Earth and Space Science Informatics Perspectives on Integrated, Coordinated, Open, Networked (ICON) Science

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Key Points:

- **Networks** across communities, with **Coordinated** data and information modeling practices, improve scientific outcomes for all involved.
- **Integrated**, **Coordinated**, and **Open** data requires sustainable support to create and maintain infrastructure for interdisciplinary **Networks**.

- **Integrated** and **Coordinated** use of data in machine learning calls for **Open** benchmark datasets, shared across **Networks** for improved outcomes.

Abstract

This article is composed of three independent commentaries about the state of ICON principles (Goldman et al., 2021) in Earth and Space Science Informatics (ESSI) and includes discussion on the opportunities and challenges of adopting them. Each commentary focuses on a different topic: **(Section 2)** Global collaboration, cyberinfrastructure, and data sharing; **(Section 3)** Machine learning and multiscale modeling; **(Section 4)** Remote sensing for advancing Earth system model development by integrating field and ancillary data. ESSI addresses data management practices, computation and analysis, and hardware and software infrastructure. Our role in ICON science therefore involves collaborative work to assess, design, implement, and promote practices and tools that enable effective data management, discovery, integration, and reuse for interdisciplinary work in Earth and space science disciplines. Networks of diverse people with expertise across Earth, space, and data science disciplines are essential for efficient and ethical exchanges of FAIR research products and practices. Our challenge is then to coordinate the development of standards, curation practices, and tools that enable integrating and reusing multiple data types, software, multi-scale models, and machine learning approaches across disciplines in a way that is as open and/or FAIR as ethically possible. This is a major endeavor that could greatly increase the pace and potential of interdisciplinary scientific discovery.

Plain Language Summary

We present commentaries on the state of "ICON principles" in Earth and Space Science Informatics. ICON principles (Integrated, Coordinated, Open, and Networked) are meant to improve the research experience for all. Ultimately, data standardized according to community conventions and formats lead to more effective and efficient collaboration, data discovery, integration, and analyses. Data standards, tools, and machine learning developed using ICON principles enhance our understanding of Earth processes. Using ICON principles improves model results and efficacy, fosters interdisciplinary research, and provides a framework by which non-experts can confidently contribute volunteered data and findings. Standardized data also provides reliable common resources to help train and benchmark machine learning algorithms. When networked communities work together to standardize and share data openly, the resulting web of research products is more readily findable, accessible, interoperable, and reusable (FAIR). Ongoing support is crucial to develop and sustain the people, systems, and tools necessary to realize ICON principles in Earth and Space Science Informatics now and in the future.

1 Introduction

Integrated, Coordinated, Open, Networked (ICON) science aims to enhance synthesis, increase resource efficiency, and create transferable knowledge (Goldman et al., 2021). This article belongs to a collection of commentaries (Leadership Team et al., 2021) spanning geoscience on the state and future of ICON science. Earth and Space Science Informatics (ESSI) encompasses a broad field that addresses data management practices, computation and analysis, and hardware and software infrastructure. ESSI's role in ICON science therefore involves collaborative work to assess, design, implement, and promote practices and tools that enable effective data management, discovery, integration, and reuse for interdisciplinary work in Earth and space science (ESS) disciplines. In this series of commentaries, we examine the current state, challenges, and opportunities of ICON science through the lenses of global collaboration, cyberinfrastructure, and data sharing (Section 2); machine learning and multiscale modeling (Section 3); and remote sensing for advancing Earth system models (ESM) development by integrating field and ancillary data (Section 4).

2 Global collaboration, cyberinfrastructure, and data sharing

2.1 Current state and challenges

Global collaboration across disciplines is essential to the development and implementation of data/metadata standards and cyberinfrastructures. Thus, many organizations have emerged to facilitate such collaboration, e.g., Research Data Alliance, World Data System, OneGeology, Earth Science Information Partners. These organizations have produced numerous active groups involved in Earth, space and environmental science data and research, and developed many data tools and services, e.g. Earth, Space and Environmental Sciences Data Vocabulary Repositories. Research is more efficient with **Networked** data practices and cyberinfrastructures that support scientific discovery. Yet, there is still a large disconnect and lack of **Coordination** across many informatics communities and the broader communities we aim to support.

