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SPECIAL ISSUE PAPER

Measuring success for a future vision: Defining impact in science gateways/virtual research environments

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Summary

Scholars worldwide leverage science gateways/virtual research environments (VREs) for a wide variety of research and education endeavors spanning diverse scientific fields. Evaluating the value of a given science gateway/VRE to its constituent community is critical in obtaining the financial and human resources necessary to sustain operations and increase adoption in the user community. In this article, we feature a variety of exemplar science gateways/VREs and detail how they define impact in terms of, for example, their purpose, operation principles, and size of user base. Further, the exemplars recognize that their science gateways/VREs will continuously evolve with technological advancements and standards in cloud computing platforms, web service architectures, data management tools and cybersecurity. Correspondingly, we present a number of technology advances that could be incorporated in next-generation science gateways/VREs to enhance their scope and scale of their operations for greater success/impact. The exemplars are selected from owners of science gateways in the Science Gateways Community Institute (SGCI) clientele in the United States, and from the owners of VREs in the International Virtual Research Environment Interest Group (VRE-IG) of the Research Data Alliance. Thus, community-driven best practices and technology advances are compiled from diverse expert groups with an international perspective to envisage futuristic science gateway/VRE innovations.

KEYWORDS

futuristic vision, measuring impact, science gateways, success metrics, virtual research environments

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1 INTRODUCTION

The term "Science Gateways" was coined in 2004 to describe the portion of the National Science Foundation (NSF) funded TeraGrid program devoted to increasing accessibility of supercomputers to all scientists. In the ensuing years, the term has acquired a much broader meaning in the United States; it now serves as a descriptor for all advanced web interfaces used for research, education and scholarship. A similar concept, namely, "virtual research environment" (VRE) was also first used in Europe to describe an online system that helps researchers to collaborate with document hosting, and domain-specific tools for analysis/visualization. Science gateways/VREs have transformed research and education endeavors spanning diverse scientific fields, and have increased the pace of innovation in research and scholarship over the last two decades. Both funding agencies and domain science/engineering user communities have worked closely to identify challenges and practical solutions that enhance the value of science gateways/VREs to serve current and pent-up needs of researchers and educators. Both financial and human resources have been the key to ensuring the success and impact of science gateways/VREs. Without adequate funding and skilled professionals, it is not possible for a science gateway/VRE to: (a) maintain persistent online presence, (b) upgrade user support and cyberinfrastructure resources, (c) ensure long-term operations sustainability, and (d) significantly increase community adoption.

Launched in 2016, the Science Gateways Community Institute (SGCI)[1] in the United States helps researchers build and discover better, more functional science gateways by documenting, developing, and disseminating best practices. The business planning training offered by SGCI to manage financial and human resources has been popular among science gateway creators. The International Virtual Research Environment Interest Group (VRE-IG) of the Research Data Alliance[2] has taken a similar leadership effort as an organization responsible for engaging VREs in tracking and contributing technologies, developing governance strategies, and best practices in community building.

Measuring and communicating impact is one of the most important factors in determining whether a given science gateway/VRE has sufficient funding (usually through research grant awards) to ensure a persistent online presence. Although critical, the definition of impact can vary widely among science gateways/VREs due to the diversity of their goals and the needs of the communities they serve. Another major factor for science gateways/VREs to serve their user communities is their ability to integrate advanced technologies and standards in cloud computing platforms, web service architectures, data management tools, and cybersecurity. Designing the pertinent system architectures with optimized resource configurations can greatly impact the cost, availability, convenience, and security/privacy of science gateways/VREs.

In this article, we feature a variety of exemplar science gateways/VREs that detail how they define impact in terms of, for example, their purpose, operation principles, and size of user base (in Section 2). The exemplars are selected from owners of science gateways in the SGCI community in the United States, and from the owners of VREs in the VRE-IG. The exemplars outline a rich set of approaches to routinely measure and communicate impact that allows us to document the key best practices (in Section 3). Further, the exemplars recognize that their science gateways/VREs will continuously evolve with technological advancements and standards in cloud computing platforms, web service architectures, data management tools and cybersecurity. Correspondingly, we present a number of technology advances that could be incorporated in next-generation science gateways/VREs in order to enhance their scope and scale of their operations for greater success/impact (in Section 4). The owners provide their futuristic visions from the roles of software developers, data engineers, resource providers, and user services experts. Thus, the contributions from this work are compiled from a diverse set of experts with an international perspective in terms of: (a) best practices for measuring success/impact, and (b) technology advances that will continue to drive the innovations in futuristic science gateways/VREs. This article concludes by summarizing how this work provides a basis for evolution of the notion of impact for current and future science gateway/VRE operators and funders (in Section 5).

2 | GATEWAY EXPERIENCES

2.1 | Ultrascan

The NIH and NSF-supported UltraScan Gateway[3] supports the Analytical Ultracentrifugation (AUC) community. AUC experiments are performed in a wide range of disciplines, encompassing biomedical life and basic science applications in biophysics, biochemistry, and molecular biology, as well as polymer chemistry, colloid, material, and nanoparticle science. The gateway, in operation since 2006, allows users to manage and perform analyses of AUC experimental data. MPI-Parallel jobs are submitted through the gateway to various compute resources, including those allocated via XSEDE. Impact metrics typically reported include number of active institutions, users, and number of publications. In the recent year time period, over 140 investigators from 116 institutions actively used the gateway based on log information. The institutions are listed on the gateway's website. In the last ten years, over 158 publications have been self-registered. The UltraScan administrators regularly ask users to submit publications through the website, but they have no guarantee that the publication list is exhaustive.

2.2 | Interactive Parallelization Toolkit

The main goals behind developing the NSF-funded Interactive Parallelization Toolkit (IPT) gateway were to lower the adoption barriers to IPT and to provide a self-paced learning environment for developing parallel programming skills.[4] While still under development, a prior version of IPT was operational for about six-months recently and accessed by approximately 40 users, the majority of whom were taking a parallel programming course at the University of Texas at Austin.

The number of users, both domain-experts and students, accessing IPT through the gateway is the key metric of success. However, it is also important to measure how well users meet their learning goals. While the number of users is captured automatically, surveys are used to get the users' feedback on their learning experience. Surveys are conducted immediately after every training event, however, as the users are not obligated to take the surveys, the amount of data collected so far has not been statistically significant. Nonetheless, the objective and subjective responses obtained thus far have indicated that the gateway is helping users to more productively learn parallel programming concepts and parallelize applications in a self-paced manner without spending time on software installations. If 70% of the software/hardware resources available to the project are being utilized at a given time, the project team considers that as a success.

2.3 | SeedMeLab

SeedMe1[5] project helps researchers to solve the "last mile" problem of sharing data and metadata as well as video generation from sets of images typically created as scientific visualization. The system provides researchers with a cloud-based service that may be used in multiple ways—via a web browser, through web services, and by application clients and command line tools. It is also integrated with scientific applications Kepler, Vapor and VisIt. SeedMe1 has been in production since 2014 and currently has over 700 users who have uploaded over 150,000 items. The website receives approximately 200 active visitors a month.

The SeedMeLab[6] (formerly SeedMe2) is a domain agnostic data platform for teams struggling with intractable data organization and data access that disrupts productivity, ensues email/attachment deluge, obscures discovery, and perpetuates poor knowledge retention. Unlike other file sharing services, SeedMeLab is an elegant approach that transforms data organization and sharing with an ability to add context, discussion and visualization while also establishing distinction for research project's data with branding and also providing them full ownership and control. The system was conservatively trialed with an early research group that grew to 18 users, 17,000 files constituting 5 GB data in two years, which in turn enabled iterative test leading up to release. SeedMeLab has been in production for over a year now and also is available as a paid subscription service. SeedMeLab's success metric includes number of active deployments and number of users, files, and aggregate data for each deployment and publications enabled. For example, the early research group after 3.5 years has grown to 24 users, 35,000 files aggregate to 28GB and has over a dozen publications supported by SeedMeLab. The project also conducts user interviews for subjective findings. Lastly, the open source software modules are currently actively being used by over 300 websites[7] worldwide.

2.4 | CyNeuro

The CyNeuro science gateway[8] has been developed at the University of Missouri-Columbia since 2017 with the goal to advance cyberinfrastructure and software automation in neuroscience. The primary focus in the development efforts is to create openly accessible software tools for data-intensive neuroscience research and education projects that benefit from advanced cyberinfrastructure resources (e.g., the Neuroscience Gateway, JetStream) and technologies (e.g., JupyterHub, CIPRES). The approach to develop and refine capacity, capability, and user support structures within CyNeuro have been through user surveys and mini-symposia of various stakeholders (e.g., researchers, resource providers, tool developers, data owners). CyNeuro hosts exemplar workflows and data sets that are being developed for exploring the potential of cyberinfrastructure and software automation in neuroscience. The gateway is connected to and leverages local MU resources, as well as Neuroscience Gateway resources to scale research productivity and develop large-scale training platforms. The ultimate purpose of CyNeuro is to support research and education use cases of neuroscientists, particularly those involving large-scale computation and image analysis, without the need for expert knowledge of programming and cyberinfrastructure configurations, which is beyond the repertoire of most neuroscience programs.

