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Investigating opportunities for global scale soil moisture studies using Cosmic-Ray Neutron Sensors

Investigating opportunities for global scale soil moisture studies using Cosmic-Ray Neutron Sensors

PhD Thesis

By

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Abstract

Soil moisture is an important aspect of the Earths hydrological system. Accurate monitoring of soil moisture is essential for advancing our knowledge of its influence on Earth system processes. Cosmic-Ray Neutron Sensing (CRNS) offers an opportunity to fill the knowledge gap between point-scale sensors and large-scale sensors (i.e., satellite remote sensing) by capturing field scale, root-zone soil moisture. However, increasing global deployment of CRNS in regional networks has led to disparate processing methods across the sensors, hindering the use of these sensors in broad scale global studies.

This thesis explores the opportunities presented in utilising CRNS stations from across the globe as a harmonized global network of sensors. Firstly, an open-source python processing tool was developed to facilitate a much-needed harmonization of CRNS data from 163 stations from across multiple networks. Using this tool, we demonstrate the problems that can come from a non-harmonized set of sensors in global studies. Utilizing this harmonized dataset, we conducted a comparative study against a satellite-derived soil moisture product (ESA-CCI) and a reanalysis product (ERA5-Land). Our analysis reveals residual biases between these products and CRNS values, which notably increases at the extremes of wet and dry conditions, whilst correlation differences increase under moderate conditions. Lastly, machine learning models were used to evaluate the role of soil moisture spatial representation in predictions of land surface fluxes of water (evapotranspiration) and photosynthesis (gross primary productivity). Our findings indicate that in-situ soil moisture data is particularly important for accurate predictions of evapotranspiration in water stressed regions., when compared to indirect estimates from empirical models or satellite remote sensing. Unlike evapotranspiration, we observe that the contribution of deeper soil moisture, in the form of soil moisture memory, plays a more significant role in predicting photosynthesis, pointing to the importance of identifying distinct mechanisms driving water and carbon fluxes at the land-atmosphere interface. Overall,

this thesis demonstrates the value of CRNS being treated as a harmonized and global network, reveals the importance of soil moisture spatial representation in modelling of land-atmosphere processes, and highlights where future soil moisture sensor deployment can be most beneficial.

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Author's Declaration

I declare that the work in this dissertation was carried out in accordance with the requirements of the University's *Regulations and Code of Practice for Research Degree Programmes* and that it has not been submitted for any other academic award. Except where indicated by specific reference in the text, the work is the candidate's own work. Work done in collaboration with, or with the assistance of, others, is indicated as such. Any views expressed in the dissertation are those of the author.

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1 Introduction

Soil moisture is an important component of the Earth system having a direct impact on numerous environmental processes. It directly influences the partitioning of water at the land surface, thereby affecting hydrological processes. Similarly, by impacting the partitioning of solar energy from the sun, it influences atmospheric processes. These interactions themselves create feedback loops that not only affect soil moisture itself but also have broader implications on the climate (Seneviratne 2010, Qiao et al., 2023). Recent research suggests that as climate change progresses, the influence of soil moisture on Earth system processes, such as through its direct coupling to evapotranspiration, is likely to intensify (Hsu and Dirmeyer 2023). Soil moisture also serves as the primary water source for plants, indicating that changes in soil moisture quantity or dynamics will directly affect both ecosystem function, as well as agricultural productivity. Given its important role, global efforts to measure and monitor soil moisture continue to grow (Romano 2014), leading to a growing source of soil moisture datasets across the globe. This growing source of data opens new avenues for a large sample hydrology approach, aiming to enhance our global understanding of soil moisture's numerous roles in global environments. Large global datasets provide opportunities to better understand the world through detailed analysis (Luo et al., 2022), validation of satellite derived soil moisture products (Crow et al., 2012), and the application of cutting-edge machine learning techniques for predictive tasks (O and Orth 2022). However, before beginning any kind of study with soil moisture it's important to first decide on the most suitable source of soil moisture data for the desired task. Numerous methods for measuring soil moisture now exist, each representing soil moisture in distinct spatial and temporal domains, and the number of available methods continues to expand. A more comprehensive discussion on various soil moisture measurement methods and their unique characteristics is presented in Chapter 2. Central to this thesis is the Cosmic-Ray Neutron Sensor (CRNS), an increasingly popular sensor that provides field scale, root-zone soil moisture values at hourly intervals (Desilets et al., 2010, Zreda et al., 2012). The spatial domain of these sensors, positioned between point-scale sensors and broader satellite remote sensing, offers new ways of understanding soil moistures role in environmental processes. In particular, it offers avenues to explore the role of spatial scaling, that is the volume of soil being represented in data, has on earth system processes. By now, these sensors have been in operation for over a decade in some cases, and their networks are expanding globally (Hawdon et al., 2017; Cooper et al., 2021; Bogena et al., 2022). Given the growing global spread and this unique spatial scale, the CRNS leads to exciting opportunities for studies into the role of soil moisture in earth system processes globally.

However, despite the opportunities presented by the growing number of CRNS stations across the globe, no studies have yet utilized a large sample hydrology approach using this globally spanning dataset. One of the key barriers to such research is the regionalisation of different CRNS networks, which can lead to inconsistencies in data processing steps across regions. As networks of these sensors have grown, so too has our understanding of the sensor technology itself. With this growing understanding, improved methods to process the raw CRNS data into soil moisture estimates have been developed. However, up to date methods have not been applied uniformly across all the networks, and in some cases, there are differences in opinion on the best practice for processing itself. These inconsistencies make it challenging to treat the increasing number of sensors as a unified network. Two main issues contribute to this. Firstly, data structure such as the naming conventions differ between networks, adding a layer of complexity to combining datasets. Second, and more critically, is the different outputs expected when using different methods for converting raw data into soil moisture estimates. As a result, these variations could influence the outcomes of subsequent research, limiting the reach and applicability of the findings. Until these issues are resolved, the full potential of a global CRNS dataset remains largely untapped.

With this in mind, there are clear opportunities to facilitate large sample hydrology type studies that will provide an understanding of the role of soil moisture in Earth system processes across the globe, covering different distinct hydroclimates. The open data policies from some of the networks ensure most raw CRNS data is publicly available. While variations in processed datasets exist, there is potential for standardizing sensor data processing to obtain a global dataset. The first step towards this is to devise a method to process raw CRNS data quickly and accurately into soil moisture estimates, leveraging the latest sensor understanding.

With a harmonized dataset, the door opens to explore the role of soil moisture in global Earth system processes. While some studies have used CRNS to validate satellite remote sensing soil moisture products (Montzka et al., 2017), none have utilized all available sensors globally in a singular study. A harmonized dataset can facilitate such comprehensive studies, enabling analysis on where large-scale gridded products agree with in situ sensors and where discrepancies remain. Additionally, growing interest in machine learning for Earth system science research, which requires large sets of quality data, positions a global and harmonized CRNS dataset as a valuable resource. As noted earlier, the intensity of coupling between soil moisture and evapotranspiration is expected to change with the changing climate. Projects are already underway leveraging machine learning and global environmental variable datasets to predict land-atmosphere exchanges like evapotranspiration (Tramontana et al., 2019). The quality of input data significantly influences these models, necessitating a deeper look into soil moisture's role in shaping their outcomes. This could help identify scenarios where different measurement techniques offer different advantages, which could itself influence decisions on where to expand sensor networks in the future. Overall, a globally spanning CRNS dataset could provide the foundation for such studies.

In summary, soil moisture is a fundamental variable in Earth system sciences, and the extensive CRNS networks across the globe provide a significant opportunity to advance our understanding of its role. The opportunities that a global dataset can provide are currently limited by the regionalisation of CRNS networks. Given this, the overall goal of this thesis is to:

> *Investigate the opportunities of a harmonized and globally spanning dataset of CRNS-derived soil moisture to increase our understanding of the role of soil moisture in Earth system sciences applications.*

To achieve this goal several steps are required which are outlined below.

Chapter 2 serves as a literature review, giving an overview on the current state of knowledge regarding soil moisture and its influence on the Earth system. It explores the methods employed to measure soil moisture, emphasizing the impact of measurement techniques on data, particularly focusing on spatial scaling. The chapter also introduces large sample hydrology, showcasing successful projects that have produced datasets facilitating such studies. Furthermore, it explores the area of large sample hydrology in the context of soil moisture specifically, discussing the potential unique benefits CRNS can offer with this in mind.

To investigate the stated goal of understanding the potential of a harmonized and global CRNS dataset for large sample hydrology studies several steps are required. The following paragraphs will outline the scope of each chapter as well as a brief description of the methods employed to achieve each chapters aim.

Firstly, there is the task of harmonizing CRNS networks worldwide which is explored in Chapter 3. The goal of this chapter is to explore the impacts of unharmonized data, and to present a new python tool (Cosmic-Ray Sensor Python tool – *crspy*) that was developed to facilitate easy harmonization of numerous sites as well as the collection of metadata about each site that can add further value to future large sample hydrology studies. Primarily, *crspy* will be presented, which is an open-source python package for processing raw CRNS data. The chapter will outline the current methods employed by the various regional CRNS networks and demonstrate the potential issues of directly comparing sites that may be processed differently. This is achieved by processing individual CRNS sites with each of the different processing methodologies currently used by regional networks (utilising *crspy*) and comparing the outputted soil moisture datasets. It is hypothesised that differences in methodology will ultimately lead to differences in soil moisture time series values demonstrating the potential benefits of harmonizing processing methods of global sites.

With access to a harmonized and global CRNS dataset, Chapter 4 explores the uncertainties between this newly harmonized global CRNS soil moisture dataset and commonly used gridded satellite and reanalysis soil moisture products. Validation studies for gridded products often use a variety of soil moisture sensors which each may have systemic differences. This leads to a primary focus on either correlation when comparing in-situ to gridded products (Gruber et al., 2020), or on rescaling techniques to account for systemic differences between the in-situ (and gridded) sensors. Utilizing a global CRNS dataset offers a unique avenue to explore the overall uncertainty between in-situ and gridded products, as well as the impact of rescaling techniques. This exploration will be carried out by directly comparing a satellite soil moisture product (ESA-CCI) and a reanalysis soil moisture product (ERA5-Land) to CRNS soil moisture data. The uncertainty characteristics between the datasets will be analysed by decomposing the mean square error (MSE) into its constituent parts: bias, correlation, and deviation. A subsequent analysis will explore how the source of uncertainty shifts in space and time. It's hypothesized that the characteristics of uncertainty will vary, particularly with the overall moisture conditions, in both spatial and temporal dimensions. Additionally, the chapter will explore the potential impact common bias correction methods might have. Comparisons between in situ soil moisture data and satellite soil moisture data often deploy bias correction approaches to tackle systemic differences between sensors. Given our global CRNS network is already harmonized, this chapter presents an opportunity to investigate the impact of bias correction methods between the in-situ data and the gridded soil moisture products, without the need to rescale the in-situ data itself.

Finally, Chapter 5 explores the impact of soil moisture spatial representation on predictions of atmospheric fluxes of energy and carbon when used in a machine learning model. Soil moisture dynamics vary based on the volume of soil measured by a specific sensor. The growing accessibility to large datasets has driven the use of machine learning models for predicting key environmental variables. Data is crucial for training a machine learning model, and the dataset choice significantly influences model performance. This chapter examines the influence of spatial scales of soil moisture on predictions of carbon and energy fluxes, by altering the source of soil moisture representation in the feature set of an established machine learning model (FLUXCOM). Comparisons will be made between soil moisture datasets ranging from point scale TDR to satellite products, to discern the impact soil moisture representation has on predictions. The hypothesis is that the comparative spatial scale of CRNS and eddy covariance towers will enhance the accuracy of predicted values. With the availability of global and harmonized CRNS data, the chapter will also investigate if this improvement is consistent across various hydroclimates. It is further hypothesized that the impact of spatial scaling will be more pronounced at arid and water-limited sites.

After these research chapters there will be three appendixes that will briefly describe research for which I was a part of, but not the lead author. Appendix A describes research into the applicability of using CRNS stations across the globe to act as an early warning system for adverse space weather events, such as Ground Level Enhancements. These events pose a particular hazard to aviation through its impact on aviation systems, and increased radiation dose for passengers and crew. For this research, crspy is used to update CRNS stations in the USA to account for the most current understanding. Appendix B describes research that utilises the newly harmonized CRNS network to validate several popular soil moisture reanalysis products. Whilst Appendix C describes research aiming to integrate CRNS stations into smart irrigation systems for precision agriculture. For this study, an updated version of crspy was developed to allow real time processing of raw CRNS data, as well as being interoperable with a wider software environment.

Overall, it is expected that this thesis will generate several key outcomes to address the gaps and challenges outlined above. Firstly, the creation of a software tool to facilitate the processing of CRNS, thus allowing the creation of a harmonized and globally spanning dataset of soil moisture values. This first step will provide a foundational resource for which to explore other topics discussed above related to soil moisture’s role in earth system sciences, in particular through the ability to harmonize the currently regional datasets into a global one. Secondly, by comparing this dataset with satellite and reanalysis products, this work will offer insights into their discrepancies, robustness, and uncertainties compared to in situ sensors across different hydroclimates. Thirdly, through the application of machine learning techniques, this research will investigate how spatial representation of soil moisture influences the accuracy of predicting land-atmosphere fluxes in diverse hydroclimatic conditions. These outcomes collectively promise to advance our understanding of soil moisture's role in earth system processes, as well as provide tools and methodologies to facilitate future large-sample hydrology studies with CRNS data. Overall, it’s expected that this thesis will emphasise the value of treating all CRNS across the globe as a single, harmonized network

2 Literature Review

2.1 Soil moisture and Earth System Processes

Soil moisture is generally defined as the water contained in the unsaturated soil zone, also known as the vadose zone (Seneviratne et al., 2010). It is a key component in various fields such as hydrology (Vereekcken et al., 2008), agriculture (Hardie, 2020), ecology (Padilla and Pugnaire, 2007), and land-atmosphere interactions (Seneviratne et al., 2010). In recognition of its significance the scientific community is committed to increasing our understanding of soil moistures' impact on the Earth system and developing accurate and robust methods to measure and monitor it. There remain challenges, however, due to the various ways that soil moisture can be defined and measured. The first step in quantifying soil moisture is to define the volume of soil of interest, whether it be at a single point in the ground, across an entire catchment, or a whole country. Each of these scales will have an influence on different processes in earth system science. Heterogeneities in the soil structure mean that choosing a relevant spatial scale will have a direct impact on the soil moisture estimate (Crow and Wood, 2002). Therefore, measurement techniques for soil moisture across multiple spatial and temporal scales continue to be an active area of research, driven by the significant environmental impacts linked with soil moisture.

Soil moisture is an important component of the Earth System, owing to its significant influence on environmental processes. Whilst soil moisture constitutes only approximately 0.05% of global fresh water (Robinson et al., 2009), it is known to have a direct impact on plant growth in both nature (Winkler et al., 2016) and agriculture (Franz et al., 2016), as well as having an influence on weather dynamics and hydrology (Koster et al., 2004, Fischer et al., 2007). Several detailed reviews are available that describe soil moistures critical influence in the earth system. Seneviratne et al. (2010) outline the varied ways soil moisture influences land atmosphere interactions, for example demonstrating the feedback that occurs leading to soil moistures influence on and by precipitation patterns, potentially leading to either floods or droughts. McColl et al., (2017) described the significant impact that surface soil moisture (~8mm depth) has on precipitation and subsequently ground water recharge across various hydroclimates. The broad influence of soil moisture on different parts of the earth system opens up numerous avenues of active research within the scientific community. To further illustrate this, the following subsections will explore the literature of some key areas where soil moisture exerts a strong influence.

A good place to start is in the field of hydrology, which is the scientific study of how water moves through the earth system. Despite constituting only a small proportion of total freshwater at any one time, soil moisture plays a large role in driving total water dynamics. For simplicity, let us consider the beginning point of the hydrological cycle as when moisture returns to the earth from the atmosphere as rainfall. Some of this moisture will return to water bodies either directly or through overland flow, or it will be intercepted by plant canopies, but a considerable amount of this moisture permeates into the soil column. Soil moisture’s downward trajectory though the soil column is known as infiltration (Vereecken et al., 2022). Soil moisture can therefore impact rainfall-runoff processes, which is the connection between precipitation and streamflow, due to its impact on the rate of infiltration (Liu et al., 2019). After a precipitation event, if the soil is dry, it has capacity to absorb the incoming moisture.

If the precipitation intensity is high, the top layer of soil will quickly reach saturation, whilst the time it takes for moisture to infiltrate deeper into the soil is dependent on the soil structure itself (Basset et al., 2023). Hence both antecedent moisture conditions and the physical structure of the soil can lead to excess runoff, ponding of water on the surface, or, in extreme cases, flooding. This describes how soil moisture can influence hydrology when water is in excess, however a lack of water can have impacts too. Droughts broadly refer to sustained periods of below normal water availability, which in the context of the environment begins as meteorological droughts (i.e., low precipitation), leading to soil moisture drought (i.e., low soil moisture), and eventually leading to hydrological droughts (i.e., low streamflow) (Van Loon 2015). It is important to note that the interaction between soil moisture and atmospheric moisture is not unidirectional; as soil moisture also exerts an influence on atmospheric processes themselves. This knowledge leads to continued efforts in the earth system science community to better understand the ways in which land-atmosphere feedback can influence ecosystem dynamics.

Given this, understanding the interplay between soil moisture and atmospheric processes is another active area of research, namely in understanding land-atmosphere interactions. These interactions encompass the cyclical feedback between atmospheric conditions—such as precipitation—and land processes, including soil moisture (Seneviratne et al 2010). At the centre of this interplay is the process of evapotranspiration, which describes how the sun’s energy converts liquid water into vapour at the Earth’s surface, and in doing so returning moisture to the atmosphere and partitioning the total energy received from the sun. This energy is generally divided into ground heat (energy absorbed into the ground), sensible heat (energy transferred from the ground to the air) and latent heat (the energy used in converting water from liquid to vapour). It is here that we can identify the crucial role of soil moisture in this process, with more soil moisture available, more energy is used in its conversion to vapour, directly reducing atmospheric temperatures at the catchment.

Equally a lack of water availability through soil moisture can drive up sensible heat, which in turn increases temperatures. This leads to higher evapotranspiration rates, potentially exacerbating reduced water levels, increasing atmospheric aridity, and generating additional heat (Vicente-Serrano et al., 2019, Zhou et al., 2019). As a direct results of this, soil moisture dynamics greatly impact droughts and heatwaves (Miralles et al., 2018). For example, it can influence drought propagation downwind via the effect on evapotranspiration and, subsequently, precipitation (Schumacher et al., 2022). Heatwaves are defined as periods of prolonged atmospheric temperatures that are above normal conditions (Stefanon et al., 2012). The link between heatwaves and droughts makes this an active area of study to better understand how a changing climate will impact future terrestrial conditions, and soil moisture's role in both warrants further investigation. Interestingly, some research contradicts the assumption that reducing moisture will lead to less available water to evaporate. Known as the 'drought-paradox', studies across Europe have found that evapotranspiration can actually increase during drought periods (Teuling et al., 2013). This is likely due to the influence plants exert on evapotranspiration through stomatal control demonstrating further the need to better understand the influence of soil moisture in the natural world. While the amount of available water in the soil heavily influences evapotranspiration, it is additionally impacted by the vapour pressure deficit (VPD), which refers to the difference in the amount of moisture in the air (water vapour) and the amount it could hold if it was fully saturated at a given temperature. Worryingly, compounding drought events, where both higher VPD and low soil moisture increase the severity of a drought, are expected to increase in the future (Zhou et al., 2019). Both droughts and heatwaves have negative implications for society, leading to excess deaths in the human population (Ellis et al., 1980), and through the impact it can have on local ecology. As an example, prolonged drought (between 1997 – 2010), along with over abstraction, in the Murray-Darling Basin in Australia led to a collapse in fish populations in the rivers of the basin, and a subsequent shift in habitat dynamics. Although water levels have since recovered, fish assemblages have not, leading to a shift in the overall ecosystem characteristics (Wedderburn et al., 2014). Additionally, sustained droughts can lead to widespread tree mortality in forests (Adams et al., 2017), which themselves provide a feedback effect on soil moisture dynamics through their control on transpiration. This highlights the need to not only understand the impact of soil moisture on the atmosphere, but also its direct impact on terrestrial ecosystems.

Living things need water to survive, and for terrestrial plants this primarily comes from moisture in the soil. Transpiration, the process of water moving through a plant and evaporating from its leaves, is driven by soil moisture. Plants sustain themselves through photosynthesis, where sunlight helps convert carbon dioxide into glucose and oxygen, with oxygen being a by-product released into the atmosphere. Through their stomata, small openings on the leaves, plants regulate photosynthesis and water uptake. These openings allow air into the leaves for photosynthesis and can close to prevent excessive water loss during water stress. However, the regulation of water and gas exchange can lead to trade-offs. In water-stressed conditions, plants may reduce water loss, but this also limits their ability to photosynthesise by reducing the availability of carbon dioxide. Respiration in plants roots, and from microorganisms that break down organic matter in the soil, lead to carbon egressing from the soil too (Kuzayakov and Gavrichkova 2010). The total flux of carbon between the land and atmosphere is referred to as net ecosystem exchange (NEE) of carbon which consists of two main components, gross primary productivity (GPP), which is the amount of carbon fixed by plants during photosynthesis, and total ecosystem respiration (TER) which is the carbon released back into the atmosphere as carbon dioxide through processes such as plant or microbial respiration. Through their stomatal control, plants directly influence overall evapotranspiration (and hence soil moisture) and carbon cycling. In return, soil moisture impacts the plants' ability to photosynthesise. The complexities of this feedback loop mean ongoing research is necessary to better understand it, especially in a changing climate. For instance, research has identified strong feedback between GPP rates and atmospheric conditions such as precipitation. This feedback additionally tends to be stronger in semi-arid and monsoonal regions (Green et al., 2017). Further studies are identifying that soil moisture dominates carbon uptake variability across the globe (Green et al., 2019, Humphrey et al., 2021). While both VPD and soil moisture influence terrestrial production, it has been shown that soil moisture has the larger influence when water stress occurs (Liu et al., 2020). GPP can occasionally increase with decreasing soil moisture, up until a threshold, whereas increasing VPD has a consistently negative impact on GPP rates (Fu et al., 2022). The occasional disconnection between soil moisture and GPP rates is due to plant adaption strategies that, for example, allow efficient use of water during periods of low moisture. Interestingly, a strong correlation has been demonstrated in data comparing soil moisture values and changes in plant biomass (estimated by using the leaf area index, LAI) with a temporal lag of around three months, demonstrating the long-term influence of soil moisture on ecosystem functioning (Li and Sawada, 2022). Evidently a complete understanding of these processes and their drivers is crucial. While individual plant mechanisms are well understood (Leegood, 2002), and how they may impact soil moisture and the climate at scale has been an active area of research for some time (Budyko, 1961, Gentine et al., 2012) the complexities involved means continued research is necessary. Plants evidently have a strong influence on, and are influenced by, soil moisture in the natural world. This complex relationship is not only important to global ecosystem dynamics, but also has significant implications for human activities, particularly in agriculture.

Agriculture is a sector critically dependent on accurate soil moisture estimates and broad understanding of soil moisture dynamics. Given its reliance on water, most of which is human controlled, the effects of soil moisture variations can be huge. Soil moisture deficits directly lead to reduced crop yields (Vough and Martin 1971, Martin et al., 1992) and in extreme cases can lead to total crop failure (Mandelsohn 2007). The societal implications of these effects are serious, considering that agriculture is the main source of our food. Consequently, research has been conducted for decades on predicting yields in relation to water (Hanks 1974). To avoid the unreliability of precipitation, irrigation is used to control the amount of water crops receive, ideally reducing water stress and optimising yields. However, given this, a 2017 census of U.S. producers found that over 75% of irrigation scheduling practices where still based on rule-of-thumb procedures such as crop calendars or visual observations (Zhang et al., 2021). Optimising irrigation can enhance water use efficiency and reduce wastage. The timing of irrigation depends on understanding how to support plant needs without excessive water use. Efforts to optimise irrigation include estimating crop water stress from weather data (Nakabuye et al., 2023), using remotely sensed indices with models to control irrigation scheduling (Zhang et al., 2023), or combining in-situ sensors in smart Internet of Things systems (Kamienski et al., 2018). Irrigation not only provides crops with moisture to use, but also provides cooling benefits at the land surface, reducing heat stress in plants, again leading to improved yields (Li et al., 2020). Irrigation can come at a cost however, as fresh water is a finite resource and so excessive irrigation can lead to water stress in the total ecosystem. For example, a large regional study using in-situ measurements across northern China has demonstrated a steady decline in topsoil moisture content (0-50cm) between 1983 and 2012, along with reduced river discharges, which is attributed to intensified agriculture over this period (Liu et al., 2015). In order to prevent future occurrences of these long-term impacts, methods are continually developed to better manage our finite water resources. One such method is precision agriculture, which is the collection of methods combining sensors, information systems, and machinery, that can lead to low input, highly efficient and sustainable agriculture, ensuring food security along with environmental sustainability (Zhang et al., 2002, Gebbers and Adamchuk 2010). Before integrating information systems and machinery together however, we must begin with one of the most basic, and arguably more difficult tasks, measuring soil moisture in a accurate manner.

The above text underscores the various ways in which soil moisture influences the Earth's systems. Each of these areas needs continued research, particularly considering the uncertain effects of climate change on our current understanding. A critical step in understanding how soil moisture dynamics might change - and how these changes might impact the topics discussed above - is the ability to measure soil moisture accurately. This task presents challenges due to both the inherent difficulties of accurate measurement and the complexities of determining the appropriate temporal or spatial resolution of interest. The subsequent subsections will explore what soil moisture is, the various methods currently employed to measure it, and the influence of temporal and spatial resolution on our choice of measurement technique.

2.2 How do we measure soil moisture?

Soil moisture values, which represents the proportion of water within a given volume of soil, are typically measured in two common units: gravimetric and volumetric soil moisture. Gravimetric soil moisture (usually given in grams per grams) refers to mass of water in a total mass soil column, whereas volumetric soil moisture (usually given in $m^3\ m^{-3}$ or $cm^3\ cm^{-3}$) refers to volume of water in a given volume of soil (Robinson et al., 2008). In theory, the only direct way to measure soil moisture is by removing soil samples from the field and using the oven drying method. In this method a core of soil of a known volume is extracted from the ground, the sample is weighed and then placed into an oven at 105 ^{o}C, usually for 24 hours, and the sample is weighed again (Romano 2014). The resulting weight loss is presumed to be the weight of water that has evaporated. Whilst an accurate process of measurement, this method is not without its limitations. The method is manual and laborious, taking a lot of time and effort, whilst it provides only a single soil moisture value at a particular point in time, and destroys the sample that is being investigated. Given these limitations the scientific community have developed numerous other methods of soil moisture measurement that tend to use properties related to water, to infer soil moisture values at a particular place. These include Reflectometers (Top et al., 1980), Ground

Penetrating Radar (Knight et al., 2001), Global Positioning Systems (Larson et al., 2008), Cosmic-ray Neutron Sensors (Zreda et al., 2008), or satellite remote sensing (Entekabi et al., 2010). Whilst an extensive review is beyond the scope of this work, several more comprehensive reviews in soil moisture sensing and measurement are available (Robinson et al., 2008, Romano 2014). The focus here will be the most relevant methods for soil moisture estimates to this thesis.

2.2.1 Point-scale soil moisture (dielectric resistance or reflectometers sensors)

Point scale soil moisture sensors that use dielectric resistance to infer soil moisture sensors are a widely accepted method for soil moisture measurement. Their functioning revolves around the unique molecular structure of water, where the opposing charges of hydrogen and oxygen lead to a permanent dipole moment, which contrasts with most other natural materials (Robinson et al., 2008). This property results in a high dielectric constant when water is present in a volume of soil, thereby affecting the propagation time of an electromagnetic pulse (Evett and Parkin, 2005). By leveraging this phenomenon, changes in propagation time can serve as a measure of soil water content. There are several different types of dielectric resistance-based soil moisture sensors, such as Time Domain Transmission sensors (Will and Rolfes 2014) or Frequency Domain Reflectometers (Skierucha and Wilczek, 2010). For the purpose of this discussion, however, focus will be directed towards one sensor in particular, the Time Domain Reflectometer (TDR). TDR sensors measure changes in the dielectric constant of soil and can infer soil moisture changes in time (Topp et al., 1980, Robinson et al., 1999). The measuring support volume is approximately a sphere with 10cm in diameter around the TDR sensor (Western and Blöschl 1999). The representativeness of this spatial scale, when compared to say a whole field, is an area of ongoing research and debate (Miralles et al., 2010). Heterogeneities in the soil structure and landscape topography can lead to different soil moisture responses to environmental conditions (Patzold et al., 2008). This leads to one of the key advantages of TDR sensors, in that they can be installed at various horizontal **and** vertical positions, allowing an understanding of soil moisture dynamics at various depths as well as at horizontal scales. Addressing the fact that individual sensors track changes in a small soil volume, multiple sensors can be installed within a catchment and combined, both vertically and horizontally, to provide an area average of soil moisture (Western and Blöschl, 1999). This desire to track soil moisture dynamics at larger spatial resolutions to than point scale measurements, such as with TDR, has led to the development of alternative techniques of soil moisture monitoring.

2.2.2 Cosmic ray neutron sensing (CRNS)

Among these methods, CRNS stands out as an in-situ sensor that can provide field scale (~250m radius around the sensor) and root zone depth soil moisture readings at hourly intervals. CRNS will be a focus in this thesis and a detailed description of how these sensors work is provided in Chapter 3, here a broad overview is given to provide context next to the other described sensors. CRNS primarily work due to some unique properties that dictate the presence of fast neutrons in the environment. Fast neutrons, which originate from space borne cosmic rays, are neutrons within a particular energy spectrum that are always present in the atmosphere (Kohli et al., 2015). Fast neutrons are thermalized (i.e., slowed down) by the presence of hydrogen atoms in the environment more so than any other atom (Zreda et al., 2012). This means that a higher presence of hydrogen atoms in the environment, such as those found in water, will lead to a reduction in the number of fast neutrons in the vicinity. When fast neutrons interact with the sensing tube filled with specific gas (either He^3 or BF_3) of a CRNS, a small electrical signal is recorded. Counting rates are usually integrated over a one-hour period, with most changes in counting rates attributed to changes in soil moisture content, after the application of appropriate corrections. There are additional correction steps required to account for additional influences on the neutron signal that originates from changes in atmospheric pressure (Zreda et al., 2012), incoming neutron intensity (Desilets et al., 2010, Hawdon et al., 2014), atmospheric water vapour (Rosolem et al., 2013), biomass (Heidbüchel et al., 2016, Tian et al., 2016), and soil organic carbon and lattice water in the soil (Franz et al., 2012, Hawdon et al., 2014). Each sensor also needs to be calibrated to the location it is placed in which is done through a campaign of oven dried samples within the sensor footprint (Zreda et al., 2012, Schrön et al., 2017). Initially this calibration campaign was conducted one time, calibrating the sensor to a single day. More recent work has established the benefit of taking calibration campaigns across multiple days, ideally across different seasons, which has led to improvements in overall data quality (Iwema et al., 2015). After calibration one of the key advantages of CRNS is that they are non-invasive and can provide an average of soil moisture over a relatively larger area than traditional point sensors, covering up to the root-zone depth. Theoretically once the site has been set up and appropriately calibrated, they can continue to run with minimal ongoing maintenance. With power being supplied by solar panels, and data being transmitted via iridium satellite meaning data is automatically collected (Desilets et al., 2010). Additionally, as our understanding of the neutron signal grows, we can re-process any collected data to account for the most current understanding. This presents us with an opportunity to monitor area average field scale soil moisture dynamics across the globe with a collection of sensors that can be harmonized in their methodology. This monitoring will be increasingly important, as we push for sub-kilometer global land surface models. Having good quality data at this spatial scale enables us to test current iterations of high spatial resolution land surface models, as well as test for improvement in the future. Although fundamentally this still relies on funding, efforts, and land, to establish and set up in situ monitoring sites across the globe. Given these challenges, the benefit of obtaining truly global soil moisture estimates becomes clear, leading to a large community of scientists seeking ways to monitor soil moisture dynamics using satellite remote sensing technology.

