In that study, the authors demonstrated that neutron intensity above the surface was inversely correlated with the amount of moisture in the soil below. This was developed further in Desilets et al., (2010), where the initial form of equation 1 was first described and applications of this technology continued to be explored within the earth sciences community (Desilets 2011; Franz et al., 2012; Rivera Villarreyes et al., 2011). A large-scale network of these sensors was subsequently deployed across the United States leading to the Cosmic-Ray Soil Moisture Observing System (COSMOS)

70 (Zreda et al., 2012).

After the establishment of the first national-scale network in the US (Zreda et al., 2012), other countries such as in Australia (Hawdon et al., 2014), Germany (Bogena et al., 2013), and the UK (Evans et al., 2016) established their individual national networks, as well as additional sensors located in smaller networks or individual sites. Sensors from these networks have in 75 some cases been running for up to 10 years, which can be potentially valuable for the understanding of soil hydrology. As these networks have grown so has the literature surrounding best practices for calibration and correction of the sensor signals, allowing us to have a lower uncertainty in CRNS soil moisture estimates (Franz et al., 2012; Rosolem et al., 2013; Hawdon et al., 2014; Baatz et al., 2015; Schrön et al., 2017). As consequence of improvements to the signal correction and sensor calibration, a divergence in methods is noticeable among different networks. Each network inevitably implements its own 80 protocol when correcting the neutron signal to give soil moisture estimates leading to a less harmonized dataset among networks.

This lack of a harmonized global dataset can ultimately lead to limitations in the global assessment of this technology from multiple CRNS networks. Discrepancies in processing methodology can leave questions around information obtained, and 85 uncertainty propagated, from analysis and comparison of sensors in different networks, such as whether soil moisture signals can be attributed solely to environmental differences or processing differences. By not necessarily following all recommended correction steps, the estimated soil moisture products from these sensors or even networks can be seen as sub-optimal, potentially undermining their true value. An example of the impact of evaluation sub-processed cosmic-ray soil moisture data from the US network against land surface models is presented by (Dirmeyer et al. 2016). There is a consensus to follow certain

- 90 steps and guidelines which are not uniformly applied across all networks. Known corrections to account for changes in atmospheric pressure, neutron intensity, atmospheric water vapour and aboveground biomass are applied differently and on occasion not at all on some networks which could lead to different estimates of soil moisture (Zreda et al., (2012), Hawdon et al., (2014), Evans et al., 2016). For example, Rosolem et al., (2013) demonstrated the influence on the neutron signal that occurs from changes in atmospheric water vapour over time. When comparing processed soil moisture estimates with, and
- without this additional signal correction, they demonstrated a difference of up to 0.1 cm<sup>3</sup>/cm<sup>3</sup> at a site at Park Falls, USA. 95 Additionally, Hawdon et al., (2014) demonstrated the different approaches available in correcting neutron counts for incoming cosmic-ray intensity and showed that there is a noticeable difference in neutron counts and ultimately soil moisture depending



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on the chosen method. Schrön et al., (2017) provided an improved approach to CRNS calibration demonstrating that their revised approach improves accuracy of soil moisture estimates. For example, at the UK site, the authors found that the Root-Mean-Squared-Error (RMSE) of soil moisture estimates from the CRNS was reduced from 5.3% volumetric, using the

conventional calibration approach, to 1.4% volumetric, using the revised calibration approach. Improvements in accuracy were identified at all the sites they analysed, however currently this revised approach is not applied across the networks.

In order to mitigate this ongoing issue of lack of harmonization in the soil moisture estimates from the CRNS technology, we 105 present here an open-source python tool to process raw CRNS data into soil moisture estimates, using the most current methods identified in the literature. It is designed to allow a user to apply consistent data processing methods across sensors that may be located in different networks. Section 2 will describe the structure of the tool along with the relevant correction and calibration methods. It will also describe the site metadata creation process which is an additional aspect to crspy that is built to facilitate data analysis of many sites. Section 3 will discuss the implications of differing processing methodologies on soil 110 moisture estimates, as well as the benefits of creating detailed metadata for post processing analysis.

#### 2 The crspy tool

The Cosmic **R**ay neutron **S**ensor **Py**thon tool (crspy, pronounced "crispy"): is a tool written in Python3 that has been developed to facilitate the processing of the global networks of CRNS data in a uniform and harmonized way. It is available through an open-source repository and can be installed into a user's python environment. The tool is designed to allow the easy implementation of the most up to date correction factors and calibration processes to any CRNS site globally, ultimately allowing for any user to access a harmonized dataset. Although it is designed for multiple sites from varied networks, crspy is versatile enough to process a single site as well. It is being provided to help facilitate research in the CRNS community and is not intended to state whether one networks processing methods are superior to another. It is the authors' opinion, however,

that it is important for the community to consider creation of a best practice, as this will allow comparison of sensor data

120 around the world in the future. In addition, crspy is structurally designed to accommodate new corrections and processing steps that may become available in the future in an easy manner. By being open source, crspy can also serve as a development and testing tool for new understanding incorporating to the CRNS technology as well as used as a teaching tool for the community.

Figure 1 is a visual representation of the processes within crspy that converts raw sensor data into corrected soil moisture estimates. Due to the varied nature of input data, such as when different networks label data differently, it is first necessary for a user to correctly format input data following crspy's naming convention (see Table A1 in Appendix). Additionally, to organise the various input and output datasets a specific working directory folder structure is necessary. This allows crspy to automatically handle the numerous sources of data. After installing the package a user can build this folder structure easily with the function crspy.initial(wd) where wd is a string representing the working directory location.





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Figure 1. The structure of crspy demonstrating all the modules that are used in creating soil moisture estimates. (1) represents the metadata table which is a collection of site descriptors (e.g., soil texture, site elevation) (see section 2.4). (2), (3) and (4) corresponds to the ERA5-Land data collection and use for gap filling, data tidying and for the computation of correction factors (see Section 2.1). (5) represents the calibration process (if this option is selected) (see Section 2.2). (6) highlights the quality assessment steps undertaken (see Section 2.3). Finally, (7) represents the step where soil moisture estimates are calculated from the neutron counting rates (refer to equation 1).

#### 2.1 Data processing and correction

- To obtain soil moisture estimates, we need to apply equation 1 at each time step in the data. The values will be obtained from time varying sensor data, external data products, static site-specific values and static values that are not site-specific. The coefficients  $[a_0 a_1 a_2]$  are constants with values of 0.0808, 0.372 and 0.115, respectively, defined in Desilets et al., (2010). These values are fitting constants that describe the shape of the relationship between neutron counts and soil moisture, obtained from neutron particle physics modelling, and are the same for all sites. These values are stored in the name\_list.py file,
- 145 which stores constant values for crspy.





#### Site-specific soil properties

- 150 The site-specific soil parameters described in Equation 1 are *LW*, *WSOM* (obtained from soil organic carbon) and  $\rho_{bd}$ . Due to the open data policies of many of the CRNS networks this data is usually available online (see data availability statement). These values should be defined prior to running the main crspy function and are stored and read from the metadata file. The parameter *LW* corresponds to the lattice water (%), which represents the hydrogen contained in the mineral structures of the soil (Hawdon et al., 2014). As fast neutrons are mitigated by hydrogen atoms, regardless of their source, this will have an
- 155 overall impact on the neutron count rate. This value is usually obtained through analysis of soil samples taken from the footprint of the site sensor (Franz et al., 2012). The parameter *WSOM* represents the water equivalent of soil organic matter (g/cm<sup>3</sup>). Soil organic carbon (SOC) is obtained through analysis of soil samples and represents the total organic carbon in the soil at the site. Hawdon et al., (2014) discuss the need to convert this value into a water equivalent. This is completed on the assumption that organic matter in the soil is cellulose which means that proportionally the water equivalent of this can be found

160 by:

$$WSOM = SOC * 0.556 \tag{2}$$

The parameter  $\rho_{bd}$  represents the dry soil bulk density (g/cm<sup>3</sup>) and is a site-specific static value. It is obtained through analysis of soil samples and is used in the conversion of gravimetric soil moisture to volumetric soil moisture values. If dry soil bulk density data is unavailable for a site, crspy includes the option to obtain this value from the global data source SoilGridsv2 (see Section 2.4). In case of missing data, crspy takes advantages of built-in routines to fill out the information. In that case, if  $\rho_{bd}$  or *SOC* (used to calculate *WSOM*) are missing, then crspy will use the estimates collected from SoilGridsv2, which is collected in the metadata process. Currently there is no way to estimate *LW* at sites that we know and so here a user should input a value of 0. Notice that the other site-specific static value is the  $N_0$  number. This number is found through the calibration process which is described in greater detail in section 2.2.