The key measures of success for CyNeuro include: (i) the number of new research/teaching tools and exemplars developed by CyNeuro developers/users, and their sustained usage by the community, (ii) development of a new undergraduate/graduate course sequence on "Cyberinfrastructure and Software Automation in Neuroscience" from biological/psychological sciences and computer science/engineering, and (iii) effective support of ongoing teacher and researcher training programs around neuroscience topics (e.g., NSF REU/RET, NIH R25). In particular, user-centered metrics such as ease-of-use, ease-of-setup, ease-of-self-service, and increased options in terms of tools/resources to complete compute/data-intensive workflows of our users are being considered as metrics. Further, additional metrics may include the number of sustainable software products (openly available via GitHub), and publishable learning outcomes through systematic evaluation studies in peer-reviewed venues.

2.5 | University of South Dakota Science Gateway

The University of South Dakota (USD) Science Gateway is a campus gateway aimed at early on-boarding of newcomers to computational research, providing a streamlined graphical interface to the most commonly used applications for emerging computational researchers at USD and across South Dakota. In South Dakota where many aspects of cyberinfrastructure and computational research are still emerging, there is not always a clear on-ramp to participation. The USD Science Gateway aims to address that by providing an accessible avenue to advanced computing on USD's Lawrence Supercomputer. With an initial focus on biology and bioinformatics applications, the Science Gateway will simplify user on-boarding to campus clusters, with a potential transition to XSEDE resources. To that end the gateway's goal is to increase productivity in groups unfamiliar with advanced digital resources and provide an accessible platform for learning scientific applications without the overhead of also learning the Unix command line and other intricacies of traditional high performance computing (HPC) practice.

The gateway, first developed in 2018, is currently in early access with approximately 10 users in two research groups, incorporating federated authentication through CILogon and offering the QIIME and Mothur applications, with plans for incorporating applications from additional scientific domains next. In South Dakota one of the greatest challenges in delivering cyberinfrastructure is simply communicating its existence. The Science Gateway will serve as an awareness-building tool, demonstrating streamlined access to popular applications in campus research communities new to advanced computing. It is expected that the user community will grow to several dozen users across multiple labs and institutions in South Dakota, with the number of groups new to advanced computing providing a key metric of the gateway's success. With a focus on lowering the bar for advanced computing, the science gateway will achieve success by increasing the number of researchers in South Dakota participating in computational research. In particular it will increase the number of new users to advanced computing, including classroom use, with awareness built by incorporating the gateway into training efforts through SD EPSCoR (NSF) and SD INBRE (NIH).

2.6 OpenTopography

The NSF-funded OpenTopography (OT) gateway[9] was initiated in 2009 to democratize access to Earth science oriented high-resolution topographic data, specifically lidar (light detection and ranging) and related compute-intensive algorithms to process these data. The primary goals of OT are to enable fundamental discoveries and innovative applications with these data by streamlining data access and processing. OT utilizes cyberinfrastructure, including large-scale data management, HPC and service-oriented architectures to provide efficient discovery, processing and visualization of large, high-resolution topographic datasets. Since inception, 129,405 unique users have run 505,076 custom processing jobs via the OT portal, processing over 6.71 trillion lidar returns. An additional 1 million+ jobs were invoked via APIs, either directly by users or via other gateways such as CyberGIS or via software applications. OT has an international user community and they self-identify as being from academia (33.3%), commercial (8.1%), non-profit (5.5%), government (4.0%), and military (1%) sectors. A conservative estimate identifies at least 386 peer-reviewed articles along with numerous theses and other publications that have been produced using OT gateway resources. These include academic works in Earth science, ecology, hydrology, geospatial and computer science, and engineering. OT data and tools are also routinely used in the classroom at the undergraduate and graduate level.

Success metrics includes a number of wide-ranging factors including growth in users and usage, growth in data holdings via growing number of partners from government and industry, national and international agencies, a growing number of software collaborations including algorithm development, and finally publications enabled by OT. User metrics and usage analytics were an important component of the gateway design from the outset and has proven to be vital for both gateway design and optimization, as well as for developing partnerships with data providers who value access to OT analytics. Additional success metrics include being an important community facilitator. As part of OT education and outreach activities, 29 short courses have been co-organized and taught on high resolution technologies, processing, and applications, reaching hundreds of students, faculty, and professionals. These courses are fully subscribed and teaching materials are popular and freely available.

2.7 CIPRES—CyberInfrastructure for Phylogenetic RESearch

The intent in creating CIPRES[10] was to make it possible for researchers around the world to access the compute resources needed to conduct phylogenetic relevant research. The need for CIPRES arose when the growing computational requirements for analyzing a wealth of new DNA data outstripped the local compute capabilities of most researchers in the field. The primary goal was to provide easy access to the most important community codes on large HPC clusters that are adequate for most analyses. The secondary goal was to create a gateway software platform that would be robust in heavy use and that could be adopted by gateway creators in support any scientific field. CIPRES has been in operation for 10 years, and is fully mature as a gateway.

Success metrics are aligned with the primary intent stated above. Currently, user-supplied information is combined with data from the XSEDE and CIPRES databases to track the number of user-submitted jobs, submission successes, number of users (new and returning), rate of user turnover, and amount of compute resources consumed per unit time. User visits, number of users on the site, and number of user accounts are no longer tracked, because historically these correlated only weakly with the gateway's intent. Through the CIPRES database, users' country and institution are tracked. This shows who CIPRES is supporting, to what extent the gateway is supporting leading edge research at prestigious institutions, research at average or under-resourced institutions, and training at teaching institutions. There is concern about user experience. User sentiment about CIPRES features and toolkit is tracked through an annual survey. Ultimately, this team believes the value of CIPRES is not that it allows users to "run jobs," but that enables creation of new knowledge. Publications are the key metric for this goal. A combination of Web of Science, Google Scholar, and self-reporting by users is used to appraise the number of publications CIPRES supports each year. Finally, the success of the software package as a platform for gateway creation is evaluated by tracking how many implementations of the CIPRES Workbench Framework are in use worldwide.

2.8 QUBES

The Quantitative Undergraduate Biology Education (QUBES) gateway[11] was launched in 2014 to address challenges in quantitative biology education. QUBES serves a community of about 7000 math and biology educators, professional societies and education projects with an infrastructure that supports the community through communication, sharing of resources, access to software tools, and professional development. The QUBES community involves a range of post-secondary institutions, including both 2- and 4-year colleges from across the country. QUBES partners with professional societies and education projects to promote their activities and resources, and connects with the discipline-based education community to encourage the use of assessment in reform efforts.

In addition to building basic services for the community, QUBES has engaged participants in professional practices including the adoption and use of Open Education Resources (OERs) as well as the incorporation of evidence-based pedagogical approaches. Discussion and exploration of emerging educational areas of emphasis such as developing inclusive and equitable learning environments are supported, as are the incorporation of new disciplinary practices such as Data Science. Services to the community include infrastructure to share educational resources as OERs, journal clubs, websites for conferences and workshops, training and support for using software tools in the classroom, and communication about upcoming opportunities.

Success metrics are largely focused on community activities, in particular, the number of participants in our professional development programming, and the demographics of those participants in terms of institution types and geographic distribution. Another important metric is the number of partner projects. These are projects designed to support quantitative biology education driven by professional societies or individuals with NSF funding. Both the number of projects on QUBES, as well as the number of times QUBES is written into projects are monitored. Partners and participants in professional development produce OERs and QUBES monitors both the generation of these materials and their use by the broader community.

2.9 | Ike Wai Gateway

The 'Ike Wai Gateway,[12] 'Ike means knowledge and Wai means water in Hawai'ian, launched in 2018 to support research in hydrology and water management by providing data and tools to address questions of water sustainability in the state of Hawai'i. The gateway currently supports 60 University of Hawai'i (UH) researchers from UH Manoa and UH Hilo. The gateway also supports a community stakeholder decision support tool developed in collaboration with the USGS to support groundwater recharge simulations for the island of O'ahu. One measure of gateway success is the number and quality of annotated data-sets, products and tools produced and made available. These products are developed by researchers and community members who see value in contributing products to the gateway and quality products require time to produce, verify and annotate properly to support FAIR data principles. Success is also measured by the use of the data and tools to support sustainable water management disseminated through papers, reports, policy, and management actions. This is tracked through a combination of usage analytics and direct outreach engagements with stakeholders and community members to gather feedback and gauge impact. The total number of users of the gateway is a measure of success, however growth in the number of users who are external to the university would demonstrate that the local and broader community stakeholders are finding value in the gateway's products and services.