Research teams often lack sufficient resources (e.g., appropriate cyberinfrastructure, expert data/software personnel, financial allotment) to effectively manage, standardize, and publish high-quality data (Mons, 2020). This hinders data from being **Open and/or Findable, Accessible, Interoperable, and Reusable** (FAIR; Wilkinson et al., 2016). Further, specific criteria to make data FAIR (Gries et al., 2019; Jones et al., 2019) inevitably vary across disciplines and data types. Because there are no widely accepted standards to evaluate FAIR-ness, data may be miscaterogized (e.g., Kinkade & Shepherd, 2021; Mons et al., 2017; Stall et al., 2019). Importantly, FAIR does not mean **Open**; data can be **Open** without being FAIR, and *vice versa* (see What is the difference between "FAIR data" and "Open data" if there is one?).

Supporting ESS research requires assessing, designing, building, and maintaining cyberinfrastructures (e.g., data repositories/archives, application programming interfaces (APIs), visualization tools, search interfaces) that are often organized around a particular data type, discipline, or organization. Interoperability issues are then minimized using bespoke or *ad hoc* conventions within that particular community (e.g., Deep Carbon Observatory, HydroShare, Long-Term Ecological Research Network, National Ecological Observatory Network). However, most cyberinfrastructures lack the resources for **Integration** and **Coordination** necessary for interdisciplinary work, including guidance and leading practices; domain semantics; technical, data, methodological, and instrumentation standards; workflow management; training; and sustainable technical and financial support. These deficits hinder **Open** data that fosters machine actionable, interdisciplinary scientific discovery.

While existing standards and practices may address similar concepts, they are not fully interoperable or **Integrated** within and across relevant disciplines. Valuable resources are spent developing/updating translators, or disciplinary standards are simply disconnected and inefficient for interdisciplinary users. **Coordination** is needed to implement standards for effective interdisciplinary data discovery and exchange. A major limitation to **Coordination** involves a lack of consistent and transparent protocols (e.g., data and code production, processing methods) across interdisciplinary teams that limits reuse and replication. These combined factors create barriers to **Open and FAIR** data.

Ever-increasing volumes of open data and tools now allow us to ask science questions that synthesize data and knowledge across scientific disciplines from globally distributed resources, thus expanding the impact of funded research (e.g., Michener, 2015; Rosenberg et al., 2019). More successful **Networked** data sharing efforts (e.g., Global Biodiversity Information Facility, Ameriflux, Consortium of Universities for the Advancement of Hydrologic Science, Inc.) have been driven by 1) demand for a specific data type (Barrett et al., 2012; Novick et al., 2018; Robertson et al., 2014); 2) reporting standards that enable global data search and integration (e.g., Wieczorek et al., 2012; Yilmaz et al., 2011); and 3) associated user-friendly tools (Clark et al., 2016; Robertson et al., 2014).

2.2. Opportunities and moving forward

Replicable and transparent research that reflects ICON principles requires sustainable investment in cyberinfrastructure to improve interoperability and **Integration**. Global high-level **Coordination** across organizations is needed to bridge siloed efforts across disciplines, organizations, and/or countries. A commitment to community engagement is needed to bring together input across disciplines, understand data management challenges and needs, and promote the adoption of shared practices. Making data as **Open and/or FAIR** as ethically possible requires key advocates who facilitate **Networked** collaboration.

Data users, code contributors, and tool developers should align with established standards or community practices. We can encourage practices that promote ICON principles, such as **Open** publication of study plans (e.g., PLOS ONE study proposals), data production and processing protocols (e.g., Common Workflow Language), and software code. We must continually evaluate how to **Coordinate** and **Integrate** across existing cyberinfrastructure from local to global scales, which involves iterative rounds of engagement; education and outreach; and feedback across data providers, tool and service creators, and scientists who use ESS data and services. **Coordinating Networks** across disciplines will involve technical approaches to connect related data (e.g., PIDs, APIs, ontologies, geospatial standards) and promoting widespread adoption of community standards that improve scientific outcomes and benefit all participants in the network.