#### Time varying values and correction methods

- The remaining values required to obtain  $\theta_{vol}$  are  $N_{raw}$  and  $f_p$ ,  $f_i$ ,  $f_h$ ,  $f_v$  which all vary with time. It is ultimately the 175 relationship between  $N_{raw}$  and  $N_0$  which gives us our ability to estimate volumetric soil moisture once the additional corrections have been applied. The parameter  $N_{raw}$  is obtained from the sensor data and will usually be representative of the number of neutrons counted over a one-hour time period. This is the measured raw (uncorrected) neutron count; however, we know that there are additional impacts on this count rate that require correction which are represented by the *f* factors in equation 1. Changes in atmospheric pressure impact the neutron counting rate, the  $f_p$  term corrects for this so that  $N_{raw} * f_p$
- 180 gives the neutron count rate as if it were taken at the reference atmospheric pressure. Changes in incoming cosmic-ray intensity will directly influence neutron count rates as this is the source of fast neutrons and so the  $f_i$  term will correct this to match a





reference date in time. Atmospheric water vapour and above ground biomass are additional sources of hydrogen, outside of the soil moisture source we are interested in, and so the  $f_h$  and  $f_v$  terms adjust the count rate in consideration of this. These correction methods have been improved upon since the technologies first implementation with additional sources of uncertainty identified and equations designed to mitigate their impact.

185 uncertainty identified and equations designed to mitigate their impact.

There are occasional data availability issues observed at some sites. For example, meteorological variables are a necessary part of converting neutron counts to soil moisture estimates because they are needed to account for the numerous impacts on the signal, such as pressure corrections and atmospheric water vapour corrections. On occasion, some of the sites do not measure all the necessary variables considered to be essential to correct for additional sources on the neutron signal. External relative humidity sensors are essential in correcting for changes in atmospheric water vapour but are not always included in site data. When data is unavailable through in-situ site sensors, ERA5-Land (<u>Muñoz Sabater, J., 2019</u>) data are used to fill values. ERA5-Land is a dataset, based upon the ERA5 reanalysis data, that combines modelled data with real world observations, resulting in a gridded, global hourly product at 9km resolution, provided publicly by the European Centre for Medium-Range Weather

- 195 Forecasts (ECMWF). Previous iterations of the ERA reanalysis datasets (such as ERA-Interim) have proved useful by other global networks for the task of gap filling missing data, such as in the FLUXNET community (Vuichard and Papale, 2015). We are implementing a similar approach used by the FLUXNET community in crspy, and consequently to the global CRNS database, as we envision the potential to a merged database incorporating both flux tower and CRNS soil moisture data in the future. As the two measurement technologies show similar temporal and spatial footprints, their combined use can eventually
- 200 lead to a better understanding of land-atmosphere interactions at the field scale, for example (Iwema et al., 2017). It is important to note that although the resolution is spatially coarser when compared with CRNS sites, the ERA5-Land dataset was chosen as a source for gap filling for three main reasons: (1) it covers the lifetime of all the CRNS sites around the world which ensures all historical data to be used for gap-filling if necessary; (2) the dataset is produced at hourly resolution which matches the standard resolution of CRNS sites; (3) this is an open data source which aligns with our desire to develop a full open-source
- 205 tool for CRNS data processing.

The ERA5-Land dataset includes key variables such as precipitation, temperature, and dewpoint temperature which can be used to correct for influence on the neutron signal, such as using dewpoint temperature when relative humidity sensors are not available at the site (Rosolem et al., 2013). Our choice also follows previous studies that demonstrated that ERA-Interim tended

210 to perform best when compared with other global reanalysis products (Decker et al., 2012). ERA5, which ERA5-Land is derived from, has benefitted from a decade of research when compared to ERA-Interim and has been shown to be a great improvement (Hersbach et al., 2020).





### (i) Atmospheric Pressure correction $(f_p)$

Changes in atmospheric pressure can have an impact on neutron counting rates measured by the CRNS (Zreda et al., 2012, Hawdon et al., 2014). This is attributed to the fact that higher atmospheric pressure reduces neutron counting rates as there are more particles in the air column that can slow fast neutrons down. In crspy this is corrected with the equation:

$$f_p = \exp(\beta(p - p0)) \tag{3}$$

where  $f_p$  is the pressure correction factor (defined in Equation 1),  $\beta$  is a coefficient to account for mass attenuation length at 225 the site, p is the atmospheric pressure at the site (hPa) and p0 is a reference atmospheric pressure (hPa) for the site, commonly taken as the mean pressure for the site's elevation. The  $\beta$  coefficient and the reference atmospheric pressure value are calculated for each location as a function of the latitude, elevation, and cut-off rigidity at the site as described in Desilets et al., (2021).

# 230 (ii) Incoming High-Energy Neutron Intensity ( $f_i$ )

It is important to correct for incoming neutron intensity as this will have a direct impact on neutron counting rates. Changes in the incoming cosmic-ray intensity will affect the number of fast neutrons in the atmosphere as increased cosmic-ray intensity will lead to an increased counting rate created through the cascade of reactions (Desilets et al., 2006). We use the data from the Neutron Monitoring Data Base (NMDB) available online, providing a collection of neutron monitoring sites from around

- 235 the world. The NMDB provides neutron counting rates at hourly resolution from monitoring stations around the world, its data is considered the official distribution from each site principal investigator. The correction method currently varies across networks. For example, the COSMOS (USA) originally corrected the data by comparing neutron intensity to a pre-defined reference date, in that case, assumed to be 01 May 2011. The Jungfraujoch neutron monitoring station in Switzerland was used as a reference site. The calculation for this is shown as follows:
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$$f_i' = \frac{I0}{Im} \tag{4}$$

where Im is the incoming cosmic-ray intensity at sensor measurement time and I0 is incoming neutron intensity at the decided reference date and  $f_i'$  here is used to define this particular incoming cosmic-ray intensity correction factor, to avoid confusion with  $f_i$  from equation 1.

The default approach in crspy, however, is to use the approach outlined in Hawdon et al., (2014) where the Jungfraujoch monitoring station is used but an additional correction for differences in site cut-off rigidity is applied with:





250 Rccorr = -0.075(Rc - Rcjung) + 1

where *Rccorr* is the correction for differences in cut-off rigidity (GV), *Rc* is the cut-off rigidity at the sensor location and *Rcjung* is the cut-off rigidity at the Jungfraujoch monitoring station (which has a value of 4.49 GV). This is applied at each time step to give a final corrected value with:

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$$f_i = (f_i' - 1)Rccorr + 1 \tag{6}$$

The Australian CosmOz network uses a different approach which does not always use the Jungfraujoch as the reference monitoring station. Instead, this network will change the reference station based on the stations which has the closest cut-off rigidity (GV) to the sensor site from the Neutron Monitor Database (Hawdon et al., 2014). This option is also available in crspy when running the main processing function crspy.process\_raw\_data(fileloc, intentype="nearestGV") by invoking intentype with the "nearestGV" option. This involves identifying the NMDB site with the nearest cut-off rigidity and applying equation 4.

# 265 (iii) Atmospheric Water Vapour $(f_h)$

Hydrogen atoms can slow down fast neutrons leading to a reduction in the count rate with increasing atmospheric water vapour. This signal needs to be removed to ensure that neutron counting rates are attributed to soil moisture and not moisture in the air. This is corrected at each time step with the following equation (Rosolem et al., 2013):

$$270 \quad f_h = 1 + 0.0054 \times \rho v \tag{7}$$

where  $f_h$  is the atmospheric water vapour correction factor and  $\rho v$  is absolute humidity (g m<sup>-3</sup>). Some sites do not have external relative humidity sensors that can be used to calculate vapour pressure, which can be used to calculate absolute humidity along with temperature. When this is the case then ERA-5 Land data can be utilised by converting dewpoint 275 temperature (°C) to vapour pressure (kPA) (for further information on the steps to obtain absolute humidity from standard meteorological variables, please refer to the appendix section in Rosolem et al., 2013).

