Data Cubes for Earth System Research: Challenges Ahead

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Abstract

Progress in Earth system science is accelerating rapidly, due to the increasing availability of multivariate datasets, often global, with moderate to high spatio-temporal resolutions. Turning these data into knowledge presents interoperability, technical, analytical, and other challenges. Earth System Data Cubes (ESDCs) have surfaced as essential tools, offering analysis-ready, cloud-optimised multivariate solutions. Coupled with advancements in Artificial Intelligence (AI), these solutions have the potential to release a wealth of information from the vast amounts of data that they contain. The application of AI methods to ESDCs promises to unpick the complexities of the Earth system, learning the underlying non-linearities to forecast its spatio-temporal behaviour. However, naive applications of such methods might lead to wrong conclusions and predictions. In this perspective paper, we discuss the methodological and conceptual challenges that AI applications of ESDCs bring. Particular risks are naive applications that ignore intrinsic properties of the Earth system, such as spatio-temporal auto-correlation issues that may deliver highly accurate but flawed predictions. Other applications may ignore known causal structures of Earth system dynamics. We also face technical challenges, such as adequate sampling strategies in ESDCs. Furthermore, documenting data cube provenance is essential to ensure end-to-end reproducible workflows. Effective visualisation tools are required to enable users to quickly navigate terabytes of data and develop an intuition for spatio-temporal dynamics encoded in these cubes. Given this, we aim to synthesise the main challenges and derive an agenda for advancing data science on data cubes to better understand global Earth system processes.

1 Introduction

Today we can observe and model most subsystems of the Earth, generating an immense amount of data with unprecedented resolution, quality, and coverage [1–3]. To understand our intricate Earth system, co-interpreting diverse datasets [e.g., 4–6] has emerged as the grand quest [7–9]. However, this wealth of heterogeneous data comes with its own challenges. The sheer volume, coupled with the high complexity of processes encoded in these multi-dimensional datasets, renders conventional data processing and interpretation methods unsuitable [10, 11]. Therefore, there is an urgent need for innovative solutions that not only tackle the enormity and complexity of these data but also provide efficient access to them, as is necessary to exploit the full potential of AI methods and their recent advances to extract novel insights into Earth system processes [12–14, 9].

Today, data cubes are widely adopted to deal with complex Earth observations [15–19, 8, 20]. Although there are significant differences between the known data cube approaches, they share the same intent: to facilitate efficient organisation, storage, and analysis of large-scale, multi-dimensional data. One key idea is to structure observations along multiple "dimensions", jointly forming a "grid", determining data resolution [8, 20]. These dimensions may encompass geographical coordinates, time, distinct variables, or even time series components. The data cube concept is closely associated with Analysis-Ready Data [ARD, 17], ideally stored in the cloud and accessible via common Application Programming Interfaces (APIs) [15]. By integrating various data types into a coherent and especially interoperable framework [21], data cubes facilitate simultaneous analysis and interpretation, transforming the data deluge into accessible and meaningful information. Furthermore, adopting FAIR Open Science principles [22] across the respective end-to-end workflows facilitates reusing information, compounding its impact. In short, data cubes advance Earth system sciences by making data management more efficient and transparent.

Various data cube initiatives have greatly enhanced the use of Earth Observations (EO) derived from satellite remote sensing and other large-scale array data, such as climate model outputs. These initiatives have showcased the immense potential of data cubes to release valuable insights from Earth system data. Going beyond research applications, data cubes have also played a pivotal role in informing governmental actions and policies, as evidenced by their integration into national data cube frameworks [23, 24]. Examples of these initiatives are, among others, the data cubes produced under the Committee on Earth Observation Satellites (CEOS) Open Data Cube [ODC, 25][1] initiative (e.g., Digital Earth Australia, 26, 27, the Colombian Data Cube, 28, the Swiss Data Cube, 29), the Semantic Austrian EO Data Cube Infrastructure [30], the Euro Data Cube[2] system (providing a platform for efficient use of ARD), as well as tailored regional [e.g., the Regional Earth System Data Lab, 20] and global data cubes [e.g., the Earth System Data Cube, 8].

Making this considerable amount of data available to the scientific community creates a bottleneck when there is an urge to perform Earth system research. Nevertheless, we can squeeze the most out of data cubes by leveraging novel advancements in cloud-based environments and standards for data processing (e.g., Google Earth Engine, GEE, 31), storage (e.g., Amazon Web Services Open Geospatial Data[3]), and specification (e.g., Spatio-Temporal Assets Catalogs, STAC[4]). Coupled with domain-specific APIs available for multiple programming languages, e.g., the emerging openEO specification for Earth Observation data [21], users can quickly request (and create) data cubes [even on demand, 16] where data are openly accessible, for instance in a public S3 bucket.

The increased availability of big data and cloud technology coincides with unprecedented advances in AI. AI has emerged as a crucial element for advancing Earth system research [32, 14], although this process has been gradual. Today, Deep Learning (DL) is a game changer [33, 9]. DL advancements offer promising opportunities for Earth system data analysis. These include the ability to perform information transformations across different domains, as demonstrated by attention mechanisms [34], which gave rise to Large Language Models (LLMs) and revolutionised the processing of text [35–38]. Additionally, generative processes in DL enable researchers to reconstruct unseen data [39, 40], while the potential for making causal inferences based solely on data is within reach [7, 41]. Integrating physical constraints and domain knowledge in the DL inference process allows for more plausible predictions [42–44]. However, the question remains whether DL can be seamlessly integrated with data cube technologies, or if its promises should be treated with caution.

Integrating big Earth system data and advanced AI data analysis techniques presents a promising opportunity to tackle complex Earth system challenges. Nevertheless, it is essential to approach this integration with a profound understanding of both the intricate nature of Earth system processes and the unique characteristics of the data cube life-cycle for representing these processes. Naive applications of DL on ESDCs may potentially deliver misleading interpretations. Pitfalls include model performance inflation caused by spatio-temporal auto-correlation, biased sampling, incorrect spatial aggregations due to the spherical nature of Earth, and inadequate sampling in the spatio-temporal and variable domains. The challenge of making Earth system data interoperable from the outset further complicates the analysis process. Data accessibility, transformations, and determining what constitutes ARD for specific application domains pose additional challenges. Disseminating Earth system data, particularly ESDCs, and effective communication of research findings remain open challenges regarding data sharing, traceability, reproducibility, and visualisation. Best practices for open data publishing in the Earth sciences are beginning to emerge and are supported by data journals (e.g., ESSD[5]) and scientific associations (e.g., AGU Open Science[6]).

This paper aims to identify the challenges ahead when exploring Earth system processes within AI applications using ESDCs. Our objective is to establish an agenda for advancing data science on ESDCs, with a focus on the complexities of the Earth system and unveiling the challenges encountered in the design, creation, and utilisation of ESDCs within AI workflows. In Section 2, we describe the specific challenges arising from the intrinsic nature of ESDCs, delineating them along various axes. Section 3 examines the challenges encompassing the entire life-cycle of data cubes while highlighting opportunities for achieving efficient Earth system data interoperability. Section 4 digs into the risks arising from uninformed applications of AI in ESDCs, offering potential solutions and emphasising the transformative potential of contemporary AI advancements in Earth system research. Section 5 presents the technical considerations in ESDCs manipulation. Lastly, in Section 6, we discuss communication challenges, encompassing visualisation hurdles encountered when working with multidimensional (and spatio-temporal) data. Through this paper, we aim to foster a deeper appreciation of the complexities and opportunities associated with employing AI techniques on ESDCs, thereby paving the way for advancements in Earth system science.

2 THE ART OF DATA CUBES

ESDCs possess unique characteristics inherent to the specific datasets representing processes in diverse subsystems of the Earth. These characteristics include spatio-temporal coverage, resolution, and the multidimensional nature of the data. Given the different purposes for which data cubes are designed, several axes can be employed to describe them. Here we present the axes that reveal challenges arising from the complexities associated with the data cube construction to the subsequent analysis processes.

2.1 *Multidimensionality*

The fundamental structure of a data cube is the grid, which defines the data resolution across various coordinates (i.e., dimensions). Although the concept of "Earth system data cubes" often relates to a spatio-temporal grid representing latitude, longitude, and time, it is not a strict requirement. Data cubes can exhibit different dimensions, and their types vary based on the number of dimensions [referred to as the order of the data cube,

[1] https://www.opendatacube.org/ceos

[2] https://www.eurodatacube.com

[3] https://aws.amazon.com/earth/

[4] https://stacspec.org/

[5] https://www.earth-system-science-data.net/policies/data_policy.html

[6] https://www.agu.org/-/media/files/publications/your-6-step-guide-for-publishing-open-access-with-agu.pdf/

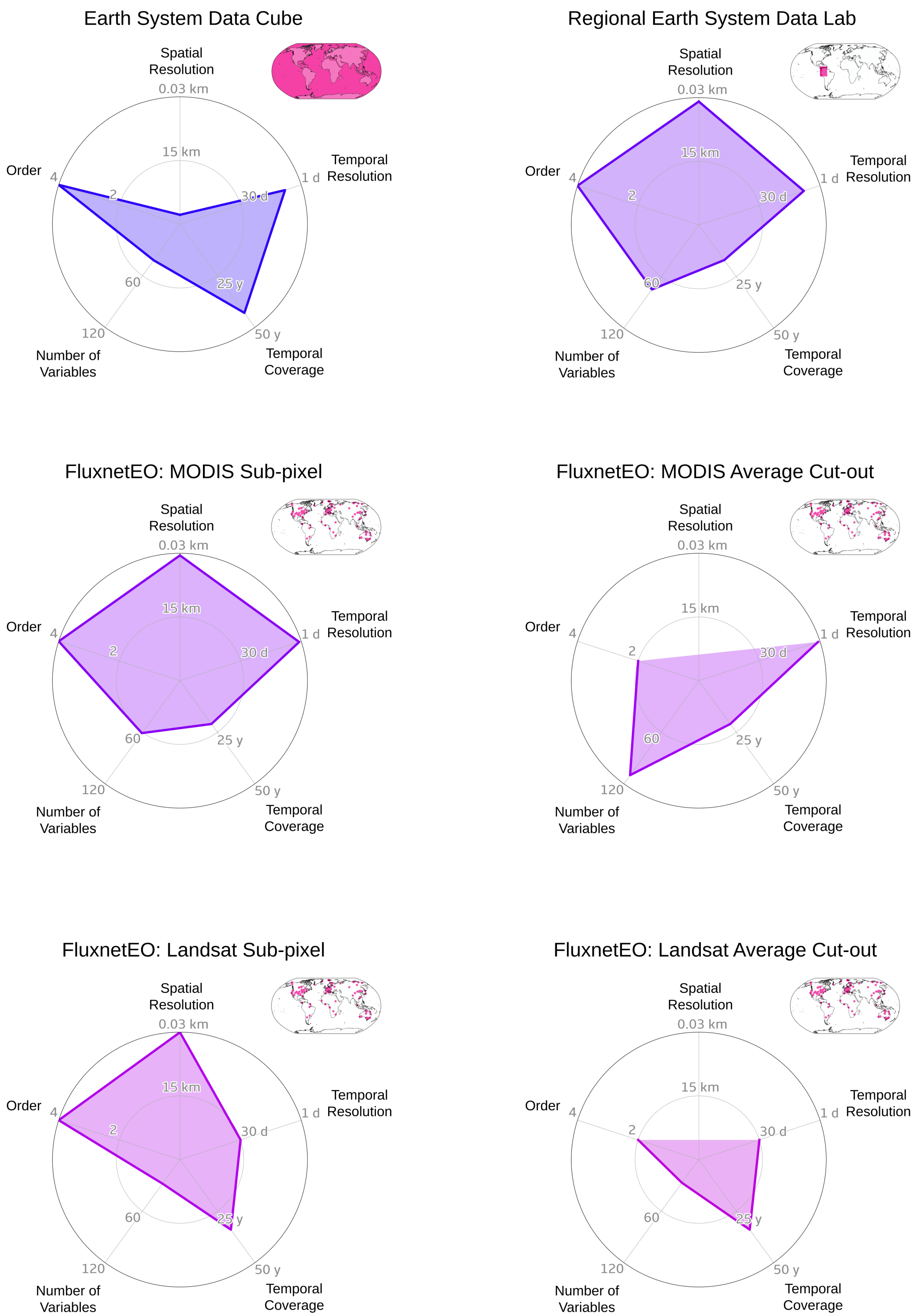

Figure 1: Radar plots representing different axes for six example ESDCs. The spatial coverage is shown for each cube in the top-right corner map. Note that for the average cut-out version of the FluxnetEO ESDCs, there is no spatial resolution value since there are no spatial dimensions in these cubes

8]. Given this, the existence of an Earth system cube of order 0 is possible (i.e., a scalar value). Thus, an increment in the cube's complexity according to its dimensions is given by their order (i.e., a spatio-temporal grid of a univariate cube has an order of 3, while the order of a multivariate cube is 4). While univariate cubes containing only one variable [e.g., precipitation dynamics over a specific region, 45], are the simplest example, most cubes comprise multiple variables. Multivariate cubes range from sets of variables of common origin, e.g., all generated by the same model or observed by the same sensor [e.g., reflectance values and derived higher-order features from specific EO sensors, 46, cf. Figure 1], to heterogeneous cubes that integrate datasets from different sources and higher-order features [8].

The creation of new dimensions instead of the conventional spatio-temporal dimensions is possible and usually required to reach a comprehensive high-level ESDC (cf. Section 2.4). For example, local spatio-temporal aggregations based on extreme events can be implemented. In this scenario, data variables can have additional sizes representing parameters related to these events, such as locations, event types, or data transformation processes. These new dimensions can prove immensely valuable in summarising vast amounts of data for specific applications. However, correct interoperability processing should be performed to ensure the quality of the cube (cf. Section 3) for these analyses. Furthermore, increasing dimensionality entails scalability costs that must be considered (cf. Section 5.3).

2.2 *Spatial scale*

ESDCs may cover various spatio-temporal scales, from local to global. Global data cubes cover the entire planet with a large range of spatial resolutions ranging from several meters to hundreds of kilometres [e.g., 8, cf. Figure 1]. Projecting these global datasets onto a plane can distort the data in terms of area, distances, and angles [47], and careful consideration should be given before conducting spatial analyses (cf. Section 4.2). Moving to a more focused scale, regional data cubes may cover entire continents, oceans, or administrative levels of zero and first order [23], with similar spatial resolutions as global data cubes [e.g., 20, cf. Figure 1]. In this case, selecting an appropriate Coordinate Reference System (CRS) is crucial to ensure minimal geometric distortion. At a local scale, mini cubes cover small areas of interest, ideally with a high spatial resolution ranging from sub-meters to meters [e.g., 46, cf. Figures 1]. These cubes exhibit negligible geometric distortions when a local CRS is used. However, georeferencing issues (e.g., co-registering images) and sampling strategies for AI training algorithms (cf. Section 4.3) should be carefully addressed.

2.3 *Temporal scale*

The temporal scale of a data cube may vary significantly according to the application domain. While some data cubes may require a time dimension with a granularity of seconds or minutes, coarser data cubes can be represented by months or even years. It is essential to recognise that the granularity of the time dimension does not necessarily indicate the sparsity of the grid in ESDCs. For example, EO images can have high temporal granularity but may have significant gaps between revisits. To effectively train DL algorithms that incorporate temporal structures, such as Recurrent Neural Networks [RNNs, 48], a regularly spaced time dimension is usually required. Hence, irregular timestamps should be aggregated or interpolated to fit into a regular temporal grid (cf. Section 3.3), a process that necessarily inserts uncertainties into the data to be considered later when interpreting results. Furthermore, these algorithms typically require much data, including an extended temporal coverage. To fulfil this requirement, variables with a limited temporal range often need to be extended by incorporating data from different sources or measurement approaches. For instance, merging the complete Landsat archive [49] can extend the temporal coverage of reflectance data by using multiple satellites and different sensors. However, this extension process is not straightforward and requires careful harmonisation procedures [e.g., 50] to ensure the consistency and quality of the data (cf. Section 3.4).