2.10 | CitSci

CitSci is a global citizen science support platform and cyberinfrastructure that advances the utility, impacts, and outcomes of field-based citizen science projects.[13] This gateway currently supports more than 760 projects ranging from those that monitor water quality and maple syrup productivity to wildlife populations and invasive species. Thousands of volunteers have contributed close to one million scientific measurements. CitSci.org is unique in that it is fully customizable; it allows projects to "create their own citizen science projects" in a do-it-yourself (DIY) approach. Projects can define what they wish to measure, document how they measure it, and build customized datasheets for real-time data entry online and via mobile applications. This saves hundreds of projects the costs and hassles associated with creating their own web frontend and backend systems as well as their own custom mobile apps. CitSci.org also provides an integrated suite of volunteer management capabilities plus data exploration and visualization tools to empower people to create their own visualizations of trends, relationships, and comparisons; and has been integrated with collaborative conservation systems for co-created citizen science and collaborative mental modeling. Tools also exist for volunteer communications, alerts and notifications, bulk uploading of legacy datasets, and download of data.

The CitSci team defines success as supporting and guiding citizen science projects toward meeting their own goals and objectives and generating their desired impacts and outcomes. The goal is to amplify the impacts of projects such that they create positive social-ecological-economic change for the communities in which the projects are taking place. Toward this end, CitSci.org aims to be change-makers by supporting projects that result in positive changes for socio-ecological systems and the quality of life for people, ecosystems, and communities. To measure success, the team looks beyond the more obvious metrics of numbers of projects, numbers of volunteers, and numbers of observations to more specifically look at harder to reach and measure metrics including percent active projects, number of peer-reviewed publications supported, number of decision-making policies informed, and the degree to which participants are being impacted through metrics of scientific literacy, behavior, attitude, and knowledge gains. A separate article[14] summarizes the analysis of 134 case studies to look at intent for use in decision-making.

2.11 | CyberGIS

CyberGIS represents the new generation of geospatial information science and systems (GIS) based on advanced computing and cyberinfrastructure while the CyberGIS Science Gateway was originated as TeraGrid GIScience Gateway that is one of the earliest science gateways operated based on NSF advanced cyberinfrastructure resources.[15] The specific goals of the gateway are to democratize access to advanced cyberinfrastructure for enabling geospatial discovery and innovation. The gateway has gone through multiple generations of research and development cycles ranging from various back-end, middleware, and front-end technologies to user environments, and has served several thousand users in diverse domains including agriculture, bioenergy, emergency management, geography and spatial sciences, geosciences, and public health. The CyberGIS success metrics relate to our stated goals in the following ways: (i) solving major scientific problems; (ii) enabling broad research advances; (iii) supporting education and training; and (iv) engaging the public to appreciate the power and value of advanced cyberinfrastructure and cyberGIS. Accordingly, major progress of related science teams is being measured in terms of the number and variety (e.g., journal papers, dissertations, data, and software) of publications, the number of students and courses/tutorials, and the number and type of general users engaged in public outreach activities.

2.12 | Data Discovery Studio

Data Discovery Studio enables resource discovery in the Earth Sciences, helping users to find data, models, and other types of resources from many different repositories and resource collections used by geoscientists. Besides searching the unified catalog, users can contribute missing data resources, edit and improve metadata, organize found data into shareable resource collections, and further explore datasets using Jupyter notebooks. DDStudio has been developed through two NSF EarthCube-funded Building Blocks projects. The CINERGI (Community Inventory of EarthCube Resources for Geoscience Interoperability) project created an automated metadata augmentation pipeline that uses text analytics and several geoscience ontologies to extract additional metadata elements and add them to dataset records. These include keywords reflecting: characteristics of resources such as measured parameters, equipment used, geospatial features analyzed, scientific domains, and geospatial processes studied; missing spatial and temporal extents; and organization identifiers. Development of the initial metadata pipeline was followed by the EarthCube Data Discovery Hub project, which expanded the inventory to over 1.6 million data resources from 40+ geoscience data repositories and from community contributions, and enabled geospatial and temporal filtering, creation of collections, and dataset exploration capability.

DDStudio success metrics ultimately reflect advancing cross-disciplinary geoscience, as enabled by comprehensive data discovery across multiple repositories, using spatio-temporal, full-text and faceted search over semantically enhanced metadata, improved ability to interpret and re-use resource descriptions, create collections, and launch Jupyter notebooks to visualize or analyze the registered resources. Translating metadata records into schema.org markup and their subsequent indexing by Google results in better visibility of geoscience data to the general public. Further, DDStudio search has been embedded in other systems (e.g., ModelMyWatershed) and on web sites. At the time of this writing, the DataDiscoveryStudio.org site has been public and active for about 9 months; in that time, the site has had 1.1K visitors in 2.6K sessions with 6.3K page views. In addition to autogenerated metrics such as the number of portal users, count of registered resources and metadata collections, number and types of metadata enhancements, and the size of the underlying integrated geoscience ontology, internal project metrics quantify search improvements through focused testing among groups of researchers from several domains.

2.13 | COSMIC2

The COSMIC2 science gateway provides HPC access to the structural biology community, allowing users to determine macromolecular structures using cryo-electron microscopy (cryo-EM) data.[16] Cryo-EM is the fastest-growing field of structural biology, where new users are now able to prepare samples and collect high-quality data at both regional and national cryo-EM facilities. Using these instruments, users collect thousands of movie files that can total up to 10-20 terabytes per project. It is expected that there are 50-100 users around the United States who have limited to no HPC background or infrastructure available to them. This number can be much more as cryo-EM becomes a go-to technique for structural biologists around the country. The role of the COSMIC2 gateway is to provide software and data management, allowing users to leverage cutting-edge algorithms with minimal effort for job submission.

The success of the COSMIC2 gateway will be evaluated by metrics related to user number as well as the number of cryo-EM structures calculated by the gateway. Because the gateway is focused on serving cryo-EM users who have limited access to HPC resources or are new the field, the number of new users are moving projects forward through their use of the gateway will be tracked. This will require on-boarding surveys, tracking of user job submissions, and final structures (if any) determined for a given user. Overall user number will also be tracked, but an emphasis on new users will help to determine whether the gateway has led to growth in the field. Beyond tracking user number, another metric is the number of cryo-EM structures deposited in the Electron Microscopy Data Bank, as well as the number of atomic coordinates that are published in the Protein Data Bank. Because published cryo-EM structures and atomic models are the goal of cryo-EM projects, tracking the number of these that cite the gateway will be critical for measuring success. Based on these metrics, the gateway will be functioning effectively if it is able to: (i) attract new users (or users without HPC infrastructure), and (ii) ensure that these new users are publishing and depositing their cryo-EM structures.

2.14 | SimCCS

The SimCCS Gateway[17,18] provides novel decision-support capabilities for evaluating carbon capture, utilization, and storage technologies (CCS) for mitigating greenhouse gas emissions to the atmosphere. Developed in 2018 by members of the U.S.-China Clean Energy Research Center, the gateway supports decision making by integrating applications in operations research, geographical information systems, carbon capture engineering, pipeline infrastructure design and reservoir performance prediction. Users are able to produce integrated CCS system designs for problems ranging from single facilities to large, regional networks involving multiple CO2 sources and geologic sinks. By harnessing the power of HPC resources, users in the research and policy communities can investigate how CCS may play a meaningful role in mitigating climate change. Users in the commercial sector are able to run large ensembles of experiments to evaluate financial risk and find optimal investment solutions for implementing CCS technologies.

Although early in the development cycle, the SimCCS Gateway has attracted users in the energy and policy research communities across the U.S., China, and Australia.[19] Feedback from multiple webinars and workshops convened in the first year of gateway operation has led to accelerated development of four core applications used to build, solve, and analyze complex optimization problems for designing integrated CCS infrastructure solutions. Early success metrics have centered on growth in user numbers and developing an international user base in the energy research and policy communities. Such metrics are inherently aligned with the developer's goals of achieving high impact scholarship and innovative educational opportunities for students at the postgraduate level. A surprising outcome to date has been the overwhelmingly positive response by the commercial sector to the novel capabilities of the gateway. Despite a multi-decadal history of substantial research and development investment in CCS technologies by governments around the world, it is clear that large-scale CCS deployment still faces significant economic, technical, and non-technical challenges (e.g., policy making, project permitting, and a social license to operate). The vision of future success includes the extent to which the gateway's user base can grow from private-sector industries.

2.15 | CUAHSI HydroShare

HydroShare is a domain specific data and model repository operated by the Consortium of Universities for the Advancement of Hydrologic Science Inc. (CUAHSI) to advance hydrologic science by enabling researchers to more easily share data, model and workflow products resulting from their research and to create and support reproducibility of the results reported in scientific publications. HydroShare was launched in June 2015 and currently has over 3650 user accounts.