# (iv) Above Ground Biomass (AGB) ( $f_v$ )

Similar to other sources of hydrogen, biomass can also affect the neutron counting signal. There have been numerous attempts to identify the relationship between AGB and neutron count rates (e.g. Rivera Villarreyes et al., (2011), Baatz et al., (2015), Heidbüchel et al., (2016) and Tian et al., 2016). Unlike other sources of hydrogen, AGB is sometimes not available from local samples at each site. In order to reduce the impact of AGB on the measured neutron signal, crspy currently uses static estimated

(5)





for each site from the European Space Agency (ESA) Climate Change Initiative (CCI) global dataset and apply the correction method based on the work of Baatz et al., (2015), who found a linear relationship between above ground biomass and neutron counting rates.

The following equation is used:

$$f_v = \frac{1}{1 - (0.009 * agb)} \tag{8}$$

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where  $f_v$  is the above ground biomass correction factor and agb is the dry above ground biomass at the site (kg/m<sup>2</sup>). The ESA CCI database provides above ground biomass estimates as a global gridded data product at 100m resolution (Santoro and Cartus, 2019). As the ESA CCI data currently used is a static value in time, it will not impact the soil moisture estimates, in principle, because the correction is applied on both the  $N_{raw}$  and  $N_0$  numbers, hence mitigating any impact. Nevertheless, we

295 have included this routine in crspy in this form as we anticipate improvements to dynamical above ground biomass corrections in the future, at which point crspy can be updated to include the latest theory that can be applied across all sites (Wahbi et al., 2018; Vather et al., 2020; Fersch et al., 2020). Further improvements to be able to dynamically account for biomass changes at all CRNS sites will be important for reliable estimation of soil moisture dynamics, especially when analysing sites with land-use changes or cropping cycles.

#### 300 2.2 Sensor calibration

The above steps give us all the values in equation 1 necessary to provide a soil moisture estimate, except for  $N_0$ . A required step in processing, and eventually using the data, is to calibrate the CRNS to the specific conditions found at the site of interest. Without this step, the soil moisture can potentially have significant biases and deemed unusable. Alternatively, the uncalibrated measurement can only give you a rough idea about the dynamics of the soil wetness conditions in relative terms. The calibration

- 305 step typically requires multiple soil samples (typically 100s) taken from within the sensor footprint and oven dried to get an accurate representation of soil moisture at the calibration time. These samples are then weighted and averaged to give a field scale soil moisture estimate of the sensor footprint (note that we use dry soil bulk density,  $\rho_{bd}$ , sampled within the footprint to estimate volumetric water content in cm<sup>3</sup> cm<sup>-3</sup>). The crspy tool uses the soil moisture averaging method obtained from field samples proposed by Schrön et al (2017), which is based upon the original work of Köhli et al., (2015). The method provides
- 310 an updated approach for weighting soil moisture samples taken within the footprint that considered spatial distance from the sensor of each sample as well as the influences of pressure and humidity during the sampling period. This allows for a more accurate estimate of independent soil moisture within the CRNS footprint for the calibration step. Schrön et al. (2017) suggested improved sampling strategies which included samples closer to the sensor (< 5m radius from the sensor) and sample locations guided by knowledge of local hydrological features. The data required for the calibration step includes the date of</p>





315 the sample, an integer to represent each soil moisture profile (a core of soil taken from within the sensor footprint), the depth of each sample within each profile, the distance from the sensor, and the volumetric soil moisture of the sample. Again, these should be named following the template requirements by crspy (see Table A2 in Appendix).

With regards to number of calibration days, crspy is flexible enough to process both single-day or multiple-day calibration

- 320 campaigns. Multiple calibration campaigns were shown to improve the CRNS signal (Iweema et al., 2015). For the case of multiple-day calibration, all calibration days should be presented in a single table, ensuring that the correct dates of each sample period are provided, and following the same formatting and naming requirements used for single-day calibration. Finally, when running crspy for a single site, the user is able to turn on or off the calibration process. This is included because
- calibration only needs to be done once, as  $N_0$  does not vary with time. When the calibration step is turned on, crspy will call 325 the calibration routine and write the output to the metadata table in the column 'N0'. If the calibration routine is turned off, crspy will skip this step and simply read the  $N_0$  number for the site from the metadata. Alternatively, the user can provide the  $N_0$  coefficient independently in the metadata table and skip the calibration step completely by always having it off in crspy.

## 2.3 Quality assessment

- 330 All data should be checked for quality to ensure that erroneous data is not included, and crspy includes some automated steps to begin this process. All networks implement quality assessment on neutron counts in order to remove poor quality data (e.g., Zreda et al., 2012; Hawdon et al., 2014; Evans et al., 2015). In crspy, we remove suspicious data points by applying flags to neutron counts that fall within four categories, the below rules are consistent with the application in other networks:
- 335 1. Counts that differ by 20% from the previous time step are removed
  - 2. Counts below 30% of N0 are removed
  - 3. Counts above N0 are removed
  - 4. Battery voltages below 10V are removed
- 340 Additionally, crspy will output time series diagnostic plots of all variables used for identifying patterns in data that point towards potential issues which may require a small subset of the data to be removed manually (this, of course, depends on the quality of the data from individual sites and, therefore, cannot be fully automated).

#### 2.4 Metadata

345 Metadata is an important piece of information that allows the user to better describe each site characteristics beyond its soil moisture dynamics. The information can be extremely useful especially when multi-site regional to global CRNS stations are



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to be analysed simultaneously. The metadata of each site is stored in a tabular format within the folder structure of the working directory, a full description of the columns is given in the Appendix (Table A3 in Appendix). It serves two main purposes. Firstly, it stores static site-specific variables that are used in computing estimated soil moisture values (e.g., *LW*, *SOC* and  $\rho_{bd}$ 

- 350 ). To provide an example,  $\rho_{bd}$  is necessary to convert gravimetric soil moisture estimates into volumetric soil moisture estimates in equation 1. The  $\rho_{bd}$  value is collected during the calibration campaign at each site and will vary between sites. It represents an averaged value taken from the soil samples and it is stored in the metadata. Each site is also be given a country code and a site number in the metadata, which is used by crspy to find any required values stored in the metadata. The country code is used to help identify geographic locations in analysis and helps when the site numbering of networks may overlap.
- 355 Raw time series data should be titled with the country code and number in the following format: *country\_SITE\_sitenum.txt*. Where *country* is a capitalised letter code and the *sitenum* is a 3-digit number. For example, sensor data for a site in the UK could be titled: UK\_SITE\_101.txt. This *sitecode* (i.e., UK\_SITE\_101) is used to identify each site when organising the outputs, as well as a lookup code for constant variable values stored in the metadata.
- 360 A second purpose of the metadata is to act as a resource when analysing many sites together. The ability to classify catchments by physical characteristics can allow us to understand key similarities and differences between sites, an important direction in hydrological research (Wagener et al., 2007). To increase the value of the metadata, as well as including data collected at the site, global data products have been integrated. These products are all public products that a user can download and store within the folder structure of the working directory. We realize that these global datasets are not a direct replacement for the invaluable information obtained at the site; however, in many cases, such pieces of information are not available, undermining any multi-site analysis. We believe the use of the datasets described in detail below can provide us key information at regional
- and global level. In crspy, a simple function is used to extract the information from the data products below when provided with the location of the CRNS (i.e., latitude and longitude):
- (i) ESA CCI Land Cover and Above Ground Biomass data: The European Space Agency (ESA) Climate Change Initiative (CCI) provides numerous global data products that are useful in the earth sciences community. Land cover data and above ground biomass data are obtained from ESA CCI and stored in metadata for each site for analysis through identifying site differences and similarities. Both products are spatial consistent with the CRNS sensor range (100m-300m) and are available globally. The usefulness of ESA CCI datasets in land surface modelling continues to be established (Li et al., 2017).
  - (ii) International Soil Reference and Information Centre (ISRIC): The ISRIC provides a global data product that gives estimates of soil properties on a 250m resolution grid. This is available as SoilGridv2 which is an updated (as of May 2020) iteration of the original SoilGrid product (Hengl et al., 2017). The properties are estimated from collections of ground measurements that are compiled by the World Soil Information Service (WoSIS). WoSIS provide standardised soil profile data to facilitate the creation of products such as SoilGrid (Batjes et al., 2020).





(iii) ERA5-Land: As discussed previously meteorological variables from ERA5-Land data can be downloaded for each site. Mean annual precipitation and temperature data is stored, along with derived Köppen-Geiger classifications.