2.4 *Readiness*

During data cube creation, data curation is crucial to prepare the data for subsequent spatio-temporal processes and ensure its compatibility with a predefined grid. This step is essential for the data cube to be considered an Analysis Ready Data Cube (ARDC). However, the level of readiness can vary depending on the variables involved and the application domain. In this context, we present an adapted version of the readiness levels proposed initially by [51] for EO data cubes tailored for ESDCs.

An ARDC can be defined as a cube that requires minimum input (or does not necessitate any additional input) from the end user to initiate analyses [52]. This readiness may, however, vary depending on the specific application domain. Achieving an ARDC level often entails essential preprocessing and data curation tasks particular to the application domain. For instance, the tasks required to achieve this level of readiness for an EO data cube include but are not limited to masking clouds and cloud shadows [53], correcting Bidirectional Reflectance Distribution Function (BRDF) effects [e.g., 54], resampling, and subsetting the data to a common spatial grid. Initially developed by CEOS, the ARD concept has recently been addressed by the Open Geospatial Consortium by a new Standards Working Group with the objective to define a generic multi-part Standard specifying a set of minimum requirements for geospatial products to be considered analysis-ready[7].

Additional post-processing of data variables may be necessary to address Earth system challenges using AI. This entails further data curation to obtain a fully gap-filled, harmonised product with evenly spaced time steps. Typically, this level of readiness involves data harmonisation [e.g., 55, 56], gap-filling, and smoothing [e.g, 57]. This enhanced readiness level is sometimes called highly Analysis Ready Data Cubes [hARDC, 51].

The readiness of a data cube can be further enhanced by incorporating higher-order features, which involve generating new products from the input data within the cube. For example, spectral indices derived from reflectance bands [58], frequencies obtained from time series decomposition [59], spatio-temporal compositions [60], or outputs from AI models [e.g., 61] can be added. This elevates the readiness level to an even higher state,

[7] https://www.ogc.org/press-release/ogc-forms-new-analysis-ready-data-standards-working-group

known as highly Analysis Ready Data Cubes plus [hARDC+, 51].

It is worth noting that when a cube's readiness level increases, the flexibility of data manipulation decreases as specific algorithms have to be selected to pre-process, curate, or further develop and transform the data.

2.5 Applicability

ESDCs can be classified according to their domain-specific study areas, each involving intricate interactions among multiple variables. While categorisation based on the application sphere is possible (e.g., lithosphere, biosphere, atmosphere, and hydrosphere), multiple sub-domain applications exist based on the targeted aspects of these spheres and considering the technical and methodological approaches employed.

Firstly, data cubes can be employed in various (and usually interdisciplinary) application domains, encompassing but not limited to the climate system [62, 6], land-atmosphere interactions [4, 5, 63], and the socioeconomic system [64, 65]. These interconnected systems have significant implications for the Earth and its inhabitants [66]. For instance, the relationships between human activities and socioeconomic dynamics directly or indirectly impact the climate system. Conversely, climate change and its extremes can, directly and indirectly, affect socioeconomic dynamics [67, 68]. In this scenario, studying climate and weather-related extreme events may necessitate data from the climate system, biosphere, and socioeconomic system simultaneously (cf. an abstract example in Figure 2).

Secondly, in a more technical aspect, it is common to encounter data cubes derived from different methodological approaches. For instance, making the data cubing process for EO data is more straightforward (primarily because higher level EO data that are typically used as inputs for ESDCs generation have already been processed onto regular spatial grids by the space agencies) than for ungridded filed measurements that need to be gridded in advance. For example, climate data cubes predominantly originate from climate models, terrestrial biosphere data cubes primarily rely on EO data, and socioeconomic data cubes largely depend on gridded products derived from statistical, administrative data, which exhibit varying levels of granularity across administrative boundaries (e.g., developing countries often feature limited data availability compared to developed countries), thereby posing challenges for data harmonisation (cf. Section 3.4).

Integrating and summarising these heterogeneous data across different application domains into single ESDCs can help streamline Earth system analyses, enabling a more focused data-driven approach via hARDC+ products (e.g., Figure 1). However, this integration process presents interoperability challenges (cf. Section 3) that require scientific expertise to overcome. Furthermore, the computational resources needed to manage and process such large-scale integrated datasets are significant, as memory limitations must be carefully addressed to ensure efficient data processing (cf. Section 5.3).

3 Interoperability of Earth system data

Enabling interoperability for Earth system data is challenging but crucial to facilitate efficient analysis through AI pipelines. This process involves several intricate tasks, including accessing the source data, performing data cubing, harmonising data across different sources, and generating comprehensive metadata. These steps create high-quality ESDCs, enabling seamless integration and analysis. However, achieving interoperability is a complex and non-trivial endeavour. Here we present the challenges (and potential opportunities) associated with the management of big data and addressing issues related to data heterogeneity, data formats, and varying data sources during the life-cycle of data cubes (Figure 3).

3.1 Accessibility of source data

Efficient access to Earth system data is crucial to achieving robust data interoperability. Data providers often employ various formats and protocols for data sharing, making it essential to establish streamlined access mechanisms. Traditionally, File Transfer Protocol (FTP) servers have been used for data sharing. However, to enhance data discoverability and usability, data providers are increasingly adopting data stores that offer persistent and standardised data storage. Repositories play a vital role in this process by standardising metadata for datasets, enabling easy search and retrieval of assets through metadata queries. Recently, more and more data providers offer APIs to facilitate efficient querying of metadata and access to the data itself.

The standardisation of metadata has also led to the development of innovative geospatial data specifications, such as the widely recognised STAC specification. This specification empowers users to query data assets based on metadata and spatio-temporal criteria, making it applicable to various use cases. Coupled with domain-specific API clients available for multiple programming languages [e.g., rstac for R, 69, as well as pystac[8] and pystac-client[9] for Python] and Geographic Information Systems (GIS) Software (e.g., QGIS STAC Plugin[10]), users can easily retrieve geospatial data. The flexibility of the STAC specification has prompted numerous data providers to adopt it for creating their own data catalogues[11], with notable examples including GEE and Microsoft's Planetary Computer[12], which have emerged as prominent cloud-based geospatial environments with comprehensive STAC catalogues.

These specifications' flexibility enhances data interoperability by enabling the development of extensions that simplify data integration. For instance, the Electro-Optical STAC-extension[13] has been created to facilitate the integration of multispectral remote sensing data by expanding the capabilities of STAC to accommodate specific requirements and metadata associated with this kind of data. Furthermore, the benefits of data interoperability extend beyond raw source data, encompassing data cubes. The datacube STAC-extension[14] has been developed specifically for data cubes, advancing integration and interoperability of this structured data representation within the STAC

[8] https://github.com/stac-utils/pystac
[9] https://github.com/stac-utils/pystac-client
[10] https://github.com/stac-utils/qgis-stac-plugin
[11] https://stacindex.org/catalogs/
[12] https://planetarycomputer.microsoft.com/
[13] https://github.com/stac-extensions/eo
[14] https://github.com/stac-extensions/datacube

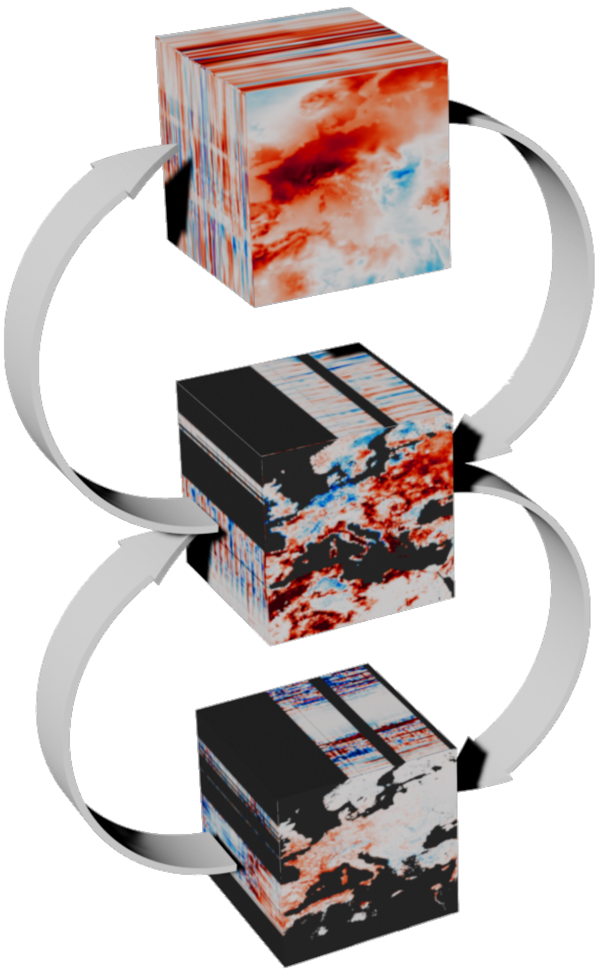

Figure 2: Abstract representation illustrating the connection between three Earth system variables in a hARDC+ (from top to bottom: anomalies in air temperature, soil moisture, and gross primary production). The arrows illustrate the interactions that can be modelled, e.g., via DL methods performing, e.g., predictive modelling (top to bottom), or interpretation (bottom to top), depending on the use case of interest

ecosystem and enhancing the opportunity of reusing data cubes for new pipelines.

3.2 Cloud readiness

GeoTIFF is arguably the most used and renowned data format for georeferenced raster data. This format adds a standard specification for the TIFF format that describes the spatial properties of the raster. It is widely used for EO products such as Landsat imagery. When the dimensionality of the data increases, formats such as NetCDF or HDF5 are typically used to encapsulate data and coordinate values. Tiling and chunking allow efficient access to big data arrays for both data formats. However, these formats are not inherently optimised for cloud environments.

The need to operate in cloud environments has driven the development of cloud-optimised geospatial data formats. Consequently, the GeoTIFF format has evolved to the Cloud-Optimized GeoTIFF (COG) format, enhanced to function efficiently in cloud environments through HTTP range requests. For multidimensional arrays, the Zarr specification can be directly used in cloud environments, enabling efficient chunk access for parallel processing. Going beyond the standardisation that file formats offer, similar specifications, e.g., the geo-zarr specification[15] or the xcube dataset convention[16], emerged with the objective to further facilitate interoperability.

Cloud data optimisation has revolutionised the exploration of the intricate and interconnected dynamics of the multivariate Earth system by providing a standardised approach to generating customised data cubes instantly. This transformative advancement, known as on-demand data cubes, empowers users to create tailored data cubes from extensive collections of Earth system datasets with minimal user input [70] on the fly. This is especially salient for applications that require rapid and efficient specialised analysis of vast amounts of data, facilitating the interoperability of multi-sourced datasets. There are already multiple tools enabling the creation of on-demand data cubes [e.g.,

[15] https://github.com/zarr-developers/geozarr-spec
[16] https://xcube.readthedocs.io/en/latest/cubespec.html

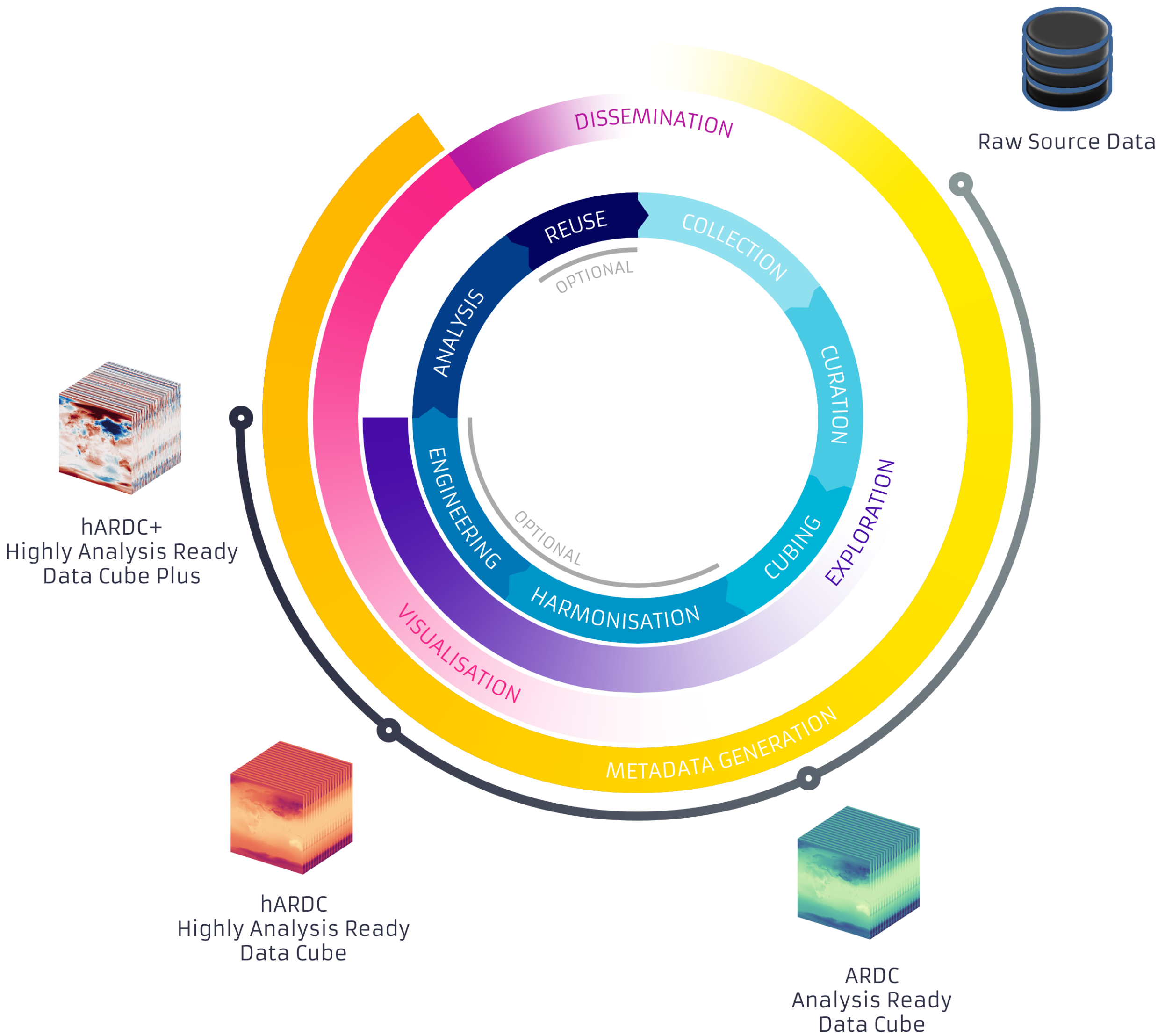

Figure 3: Earth system data cubes life-cycle. The inner circle represents data processing tasks, and the outer circles represent ancillary tasks that run parallel to the processing steps, involving activities such as data exploration, visualisation and dissemination, and metadata generation. The outermost circle of the diagram illustrates the readiness level of the processed data at specific points within the cycle

51, 16, 70], with emerging technologies already harnessing the potential of STAC and cloud-optimised formats[17,18,19,20,21].

The cloud-optimised nature of data formats used for most on-demand data cubes opens up new possibilities for data cube sampling in AI pipelines (cf. Section 4.3), including a specialised focus on mini cube sampling. This approach offers potential solutions to overcome storage and memory limitations. By leveraging the cloud infrastructure and optimised formats, data can be efficiently accessed and processed in smaller, manageable subsets, enabling more effective sampling strategies. This improves the scalability and performance of the AI pipeline and therefore delivers computational efficiency gains.

3.3 *Spatio-temporal cubing*

The core concept of an ESDC is to align data onto a unified grid. Domain experts predefine this grid, and all data sources must conform. When the grid moves in the spatio-temporal domain, the varying spatio-temporal resolutions and coverage among multiple data sources require selecting adequate methods to fit the data into the regular predefined grid.