2.2.3 Satellite remote sensing

This brings us to satellite remote sensing, which refers to sensors installed on satellites orbiting the Earth. These sensors track changes in electromagnetic radiation to infer changes in surface soil moisture (Layman et al., 2001). Satellite remote sensing can be mainly sub-divided into two main categories: passive and active remote sensing. Both measure microwave energy using instrumentation on satellites orbiting the Earth, which is highly influenced by changes in soil moisture, with a penetration depth of 2-5cm. This means that satellite remote sensing is said to track changes in surface soil moisture (Beck et al., 2020). Passive remote sensing measures changes of thermal microwave radiation emissions from the soil, which are strongly dependent on soil moisture content (Njoku et al., 1977). This detected radiation is often referred to as the "brightness temperature" which is a measurement that combines the physical temperature of the object and its emissivity, which describes how well the object emits radiation. A key benefit of passive sensing is that the changes in the signal's brightness due to changes in soil moisture content are much higher than the sensitivity of microwave radiometers. The higher signal-to-noise ratio means that the radiometer can pick up changes in soil moisture with accuracies of around 1-2% (Njoku and Entekhabi, 1999). However, it's also important to note that brightness temperature measurements are influenced by the temperature of the soil itself, as well as by other factors like the composition of the soil and the presence of vegetation. Therefore, interpreting brightness temperature data to get soil moisture information can be complex, requiring sophisticated algorithms and potentially other types of data for calibration or validation. In contrast, active remote sensing involves sensors emitting their own energy, such as microwaves, and measuring the backscatter from the Earth's surface. While they can provide a finer spatial resolution than passive remote sensing, they are more susceptible to influences from factors like vegetation canopy structure, surface roughness, and incidence angle, which is the angle of incoming radiation, leading to a need for more sophisticated algorithms to correct for this (Wagner et al., 2007, Peng et al., 2017). There are many examples of active and passive sensors onboard satellites that have been used to record soil moisture across the globe such as Sentinel (Berger et al., 2012), SMOS (Kerr et al., 2010), SMAP (Entekabi et al., 2010), ASCAT (Bartalis et al., 2007), AMSR-E (Njoku et al., 2003), to name a few. This means satellite remote sensing offer a chance to monitor global soil moisture at regular intervals (usually measurements every 1-3 days), with horizontal spatial scales ranging from ~10^1 – 10^3 km^2 (Gruber et al., 2020). Ultimately active and passive sensors each have their own positive and negative characteristics demonstrating the importance of continued development of both methods. Considering the growing number of satellites products available, each spanning different periods, attempts to merge multiple satellite products into a single product have been attempted, such as the ESA-CCI merged satellite soil moisture product (Gruber et al., 2019). Since then, evidence has shown through direct comparisons to in-situ soil moisture networks, that these merged products can outperform individual satellite sensors (Beck et al., 2020). One suggested reason behind this is that the weighted algorithm they use to merge the products considers individual data quality, allowing the merged product to compile the best of each sensor into a single dataset. More recently constellations of miniature CubeSats, which have a volume of exactly one litre, have been increasingly put into Earth orbit (Villela et al., 2019). They are increasingly used to monitor soil moisture at a global scale (Norton et al., 2016), and may offer an opportunity for quicker return times due to the higher number of satellites that can orbit the Earth. Satellite remote sensing can give truly global coverage of soil moisture, although the low sensing depth and coarse spatial resolution means the data available may not be suitable to all requirements.

2.2.4 Land Surface Modeling

Soil moisture modelling broadly refers to methods to predict soil moisture without the need for direct measurements. Land surface models are numerical models that parameterize the relationships between earth system processes and attempt to make accurate predictions on states at points in time and space (Martens et al., 2020). Originating from climate modelling, land surface models have grown in complexity as our access to both data and understanding has advanced (Fisher and Coven, 2020). There are numerous parameterizations of soil moisture within land surface models, with design choices ultimately having an impact on the overall results (Koster et al., 2009). Typically, models are divided into grid areas, each grid being assigned properties corresponding to the estimated soil type or texture. Factors like precipitation and evaporation, which could also be modelled data, regulate the soil's input and output in the grid. The level of saturation, in conjunction with the soil properties, defines the drainage volume and percolation into the soil. Additionally, models will make a choice on the number of layers of soil that are to be calculated although it should be noted that the complexity can be much greater than what is described above. For example, coupled models will attempt to model additional feedback between soil moisture and climate (Dirmeyer 2011), or soil moisture and plant growth (Schymanski et al., 2008). Reanalysis products are another type of model which often combine both land surface models and observations of state variables (e.g., through satellite remote sensing) to ensure that the predictions remain as close to the real-world values as possible (Naz et al., 2020). Ultimately, the structure of the model will have a great influence on the predicted outputs. Direct observations of soil moisture, whether in situ or remotely sensed, can also play a large role in model improvements (Koster et al., 2009). Observations are used to test the outputs or models or can be used in data assimilation of reanalysis products to ensure models are consistent with what we know from observations themselves (Williams et al., 2009). The spatiotemporal scale of models also differs ranging from tens of kilometers to only a few kilometers and with temporal aggregation ranging from hourly to daily (Zheng et al., 2023). There is a desire in the scientific community to improve the resolution of these models to represent processes at the sub-kilometre scale globally (Clark et al., 2017). However, in order to do this, we will need greater understanding of the processes that drive soil moisture (and other variables) at these finer spatial scales. For example, soil structure can have a large impact on earth system modelling outputs, impacting routines that represent infiltration and runoff. Currently this is an underrepresented aspect of global earth system models and greater understanding of soil properties and how they influence moisture dynamics will improve future model iterations (Fatichi et al., 2020). An alternative technique for predictions is that given by machine learning, which are methods that can infer statistical and nonlinear relationships between predictor variables and target variables when trained on large volumes of collected data (Naqa and Murphy, 2015).

2.2.5 Machine Learning models

Distinct from empirical or physics-based models, machine learning models discover direct, albeit abstract, relationships between predictor and target variables. These are often called "black box models", as the inner workings are largely unknown even to the individuals who trained the model—a common critique of such models (Rudin 2019). Many options of machine learning architecture are available for predictions tasks, ranging from decision tree-based models to artificial neural networks (Ray 2019). A key benefit of machine learning is that although expensive to train, once a model has been trained, they can be relatively inexpensive to run, especially when compared to large scale empirical models (Rodrigues et al., 2018). For example, in climate models the computationally expensive process of resolving clouds at the sub-grid level has been successfully replaced with a deep learning processes, increasing model accuracy without costs to efficiency (Rasp et al., 2018). However, while they hold significant potential in addressing key questions, machine learning models also have inherent disadvantages. In particular machine learning models are far poorer when presented with data not seen in the original training dataset, the so called "extrapolation problem" (Reichstein et al., 2019). This becomes especially problematic when exploring the impact of climate change, which could potentially result in unprecedented environmental scenarios. Even so, there are a growing number of products to predict soil moisture using machine learning employing a plethora of different techniques. These include extending satellite data quality through data merging (Xu et al., 2018), downscaling satellite soil moisture data with machine learning (Srivastava et al., 2013), conversion of satellite raw data to soil moisture (Rodriguez-Fernandez et al., 2017), or directly predicting soil moisture using meteorological forcing values (Adeyemi et al., 2018). A recent study for producing a global product of soil moisture through long-short term memory models (LSTM) was published that used global in situ soil moisture data as a predictor (Oh and Orth 2020). When training their model, they used a large global dataset of soil moisture observations (see section 2.3.4), which came from many unique sensor types each representing distinct spatial scales. To account for differences in individual sensors, steps were required to harmonize the in-situ network by rescaling it to match a reference reanalysis land surface model dataset (ERA5-Land). The precise impact of such statistical harmonization steps, especially in such statistically driven models, warrants future study. This means access to a globally harmonized network of the same sensor types could support our understanding of this potential impact.

2.2.6 Soil Moisture Scaling

Despite its importance, soil moisture measurement remains challenging, especially considering the unique spatial scales represented by different measurement techniques. The measurement techniques described above each represent unique horizontal and vertical scales, ranging from point, to field, to satellite/model grid. The factors driving soil moisture values change depending on what scale we are considering, and this is shown within the context of the spatial scales different sensors represent in Figure 2.1. Controlling factors on soil moisture are generally dominated by soil structures at finer spatial scales and become more dominated by topography and land cover as the scales increase, eventually being mostly driven by meteorological drivers, such as precipitation patterns, at the coarsest spatial scales. For example, research has shown differences in the mean and standard deviation of soil moisture dynamics can occur in soils under similar climates, with differing structures (Wang et al., 2015). This suggests that soil moisture dynamics can change depending on the scale of soil moisture being measured, reflecting the variations in soil structure within the spatial range. Drivers of soil moisture dynamics also change in time, depending on whether it's under either wet or dry conditions (Grayson et al., 1997). Under wet conditions soil moisture is more susceptible to so called nonlocal controls, e.g., lateral, catchment scale drainage driven by topographic changes. Under dry conditions, vertical fluxes dominate spatial patterns of soil moisture which are more correlated with soil structure itself, which can be heterogeneous across the field or catchment. The differences in both absolute values and the controlling features of soil moisture across spatial scales leads to continued efforts to bridge this gap. For example, we often use ground-based point scale networks to validate global scale models or satellite remote sensing products, but the differences between the soil moisture scales being represented by each means methods of bias correction and upscaling (from in situ to a coarse grid) are often implemented to compare the two (Crow et al., 2012). The best practices for validating coarse-scale satellite remote sensing data against point scale observations are continually being refined, with future research areas, including understanding the impacts of rescaling efforts, identified as crucial (Gruber et al., 2020). Continued research is necessary that better allows us to downscale coarse satellite remote sensing to better represent field scale, root-zone soil moisture dynamics (Peng et al., 2017). Better representation and understanding of soil moistures impact on hydrological systems at the sub-kilometre scale is necessary in the push towards hyperresolution global land surface models (Wood et al., 2011). To achieve this, we will require access to large quantities of in situ data across various hydroclimates, allowing us to develop methods that merge the global coverage of satellite and model sensing with the field-scale dynamics of in situ sensors.

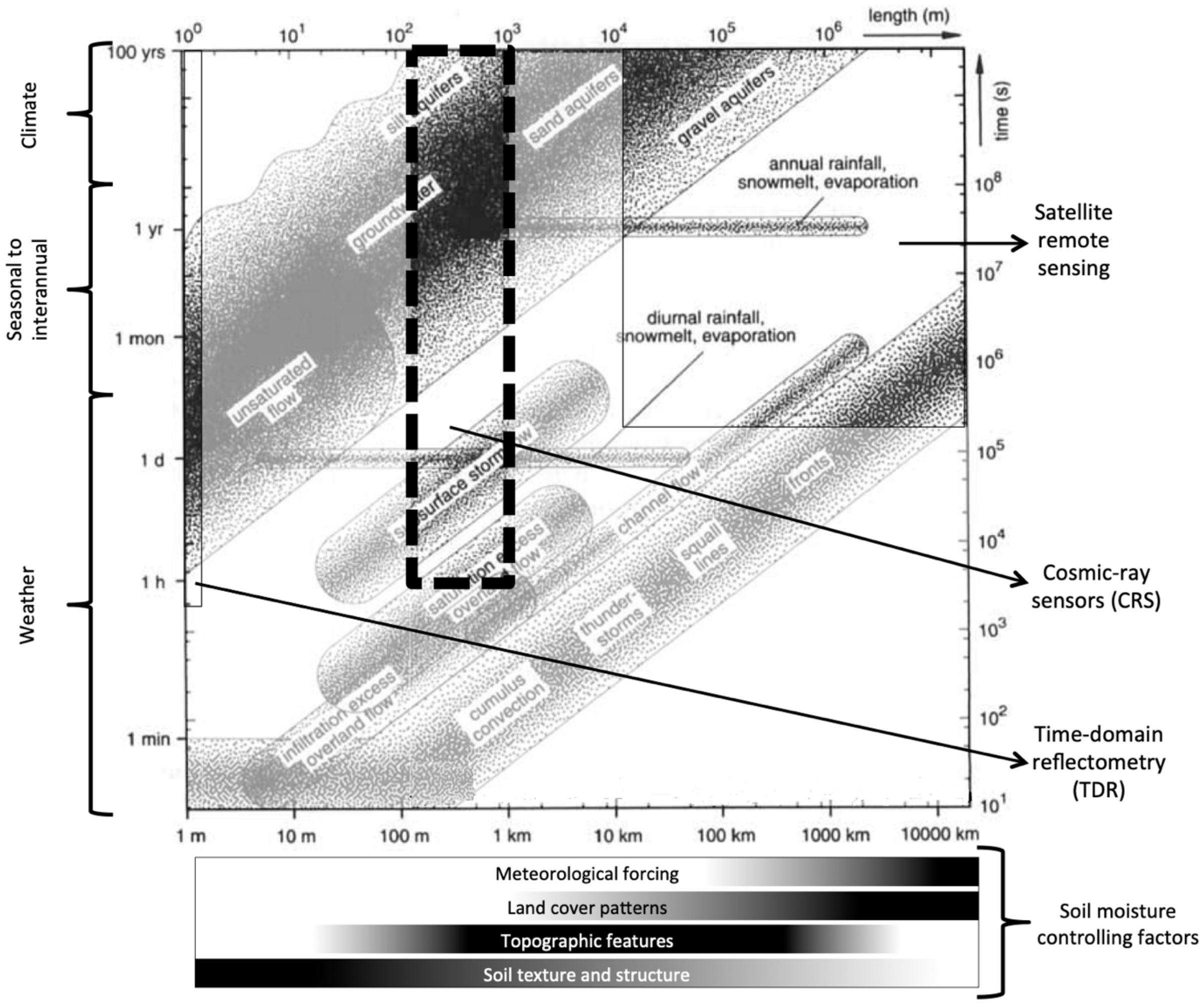

Figure 2.1 Key processes influenced by soil moisture and their dominant spatial and temporal scales. Clear areas represent available data from specific sensor types outlined above. The dashed box highlights the spatiotemporal coverage of CRNS. The main controls of soil moist are shown in the bottom with darker shading representing dominant spatial scales. Adapted from Blöschl and Sivapalan 1995 and Crow et al., 2012. Credit: Rosolem (2020)

2.3 Large Sample Hydrology and Soil Moisture

The previous subsection highlighted soil moisture's key role in earth system processes and discussed various methods to measure and predict it. This subsection will explore the potential of enhancing our understanding of soil moisture and its wider influence on the environment, using these continually growing soil moisture datasets, with an emphasis on the promise held by CRNS soil moisture networks. A description will be given describing the concept of large sample hydrology and why it is of interest to the hydrology community. Next, a review of current large sample hydrology datasets will be given, shedding light on both their achievements and challenges. Finally, the focus will be directed to soil moisture networks, their current limitations, how the CRNS networks can provide an opportunity for future studies and describe how this thesis will support this goal.

2.3.1 What is Large Sample Hydrology?

Large Sample Hydrology is a branch of hydrology that harnesses increasingly large datasets to expand our understanding of hydrology across different temporal and spatial scales (Gupta et al., 2014). As climate change continues to reshape global water resources, it is crucial to understand the differences between catchment specific characteristics and more universal behaviours. Large sample hydrology, through its use of big data, provides a robust approach for such differentiation. Given this, large sample hydrology is an increasingly important area of research. It holds the promise of enhancing our hydrological understanding, enabling us to create more dependable models that can accurately predict hydrological processes from local to global scales.

Large sample hydrology can be traced back to the research area of comparative hydrology (Gupta et al., 2014). At its core, comparative hydrology focuses on knowledge transfer between catchments across the globe (Falkenmark and Chapman, 1989). The aim of comparative hydrology is to identify sites by their similarities, be it climatological, ecological, or physiological, and to transfer acquired knowledge between catchments. More pointedly it is trying to understand when we can reasonably transfer our understanding of well gauged and studied catchments to others, when we might expect differences, and ultimately what drives those differences. Examples of such studies include examining how catchments with apparent similarities react differently to hydrological events (Woo and Liu, 1994, Araújo and Piedra, 2009, Gaál et al., 2012, Singh et al., 2014) or exploring the effects of land use changes on similar catchments, offering insights into fundamental processes behind events like floods or droughts (Burch et al., 1987, Rangecroft et al., 2019, Van Loon et al., 2019). An early goal of comparative hydrology was evaluating the appropriateness of transferring our knowledge and understanding from the predominantly temperate climates of Europe and the USA, where most early hydrologic studies were conducted, to other regions across the globe (Gupta et al., 2014). In other words, the aim was to determine the extent to which hydrological models and concepts developed in temperate zones can be applied across more diverse climatic and environmental conditions across the globe. Critically, the success of such comparisons centres on accessing a vast and varied pool of catchments for analysis.

Gupta et al., (2014) aptly sub-titled their review of large sample hydrology "*a need to balance depth with breadth*", which succinctly describes one of the key problems in large sample research. Historically, hydrology research was constrained to the catchment scale due to limitations in data and computation, allowing for in-depth exploration of catchment characteristics. Comparative hydrology emerged from this focus, seeking to transfer knowledge from one catchment to another, identifying which hydrologic responses were particular to certain catchment types, and which were more universal. While sharing objectives with comparative hydrology, large sample hydrology aims to create robust and generalized principles through the examination of large and broad datasets covering numerous catchment types, rather than isolated, in-depth studies (Addor et al., 2019). The overarching goal is to develop enough of an understanding of hydrological processes that models can be developed spanning all terrestrial ecosystems at multiple spatial and temporal scales. This can help us to tackle the goal of accurate predictions of key environmental variables in ungauged basins, as it is practically impossible to have networks of in situ sensors available in every location globally (Sivapalan 2003). With increasing access to global data, the path is open to move towards finer resolution sub-kilometre global models, vital for water resource planning and assessing climate changes impact on ecosystem function (Wood et al., 2011, Bierkens, 2015). However, this advancement hinges on the scientific community's access to long-term records at diverse spatial and temporal scales, a crucial factor in understanding environmental dynamics worldwide. Given the need to deepen our understanding of global Earth system dynamics and the growing amount of environmental data, numerous initiatives have arisen to facilitate big data type studies in this area.

2.3.2 Early initiatives from “Traditional” hydrological applications

If we aim to discover generalizable findings in hydrology, it is crucial to have access to comprehensive and good quality datasets. Addor et al., (2020) describes currently available datasets in hydrology, with an emphasis on streamflow data. In their review they addressed potential issues within large sample hydrology datasets, which affect their suitability for certain applications, as well as outlining future solutions to improve them. One of the key identified issues is a lack of common standards, leading to difficulties in comparing two catchments that happen to be from different collections of data. The impact can come from something as simple as different variable naming conventions to differences in the processing or quality control steps which will impact the actual values being investigated. With different naming conventions a need for additional steps to format data, whilst unnecessary, is fairly easily addressed. Different processing methods however can be much more difficult to correct. Such adjustments would involve additional data processing, requiring time and expertise, possibly impacting the perceived value of the dataset if the time and effort required for corrections is seen as too costly.

Take for example the growing availability of Catchment Attributes and MEterology for Large-sample Studies (CAMELS) datasets which began as a collection of 671 small to medium sized basins across the USA (Newman et al., 2015). The dataset combined streamflow data, along with meteorological forcing data such as temperature and precipitation, to facilitate large sample hydrology type studies. The meteorological data for CAMELS-USA was sourced from Daymet, a gridded product that covers the Conterminous United States (Thornton et al., 2021). Whilst gridded products are less accurate than in situ measurements, they provide a good alternative when local ground-based sensors are unavailable. Since the release of the CAMELS-USA dataset, other regional datasets have been created that replicate the overall goals of the original. There are now CAMELS datasets covering Great Britain (Coxon et al., 2020), Australia (Fowler et al., 2020), Brazil (Chagas et al., 2020), Chile (Alvarez-Garreton et al., 2018), and more recently France (Delaigue et al., 2022). However, data interoperability remains challenging due to regional datasets relying on different meteorological sources. For instance, CAMELS-GB uses CEH-GEAR for precipitation data (Keller et al., 2015), which differs from the CAMELS-USA choice of Daymet. The choice of precipitation forcing data source has been shown to influence outputs in hydrological modelling, leading to potential sources of uncertainties between the regional datasets (Try et al., 2020). This means that when comparing catchments from two different datasets the forcing data may be influencing outcomes that are down to the behaviours of the specific products used rather than actual catchment dynamics. This can lead to an additional layer of uncertainty for researchers.

Tackling this regionalization, the recently published Caravan (a collection of CAMELS datasets) dataset addresses interoperability issues of individual CAMELS datasets by making a so-called network of networks (Kratzert et al., 2023). The Caravan dataset takes previously published regional datasets and standardises them into single worldwide dataset. They standardised the naming conventions, data formats and the meteorological forcing data, with meteorological data now all being derived from the ERA5-Land model (Muñoz Sabater et al., 2021). The Caravan dataset consists of 6830 catchments across the globe covering a wide range of hydroclimates making it a rich resource for large sample type studies. Alongside the dataset publication, the software used for the data processing was released and development continues open source, allowing researchers to see exactly the steps being taken during the data creation, as well as providing the ability to easily add more sites in the future. Standardisation supports global studies, however the route to a standard dataset remains debateable. Caravan uses a single product (ERA5-Land) from which to collect ancillary data, for example precipitation data. Whilst this standardises the source of data, the quality of the data may still differ which will be attributed to the quality of the chosen model at points across the globe. Gridded products, such as ERA5-Land do not perform uniformly well across geography (You et al 2014), hydroclimates (Gomis-Cebolla et al., 2023), or seasons (Dinku et al., 2008). This means there remains a balance between uniformity and accuracy that requires ongoing study and debate. For example, is it more important to ensure consistent datasets (i.e., a single source product), or accurate datasets (i.e., regionalized data that purports higher accuracy). It has been shown that high-quality regional datasets may be preferable in hydrological models by providing higher accuracy predictions, over models driven by gridded products. (Naha et al., 2023). Attempts to benchmark the observation uncertainties in the multitude of available products may serve as a solution to this by providing a better understanding of data quality (McMillan et al., 2012). This could lead to harmonization efforts that try to harmonise to performance and uncertainties rather than source, although more research is necessary to better understand this. Even so, the Caravan dataset serves as a prime example of the path towards combining individual networks to expand the scope of global research.

2.3.3 Large sample hydrology - beyond hydrology

An earlier harmonisation project, preceding the CAMELS datasets, is associated with the eddy covariance community. Eddy covariance towers, which measure water, carbon, and energy fluxes at the land-atmosphere boundary, require complex post-processing steps to convert the measurements into data of broad interest to the earth system science community (Baldocchi 2003, Papale et al., 2006). The absence of a standardised methodology will lead to inconsistencies between the sensors across the globe, owing to the varied interpretation methods. For example, gross primary productivity quantifies the amount of carbon sequestered by plants from the atmosphere. It is determined by partitioning net ecosystem exchange – the total atmospheric carbon flux, into gross primary productivity and ecosystem respiration, a measure of carbon egressed into the atmosphere through respiration. Different methods to derive ecosystem respiration have shown different sensitivities to long term temperatures leading to differences in outputs >25% over a year (Reichstein et al., 2005). Consequently, if sensors are processed through different algorithms, then these differences may be accidently attributed to catchment dynamics rather than process differences. The AmeriFlux network, established in 1996 as a coalition of individual sites across the Americas, aimed to expand the impact of these sensors by pooling them together into a larger network (Novick et al., 2018). AmeriFlux's bottom-up organizational approach permits the fusion of independently operated sites, initially selected for particular research aims, into an extensive network suitable for large sample studies. This method's strength lies in its adaptability, facilitating the merging of diverse projects with wide-ranging objectives and funding sources. However, this approach isn't without drawbacks. One criticism is that it allows each site to establish their own operational standards, resulting in variations between the sites within the network. For example, whilst many sites include point scale soil moisture sensors such as Time-Domain Reflectometry (TDR) within the sensor footprint, the number and spread of these sensors varies widely, ranging from multiple profiles of soil moisture sensors to none. This lack of standardisation can impact the comparability of sites in certain types of studies, especially when sensors are missing entirely from otherwise valuable locations.

Several regional networks of eddy covariance towers have been developed over the years, including EuroFlux (Aubinet et al. 1999), OzFlux (Beringer et al., 2016) and Asia-Flux (Mizoguchi et al., 2009). Whilst the community of researchers operate collaboratively, regional networks will again have their own operational standards which may be influenced by internal research requirements and funding bodies. To address this, FLUXNET, an international network comprising of many regional networks of eddy covariance towers, was established to facilitate global scale studies of carbon, water, and energy fluxes (Baldocchi et al., 2001). Like AmeriFlux, FLUXNET uses a bottom-up approach where networks or individual sites can join by sharing their data to the overall project, with the emphasis being on standardising the methodologies used in post-processing data. This ensures the production of a harmonised dataset that covers the globe, facilitating global scale studies. FLUXNET periodically produces and publishes fully processed data releases, meaning a user can be confident that all the data contained within it are processed to the same quality standards (Pastorello et al., 2020). Alongside the dataset, the open-source software used to create it, ONEFLUX, was released (Pastorello et al., 2020). This transparency allows users to understand data processing steps and offers scientists the avenue to recommend enhancements for subsequent versions. Combined dataset production along with detailed instructions on the steps towards the dataset creation will be important as datasets grow in both availability and complexity.

2.3.4 Large sample hydrology and soil moisture

In addition to large sample datasets in hydrology and ecohydrology, large datasets for soil moisture are essential, given its role in both terrestrial and atmospheric processes. The International Soil Moisture Network (ISMN) was established in 2009, serving as a platform for hosting in situ soil moisture datasets from across the globe (Dorigo et al., 2011). Its design follows that of the FLUXNET project, with data provided by individual networks and researchers, and then compiled, processed, and published online by the ISMN. This centralized repository ensures that datasets from many different organisational teams are searchable and findable, thereby enhancing prospects for comprehensive studies on soil moisture and its overarching influence on earth system science. By 2021, the ISMN's significance is underscored by its reference in over 100 scientific publications and its boasting of 2842 stations worldwide (Dorigo et al., 2021). Whilst the dataset is open and findable, ensuring standardization across sensors and networks poses a significant challenge. This complexity is heightened given the myriad of sensor types that the ISMN incorporates from different networks. As previously discussed in this chapter, soil moisture measurements are typically inferential. The intrinsic attributes of each sensor type can introduce variability in soil moisture estimates. Research has shown that absolute values between sensors can differ and may not be transferable between sites (Leib et al., 2003). As such, these values may not always be transferable across sites, thereby creating additional uncertainty in certain metrics, especially those reliant on absolute values. This means that whilst the ISMN provides an opportunity for large sample type studies, additional rescaling steps are sometimes necessary to account for the different sensor types when attempting to use the entire network of sensors available (e.g., O and Orth 2021). The impact of such rescaling on the overall outcome of studies remains uncertain and warrants further investigation. The ability to organise standardized networks of sensors across the globe is restricted by the myriad sources of funding that would be required to implement such projects. This does not, however, prevent large regional networks from being implemented that can attempt to solve the above-described issues. In the United States there is the North American Soil Moisture Database (NASMD, Quiring et al., 2016) as well as the more recent National Coordinated Soil Moisture Monitoring Network (NCSMMN, Cosh et al., 2021, Baker et al., 2022). The NCSMMN was itself borne of National Integrated Drought Information System (NDIS), who's specific goal is to improve access to soil moisture information for natural resource assessment and hazard management. A key aspect of this goal is to coordinate strategies for data management, merging in-situ sensors with remote sensing or modelled soil moisture data, and expanding sensors into areas clearly identified as missing from the current network. Coordination on this scale is more likely possible with regional networks, however the benefits will be extended to global datasets such as with the ISMN. The ability to merge soil moisture data from multiple spatial scales will require understanding of how such spatial scales interact. A harmonized network of soil moisture sensors, comprising of the same sensor types (and spatial scales) and spanning diverse landscapes, could serve as an additional opportunity to answer questions surrounding soil moistures influence on earth system processes.

2.3.5 COSMOS networks as opportunity

In this respect, the CRNS offers a unique opportunity to combine the growing collection of sensors across the globe, into a single harmonized dataset, for testing large sample soil hydrology questions. Regional networks of CRNS have been expanding across the globe since 2012. The first network to be installed was the Cosmic Ray Soil Moisture Observing System (COSMOS) (Zreda et al., 2012). This network comprised of over 50 sensors, primarily located in the USA, but with additional sites in Brazil, Kenya, and Europe. Designed for long-term monitoring, these sensors transmit data to a centralized database via iridium satellite. They're strategically located to represent varied hydroclimates across the USA. The data, from raw readings to corrected soil moisture values, is publicly accessible (http://cosmos.hwr.arizona.edu/, last accessed: 02/06/2023). Subsequent networks emerged in Germany under the Terrestrial Environmental Observatory (TERENO) initiative (Bogena et al., 2006, Zacharias et al., 2011) and Australia with the growing CosmOz network (Hawdon et al., 2014). The UK's COSMOS-UK has installed over 50 sensors since 2013 (Cooper et al., 2021) and has also worked closely with researchers in India to help establish an Indian COSMOS network (Upadhyaya et al., 2021). More recently the International Atomic and Energy Agency (IAEA) has begun installing a network of CRNS sensors in locations across the globe that have been less well monitored in the past, including sites in Oman, Kuwait, Ethiopia, Morocco, Bolivia, and Peru to name a few (https://crnslab.org/, last accessed: 02/06/2023). Besides these major networks, there exist standalone sites and smaller networks globally, including in China (Tan et al., 2020), and Nebraska (https://crnslab.org/, last accessed:

02/06/2023). Furthermore, a collection of European sites recently became the COSMOS-EUROPE network, harmonising data processing methods across 66 sites spanning the European continent (Bogena et al., 2022).

One thing is clear, the CRNS is evolving into a global sensor network, offering hourly soil moisture readings over extended periods, with some sensors having accumulated over a decade's worth of data. However, there remains issues in data harmonization between networks that has yet to be addressed fully. As understanding of the neutron signal has evolved, so too has disparities between the processing methods of each network. Chapter 3 will explore the impact of these disparities, alongside prospective solutions, and tools. One key advantage of global CRNS is the potential for uniformity in calibration and processing, similar to that seen with eddy covariance towers. While the counting rate varies between sensors due to environmental or sensor-specific factors, with evolving research, we are uncovering ways to standardize and correct these variances allowing a more harmonized network of soil moisture sensors (Schrön et al., 2017, Iwema et al., 2021). However, efforts towards a more globally complete networks will require collaboration amongst all the networks currently involved, as well as the development of tools like ONEFLUX (Pastorello et al., 2020), which facilitate the processing of data in a harmonized and open way. Ultimately, a globally harmonized dataset paves the way for increased understanding of Earth system sciences, deepening our grasp of soil moisture's pivotal role in global earth system dynamics.

2.3.6 Opportunities of harmonized soil moisture data

A central aim of large-sample hydrology studies is to derive generalizable hydrological principles, aiding in model predictions in ungauged basins. Large datasets are essential for this goal, enabling rigorous testing across diverse catchments and hydroclimates. One such method to test robustness in our ability to predict environmental states is multiple hypothesis testing, through which revised model structures are tested to understand if our current presumptions are true for the wide range of hydrological catchments globally (Clark et al., 2011). This approach extends to testing modular components of models, such as those proposed in the Framework for Understanding Structural Errors (FUSE) (Clark et al., 2008). These approaches help us understand errors arising from the model structure. A related issue is discerning whether uncertainties in outputs arise from model structure or observational data (McMillan et al., 2021). By minimizing potential sources of observational uncertainties, such as those from processing differences, or alternatively at least understanding the uncertainty present, we can increase our confidence in attributing differences of predictions and test data to model structure and hypothesize improvements for future versions.