# 2.5 Running the tool.

385 Once the working environment has been prepared the be processed with data can crspy.process\_raw\_data(fileloc, Calibration=True, intentype=None). Where fileloc is the location of the raw sensor data, the Calibration process can be turned on or off as a Boolean descriptor and intentype can be left as None to enact the default process for incoming neutron intensity correction or can be changed to "nearestGV" to utilise the alternative method.

#### 390 3 Discussion

# 3.1 Benefits of data harmonization

As mentioned previously, one of the key purposes of crspy is the easy and harmonized processing of CRNS sites from around the globe, as there is currently no true consensus on what correction steps are implemented in different national networks. These technical differences can lead to changes in outputs which may result in non-optimal conditions for regional/global analysis from multiple countries. Whereas some users may wish to understand changes at one particular site, inter-site comparisons are limited when each site could be processed in a different way. In this section, we highlight such impacts with

Table 1 outlines three identified methods that are currently employed across different networks. Method  $p_{int1}$  is the method

one example related to the individual sensor corrections steps, and their impact on the final soil moisture estimates.

- 400 employed at the COSMOS (USA) network, which lacks the atmospheric water vapour correction and applies an intensity correction using only the Jungfraujoch neutron monitoring site directly. Method  $p_int2_awv$  closely resembles the CosmOz (Australia) network methodology, which does apply the atmospheric water vapour corrections and an intensity correction that differs from method  $p_int$ . In this case, the neutron monitoring station used as an incoming neutron intensity reference is changed to the nearest station with a similar cut-off rigidity to the CRNS site being corrected. Method  $p_int3_awv_agb$  is the
- 405 default crspy method, and resembles the methods used by COSMOS-UK, while also allowing for the above ground biomass correction to the neutron signal. In this final case, the intensity correction uses Jungfraujoch as its reference site but with an additional correction to account for differences in cut-off rigidity between Jungfraujoch and the site (equation 5).





Table 1. The three identified methods of correcting neutron signals in use	Table 1.	. The three	identified	methods of	correcting	neutron signals in use.
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	Method $p_int1$	Method <i>p_int2_awv</i>	Method <i>p_int3_awv_agb</i>
Atmospheric pressure correction	Yes	Yes	Yes
Incoming neutron intensity correction	Jungfraujoch NMDB (no GV correction)	Nearest GV NMDB (variable locations) (Hawdon et al., (2014))	Jungfraujoch NMDB <b>plus</b> additional correction for site GV (see equation (5) and Hawdon et al., 2014)
Atmospheric water vapour correction	None	Yes (Rosolem et al., (2013))	Yes (Rosolem et al., (2013))
Above ground biomass correction	None	None	Yes (Baatz et al., (2015))

With all these different correction approaches applied independently from each national network, we investigate both the impact on the measured neutron counts and consequently the propagated effects on the estimation of soil moisture. Figure 2

- 415 shows two sites with distinct hydroclimatic regimes, both taken from the COSMOS-USA network, that have been processed in the three identified methods (see highlighted star markers in Fig. 3 and Fig. 4). The Santa Rita Creosote site is shrubland dominated with a soil categorized predominantly by sandy loam type located in Arizona, USA. The site has a mean annual temperature of 19 °C and a mean annual precipitation of 335 mm, which primarily falls in winter storms and monsoonal summers (Köppen-Geiger climate classification BSh, a hot semi-arid climate). Climate data taken from ERA5-Land and
- 420 Köppen-Geiger classification derived from ERA5-Land data using the method outlined in Peel et al., (2007). The Wind River site is an old-growth mixed conifer forest site in Washington, USA. The site is much wetter than the Santa Rita Creosote site, with an annual precipitation of 2,200 mm, and much colder, with an average annual temperature of 8 °C. Precipitation at Wind River tends to fall all year round but with slightly lower rates in the summer period (Köppen-Geiger classification is Csb, a Mediterranean climate mild with dry, warm summers). Climate data has been extracted from ERA5-Land and Köppen-Geiger
- 425 classification derived from 10 years of ERA5-Land data using the method outlined in Peel et al., (2007). The raw neutron data from both sites were obtained directly from the COSMOS network, representing the  $p_{int}$  case in Table 1. In addition, in order to compare the impact of the different correction approaches outlined in Table 1, the raw data from the CRNS at both sites, have been processed in crspy to give the corrected signals for methods  $p_{int2}awv$  and  $p_{int3}awv_agb$ .







Figure 2. Example of CRNS data obtained at two distinct sites: Santa Rita Creosote (a, c, and e) and Wind River (b, d, and f). Neutron counting rates (raw and corrected based on the different strategies outlined in Table 1) are shown in panels (a) and (b). Derived soil moisture estimates (cm<sup>3</sup> cm<sup>-3</sup>) are shown at hourly and monthly timescales in panels (c) and (d) and panels (e) and (f), respectively.

- 435 It is clear to see the inverse relationship between neutron count rates and soil moisture, most noticeably at Santa Rita Creosote (Figures 2a and 2c). The soil moisture here tends to be low, such as in June when it was below 0.05 cm<sup>3</sup> cm<sup>-3</sup>, which is to be expected in a hot semi-arid environment. Sudden spikes in soil moisture can be attributed to precipitation events, with the summer monsoonal precipitation causing a sudden increase in the mean soil moisture values for the months of July, August, and September (and, inversely, periods corresponding to decreases neutron counting rates). It is also clear that the method
- 440 chosen has an impact on soil moisture values. This is most notable when comparing the  $p_int1$  method with both the  $p_int2\_awv$  and  $p_int3\_awv\_agb$  methods. During the summer months, the  $p_int1$  method appears to estimate higher soil moisture values compared to the other two methods (both appearing to be much more closely aligned to each other). This is likely due to the fact that the  $p_int1$  method does not account for changes in atmospheric water vapour. As a consequence, during the monsoonal summers when there is more hydrogen in the atmosphere from increased humidity, the relatively high
- 445 water vapor in the atmosphere is incorrectly attributed to additional soil moisture. This is because the CRNS records wrongly attribute the decrease (attenuation) of neutron counts due to water vapor to an increase in soil moisture, causing an over

estimated by inferring porosity of the soil:





estimation. For example, even early in March there is a sudden rise in soil moisture from the  $p\_int1$  estimates which does not appear in the other two methods (Figure 2c). This suggests that rather than a sudden rise in soil moisture, this was actually a rise in atmospheric water vapour. This demonstrates the importance of removing external impacts on the neutron signal as they could be incorrectly attributed to soil moisture dynamics. The negative effect of neglecting such correction, for example, can be pronounced even more on monthly estimates of soil moisture due to the aggregated nature of this error (Figure 2e).

The Wind River site is a much wetter site when compared to Santa Rita with its driest month matching Santa Rita Creosotes wettest month. It is worth noting in that in the case of Wind River there is a much larger difference between the neutron count
rate of method *p\_int3\_awv\_agb* compared to the other methods (Figure 2b). This is because the *p\_int3\_awv\_agb* method includes an above ground biomass correction, using the ESA CCI above ground biomass product to calculate a correction. Currently, as this correction is applied using a static aboveground biomass value (constant with time), the impact of the correction is not translated to differences in estimated soil moisture. This is due to the correction being applied to both the neutron counting rate and the N<sub>0</sub> term as well. With dynamic data, that represents changes in above ground biomass could be removed from the neutron signal. One additional noticeable feature that crspy implements is the capping of soil moisture to more realistic values, in this case 0.68 cm<sup>3</sup> cm<sup>-3</sup>. The *p\_int1* method does not do this and so there are physically impossible values of volumetric soil moisture in February and December, as seen in figure 2d. In crspy maximum values for soil moisture are

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$$sm_max = 1 - \left(\frac{\rho_{bd}}{density}\right) \tag{9}$$

where  $sm_max$  is the maximum volumetric soil moisture value (cm<sup>3</sup> cm<sup>-3</sup>),  $\rho_{bd}$  is soil bulk density (g/cm<sup>3</sup>) and *density* is the density of ground material (estimated with an assumed density of quartz at 2.65 g/cm<sup>3</sup>).