Datasets with varying spatial resolutions and coverage must be resampled onto a common spatial grid. This process often requires modifying the data [71]. While non-destructive algorithms such as nearest neighbours can preserve data values (at the cost of duplicating or ignoring values), large differences in

[17]https://github.com/opendatacube/odc-stac
[18]https://github.com/gjoseph92/stackstac
[19]https://github.com/ESDS-Leipzig/cubo
[20]https://github.com/dcs4cop/xcube
[21]https://pangeo.io

spatial resolution often require transformation through (non-) linear resampling methods, such as cubic convolution or advanced fusion techniques [72]. Complex AI methods can be employed to perform spatial transformations while preserving the quality of the measured variable [e.g., multi-image super-resolution algorithms, 73, 74]. Geometric distortions may arise when applying resampling methods at a global scale. Due to the Earth's spherical shape, traditional resampling techniques that assume planar surfaces may not accurately account for the curvature and distortions introduced by the geographic coordinates (cf. Section 4.2). This can lead to inaccuracies and artefacts in the resampled data.

When datasets differ in time, two types of issues arise: 1) datasets have the exact temporal resolution but a different granularity, and 2) datasets have different temporal resolutions. When dealing with datasets that share the exact temporal resolution but require different levels of granularity, a suitable predefined temporal granularity must be selected, and data must be interpolated (i.e., gap-filling). Determining the optimal interpolation method for achieving the desired granularity is not straightforward. Various interpolation techniques, ranging from simple linear interpolation to more complex AI-based modelling approaches, can be employed to address this [e.g., 75]. The choice of the interpolation method depends on factors such as the data's nature, the desired accuracy level, and the specific requirements of the analysis or application at hand. When working with datasets with different temporal resolutions, datasets with a finer resolution must be aggregated to match a predefined coarser temporal grid. While this process is straightforward for regularly sampled data, it can pose challenges for EO data with long revisit periods, resulting in potential uncertainties during aggregation. Significant gaps in EO data can affect the accuracy and representativeness of the aggregated results. It is essential to carefully consider the temporal characteristics of the data and employ appropriate methods, such as gap-filling techniques and incorporating uncertainty estimates (cf. Section 4.6) to account for the limitations introduced by the data gaps.

The process of spatio-temporal cubing is complex and requires meticulous expert involvement. While there is an ambition to develop systems for creating on-demand ESDCs with a hARDC+ readiness level, it is essential to consider the methodological heterogeneity based on the specific application domain and subsequent analyses. This ensures that the ESDCs generated are well-suited for the intended purposes and facilitate effective and meaningful analyses in the respective research fields.

3.4 Variable harmonisation and extrapolation

Data harmonisation is crucial to ensure the consistency and compatibility of variables obtained or generated using different methodological or technical approaches [76]. When discrepancies exist between data acquisition or creation methods, it can introduce inconsistencies that hinder subsequent analyses involving the specific variable. To address this, one approach is to create separate variables that represent the same measured quantity, highlighting the differences between them. However, to enhance spatio-temporal resolution and coverage, harmonisation of variables is often necessary [e.g., harmonising reflectance values from Sentinel-2 and Landsat, 55]. This can be achieved through simple methods that involve sampling data from the same spatio-temporal index in both variables to establish a direct conversion model. Alternatively, more advanced AI models can harmonise data by incorporating one or more additional variables. This may require the development of an entire AI pipeline to extend a variable with newly available data or reconstruct it, especially in cases where the variable was not previously measured [e.g., reconstructing Sun-Induced Fluorescence from TROPOMI, 77]. In this sense, data harmonisation also encompasses projecting data in simulated future scenarios [e.g., projecting vegetation dynamics for the rest of the century, 78]. In addition, it is crucial to incorporate uncertainty metrics to facilitate accurate and reliable future analysis using the harmonised data variables (cf. Section 4.6).

3.5 Metadata generation

Traceability and self-explanatory power are essential aspects alongside the data values themselves. When a data cube is generated, the end user can access its description through documentation such as blogs, web pages, or research papers. However, the data must carry its own encapsulated description in the form of metadata. This ensures the data contain relevant information about their characteristics and attributes, facilitating understanding and utilisation.

Metadata generation should begin at the initial stage of data acquisition, encompassing crucial information such as data descriptors (e.g., name, units, measurement methods and equipment, resolution), data transformations (e.g., resampling or interpolation methods), metadata transformations (e.g., renaming procedures, conventions conversion), and responsible producers (e.g., creator entity, data provider). This metadata generation process should be consistently maintained throughout the enhancement of the readiness level of the cube, documenting each step undertaken to derive the final product. This ensures comprehensive self-contained documentation of the history and processing of the data cube.

While flexibility exists in metadata management, conventions are crucial when dealing with Earth system data. The Climate and Forecast Metadata Conventions [CF Conventions, 79] are a comprehensive set of standards for Earth system data, facilitating clear descriptions of data variables and coordinate dimensions. Compliance with these conventions simplifies data sharing through specifications like STAC and promotes interoperability among various data sources.

3.6 Transparency, traceability and reproducibility

The advancements of cloud technologies have also enabled the creation of data cube services that abstract from the underlying file structures and formats and replace them with APIs offering varying processing functionalities, e.g., Sentinel Hub[22] or the openEO platform[23]. These services allow for the tailored specification of data cubes on-demand, and the server-side processing frees the requester from the challenges and pitfalls of the generation task. Such convenience comes, however, at a cost beyond the price for commercial services, namely transparency and reproducibility. Neither the code basis of the processing

[22] https://www.sentinel-hub.com/
[23] https://openeo.cloud

engine, processing environment, nor the input data are typically known to the requester, and any change in these specifications may yield a different result for identical requests to the data cube API.

Less convenient but more transparent are approaches that fully document the data cube generation process in so-called recipes containing the versioned source code used for the input data processing, e.g., Pangeo forge[24] or DeepESDL recipes[25]. Such recipes, together with versioned input data and fully specified processing environments, allow for full, practical reproducibility of the resulting data cubes. Efforts to provide more transparent data lineage and provenance are ongoing as part of the Copernicus Data Space Ecosystem. The "traceability" service[26] (currently in development) is planned to allow users to fully trace all modifications to the data from its origin to when it reaches the user. This should guarantee data integrity, enable reproducibility, and contributes to more explainable AI on top of the data.

The Open GeoSpatial Consortium acknowledged the increasing importance of data cube approaches for geographical data by recently establishing a GeoDataCubes Standard with the aim of facilitating interoperability of the different solutions[27]. The working group has a broad scope explicitly including API functionalities for access and processing, exchange format recommendations, profiles, and a metadata model.

4 Data Science on Data Cubes

Applying AI methods to ESDCs presents numerous challenges that must be carefully addressed. In particular, specific issues are associated with the naive application of AI techniques to ESDCs without considering the unique characteristics of Earth system data, reliability and trustworthiness of data, handling scalability issues, and more. However, amidst these challenges, some opportunities emerge when working with Earth system data. Here we present the key challenges and opportunities when doing Earth system data science, incorporating today's AI advancements and the recent boost in ESDCs.

4.1 *Adding factual knowledge via Physics-Informed Machine Learning*

A great addition to Machine Learning (ML) modelling is combining the pure data-driven approach with factual knowledge of the system under investigation [42]. Physics-Informed Machine Learning (PIML) leverages domain knowledge (typically in the form of mechanistic models or differential equations) and flexible data-driven ML methods (typically neural networks). Consequently, PIML models tend to respect physical boundaries more faithfully while being flexible enough to approximate arbitrarily complex non-linear functions from data (cf. discussion and references in 12). Data cubes provide a unique structure to access multiple data streams, and the equation-based model describes the underlying process. Thanks to this ready availability of data and equations, exploring PIML models using a wide array of baseline models would be far easier and faster. The equations detailing a given variable could be added to the cube as a sub-field of the variable of interest in the same way that space and time are. The eventual implementation should consider the multi-platform and multi-language nature of the data cubes. This requires a unified and robust approach that suits multiple use cases, as illustrated above.

4.2 *Geometric challenge on planet Earth*

Most data cubes that cover the whole globe use a simple longitude-latitude plate-carrée projection, which fits the data cube model very well. The approach also allows for efficient storage and subsetting of cubes to user-generated subsets that correspond to a bounding box. However, for advanced data analysis, equirectangular projections have two main drawbacks: 1) grid cells differing in latitude do not have equal area, and 2) the distances to nearest neighbours are not constant.

The first drawback introduces a sampling bias towards high latitudes in the data. This bias can affect the representativeness and accuracy of analyses (cf. Section 4.4), particularly for regions located closer to the equator. The most trivial cases are computations of scalars, like global means (e.g., Figure 4), which need to be weighted or approaches like principal component analyses that require area-weighed covariance matrices. Effects of this kind have been known for decades and are considered climate textbook knowledge [80]. However, they remain a challenge, as we find them often ignored in data cube analytics. Issues of this kind can be alleviated using area-weighted statistics, which are suitable for most linear algorithms [e.g., WeightedOnlineStats.jl, 63], or by performing weighted sampling from grid cells. For advanced, often non-linear data science methods, considering the spherical geometry is much more challenging, and careful consideration is advised before naive applications are performed. Even when applying area-weighted statistics correctly, oversampled areas lead to unnecessary increases in storage requirements and computation time.

The second drawback is particularly significant when applying spatial convolutions or moving window operations. To address this, several approaches can be employed. One option is to use spherical harmonics for simple convolutions, providing a transformation that respects the spherical nature of the data [81]. Another approach involves graph convolutions that consider varying distances to neighbours.

An alternative approach to solve both drawbacks mentioned here would be regridding the cube onto a Discrete Global Grid System [DGGS, 82]. These grid systems seek to minimise distortions, harmonise cell sizes and maintain consistent distances from neighbours. Although many different DGGSs have been defined, we still lack integration into libraries providing storage, IO and scalable processing on these grids. Defining standards and solutions for efficient chunk storage, subsetting, and integration into the data cube framework will be a challenging future task but could lead to significant improvements in both performance and accuracy of spatial algorithms.

4.3 *Sampling for AI in a complex system*

Sampling on ESDCs is essential for deciphering the concrete interactions of drivers, spatial conditions, timing, and other de-

[24] https://pangeo-forge.org
[25] https://github.com/deepesdl/cube-gen
[26] https://dataspace.copernicus.eu/analyse
[27] https://www.ogc.org/press-release/ogc-forms-new-geodatacube-standards-working-group

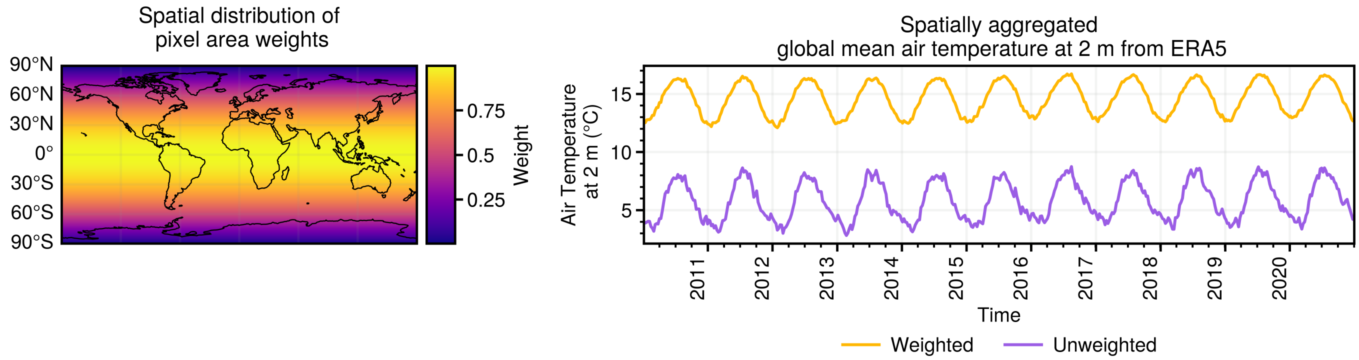

Figure 4: Comparison of air temperature at 2 m from ERA5 with and without weighting on the global mean time series computation. This rather trivial example shows how radically wrong any computation can be if the spherical nature of planet Earth is ignored

terminants of specific processes and their implications. Samples can be derived from all types of cubes, from global data cubes to mini cubes produced on-demand. In the dimensional aspect of models, they can be derived based on the algorithm type and required data dimensions. For tabular-based algorithms like tree-based methods, 2-dimensional batches (sample and variable) are selected as individual points from the spatio-temporal domain. DL methods like RNNs, e.g., Long Short-Term Memory [LSTMs, 83], which consider temporal dependencies, require 3-dimensional batches (sample, timestep, variable) and extract samples as subsets of time series from the spatial domain. Convolutional Neural Networks [CNNs, 84], focusing on spatial context, need 4-dimensional batches (sample, height, width, variable) and take spatial subsets or grids from the temporal domain. DL methods accounting for both spatio-temporal dependencies, such as 3DCNNs or Convolutional LSTMs [ConvLSTMs, 85], require 5-dimensional batches (sample, height, width, timestep, variable) and extract samples as subsets of data cubes. These samples can even represent complete mini cubes or subsets derived from them, enabling the modelling of complex spatio-temporal relationships within the data. Note that samples are taken across the same variables in the data cube.

In the multivariate aspect, constructing representative samples in Earth system processes must ensure an unbiased representation of the target variable. The multidimensional nature of Earth system processes poses sampling challenges across multiple variables. Consider, for instance, a study that aims at understanding the effects of climate extremes on the terrestrial biosphere using AI [86]. We know that climate extremes such as heatwaves, droughts, extreme precipitation, flooding, etc., are typically associated with multiple variables [87]. Additionally, such events can occur simultaneously or in unfavourable sequences, i.e., compounding heatwaves, droughts, or floods following droughts [88]. To understand such events, one should consider the full spatio-temporal extended in all relevant dimensions, including derived meta-variables that describe the characteristics of these events, such as timing, duration, extent, and intensity [89]. Often, additional factors gain significance. For example, ecosystem responses to extremes are varying in space depending on ecosystem conditions [90], land-cover types [87], and associated impacts, e.g., on the carbon cycle [86]. In order to build suitable AI models that predict such impacts requires including static data (e.g., vegetation type). Yet, the key question is then: how to obtain adequate and balanced training and validation data. Figure 5 showcases a potential workflow where event detection is performed based on global data cubes, and samples for high-resolution ML are extracted based on a systematic sampling strategy. Here, analysing land cover purity is necessary (a relatively homogeneous land cover dominated by a single vegetation type allows for easier comparisons and subsequent analyses) as well as incorporating mixed land covers (which introduces heterogeneity and interactions among land cover types), providing more comprehensive information for model training.

Representative samples that capture the complex dynamics of Earth system processes must preserve spatio-temporal representativeness and avoid auto-correlation. Earth system processes often involve rare events of extreme conditions, which may occur sporadically over time and space. This rarity can lead to imbalanced datasets, where the occurrence of the target variable is disproportionately low compared to other variables. Imbalanced datasets affect the performance and generalisation of models trained on these samples. Achieving spatio-temporal representativeness in this context can be challenging. Because Earth system datasets are often vast and high-dimensional, sample sizes must be balanced with available resources to conserve computational resources.