Additionally, when testing model performance, large sample datasets are often used as ground truth data. Model parameters are then fine-tuned by comparing how a model performs on some portion of the data and adjusting the parameters to reduce the difference between simulated and observed values. A common metric used is the mean squared error (MSE), which statistically describes the discrepancy between the actual and simulated values. It is important to understand that MSE comprises three distinct sources of error: bias (systemic over or under prediction), variability (the degree of variation), and correlation (the degree to which simulated and observed values change together). The interaction of these sources of error has been discovered to lead to the underestimation of variability when it is used as a performance metric the model is trying to adjust for (Gupta et al., 2009). As the errors are squared, large outliers can lead to greater penalization, and so the model is encouraged to underestimate variability. This has led to increasing interest in alternative ways to identify if a traditional model is working as desired through the use of hydrological signatures rather than through statistics such as MSE (McMillan 2011). Hydrological signatures are methods to define responses at catchments, for example, the response lag time between precipitation and streamflow discharge. These signatures offer alternative methods of understanding whether a model is representing the overall system response to changes and have been used to demonstrate functional differences between catchments (McMillan et al., 2022, Mathai and Mujumdar 2023). Whilst much research in this area has been more focused on streamflow signatures (Gnann et al., 2021), there are increasing efforts to expand this concept to soil moisture signatures (Branger and McMillan 2020, Araki et al., 2022, Araki et al., 2023). It is arguable that the move to a more signature-based analysis will necessitate even greater focus on sensor harmonization. Earlier in this review were descriptions of the different soil moisture sensors and how they uniquely infer soil moisture. If responses to changes differ due to inherent issues from the technology, comparing sensors could lead to false interpretations. For example, soil structure changes have been shown to impact measurements using the TDR sensor (Rothe et al., 1997), whilst wetting and drying cycles have been shown to change soil structure itself (Diel et al., 2019). This indicates that sensor readings may vary across catchments over time due to technological peculiarities. This point is less about the specific issues of TDR sensors and more a point that this may introduce structures into the data that are not present in other sensors. This includes the possibility that systemic issues from other sensors will also not be apparent in TDR sensor values.

2.4 Concluding the goals of this thesis.

Soil moisture plays a pivotal role influencing ecosystem functioning. Whilst projects such as the ISMN network are important and valuable to the community, there is an argument that differences between the sensors within the network leads to potential issues in large sample hydrology type studies. The CRNS represents a growing global resource that provides information of a key spatial and temporal scale of soil moisture, which has the potential to act as a harmonized network such as those already found through FLUXNET. Increasingly, we are realizing the need to extend soil moisture networks to places that are currently underrepresented and yet highly influenced by changes in soil moisture in the environment (Bassenbacher et al., 2023). To achieve this goal, however, will require tools and methods of harmonization and studies that help us understand the data we already have as well as where we might be missing data for future network design. A harmonized network, spanning many different hydroclimates will help facilitate improved understanding of soil moistures influence on global earth system dynamics. This thesis will fill this research gap in three ways:

1) Development of a community tool for processing and harmonising CRNS with the most recent understanding along with ancillary processes to collect metadata describing sites from available global products. Additionally, the tool will be used to understand the impacts of different methods of processing.
2) This newly harmonised global CRNS dataset will serve as an opportunity for large sample studies. A meta-analysis of global sites, along with direct comparison of soil moisture values to modelled and satellite soil moisture data to understand residual differences between this in situ network and global gridded products will be presented.
3) With the increasing application of Machine Learning in earth system science, the choice of input data becomes crucial. Given that soil moisture sensors vary in their output and scale, this research will explore the impact of different soil moisture representations, with an emphasis on the impact of representative scales, in a machine learning model predicting surface fluxes of energy and carbon.

3 Cosmic-Ray neutron Sensor PYthon tool (crspy 1.2.1): an open-source tool for the processing of cosmic-ray neutron and soil moisture data

Power, D., Rico-Ramirez, M. A., Desilets, S., Desilets, D., and Rosolem, R.: Cosmic-Ray neutron Sensor PYthon tool (crspy 1.2.1): an open-source tool for the processing of cosmic-ray neutron and soil moisture data, Geosci. Model Dev., 14, 7287–7307, https://doi.org/10.5194/gmd-14-7287-2021, 2021.

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3.1 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); 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 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 (~40 km resolution) and temporal (~3 d) scale, and at much shallower depths (~5 cm) (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 for the improvements of farming practices (such as through the process of irrigation scheduling); thus, there is a need 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 that we require measurements at a finer spatial resolution, on the order of sub-kilometre scales (Wood et al., 2011). Bierkens et al. (2015) discussed the implications of moving from a more standard resolution ~50 km model to a hyper-resolution model at the sub-kilometre scale. The study further discussed the need to move from sub-grid paradigms, which represent a conceptualised form of Earth system dynamics from within the standard 50 km resolution model, to explicit dynamics of Earth system processes at scales <50 km. This requires a 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 (CRNSs) are a relatively new technology that allows estimates of soil moisture at the field scale (~600 m diameter) at an 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) (Eq. 1). The original equation along with the above-mentioned advancements provides us with estimates of volumetric soil moisture:

$$\theta_{vol} = \left[\frac{a_0}{\frac{N_{raw} \cdot f_p \cdot f_i \cdot f_h \cdot f_v}{N_0} - a_1} - a_2 - LW - WSOM\right]\frac{\rho_{bd}}{\rho_w} \qquad (3.1)$$

where θ_{vol} is volumetric soil moisture (cm^3 cm^{-3}); a_0, a_1, and a_2 are coefficients obtained from neutron particle physics modelling (Zreda et al., 2008; Desilets et al., 2010) and are assumed to be constants; LW is the lattice (chemically bounded mineral) water (g g^{-1}); $WSOM$ is the water equivalent of soil organic carbon (gram of water per gram of soil); ρ_{bd} is the bulk density of the dry soil (g cm^{-3}); ρ_w is the density of water defined as 1 g cm^{-3}; N_{raw} is the measured raw, uncorrected, neutron count identified over the given integration time, usually set to 1 h; f_p, f_i, f_h, and f_v represent correction factors for air pressure, incoming neutron intensity, atmospheric water vapour, and above-ground biomass respectively that are applied to N_{raw} to account for additional influences on the neutron signal other than soil moisture; and 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 last term is unique to each site and is found through the calibration process, explained in detail in Sect. 2.2.

The detection of background neutrons in the atmosphere, as a method to infer estimates of field-scale soil moisture, was first 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 Eq. (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 USA, leading to the Cosmic-Ray Soil Moisture Observing System (COSMOS) (Zreda et al., 2012).

After the establishment of the first national-scale network in the USA (Zreda et al., 2012), other countries such as Australia (Hawdon et al., 2014; McJannet et al., 2021), Germany (Zacharias et al., 2011; Bogena, 2016), and the UK (Evans et al., 2016; Cooper et al., 2021) established their individual national networks, as well as additional sensors located in smaller networks or individual sites. Sensors from these networks have, in some cases, been running for up to 10 years and can provide potentially valuable information for the understanding of soil hydrology. As these networks have grown so has the literature surrounding best practices for the 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 a consequence of improvements to the signal correction and sensor calibration, a divergence in methods is noticeable between different networks. Each network inevitably implements its own protocol when correcting the neutron signal to give soil moisture estimates, leading to a less harmonised data set among networks. This is in part due to the difficulties that would be encountered in quickly changing data processing pipelines within already established databases. The benefit of such structures is that live data are available to stakeholders through online portals. Unfortunately, the interdependencies of a database mean that it does not lend itself to quick changes; thus, a post-processing method could alleviate some of these issues.

This lack of a harmonised global data set can ultimately lead to limitations in the global assessment of this technology from multiple CRNS networks. Discrepancies in processing methodology can leave questions around the information obtained and the uncertainty propagated from the 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 of the recommended correction steps, the estimated soil moisture products from these sensors or even networks can be seen as suboptimal, potentially undermining their true value. An example of the impact of evaluating with sub-processed cosmic ray soil moisture data is found in Dirmeyer et al. (2016). CRNS data from the COSMOS network were compared with both alternative in situ soil moisture instruments and land surface models. The CRNS data used in this study did not apply the atmospheric water vapour correction at the time and so can be considered less accurate than they otherwise should be. There is a consensus to follow certain 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 or, 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 $cm^3\ cm^{-3}$ at a site at Park Falls, USA. Additionally, Hawdon et al. (2014) demonstrated the different approaches available for correcting neutron counts for incoming cosmic-ray intensity and showed that there is a noticeable difference in neutron counts and ultimately soil moisture depending on the chosen method. Schrön et al. (2017) provided an improved approach to CRNS calibration, demonstrating that their revised approach improves the accuracy of soil moisture estimates. Using UK sites as an example, Schrön et al. (2017) found that the root-mean-square error (RMSE) of soil moisture estimates from the CRNS was reduced from 5.3 % vol, using the conventional calibration approach, to 1.4 % vol, using the revised calibration approach. Improvements in accuracy were identified at all of the sites that they analysed. Although this revised approach is being adopted in more recent studies (Cooper et al., 2021), this is not always the case (such as the original sites in the COSMOS network) and can mean that sites in different networks have been calibrated using different methods.

In order to mitigate this ongoing issue of lack of harmonisation in the soil moisture estimates from the CRNS technology, we 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. Section 2 will also describe the site metadata creation process, which is an additional aspect to crspy that is built to facilitate the data analysis of many sites. Section 3 will discuss the implications of differing processing methodologies on soil moisture estimates, as well as the benefits of creating detailed metadata for post-processing analysis.

3.2 The crspy tool

The Cosmic-Ray neutron Sensor PYthon 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 harmonised 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 harmonised data set. 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 the creation of a best practice, as this will allow for the comparison of sensor data 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 any new understanding of the CRNS technology, as well as a teaching tool for the community.

Figure 3.1 is a visual representation of the processes within crspy that convert 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 Supplementary below). Additionally, to organise the various input and output data sets, 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 `crspy.initial(wd)` function, where `wd` is a string representing the working directory location.

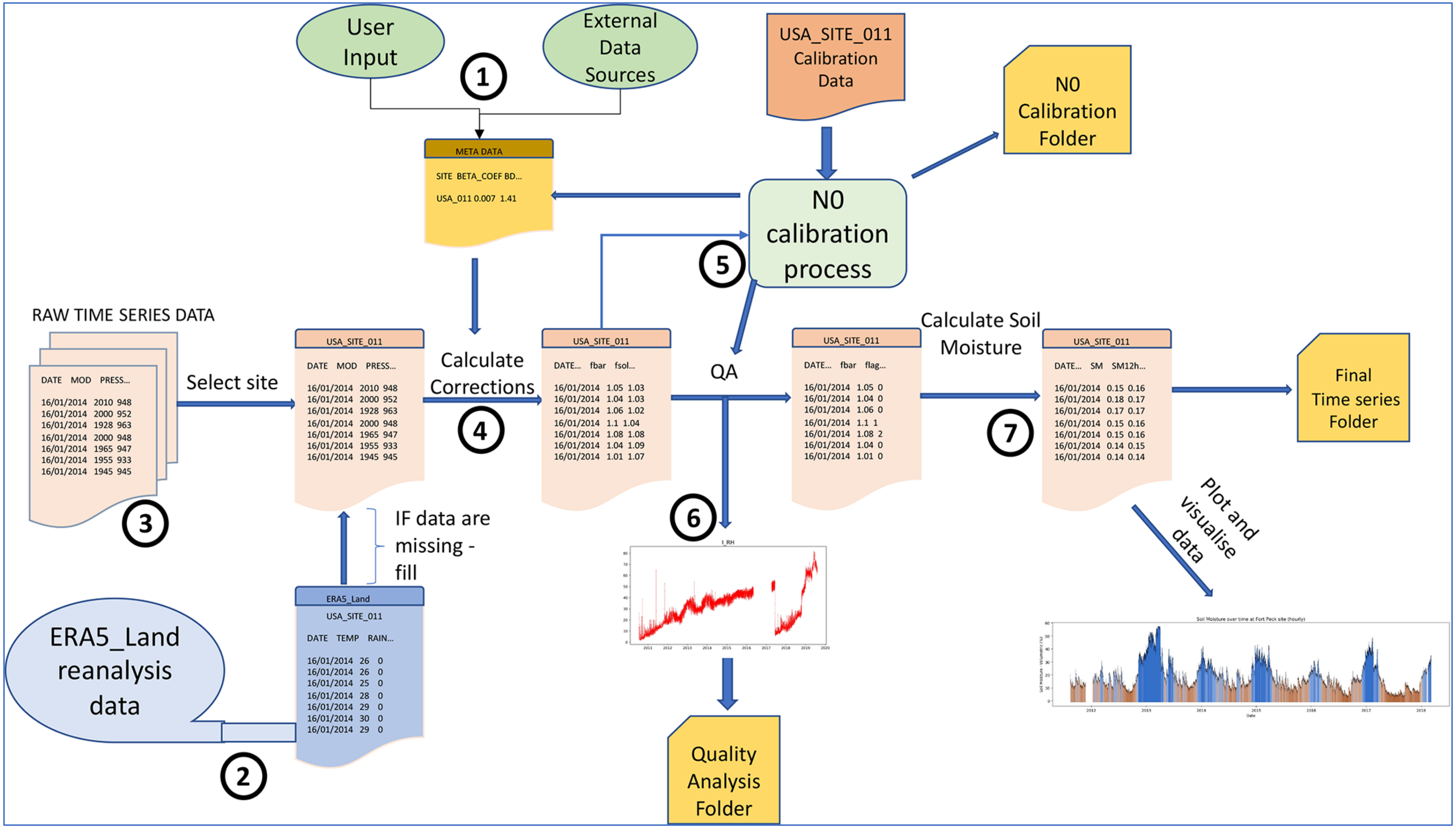

Figure 3.1 The structure of crspy, demonstrating all of the modules that are used in creating soil moisture estimates. Number 1 represents the metadata table, which is a collection of site descriptors, e.g., soil texture and site elevation (see Sect. 2.4). Numbers 2, 3, and 4 correspond to gap filling with ERA5-Land data, data tidying, and the computation of correction factors, respectively (see Sect. 2.1). Number 5 represents the calibration process, if this option is selected (see Sect. 2.2). Number 6 highlights the quality assessment steps undertaken (see Sect. 2.3). Finally, number 7 represents the step where soil moisture estimates are calculated from the neutron counting rates (refer to Eq. 1)

3.2.1 Data processing and correction

To obtain soil moisture estimates, we need to apply Eq. (3.1) 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, as 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 `config.ini` file, which stores constant values for crspy.

Site Specific soil properties

The site-specific soil parameters described in Eq. (1) are LW, $WSOM$ (obtained from soil organic carbon), and ρ_{bd}. Due to the open data policies of many of the CRNS networks, these data are usually available online (see the "Data availability" section). These values should be defined prior to running the main crspy function and are stored and read from the metadata file.

The LW parameter 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 overall impact on the neutron count rate. This value is usually obtained through the analysis of soil samples taken from the footprint of the site sensor (Franz et al., 2012). The $WSOM$ parameter represents the water equivalent of soil organic matter (g cm^{-3}). Soil organic carbon (SOC) is obtained through the 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 and provided a method for this (Eq. 3.2). This is completed on the assumption that organic matter in the soil is cellulose and means that proportionally the water equivalent of this can be found as follows:

$$WSOM = SOC \,.\, 0.556 \tag{3.2}$$

The ρ_{bd} parameter represents the dry-soil bulk density ($\mathrm{g\,cm^{-3}}$) and is a site-specific static value. It is obtained through the 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 are unavailable for a site, crspy includes the option to obtain this value from the global data source SoilGridsv2 (see Sect. 2.4). In the case of missing data, crspy takes advantages of built-in routines to fill out the information. In that case, if ρ_{bd} or SOC (used to calculate $WSOM$) are missing, crspy will use the estimates collected from SoilGridsv2, which are assembled in the metadata process. If LW is unavailable, a value of zero can be input into the metadata table by the user. Past studies have also demonstrated techniques to estimate LW using soil clay content, which could be used to provide estimates that can be input to the metadata table (Avery et al., 2016; McJannet et al., 2017). 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 Sect. 2.2.

Time-varying values and correction methods

The remaining values required to obtain θ_{vol} are N_{raw} and f_p, f_i, f_h, and f_v, which all vary with time. It is ultimately the relationship between N_{raw} and N_0 that gives us the 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 1 h 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 Eq. (3.1). Changes in atmospheric pressure impact the neutron counting rate; the f_p term corrects for this so that $N_{\mathrm{raw}} \cdot f_p$ 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; thus, 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 that 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 first implementation of this technology, with additional sources of 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 of 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 are unavailable from in situ site sensors, ERA5-Land (Muñoz Sabater, 2019) data are used to replace missing sensor data. ERA5-Land is a data set, based upon the ERA5 reanalysis data and provided publicly by the European Centre for Medium-Range Weather Forecasts (ECMWF), that combines modelled data with real-world observations, resulting in a gridded, global hourly product at a 9 km resolution. Previous iterations of the ERA reanalysis data sets (such as ERA-Interim) have proven useful for other global networks for the task of gap filling missing data, such as in the FLUXNET community (Vuichard and Papale, 2015). We implement a similar approach to that used by the FLUXNET community in crspy and, consequently, to the global CRNS database, as we envision the potential of 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 lead to a better understanding of land–atmosphere interactions at the field scale (e.g., Iwema et al., 2017). It is important to note that although the resolution is spatially coarser when compared with CRNS sites, the ERA5-Land data set was chosen as a source for replacing missing sensors for three main reasons: (1) it covers the lifetime of all of the CRNS sites around the world, which ensures that all historical data can be used for gap filling if necessary; (2) the data set is produced at an hourly resolution, which matches the standard resolution of CRNS sites; (3) it is an open data source, which aligns with our desire to develop a full open-source tool for CRNS data processing.

The ERA5-Land data set includes key variables such as precipitation, temperature and dew point temperature which can be used to correct for influences on the neutron signal, such as the impact of atmospheric water vapour on neutron count rates. Hence, we can use dew point 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 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 with 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 CRNSs (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 following equation:

$$f_p = \exp\left(\beta(p - p0)\right) \tag{3.3}$$

where f_p is the pressure correction factor (defined in Eq. 3.1), β is a coefficient to account for mass attenuation length at 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 β 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 (2021).

(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 data from the Neutron Monitor Database (NMDB; available online), which comprises a collection of neutron monitoring sites from around the world. The NMDB provides neutron counting rates at an hourly resolution from monitoring stations around the world, and its data are considered the official distribution from each site principal investigator. The correction method currently varies across networks. For example, COSMOS (USA) originally corrected the data by comparing neutron intensity to a predefined reference date, which, in that case, was to be 1 May 2011. The Jungfraujoch neutron monitoring station in Switzerland was used as a reference site. The calculation for the incoming neutron intensity correction factor is as follows:

$$f_i' = \frac{I0}{Im} \tag{3.4}$$

where Im is the incoming cosmic-ray intensity at the sensor measurement time, $I0$ is incoming neutron intensity at the decided reference date, and f_i' is used here to define this particular incoming cosmic-ray intensity correction factor (in order to avoid confusion with f_i from Eq. 3.1).

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:

$$Rccorr = -0.075(Rc - Rcjung) + 1 \tag{3.5}$$

Here, 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 as follows:

$$f_i = (f_i{'} - 1)Rccorr + 1 \tag{3.6}$$

Ultimately, f_i is similar to f_i' but contains an additional correction to account for the difference in cut-off rigidity between the CRNS site being processed and the Jungfraujoch neutron monitoring reference site.

The Australian CosmOz network employs a different approach that does not always use the Jungfraujoch as the reference monitoring station. Instead, this network changes the reference station based on the station that 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 Eq. (3.4).

(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):

$$f_h = 1 + 0.0054 \times \rho v \tag{3.7}$$

where f_h is the atmospheric water vapour correction factor, and ρv is absolute humidity ($g\ m^{-3}$). 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, ERA-5 Land data can be utilised by converting dew point 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).

Arguably, ERA5-Land data present a spatial mismatch with the cosmic-ray sensor whilst also being a non-direct measurement of environmental variables. The majority of CRNS sites in the USA have not been deployed with a set of standard meteorological measurements, and only a few are co-located with external monitoring stations. Hence, in this case, ERA5-Land data are critical to ensure that neutron counts are appropriately corrected for water vapour variations at these sites. Our preliminary analysis suggests that correcting neutron counts with ERA5-Land data provides superior results compared with not applying the correction at all due to a lack of meteorological data (Fig. 3.2). In this example, meteorological data at the Atmospheric Radiation Measurement (ARM) site in Oklahoma are available from a nearby flux tower (Biraud et al., 2021). Notice how the processed soil moisture time series corrected with ERA5-Land data closely follows the soil moisture estimates produced when using the in situ meteorological data (Fig. 3.2a). Neglecting this correction can lead to a significant underestimation of soil moisture, especially during the wet seasons. Figure 3.2c helps to visualise these impacts by showing the difference between obtained soil moisture with a correction using ERA5-Land data and that with no correction applied, both compared with soil moisture corrected with in situ data.

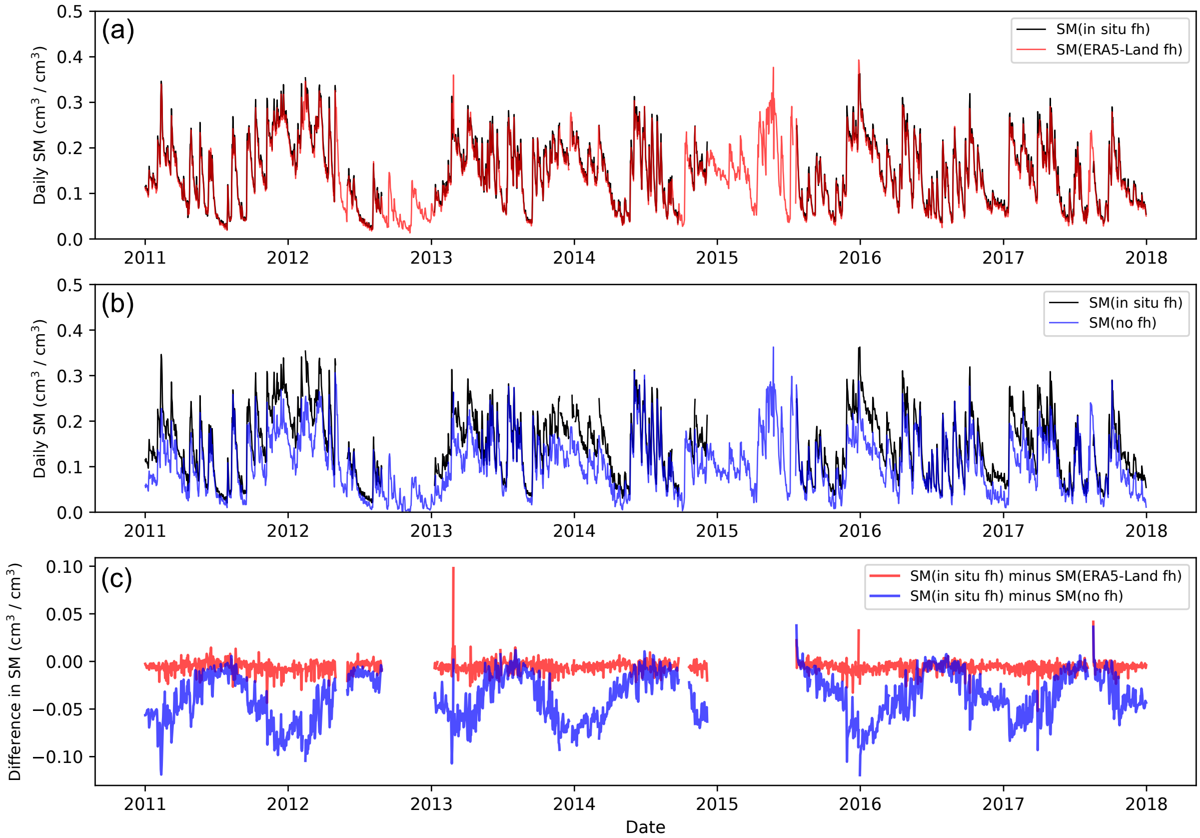

Figure 3.2 The soil moisture (SM) record at the ARM-1 CRNS site in the USA. Panels (a) and (b) show the SM product when corrected using in situ data in black. The red line in panel (a) is the SM product corrected with ERA5-Land data in place of temperature and relative humidity sensors. The blue line in panel (b) shows the SM product when not correcting for atmospheric water vapour (fh). Panel (c) shows the difference between the SM corrected with in situ data and the alternative correction methods.

(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 a static estimated value for each site from the European Space Agency (ESA) Climate Change Initiative

(CCI) global data set and applies a 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:

$$f_v = \frac{1}{1-(0.009*agb)} \tag{3.8}$$

where f_v is the above-ground biomass correction factor, and agb is the dry above-ground biomass at the site ($\mathrm{kg\,m^{-2}}$). The ESA CCI database provides above-ground biomass estimates as a global gridded data product at a 100 m resolution (Santoro and Cartus, 2019). As the ESA CCI data currently used are a static value in time, they will not impact the soil moisture estimates, in principle, because the correction is applied on both the N_{raw} and N_0 numbers, thereby mitigating any impact. Nevertheless, we have included this routine in crspy in this form because 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 (Franz 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.

3.2.2 Sensor Calibration

The above steps give us all of the values in Eq. (3.1) that are 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 may be 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 step typically requires multiple soil samples (typically >100) 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, ρ_{bd}, sampled within the footprint to estimate volumetric water content in $cm^3\ cm^{-3}$). 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 an updated approach for weighting soil moisture samples taken within the footprint that considers the spatial distance of each sample from the sensor 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 (<5 m radius from the sensor) and sample locations guided by the knowledge of local hydrological features. The data required for the calibration step include the date of 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 of crspy (see Table A2 in Appendix A). Calibration data sets are openly available from some of the networks at existing sites, such as CosmOz and COSMOS, and can be obtained from their respective websites. Alternatively, if a user was setting up their own sensor, a sampling campaign would be required such as that described in Schrön et al. (2017).

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

3.2.3 Quality assessment

All data should be checked for quality to ensure that erroneous data are 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., 2016). In crspy, we remove suspicious data points by applying flags to neutron counts that fall within four categories, and the following rules are consistent with the application in other networks:

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 ·1.075) are removed, according to Eq. (13) in Köhli et al. (2021);
4. battery voltages below 10 V are removed,

Flag 1 is applied on the raw, uncorrected neutron count, as we are interested in identifying sudden jumps in the counting rate in the sensor that are believed to be in error. Flags 2 and 3 are applied to the corrected neutron count. This is because the N_0

number is itself a corrected number (i.e., it is the maximum number of neutrons at the site under theoretical dry conditions, once additional environmental influences on the neuron count rate, N, have been taken into account and removed from the signal). In the case of flags 2 and 3 the N and N_0 number need to both be corrected in order to be comparable.

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).

3.2.4 Metadata

Metadata are important pieces of information that allow the user to better describe each site characteristics beyond its soil moisture dynamics. This information can be extremely useful, especially when multi-site regional to global CRNS stations are to be analysed simultaneously. The metadata of each site are stored in a tabular format within the folder structure of the working directory, and a full description of the columns is given in the Appendix A (Table A3). This 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 ρ_{bd}). To provide an example, ρ_{bd} is necessary to convert gravimetric soil moisture estimates into volumetric soil moisture estimates in Eq. (3.1). The ρ_{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. The user should also give each site a country code which represents the country it is located in and a unique site number for each CRNS site. The country code is used to help identify geographic locations in analysis and helps when the site numbering of networks may overlap. Raw time series data should be titled with the country code and number in the following format: *country*_SITE_*sitenum*.txt. Here, *country* is a capitalised letter code, and the *sitenum* is a three-digit number. For example, sensor data for a site in the UK could be titled: UK_SITE_101.txt. The *country* and *sitenum* variables form a *sitecode* (e.g., UK_SITE_101) which is used to label the outputs of crspy for easier identification, especially when processing many sites. The *country* and *sitenum* are also used as lookup values in the metadata to extract necessary variables.

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, which is an important direction in hydrological research (Wagener et al., 2007). To increase the value of the metadata, in addition to 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 realise that these global data sets 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 that the use of the data sets described in detail below can provide us with key information at both the 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 via identifying site differences and similarities. Both products are spatially consistent with the CRNS range (100–300 m) and are available globally. The usefulness of ESA CCI data sets 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 250 m resolution grid. This is available as SoilGridsv2 (Poggio et al., 2021), 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 provides 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 are stored along with derived Köppen–Geiger classifications.

3.2.5 Running the tool.

Once the working environment has been prepared, the data can be processed with:

```
crspy.process_raw_data(fileloc, calibrate=True, intentype=None)
```

Here, "`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. Once applied, crspy will process the raw data using the provided information to give soil moisture estimates and will output figures and tables into the folder structure of the working directory. A description of the final output file and what each of the standard columns represent is given in Table A4.

3.3 Discussion

3.3.1 Benefits of Harmonization

As mentioned previously, one of the key purposes of crspy is the easy and harmonised 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 using an example related to the individual sensor corrections steps and their impact on the final soil moisture estimates.

Table 1 outlines three identified methods that are currently employed across different networks. The *p_int*1 method is employed at the COSMOS (USA) network; it lacks the atmospheric water vapour correction and applies an intensity correction using only the Jungfraujoch neutron monitoring site directly. The *p_int*2*_awv* method closely resembles the CosmOz (Australia) network methodology, which applies the atmospheric water vapour corrections and an intensity correction that differs from the *p_int* method. 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. The *p_int*3*_awv_agb* method is the default crspy method; it 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 (Eq. 3.5).

Table 3.1 The three identified methods of correction neutron signals in use

	Method p_int1	Method p_int2_awv	Method $p\_int3\_awv\_agb$
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 and an additional correction for site GV (see Eq. 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 of these different correction approaches applied independently by 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 3 shows two sites with distinct hydroclimatic regimes, both taken from the COSMOS-USA network, that have been processed using the three identified methods (see highlighted star markers in Figs. 4 and 5). The Santa Rita Creosote site (Arizona, USA) is a shrubland-dominated region with a soil categorised predominantly by sandy loam. The site has a mean annual temperature of 19 °C and a mean annual precipitation of 335 mm, the latter of which primarily falls in winter storms and monsoonal summers (Köppen–Geiger climate classification BSh, a hot semi-arid climate). Climate data are taken from ERA5-Land, and the Köppen–Geiger classification is derived from ERA5-Land data using the method outlined in Peel et al. (2007). The Wind River site (Washington, USA) is an old-growth mixed conifer forest area. The site is much wetter than the Santa Rita Creosote site, with an annual precipitation of 2200 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 have been extracted from ERA5-Land, and the Köppen–Geiger classification is 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 CRNSs at both sites have been processed in crspy to give the corrected signals for the *p_int*2_*awv* and *p_int*3_*awv_agb* methods.

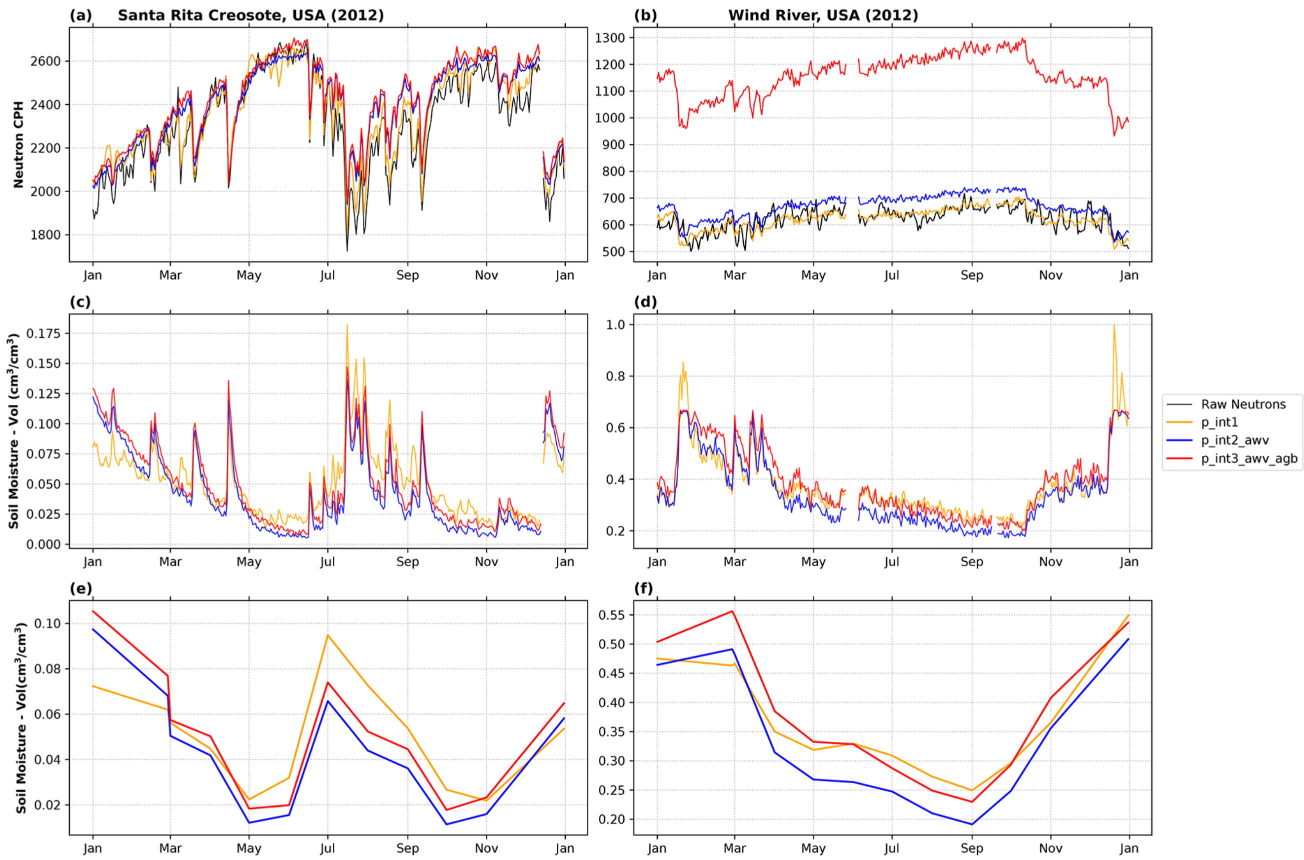

Figure 3.3 Example of CRNS data obtained at two distinct sites: Santa Rita Creosote (a, c, e) and Wind River (b, d, f). Daily neutron counting rates (raw and corrected based on the different strategies outlined in Table 1) are shown in panels (a) and (b)

It is clear to see the inverse relationship between neutron count rates and soil moisture, most noticeably at Santa Rita Creosote (Fig. 3.3a, c). The soil moisture here tends to be low, such as in June when it was below 0.05 $\mathrm{cm^3\ cm^{-3}}$, 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 chosen has an impact on soil moisture values. This is most notable when comparing the *p_int*1 method with both the *p_int*2_*awv* and *p_int*3_*awv_agb* methods. During the summer months, the *p_int*1 method appears to estimate higher soil moisture values compared with the other two methods (both appearing to be much more closely aligned with each other). This is likely due to the fact that the *p_int*1 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 water vapour 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 vapour to an increase in soil moisture, causing an overestimation. For example, even early in March, there is a sudden rise in soil moisture from the *p_int*1 estimates that does not appear in the other two methods (Fig. 3.3c). 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 even more pronounced in monthly estimates of soil moisture due to the aggregated nature of this error (Fig. 3.3e).