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At the Wind River site, the differences between  $p_int2_awv$  and  $p_int3_awv_agb$  are much more noticeable, especially when the soil moisture estimates are aggregated to monthly timescales (Figure 2f). This observed difference is due the fact that these methods do not apply the same correction for incoming cosmic-ray intensity ( $f_i$ ). Such differences are caused by the choice of correction rather than physical controls on soil water dynamics. This can lead to inaccurate comparisons across sites from different national/regional networks. For example, identifying useful soil moisture signals that can be used to categorise the hydrology of sites will be an important tool for understanding differences and similarities with regards to hydrology. Branger and McMillan (2020) demonstrated this in their paper looking to identify useful soil moisture signals that can be robust, discriminatory, and representative, with research continuing in this area of developing useful diagnostic soil moisture signatures (Araki and McMillan, 2020). When reducing large time series data into signatures, such differences can be





480 aggregated which could begin to effect conclusions. However, the authors stress here that it is not within the scope of this work, nor the intention, to identify which method is better or worse than the other, but rather highlight the potential negative impacts of the lack of a harmonized dataset for large-scale global assessment of the CRNS technology.

# 3.2 Usefulness of crspy metadata

- 485 Metadata can be used to describe the network of CRNSs around the world geographically, climatologically, and hydrologically. To achieve this, crspy compiles relevant data obtained directly from the sensor, key data descriptors provided from each site or network, and from global data products. Wagener et al. (2020) discuss the need for high quality metadata to improve our ability to understand the knowledge accumulation in the field of hydrology. The metadata can be valuable in separating relevant sites in different groups, for example researchers may be interested in understanding how soil moisture behaves at sites above
- 490 2000m elevation with certain land use types and given particular weather events (Chen et al., 2020); or sites where mean annual precipitation is above/below a certain threshold; or even grouping sites by different land cover or soil types. So called meta-analyses can help a researcher identify which sites should be included in their studies and which can be excluded (Evaristo and McDonnell, 2017). The metadata provided by crspy allows the user to quickly obtain any grouping of interest in an easy and accessible way.
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In order to demonstrate some of the features that can be easily accessed with the help of metadata, we show an example using the compiled COSMOS network data for continental USA (CONUS). Some of this data are taken directly from the network website and then processed using the crspy.fill\_metadata() function. This function collects information from global data products at specific site location (i.e., latitude and longitude), as well as using meteorological data from ERA5 Land to produce annual meteorological summaries (e.g., mean annual temperature, mean annual precipitation, Köppen-Geiger climate classification, etc). Figure 3 gives an example of how the metadata can be easily used to show the location of each sensor in the continental USA domain (CONUS) based upon the supplied with additional information, in this case, main land cover classes obtained from the CCI ESA Land Use data. An important step here is that the user is not required to download and process the land cover data separately and individually, crspy incorporates that step for the user seamlessly.







Figure 3. Map showing the location of CRNS sites from the COSMOS network across CONUS. The colours are representative of the land cover types obtained from the ESA CCI global database and the stars highlight the location of the two sites processed above (i.e., Santa Rita Creosote and Wind River).

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In addition to locating the CRNS stations and identified the main land cover type, Figure 4 shows a scatter-histogram of the sites across CONUS providing additional annual meteorological summaries, namely mean annual temperature and mean annual precipitation. The scatterplot still retains the information about the main land cover type obtained from the ESA CCI global database. In addition, both meteorological variables are shown as side-histograms and were computed using the ERA5

- 515 Land data. Initial analysis indicates that CRNS classified as shrublands tend to be relatively warmer and drier. Grassland and forests tend to be wetter while showing a wider range of temperatures. Croplands are slightly warmer than grassland and forests but still showing lower temperatures than those observed in shrublands. However, croplands also indicate a slightly wider range of wetness, when compared to the grassland and forest sites, as observed from the total annual precipitation. This could be useful when deciding which sites should be used in a particular study, such as a study on soil moisture dynamics in
- 520 shrublands with low overall precipitation. Alternatively, it can be used in big data analytics when trying to identify the dominant mechanisms on soil moisture dynamics globally.







Figure 4. Scatter-histogram showing the Continental USA CRNS sites and some of their climatological characteristics. The colours represent land use types which has been identified from ESA CCI Land Use global data set. The stars highlight the location of the two sites processed above (i.e., Santa Rita Creosote and Wind River).

# 4. Summary

Soil moisture is an important component of the hydrological cycle and understanding its dynamics at relevant spatiotemporal scales is critical especially with recent advances of global land surface and hydrological models. The CRNS technology is able

- 530 to provide estimates of soil moisture at the sub-kilometre scale and at hourly resolution. This is particularly relevant now as we continue to move towards hyper-resolution global modelling efforts. Over the years, with an increase of adoption to the technology, the CRNS community has acquired a better understanding about the benefits and limitations of this relatively novel technique. However, due to a lack of data harmonization across networks, undertaking global scale analyses is currently very limited and unexploited. Here, we introduced the crspy python package with the aim to facilitate users to process data
- 535 easily with the most current methods, and most importantly, in a harmonized fashion. crspy is an open-source tool aimed to





integrate the latest developed methodologies for CRNS to be used both for research and teaching activities. It integrates highquality global data products (such as ERA5-Land) to ensure that all sites can be included in analysis. This is done in a similar way to other well-established global environmental networks such as the Ameriflux and Fluxnet.

- Our examples of application demonstrated that when CRNS data is processed with different methodologies, it can ultimately lead to divergences in soil moisture estimates. This could potentially have a negative impact on the analysis and overall findings, especially when sites across multiple networks are evaluated simultaneously. By harmonizing data processes, we envisage that CRNS data will be used more widely by the global modelling and experimental communities, leading to further adoption of the technology. The objective of crspy is to provide an open and easy-to-use data processing platform that can enable initially. Additionally, crspy data collection relies on the production of an extensive metadata archive. This archive can
- 545 be shared and used within the community to better understand key aspects about soil moisture from typical sampling locations, to inform on signature behaviour by different groupings. crspy has been developed to open up the debate and use of free and public open CRNS data, and we invite the general community to engage with us to improve this platform in future years.

# **5** Data availability statement

Raw CRNS data are publicly available from several sources, including the US COSMOS network 550 (http://cosmos.hwr.arizona.edu/), the Australian CosmOz (https://cosmoz.csiro.au/) **UK-COSMOS** network and (https://doi.org/10.5285/b5c190e4-e35d-40ea-8fbe-598da03a1185). We acknowledge the NMDB database (https://www.nmdb.eu), founded under the European Union's FP7 programme (contract no. 213007) for providing neutron count data. ESA CCI data including above ground biomass data and land cover data are available from (http://cci.esa.int/data last accessed 26/02/2021). The soil grids data are accessible online from https://soilgrids.org/. The ERA5-Land data are 555 provided by ECMWF and are available at https://doi.org/10.24381/cds.e2161bac.

#### 6 Code availability

The code discussed in this paper can be found at <u>https://doi.org/10.5281/zenodo.4585513</u>. The GitHub repository, where future updates will be uploaded can be found at <u>https://github.com/danpower101/crspy</u>. The GitHub repository also includes a wiki page which goes into greater detail on how to run the package and includes a walkthrough jupyter notebook (run\_crspy\_workthrough.ipynb) that will walk through processing an example site.





# 7 Author contributions

All authors were involved in the conceptualisation of this work. Data curation was undertaken by DD, SD, and DP. Investigation undertaken by RR, MRR, and DP. Software was written by DP. Manuscript drafted primarily by DP and subsequently written together with RR and MRR.

# 565 8 Competing Interests

The authors declare that they have no conflict of interest.

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# **10 Appendix**

575 The appendix section consists of 4 tables that outline the naming conventions required for crspy to run as well as the output table along with a description of each variable. When labelling input data, columns titles should match the styles below in the 'COLUMN NAME' column. This initial step will then allow crspy to run smoothly, as it uses column titles to identify relevant data sources.





Table A1. The naming convention for CRNS input data. Networks can occasionally have different naming conventions590(e.g., temperature is referred to as t1). Changing the column titles to the following format will allow crspy to function

correctly.

COLUMN NAME	UNITS	DESCRIPTION
TIME	datetime	Datetime of the observation. Format: "yyyy-mm-dd hh:mm:ss"
MOD	count	Moderated neutron count for time interval
UNMOD	count	Unmoderated neutron count for time interval
PRESS1	hPa	Pressure sensor number 1. Usually the older analogue version that is somewhat less accurate
PRESS2	hPa	Pressure sensor number 2. This will be used primarily and if unavailable PRESS1 will be used in place.
I_TEM	Celsius	Internal Temperature of the sensor box
I_RH	%	Relative humidity inside the sensor box
BATT	Voltage	Voltage of the battery
E_TEM	Celsius	External Temperature at the site. This would be an external reading. If not available then ERA5-Land data is used
E_RH	%	External Relative Humidity at the site. If not available then dewpoint temperature is used to find absolute humidity
RAIN	mm	Rainfall at the site. If local is available this is used - if not available it is obtained from ERA5-Land data





Table A2. The naming convention for the calibration data. This format should be followed and will allow the calibration module to be utilised.