4.4 *Spatio-temporal representativeness for an accurate model evaluation*

Diagnostics on predictive modelling with data cubes can be challenged by the representativeness and spatio-temporal structure of training data [91–94]. Assessing the accuracy of a prediction is statistically straightforward as long as reference data is available for the entire population or if a respective sample represents the spatio-temporal structure of the population [95, 96]. However, many modelling tasks build on observations not representative of underlying temporal dynamics or an entire land surface variability (e.g., upscaling functional ecosystem properties from sparse and clustered FLUXNET sites). Such an imbalance in reference data may not necessarily lead to a bias in model coefficients [97]. However, it may lead to inflated prediction accuracy estimates, given the commonly limited capacities of ML to extrapolate

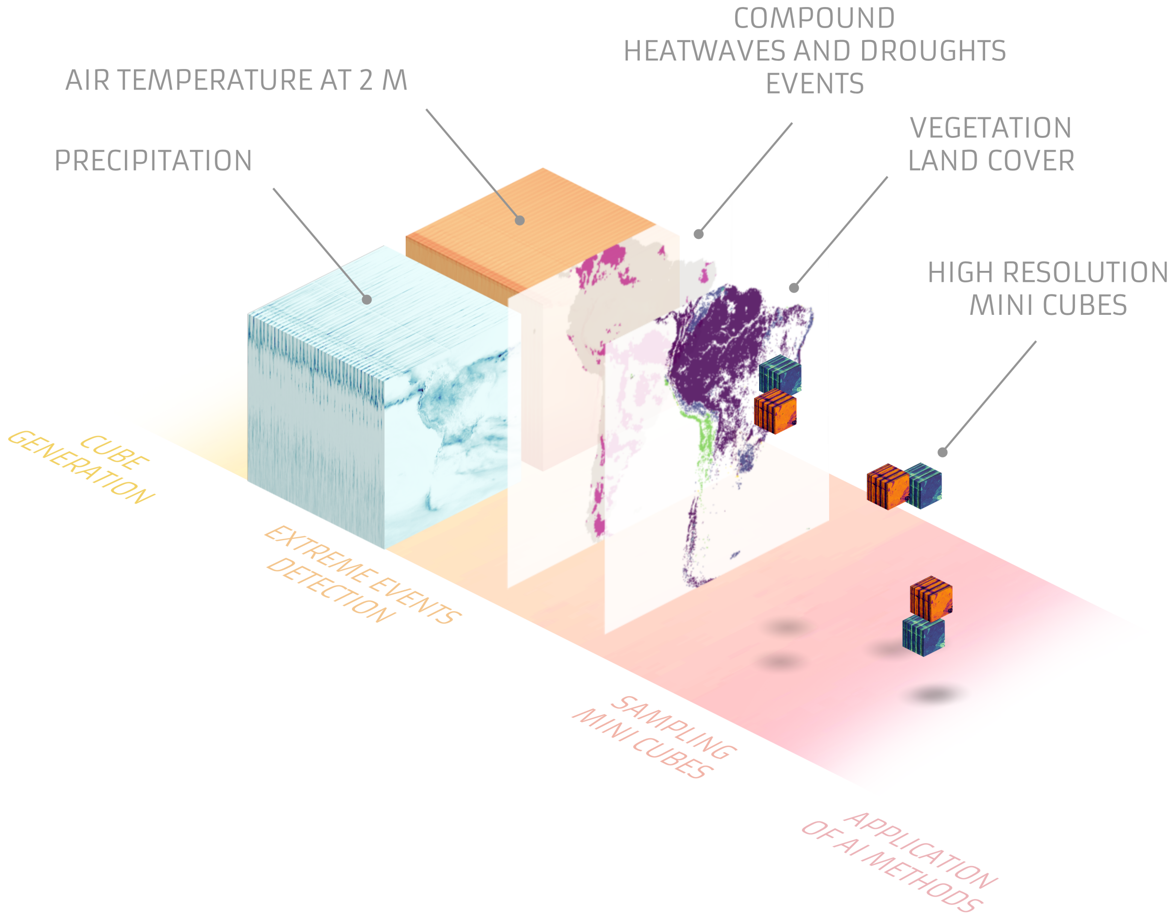

Figure 5: Abstract representation illustrating the process of sampling high-resolution mini cubes for further analysis by considering vegetation land covers and extreme events detected via a global data cube. Note that sample mini cubes are specified in the spatial and temporal ranges of the detected extreme events (also considering their occurrence)

into the unknown, where the predictor-response relationship may depart [98]. Thus, the accuracy assessment of a prediction estimated from clustered samples will not represent the factual accuracy of predictions beyond the reference data availability. This is critical for assessing the quality of a prediction itself and potential error propagation in subsequent analysis [99, 92, 100]. It is advised that predictions should inform on the Area of Applicability [92], i.e., the area in which the predictor-space is covered by the reference data and obtained predictive accuracies thereof are assumed to hold.

The predictive performance of a model outside the area of applicability may be estimated by assessing the model's accuracy (i.e., the predictive performance of a model on unseen observations). However, assessing the model's accuracy can also be challenged by the spatio-temporal structure of the training and test data. Commonly, adjacent observations (both in time and space) are more similar (autocorrelated in space and time), and therefore accuracies determined from test observations near the training data will be more accurate [101, 102]. However, dependence among training and reference data results in any case on optimistic estimates of model performance, meaning that such accuracies do not reflect the actual transferability of the model to unseen areas or time steps [101]. For instance, [93] showed that ML-based models found accurate in the presence of spatial dependent training and validation data may learn spatial data structures instead of transferable relationships between a response (biomass) and the predictors (environmental variables and optical reflectance). This may not only lead to erroneous model transferability and extrapolation to new spatial or temporal domains but also prevent an adequate interpretation of model functioning and attribution to variables and processes (cf. Section 4.5). Therefore, model performance should be assessed by minimising training and test data dependence using spatial cross-validation strategies [cf. 101, 93, 94].

4.5 *Leveraging data cubes as tensors*

ML, particularly DL through neural networks, has revolutionised Earth system sciences [103, 104] and promises to continue doing so [105, 9]. ARDCs are crucial in many AI applications as they provide a structured and efficient way to organise and analyse multidimensional data. Interpreting data cubes as a representation of tensors, AI algorithms can extract valuable insights from Earth system data. This includes methods such as regression, classification, anomaly and object detection.

The tensor-based representation facilitates the exploitation of the multidimensional nature of ESDCs. Additionally, sub-groups such as subset cubes, matrices, and vectors can be identified, reflecting the underlying tensor structure. The integration of AI and data cubes opens up possibilities for analytical techniques, such as tensor decomposition [106, 63] or ML algorithms which are based on tensors like CNNs or related architectures. These techniques can help uncover latent patterns and dependencies within the data (spatial, temporal, and mixed), improving the accuracy and interpretability of AI models [107]. This basic structure is enforced not only in the software but also in the hardware[28].

In summary, the relationship between tensors and data cubes in AI applications is crucial for effectively handling and analysing multidimensional data. Tensors provide a flexible and efficient representation of data cubes, enabling AI algorithms to leverage their inherent structure and extract valuable insights. This integration advances AI techniques across various domains, empowering researchers to make data-driven decisions and achieve robust results.

4.6 *Uncertainty quantification and propagation*

Uncertainty quantification is crucial to Earth science, providing a comprehensive assessment of the reliability and confidence associated with scientific predictions, model simulations, and observational data. Capturing and modelling uncertainty is a complex task as it arises from various sources such as data limitations, model approximations, and the inherent complexity of Earth system dynamics.

Uncertainty can be broadly categorised into two types: epistemic uncertainty and aleatoric uncertainty [108]. Epistemic uncertainty refers to the model's confidence in its predictions and is related to the choice of model parameters. Techniques such as Bayesian inference or Dropout can estimate epistemic uncertainty [109, 110]. Bayesian methods assign probability distributions to model parameters, directly quantifying uncertainty. Dropout-based methods create model ensembles by randomly dropping out units during training, providing a measure of uncertainty based on the variability among the ensemble members. While these techniques may not completely capture the underlying uncertainty due to assumptions made during modelling or training, they are practical and can be employed to estimate uncertainty. These methods can be computationally demanding and time-consuming, especially when applied to real-time applications. However, advancements in cloud platforms (cf. Section 5.1) and the Monte Carlo (MC)-Dropout technique have enabled reliable uncertainty estimates, even when working with massive amounts of data [111]. On the other hand, aleatoric uncertainty is associated with the inherent noise or variability present in the data (e.g., data affected by natural variability, measurement errors, or other sources of noise) and cannot be reduced. Instead, it can be identified and quantified as part of the uncertainty characterisation.

ESDCs involving measurements or modelled data must be accompanied by associated uncertainty values. Data assimilation techniques play a key role in incorporating data into ESDCs while considering the associated uncertainties. Approaches such as Kalman filtering, variational data assimilation, or ensemble-based assimilation can effectively merge different data sources and quantify the resulting uncertainties [112]. Once the uncertainties associated with individual data points are estimated, the next step is to propagate these uncertainties throughout the data cube. By incorporating uncertainty quantification into ESDCs, valuable insights can be gained regarding the reliability and confidence of the data.

5 Technical considerations for managing Earth system data cubes

Managing ESDCs throughout their entire life cycle is complex and resource-intensive. In this section, we outline the technical considerations and limitations associated with the current state-of-the-art technological resources for ESDCs management. This encompasses aspects such as computing resources, software tools, and scalable solutions that are crucial for effectively handling the challenges involved in ESDC management.

5.1 *Computing resources*

Data processing feasibility throughout the data cube life-cycle is determined by the data size and available computing resources. Computing resources vary from a single laptop to a local cluster with multi-threaded or distributed processing capabilities and can extend to cloud computing environments composed of multiple clusters. Computation on local systems typically involves single-threaded computations with a higher level of interactivity. In High-Performance Computing (HPC) environments, software primarily operates in a multi-threaded or multi-core manner and is usually installed by a local system administrator. HPC environments are well-suited for extensive processing tasks but offer reduced interactivity due to the involvement of job schedulers for managing computation resources. Cloud computing environments offer a promising solution for effectively managing vast amounts of Earth system data. Platforms such as GEE, the European Open Science Cloud (EOSC)[29], Google Colaboratory[30], Amazon SageMaker[31], DeepESDL[32], and Kaggle[33] provide opportunities for efficient data storage, processing, and collaboration in scientific research. However, it is important to note that these platforms often have certain limitations imposed on users. These limitations include storage capacity, computational resources, available tools, access permissions, and usage restrictions.

5.2 *Software capabilities*

In the context of processing ESDCs, diverse tools are available in different programming languages. These tools enable direct access to data stored in formats like GeoTIFF, NetCDF, or Zarr, as well as through databases such as Rasdaman [17] and ODC [25]. While databases streamline data access, they require setup and maintenance. Examples of tools for direct ESDCs management include xarray [113] and xcube in Python, gdalcubes [16], stars [114], and terra[34] (for 3 dimensions) in R, and YAXAr-

[28] https://developer.nvidia.com/blog/nvidia-research-tensors-are-the-future-of-deep-learning/

[29] https://eosc-portal.eu/

[30] https://colab.research.google.com/

[31] https://aws.amazon.com/sagemaker/

[32] https://www.earthsystemdatalab.net/

[33] https://www.kaggle.com/

[34] https://github.com/rspatial/terra

rays.jl[35] and Rasters.jl[36] in Julia. These tools facilitate ESDC manipulation on local machines and computing clusters, offering diverse processing capabilities. In the context of combining datasets, these tools support grid interoperability operations and employ efficient data chunking techniques to ensure fast data access and processing [e.g., using dask, 115].

During the analysis step, which often involves the application of AI methods, Python-based tools are commonly chosen for ML approaches. Scikit-learn [116] is widely used as a general-purpose ML library (typically with tabular data). In the realm of DL techniques, popular choices include TensorFlow [117] and PyTorch [118]. While achieving easy ESDC analysis remains a challenge (particularly when applying AI techniques), there is already software tailored for specific geospatial operations using ML, such as verde [119] and AiTLAS [120]. In the case of DL, several torch-based developments have been created for geospatial data (e.g., torchgeo, 121, GeoTorchAI, 122, and rastervision[37]), as well as domain-specific libraries for pre-trained models (e.g., moonshine[38]), xarray-based batching (i.e., xbatcher[39]), and EO-based classifications (e.g., DELTA[40]). Tools are also available in R (e.g., SITS, 123) and Julia (e.g., Flux.jl, 124, DiffEqFlux.jl, 125, ReservoirComputing.jl, 126) that incorporate ML and DL techniques, which can be utilised for geospatial data analysis, including state-of-art advanced methods, such as PIML.

5.3 Scalability obstacles

The size of data cubes poses several challenges for analysis. Generally, in most programming languages for data science (e.g., Python, Julia, R), data has to be completely loaded into memory before calculating a simple statistic (e.g., median). However, data cubes often surpass the memory limit, hindering computations or resulting in significant slowdowns due to frequent disk read-write operations. Instead, users can apply specialised algorithms that calculate statistics iteratively [127, 128]. $\mathcal{O}(1)$ memory algorithms allow the user to track statistics (e.g., mean, sums, and standard deviations) iteratively. They give the user complete control (and responsibility) over the order of the data reads. Because of the spherical nature of the Earth, and the resulting differences in the area covered by pixels, these computations require weighted versions of the statistics (cf. Section 4.2). Errors arising from floating-point arithmetic must be minimised, including the potential for catastrophic cancellation [129, 130]. Software that implements such statistics include OnlineStats.jl[41] [131] and WeightedOnlineStats.jl[42] [63].

Often analyses can be performed independently on timesteps, maps, or any other discrete pieces of a data cube (e.g., dimensions, periods, spatial slices). First, users *split* the data into those pieces, and then *apply* the transformation. In the end, users *combine* the elements back together into a new cube (see fig. 6). Many analyses can be expressed in terms of *split-apply-combine* [132, 8], such as calculating mean seasonal cycle maps from a time axis to a day-of-year axis, or a global mean temperature time series that collapses latitude and longitude into a scalar value per timestep. This method is also known as *map-reduce* in distributed data processing. Still, in contrast, it is made for array-like or tabular data (and the *reduce* step always consists in concatenating the results of the *map* step, cf. 132). Implementations of *split-apply-combine* can trade off between memory consumption and performance by adjusting the amount of data being loaded into memory at the same time. They may also take advantage of parallel reading, processing, and writing of data, which is especially important if the data is not stored on local storage but on object stores with high access latency.

The chunked storage format typically employed by data cubes, where reading a single element requires loading an entire chunk into memory, presents an opportunity for optimising sampling during ML training. Reading points individually is inefficient, as sampling two points from the same chunk necessitates reading the entire chunk twice. To mitigate this, reordering the points within a batch enables reading points from the same chunk jointly, reducing the number of reading operations. Adopting this approach makes it possible to limit the need to read the entire data cube only once per batch, optimising the data access process. Libraries such as YAXArrays.jl, which offer improved efficiency for working with data cubes, use this technique.

Ensuring that scalability obstacles are transparent for end users during Earth system data analysis is essential. While experienced users may be able to address scalability issues effectively, less experienced users may struggle with the process if it is not fully transparent. It is important to provide a user-friendly interface that hides the complexities of scalability, allowing users to focus on their analysis tasks. Additionally, not all users can access sufficient computing resources for scaling processes, resulting in additional processing costs. Therefore, providing accessible and cost-effective solutions for scalability, such as cloud-based platforms, is crucial to enable a broader range of users to harness the benefits of scaling in Earth system data analysis.

6 Visual interaction with Data Cubes

Data and process visualisation are critical for communicating Earth system science because big data are often hard to understand intuitively based on metadata alone, especially for non-expert audiences [133–135]. The gap between analytic capability and the means to effectively visualise results slows our progress in understanding complex Earth system phenomena. Specialised tools are needed to visualise data cubes and address their specific needs. Helbig et al. [136] defined the key challenges of data visualisation for advancing Earth system sciences. Their ambition was to use data cube visualisation for visual data exploration, facilitating multidisciplinary and collaborative research, and also emphasising their educational role.