The Wind River site is a much wetter site when compared with Santa Rita, with its driest month matching Santa Rita Creosote's wettest month. In the case of Wind River, it is worth noting that there is a much larger difference between the neutron count rate of the *p_int*3_*awv_agb* method compared with the other methods (Fig. 3.3b). This is because the *p_int*3_*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_0 term. With dynamic data, which represent changes in above-ground biomass over time, we would be able to improve our estimates of soil moisture, as the impact of changing 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 $cm^3\ cm^{-3}$. The *p_int*1 method does not do this, and so there are physically impossible values of volumetric soil moisture in February and December, as seen in Fig. 3.3d. In crspy, maximum values for soil moisture are estimated by inferring the porosity of the soil:

$$sm\_max = 1 - \left(\frac{\rho_{bd}}{density}\right) \tag{3.9}$$

where sm_max is the maximum volumetric soil moisture value ($cm^3\ cm^{-3}$), ρ_{bd} is soil bulk density ($g\ cm^{-3}$), and density is the density of ground material (estimated with an assumed density of quartz at 2.65 $g\ cm^{-3}$). If a user did not wish to enable this cut-off value, the value for sm_max can be set to one in the metadata.

At the Wind River site, the differences between *p_int*2_*awv* and *p_int*3_*awv_agb* are much more noticeable, especially when the soil moisture estimates are aggregated to monthly timescales (Fig. 3.3f). This observed difference is due to 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 which looked to identify useful soil moisture signals that can be robust, discriminatory, and representative, and research into developing useful diagnostic soil moisture signatures is ongoing (Araki and McMillan, 2020). When reducing large time series data into signatures, such differences can be aggregated, which could begin to affect conclusions. However, the authors stress here that it is not within the scope of this work nor the intention of this study to identify which method is better or worse than the other; rather, we intend to highlight the potential negative impacts of the lack of a harmonised data set for large-scale global assessment of CRNS technology.

3.3.2 Usefulness of crspy metadata

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. (2021) discuss the need for high-quality metadata to improve our ability to understand the knowledge accumulation in the field of hydrology. 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 2000 m elevation with certain land use types and given particular weather events (Chen et al., 2020), how it behaves at sites where mean annual precipitation is above/below a certain threshold, or they may even wish to group 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 allow the user to quickly obtain any grouping of interest in an easy and accessible way.

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 the continental USA (CONUS). Some of these 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 a 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, and Köppen–Geiger climate classification). Figure 3.4 gives an example of how the metadata can be easily used to show the location of each sensor in the CONUS domain based upon the supplied additional information – in this case, the 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.

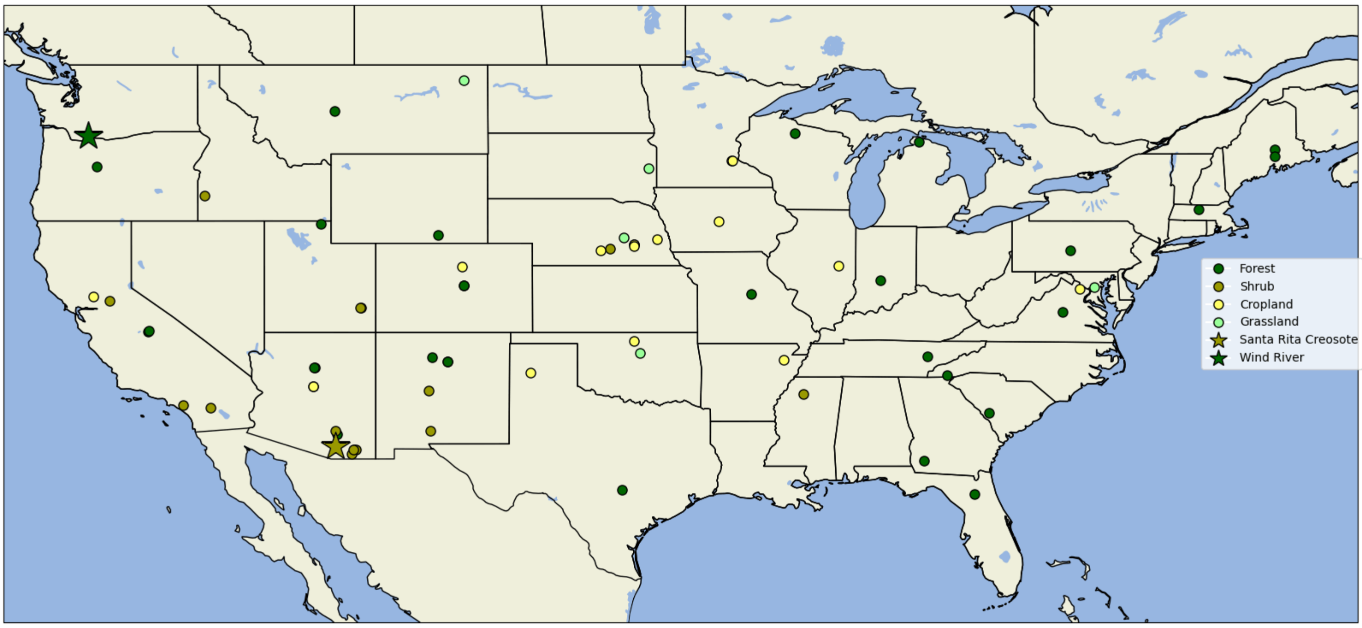

Figure 3.4 Map showing the location of CRNS sites from the COSMOS network across continental USA (CONUS). The colours are representative of the land cover types obtained from the ESA CCI global database, and the stars highlight the location of the two sites processed above (i.e. Santa Rita Creosote and Wind River).

In addition to locating the CRNS stations and identified the main land cover type, Fig. 3.5 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 ERA5-Land data. The initial analysis indicates that CRNSs 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 show lower temperatures than those observed in shrublands. However, croplands also indicate a slightly wider range of wetness compared with 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 shrublands with low overall precipitation. Alternatively, it can be used in big-data analytics when trying to identify the dominant mechanisms in soil moisture dynamics globally.

The objective of metadata in crspy is to easily collect a wide range of information on site characteristics that can be used to improve our knowledge of soil moisture and, consequently, other hydrological and environmental processes beyond just a single site. This allows for knowledge accumulation across multiple sites (from local to regional and even global), highlighting key similarities and any emergent patterns (e.g. hydroclimatic and ecological). Metadata analysis has not yet been fully exploited in hydrological sciences (Evaristo and McDonnell, 2017), but it can also contribute to knowledge accumulation, which can be translated to aid in the design of improved or new perceptual or conceptual models (Wagener et al., 2021). An early example of that within the cosmic-ray neutron sensing community is clearly demonstrated by Shuttleworth et al. (2013) during the conceptual development of the COsmic-ray Soil Moisture Interaction Code (COSMIC). COSMIC was developed as a forward observational operator, allowing for the conversion of simulated soil moisture profile by land surface or hydrological models into equivalent neutron counting rates, facilitating data assimilation applications (Rosolem et al., 2014). By collecting and accumulating information from (at that time) 42 available COSMOS sites (see Table 1 in Shuttleworth et al., 2013), the authors were able to simplify the requirement for two of the prescribed parameters by establishing relationship with dry-soil bulk density (see Fig. 6 and Eqs. 6 and 7 in Shuttleworth et al., 2013). crspy will certainly facilitate such efforts in the future to help both experimental and modelling scientists, with the potential to reach other disciplines beyond traditional hydrological and environmental sciences. For example, a prototype version of crspy has recently been used for space weather application (Hands et al., 2021).

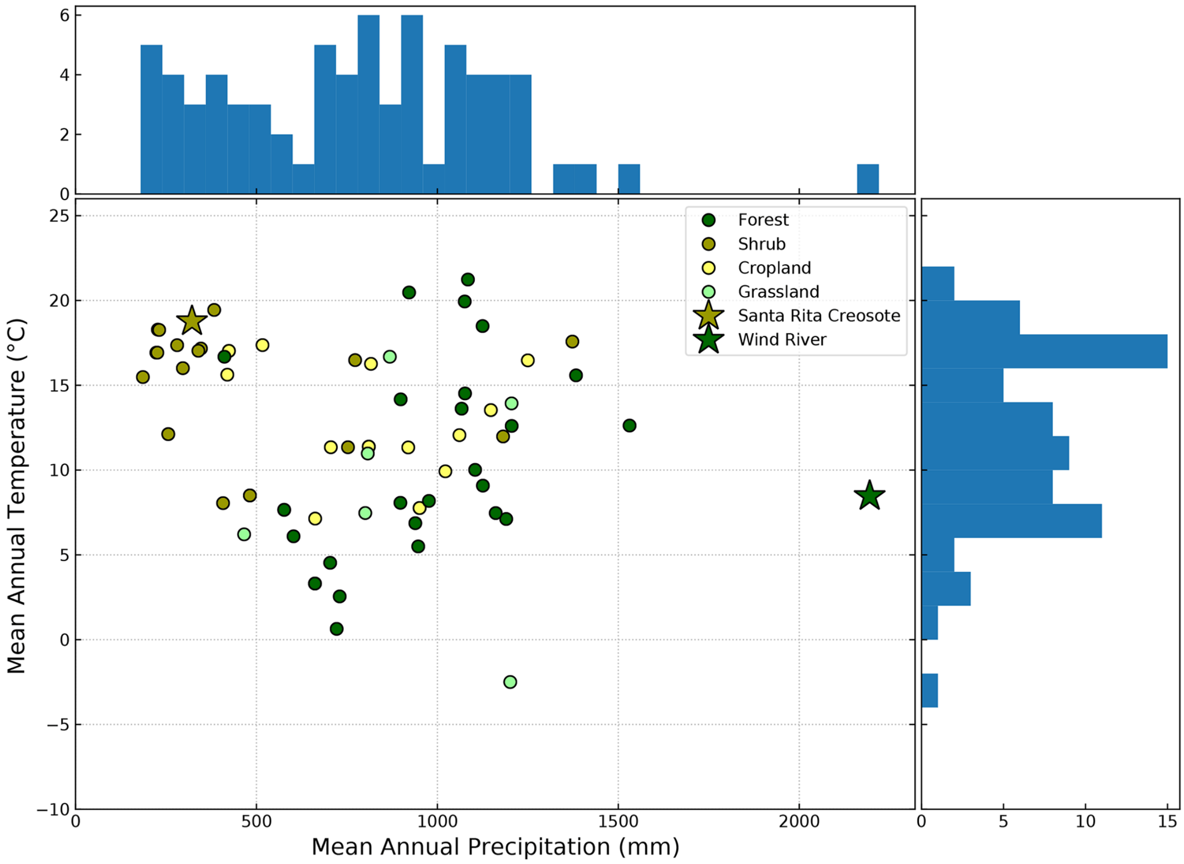

Figure 3.5 Scatter histogram showing the CONUS CRNS sites and some of their climatological characteristics. The units for the histograms are the number of sites for each bin. The colours represent land use types identified from the ESA CCI Land Use global data set. The stars highlight the location of the two sites processed above (i.e. Santa Rita Creosote and Wind River).

3.4 Future direction

In this paper, we have presented crspy, an open-source Python tool for the processing of cosmic-ray neutron sensors. Our aim in developing crspy is to provide a tool to the community that can provide methods to process CRNS data easily and that can be updated in the future to keep pace with our increasing understanding of the sensor signal. Due to this evolving understanding of the sensor, we expect to be updating crspy regularly in the future to accommodate our new understanding of the technology along the years.

Köhli et al. (2021) recently presented research that demonstrates a revised formulation of the key equation that converts neutron counts into soil moisture estimates (see Eq. 3.1). This emphasises the need to be able to update CRNS estimates to keep pace with the research as well as to test newer formulations across a range of sites quickly. In version 1.2.1 of crspy, we maintain the Desilets et al. (2010) version of Eq. (3.1) as the default setting but provide a document that describes how a user could update crspy on their home machine to implement the revised approach (see the Supplement). This document serves two functions: it demonstrates how to update crspy so that researchers may be able to test newer methods on a broad range of sites, but it also speaks of a more general need to agree on a standard approach for processing CRNS data. We believe it will be an important step in the future for the numerous stakeholders in CRNS measurements to agree upon a standard approach. This must be decided as a community, and we should look towards the positive steps other communities have taken in this regard, such as the flux community (Novick et al., 2018).

Another aspect of development in crspy will be making it more accessible and user-friendly. We consider that one of the key functions of crspy is to act as a tool for researchers, providing a way to update processing methods and apply them quickly to a collection of data. On top of this, we would hope that it can be used as an education tool, helping newer users understand how the sensor functions and what is required to fully correct it based on our current understanding. This could include developing crspy into frameworks such as Python Dash, which are powerful tools for exploring data.

3.5 Summary

Soil moisture is an important component of the hydrological cycle, and understanding its dynamics at relevant spatio-temporal scales is critical especially with recent advances of global land surface and hydrological models. The CRNS technology is able to provide estimates of soil moisture at the sub-kilometre scale and at an hourly resolution. This is particularly relevant now as we continue to move towards hyper-resolution global modelling efforts. Over the years, with increased adoption of the technology, the CRNS community has acquired a better understanding of the benefits and limitations of this relatively novel technique. However, due to a lack of data harmonisation across networks, undertaking global-scale analyses is currently very limited and unexploited. Here, we introduced the crspy Python package with the aim of facilitating user data processing easily and with the most current methods and, most importantly, in a harmonised fashion. crspy is an open-source tool aimed at integrating the latest developed methodologies for CRNSs for use in both research and teaching activities. It integrates high-quality global data products (such as ERA5-Land) to ensure that all sites can be included in the analysis. This is done in a similar way to other well-established global environmental networks such as the AmeriFlux and FLUXNET.

Our application examples demonstrated that processing CRNS data with different methodologies 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 harmonising 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 easy processing of CRNS data. Additionally, crspy data collection relies on the production of an extensive metadata archive. This archive can be shared and used within the community to better understand key aspects of soil moisture from typical sampling locations, in order to provide information on signature behaviour by different groupings. crspy has been developed to show the potential to easily and efficiently process CRNS data in a harmonised way. The aim is to promote the usefulness of free and open-access data and engage the CRNS and research communities in the continued improvement of this product in the coming years.

3.6 Appendixes of Chapter 3

Appendix A: Tables to describe variables' names and outputs.

Appendix A consists of four tables that outline the naming conventions required for crspy to run; it also presents the output table and a description of each variable. When labelling input data, column titles should match the style used in the "Column name" column below. 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 conventions (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	Date and time	Date and time of the observation in UTC (format: yyyy-mm-dd hh:mm:ss)
MOD	Count	Moderated neutron count for time interval – the sensor tube is surrounded by a high-density polyethylene shield to remove thermal neutrons from the count rate
UNMOD	Count	Unmoderated neutron count for time interval – a bare tube without the shield which will include thermal neutrons in the count
PRESS1	hPa	Pressure sensor number 1: usually the older analogue version that is somewhat less accurate
PRESS2	hPa	Pressure sensor number 2: the sensor that will be primarily used. If it is unavailable, PRESS1 will be used in its place.
I_TEM	oC	Internal temperature of the sensor box
I_RH	%	Relative humidity inside the sensor box
BATT	V	Voltage of the battery
E_TEM	oC	External temperature at the site: this would be an external reading. If it is unavailable, ERA5-Land data are used
E_RH	%	External relative humidity at the site. If it is unavailable, dew point temperature is used to find absolute humidity
RAIN	mm	Rainfall at the site. If local information is available, it is used; if local information is not available, rainfall 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/yyyy)	Date that the data were collected from the site
PROFILE	int	Integer (int) to differentiate profiles, with a profile being a single core. The core could then have multiple “layers”.
LOC_rad	m	Distance from the sensor for each sample in metres.
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, which should be given as a decimal (i.e. 0.3). If it is given as a numeric percent (e.g. 30 %), crspy will attempt to identify this and convert it to a decimal

Table A3 The naming convention of the metadata table.

Column name	Units	Description	Required at start?
COUNTRY	–	Country code for the location of the site, e.g. “USA”	Yes
SITENUM	–	Assigned three-digit number for the site, e.g. 001	Yes
INSTALL_DATE	–	Date of site installation	No
LONGITUDE	Decimal degrees	Longitude of the site	Yes
LATITUDE	Decimal degrees	Latitude of the site	Yes
ELEV	m	Elevation of the site above sea level	Yes
TIMEZONE	–	Time zone of the site	No
GV	GV	Cut-off rigidity (GV) of the site	Yes
LW	%	Lattice water from site-specific calibration data	Yes
SOC	%	Soil organic carbon from site-specific calibration data	Yes

BD	g cm−3	Dry-soil bulk density from site-specific calibration data	Yes
N0	–	Theoretic maximum neutron count for site (dry conditions), calculated in tool and written	No
AGBWEIGHT	kg m−2	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 β coefficient (see pressure calculations) for each individual site	No
REFERENCE_PRESS	hPa	Reference pressure calculated using elevation	No
BD_ISRIC	g cm−3	Bulk density estimates taken from the International Soil Reference and Information Centre (SoilGrids250m; https://soilgrids.org/, last access: 11 November 2021)	No
SOC_ISRIC	g dm−3	Soil organic carbon estimates from ISRIC	No
pH_H20_ISRIC	pH	pH of water estimates from ISRIC	No
CEC_ISRIC	mmol(c) kg−1	Cation exchange capacity at pH 7 from ISRIC	No
CFVO_ISRIC	cm3 dm−3	Coarse fragments from ISRIC	No
NITROGEN_ISRIC	cg kg−1	Nitrogen in soil from ISRIC	No
SAND_ISRIC	g kg−1	Sand in soil from ISRIC	No
SILT_ISRIC	g kg−1	Silt in soil from ISRIC	No
CLAY_ISRIC	g kg−1	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	Date and time	Date and time of the observation (format: yyyy-mm-dd hh:mm:ss)
MOD	Counts h^{-1}	Moderated neutron count
UNMOD	Counts h^{-1}	Unmoderated neutron count
PRESS	hPa	Atmospheric pressure recorded by the sensors at the site
TEMP	∘C	Atmospheric temperature. If sensors are missing, ERA5-Land data are used
I_TEM	∘C	Internal temperature of the sensor box
I_RH	%	Relative humidity inside the sensor box
E_TEM	∘C	External (atmospheric) temperature
E_RH	%	External (atmospheric) relative humidity
RAIN	mm	Rainfall recorded at the site. If local data are unavailable, ERA5-Land data will be used in their place
BATT	V	Voltage of the battery
fbar	–	The pressure correction factor
DEWPOINT_TEMP	∘C	Dew point 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 h^{-1}	Neutron count rate from neutron monitoring database – usually Jungfraujoch
pv	kg m^{-3}	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 Sect. 2.3 for definitions)
MOD_CORR	Counts h^{-1}	The corrected neutron count rate after the correction factors have been applied
MOD_ERR	Counts h^{-1}	The statistical error of the neutron count rate
SM	Volumetric soil moisture cm^3 cm^{-3}	Estimated soil moisture

SM_PLUS_ERR	Volumetric soil moisture cm3 cm−3	Estimated soil moisture error above the estimated value – this is calculated by subtracting the MOD_ERR value (due to the inverse relationship) from the MOD_CORR value and calculating what the SM would then be
SM_MINUS_ERR	Volumetric soil moisture cm3 cm−3	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 cm3 cm−3	The SM value with a 12 h rolling average applied to it. Minimum number of values to calculate the 12 h average is 6 h of data within the 12 h window
D86avg	cm	The depth of the measurement – taken as the depth from which 86 % of neutrons are estimated to be sourced from (Schrön et al., 2017)
D86avg_12h	cm	The D86 value with a 12 h rolling average applied to it. Minimum number of values to calculate the 12 h average is 6 h of data within the 12 h window

Appendix B: Examples of standard outputs of crspy

Appendix B provides some examples of the automatically generated outputs of crspy along with a description of their purpose.

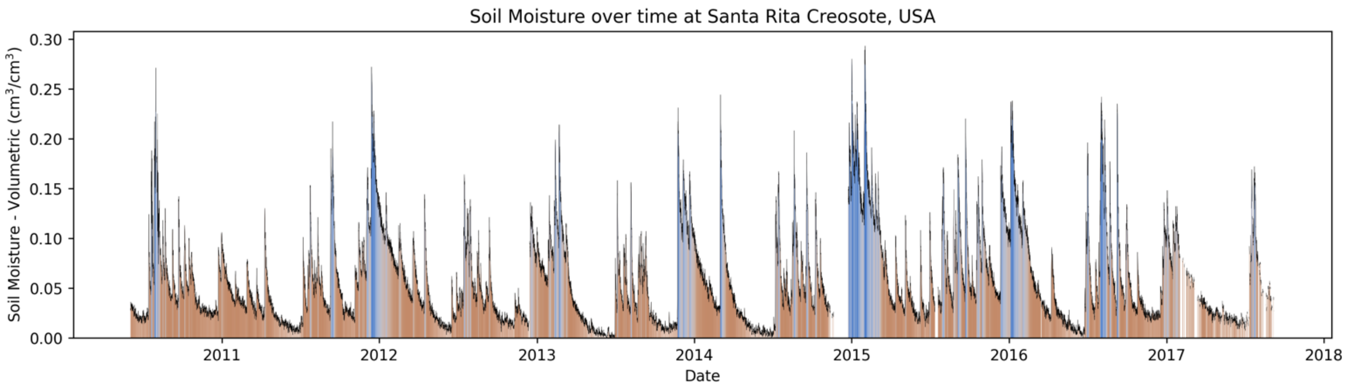

Figure 3.6 Charts that take the fully corrected SM data and plot them over the entire time series are output automatically. Optional yearly plots are also possible. The colouring is used to visually see the difference between wet (dark blue) and dry (dark brown) periods (code is found in "graphical_functions.py" under the "colourts()" function).

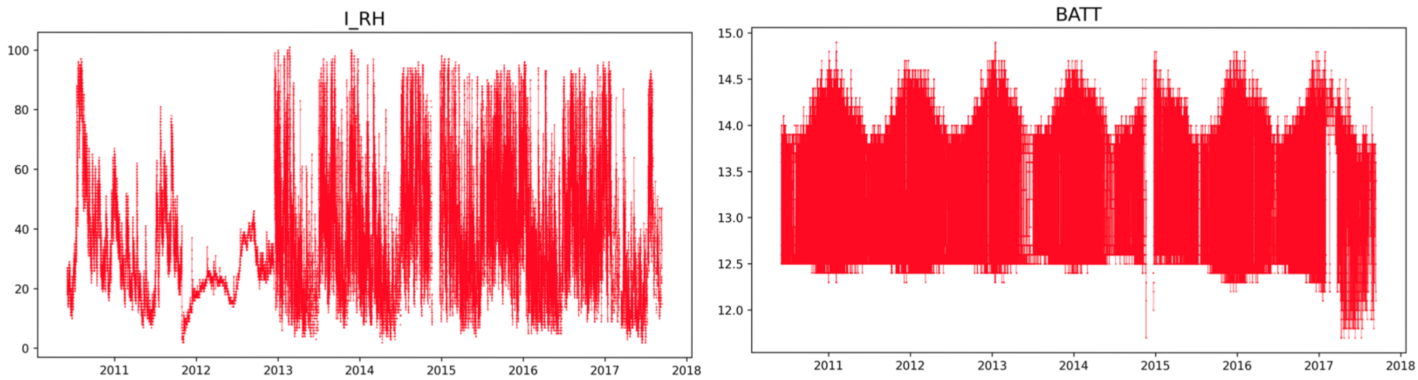

Figure 3.7 Diagnostic plots that create time series of the data columns are generated. Here, two are presented (titles match variables from Table A4): I_RH is the internal relative humidity, and BATT is the battery voltage. These allow a user to quickly visually understand possible periods where more investigation is necessary. For example, the BATT variable begins to fall around 2017 which demonstrates an issue with the battery (right panel).

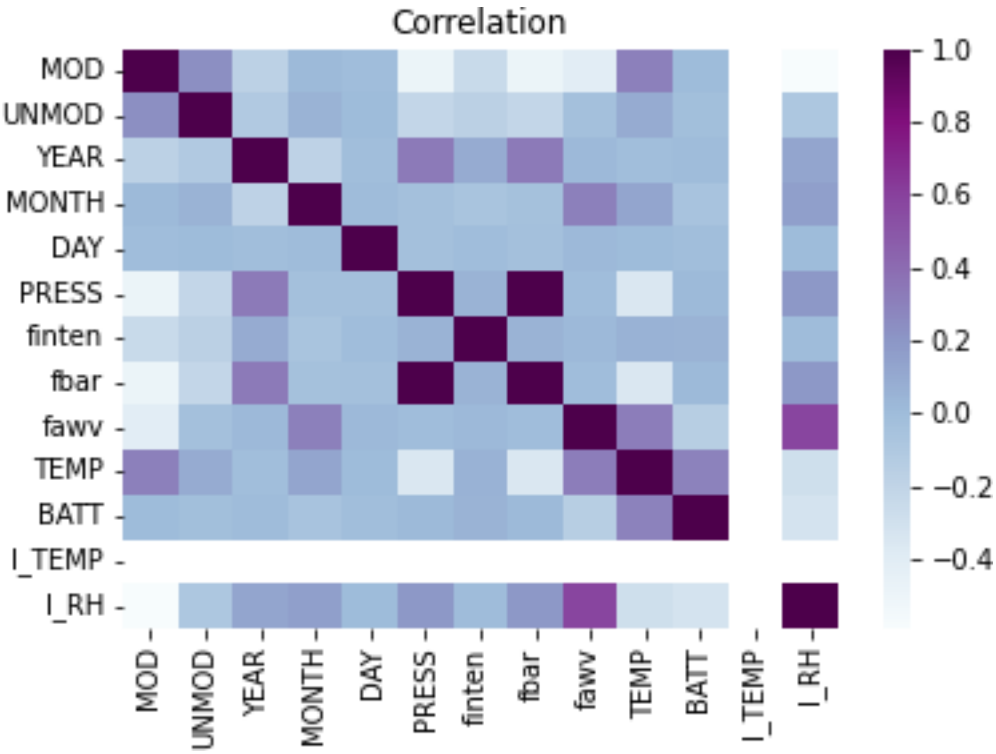

Figure 3.8 A correlation heat map is generated during quality analysis. We would expect correlation between certain variables (such as fbar and PRESS), but other correlations may point towards issues with the sensor that require investigation.

4 Validation of satellite and reanalysis soil moisture products using global Cosmic-Ray Neutron Sensors

4.1 Introduction

Global soil moisture estimations from satellite remote sensing and land surface modelling products are increasingly popular in hydrological studies, as our need for globally available data grows. Soil moisture is highly influential on numerous parts of the ecosystem, as described in Chapter 2, making it essential to understand global hydrological dynamics amidst a changing climate. This necessitates high quality data with good spatial and temporal resolutions that covers as much of the globe as possible. Despite its significance, soil moisture is challenging to measure, and while in-situ networks continue to expand, their coverage can never be truly global due to the high costs of setup and maintenance, and the fine spatial scale most current sensors represent. In light of this, gridded soil moisture modelling products, such as the ERA5-Land model (Muñoz-Sebater, 2019), or satellite soil moisture products, such as Soil Moisture Active Passive (SMAP, Entekabi et al., 2010) or European Space Agency Climate Change Initiative soil moisture product (ESA-CCI, Dorigo et al., 2017), present an opportunity for truly global coverage of soil moisture values. Satellite products are particularly effective for monitoring global dynamics of soil moisture and have been used to tackle issues such as agricultural drought monitoring (Bolton et al., 2009, Martinez-Fernandez et al., 2016), landslide susceptibility monitoring (Ray et al., 2010, Brocca et al., 2016, Zhao et al., 2021), ecohydrological modelling (Duethmann et al., 2022), or to constrain the algorithms of other products such as those predicting evapotranspiration (Bust et al., 2021).

Modelling products such as ERA5-Land, model ecosystem processes across the globe of which soil moisture is just one part and whilst they are not direct measurements it has been shown to compare well with in situ data or satellite data (Lal et al., 2022). Just as satellite products, ERA5-Land soil moisture products are used in studies to better understand global soil moisture dynamics (Tramblay et al., 2021, Shangguan et al., 2022). The ability of both models and satellites to monitor soil moisture dynamics in ungauged locations is of enormous value to hydrologists. However, to ensure that soil moisture values are being accurately described by satellite and modelling efforts, validation studies are required. These studies compare the reported soil moisture values with in-situ soil moisture values necessitating high quality ground-based monitoring stations.

Validation studies play a crucial role in the analysis of satellite and gridded soil moisture products, ensuring the values align with in-situ measurements. In validation studies, in-situ ground-based measurements are typically employed, being a more direct source of soil moisture information (Beck et al., 2021). A challenge in comparing different soil moisture datasets is the inherent differences in the spatial and temporal scales of measurements. The differences in spatial scales between sensors can be both in the horizontal and in the vertical domain. Satellite soil moisture's horizontal resolution can differ depending on the product, often spanning several kilometers horizontally and usually representing surface soil moisture (2-5cm in depth) in the vertical domain (Beck et al., 2021). Temporally, values are usually presented as daily. The spatial representation of modelled products also varies, depending on the chosen model parameterization. For instance, the ERA5-Land model employed in this chapter, has a 9km horizontal resolution and provides multiple soil moisture depths at hourly intervals (Muñoz-Sabater et al., 2019, more detail in Section 4.2.4). Within the field of soil sensing hydrology, it is accepted that systemic differences between in-situ and gridded data will be apparent in their bias and deviation, and likely the result of differences in the represented soil moisture domain (Su et al., 2013). This means caution should be given when directly comparing two distinct sources of soil moisture. However, soil moisture variations are known to be correlated; measurements taken closer together in both time and space tend to resemble each other more than those taken at greater distances (Crow et al., 2012). This means that whilst we know two different sensors might represent different spatial scales, the dynamics between different sources of soil moisture taken within the same area are likely related. Commonly this means that when comparing two sources of SM data, bias and standard deviation are considered systemic differences (to be removed), whilst correlation differences are considered more likely due to sensor quality. Due to this, validation studies will often compare in situ networks with satellite and gridded products, but with greater focus on testing temporal dynamics, for example, by evaluating metrics such as Pearson correlation (R) values. The assumption is that systemic differences are likely due to inherent differences in representativeness (i.e., the volume of soil influencing the measurement), with more focus given to validating temporal dynamics (Gruber et al., 2020). This has led to numerous methods to adjust datasets that eliminate observed systemic differences.