HydroShare metrics are ultimately targeted at quantifying the impact of HydroShare on advancing hydrologic knowledge. This is a challenge, as impact and advances in knowledge are hard to quantify. The project measures the number and type of users, how long they have had their account, and how active they are. New users with an account created in an adjustable reporting period (e.g., last 30 or 180 days) quantify how the user pool is broadening and how capabilities and practices that HydroShare supports are penetrating into the field (750 new users were recorded for a recent 180-day test period). Returning users are defined as users who were active (logged in and used the gateway) in the most recent reporting period but created their account prior to its start (450 returning users were recorded for a recent 180-day test period). This metric quantifies sustained adoption. Also tracked are the number of resources (8784 total were recently recorded). A resource is the discrete unit of digital content within HydroShare and may include observation data, model and analysis results, and models and scripts.

App launches for different apps (any web-based tool that connects to HydroShare through the API) help us know what users are doing and what apps are having an impact. One of the motivations for HydroShare is reuse of the data shared and published. Participation in schema.org to enable discovery of public content through systems harvesting this metadata (most notably Google data) and enable linkages between Google Data and Google Scholar that are part of the Google information ecosystem. The project also participates in the Clarivate Data Citation Index (DCI). The digital object identifier (DOI) for permanently published HydroShare resources enables tracking of papers indexed in the Web of Science that cite data in HydroShare. While citation does not actually imply reuse and there can be reuse without citation, the team feels that this is the best metric available that quantifies impact on the advances in knowledge that have come about through HydroShare.

2.16 | Chem Compute

The Chem Compute science gateway provides a web-based interface for undergraduate students to submit computational chemistry jobs to the XSEDE supercomputing resources. The gateway allows undergraduate students to perform electronic structure calculations and molecular dynamics simulations. Both of these software packages are free to download and use but require a great deal of computer expertise to install, maintain, and use correctly. The Chem Compute interface and its XSEDE backing eliminate the need for undergraduate chemistry departments to commit computing resources for these computations, it eliminates the need for faculty to design and test computational labs, and makes it significantly easier for students to perform computations.

By providing no-cost access to high-quality computational packages, this gateway aims to build students' confidence in their computational abilities and narrow the education gap in chemistry between schools that can afford expensive computational packages and those that cannot. Many schools are limited by: (1) the high cost of commercial computational packages, (2) the lack of computer expertise to maintain these packages or to install free or low-cost alternatives, (3) the lack of a University cluster to use these packages, (4) the lack of computational chemistry expertise in small departments, especially in primarily undergraduate institutions and 2-year colleges. Recently, COVID-19 has prevented schools from offering any Chemistry labs, and Chem Compute has provided a platform to help students keep learning. Chem Compute has been accessed by 21,000 users since 2014. These users (mostly undergraduate Chemistry students) have run 125,000 computational jobs. All calculations are run on XSEDE servers (Jetstream, Comet, and Bridges), and the gateway is hosted on Jetstream. Most users are from the US, but students from all over the world use the gateway. Because the goal of the gateway is to provide access to Computational Chemistry, the geographic diversity of our users (including 14 Minority Serving Institutions) is an important success metric.

As an educational gateway our main goals are to provide undergraduate students access to Computational Chemistry, thereby increasing learning and building students' confidence in using computers in Science. Chemistry often proves to be a difficult subject for students because it is not intuitive for them to conceptualize what is occurring on a molecular level[20,21] leading to many common misconceptions.[22] Computer based visualizations have been shown to increase student engagement and understanding of chemical representations. Confidence and self-esteem are important predictors of engagement, motivation, and academic achievement.[23-26] Students have reported informally that use of the gateway does help their Chemistry learning by allowing them to visualize molecules and molecular orbitals. Many students have remarked that they wished they had used the gateway in Organic Chemistry, which relies heavily on 3d structure and Molecular Orbital Theory. In the role of faculty, student misconceptions have been uncovered, such as the difference between valence and core electrons, the Schrodinger equation, and vibrational energies. Knowing these misconceptions has informed the efforts to improve teaching of future students.

2.17 | D4Science

The D4Science infrastructure is operational since 2006. One of the distinguishing features of this infrastructure is the support for the development and operation of VREs with the "as-a-Service" delivery model.[27,28] Each VRE is a dedicated working environment specifically designed to serve the needs of its designated community. D4Science-based VREs are web-based, community-oriented, collaborative, user-friendly, open-science-enabler working environments for scientists and practitioners willing to work together to perform a certain (research) task. From the end-user perspective, each VRE manifests in a unifying web application (and a set of application programming interfaces (APIs)): (a) comprising several components and (b) running in a plain web browser. Every component is aiming at providing VRE users with facilities implemented by relying on one or more services provisioned by diverse providers.

The impact of D4Science can be measured by its overall usage indicators. At the time of writing this article a total of 155 VREs are operational with others to come. These VREs are serving a great variety of communities of practice from domains including Agri-food, Earth Science, Marine Science, Social Sciences, and Humanities. These VREs are overall serving more than 10,000 users on a daily basis. The number of users is constantly growing from the 7799 active users of April 2019 up to the 11,110 active users in March 2020. In the period April 2019–March 2020, a total of 87,566 working sessions have been performed (with an average of 7297 sessions per month), and a total of 238,595,868 analytics tasks have been executed (with an average of 19,882,989 analytics tasks per month). Several research results are produced and published (be them publications, datasets, processes, etc.) by using D4Science VREs. The support received by D4Science has to be recognized according to specific acknowledgment and citation policies. By relying on this, D4Science is working with OpenAIRE[29] to develop and calculate indicators of the impact of D4Science in the scholarly communication cloud.

2.18 | Lifewatch

LifeWatch ERIC[30] (The e-Science European Research Infrastructure for Biodiversity and Ecosystem Research) is a distributed Research e-Infrastructure to advance biodiversity research and to provide major contributions to addressing the big environmental challenges, including knowledge-based solutions to environmental managers for its preservation. This goal is achieved by providing access through a single infrastructure to a multitude of sets of data, services, and tools enabling the construction and operation of VREs, which allow the accelerated capture of data with new innovative technologies and knowledge-based decision-making support for the management of biodiversity and ecosystems.[31]

LifeWatch has been established as an ERIC since March 2017, which includes seven countries as full members: Belgium, Greece, Italy, The Netherlands, Portugal, Slovenia, and Spain. LifeWatch ERIC provides tangible integrations of all the Biodiversity and Ecosystem Research relevant components, and provide the interface for synthetic research at global scales. At the same time, it also attempts to engage the research communities, stakeholders, SMEs and Industry in a collaborative environment toward sustainability in order to meet demanded Societal Challenges.[32] In particular, links with the Global Biodiversity Information Facility (GBIF)[33] are essential as LifeWatch ERIC is supporting GBIF in a collaborative way by integrating and providing e-Services. Currently, LifeWatch ERIC success had led to offerings that are more than VREs, such as Virtual Micro-CtvLabL for micro-CT data-based exploration of natural history specimens, Marine VRE for data resources holding marine biodiversity and ecosystem data, Phyto VRE for harmonised data on taxonomy and morpho functional traits, and Alien Species VRE for studying the occurrence of alien species in various types of ecosystem.[30]

2.19 | CSDMS

The Community Surface Dynamics Modeling System (CSDMS) promotes, coordinates, and provides enabling technology for the computational study of earth-surface processes. These include human time-scale processes such as landsliding, flooding, coastal erosion, and undersea gravity currents, as well as geologic-time phenomena such as land form evolution and the formation of river deltas and other sedimentary deposits. Established in 2007 with support from NSF, CSDMS works to nurture a community of practice in numerical modeling, with members both benefitting from and contributing to a modeling framework composed of freely available, every-improving software modules that simulate a variety of different processes and phenomena. CSDMS' efforts focus on three pillars: community, computing, and education. Community activities include meetings and workshops, as well as a web portal (gateway) that provides, among other resources, an open repository for sharing numerical modeling programs and tools. In terms of computing, the CSDMS Integration Facility creates and maintains software infrastructure, helps community members with software development, and promotes interoperability standards for numerical models.

CSDMS has relied on a variety of success metrics, and many of these have evolved over time in response to technological change and community growth. Over the last 10 years (2010 to 2020), membership in CSDMS has grown by about factor of four; as of mid-year 2020 membership was close to 1900. Originally established as a US-based effort centered in the sub-disciplines of sedimentary geology and geomorphology, the membership now spans about 70 countries, and includes representation from disciplines ranging from ecosystem dynamics to solid-earth geophysics. The membership and its disciplinary breadth are among the metrics used to track success in community building. CSDMS also tracks the number of attendees at annual meetings and special-topic workshops. Post-event surveys provide information about participants' experience and suggestions for future events. Success of the Model Repository is measured in part by the number of model programs and tools contributed, and the year-to-year growth in this number. To provide would-be users of these codes with evaluation metrics, CSDMS tracks an "h-index" for each program, based on citations to publications that reference that particular program. Educational activities and resources involve a different set of metrics: the number of person-hours of instruction provided in workshops and short courses, the number of educational resources contributed in a given time span, and the number of views of educational videos.