Much progress has been made in visualising data cubes in Earth system research. Several viewers now have provided researchers with the means to explore and visualise multidimensional environmental datasets and generate scientific illustrations for publi-

[35] https://github.com/JuliaDataCubes/YAXArrays.jl
[36] https://github.com/rafaqz/Rasters.jl
[37] https://github.com/azavea/raster-vision
[38] https://github.com/moonshinelabs-ai/moonshine
[39] https://github.com/xarray-contrib/xbatcher
[40] https://github.com/nasa/delta
[41] https://github.com/joshday/OnlineStats.jl
[42] https://github.com/gdkrmr/WeightedOnlineStats.jl

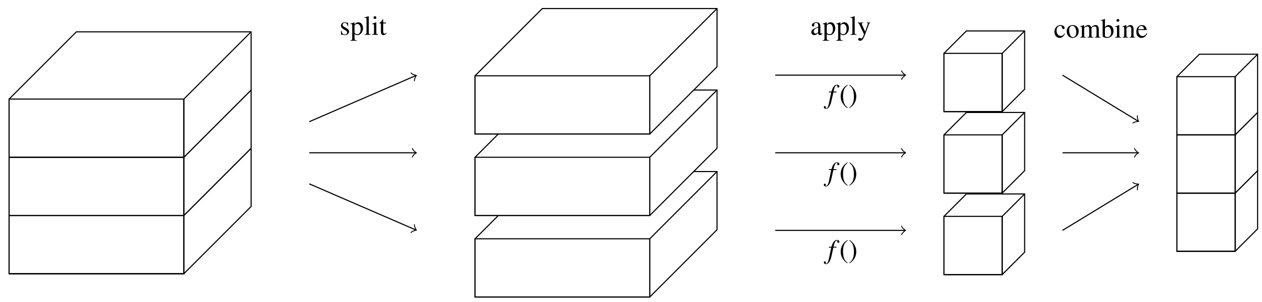

Figure 6: *Split-apply-combine*: *split* a data cube along arbitrary axes, *apply* a function f to each sub-cube, and then *combine* the results along the same axes that have been used to split the original cube

cations[43,44]. However, most approaches still rely on the classical geographical interpretation of georeferenced data and are restricted to displaying maps, extracting singular time series, or Hovmöller diagrams. Little advances have been made to visualise data cubes, in particular multivariate data cubes, for a better data understanding [cf. static attempts, 59, 137, 8]. The long-standing challenge is the trade-off between data interactions not designed for cubes and reliance on standard libraries that generate only static visualisations. Recent developments like Lexcube [138, cf. interactions in Figure 7][45] and xcube-viewer[46] enable interactive and barrier-free visualisation, allowing users to inspect any cube dimension (especially space, time, and variable) interactively. Enabling interactions on large-scale spatio-temporal data in the web is key to democratising our science [139].

A major challenge will be the integration of data analytics with interactive visualisations through visual analytics (cf. the review of 140). The existing suite of methods is only partially suited for dealing with highly multivariate data cubes, and most sophisticated visual analytic tools depend on a highly developed local computing infrastructure. There is a pressing need for web-based solutions to address this limitation. The goal should be to incorporate visualisations into any complex workflow to enhance comprehension of data inputs, monitor intermediate outcomes, and observe spatio-temporally structured results. One approach could be the tight integration of visualisation in developer workflows, particularly in popular environments like Jupyter Notebooks.

Integrating analytics tools with visualisation frameworks would allow researchers to dynamically explore, analyse, and visualise data cubes in a unified environment in real-time. This would empower researchers to gain immediate insights into the relationships and patterns within the data. Additionally, incorporating visualisation into developer workflows would facilitate seamless visualisation generation at any stage of the data cube life-cycle, allowing researchers to visualise intermediate and final results and facilitating a more intuitive, iterative exploration of Earth system data.

[43]https://github.com/carbonplan/maps
[44]https://cfs.climate.esa.int/
[45]https://www.lexcube.org/
[46]https://github.com/dcs4cop/xcube-viewer

Beyond the scientific community, data cube visualisation holds immense potential to engage and inform a wider audience. Interactive open-access visualisations, exemplified by tools like Lexcube, facilitate the exploration of Earth system data by the general public. These platforms provide an avenue for political stakeholders and the general public to directly access and examine climate data, e.g., global or regional climate anomalies and trends. By visualising anomalies, trends, and the interplay of variables, open-access interactive visualisations enable scientifically literate individuals and those with less technical expertise to delve into data cubes easily and rapidly. Such accessibility encourages a broader understanding and appreciation of Earth system research among diverse stakeholders, fostering a more informed and constructive dialogue about climate-related issues.

7 Conclusions and perspective

This paper reviews and explores the challenges and opportunities associated with leveraging data cubes for Earth system research. These challenges and opportunities might become of particular importance in the development of Earth Digital Twins (i.e., “a digital replication of the state and temporal evolution of the Earth system”, 141). In this sense, the technological challenges discussed here can be of significance in initiatives like Destination Earth (DestinE)[47]. However, data cubes’ potential also extends beyond the domain of Earth system sciences. Their applicability and benefits can be harnessed in various fields, such as fluid dynamics and mechanics, astrophysics, and health. By embracing the concept and structure of data cubes in these disciplines, researchers can unlock new opportunities for multidimensional analysis. The inherent simplicity and versatility of data cubes enable a comprehensive exploration of complex systems, facilitating a deeper understanding of intricate processes and phenomena. For advancing our understanding of the Earth system, the following main challenges emerge and need to be addressed by the research community to tap into the full potential of data cubes:

1. **Artificial Intelligence on data cubes:** The abundance of large-scale Earth system data, coupled with the recent advancements in AI methods, compels the application of the latest developments in DL on ESDCs. Capitalising on the tensor-like structure of data cubes in DL

[47]https://digital-strategy.ec.europa.eu/en/policies/destination-earth

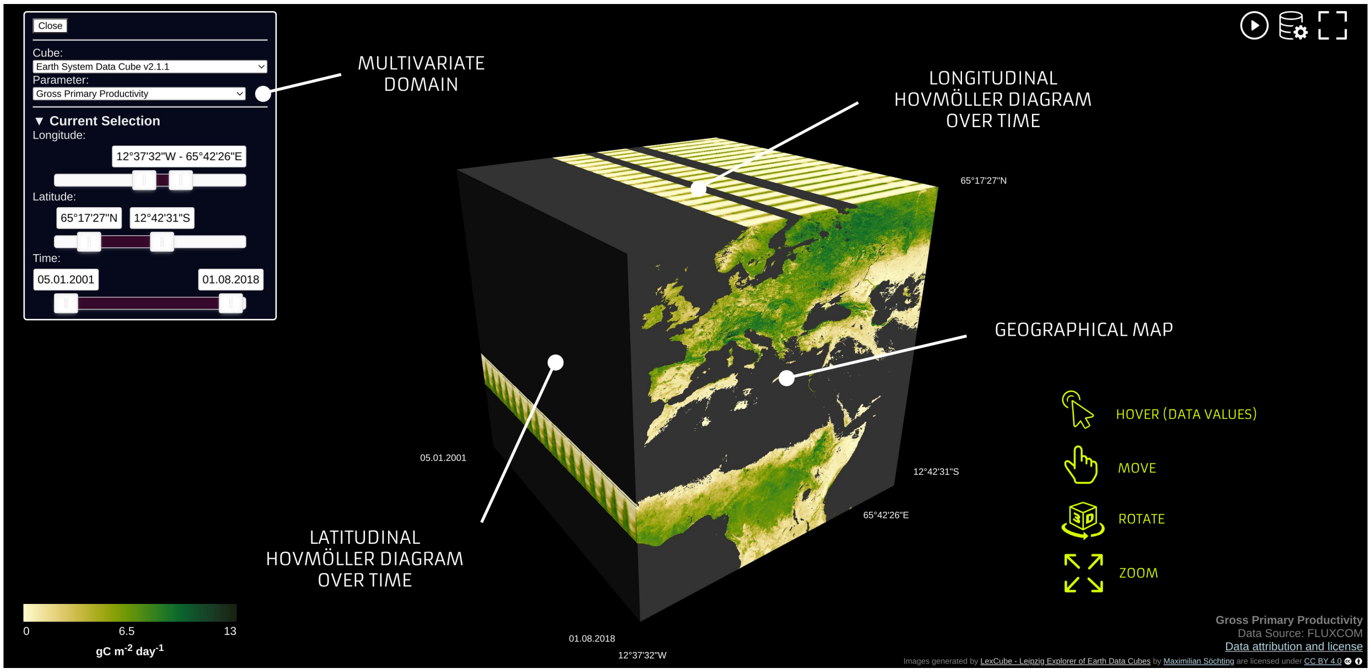

Figure 7: Interactions within an example data cube in Lexcube, showcasing a geographical map on the front side and Hollmöver diagrams depicting temporal changes on the lateral sides. The data cube allows for interactive subset operations on any side

and incorporating factual knowledge through Physics-Informed Machine Learning approaches promise great advances in modelling and understanding. Recent advancements in AI, particularly in attention mechanisms, have opened up new possibilities for Earth system research. Techniques such as LLMs, image generative models [e.g., Stable Diffusion, 142], as well as recent image segmentation models [e.g., Segment Anything Model, SAM, 143], may hold the potential to significantly advance our understanding of the Earth system. The ability to 'communicate' to ESDCs to extract valuable insights is within reach (e.g., using text prompts to extract variable anomalies from a specific land cover over a specific region in the world). Furthermore, there is potential to generate ESDCs using text prompts, images, videos, or additional data inputs simultaneously by leveraging the power of multi-modal attention mechanisms [e.g., ImageBind, 144], e.g., simulating the impact on vegetation due to an extreme event over a real ESDC using text prompts and geographical data. However, caution must be exercised when applying AI methods to ESDCs to avoid erroneous predictions and interpretations. Factors such as spatio-temporal autocorrelation, the spherical nature of the Earth, and biased sampling in the spatio-temporal and multivariate domains pose risks. Still, the abstract nature of data cubes provides an opportunity to establish a de facto standard for AI in Earth system science, benefiting from optimised data access and technical enhancements. To ensure reliable outcomes, standardised methods are needed to address spatial dependency, the model's area of applicability, and model uncertainty within data cube structures.

2. **Interacting with with data cubes:** The heterogeneity, size, and multivariate nature of datasets also may imply that the usage of ESDCs' is unintuitive, which hampers interpretation. Effective opportunities to communicate with such data are crucial throughout the data cubes' life cycle, both for scientists and a wider audience. Visualisation plays a key role in this regard [138]. While there are visualisation tools available to support the analysis process and scientific dissemination, there is still considerable potential for further exploration and development of visualisations. We believe that interactive visualisations are one key, as demonstrated by Lexcube. One promising avenue is the integration of visualisation directly into the analytics workflow (e.g., within Jupyter Notebooks or similar environments), and another is enabling visual analytics of data cubes. In both cases, the challenge is making such interactions possible during the analysis process in order to enable the scientific exploitation of big earth data cubes.

3. **Technical challenges of large data cubes:** The multidimensional nature, varying spatio-temporal scales and resolutions, and applicability of Earth system data cubes imply a series of technical challenges. These include interoperability issues, different geographical projections, questions of interpolation and aggregation, and varying levels of readiness for different analyses. Ensuring data integrity and interpretability while making Earth system data analysis-ready and interoperable requires tracing and encoding all data transformations and modifications in ESDC metadata. To address these challenges, the development of guidelines and standards for geospatial datacubes is crucial for pro-

moting FAIR and Open Earth System Science. The ever-increasing size and complexity of datasets demand scalable solutions to tackle associated challenges. The ongoing efforts of the open-source software community are commendable in this regard, as they contribute to the advancement of tools and frameworks tailored to handle big Earth system data. Furthermore, cloud environments present a possible solution to quickly scale workloads when processing ESDCs within the data cube life-cycle. They offer the advantages of on-demand resource allocation and scalability, allowing researchers to access the necessary computational power and storage capacity when needed.

4. **Integrating (geospatial) data beyond cubes:** Data cubes already offer the potential for advancing Earth system research and analysis in multiple domains. However, ESDCs can further benefit from the integration of different methodological approaches or data sources at different scales. One example is the integration of Unoccupied Aerial Vehicle (UAV)- and Light Detection and Ranging (LiDAR)-based data. This kind of data provides a means to collect highly localised and high-resolution measurements, making them particularly suitable for localised studies, and gaining valuable insights into fine-scale processes. Another example is the integration of vector data, which typically represents categorical information and carries great importance in multiple Earth system spheres (e.g., socioeconomic features). Additionally, in-situ collections of any process (e.g., via ecological monitoring data) are key. Today, the quest is that users request the integration of any additional data sources while remaining fully valid. Yet it poses a challenge as it raises important questions regarding interoperability and the encapsulation of multi-resolution cubes that incorporate multi-scale raster data and the combination of raster and vector data within a unified framework.

5. **Towards flexible cube-based structures:** To advance ESDCs' benefits, it is essential to advance the standards of data cube structures and start considering hierarchical data structures, including data cubes as "leaves" (e.g., xarray's DataTree structure). This would enhance Earth system research given the abundance of insightful (but heterogeneous) datasets, regardless of their resolution or dimensionality. Nevertheless, this implies that we must ensure data traceability and interpretability as heterogeneity increases in the resolution or dimensionality domains. A prime example lies in the integration of AI models' predictions within ESDCs. In such instances, additional dimensions must be incorporated to capture uncertainties (or quality flag systems) associated with AI-based predictions. This provides valuable insights into the reliability and robustness of the data.

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References

[1] Adrian Simmons, Jean-Louis Fellous, Venkatachalam Ramaswamy, Kevin Trenberth, Ghassem Asrar, Magdalena Balmaseda, John P Burrows, Philippe Ciais, Mark Drinkwater, Pierre Friedlingstein, et al. Observation and integrated Earth-system science: A roadmap for 2016–2025. *Advances in Space Research*, 57(10):2037–2103, 2016.

[2] Jian Peng, Clement Albergel, Anna Balenzano, Luca Brocca, Oliver Cartus, Michael H Cosh, Wade T Crow, Katarzyna Dabrowska-Zielinska, Simon Dadson, Malcolm WJ Davidson, et al. A roadmap for high-resolution satellite soil moisture applications–confronting product characteristics with user requirements. *Remote Sensing of Environment*, 252:112162, 2021.

[3] Peter Bauer, Peter D Dueben, Torsten Hoefler, Tiago Quintino, Thomas C Schulthess, and Nils P Wedi. The digital revolution of earth-system science. *Nature Computational Science*, 1(2):104–113, 2021.

[4] G. Tramontana, M. Jung, C. R. Schwalm, K. Ichii, G. Camps-Valls, B. Ráduly, M. Reichstein, M. A. Arain, A. Cescatti, G. Kiely, L. Merbold, P. Serrano-Ortiz, S. Sickert, S. Wolf, and D. Papale. Predicting carbon dioxide and energy fluxes across global FLUXNET sites with regression algorithms. *Biogeosciences*, 13(14):4291–4313, 2016. doi: 10.5194/bg-13-4291-2016. URL https://bg.copernicus.org/articles/13/4291/2016/.

[5] B. Martens, D. G. Miralles, H. Lievens, R. van der Schalie, R. A. M. de Jeu, D. Fernández-Prieto,

H. E. Beck, W. A. Dorigo, and N. E. C. Verhoest. GLEAM v3: satellite-based land evaporation and root-zone soil moisture. *Geoscientific Model Development*, 10(5):1903–1925, 2017. doi: 10.5194/gmd-10-1903-2017. URL https://gmd.copernicus.org/articles/10/1903/2017/.

[6] J. Muñoz Sabater, E. Dutra, A. Agustí-Panareda, C. Albergel, G. Arduini, G. Balsamo, S. Boussetta, M. Choulga, S. Harrigan, H. Hersbach, B. Martens, D. G. Miralles, M. Piles, N. J. Rodríguez-Fernández, E. Zsoter, C. Buontempo, and J.-N. Thépaut. ERA5-Land: a state-of-the-art global reanalysis dataset for land applications. *Earth System Science Data*, 13(9):4349–4383, 2021. doi: 10.5194/essd-13-4349-2021. URL https://essd.copernicus.org/articles/13/4349/2021/.

[7] Jakob Runge, Sebastian Bathiany, Erik Bollt, Gustau Camps-Valls, Dim Coumou, Ethan Deyle, Clark Glymour, Marlene Kretschmer, Miguel D. Mahecha, Jordi Muñoz-Marí, Egbert H. van Nes, Jonas Peters, Rick Quax, Markus Reichstein, Marten Scheffer, Bernhard Schölkopf, Peter Spirtes, George Sugihara, Jie Sun, Kun Zhang, and Jakob Zscheischler. Inferring causation from time series in Earth system sciences. *Nature Communications*, 10 (1), June 2019. doi: 10.1038/s41467-019-10105-3. URL https://doi.org/10.1038/s41467-019-10105-3.

[8] Miguel D Mahecha, Fabian Gans, Gunnar Brandt, Rune Christiansen, Sarah E Cornell, Normann Fomferra, Guido Kraemer, Jonas Peters, Paul Bodesheim, Gustau Camps-Valls, et al. Earth system data cubes unravel global multivariate dynamics. *Earth System Dynamics*, 11(1):201–234, 2020.