3 Machine learning and multiscale modeling

3.1 Success and current status of AI/ML

Over the past decade, artificial intelligence approaches, including machine learning (AI/ML), have revolutionized scientific discovery across disciplines, including ESSI (Maskey et al., 2020a). The AI/ML revolution, driven by a wealth of **Open** data and rapid technological development in computational cyberinfrastructure, has led to more processing power and greater **Networking** which allows unprecedented resource and data sharing. There are many success stories demonstrating how AI/ML has been used to address challenging issues in ESS, e.g., extreme weather prediction (Maskey et al., 2020b; Pradhan et al., 2018; Wimmers et al., 2019), land use/land cover change monitoring (Hansen et al., 2013), earth system modeling (Reichstein et al., 2019), endangered species identification (Allen et al., 2021), spatial downscaling of climate models and satellite observations (López López et al., 2018; Vandal et al., 2019), space weather forecasting (Wintoft et al., 2017), and lunar and planetary landform classification (Palafox et al., 2017; Silburt et al., 2019). Various funding agencies worldwide have recently released their strategic plans and guidelines to expand the investment in AI/ML research which will further its adoption within ESSI for at least the next decade.

3.2 Common challenges in AI/ML

To accelerate this adoption, the ESS community needs to collectively address three key challenges. First, most AI/ML applications in ESS are *ad hoc* research that lacks system-wide **Coordination** and is time-consuming. There are little AI-ready data (e.g., cleaned, harmonized, formatted, well understood) that can be efficiently **Integrated** across domains or applications and few recommended practices on proper model development and documentation (Maskey et al., 2020a). Thus, amplifying the value of AI/ML in ESS requires an ecosystem including AI-ready training datasets and standardized model development practices. This ecosystem would enable the ESS community to collaboratively develop open AI/ML applications at scale. A second challenge is related to the wealth of **Open** data in ESS. Currently, there are no community-recommended practices on how to properly develop, document, and share the AI/ML applications that track provenance and enable reproducibility (Sun et al., 2020). Third, the explainability and generalizability of AI/ML models are also major concerns for the ESS community (McGovern et al., 2019; Toms et al., 2020). To address complex questions in ESS systems, we need to better understand why AI/ML models perform in a certain way, their consistency with domain knowledge, and how models developed using a specific set of data can adjust dynamically to shifts in ESS data. Additionally, ethical awareness, conduct, and responsibility in AI/ML and related activities are essential to the practice of principled research.

3.3 Opportunities and moving forward

We identify five opportunities where researchers may focus their efforts to make ESS AI/ML more efficient. One opportunity relates to big data in ESS. Because the capacity and application scope of AI/ML heavily depends on patterns in training data, it should be as representative as possible. The requirements for big training datasets have led to calls for libraries of **Open** and FAIR benchmark datasets (WILDS, Koh et al., 2020; Radiant Earth Foundation; Rasp et al., 2020) related to questions within ESS (Crystal-Ornelas et al., 2021). A second opportunity is increased **Networking** through cloud computing (Gorelick et al., 2017; Mayer-Schönberger & Cukier, 2013). By sharing data and models in the cloud, researchers around the world can access these resources without being limited by local computing power. More work needs to be done to make cloud computing more accessible for ESS despite recent progress. Increased **Openness** in the exchange of data handling practices to allow sharing common workflows while handling large datasets is a third opportunity. A fourth opportunity is to improve interpretability through **Integration** across disciplines by: (1) including physics in ML models (Jia et al., 2019; Raissi et al., 2019), (2) leveraging machine learning exploratory tools (Montavon et al., 2017; Ying et al., 2019), and (3) involving domain experts into AI/ML pipelines. A final opportunity for growth is to automate workflows to improve the development efficiency (e.g., auto-sklearn, AutoKeras) (He et al., 2021). To improve AI engineering efficiency and reduce data collection and processing costs, modelers may also use data augmentation methods such as mixup (Zhang et al., 2017) to fill in the missing data and enhance data quality (Alexandrov & Vesselinov, 2014; Vesselinov et al., 2018). We emphasize that these opportunities for ESS to inform and apply AI/ML models is not exhaustive; rather it is a starting point for exploring how ICON science can benefit the future of this rapidly growing field within ESS.