COLUMN NAME	UNITS	DESCRIPTION
DATE	Date. Format "dd/mm/yyy"	Date that the data was collected from the site
PROFILE	int	Integer to differentiate profiles. A profile being a single core. The core could then have multiple "layers".
LOC_rad	meters	Distance from the sensor for each sample in meters.
DEPTH_AVG	cm	The depth of the soil sample for each layer. Taken as the mid point of the layer.
SWV	%	The volumetric soil moisture of the sample. Should be given as decimal (i.e. 0.3). If it is given as a numeric percent (e.g. 30%) crspy will attempt to identify this and convert to decimal

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Table A3. The naming convention of the metadata table.

COLUMN NAME	UNITS	DESCRIPTION	Required at start?
COUNTRY	-	Country code for location of site e.g. "USA"	Yes
SITENUM	-	Assigned 3 digit number for site: e.g. 001	Yes
INSTALL_DATE	-	Date of site installation	No
LONGITUDE	degrees	Longitude of site	Yes
LATITUDE	degrees	Latitude of site	Yes
ELEV	m	Elevation above sea level of site	Yes
TIMEZONE	-	Time zone of the site	No
GV	gv	Cut-off Rigidity of site	Yes
LW	%	Lattice Water from site specific calibration data	Yes
SOC	%	Soil Organic Carbon from site specific calibration data	Yes
BD	g/cm <sup>3</sup>	Bulk Density from site specific calibration data	Yes
NO	-	Theoretic maximum neutron count for site (dry conditions), calculated in tool and written.	No
AGBWEIGHT	kg/m2	Live woody above ground biomass estimates from ESA CCI biomass data	No
RAIN_DATA_SOURCE	-	Declaration of the source of rain data. Currently this will be either "Local" or "ERA5_Land"	No
TEM_DATA_SOURCE	-	Declaration of the source of temperature data. Currently this will be either "Local" or "ERA5_Land"	No
BETA_COEFF	-	Store of the calculated beta coefficient (see pressure calculations) for each individual site	No





REFERENCE_PRESS	hPa	Reference pressure calculated using elevation	No
BD_ISRIC	g/cm³	Bulk Density estimates taken from the International Soil Reference and Information Centre (SoilGrids250m <u>https://soilgrids.org/ )</u>	No
SOC_ISRIC	g/dm³	Soil Organic Carbon estimates from ISRIC	No
pH_H20_ISRIC	рН	pH of water estimates from ISRIC	No
CEC_ISRIC	mmol(c )/kg	Cation exchange capacity at ph7 from ISRIC	No
CFVO ISRIC	cm³/dm³	Coarse fragments from ISRIC	No
NITROGEN ISRIC	cg/kg	Nitrogen in soil from ISRIC	No
SAND_ISRIC	g/kg	Sand in soil from ISRIC	No
SILT_ISRIC	g/kg	Silt in soil from ISRIC	No
CLAY_ISRIC	g/kg	Clay in soil from ISRIC	No
*_ISRIC_UC	varied	The uncertainty bounds of each of the ISRIC variables, in absolute terms.	No
TEXTURE	-	Soil texture identified from Sand/Silt/Clay percentages using the USDA soil texture triangle	No
WRB_ISRIC	-	World Reference Base (2006) soil class from ISRIC. Provided as a table of probable classes - this is the most probable class.	No
LAND_COVER	-	Land Cover type taken from Copernicus data set.	No





Table A4. crspy final output table from a given CRNS site. Note that there may be additional columns when run as different networks may have additional variables.

COLUMN NAME	UNITS	DESCRIPTION
DT	datetime	Datetime of the observation. Format: "yyyy-mm-dd hh:mm:ss"
MOD	counts per hour	Moderated neutron count
UNMOD	counts per hour	Unmoderated neutron count
PRESS	hPa	Atmospheric pressure recorded by the sensors at the site
TEMP	Celsius	Atmospheric temperature - if sensors are missing ERA5-Land data is used
I_TEM	Celsius	Internal Temperature of the sensor box
I_RH	%	Relative humidity inside the sensor box
E_TEM	Celsius	External (atmospheric) temperature
E_RH	%	External (atmospheric) relative humidity
RAIN	mm	Rainfall recorded at the site. If local data is unavailable, then ERA5-Land data will be used in its place
BATT	Voltage	Voltage of the battery
fbar	-	The pressure correction factor
DEWPOINT_TEMP	Celsius	Dewpoint temperature - from ERA5-Land data
SWE	mm	Snow water equivalent - from ERA5-Land data
ERA5L_PRESS	hPa	Atmospheric pressure - from ERA5-Land data
VP	hPa	Vapour Pressure - calculated
NMDB_COUNT	counts per hour	Neutron count rate from neutron monitoring database - usually Jungfraujoch
pv	kg/m <sup>3</sup>	Absolute humidity - calculated
fawv	-	The atmospheric water vapour correction factor
finten	-	The incoming cosmic-ray intensity correction factor
fagb	-	The above ground biomass correction factor
FLAG	-	The flag assigned to data in error (see Section 2.3 for definitions)
MOD_CORR	counts per hour	The corrected neutron count rate after the correction factors have been applied





MOD_ERR	counts per hour	The statistical error of the neutron count rate
SM	volumetric soil moisture cm <sup>3</sup> cm <sup>-3</sup>	Estimated soil moisture
SM_PLUS_ERR	volumetric soil moisture cm <sup>3</sup> cm <sup>-3</sup>	Estimated soil moisture error above the estimated value - this is calculated by subtracting the MOD_ERR value (due to the inverse relationship) to the MOD_CORR value and calculating what the SM would then be
SM_MINUS_ERR	volumetric soil moisture cm <sup>3</sup> cm <sup>-3</sup>	Estimated soil moisture error below the estimated value - this is calculated by adding the MOD_ERR value (due to the inverse relationship) to the MOD_CORR value and calculating what the SM would then be
SM_12h	volumetric soil moisture cm <sup>3</sup> cm <sup>-3</sup>	The SM value with a 12-hour rolling average applied to it. Minimum number of values to calculate the 12-hour average is 6 hours of data within the 12-hour window
D86avg	cm	The depth of the measurement - taken as the depth from which 86% of neutrons are estimated to be sourced from (Schron et al., 2017)
D86avg_12h	cm	The D86 value with a 12-hour rolling average applied to it. Minimum number of values to calculate the 12-hour average is 6 hours of data within the 12-hour window





# References

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Addor, N., Do, H. X., Alvarez-Garreton, C., Coxon, G., Fowler, K., & Mendoza, P. A. (2020). Large-sample hydrology: recent progress, guidelines for new datasets and grand challenges. *Hydrological Sciences Journal*, 65(5), 712–725. https://doi.org/10.1080/02626667.2019.1683182

Araki, R and McMillan HK (2020) Developing diagnostic signatures from in-situ soil moisture networks under different landuses. AGU Fall Meeting 2020 (H195-0005)

640 Baatz, R., Bogena, H. R., Franssen, H. H., Huisman, J. A., Montzka, C., & Vereecken, H. (2015). An empirical vegetation correction for soil water content quantification using cosmic ray probes. *Water Resources Research*, 2030–2046. https://doi.org/10.1002/2014WR016443.Received

Batjes, N. H., Ribeiro, E., & Van Oostrum, A. (2020). Standardised soil profile data to support global mapping and modelling (WoSIS snapshot 2019). *Earth System Science Data*, *12*(1), 299–320. <u>https://doi.org/10.5194/essd-12-299-2020</u>

Bierkens, M. F. P., Bell, V. A., Burek, P., Chaney, N., Condon, L. E., David, C. H., de Roo, A., Döll, P., Drost, N., Famiglietti, J. S., Flörke, M., Gochis, D. J., Houser, P., Hut, R., Keune, J., Kollet, S., Maxwell, R. M., Reager, J. T., Samaniego, L., ... Wood, E. F. (2015). Hyper-resolution global hydrological modelling: What is next?: "Everywhere and locally relevant" M. F.