[9] Devis Tuia, Konrad Schindler, Begüm Demir, Gustau Camps-Valls, Xiao Xiang Zhu, Mrinalini Kochupillai, Sašo Džeroski, Jan N van Rijn, Holger H Hoos, Fabio Del Frate, et al. Artificial intelligence to advance Earth observation: a perspective. *arXiv preprint arXiv:2305.08413*, 2023.

[10] Geoffrey Boulton. The challenges of a big data earth. *Big Earth Data*, 2(1):1–7, 2018.

[11] Martin Sudmanns, Dirk Tiede, Stefan Lang, Helena Bergstedt, Georg Trost, Hannah Augustin, Andrea Baraldi, and Thomas Blaschke. Big Earth data: disruptive changes in Earth observation data management and analysis? *International Journal of Digital Earth*, 13(7):832–850, 2020.

[12] Markus Reichstein, Gustau Camps-Valls, Bjorn Stevens, Martin Jung, Joachim Denzler, and Nuno Carvalhais. Deep learning and process understanding for data-driven Earth system science. *Nature*, 566(7743):195–204, 2019.

[13] Christopher Irrgang, Niklas Boers, Maike Sonnewald, Elizabeth A Barnes, Christopher Kadow, Joanna Staneva, and Jan Saynisch-Wagner. Towards neural earth system modelling by integrating artificial intelligence in earth system science. *Nature Machine Intelligence*, 3(8):667–674, 2021.

[14] Ziheng Sun, Laura Sandoval, Robert Crystal-Ornelas, S Mostafa Mousavi, Jinbo Wang, Cindy Lin, Nicoleta Cristea, Daniel Tong, Wendy Hawley Carande, Xiaogang Ma, et al. A review of earth artificial intelligence. *Computers & Geosciences*, page 105034, 2022.

[15] Stefano Nativi, Paolo Mazzetti, and Max Craglia. A view-based model of data-cube to support big earth data systems interoperability. *Big Earth Data*, 1(1-2):75–99, 2017.

[16] Marius Appel and Edzer Pebesma. On-demand processing of data cubes from satellite image collections with the gdalcubes library. *Data*, 4(3):92, 2019.

[17] Peter Baumann, Dimitar Misev, Vlad Merticariu, and Bang Pham Huu. Datacubes: Towards space/time analysis-ready data. *Service-Oriented Mapping: Changing Paradigm in Map Production and Geoinformation Management*, pages 269–299, 2019.

[18] Gregory Giuliani, Joan Masó, Paolo Mazzetti, Stefano Nativi, and Alaitz Zabala. Paving the way to increased interoperability of earth observations data cubes. *Data*, 4 (3):113, 2019.

[19] Steve Kopp, Peter Becker, Abhijit Doshi, Dawn J Wright, Kaixi Zhang, and Hong Xu. Achieving the full vision of earth observation data cubes. *Data*, 4(3):94, 2019.

[20] Lina M Estupiñan Suarez, Fabian Gans, Alexander Brenning, Victor H Gutierrez-Velez, Maria C Londono, Daniel E Pabon-Moreno, Germán Poveda, Markus Reichstein, Björn Reu, Carlos A Sierra, et al. A regional Earth system data lab for understanding ecosystem dynamics: An example from tropical South America. *Frontiers in Earth Science*, page 574, 2021.

[21] Matthias Schramm, Edzer Pebesma, Milutin Milenković, Luca Foresta, Jeroen Dries, Alexander Jacob, Wolfgang Wagner, Matthias Mohr, Markus Neteler, Miha Kadunc, et al. The openeo api–harmonising the use of earth observation cloud services using virtual data cube functionalities. *Remote Sensing*, 13(6):1125, 2021.

[22] Mark D. Wilkinson, Michel Dumontier, IJsbrand Jan Aalbersberg, Gabrielle Appleton, Myles Axton, Arie Baak, Niklas Blomberg, Jan-Willem Boiten, Luiz Bonino da Silva Santos, Philip E. Bourne, Jildau Bouwman, Anthony J. Brookes, Tim Clark, Mercè Crosas, Ingrid Dillo, Olivier Dumon, Scott Edmunds, Chris T. Evelo, Richard Finkers, Alejandra Gonzalez-Beltran, Alasdair J.G. Gray, Paul Groth, Carole Goble, Jeffrey S. Grethe, Jaap Heringa, Peter A.C 't Hoen, Rob Hooft, Tobias Kuhn, Ruben Kok, Joost Kok, Scott J. Lusher, Maryann E. Martone, Albert Mons, Abel L. Packer, Bengt Persson, Philippe Rocca-Serra, Marco Roos, Rene van Schaik, Susanna-Assunta Sansone, Erik Schultes, Thierry Sengstag, Ted Slater, George Strawn, Morris A. Swertz, Mark Thompson, Johan van der Lei, Erik van Mulligen, Jan Velterop, Andra Waagmeester, Peter Wittenburg, Katherine Wolstencroft, Jun Zhao, and Barend Mons. The FAIR Guiding Principles for scientific data management and stewardship. *Scientific Data*, 3(1), March 2016. doi: 10.1038/sdata.2016.18. URL https://doi.org/10.1038/sdata.2016.18.

[23] Trevor Dhu, Gregory Giuliani, Jimena Juárez, Argyro Kavvada, Brian Killough, Paloma Merodio, Stuart Minchin, and Steven Ramage. National Open Data

Cubes and Their Contribution to Country-Level Development Policies and Practices. *Data*, 4(4):144, November 2019. doi: 10.3390/data4040144. URL https://doi.org/10.3390/data4040144.

[24] Martin Sudmanns, Hannah Augustin, Brian Killough, Gregory Giuliani, Dirk Tiede, Alex Leith, Fang Yuan, and Adam Lewis. Think global, cube local: an Earth Observation Data Cube's contribution to the Digital Earth vision. *Big Earth Data*, pages 1–29, July 2022. doi: 10.1080/20964471.2022.2099236. URL https://doi.org/10.1080/20964471.2022.2099236.

[25] Brian Killough. Overview of the Open Data Cube Initiative. In *IGARSS 2018 - 2018 IEEE International Geoscience and Remote Sensing Symposium*. Ieee, July 2018. doi: 10.1109/igarss.2018.8517694. URL https://doi.org/10.1109/igarss.2018.8517694.

[26] Adam Lewis, Simon Oliver, Leo Lymburner, Ben Evans, Lesley Wyborn, Norman Mueller, Gregory Raevksi, Jeremy Hooke, Rob Woodcock, Joshua Sixsmith, Wenjun Wu, Peter Tan, Fuqin Li, Brian Killough, Stuart Minchin, Dale Roberts, Damien Ayers, Biswajit Bala, John Dwyer, Arnold Dekker, Trevor Dhu, Andrew Hicks, Alex Ip, Matt Purss, Clare Richards, Stephen Sagar, Claire Trenham, Peter Wang, and Lan-Wei Wang. The Australian Geoscience Data Cube — Foundations and lessons learned. *Remote Sensing of Environment*, 202:276–292, December 2017. doi: 10.1016/j.rse.2017.03.015. URL https://doi.org/10.1016/j.rse.2017.03.015.

[27] Trevor Dhu, Bex Dunn, Ben Lewis, Leo Lymburner, Norman Mueller, Erin Telfer, Adam Lewis, Alexis McIntyre, Stuart Minchin, and Claire Phillips. Digital earth Australia – unlocking new value from earth observation data. *Big Earth Data*, 1(1-2):64–74, December 2017. doi: 10.1080/20964471.2017.1402490. URL https://doi.org/10.1080/20964471.2017.1402490.

[28] Christian Ariza-Porras, Germán Bravo, Mario Villamizar, Andrés Moreno, Harold Castro, Gustavo Galindo, Edersson Cabera, Saralux Valbuena, and Pilar Lozano. CDCol: A Geoscience Data Cube that Meets Colombian Needs. In *Communications in Computer and Information Science*, pages 87–99. Springer International Publishing, 2017. doi: 10.1007/978-3-319-66562-7_7. URL https://doi.org/10.1007/978-3-319-66562-7_7.

[29] Gregory Giuliani, Bruno Chatenoux, Andrea De Bono, Denisa Rodila, Jean-Philippe Richard, Karin Allenbach, Hy Dao, and Pascal Peduzzi. Building an Earth Observations Data Cube: lessons learned from the Swiss Data Cube (SDC) on generating Analysis Ready Data (ARD). *Big Earth Data*, 1(1-2):100–117, November 2017. doi: 10.1080/20964471.2017.1398903. URL https://doi.org/10.1080/20964471.2017.1398903.

[30] Martin Sudmanns, Hannah Augustin, Lucas van der Meer, Andrea Baraldi, and Dirk Tiede. The Austrian semantic EO data cube infrastructure. *Remote Sensing*, 13(23): 4807, 2021.

[31] Noel Gorelick, Matt Hancher, Mike Dixon, Simon Ilyushchenko, David Thau, and Rebecca Moore. Google Earth Engine: Planetary-scale geospatial analysis for everyone. *Remote Sensing of Environment*, 202:18–27, December 2017. doi: 10.1016/j.rse.2017.06.031. URL https://doi.org/10.1016/j.rse.2017.06.031.

[32] William W. Hsieh. Evolution of machine learning in environmental science—A perspective. *Environmental Data Science*, 1, 2022. doi: 10.1017/eds.2022.2. URL https://doi.org/10.1017/eds.2022.2.

[33] Claudio Persello, Jan Dirk Wegner, Ronny Hänsch, Devis Tuia, Pedram Ghamisi, Mila Koeva, and Gustau Camps-Valls. Deep learning and earth observation to support the sustainable development goals: Current approaches, open challenges, and future opportunities. *IEEE Geoscience and Remote Sensing Magazine*, 10(2):172–200, 2022.

[34] Dzmitry Bahdanau, Kyunghyun Cho, and Yoshua Bengio. Neural Machine Translation by Jointly Learning to Align and Translate, May 2016.

[35] Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Lukasz Kaiser, and Illia Polosukhin. Attention is all you need, 2017. URL https://arxiv.org/abs/1706.03762.

[36] Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding. *arXiv:1810.04805 [cs]*, May 2019.

[37] Alec Radford, Jeffrey Wu, Rewon Child, David Luan, Dario Amodei, and Ilya Sutskever. Language Models Are Unsupervised Multitask Learners, 2019.

[38] Tom B. Brown, Benjamin Mann, Nick Ryder, Melanie Subbiah, Jared Kaplan, Prafulla Dhariwal, Arvind Neelakantan, Pranav Shyam, Girish Sastry, Amanda Askell, Sandhini Agarwal, Ariel Herbert-Voss, Gretchen Krueger, Tom Henighan, Rewon Child, Aditya Ramesh, Daniel M. Ziegler, Jeffrey Wu, Clemens Winter, Christopher Hesse, Mark Chen, Eric Sigler, Mateusz Litwin, Scott Gray, Benjamin Chess, Jack Clark, Christopher Berner, Sam McCandlish, Alec Radford, Ilya Sutskever, and Dario Amodei. Language Models Are Few-Shot Learners. *arXiv:2005.14165 [cs]*, June 2020.

[39] Mario Rüttgers, Sangseung Lee, Soohwan Jeon, and Donghyun You. Prediction of a typhoon track using a generative adversarial network and satellite images. *Scientific Reports*, 9(1), April 2019. doi: 10.1038/s41598-019-42339-y. URL https://doi.org/10.1038/s41598-019-42339-y.

[40] Norihiro Oyama, Noriko N. Ishizaki, Satoshi Koide, and Hiroaki Yoshida. Deep generative model super-resolves spatially correlated multiregional climate data. *Scientific Reports*, 13(1), April 2023. doi: 10.1038/s41598-023-32947-0. URL https://doi.org/10.1038/s41598-023-32947-0.

[41] Gustau Camps-Valls, Andreas Gerhardus, Urmi Ninad, Gherardo Varando, Georg Martius, Emili Balaguer-Ballester, Ricardo Vinuesa, Emiliano Diaz, Laure Zanna, and Jakob Runge. Discovering causal relations and equations from data. *arXiv preprint arXiv:2305.13341*, 2023.

[42] George Em Karniadakis, Ioannis G Kevrekidis, Lu Lu, Paris Perdikaris, Sifan Wang, and Liu Yang. Physics-

informed machine learning. *Nature Reviews Physics*, 3 (6):422–440, 2021.

[43] Gustau Camps-Valls, Daniel H. Svendsen, Jordi Cortes-Andres, Alvaro Mareno-Martinez, Adrian Perez-Suay, Jose Adsuara, Irene Martin, Maria Piles, Jordi Munoz-Mari, and Luca Martino. Physics-Aware Machine Learning for Geosciences and Remote Sensing. In *2021 IEEE International Geoscience and Remote Sensing Symposium IGARSS*. Ieee, July 2021. doi: 10.1109/igarss47720.2021.9554521. URL https://doi.org/10.1109/igarss47720.2021.9554521.

[44] Jordi Cortés-Andrés, Gustau Camps-Valls, Sebastian Sippel, Enikő Székely, Dino Sejdinovic, Emiliano Diaz, Adrián Pérez-Suay, Zhu Li, Miguel Mahecha, and Markus Reichstein. Physics-aware nonparametric regression models for earth data analysis. *Environmental Research Letters*, 17(5):054034, 2022.

[45] Cesar Aybar, Carlos Fernández, Adrian Huerta, Waldo Lavado, Fiorella Vega, and Oscar Felipe-Obando. Construction of a high-resolution gridded rainfall dataset for Peru from 1981 to the present day. *Hydrological Sciences Journal*, 65(5):770–785, 2020. doi: 10.1080/02626667.2019.1649411.

[46] S. Walther, S. Besnard, J. A. Nelson, T. S. El-Madany, M. Migliavacca, U. Weber, N. Carvalhais, S. L. Ermida, C. Brümmer, F. Schrader, A. S. Prokushkin, A. V. Panov, and M. Jung. Technical note: A view from space on global flux towers by MODIS and Landsat: the FluxnetEO data set. *Biogeosciences*, 19(11):2805–2840, 2022. doi: 10.5194/bg-19-2805-2022. URL https://bg.copernicus.org/articles/19/2805/2022/.

[47] John P. Snyder and Philip M. Voxland. *An album of map projections*. US Geological Survey, 1989. doi: 10.3133/pp1453. URL https://doi.org/10.3133/pp1453.

[48] Alex Sherstinsky. Fundamentals of Recurrent Neural Network (RNN) and Long Short-Term Memory (LSTM) network. *Physica D: Nonlinear Phenomena*, 404:132306, March 2020. doi: 10.1016/j.physd.2019.132306. URL https://doi.org/10.1016/j.physd.2019.132306.

[49] Michael A. Wulder, Joanne C. White, Thomas R. Loveland, Curtis E. Woodcock, Alan S. Belward, Warren B. Cohen, Eugene A. Fosnight, Jerad Shaw, Jeffrey G. Masek, and David P. Roy. The global Landsat archive: Status, consolidation, and direction. *Remote Sensing of Environment*, 185:271–283, November 2016. doi: 10.1016/j.rse.2015.11.032. URL https://doi.org/10.1016/j.rse.2015.11.032.

[50] Jody C. Vogeler, Justin D. Braaten, Robert A. Slesak, and Michael J. Falkowski. Extracting the full value of the Landsat archive: Inter-sensor harmonization for the mapping of Minnesota forest canopy cover (1973–2015). *Remote Sensing of Environment*, 209:363–374, May 2018. doi: 10.1016/j.rse.2018.02.046. URL https://doi.org/10.1016/j.rse.2018.02.046.

[51] David Frantz. FORCE—Landsat + Sentinel-2 Analysis Ready Data and Beyond. *Remote Sensing*, 11(9), 2019. ISSN 2072-4292. doi: 10.3390/rs11091124. URL https://www.mdpi.com/2072-4292/11/9/1124.

[52] John L. Dwyer, David P. Roy, Brian Sauer, Calli B. Jenkerson, Hankui K. Zhang, and Leo Lymburner. Analysis Ready Data: Enabling Analysis of the Landsat Archive. *Remote Sensing*, 10(9), 2018. ISSN 2072-4292. doi: 10.3390/rs10091363. URL https://www.mdpi.com/2072-4292/10/9/1363.