Given the inherent differences between satellite, modelled, and in situ measurements, it is common to employ statistical techniques to account for these discrepancies. The accuracy of a sensor is defined as the difference between the true value and the measured value. Defining a truth becomes difficult as each sensor will have different sources of error depending on the technology being use (Webster 1998). Systemic differences, such as the overall mean and standard deviation, can come from representative differences (i.e., what volume of the soil is being measured), or from instrument error (i.e., sensor drift from a deteriorating sensor). Random errors on the other hand are more likely down to instrument error or quality. Given this understanding, when comparing two sensors directly effort is employed to correct for systemic differences between the sensors whilst the random errors based on the instrumentation remain (Gruber et al., 2013). With this, statistical rescaling methods are employed to correct for such systemic differences in soil moisture sensors representative of differing scales. Two popular methods are z-scaling and matching cumulative distribution functions (CDF). Z-scaling refers to matching the temporal mean and standard deviation of the data to a chosen reference dataset (Dorigo et al., 2012), whereas CDF matching involves matching the entire cumulative distribution of a dataset to a chosen reference dataset (Kumar et al., 2012). For example, when blending multiple satellite soil moisture datasets that will each have different systemic biases and differences, CDF matching has been used to correct each data source to match a common modelled soil moisture dataset to make blending smoother (Liu et al., 2011). Whilst more simple statistical adjustments such as z-scaling and CDF matching are still widely used, there is growing interest in more complex methods that leverage advancements in machine learning (Yuan et al., 2023). Machine learning methods use large amounts of data to train models that can find non-linear connections between two sources of data. For example, training an artificial neural network to downscale coarser satellite soil moisture data to match the finer resolution of another related data source has been successful (Srivastava et al., 2013). The ability of such models to find non-linear relationships between data sources shows great promise. However, the models may not be explainable due to the abstract way that predictions of the downscaled dataset are produced, and so there is continued interest in simpler methods such as CDF matching. Whatever method is decided upon a first and important step is to decide in what direction, and to what data, rescaling should take place.

Due to the growing number of gridded products, both satellites derived SM and modelled SM, efforts to compare or validate them usually begins by rescaling each product to a reference. This can involve scaling satellite data to match another source of satellite data (Beck et al., 2020), or scaling satellite data to match that of a model (Dorigo et al., 2017). However, it is also important to be able to validate such products and compare them to ground based in situ SM data. The largest and most popular in situ soil moisture network is the ISMN network previously described in Chapter 2. Whilst the network covers much of the globe, and undergoes quality assessment to remove outliers, and harmonize data format, it is not truly a harmonized database considering it is made up of different types of sensors with their unique error profile. The broad variety of sensors, each with their own sources of error and representative spatial and temporal scale means that care should be given when using this dataset in global studies. Beck et al., (2020) employed a large-scale analysis of 18 different satellite and model-based products using the in-situ data from the ISMN network. They note that whilst the network is considered harmonized, it is still made up of many different sensors, each with their own potential uncertainties. In validation the focus was given on comparing temporal correlation of gridded product and in situ data through the Pearson correlation coefficient, ignoring the potential impact from systemic differences. Additionally, Gruber et al., (2020) outline a set of best practices for validating satellite soil moisture retrievals, in which the recommendation is to rescale in situ soil moisture data in pre-processing to remove the influence of systemic differences between the reference datasets. However, whilst rescaling appears as an essential part of comparing products representative of different domains, this does not prevent absolute values for satellite soil moisture estimates (Chen et al., 2014, Bassiouni et al., 2020), or modelled soil moisture estimates (Zhang et al., 2021) being used directly in studies aimed at understanding soil moisture dynamics across the globe. Given this it remains important to continue to understand the total uncertainty we might find in gridded products when compared to in situ networks. Researchers could find benefit in using a truly harmonized network of soil moisture sensors, meaning we can treat the soil moisture data as a harmonized dataset, without the influence of rescaling methods.

CRNS have been growing in number across the globe and present a unique opportunity for studies using a network of harmonized soil moisture sensors that span the globe. In Chapter 2 a description was given of how these networks have been gradually expanding across the globe, in both regional networks and as individual sensors. The continued expansion has led to opportunities to assess soil moisture through large sample hydrology type studies. In Chapter 3 an open-source python tool was developed, and it was demonstrated that currently regional networks are not uniformly processed, leading to uncertainties in the impacts from correction methods. Through crspy, we can process all sites quickly and easily in a harmonized way and treat these individual networks as a single, harmonized, and global one. A major advantage of the newly established global CRNS dataset is its elimination of a key limitation present in the ISMN network - the incorporation of multiple, varied types of sensors within the dataset with unique sources of error and represented domain. Another advantage is the spatial representation of CRNS as it represents a horizontal spatial scale between traditional point measurements such as TDR and satellite remote sensing (or modelled) products (Chapter 2, Figure 2.1). Earlier research, such as those conducted by Montszka et al. (2017) and Duygu and Akyürek (2019), validated satellite soil moisture products using CRNS. These studies underscored the merits of field-scale soil moisture sensors over point-scale ones in such validation research. However as outlined in Chapter 3, the processing of some sites in the USA would not have been implementing all the corrections, missing atmospheric humidity adjustment, and therefore causing a bias between the seasons. Recent advancements in the dissemination of CRNS data, as well as the development of crspy (Power et al. 2021; also described in Chapter 3), has led to an opportunity to undertake analysis with a more globally complete dataset, that fully corrects the CRNS in a harmonized way, using our most up to date understanding of the sensor signal.

The focus of the chapter is to understand the benefits in evaluating gridded products against a newly harmonized global database of CRNS soil moisture data.. A collection of 163 global CRNS sites are combined into a single harmonized group of sites, ensuring that processing methodologies are the same across the sites. This newly established globally spanning network of sensors will be used to better understand the inherent uncertainties that can remain in satellite and gridded products. First this global network will be described to ascertain its global coverage and the types of sites present, and a description of the methods is given (Section 4.2). Next, the Global CRNS sites are compared to two gridded datasets one representing satellite data and one representing modelled soil moisture data (Section 4.3). The absolute values will be compared to our reference CRNS dataset with the source of uncertainty further divided into bias, deviation, and correlation. Additional analysis will explore the temporal shifts in the sources of uncertainty between sensors and gridded products. Finally, a commonly applied bias correction technique will be tested by rescaling the datasets and comparing these to the harmonized reference CRNS data to understand the impacts this has. It is hypothesized that sources of uncertainty will differ between the sites, in particular dependent on the overall moisture characteristics of the site.

Given the vital role soil moisture plays in our understanding of global hydrological dynamics, particularly in the context of climate change, this research can offer valuable insights. By harnessing a newly harmonized global database of CRNS soil moisture data, our work has the potential to enhance our understanding of uncertainties in gridded soil moisture products and facilitate improved soil moisture monitoring on a global scale. This study assesses uncertainties in gridded soil moisture datasets, employing a comprehensive, harmonized global CRNS dataset produced with our newly developed open-source python tool, crspy. This tool offers a streamlined, uniform method of processing CRNS data, mitigating inconsistencies found in regional networks of CRNS. Furthermore, our approach marks the first time such an expansive and harmonized global CRNS dataset has been used to evaluate the accuracy of gridded satellite and modelled products together. These innovations can offer new opportunities for improving our understanding of global soil moisture dynamics and the remaining errors that are in global gridded products.

4.2 Data and Methods

4.2.1 Global CRNS Network Description

The newly harmonized global network of CRNS, displayed in Figure 4.1, comprises of 163 sites. It includes 41 sites from COSMOS (USA, Brazil, Kenya) (Zreda et al., 2012), 12 sites from CosmOz (Australia) (Hawdon et al., 2014), 58 sites from COSMOS-UK (Stanley et al., 2023), and 53 sites from COSMOS-EUROPE (Bogena et al., 2022). The sites from COSMOS and CosmOz were reprocessed using the crspy tool to harmonize their processing methodologies with those used at COSMOS-UK and COSMOS-EUROPE. Soil moisture values were temporally adjusted to a daily time scale and only sites with over one year of data were included in the analysis. The sites were categorized based on their annual average soil moisture values into 'dry', 'moderate', and 'wet'. First an average annual soil moisture value is created for each site. The 'dry' category includes sites in the lowest 25th percentile of average annual soil moisture, the 'wet' category includes sites in the highest 25th percentile, and the 'moderate' category includes all other sites (i.e., in between 25th and 75th percentiles). This categorization was designed to help understand how temporal shifts in uncertainty impact sites with different average wetness conditions (see section 4.3.2).

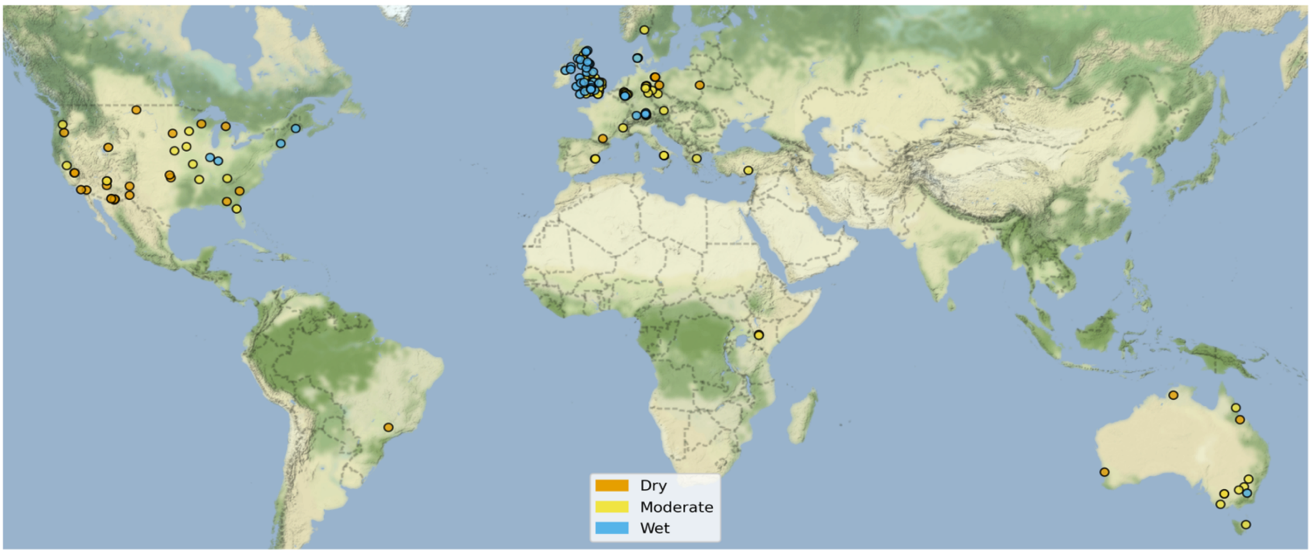

Figure 4.1 a global map showing all 163 sites used in this study. The colour of each dot is representative of whether it is a wet, moderate, or dry site, defined by the overall soil moisture average at the site.

It should be noted, whilst we refer to this as a global CRNS network, it does not include all currently available sites. This study combines four of the largest regional networks into a preliminary global CRNS network. It's important to note that there are more sites globally, but we have limited our study to those with full calibration and correction data available. For instance, the International Atomic and Energy Agency (IAEA) is currently expanding a network of sensors in previously unmonitored locations such as Oman or Senegal (https://crnslab.org/network-maps/networks/iaea/, last accessed 29/07/2023). Future research should aim to incorporate more CRNS sensors into the network, transforming it into a truly global dataset.

4.2.2 Metadata collection and site descriptions

The metadata collected using crspy (Power et al., 2021; also refer to Chapter 3) provides insights into the characteristics of the CRNS sites beyond just their geographical location, instead including attributes related to the climate, land cover and soil type of the site. The climatological and physical features of the global CRNS sites assembled for this study are shown in Figure 4.2. Figure 4.2a presents a scatter histogram, as introduced in Chapter 3, but now applied to the expanded dataset of the global CRNS network. Notably, a larger prevalence of grassland sites within the global network is evident compared to the US-only sites, alongside an increased number of sites featuring temperate climates with average temperatures around 10°C. The dataset reveals a broad array of climatological conditions across the sites, spanning from hot and dry to wet and cold. In Figure 4.2b, soil texture data derived from SoilGrids v2 are plotted on the United States Department of Agriculture (USDA) soil texture triangle for each site, with the colour of each point corresponding to the site's aridity index (calculated as Precipitation divided by Potential Evapotranspiration).

The global CRNS network demonstrates its coverage of diverse soil types and climatological conditions, thereby enabling large-scale hydrological studies.

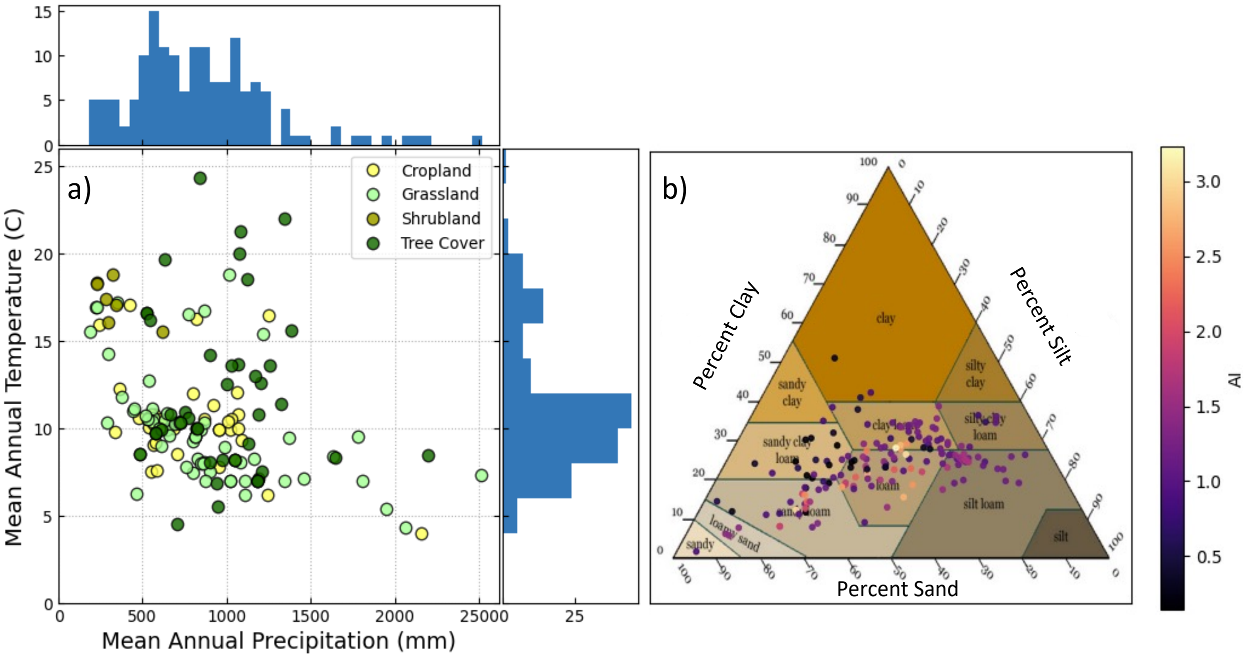

Figure 4.2 a) Scatter histogram of global CRNS sites illustrating mean annual temperature against mean annual precipitation, with colour indicating land use type (data sourced from ESA). b) USDA soil texture triangle overlaid with the soil texture of each site (data obtained from SoilGrids v2, as described in the previous chapter), where colour denotes the Aridity Index of each site.

4.2.3 Data Availability

Figure 4.3 illustrates the expansion of data availability within the newly established global CRNS network. The figure shows days when data was available between 2010 and 2020. The data is colour coded on each day of the year, with the colour representing the quantity of sites that were operational and generating data on those each day. As the networks have expanded and more sites were brought online, we can observe a consistent increase in data availability over the years. However, interestingly we do see a pattern emerge during the winter months with a reduction in data availability. This can be attributed to the impact snowfall has on CRNS measurements, leading to data being removed in quality control when snow is on the ground (Bogena et al., 2021). Importantly, the increasing volume of datasets, along with their expansive coverage of diverse hydroclimatic conditions, presents the potential to undertake large-scale hydrological studies, enhancing our understanding of global soil moisture dynamics.

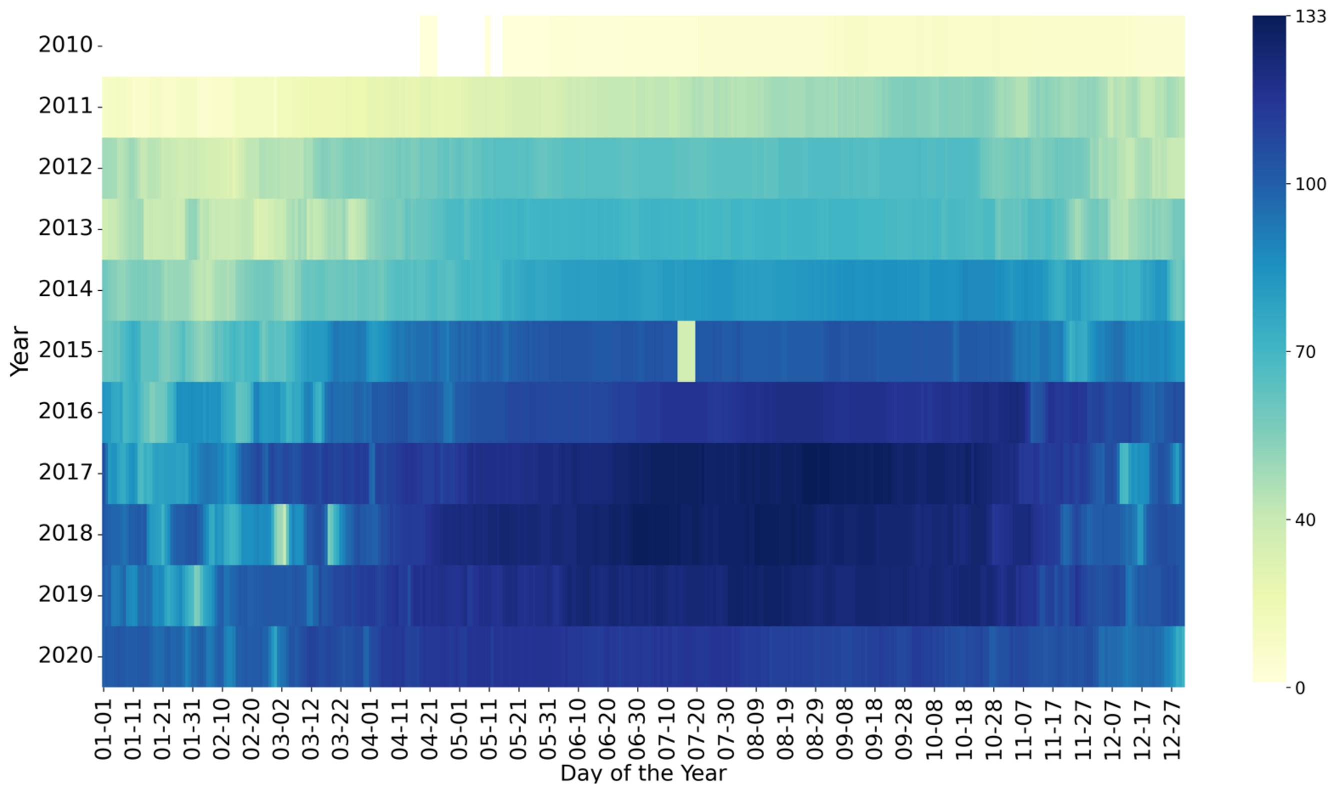

Figure 4.3: Daily data availability from the global CRNS database, 2010-2020. The colour scale denotes the number of operational sites contributing data on each day.

4.2.4 Satellite and Model data – collection and methods

The European Space Agency's Climate Change Initiative (ESA-CCI) soil moisture product combines multiple active and passive satellite remote sensing products and merges them into a single harmonized dataset that spans numerous decades (Dorigo et al., 2017). Over the years, various versions of ESA-CCI SM have been developed, with version 7 used in this study. To summarize, the project collects numerous satellite soil moisture products, standardizes them to a common daily temporal resolution, and creates three distinct merged products: active, passive, and combined. First, active sensors are merged into a single product, and passive sensors are separately merged into a single product. The active satellites are each temporally re-binned into daily time steps and rescaled using CDF matching (see 4.2.6) to match the ASCAT satellite soil moisture data. The same is done to passive satellites however they are rescaled to the AMSR-E satellite. The quality of each satellites data is identified by identifying the random error associated with the outputs, achieved using triple collocation analysis (TCA) (Gruber et al., 2016). TCA helps identify the proportion of random error associated with a reading by combining three sources of data with unique error characteristics and comparing them (McColl et al., 2014). With this, weightings are given to each satellite data source and the data is merged into separate products for active and passive satellites (Dorigo et al., 2017). Next, a combined product merging the active and passive products is created. The active and passive products are each rescaled to Global Land Data Assimilation System (GLDASv2.1) through CDF matching. Error characterization through TCA is once again undertaken and a weighting is given when merging the two products into the Combined product. The result is a combined product leveraging advantages of each type of sensor, such as the increased reliability of active sensors over areas with dense vegetation (Chen et al., 2018). The merging process has been outlined in several papers in detail, reflecting the advancements in the merging algorithm over time (Dorigo et al., 2017, Gruber et al., 2019, Preimesberger et al., 2021). It is important to note, however, that due to the rescaling to GLDAS data for the combined product (used in this study), it should not be considered a direct observation, despite this ESA CCI SM still recommends the combined product for model validation studies. This leads to a need for continued understanding of the total uncertainty profile. For the purposes of our research, we will directly compare this combined dataset with the CRNS dataset and the ERA5-Land soil moisture data.

The ERA5-Land model is a reanalysis product developed by the European Center for Medium Range Weather Forecasts (ECMWF) (Muñoz-Sabater et al., 2021). As the name suggests, it is aimed at better representing the terrestrial land-based processes when compared to the original ERA5 model (Hersbach et al., 2020). The numerical model is forced with downscaled meteorological outputs of the ERA5 model, giving an improvement in horizontal spatial resolution from 35km (ERA5) to 9km (ERA5-Land). Whereas ERA5 is an online or coupled model, meaning that feedback between atmosphere and land processes can occur, ERA5-Land is an offline model. This means that the outputs from ERA5-Land drive the land processes without feedback impacting atmospheric processes. ERA5-Land introduced a revised soil hydrology scheme, with improved formulation to account for hydraulic conductivity. After this update, evaluations against in situ observations has demonstrated that the ERA5-Land model performs better when compared to the original ERA5 model, with soil moisture representation in particular showing improvements vs ERA5 (Muñoz-Sabater et al., 2021). In terms of structure the soil moisture representation within the model is divided into four layers; 0-7cm, 7-28cm, 28-100cm, and 100-289cm. This provides users of the product multiple depths to choose from.

Due to the differences in representation between sources of soil moisture some steps are required to account for such differences. When comparing modelled soil moisture values with the other data sets, the depth of measurement is considered. Comparisons of satellite soil moisture and CRNS are made directly, without rescaling. CRNS measurements are influenced by deeper soil moisture values, with the depth of measurement changing due to the conditions at the site, as described in Chapter 3 when discussing calibration of the sensors. As we can calculate the sensor depth of CRNS at any given time, we used the weighting methodology described by Schrön et al. (2017), and implemented in *crspy*, to weight the ERA5-Land layers appropriately to match the measurement depth of the CRNS along with the proportional influence of each layer to the overall value. For completeness a comparison will be undertaken to compare the source of uncertainty between ERA5-Land soil moisture values and ESA-CCI soil moisture values. In this case the top layer of ERA5-Land will be compared to the ESA-CCI soil moisture data.

4.2.5 Comparing the datasets.

The mean squared difference (MSD) is a commonly used criterion for defining the difference between two datasets that represent the same attribute. MSD calculates the square of the difference between two datapoints at a given time, then averages these squared values across the entire dataset. By computing the square root of MSD, we obtain a difference criterion in the original units of the data set, yielding the root mean square difference (RMSD). MSD consists of three additive sources of uncertainty: bias, deviation, and correlation (Gupta et al. 2009). The additive nature of this uncertainty indicates that a single MSD value can incorporate numerous combinations of these relative sources of uncertainty. Gupta et al., (2009) outlined a method to decompose MSD into each of these sources of uncertainty, enabling clear identification of the origins of differences between two data sets (i.e., bias, deviation, or correlation)

MSD can be decomposed using the following equation:

$$MSD = 2 \cdot \sigma_e \cdot \sigma_o \cdot (1 - r) + (\sigma_e - \sigma_o)^2 + (\mu_e - \mu_o)^2 \tag{4.1}$$

where e and o, represent the estimated and observed datasets respectively, σ represents standard deviation, r is the linear correlation coefficient, and μ denotes the means of the datasets. The relative contributions of each of these components to the overall MSD can be computed using the following equation:

$$f_i = \frac{F_i}{\sum_{j=1}^{3} F_j} \tag{4.2}$$

with

$$F_1 = 2 \cdot \sigma_e \cdot \sigma_o \cdot (1 - r) \tag{4.3}$$

$$F_2 = (\sigma_e - \sigma_o)^2 \tag{4.4}$$

$$F_3 = (\mu_e - \mu_o)^2 \tag{4.5}$$

Using the above equations, we can identify the main source of uncertainty between each of the datasets analysed in this study.

4.2.6 Soil moisture rescaling (Bias Correction)

In this study, we will test a common rescaling technique, that adjusts systemic differences between datasets, by implementing empirical cumulative distribution function (CDF) matching to harmonize the satellite dataset with the modelled dataset. We will then use our reference CRNS dataset to compare the outputted results. CDF matching is a statistical procedure to harmonize two distinct datasets (Gudmundsson et al., 2012). First, the empirical CDFs (ECDF) of each dataset are calculated. Given a dataset $[x_1, x_2, \dots, x_n]$ the ECDF is given in ordered pairs with:

$$x_{(i)}\text{: sorted values of the data} \tag{4.6}$$

$$y_{(i)} = \frac{i}{n} \tag{4.7}$$

where n is the number of data points. Next, the ECDF of one dataset (the source) is adjusted to match the second dataset (the target). This is completed using the numpy interpolation package in python. This process effectively transforms the statistical distribution of the source dataset (in this case satellite soil moisture data) to align with the distribution of the target dataset (here using ERA5-Land SM). The result is a source dataset that reflects the statistical properties of the target dataset.

4.3 Results

4.3.1 SM estimates and relative uncertainties

A comparative analysis of each soil moisture dataset is shown in Figure 4.4. The figure comprises of sub-figures that group sites based on the average soil moisture values, which are inferred from the reference CRNS data. The sites range from driest to wettest, in increments of 0.02 cm^3-cm^3. When a group includes multiple sites, the results are averaged. Figure 4.4a shows the total Root Mean Squared Difference

(RMSD) of each bin for each of the three comparisons being made: CRNS and Satellite soil moisture (blue), CRNS and ERA5-Land data (yellow), and Satellite soil moisture and ERA5-Land soil moisture data (green). The RMSD between our reference CRNS dataset, and the modelled and satellite datasets, appears noticeably higher at the extremes (i.e., RMSD increases at the wetter sites, and the drier sites). Interestingly, we find that the ERA5-Land data and Satellite soil moisture data have an almost uniform RMSD across all sites. Figure 4.4b shows the decomposed RMSD, illustrating the proportional contribution from bias, standard deviation, and correlation, for CRNS soil moisture vs Satellite soil moisture. There is a noticeable shift in uncertainty characteristics across the ordered sites. Bias dominates at sites with average soil moisture less than 0.2 cm^3-cm^3 and greater than 0.4 cm^3-cm^3, whilst deviation and correlation are more influential at sites between these values. Figure 4.4c shows the comparison of CRNS soil moisture and ERA5-Land soil moisture, where we see slightly different results. Though we see similar uncertainty source as with Satellite soil moisture, such as bias dominating at the drier and wetter sites, the proportion of uncertainty from standard deviation differences appears considerably reduced, possibly due to the more comparable representative depths, given that CRNS measures deeper than the surface soil moisture represented by satellites. Interestingly, Figure 4.4d shows that the source of uncertainty between the satellite soil moisture and the ERA5-Land soil moisture are much more consistent across all the tested sites, only showing a general pattern of greater bias domination as sites get wetter. This demonstrates that whilst there is greater agreement between satellite and modelled SM data, as well as a more similar uncertainty contribution, there is a remaining residual bias between the in situ CRNS data and both gridded SM datasets. This is particularly prevalent at either dryer or wetter sites. The results in Figure 4.4 clearly show source of uncertainty shifts depending on the average moisture conditions of a site, we will now look to understand how these sources of uncertainty might shift in time.

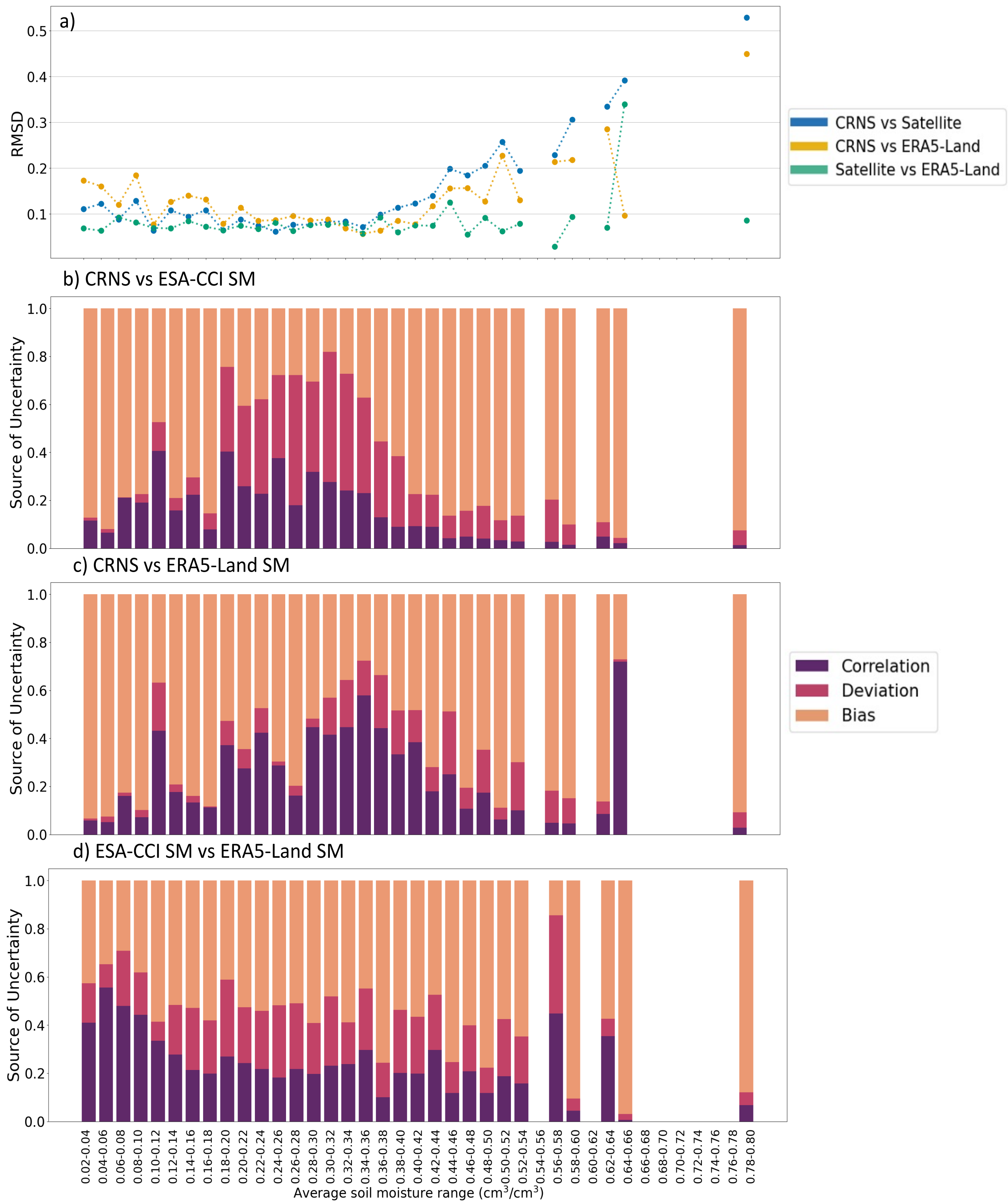

Figure 4.4: Root Mean Squared Difference (RMSD) and uncertainty decomposition across soil moisture datasets. (a) Comparative RMSD across CRNS vs Satellite Soil Moisture (SM) (blue), CRNS vs ERA5-Land SM (yellow), and Satellite SM vs ERA5-Land SM (green). (b-d) Proportional distribution of uncertainty, attributed to bias, standard deviation, and correlation, between CRNS vs Satellite SM (b), CRNS vs ERA5-Land SM (c), and Satellite SM vs ERA5-Land SM (d)

4.3.2 How uncertainty characteristics change in time.

To analyse how uncertainty characteristics might change in time, we conducted an examination of extreme soil moisture values at the sites. By focusing on extreme values of wet and dry we can discern shifts in uncertainty characteristics that might occur as seasons change. Figure 4.5 shows the results from a comparison of CRNS and Satellite soil moisture data. Each of the sites was assigned into one of three groups, representative of dry, moderate, and wet sites. The categorization was based on their site-specific average CRNS soil moisture, with the lower 25^{th} percentile deemed dry, the upper 25^{th} percentile regarded as wet, and the remainder classified as moderate (i.e., between 25^{th} and 75^{th} percentiles). The geographical locations of the sites within each group are shown in Figure 4.2 above. After groups are established, data from each group was collated into a dataset. Meaning that there is a single table for dry sites, moderate sites, and wet sites respectively. The soil moisture values of each dataset were subdivided into the lowest 10^{th} percentile, the highest 10^{th} percentile, and the rest of the data. This allows us to explore how uncertainty characteristics might differ at the extremes of soil moisture, whilst ensuring we are exploring characteristics of similar sites. Starting with the dry sites, we found that during the driest periods (i.e., lowest 10^{th} percentile), bias uncertainty primarily contributed to the difference, accounting for ~90%. In contrast, the wettest periods of the dry sites displayed different characteristics, with almost 70% of the difference coming from correlation uncertainty. When analysing the group of wet sites, we observed opposing characteristics, with bias dominating the wettest periods and correlation dominating the driest periods. Interestingly, for the moderate sites, we find that bias dominates at both the 10^{th} and 90^{th} percentile and is almost absent from the bulk of the data. We can see from Figure 4.4b that for the more moderate sites, bias is accounting for ~30% of the uncertainty, but the temporal results here suggest that this is mostly originating from the most extreme wet and dry periods of soil moisture readings. The results evidently show that the uncertainty characteristics, such as the bias, change over time at the sites, and interestingly, we found that these shifts heavily depend on the soil moisture conditions at the site.