650 P. Bierkens et al. Invited Commentary. *Hydrological Processes*, 29(2), 310–320. <u>https://doi.org/10.1002/hyp.10391</u>

Bogena, H. R., Huisman, J. A., Baatz, R., Franssen, H. H., & Vereecken, H. (2013). Accuracy of the cosmic-ray soil water content probe in humid forest ecosystems: The worst case scenario. 49(September), 5778–5791. https://doi.org/10.1002/wrcr.20463

655

Bonan, G. B. (2008). Forests and climate change: Forcings, feedbacks, and the climate benefits of forests. *Science*, *320*(5882), 1444–1449. <u>https://doi.org/10.1126/science.1155121</u>

Branger, F., & McMillan, H. K. (2020). Deriving hydrological signatures from soil moisture data. *Hydrological Processes*,
34(6), 1410–1427. <u>https://doi.org/10.1002/hyp.13645</u>

Chen, M., Zeng, C., Zhang, F., Kang, S., & Li, C. (2020). Characteristics of Dissolved Organic Matter from a Transboundary Himalayan Watershed: Relationships with Land Use, Elevation, and Hydrology. *ACS Earth and Space Chemistry*, *4*(3), 449– 456. <u>https://doi.org/10.1021/acsearthspacechem.9b00329</u>





#### 665

Desilets, D. (2011). Radius of influence for a cosmic-ray soil moisture probe : Theory and Monte Carlo simulations. March.

Desilets, D., (2021), Intensity correction factors for a cosmic ray neutron sensor, *Hydroinnova Technical Document* 21-01, doi: 10.5281/zenodo.4569062.

670

Desilets, D., Zreda, M., & Ferré, T. P. A. (2010). Nature's neutron probe: Land surface hydrology at an elusive scale with cosmic rays. *Water Resources Research*, *46*(11), 1–7. https://doi.org/10.1029/2009WR008726

Dirmeyer, P. A., Wu, J., Norton, H. E., Dorigo, W. A., Quiring, S. M., Ford, T. W., Santanello, J. A., Bosilovich, M. G., Ek,
M. B., Koster, R. D., Balsamo, G., & Lawrence, D. M. (2016). Confronting weather and climate models with observational data from soil moisture networks over the United States. *Journal of Hydrometeorology*, *17*(4), 1049–1067. https://doi.org/10.1175/JHM-D-15-0196.1

Dobriyal, P., Qureshi, A., Badola, R., & Hussain, S. A. (2012). A review of the methods available for estimating soil moisture

680 and its implications for water resource management. *Journal of Hydrology*, 458–459(January 2018), 110–117. https://doi.org/10.1016/j.jhydrol.2012.06.021

Dong, J., Ochsner, T. E., Zreda, M., Cosh, H., & Zou, C. B. (2014). *Calibration and Validation of the COSMOS Rover for Surface Soil Moisture Measurement*. <u>https://doi.org/10.2136/vzj2013.08.0148</u>

685

Dutta, R., Morshed, A., Aryal, J., Este, C. D., & Das, A. (2014). Environmental Modelling & Software Development of an intelligent environmental knowledge system for sustainable agricultural decision support. *Environmental Modelling and Software*, 52, 264–272. https://doi.org/10.1016/j.envsoft.2013.10.004

- 690 Entekhabi, D., Njoku, E. G., O'Neill, P. E., Kellogg, K. H., Crow, W. T., Edelstein, W. N., Entin, J. K., Goodman, S. D., Jackson, T. J., Johnson, J., Kimball, J., Piepmeier, J. R., Koster, R. D., Martin, N., McDonald, K. C., Moghaddam, M., Moran, S., Reichle, R., Shi, J. C., ... Van Zyl, J. (2010). The soil moisture active passive (SMAP) mission. *Proceedings of the IEEE*. <u>https://doi.org/10.1109/JPROC.2010.2043918</u>
- 695 Evans, J. G., Ward, H. C., Blake, J. R., Hewitt, E. J., Morrison, R., Fry, M., Ball, L. A., Doughty, L. C., Libre, J. W., Hitt, O. E., Rylett, D., Ellis, R. J., Warwick, A. C., Brooks, M., Parkes, M. A., Wright, G. M. H., Singer, A. C., Boorman, D. B., Jenkins, A., ... Doughty, L. C. (2016). Soil water content in southern England derived from a cosmic-ray soil moisture observing system COSMOS-UK. *Hydrological Processes*, *30*(26), 4987–4999. <u>https://doi.org/10.1002/hyp.10929</u>





Evaristo, J., & McDonnell, J. J. (2017). A role for meta-analysis in hydrology. *Hydrological Processes*, 31(20), 3588–3591.
 <a href="https://doi.org/10.1002/hyp.11253">https://doi.org/10.1002/hyp.11253</a>

Fang, B., & Lakshmi, V. (2014). Soil moisture at watershed scale: Remote sensing techniques. *Journal of Hydrology*, *516*, 258–272. <u>https://doi.org/10.1016/j.jhydrol.2013.12.008</u>

705

Fersch, B., Francke, T., Heistermann, M., Schrön, M., Döpper, V., Jakobi, J., Baroni, G., Blume, T., Bogena, H., Budach, C., Gränzig, T., Förster, M., Güntner, A., Franssen, H. J. H., Kasner, M., Köhli, M., Kleinschmit, B., Kunstmann, H., Patil, A., ... Oswald, S. (2020). A dense network of cosmic-ray neutron sensors for soil moisture observation in a highly instrumented pre-Alpine headwater catchment in Germany. *Earth System Science Data*, *12*(3), 2289–2309. <u>https://doi.org/10.5194/essd-12-</u>

710 <u>2289-2020</u>

Fontanet, M., Fernàndez-Garcia, D., & Ferrer, F. (2018). The value of satellite remote sensing soil moisture data and the DISPATCH algorithm in irrigation fields. *Hydrology and Earth System Sciences*, 22(11), 5889–5900. https://doi.org/10.5194/hess-22-5889-2018

## 715

720

Franz, T. E., Zreda, M., Rosolem, R., & Ferre, T. P. A. (2012). Field Validation of a Cosmic-Ray Neutron Sensor Using a Distributed Sensor Network. *Vadose Zone Journal*. https://doi.org/10.2136/vzj2012.0046

Green, J. K., Seneviratne, S. I., Berg, A. M., Findell, K. L., Hagemann, S., Lawrence, D. M., & Gentine, P. (2019). Large influence of soil moisture on long-term terrestrial carbon uptake. *Nature*, *565*(7740), 476–479. <u>https://doi.org/10.1038/s41586-018-0848-x</u>

Hamed Alemohammad, S., Kolassa, J., Prigent, C., Aires, F., & Gentine, P. (2018). Global downscaling of remotely sensed soil moisture using neural networks. *Hydrology and Earth System Sciences*, 22(10), 5341–5356. <u>https://doi.org/10.5194/hess-</u>22-5341-2018

# 725

Hawdon, A., Mcjannet, D., & Wallace, J. (2014). Calibration and correction procedures for cosmic-ray neutron soil moisture probes located across Australia. *Water Resources Research*, 1–17. <u>https://doi.org/10.1002/2013WR014333.Received</u>

Heidbuchel, I., Guntner, A., & Blume, T. (2016). Use of cosmic-ray neutron sensors for soil moisture monitoring in forests. *Hydrology and Earth System Sciences*, 20(3), 1269–1288. <u>https://doi.org/10.5194/hess-20-1269-2016</u>





Hengl, T., De Jesus, J. M., Heuvelink, G. B. M., Gonzalez, M. R., Kilibarda, M., Blagotić, A., Shangguan, W., Wright, M. N., Geng, X., Bauer-Marschallinger, B., Guevara, M. A., Vargas, R., MacMillan, R. A., Batjes, N. H., Leenaars, J. G. B., Ribeiro, E., Wheeler, I., Mantel, S., & Kempen, B. (2017). SoilGrids250m: Global gridded soil information based on machine learning. In PLoS ONE (Vol. 12, Issue 2). https://doi.org/10.1371/journal.pone.0169748

735

Hersbach, H., Bell, B., Berrisford, P., Dee, D., Horanyi, A., Muñoz-sabater, J., Nicolas, J., Radu, R., Schepers, D., Simmons, A., & Soci, C. (n.d.). ERA5 : STATE-OF-THE-ART GLOBAL ATMOSPHERIC REANALYSIS AT ECMWF.