[53] Sergii Skakun, Jan Wevers, Carsten Brockmann, Georgia Doxani, Matej Aleksandrov, Matej Batič, David Frantz, Ferran Gascon, Luis Gómez-Chova, Olivier Hagolle, Dan López-Puigdollers, Jérôme Louis, Matic Lubej, Gonzalo Mateo-García, Julien Osman, Devis Peressutti, Bringfried Pflug, Jernej Puc, Rudolf Richter, Jean-Claude Roger, Pat Scaramuzza, Eric Vermote, Nejc Vesel, Anže Zupanc, and Lojze Žust. Cloud Mask Intercomparison eXercise (CMIX): An evaluation of cloud masking algorithms for Landsat 8 and Sentinel-2. *Remote Sensing of Environment*, 274:112990, June 2022. doi: 10.1016/j.rse.2022.112990. URL https://doi.org/10.1016/j.rse.2022.112990.

[54] D.P. Roy, H.K. Zhang, J. Ju, J.L. Gomez-Dans, P.E. Lewis, C.B. Schaaf, Q. Sun, J. Li, H. Huang, and V. Kovalskyy. A general method to normalize Landsat reflectance data to nadir BRDF adjusted reflectance. *Remote Sensing of Environment*, 176:255–271, April 2016. doi: 10.1016/j.rse.2016.01.023. URL https://doi.org/10.1016/j.rse.2016.01.023.

[55] Martin Claverie, Junchang Ju, Jeffrey G. Masek, Jennifer L. Dungan, Eric F. Vermote, Jean-Claude Roger, Sergii V. Skakun, and Christopher Justice. The Harmonized Landsat and Sentinel-2 surface reflectance data set. *Remote Sensing of Environment*, 219:145–161, 2018. ISSN 0034-4257. doi: https://doi.org/10.1016/j.rse.2018.09.002. URL https://www.sciencedirect.com/science/article/pii/S0034425718304139.

[56] George C. Hurtt, Louise Chini, Ritvik Sahajpal, Steve Frolking, Benjamin L. Bodirsky, Katherine Calvin, Jonathan C. Doelman, Justin Fisk, Shinichiro Fujimori, Kees Klein Goldewijk, Tomoko Hasegawa, Peter Havlik, Andreas Heinimann, Florian Humpenöder, Johan Jungclaus, Jed O. Kaplan, Jennifer Kennedy, Tamás Krisztin, David Lawrence, Peter Lawrence, Lei Ma, Ole Mertz, Julia Pongratz, Alexander Popp, Benjamin Poulter, Keywan Riahi, Elena Shevliakova, Elke Stehfest, Peter Thornton, Francesco N. Tubiello, Detlef P. van Vuuren, and Xin Zhang. Harmonization of global land use change and management for the period 850–2100 (LUH2) for CMIP6. *Geoscientific Model Development*, 13(11):5425–5464, November 2020. doi: 10.5194/gmd-13-5425-2020. URL https://doi.org/10.5194/gmd-13-5425-2020.

[57] Álvaro Moreno-Martínez, Emma Izquierdo-Verdiguier, Marco P. Maneta, Gustau Camps-Valls, Nathaniel Robinson, Jordi Muñoz-Marí, Fernando Sedano, Nicholas Clinton, and Steven W. Running. Multispectral high resolution sensor fusion for smoothing and gap-filling in the cloud. *Remote Sensing of Environment*, 247:111901, September 2020. doi: 10.1016/j.rse.2020.111901. URL https://doi.org/10.1016/j.rse.2020.111901.

[58] David Montero, César Aybar, Miguel D. Mahecha, Francesco Martinuzzi, Maximilian Söchting, and Sebastian Wieneke. A standardized catalogue of spectral indices to advance the use of remote sensing in Earth system research. *Scientific Data*, 10(1), April 2023. doi: 10.1038/s41597-023-02096-0. URL https://doi.org/10.1038/s41597-023-02096-0.

[59] Miguel D Mahecha, Lina M Fürst, Nadine Gobron, and Holger Lange. Identifying multiple spatiotemporal patterns: A refined view on terrestrial photosynthetic activity. *Pattern Recognition Letters*, 31(14):2309–2317, 2010.

[60] Patrick Griffiths, Sebastian van der Linden, Tobias Kuemmerle, and Patrick Hostert. A Pixel-Based Landsat Compositing Algorithm for Large Area Land Cover Mapping. *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, 6(5):2088–2101, 2013. doi: 10.1109/jstars.2012.2228167.

[61] Christopher F. Brown, Steven P. Brumby, Brookie Guzder-Williams, Tanya Birch, Samantha Brooks Hyde, Joseph Mazzariello, Wanda Czerwinski, Valerie J. Pasquarella, Robert Haertel, Simon Ilyushchenko, Kurt Schwehr, Mikaela Weisse, Fred Stolle, Craig Hanson, Oliver Guinan, Rebecca Moore, and Alexander M. Tait. Dynamic World, Near real-time global 10 m land use land cover mapping. *Scientific Data*, 9(1), June 2022. doi: 10.1038/s41597-022-01307-4. URL https://doi.org/10.1038/s41597-022-01307-4.

[62] Richard C. Cornes, Gerard van der Schrier, Else J. M. van den Besselaar, and Philip D. Jones. An Ensemble Version of the E-OBS Temperature and Precipitation Data Sets. *Journal of Geophysical Research: Atmospheres*, 123(17):9391–9409, 2018. doi: https://doi.org/10.1029/2017JD028200. URL https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/2017JD028200.

[63] Guido Kraemer, Gustau Camps-Valls, Markus Reichstein, and Miguel D. Mahecha. Summarizing the State of the Terrestrial Biosphere in Few Dimensions. *Biogeosciences*, 17(9):2397–2424, May 2020. ISSN 1726-4170. doi: 10.5194/bg-17-2397-2020.

[64] Christopher T. Lloyd, Alessandro Sorichetta, and Andrew J. Tatem. High resolution global gridded data for use in population studies. *Scientific Data*, 4(1), January 2017. doi: 10.1038/sdata.2017.1. URL https://doi.org/10.1038/sdata.2017.1.

[65] Matti Kummu, Maija Taka, and Joseph H. A. Guillaume. Gridded global datasets for Gross Domestic Product and Human Development Index over 1990–2015. *Scientific Data*, 5(1), February 2018. doi: 10.1038/sdata.2018.4. URL https://doi.org/10.1038/sdata.2018.4.

[66] Miguel D. Mahecha, Ana Bastos, Friedrich J. Bohn, Nico Eisenhauer, Hannes Feilhauer, Henrik Hartmann, Thomas Hickler, Heike Kalesse-Los, Mirco Migliavacca, Friederike E. L. Otto, Jian Peng, Johannes Quaas, Ina Tegen, Alexandra Weigelt, Manfred Wendisch, and Christian Wirth. Biodiversity loss and climate extremes — study the feedbacks. *Nature*, 612(7938):30–32, November 2022. doi: 10.1038/d41586-022-04152-y. URL https://doi.org/10.1038/d41586-022-04152-y.

[67] Markus Reichstein, Michael Bahn, Philippe Ciais, Dorothea Frank, Miguel D. Mahecha, Sonia I. Seneviratne, Jakob Zscheischler, Christian Beer, Nina Buchmann, David C. Frank, Dario Papale, Anja Rammig, Pete Smith, Kirsten Thonicke, Marijn van der Velde, Sara Vicca, Ariane Walz, and Martin Wattenbach. Climate extremes and the carbon cycle. *Nature*, 500(7462):287–295, August 2013. doi: 10.1038/nature12350. URL https://doi.org/10.1038/nature12350.

[68] Jiabo Yin, Pierre Gentine, Louise Slater, Lei Gu, Yadu Pokhrel, Naota Hanasaki, Shenglian Guo, Lihua Xiong, and Wolfram Schlenker. Future socio-ecosystem productivity threatened by compound drought–heatwave events. *Nature Sustainability*, 6(3):259–272, January 2023. doi: 10.1038/s41893-022-01024-1. URL https://doi.org/10.1038/s41893-022-01024-1.

[69] Rolf Simoes, Felipe Carvalho de Souza, Matheus Zaglia, Gilberto Ribeiro de Queiroz, Rafael D. C. dos Santos, and Karine Reis Ferreira. Rstac: An R Package to Access Spatiotemporal Asset Catalog Satellite Imagery. In *2021 IEEE International Geoscience and Remote Sensing Symposium IGARSS*. Ieee, July 2021. doi: 10.1109/igarss47720.2021.9553518. URL https://doi.org/10.1109/igarss47720.2021.9553518.

[70] Gregory Giuliani, Bruno Chatenoux, Thomas Piller, Frédéric Moser, and Pierre Lacroix. Data Cube on Demand (DCoD): Generating an earth observation Data Cube anywhere in the world. *International Journal of Applied Earth Observation and Geoinformation*, 87:102035, May 2020. doi: 10.1016/j.jag.2019.102035. URL https://doi.org/10.1016/j.jag.2019.102035.

[71] A. P. Cracknell. Review article Synergy in remote sensing-what's in a pixel? *International Journal of Remote Sensing*, 19(11):2025–2047, January 1998. doi: 10.1080/014311698214848. URL https://doi.org/10.1080/014311698214848.

[72] Konstantinos G. Nikolakopoulos. Comparison of Nine Fusion Techniques for Very High Resolution Data. *Photogrammetric Engineering & Remote Sensing*, 74(5):647–659, May 2008. doi: 10.14358/pers.74.5.647. URL https://doi.org/10.14358/pers.74.5.647.

[73] Julien Michel, Juan Vinasco-Salinas, Jordi Inglada, and Olivier Hagolle. SEN2VENUS, a Dataset for the Training of Sentinel-2 Super-Resolution Algorithms. *Data*, 7(7), 2022. ISSN 2306-5729. doi: 10.3390/data7070096. URL https://www.mdpi.com/2306-5729/7/7/96.

[74] Muhammed T. Razzak, Gonzalo Mateo-García, Gurvan Lecuyer, Luis Gómez-Chova, Yarin Gal, and Freddie Kalaitzis. Multi-spectral multi-image super-resolution of Sentinel-2 with radiometric consistency losses and its effect on building delineation. *ISPRS Journal of Photogrammetry and Remote Sensing*, 195:1–13, 2023. ISSN 0924-2716. doi: https://doi.org/10.1016/j.isprsjprs.2022.10.019. URL https://www.sciencedirect.com/science/article/pii/S0924271622002878.

[75] Huiying Ren, Erol Cromwell, Ben Kravitz, and Xingyuan Chen. Technical note: Using long short-term memory models to fill data gaps in hydrological monitoring networks. *Hydrology and Earth System Sciences*,

26(7):1727–1743, April 2022. doi: 10.5194/hess-26-1727-2022. URL https://doi.org/10.5194/hess-26-1727-2022.

[76] Michael A. Wulder, Thomas Hilker, Joanne C. White, Nicholas C. Coops, Jeffrey G. Masek, Dirk Pflugmacher, and Yves Crevier. Virtual constellations for global terrestrial monitoring. *Remote Sensing of Environment*, 170:62–76, December 2015. doi: 10.1016/j.rse.2015.09.001. URL https://doi.org/10.1016/j.rse.2015.09.001.

[77] Xingan Chen, Yuefei Huang, Chong Nie, Shuo Zhang, Guangqian Wang, Shiliu Chen, and Zhichao Chen. A long-term reconstructed TROPOMI solar-induced fluorescence dataset using machine learning algorithms. *Scientific Data*, 9(1), July 2022. doi: 10.1038/s41597-022-01520-1. URL https://doi.org/10.1038/s41597-022-01520-1.

[78] Natalie Mahowald, Fiona Lo, Yun Zheng, Laura Harrison, Chris Funk, Danica Lombardozzi, and Christine Goodale. Projections of leaf area index in earth system models. *Earth System Dynamics*, 7(1):211–229, March 2016. doi: 10.5194/esd-7-211-2016. URL https://doi.org/10.5194/esd-7-211-2016.

[79] D. Hassell, J. Gregory, J. Blower, B. N. Lawrence, and K. E. Taylor. A data model of the Climate and Forecast metadata conventions (CF-1.6) with a software implementation (cf-python v2.1). *Geoscientific Model Development*, 10(12):4619–4646, 2017. doi: 10.5194/gmd-10-4619-2017. URL https://gmd.copernicus.org/articles/10/4619/2017/.

[80] H von Storch, FW Zwiers, and RE Livezey. Statistical analysis in climate research. *Nature*, 404(6778):544, 2000.

[81] Mark A. Wieczorek and Matthias Meschede. SHTools: Tools for Working with Spherical Harmonics. *Geochemistry, Geophysics, Geosystems*, 19(8):2574–2592, August 2018. doi: 10.1029/2018gc007529. URL https://doi.org/10.1029/2018gc007529.

[82] Alexander Kmoch, Ivan Vasilyev, Holger Virro, and Evelyn Uuemaa. Area and shape distortions in open-source discrete global grid systems. *Big Earth Data*, 6(3):256–275, July 2022. doi: 10.1080/20964471.2022.2094926. URL https://doi.org/10.1080/20964471.2022.2094926.

[83] Sepp Hochreiter and Jürgen Schmidhuber. Long Short-Term Memory. *Neural Computation*, 9(8):1735–1780, November 1997. doi: 10.1162/neco.1997.9.8.1735. URL https://doi.org/10.1162/neco.1997.9.8.1735.

[84] Y. LeCun, B. Boser, J. S. Denker, D. Henderson, R. E. Howard, W. Hubbard, and L. D. Jackel. Backpropagation Applied to Handwritten Zip Code Recognition. *Neural Computation*, 1(4):541–551, December 1989. doi: 10.1162/neco.1989.1.4.541. URL https://doi.org/10.1162/neco.1989.1.4.541.

[85] Xingjian Shi, Zhourong Chen, Hao Wang, Dit-Yan Yeung, Wai-kin Wong, and Wang-chun Woo. Convolutional LSTM Network: A Machine Learning Approach for Precipitation Nowcasting, 2015. URL https://arxiv.org/abs/1506.04214.

[86] Sebastian Sippel, Markus Reichstein, Xuanlong Ma, Miguel D Mahecha, Holger Lange, Milan Flach, and Dorothea Frank. Drought, heat, and the carbon cycle: a review. *Current Climate Change Reports*, 4:266–286, 2018.

[87] Milan Flach, Alexander Brenning, Fabian Gans, Markus Reichstein, Sebastian Sippel, and Miguel D Mahecha. Vegetation modulates the impact of climate extremes on gross primary production. *Biogeosciences*, 18(1):39–53, 2021.

[88] Jakob Zscheischler, Olivia Martius, Seth Westra, Emanuele Bevacqua, Colin Raymond, Radley M Horton, Bart van den Hurk, Amir AghaKouchak, Aglaé Jézéquel, Miguel D Mahecha, et al. A typology of compound weather and climate events. *Nature reviews earth & environment*, 1(7):333–347, 2020.

[89] Milan Flach, Fabian Gans, Alexander Brenning, Joachim Denzler, Markus Reichstein, Erik Rodner, Sebastian Bathiany, Paul Bodesheim, Yanira Guanche, Sebastian Sippel, et al. Multivariate anomaly detection for earth observations: a comparison of algorithms and feature extraction techniques. *Earth System Dynamics*, 8(3):677–696, 2017.

[90] Miguel D Mahecha, Fabian Gans, Sebastian Sippel, Jonathan F Donges, Thomas Kaminski, Stefan Metzger, Mirco Migliavacca, Dario Papale, Anja Rammig, and Jakob Zscheischler. Detecting impacts of extreme events with ecological in situ monitoring networks. *Biogeosciences*, 14(18):4255–4277, 2017.

[91] Waldo R Tobler. A computer movie simulating urban growth in the Detroit region. *Economic geography*, 46 (sup1):234–240, 1970.

[92] Hanna Meyer and Edzer Pebesma. Predicting into unknown space? Estimating the area of applicability of spatial prediction models. *Methods in Ecology and Evolution*, 12(9):1620–1633, 2021.