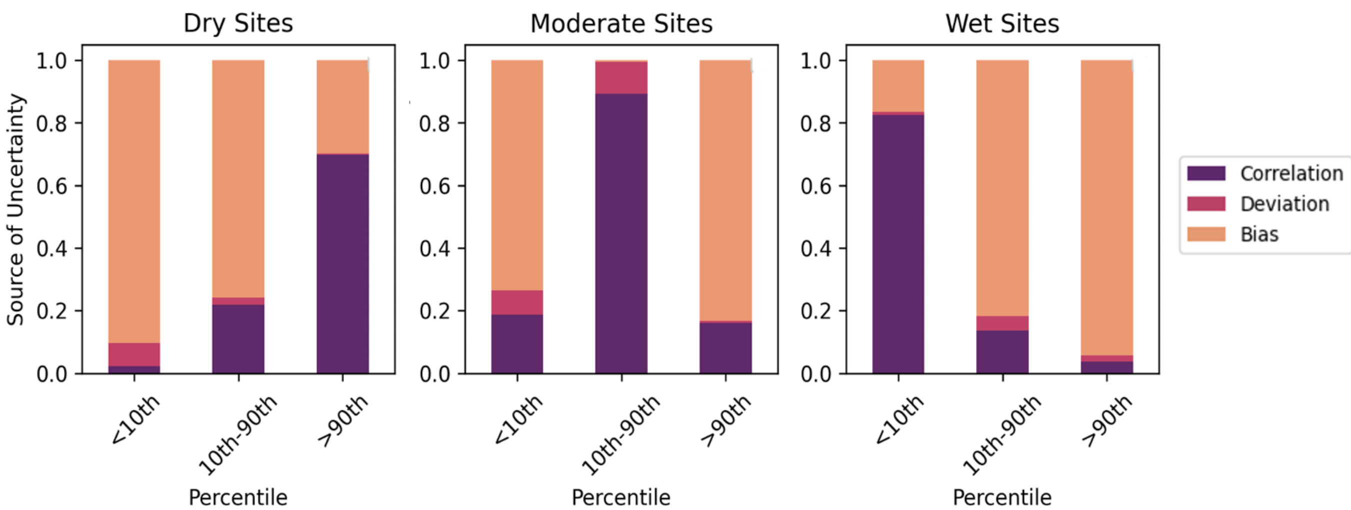

Figure 4.5: the proportion of uncertainty between CRNS and Satellite SM attributed to extreme values of soil moisture (highest and lowest 10^{th} percentile of estimates). Sites are grouped into dry, moderate, and wet based on their average CRNS SM values.

4.3.3 Impacts of bias correction (CDF matching) on time series data

As previously discussed, bias correction, often achieved by rescaling values from one dataset to match the systemic characteristics of another, is a common practice when comparing sensors of different support volumes. The above analysis did not undertake this step, as we were interested in understanding the total uncertainty characteristics at the reference CRNS sites. Here we explore the influence of bias correction techniques, specifically, the impact of CDF matching on soil moisture values. Figure 4.6 below presents a collection of figures demonstrating the impact of CDF matching on a soil moisture dataset. Figures 4.6a and 4.6b demonstrate analysis between CRNS vs Satellite soil moisture, and CRNS vs ERA5-Land, respectively. The results echo those shown for Figures 4.4a and 4.4b, respectively, but in this case, results are not normalized. Figure 4.6c shows a comparison of the reference CRNS data, with Satellite soil moisture data that has been CDF matched to resemble the systemic characteristics of ERA5-Land soil moisture (termed Sat-CDF), whilst Figure 4.6d shows the RMSD decomposition results when comparing the ERA5-Land soil moisture data and the Sat-CDF soil moisture data. It is clear from this bottom figure that the CDF matching process is performing as we would expect, eliminating most of the bias and deviation differences, and what remains are the correlation differences (i.e., the temporal dynamics of the satellite data has been retained). What is immediately obvious is that when we compare both the ERA5-Land soil moisture data (4.4b) and the Sat-CDF soil moisture data (4.4c) to the reference CRNS soil moisture data, the overall RMSD and uncertainty decomposition are now markedly similar. Whilst the temporal dynamics have been retained, the total uncertainty characteristics have been almost entirely transferred from the ERA5-Land SM data to the Satellite SM data, when both datasets are compared to the reference CRNS data.

Figure 4.6 shows the influence of rescaling methods on data. 4.6a and 4.6b show the CRNS vs ESA-CCI SM and CRNS vs ERA5-Land SM respectively. The data is the same as in Figure 4.4 although not normalized and the fractional contribution to MSD is projected onto RMSD. Figure 4.6c shows a comparison of CRNS data with ESA-CCI data that has been CDF matched to ERA5-Land data. Figure 4.6d shows a comparison of ERA5-Land SM data and the ESA-CCI data CDF matched with ERA5-Land data.

Figure 4.7 below shows a one-year SM time series taken from a site from each of the dry (top), moderate (middle), and wet (bottom) groups. The top figure is the Santa Rita Creosote site in the USA (COSMOS), a semi-arid location that sees monsoonal rains and extremely dry conditions. Between January to March, all the soil moisture records show relatively strong agreement, however when the drier months from March onwards approach the Satellite and Modelled soil moisture datasets start to disagree with the CRNS data. As indicated in Figure 4.5, dry sites tend to be dominated by bias errors during their driest periods. This suggests that this is partly due to a disconnect between the in situ CRNS data and the gridded products during these driest periods. The middle figure shows the Holme Lacy site (COSMOS-UK) located in the UK with a moderate soil moisture average. Interestingly, we see greater agreement between the original satellite soil moisture data and the CRNS soil moisture data, although again we find greater biases and disagreement when the soil becomes driest. The bottom figure shows the Redmere site (COSMOS-UK) in the UK, which is in the wet grouping of sites. We see that the Sat-CDF soil moisture data has relatively low deviations during the wetter periods, but during the driest period in July the changes in soil moisture are greatly exaggerated. Interestingly, this seems to be counter to what we are seeing in the CRNS soil moisture data, where deviations are greater during the wetter periods and decrease during the summer months.

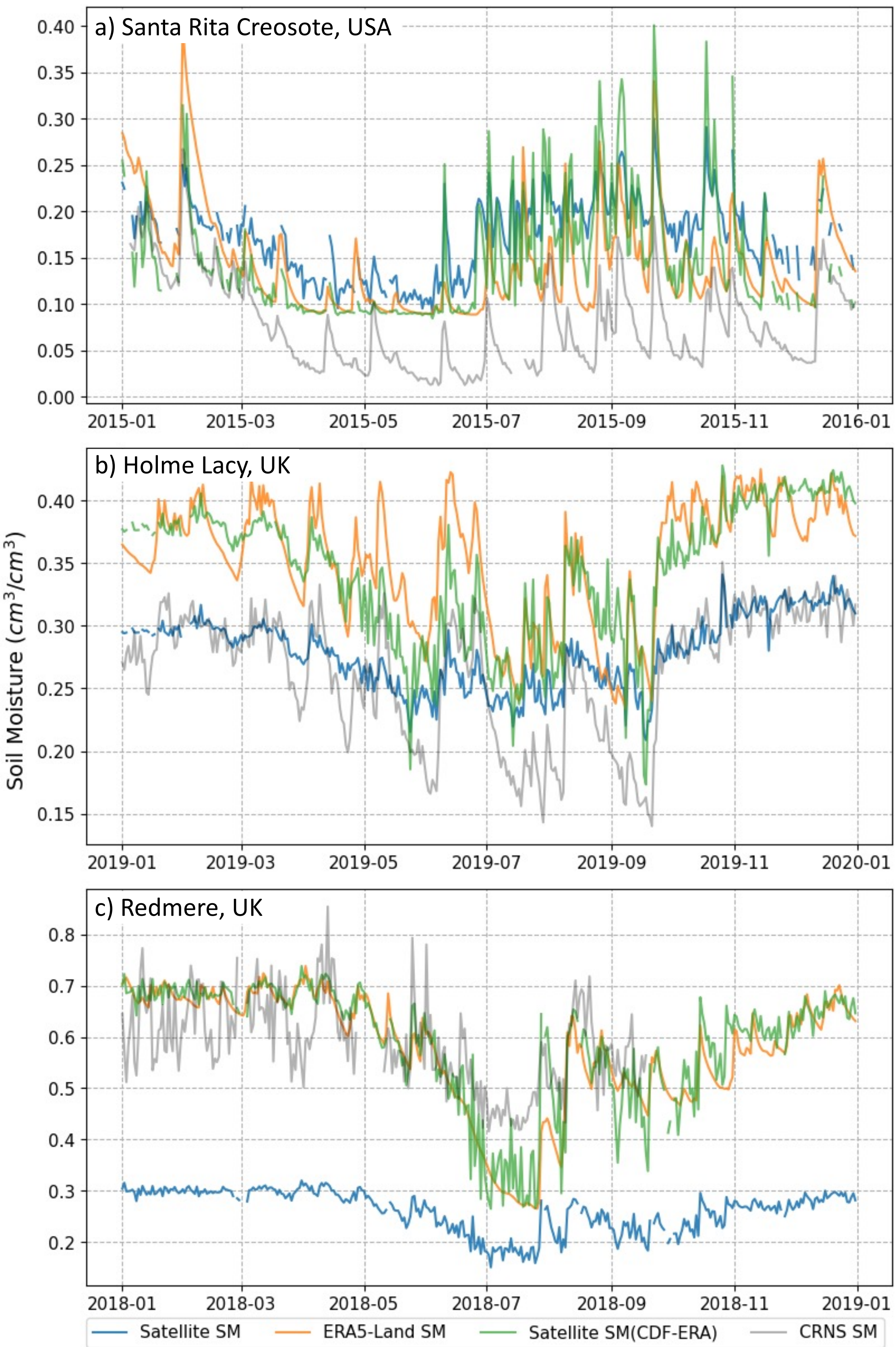

Figure 4.7 shows the actual time series of three sites one from each of the groups: wet, moderate, and dry. Fig 4.7a shows the semi-arid Santa Rita Creosote, USA. Fig 4.7b shows the moderate Holme Lacy, UK, and Fig 4.7c shows a wet site Redmere, UK. The blue line represents ESA-CCI SM data, orange is ERA5-Land SM data, green is the ESA-CCI data CDF matched to ERA5-Land and the grey represents the CRNS data at each site.

4.4 Discussion

Validating the performance of global gridded soil moisture products, which hold immense value for the environmental science community, critically relies on access to high quality in situ data. Global CRNS sensors provide field scale soil moisture values. Their horizontal resolutions effectively bridge the gap between point scale sensors and larger gridded products, such as those used in this study. Recognizing their potential, studies have already utilized CRNS sensors to validate spaceborne and modelled products (Montzka et al., 2017, Duygu and Akyürek 2019). Here we expand the spread of available sensors to the global scale by harmonizing multiple networks with the python tool crspy. This ensures that uncertainties are not related to processing methodologies. As evidence of the need for this harmonization, Chapter 3 highlighted how the USA COSMOS network's failure to apply the atmospheric humidity correction introduced a seasonal bias. By addressing such uncertainties, we ensure that observed differences in data truly reflect soil moisture conditions, not the differences of processing methodologies. With this newly harmonized global CRNS dataset we can investigate where differences arise with a global perspective.

A key observation from our study is that the characteristics of uncertainty between CRNS soil moisture data and gridded products are significantly influenced by a site's overall moisture content—particularly showing pronounced biases emerge at the extremes of soil moisture conditions. Notably, these biases aren't static; they evolve over time and are heightened during extreme dry and wet phases. Why these biases occur remains uncertain, however one possibility is the different sensing depths of each of the products in the study. The CRNS estimates soil moisture from a deeper profile, and the depth of measurement increases in dry conditions (Zreda et al., 2012). This could explain why bias increases as sites get drier, as the difference in sensing depth widens between satellite and CRNS SM estimates. However, in this study we weighted the ERA5-Land reanalysis soil moisture product to match the sensing depth of the CRNS at each given point in time, and we still find biases increase as soil moisture is at the extremes. This might point towards alternative reasons behind these changing uncertainty profiles. One such possibility is that the current generation of algorithms for converting raw data from satellite remote sensing into soil moisture estimates is not capturing dynamics at the extremes of wet and dry.

The remote sensing community acknowledges discrepancies between in situ and gridded data. However, many validation studies sidestep these biases using rescaling techniques, focusing predominantly on temporal dynamics. Such an approach leaves residual biases that can skew subsequent studies. The need to better represent SM dynamics at the extremes of wet and dry periods has previously been identified as a key area requiring continued study (Vreeckan et al., 2013). Our findings corroborate this sentiment: both satellite and modelled data exhibit marked disagreements with harmonized CRNS sensors during the most severe moisture conditions. This is of particular concern given that soil moisture droughts are expected to increase in the coming years due to climate change (Grillakis 2019), with the propagation of drought, from meteorological drought to agricultural (soil) drought highly dependent on antecedent soil moisture conditions (Kwon et al., 2019). Not only this, but due to soil moisture's role in land-atmosphere feedback, this will concurrently lead to increased maximum temperatures, potentially further driving extreme drought scenarios (Whan et al., 2015). With expected increases in drought events and the significant influence soil moisture can have on it, the scientific community remains committed to better understanding the main causes of extreme events, as well as better ways to predict them through modelled or satellite derived data (Champagne et al., 2011, Eswar et al., 2018, Zhang et al., 2021). Nicolai-Shaw et al. (2017), for instance, employed global satellite data to evaluate drought occurrences worldwide. However, based on our findings, such studies might overlook crucial dynamics at the soil moisture extremes. Whether the differences can be attributed to error due to sensor technology, or more related to the difference in representative soil moisture domain remains uncertain. Bridging the gap between point-scale data and gridded products often necessitates scaling adjustments (Crow et al., 2012), typically achieved via statistical rescaling and bias correction techniques, like the CDF matching method highlighted earlier.

Given the prevalence of rescaling methods, our results suggest that prevailing techniques used to amend systemic differences in soil moisture records might not be entirely suitable, particularly at the soil moisture extremes. This potential shortcoming is also highlighted by Gruber et al., (2020) in their satellite validation review. They underscore that because biases may evolve over time, applying blanket corrective methods might not always be ideal. Our results appear to agree with this claim. Uncertainty characteristics are not static in time as seen in Figure 4.5. Consequently, adjusting for systemic biases derived from the whole data period, and not specific to certain periods, may be introducing systemic biases itself. For example, if a specific dry site predominantly exhibits bias during its driest phases, this bias will be reflected in overall uncertainty metrics. Our data suggests that as these dry sites become moister, the bias diminishes. However, applying a consistent bias correction could unintentionally introduce a new bias during these moister intervals. Interestingly this seems to be the case whether we were looking at the satellite soil moisture product, or the ERA5-Land soil moisture product. One reason behind this could be that the linkage between modelled and satellite products are closely aligned due to the ways that data assimilation takes place. In the case of ERA5-Land data used in this study, whilst the model itself does not assimilate data, the driving data (ERA5 data) does assimilate data from satellite products (Hersbach et al., 2020). Recent research has suggested that the differences between satellite soil moisture and modelled soil moisture datasets is falling (Xing et al., 2023), however if the reanalysis products themselves continue to have the residual biases shown in satellite products, then this may not be so desirable.

Building on this, we also find that CDF matching is potentially altering datasets in ways that make them undesirable for more statistically driven studies such as those using machine learning. In this study we rescaled the satellite data to match the systemic metrics of the modelled data through CDF matching. When we then compared the corrected satellite dataset with our reference CRNS the overall RMSD and the decomposed uncertainty much more closely resembled that of the modelled data. This may present problems in certain studies if the full impact of this is not considered. For example, whilst assimilation of satellite soil moisture into hydrological models, which usually involves scaling techniques, has been demonstrated to show improvements for hydrological modelling (Alvarez-Garreton et al., 2014), the impact of these methods on more statistically driven machine learning techniques remains uncertain. This means caution should be given when considering rescaling methods in machine learning models. Machine learning methods are abstract in nature and will find statistical ways to predict a target from a set of input features. Given this, statistical rescaling techniques may be itself influential on the performance of such models. For example, studies have been conducted using rescaling to account for differences in the ISMN network of sensors, by rescaling them to match the systemic metrics of ERA5-Land data (O and Orth 2021). If we consider for the sake of argument that the CRNS data is closer to the "truth" soil moisture, the RMSD and decomposed uncertainty is now closer in resemblance to the modelled data used for rescaling. Given also that regression-based machine learning methods commonly use MSD as the loss function for model training, it is uncertain whether this means the model is being trained to be more like the original data or the data used for scaling. Further investigations towards understanding the impacts of this are warranted.

As with many studies there are limitations that should be considered in this analysis. One limitation of this study is that the ESA-CCI SM dataset is a combined product that itself uses CDF matching to merge multiple satellites into a single consistent time series. On top of this the combined product is rescaled to match GLDAS soil moisture values. Given this double adjustment, it's important to exercise caution before attributing discrepancies solely to satellite products. Even so, it is a popular product that is used widely in the community to understand the influence of SM on various environmental impacts, for example in studies investigating the propagation of agricultural drought (Chen et al., 2014). Given this, it remains important to continue to understand where these products remain uncertain in comparison to in-situ sensors so that we might improve future iterations. Another consideration is that this study didn't address spatial domain scaling. It's known that each soil moisture estimation relates to a specific spatial domain, both horizontally and vertically—especially considering CRNS captures soil moisture values within the root zone.

The global CRNS network presents opportunities to further our understanding of global soil moisture dynamics and validate other soil moisture products. In this study we have looked at how we might validate the performance of other global products such as satellite and modelling products using a globally harmonized network of CRNS sensors. Future studies should continue to explore the reasons behind greater uncertainties at specific sites, such as those exhibiting extreme dry or wet conditions, and strategize ways to address these differences. An interesting research direction would also be to further investigate the impact common rescaling strategies might have on study outputs, with a particular focus on machine learning methods. Such investigations could lead to refined rescaling methods that better account for the inherent variances in soil moisture datasets. This becomes particularly significant at the extremes of soil moisture values. From this improved understanding we would be able to further improve global soil moisture products.

4.5 Conclusions

Global gridded satellite and reanalysis soil moisture products require validation with in-situ soil moisture stations, and a harmonized global CRNS network of sensors presents a unique opportunity to investigate residual uncertainties between such products and the CRNS data. The regional networks of CRNS data were reprocessed through crspy, providing a unified and harmonized dataset of CRNS soil moisture estimates that span hydroclimates across the globe. The analysis in this chapter provides several key insights into the relative uncertainties of soil moisture estimates from CRNS, satellite, and modelled data, particularly looking at their spatial and temporal variations. One of the key conclusions of this chapter is that when comparing the satellite soil moisture to the reference CRNS soil moisture data, the source of uncertainty fluctuates with overall site wetness. Bias notably dominates at the extremities, i.e., at wetter and drier sites, while correlation and deviation become more influential at moderate sites. A similar pattern is seen for modelled data, with biases dominating at the most arid and saturated sites. This finding raises concerns regarding the accurate detection of extreme hydrological events such as floods and droughts, as the gridded products appear to be showing greater disagreement with our reference CRNS data during extreme periods of dry or wet soil moisture conditions. Moreover, the study reveals that error propagation is not only spatially variable but temporally variable as well, showing distinct characteristics for generally wet and generally dry sites. One key implication of these findings is that common bias correction and rescaling methods, such as CDF matching, may be suboptimal, particularly at the extremes of soil moisture, both spatially and temporally. By bias-correcting datasets to conform to the overall average statistics of a reference dataset, the dynamic nature of systemic biases across time is not properly accounted for. Furthermore, it is observed that when the Satellite soil moisture dataset that was CDF matched to ERA5-Land soil moisture data (Sat-CDF) is compared with our reference CRNS data, the overall statistics of the source dataset, in this case, the ERA5-Land soil moisture, are almost entirely transferred to the scaled dataset. This is evidenced by the similar sources of uncertainty between ERA5-Land soil moisture data and Sat-CDF soil moisture data, when compared to the reference CRNS soil moisture data. While temporal soil moisture dynamics from the satellite data are preserved, the overall RMSD profile bears a closer resemblance to the target ERA5-Land SM data. This could have implications when training models, particularly machine learning-based models, as we may inadvertently train them to match our target dataset more than our source. With the growing popularity of machine learning methods to tackle key questions in hydrology, further investigations will be necessary to fully understand these implications. The analysis clearly shows that both modelled and satellite products exhibit greater error, especially bias, at both ends of the soil moisture spectrum. Given that CRNS performs particularly well at arid sites, there is an opportunity for understanding differences from both model and satellite datasets and potential for future improvements. Knowing that the global CRNS sensors are harmonized in their processing methods, means that they can be treated as a reference dataset without additional scaling needed between them. Even so, there remains uncertainty related to the different spatial domains of the sensors when directly comparing them, and improvements to the commonly applied scaling methods are required. The newly formed global CRNS dataset presents a unique opportunity to further our understanding in this regard. In summary, residual biases remain between soil moisture products that appear to be more prevalent at the extremes of wet and dry periods. Current methods to address for this may be sub-optimal and additional research is required to better understand this impact and mitigate it in future products. The global CRNS network presents a unique opportunity to support research aiming to improve as a globally spanning and harmonized network of soil moisture sensors.

5 Exploring the role of soil moisture footprint in predictions of evapotranspiration and photosynthesis.

This chapter has been submitted to Environmental Research Letters for review. Rafael Rosolem, Miguel Angel Rico-Ramirez, and Pierre Gentine acted as co-supervisors throughout the development of this chapter. David McJannet, Humberto de la Rocha, Corinna Rebmann, and Martin Schrön all contributed with data processing, discussions, and development of the manuscript.

5.1 Introduction

Evapotranspiration (ET) and photosynthesis are important processes influencing ecosystem function. Gross Primary Productivity (GPP), for example, represents how much carbon dioxide is taken up by plants from the atmosphere via photosynthesis; while ET corresponds to the phase change of liquid water at the land surface to vapor back to the atmosphere. The magnitude and dynamics of both fluxes are controlled by a range of environmental factors. Here, we are particularly interested in understanding how the spatial representation of soil moisture (SM) can influence the predictions of ET and GPP simultaneously.

SM potentially serves as a strong regulator of fluxes at the land-atmosphere boundary (Seneviratne et al., 2010, Novick et al., 2016). For example, SM can directly impact ET, acting as the main source of water for soil evaporation or plant transpiration. When SM is limited, a reduction in ET leads to increased sensible heat flux, and consequently higher near surface temperatures. This ultimately leads to land-atmospheric feedback mechanisms that further constraints ET (Gentine et al., 2019; Green et al., 2019, Zhou et al., 2019), which can lead to further ecological and hydrometeorological stresses such as droughts and heatwaves that are potentially getting worse and more frequent under climate change (Miralles et al., 2019). Furthermore, the ability of plants to uptake carbon dioxide comes at a cost of losing water (vapor) at the leaf-air interface. This biophysical process is controlled by the stomatal functioning of plants, which is also governed by responses to environmental conditions, including SM (Bunce 2008). Overall, the influence SM can have on the land surface fluxes also depends on the local hydroclimate, with drier sites likely being strongly driven by changing SM conditions when compared to humid/tropical sites (Seneviratne et al., 2019). In addition, for relatively drier conditions, SM heterogeneity can result in challenges regarding accurately estimating SM at the ecosystem level (i.e., flux footprint) (Iwema et al., 2017).

The inter-relationship between ET, GPP, and SM have been and continue to be studied extensively with the success of in situ monitoring networks. The Ameriflux and FLUXNET are good examples of initiatives utilizing the eddy covariance technique around the globe and spanning decades of coverage (Baldocchi et al., 2001; Pastorello et al., 2020). Understanding the controlling factors of ET and GPP also plays a crucial role in improving the interactions between hydrology and biogeochemistry parameterized in Earth system models. However, despite its continuing growth, the spatial coverage of flux monitoring networks will always correspond to a small fraction of the actual land cover of the Earth. Hence, our ability to predict land surface fluxes everywhere globally relies on methodologies for extrapolating and upscaling our knowledge from the site level to larger areas. This can be achieved either through (physics-based) modelling (Clark et al., 2011, Best et al., 2011) or via data-driven, statistical, approaches (Tramontana et al., 2016). There are recent attempts to leverage machine learning methods, and the growing body of open data, to train machine learning models to make predictions of surface fluxes based on data from eddy covariance flux sites (Dou and Yang, 2018; Cui et al., 2021; Bodesheim et al., 2018; Jung et al., 2020; Barnes et al., 2021; Zeng et al., 2020). A popular approach is the FLUXCOM project (Tramontana et al., 2016) which provides global predictions of energy and carbon fluxes using several machine learning methods.

Whether using physics-based models or machine learning algorithms, the robustness of any approach ultimately relies on the volume and quality of available data. Particularly, SM can be estimated in various ways, each representing a distinct spatial coverage (i.e., SM "footprint"). For instance, Time Domain Reflectometry (TDR), Frequency Domain Reflectometry (FDR), and Time Domain Transmissivity (TDT) are all common methodologies employed for in situ (local) SM measurements and are usually referred to as point-scale methods (Robinson et al. 2008). We recognize that the above methods operate slightly differently, but for simplicity of the language, we refer to them here more generally as TDR. These sensors can be installed at various depths to monitor vertical SM changes, but only measure a small spatial footprint around the sensor, on the order of 10s of cm. Field scale SM estimates have become more accessible with the establishment of the Cosmic Ray Neutron Sensors (CRNS) (Zreda et al., 2008). The CRNS technology estimates root-zone SM at the so-called field scale (i.e., ~400-600 m diameter around the sensor and up to 0.5 m depth). A key aspect of the CRNS is that its footprint is similar in size with that of eddy covariance towers (Iwema et al., 2017). Previous studies investigated the potential of CRNS data in combination with eddy covariance fluxes, to close the water balance in semi-arid and agricultural sites (Schreiner-McGraw et al. 2016, Wang et al. 2018), and to estimate actual ET from SM measurements (Foolad et al. 2017). However, the use of this technology with several flux sites covering a wide range of biomes across the globe has not been previously explored. Large scale global SM estimates can be achieved with satellite remote sensing products, such as the Soil Moisture Active Passive (SMAP) (Entekhabi et al., 2010) or the ESA CCI SM remote sensing product (Dorigo et al., 2017; Gruber et al., 2019), two examples of many available products. Active remote sensing emits microwaves and measures the scattering of the signal, whereas passive remote sensing uses natural emissions of radiation from the Earth surface. These products tend to have a coarser horizontal resolution (several kms) and only estimate the surface SM layer (2-5cm depth) which can be somewhat decorrelated from deeper SM, more important for root zone regulation of surface fluxes.

Fundamentally, distinct SM estimates range from very localized spatial scales likely governed by differences in soil texture and properties, to field scales in which spatial variability of land cover and microtopography influences SM, and ultimately reaching large spatial coverage which is likely governed by variability of large meteorological features such as frontal systems. Each methodology, therefore, measures the different responses of SM to environmental conditions according to their spatial footprint (see Supplemental S1). However, despite having distinct SM "footprints", the estimates from different technologies are too often used interchangeably for spatial scaling without carefully evaluating the inherent impacts of their unique spatial representation.

In this study, we use machine learning to quantify how the spatial representation of SM (i.e., SM "footprint") can influence the ability to predict ET and GPP fluxes at the multiple sites located across a wide range of hydroclimates. We replicate the feature set from the established and widely used global upscaling model, FLUXCOM (Tramontana et al., 2016). In doing so, we keep the same attributes from FLUXCOM except for the attribute related to SM, which gets replaced by different sources of SM estimates representing distinct footprints. We expect the results can provide new insights into the benefits and limitations of scaling SM information in Earth systems applications.

5.2 Methods and data

5.2.1 Study sites

We identified 20 sites covering a wide range of biomes and hydroclimates globally with co-located TDR, CRNS sensors and eddy covariance towers, while satellite SM products are globally available (Table 1 and Supplemental S2). CRNS sites were available as part of the US COsmic-ray Soil Moisture Observing System (COSMOS) (Zreda et al., 2012), the Australian CosmOz (Hawdon et al., 2014), and the German TERENO project (Bogena et al., 2016, Wollschläger et al., 2016). We used FLUXNET

(Baldocchi et a., 2001) base data and further processed at each site to collect the appropriate flux variables for the sites in the USA. GPP was calculated by removing ecosystem respiration obtained from night-time Net Ecosystem Exchange (Reichstein et al. 2005), defined when incoming solar radiation was less than 5 W m^{-2} following Rosolem et al. (2010). Half-hourly flux data was aggregated to daily only if data gaps were less than 30% for that day. For the rest of the sites (one in Brazil, five in Australia, and two in Germany), the data were processed by local site investigators following similar steps.

We anticipate that the importance of SM representation will vary amongst different hydroclimates (i.e., more pronounced with increasing dryness conditions). To help us better characterize the hydroclimatology of each site, we computed the aridity index (AI) which is defined as the ratio of the mean annual precipitation over mean annual potential evapotranspiration. We use long-term annual means of precipitation and potential evapotranspiration calculated from 30-year data using the ERA5-Land reanalysis (Muñoz Sabater, 2019) and global potential ET (hPET, Singer et al., 2021) data products, respectively.

Table 5.1 provides information on each of the sites in this study. The site code is used in Figure 1 and 2 to differentiate each site. Included is the latitude and longitude, the FLUXNET eddy covariance tower name, data source for FLUXNET data, the aridity index (AI), land cover information, the Köppen-Geiger classification, and the plant functional type.