3 | SUMMARY AND INSIGHTS ACROSS THE SCIENCE GATEWAYS/VRES

This article represents a first attempt at collecting success metrics across a diverse collection of science gateways/VREs, in this case, clients of the SGCI and members of the VRE-IG. The variety of metrics from these international efforts provides valuable insights both for new and experienced science gateway/VRE designers. These deeper success metrics are inexorably linked to the deeper goals of the principal investigator leading the science gateway/VRE in partnership with their funding entity. The definition of success is also fluid, and each effort's constituents likely represents a fluid set of needs. As each community evolves and technologies change, the metrics may change as well. It is of critical importance for science gateway/VRE designers to think about metrics at all levels while the operations are still in the planning stage, and at least annually throughout the operational existence. It is incumbent on developers to establish a clear alignment of their goals with their funding sources, and their users, then create plans and tools to collect, track, publicize these metrics, while considering how they might adapt these metrics over time. Four primary areas for metrics emerge from analysis of the science gateways/VREs, which are listed and detailed in the following subsections and summarized in Tables 1 to 4 in increasing complexity - *user type and count*, *user behavior*, *user satisfaction*, and *long-term impacts*.

TABLE 1 Mapping of user type and count metric to proposed improvements along with exemplar adopters of improvements

Proposed Improvements	Exemplar SG/VRE Cases
Understand types of users	- *QUBES* tracks users from diverse fields and institutions, for example, they serve a community of about 7000 math and biology educators, professional societies, and education projects.
	- *SeedMeLab* tracks adopters who deploy it as a data sharing hub, customize it as a gateway, or use the software modules on their websites.
	- *OpenTopography* tracks users who utilize the platform to run processing jobs for downloading high resolution topography data and generating derived products.
	- *University of South Dakota (USD) Science Gateway* tracks newcomers to computational research around a geo-graphical region, that is, at USD and across South Dakota.
Publicize counts of users	- *UltraScan* use log information to track counts of users, for example, they found in a recent annual time period that over 140 investigators from 116 institutions actively used the gateway. They also publicize their user activity through self-registered publications, that is, they reported over 158 publications in the last ten years.
	- *SeedMe1* that has been in production since 2014 not only tracks their over 700 users and ∼200 active visitors per month, but they also publicize over 150,000 items uploaded by the users.
	- *COSMIC2* is interested in tracking new users counts in order to help them publicize whether the gateway has led to growth in the field.
	- *OpenTopography* captures detailed metrics of its users, data holding and usage and makes these available publicly via a live analytics dashboard on the gateway. It has been in operation since 2009 and currently has over 129,405 unique users who have run jobs via the gateway. At least 386 peer-reviewed articles along with numerous theses and other publications have been produced using OpenTopography resources. These include academic works in Earth science, ecology, hydrology, geospatial and computer science, and engineering.
	- *CitSci* goes beyond the more obvious metrics of numbers of projects, numbers of volunteers, and numbers of observations to more specifically look at harder to reach and measure metrics including percent active projects, number of peer-reviewed publications supported, number of decision-making policies informed, and the degree to which participants are being impacted through metrics of scientific literacy, behavior, attitude, and knowledge gains. For instance, they publicized 134 case studies to look at intent for use in decision-making and their impact to create positive social-ecological-economic changes for the communities.
Failure investigations and growth actions	*SeedMeLab* used a strategy that involved an early access to work with limited partners to de-risk their gateway development, for example, they first worked with a research group that heavily used their gateway for over two years with 18 users who shared over 17,000 items with an aggregate size of approximately 5GB. Based on the early adopter experiences, they released their framework and transitioned to production.
	- *University of South Dakota (USD) Science Gateway* observed that one of the greatest challenges in delivering cyberinfrastructure is simply communicating its existence. Hence, they have used their gateway as an awareness-building tool to increase their user impact/engagement by demonstrating streamlined access to popular applications in campus research communities new to advanced computing. Similarly, *COSMIC2*gateway found user adoption success by making software and data management for cutting-edge algorithms requiring users to expend minimal effort for job submission.

3.1 User type and count

There are several common and obvious steps that can be taken to help grow usage: count users, publicize user counts, disseminate stories about what the counts mean, investigate and take action if a science gateway/VRE is not growing as envisioned. A significant observation in this context relates to understanding the types of users. Are they from diverse fields? Diverse geographical locations? Diverse educational institutions? Commercial companies? Is user turnover high? How do their needs vary? How does that information fit with the science gateway/VREs' goals? How important is each group to the intent and success? Several science gateways/VREs have a clear idea of success—whether that means serving users from both prestigious research institutions and teaching institutions, serving users from geographical areas internationally outside the science

TABLE 2 Mapping of user behavior metric to proposed improvements along with exemplar adopters of improvements

Proposed Improvements	Exemplar SG/VRE Cases
Method to profile user behavior	- *SeedMeLab* used the data on a per-deployment basis, that is, they profiled the number of users, number of items, total storage and publications supported for each deployment and conducted user interviews for subjective feedback.
	- *OpenTopography* was designed and developed from the very onset with the capability to capture detailed metrics on usage. Analysis of usage metrics over the years has shown some predictable patterns on user behaviour. They were able to identify consistent spikes in usage and new users when new topography datasets become available in OpenTopography as well as specific datasets that are popular with users and see consistent usage over the years.
	- *CitSci* was developed as a global citizen science support platform and cyberinfrastructure that advances the utility, impacts, and outcomes of field-based citizen science projects. They studied their user's behavior in their platform in terms of real-time data entry and mobile application needs and found costs and hassles associated with users creating their own web frontend/backend systems and custom mobile apps. Using this information, they developed volunteer management capabilities with customizable do-it-yourself (DIY) features such as, for example, 'create your own citizen science project'. Due to this approach, their gateway currently supports more than 760 projects ranging from those that monitor water quality and maple syrup productivity to wildlife populations and invasive species.
Track usage patterns of the offered feature	- *SeedMeLab* gateway used their experiences of SeedMe1 to develop from scratch (in part due to breaking changes in the underlying Drupal framework) as a distributable set of modular building blocks for creating data sharing and data management websites. They identified and developed features that research teams need to manage, share, search, visualize, and present their data in a web-based environment using an access-controlled, branded, and customizable website that the research group owns and controls.
	- *OpenTopography* captures metrics on not just which topography datasets are used but also spatial "hot zones" within a dataset that users are interested in along with processing algorithms that are most commonly used. Analysis of usage over the years allows the gateways to identify patterns of usage and allocate the limited compute resources in an efficient manner to meet the user demand.
	- *CIPRES* tracks user patterns by combining user-supplied information with data from the XSEDE and CIPRES databases to track the number of user-submitted jobs, submission successes, number of users (new and returning), rate of user turnover, and amount of compute resources consumed per unit time.
Failure to prepare for evolution in user behavior and remediation actions	- *CIPRES* found that tracking user visits, number of users on the site, and number of user accounts were not useful because they historically weakly correlated with the particular user behavior they were interested in, that is, the gateway's intent.
	- *'Ike Wai Gateway* found that supporting FAIR data principles leads to quality products but they require time to produce, verify and annotate properly. They have been successful to attract quality products by researchers and community members who see value in contributing products to the gateway despite the time burden involved.
	- *OpenTopography* continued to see growth in users as well as usage (processing jobs). This growth corresponded to the increase in its data holdings and services. As new datasets beaome available in OpenTopography along with new compute intensive processing algorithms such as topography differencing (change detection), they needed to address the growing limitations of on-premise infrastructure. They have thus begun investigations to migrate to the commercial cloud and become more efficient in leveraging of XSEDE resources to keep up with the demand from the user community.
	- *SimCCS* found that evolution in user behavior can be profiled from feedback from multiple webinars and workshops convened early in the gateway operation. This led to accelerated development of four core applications in their integrated CCS infrastructure solutions. A surprising outcome of this approach was seen in the overwhelmingly positive response by the commercial sector to the novel capabilities of the SimCCS gateway. Similarly, *CyNeuro*used user surveys and mini-symposia of various stakeholders (e.g., researchers, resource providers, tool developers, data owners) early in their development to implement and refine infrastructure capacity, tools capability, and user support structures.