[93] Pierre Ploton, Frédéric Mortier, Maxime Réjou-Méchain, Nicolas Barbier, Nicolas Picard, Vivien Rossi, Carsten Dormann, Guillaume Cornu, Gaëlle Viennois, Nicolas Bayol, et al. Spatial validation reveals poor predictive performance of large-scale ecological mapping models. *Nature communications*, 11(1):1–11, 2020.

[94] Teja Kattenborn, Felix Schiefer, Julian Frey, Hannes Feilhauer, Miguel D Mahecha, and Carsten F Dormann. Spatially autocorrelated training and validation samples inflate performance assessment of convolutional neural networks. *ISPRS Open Journal of Photogrammetry and Remote Sensing*, 5:100018, 2022.

[95] Alexandre MJ-C Wadoux, Gerard BM Heuvelink, Sytze De Bruin, and Dick J Brus. Spatial cross-validation is not the right way to evaluate map accuracy. *Ecological Modelling*, 457:109692, 2021.

[96] Dick J Brus. Statistical approaches for spatial sample survey: Persistent misconceptions and new developments. *European Journal of Soil Science*, 72(2):686–703, 2021.

[97] Daniel E Pabon-Moreno, Mirco Migliavacca, Markus Reichstein, and Miguel D Mahecha. On the potential of sentinel-2 for estimating gross primary production. *IEEE Transactions on Geoscience and Remote Sensing*, 60:1–12, 2022.

[98] Marvin Ludwig, Alvaro Moreno-Martinez, Norbert Hölzel, Edzer Pebesma, and Hanna Meyer. Assessing and improving the transferability of current global spatial prediction models. *Global Ecology and Biogeography*, 32(3):356–368, 2023.

[99] Katherine L Yates, Phil J Bouchet, M Julian Caley, Kerrie Mengersen, Christophe F Randin, Stephen Parnell, Alan H Fielding, Andrew J Bamford, Stephen Ban, A Márcia Barbosa, et al. Outstanding challenges in the transferability of ecological models. *Trends in ecology & evolution*, 33(10):790–802, 2018.

[100] Carles Mila, Jorge Mateu, Edzer Pebesma, and Hanna Meyer. Nearest neighbour distance matching Leave-One-Out Cross-Validation for map validation. *Methods in Ecology and Evolution*, 13(6):1304–1316, 2022.

[101] David R Roberts, Volker Bahn, Simone Ciuti, Mark S Boyce, Jane Elith, Gurutzeta Guillera-Arroita, Severin Hauenstein, José J Lahoz-Monfort, Boris Schröder, Wilfried Thuiller, et al. Cross-validation strategies for data with temporal, spatial, hierarchical, or phylogenetic structure. *Ecography*, 40(8):913–929, 2017.

[102] Carsten Dormann, Jana M. McPherson, Miguel B. Araújo, Roger Bivand, Janine Bolliger, Gudrun Carl, Richard G. Davies, Alexandre Hirzel, Walter Jetz, W Daniel Kissling, et al. Methods to account for spatial autocorrelation in the analysis of species distributional data: a review. *Ecography*, 30(5):609–628, 2007.

[103] Gustau Camps-Valls, Devis Tuia, Xiao Xiang Zhu, and Markus Reichstein. *Deep learning for the Earth Sciences: A comprehensive approach to remote sensing, climate science and geosciences*. Wiley & Sons, 2021. ISBN 9781119646143. URL https://github.com/DL4ES.

[104] Teja Kattenborn, Jens Leitloff, Felix Schiefer, and Stefan Hinz. Review on convolutional neural networks (cnn) in vegetation remote sensing. *ISPRS journal of photogrammetry and remote sensing*, 173:24–49, 2021.

[105] Gustau Camps-Valls. Perspective on deep learning for earth sciences. In Min Wu Zhenghua Chen, Xiaoli Li, editor, *Generalization with Deep Learning: for Improvement on Sensing Capability*, pages 159–173. World Scientific Pub Co Inc, 2021. ISBN 978-9811218835.

[106] Tamara G. Kolda and Brett W. Bader. Tensor Decompositions and Applications. *SIAM Review*, 51(3):455–500, August 2009. ISSN 0036-1445, 1095-7200. doi: 10.1137/07070111x.

[107] Christoph Molnar. *Interpretable Machine Learning*. 2 edition, 2022. URL https://christophm.github.io/interpretable-ml-book.

[108] Armen Der Kiureghian and Ove Ditlevsen. Aleatory or epistemic? does it matter? *Structural Safety*, 31(2):105–112, 2009. ISSN 0167-4730. doi: https://doi.org/10.1016/j.strusafe.2008.06.020. URL https://www.sciencedirect.com/science/article/pii/S0167473008000556. Risk Acceptance and Risk Communication.

[109] Nitish Srivastava, Geoffrey Hinton, Alex Krizhevsky, Ilya Sutskever, and Ruslan Salakhutdinov. Dropout: a simple way to prevent neural networks from overfitting. *The journal of machine learning research*, 15(1):1929–1958, 2014.

[110] Yarin Gal and Zoubin Ghahramani. Dropout as a bayesian approximation: Representing model uncertainty in deep learning. In *international conference on machine learning*, pages 1050–1059. Proceedings of Machine Learning Research, 2016.

[111] Laura Martínez-Ferrer, Álvaro Moreno-Martínez, Manuel Campos-Taberner, Francisco Javier García-Haro, Jordi Muñoz-Marí, Steven W. Running, John Kimball, Nicholas Clinton, and Gustau Camps-Valls. Quantifying uncertainty in high resolution biophysical variable retrieval with machine learning. *Remote Sensing of Environment*, 280:113199, 2022. ISSN 0034-4257. doi: https://doi.org/10.1016/j.rse.2022.113199. URL https://www.sciencedirect.com/science/article/pii/S0034425722003091.

[112] Pierre-Philippe Mathieu and Alan O'Neill. Data assimilation: From photon counts to earth system forecasts. *Remote Sensing of Environment*, 112(4):1258–1267, 2008. ISSN 0034-4257. doi: https://doi.org/10.1016/j.rse.2007.02.040. URL https://www.sciencedirect.com/science/article/pii/S0034425707003240. Remote Sensing Data Assimilation Special Issue.

[113] Stephan Hoyer and Joe Hamman. xarray: N-d labeled arrays and datasets in python. *Journal of Open Research Software*, 5(1):10, April 2017. doi: 10.5334/jors.148. URL https://doi.org/10.5334/jors.148.

[114] Edzer Pebesma and Roger Bivand. *Spatial Data Science: With applications in R*. Chapman and Hall/CRC, London, 2023. doi: 10.1201/9780429459016. URL https://r-spatial.org/book/.

[115] Matthew Rocklin. Dask: Parallel computation with blocked algorithms and task scheduling. In Kathryn Huff and James Bergstra, editors, *Proceedings of the 14th Python in Science Conference*, pages 130–136, 2015.

[116] F. Pedregosa, G. Varoquaux, A. Gramfort, V. Michel, B. Thirion, O. Grisel, M. Blondel, P. Prettenhofer, R. Weiss, V. Dubourg, J. Vanderplas, A. Passos, D. Cournapeau, M. Brucher, M. Perrot, and E. Duchesnay. Scikit-learn: Machine learning in Python. *Journal of Machine Learning Research*, 12:2825–2830, 2011.

[117] Martín Abadi, Ashish Agarwal, Paul Barham, Eugene Brevdo, Zhifeng Chen, Craig Citro, Greg S. Corrado, Andy Davis, Jeffrey Dean, Matthieu Devin, Sanjay Ghemawat, Ian Goodfellow, Andrew Harp, Geoffrey Irving, Michael Isard, Yangqing Jia, Rafal Jozefowicz, Lukasz Kaiser, Manjunath Kudlur, Josh Levenberg, Dan Mane, Rajat Monga, Sherry Moore, Derek Murray, Chris Olah, Mike Schuster, Jonathon Shlens, Benoit Steiner, Ilya Sutskever, Kunal Talwar, Paul Tucker, Vincent Vanhoucke, Vijay Vasudevan, Fernanda Viegas, Oriol

Vinyals, Pete Warden, Martin Wattenberg, Martin Wicke, Yuan Yu, and Xiaoqiang Zheng. Tensorflow: Large-scale machine learning on heterogeneous distributed systems, 2016. URL https://arxiv.org/abs/1603.04467.

[118] Adam Paszke, Sam Gross, Francisco Massa, Adam Lerer, James Bradbury, Gregory Chanan, Trevor Killeen, Zeming Lin, Natalia Gimelshein, Luca Antiga, Alban Desmaison, Andreas Köpf, Edward Yang, Zach DeVito, Martin Raison, Alykhan Tejani, Sasank Chilamkurthy, Benoit Steiner, Lu Fang, Junjie Bai, and Soumith Chintala. Pytorch: An imperative style, high-performance deep learning library, 2019. URL https://arxiv.org/abs/1912.01703.

[119] Leonardo Uieda. Verde: Processing and gridding spatial data using Green's functions. *Journal of Open Source Software*, 3(29):957, 2018. ISSN 2475-9066. doi: 10.21105/joss.00957.

[120] Ivica Dimitrovski, Ivan Kitanovski, Panče Panov, Ana Kostovska, Nikola Simidjievski, and Dragi Kocev. Aitlas: Artificial intelligence toolbox for earth observation. *Remote Sensing*, 15(9), 2023. ISSN 2072-4292. doi: 10.3390/rs15092343.

[121] Adam J. Stewart, Caleb Robinson, Isaac A. Corley, Anthony Ortiz, Juan M. Lavista Ferres, and Arindam Banerjee. TorchGeo: Deep learning with geospatial data. In *Proceedings of the 30th International Conference on Advances in Geographic Information Systems*, SIGSPATIAL '22, pages 1–12, Seattle, Washington, 11 2022. Association for Computing Machinery. doi: 10.1145/3557915.3560953. URL https://dl.acm.org/doi/10.1145/3557915.3560953.

[122] Kanchan Chowdhury and Mohamed Sarwat. Geotorch: A spatiotemporal deep learning framework. In *Proceedings of the 30th International Conference on Advances in Geographic Information Systems*, SIGSPATIAL '22. Association for Computing Machinery, 2022. ISBN 9781450395298. doi: 10.1145/3557915.3561036. URL https://doi.org/10.1145/3557915.3561036.

[123] Rolf Simoes, Gilberto Camara, Gilberto Queiroz, Felipe Souza, Pedro R. Andrade, Lorena Santos, Alexandre Carvalho, and Karine Ferreira. Satellite image time series analysis for big earth observation data. *Remote Sensing*, 13(13):2428, June 2021. doi: 10.3390/rs13132428. URL https://doi.org/10.3390/rs13132428.

[124] Mike Innes. Flux: Elegant machine learning with julia. *Journal of Open Source Software*, 3(25):602, May 2018. doi: 10.21105/joss.00602. URL https://doi.org/10.21105/joss.00602.

[125] Chris Rackauckas, Mike Innes, Yingbo Ma, Jesse Bettencourt, Lyndon White, and Vaibhav Dixit. Diffeqflux.jl - a julia library for neural differential equations, 2019. URL https://arxiv.org/abs/1902.02376.

[126] Francesco Martinuzzi, Chris Rackauckas, Anas Abdelrehim, Miguel D. Mahecha, and Karin Mora. Reservoircomputing.jl: An efficient and modular library for reservoir computing models. *Journal of Machine Learning Research*, 23(288):1–8, 2022. URL http://jmlr.org/papers/v23/22-0611.html.

[127] B. P. Welford. Note on a Method for Calculating Corrected Sums of Squares and Products. *Technometrics*, 4 (3):419–420, August 1962. ISSN 0040-1706, 1537-2723. doi: 10.1080/00401706.1962.10490022.

[128] Erich Schubert and Michael Gertz. Numerically Stable Parallel Computation of (Co-)Variance. In *Proceedings of the 30th International Conference on Scientific and Statistical Database Management*, Ssdbm '18, pages 1–12, New York, NY, USA, July 2018. Association for Computing Machinery. ISBN 978-1-4503-6505-5. doi: 10.1145/3221269.3223036.

[129] W. Kahan. Further Remarks on Reducing Truncation Errors. *Communications of the ACM*, 8(1):40, January 1965. ISSN 0001-0782, 1557-7317. doi: 10.1145/363707.363723.

[130] David Goldberg. What Every Computer Scientist Should Know about Floating-Point Arithmetic. *ACM Computing Surveys*, 23(1):5–48, March 1991. ISSN 0360-0300. doi: 10.1145/103162.103163.

[131] Josh Day and Hua Zhou. OnlineStats.Jl: A Julia Package for Statistics on Data Streams. *Journal of Open Source Software*, 5(46):1816, February 2020. ISSN 2475-9066. doi: 10.21105/joss.01816.

[132] Hadley Wickham. The Split-Apply-Combine Strategy for Data Analysis. *Journal of Statistical Software*, 40(1): 1–29, April 2011. ISSN 1548-7660. doi: 10.18637/jss.v040.i01.

[133] Bill Hibbard, Michael Böttinger, Martin Schultz, and Joachim Biercamp. Visualization in earth system science. *Acm Siggraph Computer Graphics*, 36(4):5–9, 2002.

[134] Wesley Kendall, Markus Glatter, Jian Huang, Forrest Hoffman, and David E Bernholdt. Web enabled collaborative climate visualization in the earth system grid. In *2008 International Symposium on Collaborative Technologies and Systems*, pages 212–220. IEEE, 2008.

[135] Johannes Kehrer and Helwig Hauser. Visualization and visual analysis of multifaceted scientific data: A survey. *IEEE transactions on visualization and computer graphics*, 19(3):495–513, 2012.

[136] Carolin Helbig, Doris Dransch, Michael Böttinger, Colin Devey, Antonie Haas, Mario Hlawitschka, Claudia Kuenzer, Karsten Rink, Christian Schäfer-Neth, Gerik Scheuermann, et al. Challenges and strategies for the visual exploration of complex environmental data. *International Journal of Digital Earth*, 10(10):1070–1076, 2017.

[137] Miguel Mahecha. Earth system data cube. figshare. Figure., 2017. URL https://doi.org/10.6084/m9.figshare.4822930.v2. DOI: 10.6084/m9.figshare.4822930.v2.

[138] Maximilian Söchting, Miguel D Mahecha, David Montero, and Gerik Scheuermann. Lexcube: An interactive earth science data cube visualization. Technical report, EGU General Assembly, 2023.

[139] Chad A Steed, Katherine J Evans, John F Harney, Brian C Jewell, Galen Shipman, Brian E Smith, Peter E Thornton, and Dean N Williams. Web-based visual analytics

for extreme scale climate science. In *2014 IEEE International Conference on Big Data (Big Data)*, pages 383–392. IEEE, 2014.

[140] Wenqiang Cui. Visual analytics: A comprehensive overview. *IEEE access*, 7:81555–81573, 2019.

[141] Peter Bauer, Bjorn Stevens, and Wilco Hazeleger. A digital twin of earth for the green transition. *Nature Climate Change*, 11(2):80–83, February 2021. doi: 10.1038/s41558-021-00986-y. URL https://doi.org/10.1038/s41558-021-00986-y.

[142] Robin Rombach, Andreas Blattmann, Dominik Lorenz, Patrick Esser, and Björn Ommer. High-resolution image synthesis with latent diffusion models, 2021. URL https://arxiv.org/abs/2112.10752.

[143] Alexander Kirillov, Eric Mintun, Nikhila Ravi, Hanzi Mao, Chloe Rolland, Laura Gustafson, Tete Xiao, Spencer Whitehead, Alexander C. Berg, Wan-Yen Lo, Piotr Dollár, and Ross Girshick. Segment anything, 2023. URL https://arxiv.org/abs/2304.02643.

[144] Rohit Girdhar, Alaaeldin El-Nouby, Zhuang Liu, Mannat Singh, Kalyan Vasudev Alwala, Armand Joulin, and Ishan Misra. Imagebind: One embedding space to bind them all, 2023. URL https://arxiv.org/abs/2305.05665.