Site Code	Site name	FLUXNET Code	Latitude	Longitude	Aridity Index (P/PET)	Land Cover	Plant Functional Type	Flux Data Source
AUS2	Daly	AU-DaP	-14.16	131.39	0.57	shrubland deciduous	SAV	Beringer (2013)
AUS3	Gnangara	AU-Gin	-31.38	115.71	0.32	tree broadleaved deciduous open	WSA	Silberstein (2015)
AUS6	Robson	AU-Rob	-17.12	145.63	0.86	tree broadleaved evergreen closed to open	EBF	Liddell (2013)
AUS9	Tumbarumba	AU-Tum	-35.66	148.15	1.09	tree broadleaved evergreen closed to open	EBF	Woodgate (2013)
AUS11	Yanco	-	-35.01	146.3	0.33	mosaic cropland	GRA	Beringer (2013)
BRZ44	Pe-de-Gigante	BRZ-PdG	-21.62	-47.63	0.96	tree broadleaved evergreen closed to open	WSA	-
DEU20	Grosses Bruch	-	52.03	11.11	1.02	Cropland	CRO	Rebmann et al., (2023)
DEU28	Hohes Holz	-	52.09	11.22	0.96	Forest	DBF	Rebmann et al., (2023)
USA10	Kendall	US-Wkg	31.74	-109.94	0.16	Shrubland	GRA	Scott (2022)
USA11	Santa Rita Creosote	US-SRC	31.91	-110.84	0.2	Shrubland	OSH	Kurc (2019)
USA15	ARM-1	US-ARM	36.61	-97.49	0.68	Cropland rainfed	CRO	Biraud et al., (2021)

						herbaceous cover		
USA23	Pinyon/Juniper	US-SCw	33.61	-116.45	0.2	Shrubland	OSH	Goulden (2018)
USA24	Coastal Sage	US-SCs	33.73	-117.7	0.31	Shrubland	OSH	Goulden (2018)
USA27	Morgan Monroe	US-MMS	39.32	-86.41	1.21	tree broadleaved deciduous closed to open	DBF	Novick and Phillips (2022)
USA28	Mozark	US-Moz	38.74	-92.2	1.07	tree broadleaved deciduous closed to open	DBF	Wood and Gu (2022)
USA29	Neb Field 3	US-Ne3	41.18	-96.44	0.85	Cropland rainfed herbaceous cover	CRO	Suyker (2022)
USA32	Tonzi Ranch	US-Ton	38.43	-120.97	0.63	Shrubland	WSA	Ma and Xu (2022)
USA33	Soaproot	US-CZ2	37.03	-119.26	0.72	tree needleleaved evergreen closed to open	ENF	Goulden and Kelly (2019)
USA38	Metolius	US-Me2	44.45	-121.56	0.96	tree needleleaved evergreen closed to open	ENF	Law (2022)
USA60	Lucky Hills	US-Whs	31.74	-110.05	0.16	Shrubland	OSH	Scott (2022)

5.2.2 Feature list for ET and GPP predictions

To focus on the influence the SM spatial representation (i.e., footprint) has on regulating ET and GPP, we replicated an established set of features for predicting energy and carbon fluxes following the methodology from the FLUXCOM project

(Tramontana et al., 2016; Jung et al., 2019). To select the most important features for model training, the FLUXCOM team used a guided hybrid genetic algorithm (Jung and Zscheischler, 2013), leading to two unique sets of features developed for energy and carbon fluxes separately (see Table 2 in Tramontana et al., 2016). The feature list is further divided into three types: spatial features (site-specific), long-term climate features (averaged yearly and seasonal values), and short-term features (daily weather values). We did not use any spatial features in this study since our goal is to isolate the impact of SM representation on these surface fluxes at each site individually. This means that we trained separate machine learning models for each site. Site-specific mean seasonal cycles of the variables were derived from long-term (2001-2021) products available from the MODIS satellite data such as the Normalized Difference Vegetation Index (NDVI), Land Surface Temperature Day (LST_{day}), and fraction of photosynthetically active radiation (fPAR). Finally, short-term features were derived from in-situ sensors (such as air temperature) collected at each site (see Supplemental S3 for more details).

5.2.3 Soil moisture spatial representation (footprint)

Our study focuses on evaluating how distinct SM estimates can influence the prediction of both water vapor and carbon fluxes at the land surface. FLUXCOM uses a simple soil water balance approach aimed at capturing water stress effects. The Water Availability Index (WAI) is a simple bucket type model, here produced using ERA5-Land data, and used in the predictions of GPP; whereas the Index of Water Availability (IWA) is analogous to evaporative fraction and was used in the predictions of ET (Tramontana et al., 2016). Jung and Zscheischler (2013) did note that direct SM measurements could provide additional benefits over simulated representation of SM but were unable to integrate direct observations to the FLUXCOM platform at the time due to limited availability of data. For this paper, we will refer to both WAI and IWA approaches together as ‘empirical’ representation of SM.

For point-scale representation, we simplify the choice by using a single TDR sensor from each site, selected as the shallowest depth. Satellite remote sensing products measure SM at shallow depths and, while the CRNS can effectively reach deeper soils, its SM contribution to the signal decays exponentially from the surface towards deeper soils (Schrön et al. 2017). In contrast to point-scale TDR measurements, a single CRNS station can provide an area-average measurement of SM, thereby being insensitive to small-scale heterogeneity (Franz et al. 2013). For the CRNS sensors, raw data were processed using the *crspy* package (Power et al., 2021) to ensure a fully harmonised methodology across all sites. Finally, we used the ESA CCI soil moisture remote sensing product (Dorigo et al., 2017; Gruber et al., 2019) for the satellite SM product. This product merges multiple satellite remote sensing datasets over a long time period, spanning 1978 to today with a horizontal resolution of 25km.

5.2.4 Study aims and hypothesis

Our study aims to evaluate the impact of distinct spatial SM representation on the ability to predict ET and GPP. For that, we retain all input from the FLUXCOM feature list with the exception of factors associated with SM. Instead, we introduce four distinct ways to represent SM:

1. Empirical - Replicating the FLUXCOM method with WAI and IWA.
2. TDR - Time Domain Reflectometry point-scale sensor, often deployed at flux sites.
3. CRNS - Cosmic-Ray Neutron Sensors that provide field scale SM measurements.
4. Satellite - the ESA CCI merged product of multiple satellite sensors.

In addition, we added a final option, called “Null”, in which we completely remove any SM representation and use it as a reference comparison among all other options. Although we replicate our feature list from the FLUXCOM method, we have implemented slightly different steps from its original approach to better suit this study. Unlike the original FLUXCOM, we have not used any gap filled data. While gap-filling may result in a more balanced representation of the full seasonal behaviour of these fluxes, it can arguably lead to duplicated data within the training and validation datasets. This can result in data leakage issues impacting the overall performance scores of the model (Allamanis, 2018) because the proportion of gap-filled data in a dataset may become correlated with the overall performance. As our main goal here is to better understand the impacts of spatial representation of SM, we have chosen to trade data volume with robustness, by training our machine learning model on fewer but more reliable non-gap filled data points. When building the dataset of daily observations, if gaps in the data were found for any of the input features (e.g., the TDR sensor value is missing but the CRNS is available), the day was excluded from the training dataset entirely for all model runs. We believe this choice ensures that results more strongly represent the relationships from the measurements directly. A machine learning model is trained for each individual hypothesis listed above at each individual site separately. This allowed us to identify how different sites respond to SM data input.

The original FLUXCOM methodology was tested using multiple methods such as Random Forest and Neural Networks. Instead, our study employs an extreme gradient-boosted regression tree model known as XGBoost (Chen and Guestrin, 2016). XGBoost has been proven to be a powerful machine learning method for tabular data often outperforming artificial neural networks whilst being efficient and quick to apply, with minimum hyperparameter tuning (Shwartz-Ziv and Armon, 2022). Having an algorithm more suitable for limited data is important as our strict quality-flag conditions led to fewer available observations for training.

Our study is based on some key initial hypotheses. First, we hypothesize that the representation of the SM scale will be important, especially as site conditions get drier. Secondly, under relatively drier conditions, we also hypothesize that the knowledge obtained with directly observed SM at the site (i.e., in situ measurements from TDR or

CRNS) will result in better predictions of the fluxes compared to when using empirical methods or satellite remote sensing. Finally, with regards to the representation of in-situ direct observations of SM, we hypothesize that the improvements obtained with the CRNS will be superior to those obtained via TDR estimates, given the more comparable spatial scale obtained for SM with the CRNS to the fluxes measured at the sites.

5.3 Results

The performance of the machine learning models was assessed through k-folds cross validation at each site. Data from each site were randomly split into 10 equal bins, always leaving one out for testing. This process was repeated until all data have been treated as both training and testing data, with the average performance of the 10 models then calculated. To facilitate comparisons between the sites which have different magnitudes of fluxes, the results were normalised by dividing the models RMSE by the interquartile range of the predicted data, which is less sensitive to the influence of extreme values and allows us to see relative changes in RMSE from each model (Otto, 2019).

The results for ET predictions as presented in Figure 5.1. The sites have been ordered from most humid (left) to most arid (right) according to the Aridity Index whose classes are shown in the background (see Table 5.1 for individual values). There are key noticeable findings from this analysis. First, we found that the way we represent SM footprint at humid sites is unimportant. The results suggest that SM information at humid sites has a low impact on ET predictions overall. This is supported by the lack of spread in model performance from each tested representation, including the "Null" case.

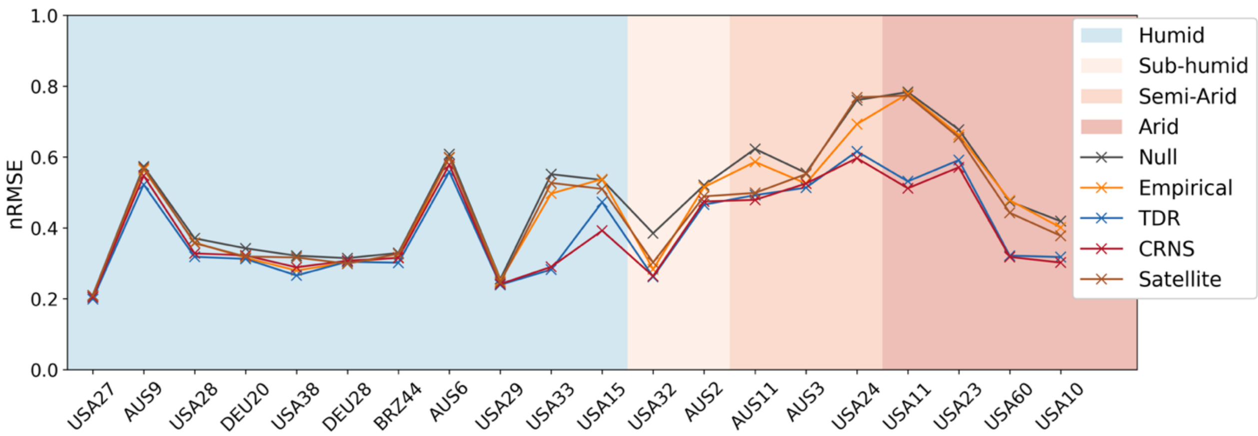

Figure 5.1 Average performance of ET predictions at each site using nRMSE obtained from different spatial representations of soil moisture. The sites are ordered from most humid (left) to most arid (right) according to Aridity Index classes shown in the background. The country of origin for each site is given in the name with sites being located in USA (USA), Australia (AUS), Germany (DEU), and Brazil (BRZ)

As initially hypothesized, the spatial representation of SM does indeed impact the prediction of ET fluxes as site conditions becomes drier. This is evident by a wider spread in model performance going from sub-humid to arid classes in Figure 5.1. In addition, ignoring the information obtained from SM can be highly detrimental as seen by the worst performance shown for the Null SM representation case. These findings likely indicate that knowledge of SM footprint is important for spatial scaling applications, as the SM information depends on its representation spatially. Our results further support our initial hypothesis that direct (in situ) observations of SM perform better in predicting ET fluxes. This is evident by the consistent lower nRMSE obtained at relatively drier sites from both CRNS and TDR cases in comparison to the empirical and satellite cases. We notice that empirical and satellite cases initially showed comparable performances to CRNS and TDR at sub-humid conditions, but both tend to deteriorate, and more closely compare with the Null SM representation, as aridity increases. Interestingly, our results could not support our initial hypothesis that ET predictions would show better performance using CRNS SM when compared to TDR SM. This initially suggests that SM footprint on the order of a few 100s of meters or smaller are equally beneficial for accurate predictions of ET fluxes.

While the results for GPP at humid sites follow the same pattern as seen with ET, the performance of the machine learning models are clearly different as aridity increases (Figure 5.2a). Although ignoring SM representation (i.e., Null case) has the same negative impact on nRMSE values for GPP, we did not find a clear performance benefit from cases where SM representation is obtained from in-situ direct measurements (i.e., CRNS and TDR) when compared to indirect SM representation (i.e., empirical) were used. In fact, the performance of the model using empirical estimates of SM is almost always superior at all sites from sub-humid to arid conditions. We also noted relatively poor performance of GPP prediction by machine learning models using the satellite remote sensing measurements.

Figure 5.2 Average performance of GPP predictions at each site using nRMSE obtained from different spatial representations of soil moisture without (a) and with (b) the addition of a soil moisture memory term. The sites are ordered from most humid (left) to most arid (right) according to Aridity Index classes shown in the background. Note fewer sites shown here due to unavailability of data. The country of origin for each site is given in the name with sites being located in USA (USA), Australia (AUS), Germany (DEU), and Brazil (BRZ).

For GPP predictions at relatively drier sites, our findings indicate a more pronounced role exhibited by the integrated depth-profile of SM. This is strongly evident with the highest performance obtained with the 2-layer bucket type empirical model used by

FLUXCOM which acts as an indirect buffer (i.e., memory from deeper soils) for SM available for photosynthesis. On the other hand, shallow and instantaneous estimates of SM from satellite remote sensing offer the overall least improvements on GPP predictions from all cases where SM is represented in some way.

To test this assumption, we trained additional machine learning models for each of the original soil moisture representations, in which an explicit SM memory factor is included in the original feature list. We calculated SM memory by taking a rolling-average of CRNS SM over the previous 30-days. We chose CRNS to calculate SM memory because it is a direct in situ estimate which can reach slightly deeper soils, compared with TDR, especially at drier sites (Zreda et al., 2008, Schrön et al. 2017). The memory period of 30 days was obtained based on our analysis of varying memory lengths (Figure 5.3). For that, we retrained the XGBoost models for each site, with increasing lengths of memory period (from 0 to 80 days in two-day increments). The more arid sites show a greater improvement from increasing memory lengths up until 30 days, at which model improvements stop, or in some cases performance even degrades. Performance at humid sites also improves although at a smaller rate, as shown in the lower plot showing relative improvement against no SM memory.

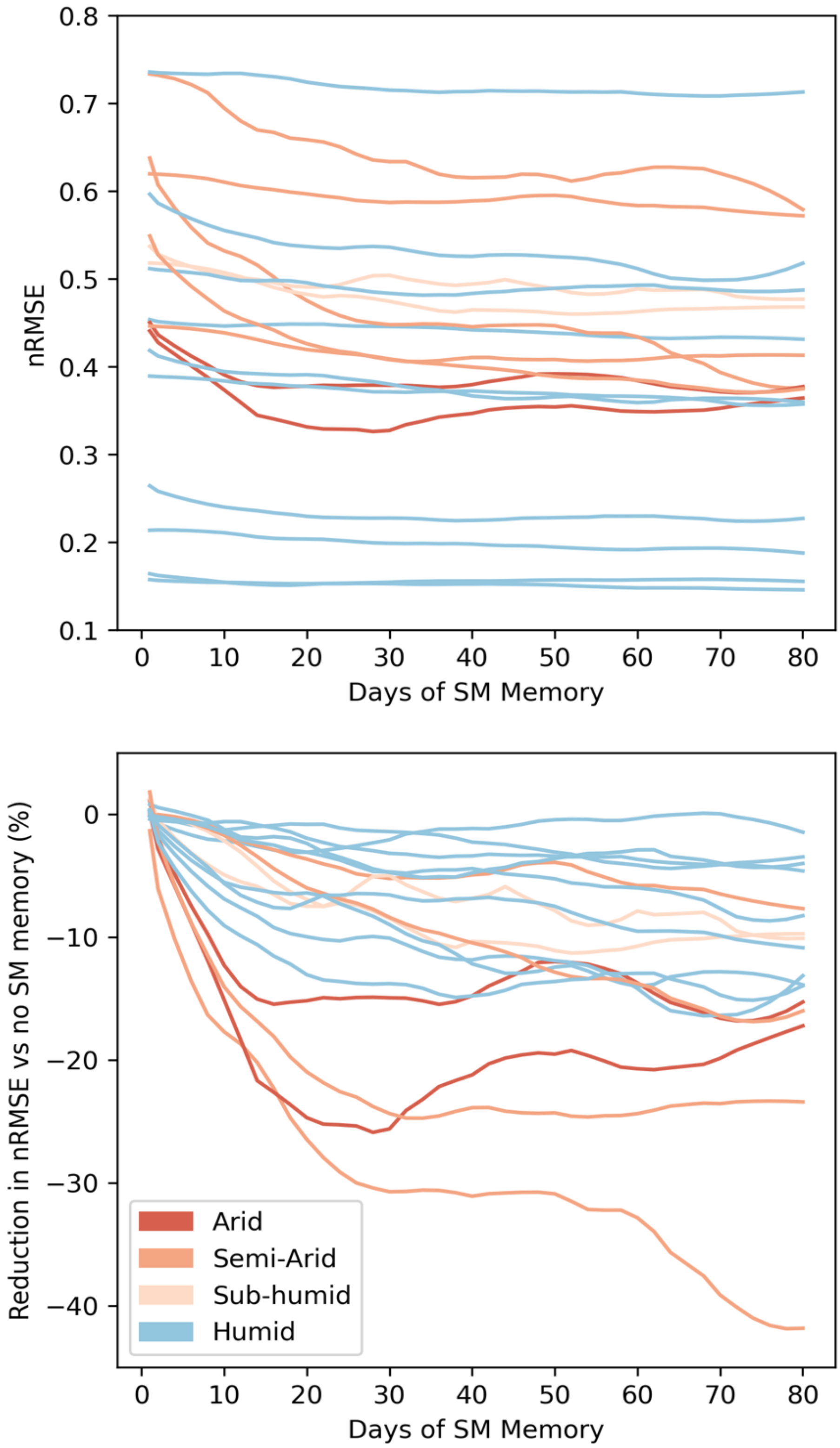

Figure 5.3 (a) Model performance (nRMSE) in predicting GPP for increasing length of soil moisture memory. (b) Relative reduction in nRMSE when compared to same model performance with no soil moisture memory provided (i.e., daily soil moisture only). Individual lines represent one site, colour-coded by their aridity classes. The CRNS soil moisture data were used for this analysis.

Interestingly, when the 30-day SM memory is included in the prediction of GPP, model performance is improved across almost all instances (Figure 5.2b), with arid and semi-arid sites showing improvements in RMSE of up to 30% or more (Figure 5.3). The spread in model performance from all different representations of SM is almost entirely removed across all aridity classes, from humid to arid. This is even evident when SM memory is used but without actual instantaneous knowledge of SM (i.e., our Null SM case). Surprisingly, this feature did not appear to be as important for ET predictions, particularly at the more arid sites (Supplemental S4) which could indicate a distinct role of SM when predicting ecosystem-based quantities (i.e., ET) versus plant-based quantities (i.e., GPP).

5.4 Discussion

Our findings suggest that the way we spatially represent SM can play a key role in improving the performance of land surface flux predictions, but it does so differently for ET and GPP fluxes. We found that ET predictions, particularly at arid sites, perform best when in-situ SM estimates are used by the machine learning model, in contrast to indirect estimates (i.e., empirical, or remote sensing) (Figure 5.1). On the other hand, the lower impact of SM representation observed at humid sites is not surprising as these sites are usually not water limited and so other features provided more strongly influence ET predictions.

Originally, we expected a stronger delineation, in terms of overall predictive power, between the two representations of in-situ data (CRNS and TDR), as found by Schreiner-McGraw et al. 2016. That is because TDR and CRNS observations correspond to different spatial scales (Iwema et al., 2017, Schrön et al., 2017), with the latter being more comparable to the typical footprint of flux towers. Our findings did not support this hypothesis, as demonstrated by the fact that the difference between the performance of ET predictions obtained with point-scale (TDR) and field scale (CRNS) is small (Figure 5.1). This remains the case even though we can see that the absolute values are different (Supplemental S1). As flux sites are typically setup at largely homogeneous areas (Rebmann et al., 2018), this resulted in limited spatial heterogeneity at field scale, possibly diminishing the benefits of using CRNS, compared to TDR, under such conditions. Additionally, machine learning models are powerful tools for bias correction and have been used for this specific purpose already (Lary et al., 2019). It is possible that the differences between CRNS and TDR are less pronounced than found between in situ sensors and empirical or satellite products.

The satellite SM data did not show the same improvement in predicting ET when compared against our Null SM representation, as we find for the in-situ datasets (Figure 5.1). We are not applying bias correction to the satellite SM data in this study as we are primarily interested in understanding the role of spatial scales and how they may impact our results. As previously noted, machine learning models are demonstrated as good bias correctors themselves (Lary et al., 2019), but in our study, the dynamics of satellite SM do not correlate as strongly with in-situ datasets. This may explain its relatively lower performance when compared to the in-situ SM measurements, due to satellite products being associated with shallower, more dynamic, SM representation than in-situ SM. The satellite product used here is the ESA-CCI Soil Moisture, a merged product of multiple satellites, with physical SM ranges constrained by GLDAS v2.1 (Dorigo et al., 2017), which suggested superior performance than single satellite products when compared to in-situ measurements (Beck et al., 2020). The resolution of ESA CCI is 25km which may also be too coarse horizontally to provide information on SM conditions at the field scale. For instance, a recent study has shown that we can lose up to 80% of the information contained in SM when moving from a 30m resolution to a 1km resolution (Vergopolan et al., 2022).

For GPP predictions, whilst SM representation is important, we found that the empirical SM representation with a simple 2-layer bucket model yielded overall best results, especially as aridity increases (Figure 5.2a). This result possibly indicated a potential buffering effect from the empirical model indirectly acting as SM memory. By explicitly introducing a 30-day soil memory, we demonstrated the improvement in predicting GPP across all models trained (Figure 5.2b). This improvement is more noticeable at transitional to arid sites, with little impact from SM representation at the humid sites. Our results concur with a more recent machine learning GPP product (DryFlux) which also includes antecedent moisture conditions in the form of the previous months of precipitation in its machine learning model (Barnes et al., 2021). We further tested this by training our GPP models using a rain memory feature (i.e., an average of rainfall over previous 30 days), instead of SM. We found similar improvements to GPP predictions demonstrating that antecedent conditions of moisture are important more broadly (Supplemental S4). For completeness, we also carried out the same analysis including the SM memory feature for ET predictions. In this case, we found that although this new feature led to slightly improved predictions compared to no SM memory, the ET predictions using instantaneous in-situ SM still performed better at drier sites (Supplemental S5).

When considering why GPP and ET predictions respond so differently to the various SM representations tested in our study, an important distinction to make is that GPP is related to plant-only processes, whereas ET is an integrated ecosystem quantity with contributions from both vegetation and soil (i.e., ground evaporation, plant transpiration, and canopy interception loss). This is especially relevant considering that the semi-arid sites contain lower ecosystem biomass overall. In this case, our findings point to the fact that direct in-situ estimates of SM are strongly associated with the local evaporation portion of the ET process, particularly from the ground. Our findings show, however, that a different SM mechanism, in which memory plays a primary role, is more important for better predictions of plant-related fluxes, such as GPP. We interpret this as the water reaching the surface taking sufficient time to be transported down to deeper soils, even beyond the sensing depth of the measurement technologies tested in this study. Given the strong relationship between photosynthesis and transpiration via stomatal control (Scott et al., 2006), our results suggest that the role of SM memory may also be important for predictions of transpiration flux only.

We found the sites with the greatest impact from SM representation to be the semi-arid and arid sites, which all have a land cover primarily made up of shrubland. Rooting systems in shrublands can vary from shallow laterally expanding roots, to deeper penetrating tap roots (Silva and Rego, 2003, Sivandran and Bras, 2013). It is possible that even the deepest SM in-situ representation in our study (i.e., CRNS) fails to sense the deeper SM that the tap roots of these plants have access to. This could explain why similar sites show different responses to SM representation. For example, USA60 and USA10 are both sites within the Walnut Gulch experimental area in Arizona (AI=0.16), but USA60 appears to have a greater dependence on SM memory conditions when compared to USA10 for GPP predictions, apparent due to the larger spread between the trained models (Figure 5.2b). Whilst the landcover between both sites is broadly similar the exact composition of plants differs (see site descriptions at https://fluxnet.org/sites/site-list-and-pages/, last accessed 14/06/2023). While, the USA60 site consists of a greater proportion of sagebrush shrubs, the USA10 consists of less than 10% shrub cover, being more dominated by grasses. This example suggests that plant rooting strategies may be playing a large part in whether longer term, deeper SM is more important for GPP predictions in comparison to how we horizontally represent SM footprints. In summary, our findings strongly suggest caution must be taken when scaling of land fluxes are carried out in places where SM is expected to play a role, especially as site aridity increases. In those circumstances, the replacement of SM products should carefully be carried out with knowledge of their SM footprint for ET predictions, while a SM memory term should be considered (directly or indirectly) for prediction of plant-only fluxes such as GPP and even transpiration.

5.5 Conclusion

Upscaling land surface fluxes of water, energy, and carbon for global coverage is of utmost importance for our better understanding of Earth system processes and associated feedback. Yet, when it comes to the role SM plays in influencing those predictions, little effort is devoted to better understand how different spatial footprint of SM impacts those fluxes. This results in different SM estimates being used interchangeably despite their distinct spatial representation. In this study, we have demonstrated using machine learning techniques that SM footprint does exert a strong influence on land-atmosphere fluxes of carbon and water, especially in transitional to arid climates. We found that for relatively dry sites (semi-arid to arid), the spatial footprint of SM is an important aspect that needs consideration.

Interestingly, our results suggest distinct SM mechanisms are driving GPP and ET predictions. For ET predictions, SM footprint is important and particularly knowledge of in-situ (direct) SM measurements provides the best performance. However, we were not able to quantify any benefit of using field-scale estimates from CRNS, arguably with a more similar footprint to flux towers, in comparison to point-scale (TDR) representation. Our findings also suggest there are still significant benefits in relying on direct (in-situ) SM observations over new satellite remote sensing or empirical models, especially at semi-arid and arid sites. Despite its importance, SM monitoring networks are still far from providing optimal coverage worldwide, especially in regions where changes due to climate are expected to be of significant impact (Bassenbacher et al., 2023), and continued efforts to improve this are crucial. At transitional to arid sites, GPP is primarily influenced by SM memory which is more related to deeper SM dynamics. Here, we assume GPP acts as a function of plant-only activity, hence the increased importance of root water up takes from deeper soils. Importantly, we expect a similar mechanism takes place for the transpiration flux due to intrinsic stomatal regulation influenced by root zone moisture with longer memory. Unlike GPP, the ecosystem-based ET comprises contributions from soil and plants, and at semi-arid and arid sites, soil evaporation plays an important role together with transpiration from shrublands. Our study provides additional insights on understanding the true nature of SM footprint for land surface fluxes predictions and urges caution when spatial scaling approaches are implemented if SM from different products, representing different spatial scales, are used interchangeably.

5.6 Supplemental Material

S1 – Examples of soil moisture data

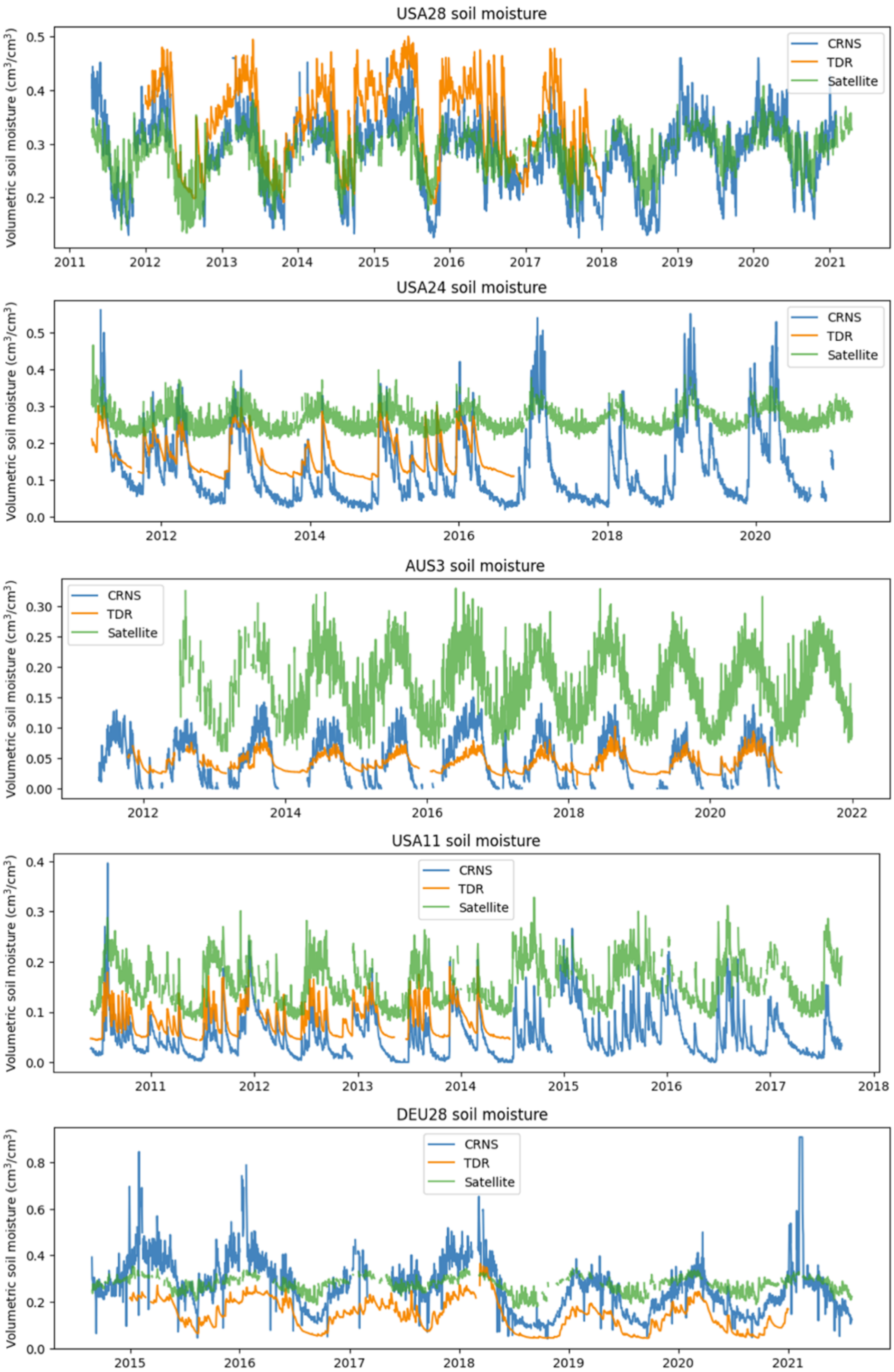

Figure 5.4. Example from selected sites of daily soil moisture time-series obtained with point-scale Time Domain Reflectometers (TDR), Cosmic-ray Neutron Sensor (CRNS), and the ESA CCI Soil Moisture satellite product (Satellite).