TABLE 3 Mapping of user satisfaction metrics to proposed improvements along with exemplar adopters of improvements

Proposed Improvements	Exemplar SG/VRE Cases
User satisfaction and impacts on productivity/usability measurement	- *CIPRES* uses an annual user survey to analyze user sentiment about CIPRES features and toolkit. Publications of users are a key metric for user satisfaction and related information is mined from a combination of Web of Science, Google Scholar, and self-reporting data of users on an annual basis. Finally, the success of the software package as a platform for gateway creation is evaluated by tracking how many implementations of the CIPRES Workbench Framework are in use worldwide.
	- *OpenTopography* measures user satisfaction by considering multiple factors, including number of users, usage of the platform for education in classrooms, publications resulting from platform use as well as adoption from data providers to utilize the platform for delivery of their datasets.
	- *Interactive Parallelization Toolkit (IPT)* measures user satisfaction based on the number of users, both domain-experts and students, accessing IPT through the gateway. Additionally usability measurement is done in terms of how well users meet their learning goals. While the number of users is captured automatically, surveys are used to get the users' feedback on their learning experience. Objective and subjective responses obtained thus far have indicated that the gateway is helping users to more productively learn parallel programming concepts and parallelize applications in a self-paced manner without spending time on software installations.
Recruitment of usability consultants for assistance	- *SGCI* offers a popular service of providing usability consultants for assistance with usability studies in science gateway efforts. Particularly, such a service is found to be highly recommended as a best practice for new science gateway/VRE efforts.
	- *Data Discovery Studio* uses focused testing among groups of researchers from several domains to quantify search improvements.

gateway/VREs' home region. In any of these cases, it is important to know about the users so that relevant information can be collected from the outset. In addition, knowing which user group(s) a funding entity considers essential can help focus on increase engagement of those users to foster higher impact.

3.2 | User behavior

It can be observed that it is important to profile user behavior in science gateways/VREs. For many science gateways/VREs, this was noted from the number of jobs run. However, more subtle behaviors can also be noted such as: classroom use, sustained use over time, bursty use, types of tools used, content accessed created and shared, citizen science observations made, student test scores. Some science gateways/VREs focus on the usage. For example, they track usage patterns of the offered features in terms of—are users using datasets across multiple repositories or reusing data in new ways? In this way, it is important to think about what success means at the outset to plan the necessary tracking mechanisms that need to be set up. At the same time, designers must be prepared for evolution in user behavior. In one example, the team was surprised by industry use. Identifying such a new user group adoption changes how the science gateway/VRE resources are managed to meeting emerging user needs. It would have been difficult to back-populate such data if the user's institution information was not collected from the outset.

3.3 | User satisfaction

For all science gateways/VREs, user satisfaction, and impacts on productivity are of primary importance. Science gateways/VREs use a variety of approaches to ascertain this. Some study user behavior through surveys to gather feedback on user experience. Others use methods such as in-person shoulder-surfing or remote tracking tools such as Google Analytics to improve usability. An increasing number are turning to usability consultants for assistance. This has become perhaps the most popular service provided by SGCI and is highly recommended as a best practice for new science gateway/VRE efforts. Evaluating impacts on productivity can be accomplished in surveys that include questions such as: Does the science gateway/VRE help you do something that would be difficult or impossible otherwise? What would be the impact on your research if the science gateway/VRE ceased to exist? How much longer would it take to achieve the same result without the science gateway/VRE?

TABLE 4 Mapping of long-term impacts metric to proposed improvements along with exemplar adopters of improvements

Proposed Improvements	Exemplar SG/VRE Cases
Measurement methods	- *Interactive Parallelization Toolkit (IPT)* measures success of a project adoption on the basis of the consumption of the available software and hardware resources. If 70% of the available resources are used up, then the project deems that as a success.
	- *QUBES* measures based on how their services are used to share educational resources such as Open Education Resources (OERs), journal clubs, websites for conferences and workshops, training and support for using software tools in the classroom, and communication about upcoming opportunities.
	- *SeedMeLab* tracks the number of deployments (not end users), active use of open source modules and publications enabled by use of the gateway.
	- *CyNeuro* measures the number of supported research and education use cases of neuroscientists, particularly those involving large-scale computation and image analysis, without the need for expert knowledge of programming and cyberinfrastructure configurations, which is beyond the repertoire of most neuroscience programs. Similarly, *'Ike Wai Gateway* measures the number and quality of annotated data-sets, products and tools produced and made available.
Tracking types of products	- *CUAHSI HydroShare* tracks products that quantify their impact on advancing hydrologic knowledge. For instance, they track new users and returning users and their related number of created resources such as observation data, model and analysis results, and models and scripts.
	- *CyNeuro* tracks products based on the number of new research/teaching tools and exemplars developed by users, and their sustained usage by the community. Development of new undergraduate/graduate course sequences is also tracked. In addition, user-centered metrics such as ease-of-use, ease-of-setup, ease-of-self-service and increased options in terms of tools/resources to complete compute/data-intensive workflows of our users are considered as success metrics.
	- *CIPRES* measures success if they can provide easy access as well as support for robust and heavy use of their gateway software for the most important community codes on large HPC clusters irrespective of the scientific field. Similarly, CyberGIS also measures success by their ability to serve thousands of users across diverse domains including agriculture, bioenergy, emergency management, geography and spatial sciences, geosciences, and public health.
	- *CSDMS* - To provide would-be users of these codes with evaluation metrics, CSDMS tracks an “h-index” for each program, based on citations to publications that reference that particular program. Educational activities and resources involve a different set of metrics: the number of person-hours of instruction provided in workshops and short courses, the number of educational resources contributed in a given time span, and the number of views of educational videos.
Failure noted that led to major actions	- *Chem Compute* team recognized that schools are limited by challenges such as high cost of commercial computational packages, lack of computer expertise to maintain these packages or to install free or low-cost alternatives and the lack of a University cluster to use these packages. Based on these observations, their gateway was developed to help faculty (especially in undergraduate institutions and two-year colleges including minority serving institutions) to design and test computational labs, and make it significantly easier for students to perform computations. Chem Compute succeeded in their efforts and has been accessed by 21,000 users since 2014. These users (mostly undergraduate Chemistry students) have run 125,000 computational jobs.
	- *SimCCS* has observed that large-scale carbon capture, utilization and storage technologies deployment still faces significant economic, technical, and non-technical challenges (e.g., policy making, project permitting). Hence, their vision of future gateway success is to address user base growth from private-sector industries.

3.4 Long-term impacts

Finally, longer term impacts are the most important and often the most difficult to measure. To one science gateway in this article, the degree to which citizen science participants are being impacted through metrics of scientific literacy, behavior, attitude, and knowledge gains is important, as is whether the findings are used to influence policy and management decisions. Painstaking case studies were conducted solely for this purpose,[14] and the knowledge gained is invaluable in science gateway/VRE promotion. To another VRE in this article, the extent of new offerings that go beyond the basic VRE offerings to their users is important to measure success and impact. Science gateways/VREs are designed for use by students to look at how well students meet their learning goals. For some efforts, the number and depth of collaborations and partnerships enabled by their science gateway/VRE are important. As part of impact measurement, many science gateways/VREs also look at what their users produce—publications, educational materials, reports, datasets and software products, as well as how these are shared with and used by others. A proactive approach where personnel conduct literature searchers is an important addition to regular reminders to users to notify the science gateways/VREs about publications. Some science gateways in this article proactively use the Clarivate Data Citation Index, the Web of Science, and Google Scholar.

4 ENVISIONING NEXT-GENERATION SCIENCE GATEWAY/VRE ADVANCES

Science gateways/VREs are becoming part of everyday scientific practice, and best practices in their creation will continue to evolve. In this section, we present a number of advances that can be used in next-generation science gateways/VREs to enhance the reach and scale of the success metrics summarized in Section 3. In addition, the advances detailed in the following subsections also help increase the development and adoption of standards across user communities. As the advances we discuss below are integrated in the future, we expect success metrics will become more vibrant from multiple roles of: software developers, data engineers, resource providers, user services experts.

4.1 Open reference architectures

Open reference architectures can encourage people and organisations constructing science gateways/VREs to follow the same pattern so that interoperation between SG/VREs can be effective. Thus, open reference architectures can help in increasing the *user type and count* as well as *long-term impacts* success metrics. Particularly, should new and improved components become available, they can be "plugged in" widely across implementations to rapidly benefit a larger set of users. Years of observation confirm that science gateways/VREs have similar architectural structures, based on generalised comparable requirements. In Europe, the VRE4EIC project[34] attempts to produce a VRE open reference architecture that can be used to consider a diverse set of user types and even *user behavior*. It comprises of three tiers that provide one view of the architecture and represent (respectively) the application (what the user is trying to achieve), the interoperability (interactions of components and assets) and resource access (interfacing to asset sources). The VRE4EIC reference architecture has been discussed widely, cited, and various projects (e.g., EPOS[35]) are using components of it.