Hersbach, H., Bell, B., Berrisford, P., Hirahara, S., Horányi, A., Muñoz-Sabater, J., Nicolas, J., Peubey, C., Radu, R., Schepers, 740 D., Simmons, A., Soci, C., Abdalla, S., Abellan, X., Balsamo, G., Bechtold, P., Biavati, G., Bidlot, J., Bonavita, M., ... Thépaut, J. N. (2020). The ERA5 global reanalysis. Quarterly Journal of the Royal Meteorological Society, 146(730), 1999-2049. https://doi.org/10.1002/qj.3803

Iwema, J., Rosolem, R., Baatz, R., Wagener, T., & Bogena, H. R. (2015). Investigating temporal field sampling strategies for 745 site-specific calibration of three soil moisture – neutron intensity parameterisation methods. 3203–3216. https://doi.org/10.5194/hess-19-3203-2015

Kerr, Y. H., Waldteufel, P., Wigneron, J. P., Martinuzzi, J. M., Font, J., & Berger, M. (2001). Soil moisture retrieval from space: The Soil Moisture and Ocean Salinity (SMOS) mission. IEEE Transactions on Geoscience and Remote Sensing. https://doi.org/10.1109/36.942551

Köhli, M., Schrön, M., Zreda, M., Schmidt, U., Dietrich, P., & Zacharias, S. (2015). Footprint characteristics revised for fieldscale soil moisture monitoring with cosmic-ray neutrons. Water Resources Research, 5772-5790. https://doi.org/10.1002/2015WR017169.Received

755

750

Koster, R. D., Guo, Z., Bonan, G., Chan, E., & Cox, P. (2014). Regions of Strong Coupling Between. Science, 1138(2004), 10-13.

Li, W., MacBean, N., Ciais, P., Defourny, P., Lamarche, C., Bontemps, S., Houghton, R. A., & Peng, S. (2017). Gross and net 760 land cover changes based on plant functional types derived from the annual ESA CCI land cover maps. Earth System Science Data Discussions, 1-23. https://doi.org/10.5194/essd-2017-74

Muñoz Sabater, J., (2019): ERA5-Land hourly data from 1981 to present. Copernicus Climate Change Service (C3S) Climate Data Store (CDS). (<date of access>), 10.24381/cds.e2161bac





Peel, M. C., Finlayson, B. L., and McMahon, T. A.: Updated world map of the Köppen-Geiger climate classification, Hydrol. Earth Syst. Sci., 11, 1633–1644, https://doi.org/10.5194/hess-11-1633-2007, 2007.

Peters-Lidard, C. D., Clark, M., Samaniego, L., Verhoest, N. E. C., Van Emmerik, T., Uijlenhoet, R., Achieng, K., Franz, T.
E., & Woods, R. (2017). Scaling, similarity, and the fourth paradigm for hydrology. *Hydrology and Earth System Sciences*, 21(7), 3701–3713. <u>https://doi.org/10.5194/hess-21-3701-2017</u>

Portal, G., Jagdhuber, T., Vall-llossera, M., Camps, A., Pablos, M., Entekhabi, D., & Piles, M. (2020). Assessment of multiscale SMOS and SMAP soil moisture products across the Iberian Peninsula. *Remote Sensing*, *12*(3). https://doi.org/10.3390/rs12030570

Rosolem, R., Shuttleworth, W. J., Zreda, M., Franz, T. E., Zeng, X., & Kurc, S. A. (2013). The effect of atmospheric water vapor on neutron count in the cosmic-ray soil moisture observing system. *Journal of Hydrometeorology*, *14*(5), 1659–1671. https://doi.org/10.1175/JHM-D-12-0120.1

780

775

Santoro, M.; Cartus, O. (2019): ESA Biomass Climate Change Initiative (Biomass\_cci): Global datasets of forest above-ground biomass for the year 2017, v1. Centre for Environmental Data Analysis, *02 December 2019*. doi:10.5285/bedc59f37c9545c981a839eb552e4084. http://dx.doi.org/10.5285/bedc59f37c9545c981a839eb552e4084

785 Schrön, M., Köhli, M., Scheiffele, L., Iwema, J., Bogena, H. R., Lv, L., Martini, E., Baroni, G., Rosolem, R., Weimar, J., Mai, J., Cuntz, M., & Rebmann, C. (2017). *Improving calibration and validation of cosmic-ray neutron sensors in the light of spatial sensitivity*. 5009–5030.

Tian, Z., Li, Z., Liu, G., Li, B., & Ren, T. (2016). Soil water content determination with cosmic-ray neutron sensor : Correcting
aboveground hydrogen effects with thermal / fast neutron ratio. *Journal of Hydrology*, 540, 923–933. https://doi.org/10.1016/j.jhydrol.2016.07.004

Van Loon, A. F. (2015). Hydrological drought explained. Wiley Interdisciplinary Reviews: Water, 2(4), 359–392. https://doi.org/10.1002/wat2.1085

795

Vather, T., Everson, C. S., & Franz, T. E. (2020). The applicability of the cosmic ray neutron sensor to simultaneously monitor soil water content and biomass in an acacia mearnsii forest. *Hydrology*, 7(3). https://doi.org/10.3390/HYDROLOGY7030048



830



Villarreyes, C. A. R., Baroni, G., & Oswald, S. E. (2011). *Integral quantification of seasonal soil moisture changes in farmland by cosmic-ray neutrons*. 3843–3859. <u>https://doi.org/10.5194/hess-15-3843-2011</u>

Vuichard, N., & Papale, D. (2015). Filling the gaps in meteorological continuous data measured at FLUXNET sites with ERA-Interim reanalysis. *Earth System Science Data*, 7(2), 157–171. <u>https://doi.org/10.5194/essd-7-157-2015</u>

805 Wagener, T., Gleeson, T., Coxon, G., Hartmann, A., Howden, N., Pianosi, F., Rahman, S., Rosolem, R., Stein, L., & Woods, R. (2020). On doing large-scale hydrology with Lions: Realising the value of perceptual models and knowledge accumulation. https://doi.org/10.31223/OSF.IO/ZDY5N

Wagener, T., Sivapalan, M., Troch, P., & Woods, R. (2007). Catchment Classification and Hydrologic Similarity. *Geography Compass*, 1(4), 901–931. <u>https://doi.org/10.1111/j.1749-8198.2007.00039.x</u>

Wahbi A et al., Cosmic Ray Neutron Sensing: Estimation of Agricultural Crop Biomass Water Equivalent, https://doi.org/10.1007/978-3-319-69539-6\_4

Western, A. W., Grayson, R. B., Blöschl, G., Willgoose, G. R., & McMahon, T. A. (1999). Observed spatial organization of 815 soil moisture and its relation to terrain indices. Water Resources Research. 35(3). 797-810. https://doi.org/10.1029/1998WR900065

Wood, E. F., Roundy, J. K., Troy, T. J., van Beek, L. P. H., Bierkens, M. F. P., Blyth, E., de Roo, A., Döll, P., Ek, M.,

- 820 Famiglietti, J., Gochis, D., van de Giesen, N., Houser, P., Jaffé, P. R., Kollet, S., Lehner, B., Lettenmaier, D. P., Peters-Lidard, C., Sivapalan, M., … Whitehead, P. (2011). Hyperresolution global land surface modeling: Meeting a grand challenge for monitoring Earth's terrestrial water. *Water Resources Research*, 47(5), 1–10. https://doi.org/10.1029/2010WR010090
- Zhuo, L., Dai, Q., Han, D., Chen, N., Zhao, B., & Berti, M. (2019). Evaluation of Remotely Sensed Soil Moisture for Landslide
   Hazard Assessment. *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, 12(1), 162–173. https://doi.org/10.1109/JSTARS.2018.2883361

Zreda, M., Shuttleworth, W. J., Zeng, X., Zweck, C., Desilets, D., Franz, T., & Rosolem, R. (2012). COSMOS: The cosmicray soil moisture observing system. *Hydrology and Earth System Sciences*, *16*(11), 4079–4099. <u>https://doi.org/10.5194/hess-</u> 16-4079-2012





Zreda, M., Desilets, D., Ferré, T. P. A., & Scott, R. L. (2008). Measuring soil moisture content non-invasively at intermediate spatial scale using cosmic-ray neutrons. *Geophysical Research Letters*, *35*(21), 1–5. https://doi.org/10.1029/2008GL035655