S2. Site locations

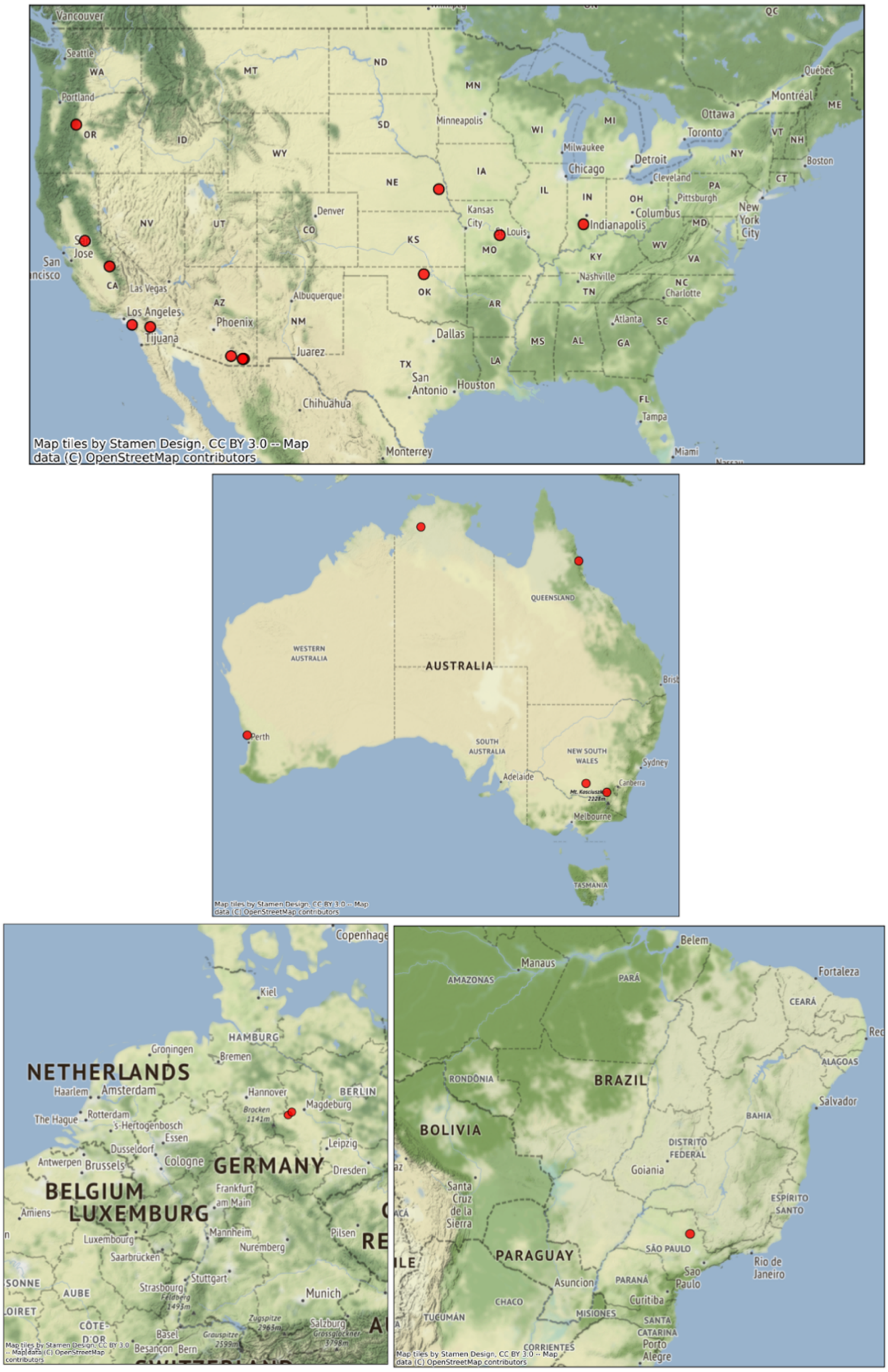

Figure 5.5. Geographic location of the sites used in this study. Please refer to Table 1 in the main manuscript for site summary.

S3. Features used in XGBoost model.

Table S3 lists input features used in training the XGBoost models to predict either Gross Primary Productivity (GPP) or Evapotranspiration (ET) fluxes. The feature list is adapted from Tramontana et al (2016) for the FLUXCOM methodology. One of the key differences in our work, in comparison to the FLUXCOM methodology, is that we train machine learning models for each site separately. Therefore, we do not use the spatial (static) site descriptors available in the original feature list as such information becomes irrelevant at each site individually.

Table 5.2 Features used in the machine learning model implementation adapted from the original definitions by Tramontana et al (2016). MSC refers to the Mean Seasonal Cycle derived from 20 years of data collected from the MODIS satellite datasets. LST refers to Land Surface Temperature, Rpot refers to Potential Top of Atmosphere Radiation, NDWI refers to the Normalized Difference Water Index, EVI refers to the Enhanced Vegetation Index, NDVI refers to the Normalized Difference Vegetation index, fPAR refers to the fraction of photosynthetically active radiation, SW_IN refers to Incoming Shortwave Radiation measured at each flux site. In our case, SM refers to Soil Moisture which changed depending on which representation was tested (see Methods and data in the main article), and SM_MEM is the Memory aspect of Soil Moisture used at specific cases as discussed in the main paper.*

Gross Primary Productivity (GPP)	**Evapotranspiration (ET)**
MSC of LSTnight	Rpot
MSC of (fPAR, LSTday)	MSC of NDWI
MSC (EVI, Rpot)	MSC of LSTnight
Temperature (air)	MSC of (EVI, SW_IN)
(SW_IN, MSC of NDVI)	Rain
SM*	
SM_MEM	SW_IN
	Relative Humidity
	SM*
	SM_MEM

The different MODIS datasets were obtained using the Google Earth Engine platform (https://earthengine.google.com/, last accessed 19/07/2023). Below lists the specific products used in compiling the features described above:

EVI/NDVI: MOD12A2.061 Terra Vegetation Indices 16-Day Global 1km
LSTday/LSTnight: MOD11A2.061 Terra Land Surface Temperature and Emissivity 8-Day Global 1km
fPAR: MOD15A2H.061 Terra Leaf Area Index/FPAR 8-Day Global 500m
NDWI: MCD43A4_006_NDWI MODIS Combined16-Day NDWI

S4. Comparison between rain memory and soil moisture memory on Gross Primary Productivity (GPP) predictions

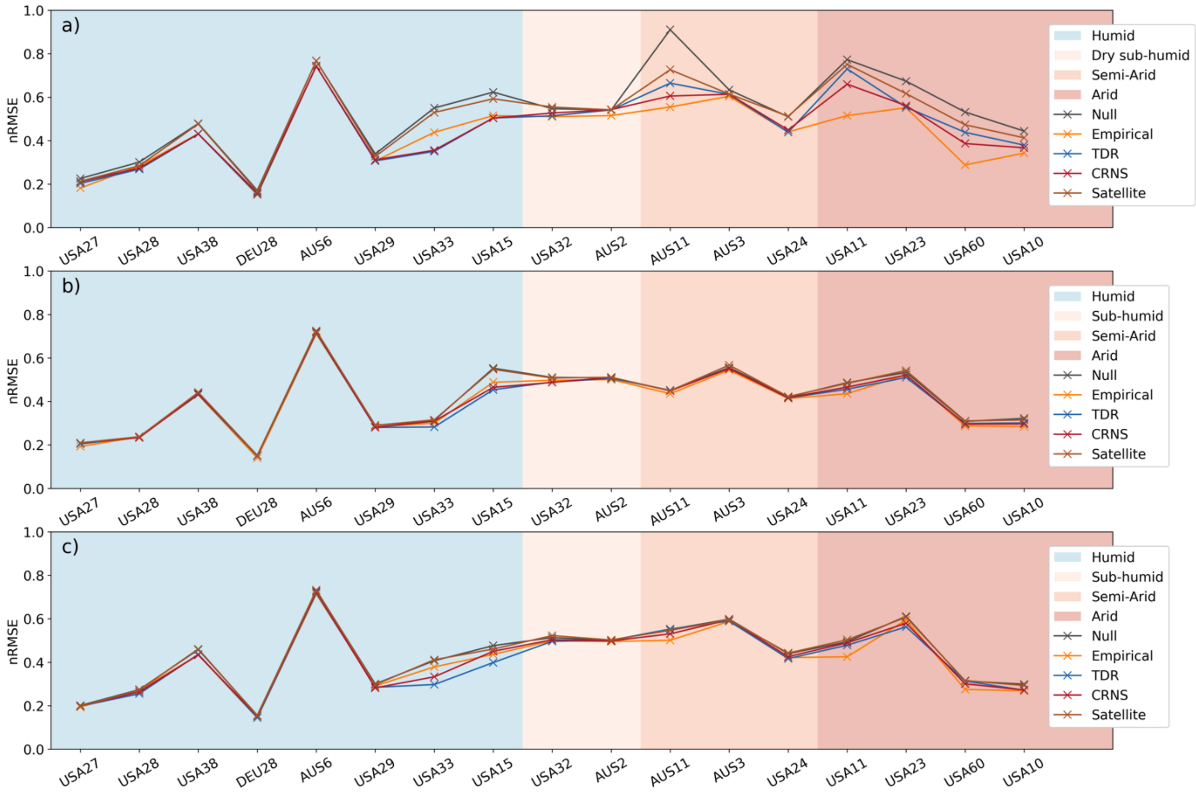

Figure 5.6. The first two panels (a) and (b) are the same as shown in Figure 2: Average performance of GPP predictions at each site without (a) and with (b) the addition of a soil moisture memory term. The bottom panel (c) shows the average performance of GPP predictions at each site with the addition of a 30-day rainfall memory attribute instead of a SM memory

S5. The impact of soil moisture memory on Evapotranspiration (ET) predictions

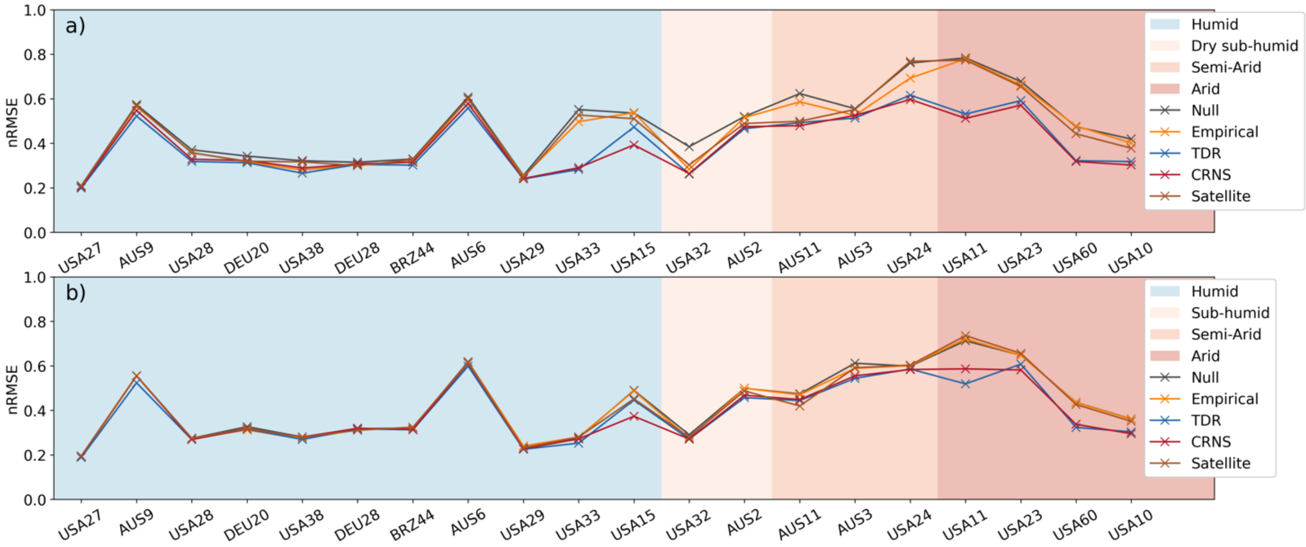

Figure 5.7 ET predictions using the standard feature sets (a) and including a 30-day soil moisture memory (b). Whilst we find broad improvements in model performance when including the SM memory feature (b), we still find an additional improvement from including daily in situ soil moisture values, (e.g., at sites USA11, USA23, USA60, and USA10).

6 Conclusions and Outlook

Soil moisture plays a critical role in earth system processes, including hydrology, atmospheric interactions, and ecosystem health. The growing availability of Cosmic-Ray Neutron Sensor (CRNS) data offers exciting new opportunities for conducting "large-sample hydrology" studies aimed at enhancing our understanding of soil moisture's role in global Earth system processes. This is increasingly important as Earth system models evolve with finer spatial resolutions, making obtaining soil moisture data at relevant scales increasingly important. CRNS stands out for its ability to capture field-scale soil moisture dynamics, thanks to its spatiotemporal coverage and the growing number of sensors worldwide. Despite its promise, CRNS data utilization faces challenges, such as differences between regional CRNS networks leading to inconsistent data processing methods. These variations introduce uncertainties in data comparisons, hindering their application in large scale and global studies. To date, no studies have successfully employed a globally harmonized CRNS dataset for this purpose. This thesis serves to improve our ability to utilize CRNS in a large sample hydrology way, conduct the first large sample type studies with this newly harmonized resource and further our understanding of soil moisture's role in key Earth system processes with machine learning.

The goal of this thesis was to:

> *Investigate the opportunities of a harmonized and globally spanning dataset of CRNS-derived soil moisture to increase our understanding of the role of soil moisture in Earth system sciences applications.*

This was achieved through the research presented in Chapters 3, 4, and 5. The key overall contribution of this thesis is in demonstrating the value of a harmonized global CRNS dataset for exploring soil moisture’s role in Earth system dynamics and presenting methods to facilitate such research in future studies. Individual contributions from each chapter, as well as a final summary of this thesis's overall contribution to the field, are detailed below.

To address the existing issue of a lack of harmonization between CRNS data across various networks, Chapter 3 introduces *crspy*, the first open-source Python package designed to easily process CRNS data. Until now, each CRNS network or sensor owner handled data processing individually, adhering to their own protocols, which led to inconsistencies when comparing data beyond a regional scale. One of the key contributions of this chapter is the building, testing, and release of the first open-source python package, specifically designed to facilitate processing of multiple CRNS stations at once. A second key contribution of this chapter is using *crspy* to highlight how regional discrepancies in CRNS networks could impact the validity of global studies. As shown in Chapter 3, differences between each network's decision for processing incoming neutron intensity leads to changes in calculated soil moisture values. Crspy is designed to facilitate the processing of large batches of sites at once, with the flexibility to choose which correction steps to apply. It additionally integrates with other products for correction steps, such as the nmdb.eu database for incoming neutron correction or ERA5-Land to address missing data. The tool allows for harmonization which ultimately facilitates multi-site comparison at continental to global scale. Another key aspect of crspy is its metadata component, specifically designed to support large-sample hydrology studies by detailing descriptions of available sites. The open-source nature of crspy encourages the CRNS research community to adapt the tool for various research needs, such as testing revised theories of sensor correction and calibration. In short, crspy unlocks the potential of conducting large-sample hydrology studies using a harmonized CRNS network.

Next in Chapter 4, it is shown that there are varying sources of uncertainty in soil moisture estimations by comparing a harmonized global CRNS dataset to satellite and model-based soil moisture products. The key contribution of this chapter is showing that there remain residual biases in global gridded soil moisture products, when compared to harmonized CRNS data, and revealing the potential limitations of common rescaling techniques like CDF matching. Utilizing crspy, 163 CRNS stations were harmonized into a single, global dataset for comparison. The soil moisture data of each site were then compared to the corresponding values obtained from satellite remote sensing (ESA-CCI) and land surface model (ERA5-Land) products of soil moisture. The overall mean squared error was further decomposed into its three constituent parts; bias, deviation, and correlation, to better understand what source of error is dominant at each site, and how these change in space and time. The analysis reveals that dry and wet extremes are mainly influenced by bias, whereas transitional sites show a higher prevalence of correlation and deviation errors. Interestingly, this pattern does not hold when comparing satellite remote sensing to land surface models, where uncertainty sources are largely consistent across the sites. Seasonal variations also influence the dominant source of error; drier sites have more correlation and deviation errors during wet periods, and wetter sites display the opposite pattern. This is particularly important given that many common bias correction techniques, such as CDF matching, correct a time series to the total error profile, meaning that additional biases may be introduced to the dataset at some points of the year. Ultimately, the chapter highlights that while global soil moisture products like satellite remote sensing and land surface models hold great value, they come with uncertainties that are spatially and temporally inconsistent.

Chapter 5 explores the role of spatiotemporal soil moisture representation in predicting land-atmosphere fluxes of carbon and water. The key contribution of this chapter is showing that soil moisture data source is highly influential on the accuracy of machine learning predictions of evapotranspiration (ET) and gross primary productivity (GPP), particularly in water limited regions. Another key contribution is showing the contrasting mechanisms driving ET and GPP; with deeper soil moisture values (proxied through soil moisture memory) improving GPP predictions, and surface soil moisture being more closely linked to accurate ET predictions. Increasingly data driven, machine learning methods are being applied in the prediction of key environmental processes.

To achieve these outcomes, the methodology of an established machine learning model for land-atmosphere flux predictions (FLUXCOM) was used. We showed that in-situ soil moisture representation can particularly improve predictions in more arid and water stressed regions. Daily in-situ measurements of soil moisture increased model performance for ET predictions. On the other hand, GPP predictions benefit from considering longer-term and deeper soil moisture values. Deeper soil moisture values can be inferred in ML models through the soil moisture memory, which is in this study is an average of soil moisture over the previous month. The memory period was shown to incrementally improve predictions up until around 30 days, although the exact memory period impact varied between sites. Feature selection and engineering are crucial in machine learning models, emphasizing the need for high-quality, in-situ soil moisture data. Care should be given when selecting a source of soil moisture data for such tasks, as the selection has been shown to have a large impact on model outcomes. This chapter ultimately advocates for the expansion of in situ soil moisture monitoring networks, particularly in water-limited areas like semi-arid and arid regions, to improve predictive accuracy where soil moisture has the highest impact.

Overall, this thesis highlights the potential in applying a large sample hydrology approach to harmonized CRNS networks on a global scale. CRNS sensors are crucial in monitoring and understanding field-scale soil moisture dynamics worldwide. While global expansion of these sensors is continuing, a critical barrier has been the absence of harmonized data processing methods. To address this, Chapter 3 introduced the first open-source tool designed for batch processing of multiple CRNS sites, thereby enabling large-scale and global studies. Chapter 4's analysis demonstrated that the now harmonized CRNS network, when compared to established satellite and reanalysis products, revealed varying sources of error dependent on site soil moisture conditions. Whilst satellite-based soil moisture products offer global data availability, they still come with uncertainties, especially when compared to in-situ CRNS measurements. Chapter 5 shows that machine learning predictions of surface fluxes like ET and GPP improved significantly with in situ sensor data, but not so much with satellite or modeled data. In particular, deeper soil moisture values were shown to be important for predictions of GPP, and by extension transpiration. A global and harmonized soil moisture dataset, such as that available with CRNS, can facilitate global soil moisture research.

Through the research of this thesis there are various implications to soil moisture science, plus several directions that could provide additional insights to those already shown above. First off, the open-source tool, *crspy*, has proven to be valuable and should continue to evolve in two main directions: simplified versions for newcomers and advanced versions for cutting-edge research. Such software not only educates the next generation of CRNS researchers but also serves as a valuable resource for real-world applications, as demonstrated in Appendix C through smart agriculture irrigation. Recent work by McJannet and Desilets (2023), which revisits how to correct for incoming neutron intensity, further underscores the need for modular software components that can easily integrate emerging theories or formula revisions, thus benefiting global research with CRNS. Beyond software, this thesis underscores the value of in situ soil moisture networks, especially in water-stressed regions. Bassenbacher et al., (2023) have already stressed the importance of optimizing sensor placements in the future, something further validated by Chapters 4 and 5 of this thesis. Future work should employ the harmonized, global CRNS dataset to identify gaps in current monitoring, integrating concepts, such as soil moisture signatures, to pinpoint underrepresented areas (Branger and McMillan 2019, Araki et al., 2021). While global in-situ coverage may be unfeasible, we can leverage the unique strengths of both satellite and in-situ data. Future research should continue focus on exactly how and why satellite remote sensing soil moisture estimates differ from in-situ sensors and seek methods to correct the globally spanning satellite datasets to better match in-situ dynamics. Ultimately, a harmonized global CRNS network will present unique opportunities for understanding soil moisture's earth system impact, and continued efforts to expand, support, and grow such networks are crucial.

Co-Authored Works

The following section briefly outlines the contribution I made to three pieces of research of which I was not the main author.

Appendix A – Detecting Ground Level Enhancements Using Soil Moisture Sensor Networks

Hands, A. D. P., Baird, F., Ryden, K. A., Dyer, C. S., Lei, F., Evans, J. G., Wallbank, J. R., Szczykulska, M., Rylett, D., Rosolem, R., Fowler, S., Power, D., and Henley, E. M.: Detecting Ground Level Enhancements Using Soil Moisture Sensor Networks, Adv Space Res, 19, https://doi.org/10.1029/2021sw002800, 2021.

For this work I utilised the newly developed crspy tool to reprocess sites across the COSMOS (USA/Canada) network to update missing corrections in the original dataset. Datasets were developed with and without certain corrections based on the project needs, demonstrating the versatility of crspy.

Ground Level Enhancements (GLE) are space weather events that have huge negative consequences for the aviation industry. Solar activity increases atmospheric radiation to levels, leading to higher levels of neutrons in the atmosphere, which cause problems with avionic equipment and pose a danger to passengers and crew. Given this, there are ongoing efforts to monitor space weather activities such as this, which can lead to earlier detection and prevention of the worst impacts of such events. However due to the prohibitive cost of such detectors there are relatively few active across the world, with none currently operating in the UK. CRNS effectively measure the same thing as these larger detectors, albeit on a smaller scale. This leads to an opportunity to explore whether this network of CRNS could be used to monitor and detect adverse space weather events. The goal of this research was to investigate the feasibility of converting the CRNS network across the UK (and the globe) into a space weather monitoring network giving it a dual purpose.

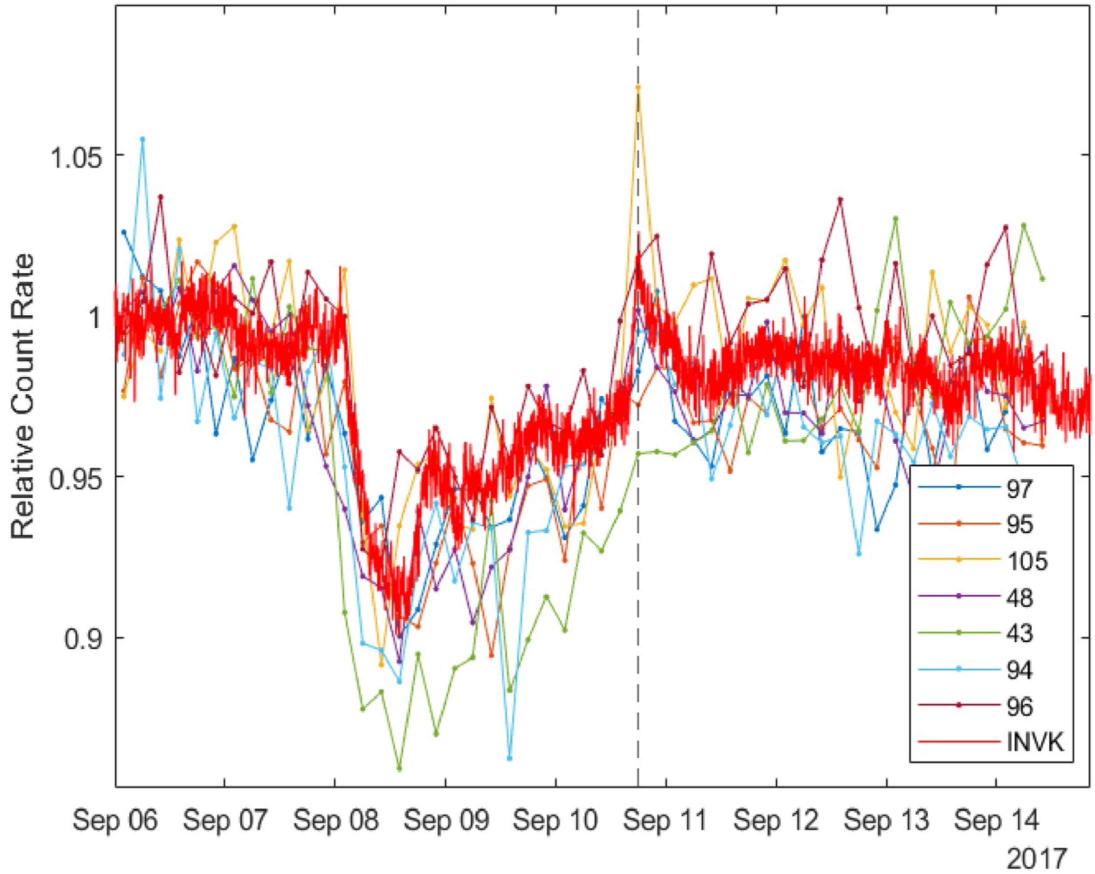

Figure A1 Renormalized COsmic-ray Soil Moisture Observing System data from seven stations during ground level enhancement (GLE72) in September 2017 (lines with dotted points). Equivalent renormalized count rates from the Inuvik (INVK) neutron monitor station are also plotted (red line). GLE72 is represented by a dashed vertical black line.

Hands et al., (2021)

The key outcome of this research was in demonstrating that the current CRNS network can compliment the global neutron monitor network to provide space weather detection at finer spatial resolutions. Whilst recent GLEs where shown to be only barely noticeable, simulations showed that larger GLEs, that have occurred historically, could be detected by the network of CRNS. Given this it is suggested that work starts quickly on extending CRNS sensors to sites that could further support such activities, whilst also providing valuable soil moisture data concurrently.

Appendix B - Evaluation of reanalysis soil moisture products using Cosmic Ray Neutron Sensor observations across the globe.

Zheng, Y., Coxon, G., Woods, R., Power, D., Rico-Ramirez, M. A., McJannet, D., Rosolem, R., Li, J., and Feng, P.: Evaluation of reanalysis soil moisture products using Cosmic Ray Neutron Sensor observations across the globe, Hydrol. Earth Syst. Sci. Discuss. [preprint], https://doi.org/10.5194/hess-2023-224, in review, 2023.

For this project I processed CRNS data using crspy to provide a global harmonized dataset. I also provided my expertise on the sensor technology and data structure in discussions on how best to approach the analysis in the paper. It is currently under review at the journal of Hydrology and Earth System Sciences.

Information on soil moisture is critical for hydrological sciences, such as in the prediction of drought or flood events. Given this importance there is continued emphasis on the expansion of soil moisture monitoring stations across the globe. However, it would be impossible to monitor every part of the globe due to the prohibitive cost of setting up and maintaining monitoring stations. Given this, there is a growing number of reanalysis products that attempt to fill the gaps, spatially and temporally, where soil moisture data is missing in historical records. With these products research can be conducted across the globe in previously unmonitored locations. However, it is important to continue to validate such models against in situ sensors to ensure that the estimated values are consistent with more directly measured values. The CRNS serves as a great opportunity for such studies due to its field scale, root-zone spatial coverage and growing number of sites across the globe. However, a lack of harmonization between the networks has limited such studies in the past. Here we use globally spanning and harmonized CRNS stations to validate multiple reanalysis soil moisture products to test the performance against various metrics.

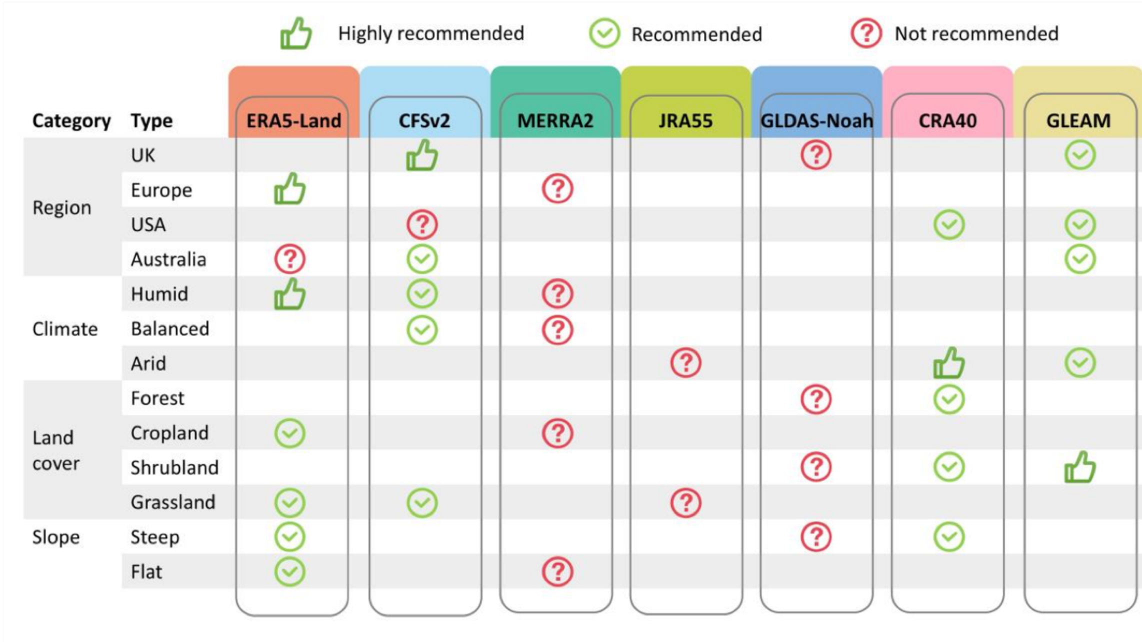

Figure A2 shows recommendations for 7 different reanalysis products based on their performance under various regions, climates, land cover, and topographic slope conditions.

Zheng et al., (2023)

One of the key conclusions of this study was that the performance of different reanalysis products varied based on different conditions. Figure A2 above shows the overall suggestions for which product to choose if a study is interest in a particular area of interest. This study paves the way for future research into exactly why different products perform well, or not well, under certain conditions, whilst also assisting researchers in deciding on a suitable source of data for future studies.

Appendix C – COSMIC-SWAMP

The COSMIC-SWAMP project is an ongoing project of which I've been a part of. Led by Patrick Stowell (University of Durham) and including partners from the UK, Germany, and Brazil, the overall goal of this project is to interface newly developed CRNS soil moisture sensors into an Internet of Things smart irrigation system (SWAMP) for smart irrigation. As part of this project, I have been primarily involved in leading the development of a new version of crspy that could tackle real time processing of CRNS data and easily fit into an already developed system. To achieve this the crspy software was converted into an Application Interface Program (API) and rewritten into a Docker container. This allows the server version of crspy (crspy-server) to be easily integrated into already established set of software.

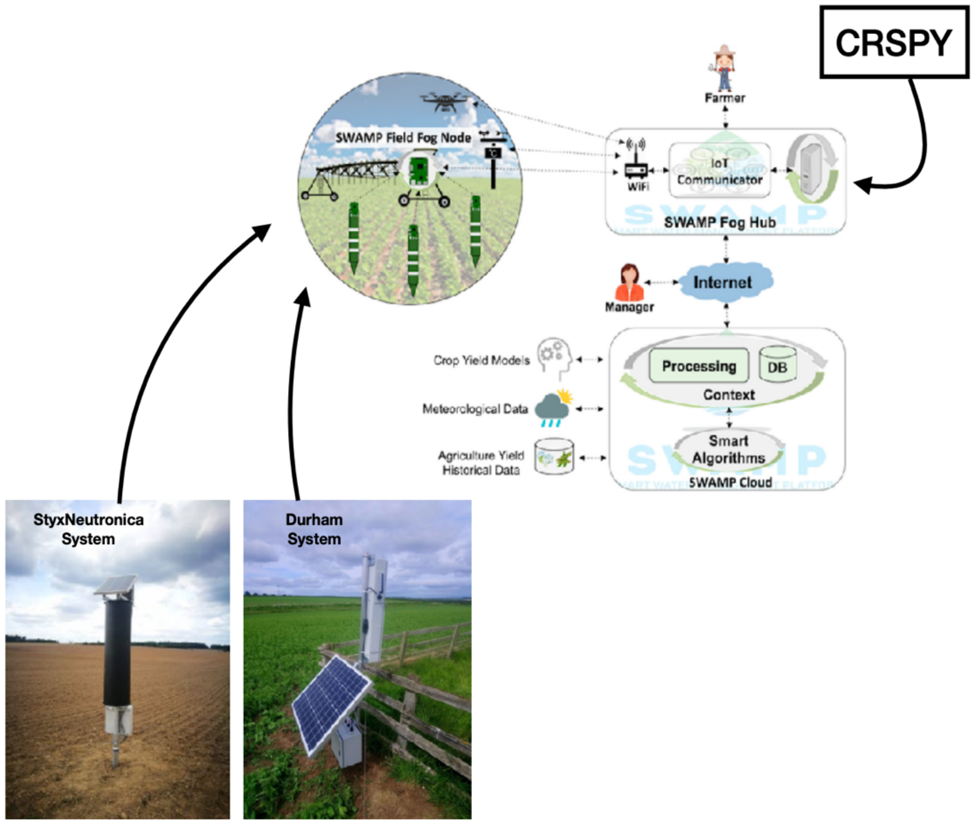

Figure A3 shows a schematic diagram of how the whole COSMIC-SWAMP ecosystem will work. Stowell (2021)

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