The ultimate impact is in further knowledge, further research, education, citizen science and commercial success using the assets, the output products of research such as publications, datasets, software or patented outputs. This was foreseen, and VRE4EIC uses asset catalog metadata based on the "standard" CERIF[36] (Common European Research Information Format: an EU Recommendation to Member States) used widely in Current Research Information Systems (CRIS). CERIF is an open data model built on the extended entity-relationship model with temporal duration—thus providing provenance automatically. Furthermore, CERIF includes specific entities for measuring not only research outputs but also their impact based on indicators and associated measurements[37] that tangibly relate to the success metrics we consider in this work that include: *user type and count*, *user behavior*, *user satisfaction*, and *long-term impacts*. Hence, one key aspect of VRE4EIC was that by using this metadata standard, people at a given institution/university can be encouraged to link up with the CRIS (in Europe commonly using CERIF) recording their research outputs and their impact. In the UK, universities are assessed every few years by the Research Excellence Framework (REF) and its predecessor exercises. Universities report huge savings by having the requisite information available automatically using CERIF and a cooperation among universities and Elsevier incorporates the "snowball metrics"[38] as a mapping from the specification of these metrics onto the indicator and measurement structure within CERIF.

4.2 Framework building blocks

Experience over the last decade shows that science gateways/VREs that are successful in terms of *user type and count*, *user behavior*, *user satisfaction*, and *long-term impacts* adhere to one of the following concepts: (i) widely used complete frameworks such as Galaxy,[39] HUBzero,[40] and gCube/D4Science;[28] (ii) RESTful APIs, microservices and support of multiple programming languages in widely used frameworks such as TAPIS;[41] (iii) reused interface implementations like the one CIPRES[10] offers, or (iv) generic middleware such as Agave,[42] SciGaP[43] that support multi-tenancy in science gateways/VREs. Additionally, software frameworks and platforms have never faster evolved than in current times evident in the growing number of mature JavaScript libraries, environments such as the Jupyter notebook or containerizations with Docker supporting reproducibility. Current and upcoming technologies allow for agile software development and could lead to a faster turn-over of "building blocks" for science gateway instances.

The science gateway/VRE landscape is rich with the diverse available frameworks and services and each of them have their strengths and foci. The landscape is scattered though—the interoperability between the different systems is rarely given, which hinders *long-term impacts*. Thus, researchers and science gateway/VRE designers may still develop their own solutions despite the availability of mature and well-designed solutions because they miss a certain feature or option in existing frameworks. The ideal would be a set of building blocks for science gateways/VREs that combine the strengths of the existing ones and can be applied as plug-and-play architecture. The vision of SGCI and VRE-IG initatives is that such building blocks for science gateways/VREs work like the Internet: they follow a protocol and concept to deliver services and features while leaving much freedom on content level. Such a reference architecture would allow novel features to be integrated faster in a science gateway/VRE and foster *user satisfaction*metrics more flexibly. Moreover, the *long-term impacts* success metric would be addressed when relatively small amount of effort needed is expended on reference architecture implementations to integrate add-on features. Such add-on efforts in turn promote *user type and count* metric by increasing community adoption diversity. They also help with faster reaction to changing *user behavior* in user communities' and help researchers publish results earlier in the research life-cycle.

4.3 | Integration of analysis, modeling, and sensing

Future science gateways will encompass new and transdisciplinary approaches to bringing three distinctive scientific paradigms—analysis, modeling, and sensing—under one convergent umbrella through innovative cyberinfrastructure capabilities. The interaction and integration of these three paradigms are often approached in a fragmented way that affects *user type and count*, *user satisfaction*, and *long-term impacts*. Therefore, future science gateways will have great opportunities to integrate: (a) data-intensive analytics with computation-intensive simulation modeling enabled by cyberinfrastructure; (b) scientific models for understanding both natural processes and human-environment interactions; and (c) diverse and dynamic data sources. This integration can be approached to improve *user type and count*, *user satisfaction*, and *long-term impacts* through the following four general strategies: integrative science frameworks, open platforms, computationally reproducible notebooks, and community-driven participatory processes for collaborative research and education.

As an example, "Where COVID-19"[44] has been developed as a new-generation science gateway that combines big data analytics, computationally intensive simulation modeling, and near real-time sensing into computationally reproducible notebooks. These notebooks achieve scalable integration of heterogeneous cyberGIS and cyberinfrastructure capabilities, and have been developed based on advanced geospatial analysis and modeling methods. This science gateway is well positioned to host notebooks contributed and shared by pertinent communities. The user interface is friendly for presenting geospatial information that is produced by scientifically validated geospatial analysis and modeling methods encapsulated in the notebooks. No in-depth technical knowledge of cyberGIS or cyberinfrastructure is required of end users. The gateway is designed to support exploration and discovery of spatiotemporal patterns of the COVID-19 pandemic based on advanced geospatial analysis and modeling research. Engaging graphical interfaces as seen in the "Where COVID-19" gateway will always be a critical aspect of data analysis/visualization for interdisciplinary fields. Allowing easy-to-use programs with drag-and-drop interfaces will enable users at all levels of expertise to access cutting-edge algorithms thus directly improving outcomes in terms of *user type and count* and *user satisfaction* metrics. Building algorithm agnostic graphical web interfaces will enable analysis and modeling tools to have standardized interfaces, which improves *long-term impacts* by serving a broader set of users with varied backgrounds.

4.4 | Seamless multi-factor authentication

Typically, science gateways are allowed to execute applications on high-performance computing (e.g., XSEDE) resources through an account that is designated as a "community account" to promote *user type and count* tracking. It is a common account through which all the batch computing jobs are submitted from a science gateway. Some science gateways also provide a mechanism through which the users can run jobs under their own allocation on, for example, XSEDE resources. Irrespective of whether a community account and allocation are used for running jobs, or a user's own allocation is used, the science gateway operators may have to request for exemption from multi-factor authentication (MFA) if the XSEDE system of their interest has the MFA policy. For instance, the Stampede2 system requires MFA and the related science gateways interested in running jobs on Stampede2 need to submit MFA exemption requests. While such exemptions facilitate the smooth usage of the XSEDE systems through the science gateways to foster *long-term impacts*, they have the potential of being a security-risk if the server on which the gateways are running get compromised. Hence, to be better prepared for handling any security-risk to account for *user behavior*, and to be prepared for any policy changes regarding exemptions that impact *user satisfaction*, the next-generation science gateways will have to consider investigating approaches for supporting seamless MFA.

4.5 | Integrated FAIR data support

Granting agencies invest millions of dollars on the generation and analysis of data, making related products extremely valuable in terms of *long-term impacts*. However, without sufficient annotation of the methods used to collect and analyze the data, the ability to reproduce and reuse those products suffers. This lack of assurance of quality and credibility of the data at the different stages in the research process essentially wastes much of the investment of time/funding and also impacts *user satisfaction*. Moreover, it fails to drive research forward to the level of greatest potential if research products were effectively annotated and disseminated to the wider research community. Future science gateways/VREs will be required to have features that enable FAIR (Findable, Accessible, Interoperable, and Reproducible)[45] data principles guideline aiming to enhance the reusability of data and metadata and overall reproducibility of science to foster *user type and count*. The FAIR principles put specific emphasis on enhancing the ability of machines to automatically find and use the data, in addition to supporting its reuse by individuals based on *user behavior*. These future science gateways/VREs will need to incorporate workflows and tools, such as algorithms using deep learning and artificial intelligence, which assist in automating the capture and annotation of data/metadata within the environment and ultimately to the wider community. Further, these FAIR features will enable connected-ness with other science gateways/VREs, services, and workflow tools to be applied to raw, intermediate and end data products for *long-term impacts*.

4.6 | Self-learning and adapting nature

There is a quote from William Gibson, American-Canadian science fiction writer, that the future is already here, it is just not evenly distributed. Indeed, several elements of a next-generation science gateway/VRE already exist and can be observed in various efforts reviewed in Section 2 of this article. These include futuristic-looking 3D visualizations, interactive user interfaces, the ability to command and pool together powerful HPC resources for complex model simulations, and the ability to chain operations into distributed workflows. Scientific and technological innovations will get increasingly integrated into science gateways/VREs in the form of AI/ML tools, and foster the increased availability of well-described and analysis-ready datasets to create *long-term impacts*.

The next-generation science gateways/VREs will be self-learning through interactions with users and adapting to changing user needs based on *user behavior*. User interactions will be supported by AI/ML tools such as chatbots with knowledge bases, designed to recommend additional operations on the data (e.g., next steps in processing workflows, or suitable analysis, visualization and reporting components) or adapt underlying computing resources[46] to increase *user satisfaction*. The recommendations will be based on which operations have been selected by previous users. This additional information obtained through user interaction, could be managed in knowledge graphs associated with each science gateway/VRE so that user actions actions can be anticipated to pre-allocate resources. In addition, extracting information and knowledge from previous runs would lead to the ability to answer questions through guided interfaces of web-pages with chatbots more efficiently and avoid duplication. Further, a next-generation science gateway/VRE may provide services for "precomputing" to address *user type and count*needs in certain domains. For example, addressing needs in computational genomics benefit when pre-computing of the results is followed by storing them in a database for shortening the turn-around time of jobs. Ultimately, the knowledge base driven approaches with guided interfaces will make working with science gateways/VREs easier and more intuitive for *long-term impacts*.