4 Remote sensing for advancing Earth system model development by integrating field and ancillary data

4.1 Current Status

Remote sensing technology combined with field and ancillary data (e.g., field measurements, other imagery; Acton, 1996) has transformed the development of ESMs as they have advanced from aerial imagery of the early nineteenth century (Necsoiu et al., 2013) to the present-day's Google Earth Engine (Gorelick et al., 2017) and Unmanned Aerial Vehicles (Singh & Frazier, 2018). Most publicly-funded remote sensing datasets are **Open** and hosted on public repositories (e.g., government-sponsored repositories, Github, Zenodo). In addition, this data is collected through **Coordinated** standards between government agencies across the globe (Alameh, 2020). **Integration** of remote sensing technology with independent field measurements and high spatial resolution satellite imagery has been essential for ESM validation. This also includes estimating derived data products (e.g., from satellites) accuracy and quantifying uncertainty (Strahler et al., 2006). Crowdsourcing and citizen science have further advanced the integration of remote sensing with field data (e.g., RaspberryShake, Khan et al., 2018; Saralioglu & Gungor, 2020; Worldwide Hydrobiogeochemistry Observation Network for Dynamic River Systems [WHONDRS], Stegen & Goldman, 2018), resulting in broader **Networked** efforts that benefit researchers and a wide variety of data users. We note that agencies in the US and Europe have open-sourced their data to all users internationally. Some popular open data sources, associated cyberinfrastructure, and tools are included in an associated github repository.

4.2 Challenges and call to action

Two primary challenges which the ESSI community faces are limited global data collection and inadequate cyberinfrastructure. Despite advances in sensors, crowdsourcing, and citizen science (e.g., RaspberryShake, WHONDRS), collecting and hosting high-quality global data present immense challenges. For example, RaspberryShake has collected more than 30TB of seismographic data over the past decade but lacks the necessary cyberinfrastructure to reliably and sustainably store it.

Recent progress in AI/ML has improved the representation of Earth system processes (e.g., thermal, land physics and hydrology, radiation, atmospheric ocean circulation) in ESMs (Rasp et al., 2018). ML, in particular, requires massive datasets to represent processes at both normal and extreme events (e.g., hurricanes, wildfires); however, extreme event data are rare due to the unique challenges faced during collection. Thus, the concept of crowdsourcing data collection, using **Coordinated** methods (e.g., RaspberryShake, WHONDRS) on extreme events, is an attractive option that improves **Networked** research.

There has been a **Coordinated** effort from US and European agencies to develop cyberinfrastructure that improves and increases access to data to enhance predictions and understanding of various Earth system processes. For example, the European Space Agency Sentinel data products are recently available in the Copernicus Data and Information Access Service cloud environments. In addition, the US Geological Survey Landsat satellite data inventory has been open to the public since 2008 and has been in the cloud since 2020 (U.S. Geological Survey, 2008). Furthermore, the National Aeronautics and Space Administration (NASA) and the National Oceanic and Atmospheric Administration (NOAA) have adopted a strategic vision to leverage cloud computing and operate multiple components of their data systems in a retail cloud environment. This calls for action to identify the opportunities to improve policy and strategy planning across various countries to make satellite data products accessible to all users in open data portals. In addition, automated quality assurance of satellite observations is needed to support global, regional, or local data services. **Coordinated** across international agencies, a standard open data cyberinfrastructure will help to assure ESM data from multiple sources (national, regional, governments, academia, and the private sector) are available and easily **Integrated** into open-source platforms and networks.

4.3 Opportunities and moving forward

First, close coordination would help international agencies and organizations build a standard open data cyberinfrastructure to ensure that earth science data are free, open, and easily integrated into ESMs. Second, we need next-generation sensors and satellites which provide more fine resolution data to increase the accuracy of ESMs. For example, the joint NASA-Indian Space Research Organization (ISRO) Synthetic Aperture Radar (SAR) (NISAR) mission is anticipated to provide fine-scale resolution radar data with a spatial resolution of less than a centimeter to study the earth's features and processes. Third, the role of AI/ML needs to be expanded to plug in the gaps of remote sensing data.

5 Concluding remarks

ESSI science that utilizes ICON principles enables data synthesis, increases resource efficiency, and creates knowledge that transcends individual systems (Goldman et al., 2021). ESSI can work to ensure that diverse scientists have user-friendly resources to contribute and use data that follows community conventions. Such collections of **Open and/or FAIR** data, shared across **Networks** for mutual benefit, are critical to appropriately train AI/ML, which furthers **Integration** and **Coordination** in ESSI science. Cross-community **Networks** improve scientific outcomes for all involved. Communities must work together to share data openly using community standards, to produce **Open and/or FAIR** data that enables data synthesis and can revolutionize fields of research (e.g., Kelling et al., 2009). Ongoing, sustainable support is vital to create and maintain the cyberinfrastructure and human resources necessary for **Integrated**, **Coordinated**, and **Open and/or FAIR** data (as much ethically as possible) for interdisciplinary **Networks**.

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