4.7 | Decoupling application code

Science-focused researchers typically do not have the staff or funding to maintain a science gateway/VRE, yet do have valuable contributions embodied in domain-specific code. This situation contributes to publicly funded software development ending up as "dark code" that does not contribute to *long-term impacts*. GenApp[47] was created to address this issue and simplify the task of a researcher to widely deploy applications to increase *user type and count* and account for diverse *user behavior*. The GenApp solution divorces the application code from the science gateway by having the researcher create a definition file completely describing the inputs, outputs, and any details needed to execute the underlying code and to wrap or modify their code to conform to the definition. Thinking in these terms, if a standard were to be adopted by the community for such a definition file, many community ecosystems could arise utilizing this standard to incorporate defined modules within their science gateway, thus improving *long-term impacts*. This would also enable a researcher to define their code depending upon *user behavior* and share it privately or publicly. The shared code could be community vetted and seamlessly integrated into multiple science gateways that support the standard. Science gateway hosting clouds could provide dynamic organized collections of modules (or “applications”) with a uniform look-and-feel, simplifying user experience and simplifying domain researchers’ effort to increase *user satisfaction*.

Decoupling application code in future science gateways/VREs will also allow users to create: (i) modular analysis tools, (ii) engaging graphical interfaces, and (iii) access to affordable computing resources. This vision is being investigated in another case study involving user-curated data analysis pipelines for single-particle cryo-electron microscopy (cryo-EM) image analysis. In this effort, users are allowed to mix-and-match algorithms between software packages. However, in this hybrid processing environment, users lose meta-data tracking, intuitive interfaces, and real-time feedback to help them navigate through their workflows. The difficulty in switching between software leads to siloing of data analysis routines, leaving users with less-than-optimal tools because: (a) they do not know about better-performing tools, or (b) they do not know how to execute these tools on their data. By connecting tools through modular architectures that allow application decoupling, users will be equipped to mix-and-match algorithms to enable improved scientific outcomes and create *long-term impacts*.

4.8 | Scaling with cloud integration

The role of commercial clouds in helping science gateways address the issues of scalability and sustainability is only beginning to be explored. Recently, the CIPRES science gateway[10] developed tools to access a commercial cloud, and found it offered the following benefits to enhance *user type and count* and *user satisfaction*: (i) it expanded the number of resources available to meet surges in community demand (e.g., GPU nodes), thus decreasing queue wait times by as much as 41 hours; (ii) it provided access to the latest processors/GPUs, thus increasing the speed of job runs relative to those on locally available hardware; and (iii) it allowed jobs to run much longer than scheduler policies on available XSEDE resources allow (up to 22 days in this case), which benefits job runs using codes that do not checkpoint. In short, access to commercial clouds provided a new level of scalability that can accelerate science along at least three dimensions. The project also made clear that a high level of local technical expertise was essential to create, sustain, and support functional submissions to a commercial cloud, and this is a place where developing a common infrastructure could be very helpful for increasing *user type and count* and enhancing *long-term impacts*.

4.9 | Economic model for cloud integration

While the potential value of commercial clouds to gateway users is clear, their role in scalability and sustainability remains contingent on developing a viable economic model, that is, “who will pay for computing in the commercial cloud?”. For compute-intensive analysis routines in, for example, cryo-EM image analysis case, using the public cloud resources can be prohibitively expensive for both computing and storage. Two parameters that are key in achieving economic viability and *long-term impacts* are: (i) maximizing efficiency of use, and (ii) establishing a funding model for commercial cloud computing. To improve efficiency, science gateways/VREs must develop tools that take advantage of the deep discounts offered by commercial providers on instances where running jobs can be interrupted at any time. The ability in *user behavior* to capture and restart jobs automatically will be critical to minimizing instance charges. The second critical issue is developing a mechanism to make research funds available and to simplify the use of such funds for cloud computing to increase *user satisfaction*. Specifically, future science gateways/VREs will need access to new cloud resources for academic purposes that leverage: (i) governmental funding support, and (ii) economies of scale to create a subsidized cloud platform that is price-point competitive with local on-premises solutions but is remotely hosted. The Cloud Bank[48] project represents a first step toward creating such an infrastructure. The project enables cloud funds to be included in a proposal budget for some NSF solicitations and if awarded, Cloud Bank will broker and simplify researchers’ access to commercial clouds with efficient on-boarding processes and financial services. Emerging efforts such as the European Open Science Cloud are another direction where governmental funding support can be leveraged by future VREs to link with subsidized community cloud resources.

4.10 | Distributed microservices for data management

There is an explosion in the amount of data being generated in the earth sciences and especially in the area of high-resolution topography, largely driven by faster sensors, new methods of collection, and lowering costs of acquisition. The need to effectively manage, distribute, and process these massive volumes of data based on *user behavior* requires a shift to newer data management architectures. The recent trend in wide area (e.g., statewide) lidar acquisitions also illustrate the need for large scale computations on entire datasets (e.g., statewide flood mapping). In order to address these new requirements as well as to handle growth in *user type and count*, the OpenTopography[9] science gateway is planning to migrate to the commercial cloud with a more distributed microservices architecture. The underlying vision is to democratize access and processing of the data collections at a much larger scale, empowering users to do more custom analysis-in-place without the need to transfer data that in turn increases *user behavior*. While a majority of the user community will be satisfied by the curated workflows available within the OpenTopography science gateway, enabling more access pathways to the data in the cloud opens opportunities for rapid access, experimentation, and large-scale computation. Researchers will contribute to *long-term impacts* by having the ability to run custom computations and test prototype implementations of algorithms by spinning up their own compute resources and accessing OpenTopography's datasets via available cloud APIs. By placing OpenTopography's processing services and data catalog along with these large, government funded, geospatial datasets in the cloud, other groups are able to more effectively leverage them, thereby further expanding *long-term impacts*.

4.11 | Middleware for cloud portability and orchestration

As data is becoming increasingly large within science gateways/VREs based on *user type and count* as well as *user behavior* factors, deploying microservices and managing the workload using cloud platforms becomes crucial and provides benefits as described in the preceding three subsections. The computing infrastructures in next-generation science gateways/VREs will increasingly shift to using federated private and public cloud resources, utilizing the scalable and elastic nature of clouds. Additionally, microservices architectures based on interconnected containers enable platform independence and support portability of science gateway/VRE applications that cater to diverse *user behavior*, and contributes to *user satisfaction*. Such a federated cloud adoption vision will require integration of cloud middleware for portability and orchestration using standardized description languages, for example, TOSCA—Topology and Orchestration Specification for Cloud Applications.[49] The standards help express complex application topologies and user-defined quality of service (QoS) requirements (e.g., dynamic and potentially complex scaling policies and also dynamically adaptable security requirements). On top of such standardized description formats, a new suite of automated deployment and run-time orchestration solutions can be developed that rely on open-source building blocks supporting modularity, dynamically programmable scaling and security policies for *long-term impacts*. An example and a step toward this direction is the MiCADO (Microservices-based Cloud Application-level Dynamic Orchestrator)[50] automated deployment and autoscaling framework that utilizes widely applied open-source components as building blocks (e.g., Kubernetes, Terraform, and Prometheus). MiCADO relies on a tool-independent TOSCA-based input describing application topology and QoS policies, and supports autoscaling.[51] Thus, there is a need for novel middleware that will enable next-generation science gateways with innovative methodologies to deliver fast, automatic and flexible resource provisioning services. The middleware should provide a rich set of APIs supporting diverse *user behavior* that allow flexible portability and orchestration across federated private and public cloud resources, especially for domain science users with limited expertise in using advanced cyberinfrastructure tools.[52]

5 | CONCLUSION

Science gateways/VREs are becoming part of everyday scientific practice, and are increasing the reach of advanced cyberinfrastructure tools, distributed resources and federated data sets to larger user groups in the science and engineering communities. Accordingly, success metrics for measuring impact will remain an important and vibrant topic among science gateway/VRE developers to ensure planning of financial and human resources in collaboration with funding agencies. Using a number of exemplar science gateways/VREs from SGCI and VRE-IG communities, we detailed how impact can be defined in terms of, for example, purpose, operation principles, and size of user base. The exemplars outlined a rich set of approaches to routinely measure and communicate impact that then allowed us to document the key best practices. This article thus represents a first step in what must necessarily be a long evolutionary process in establishing known practices for setting and measuring individual science gateway/VRE goals. In addition, we also presented a number of technology advances that could be incorporated in next-generation science gateways/VREs in order to enhance their scope and scale of their operations for greater success/impact. This article thus also serves as a starting point for projecting the types of technology advances whose integration will significantly increase the impact and sustainability of science gateways/VREs in the future.

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