Facilitating collaborative science through portals connected to high-performance computing

James P. Carson[ϕ1], John Fonner[1], Matthew Vaughn[1], Niall Gaffney[1], Tracy Brown[1], Joe Stubbs[1], Jake Rosenberg[1], Sal Tijerina[1], William J. Allen[1], Erik Ferlanti[1], Joshua Urrutia[1], Ethan Ho[1], Jawon Song[1], Shweta Gopaulakrishnan[1], Hedda Prochaska[1], Joon-Yee Chuah[1], Mark Weston[2], Terrance Sejnowski[3], Kristen Harris[4], Maytal Dahan[1]

[ϕ]jcarson@tacc.utexas.edu

[1]The University of Texas at Austin, Texas Advanced Computing Center, Austin, TX, USA
[2]Netrias, Cambridge, MA, USA
[3]Salk Institute for Biological Studies, La Jolla, CA, USA
[4]The University of Texas at Austin, Center for Learning and Memory, Austin, TX, USA

***Abstract*—Large scale collaborative science requires ways to facilitate sharing of data, protocols, analysis tools, as well as data products and their provenance. We describe here two recent science gateways successfully deployed from a common platform to accomplish collaborative research in different domains. The first is the Synergistic Discovery and Design Environment (SD2E), which was a web-based analysis platform for collaborative analysis, data sharing, and application development. The second is the 3D Electron Microscopy (3DEM) portal, which is an active web-based research platform focused on developing and disseminating new technologies for enhanced resolution 3DEM. Both gateways connect to high-performance computing resources at the Texas Advanced Computing Center.**

Keywords—science gateways, collaboration, FAIR data, supercomputing

I. Introduction

Many of the Findability, Accessibility, Interoperability, and Reusability (FAIR) principles [1] that we strive for in the public sphere across the scientific data community today are also important within a developing project, especially one with widely distributed collaborators that are addressing data or computationally intensive challenges. The Texas Advanced Computing Center (TACC) Core Experience Portal (CEP) was developed as a template science gateway, and at this time has been deployed to a large number of science gateways across a wide variety of disciplines. The TACC Application Programming Interface (API) known as Tapis (https://tapis-project.org/) is the RESTful API layer that serves as the secure connection between the web gateway and the data storage and computing resources, as well as managing user access [2].

We describe here the application of the CEP and Tapis to two different large-scale collaborative efforts.

II. SD2E.org

DARPA's Synergistic Discovery and Design (SD2) program operated from 2017 until 2021 and was designed to "develop data-driven methods to accelerate scientific discovery and robust design in domains that lack complete models" [3]. This was realized as a quarterly cycle of experimental design, data collection, and data analysis that would iterate repeatedly over the four years and across multiple scientific domains of discovery. These novel domains ranged from developing genetic circuits, protein design, and solar material discovery [4]. The SD2E project's primary mission was serve the SD2 teams during the project, and to stop service at the end of the project.

SD2 teams included Data-Centric Scientific Discovery (TA1), Design in the Context of Uncertainty (TA2), Hypothesis and Design Evaluation (TA3), and Challenge Problem Integrator (TA5) [5]. TACC led the SD2 Technical Area 4 (TA4): Data and Analysis Hub, and to this end, TACC developed the Synergistic Discovery and Design Environment (SD2E), an integrated cyberinfrastructure that enabled investigators to deploy analysis tools and aggregate data resources. Leveraging Tapis, alongside a number of other services, SD2E provided a diverse and expressive set of interfaces backed by high performance computing (HPC), high performance data storage, high throughput computing, and cloud computing systems.

III. 3DEM.org

The 3DEM.org web-based research platform was developed beginning in 2017 as part of the Next Generation Network for Neuroscience (NeuroNex) program [6]. 3DEM.org is focused on supporting and disseminating new technologies for enhanced resolution 3-dimensional electron microscopy, with a specific emphasis—but not limitation—on applications involving the ultrastructure of synapses [7]. By integrating this new data collection technology with publicly funded high-performance computing, the additional computational power is leveraged to process even larger datasets, and to promote reproducibility and sharing of techniques. This NeuroNex project is designed to serve not only the project team, but all researchers interested in the tools and capabilities.

All visitors to 3DEM.org may download the latest public datasets. Users with active TACC accounts and allocations may request access to the interactive 3DEM Workbench. Within the Workbench, users can access community datasets, workflows, and applications. Applications are focused on those that support processing for enhanced resolution 3DEM. Users may also share their data and processes with other users.

IV. Analytical Environment

1) Graphical user interface with usage-tailored views.

These projects include investigators possessing a wide variety of backgrounds and expertise. To facilitate access to data and analysis resources for all members of the programs, each project provides a customized web–based graphical user interface (GUI) and Discovery Workspace (Figure 1). Through a laptop or even a smartphone, users can access data and run registered applications on HPC systems. Addressing project security needs, users can keep their data and applications fully private, share with specific users, or share with all members of the program. The infrastructure supports batch applications that submit jobs to HPC systems to run when resources are available, as well as interactive applications that open direct web-access to HPC nodes for more exploratory analysis.

2) Dynamic Data Library for exploration and discovery.

Ingested data, metadata, and data products are browsable using the Data Depot graphical interface accessible using a web browser. Using this interface, each project member can access their private data, their project data shared among a limited number of collaborators, and community data made available to every member of the project. Browser-supported files can be viewed in-browser, and all files can be downloaded to users' local systems. The Data Depot is also browsable from the Workspace interface for selecting input files for processing. For 3DEM.org, published datasets are available for general use or download, and published with a DOI provided through the Texas Data Repository.

For the SD2 program, we developed an SD2 Data Catalog to support rapid development of data types, structures, and workflows. This data repository was constructed using MongoDB, a NoSQL database program [8]. Ingested data, metadata, and data products were automatically captured and made available through the Data Catalog via search in support of data discovery and exploration. Using a NoSQL approach allowed facile application to the variety of projects in SD2 and their various data components, without requiring structural changes to the Data Catalog. Users could sort and search for datasets, and export data locations for analysis.

3) Interactive high performance analysis notebooks.

Reproducibility is of critical importance for workflows and analysis. Project members can create, access, and share Jupyter notebooks. These can run on shared virtual machines or on high performance computing nodes with the latest GPU and CPU components, as well as large memory capacity nodes. This enables high-powered real-time analysis using an electronic notebook-based interface that captured the scripts, programs, data products, and data visualizations all in one interface.

V. API Tools

Agility and portability can be critical to achieving a rapid pace of iteration and discovery. Toward this end, these gateways use Tapis version 2 as a common, unifying platform to harmonize the presentation of data, the automation of extract, transform, load (ETL) processes, the publication of software applications, and the provenance of analyses [2]. As discussed in section IV, the portals provide a graphical, browser-based interface to the hardware infrastructure. These views were built on Tapis endpoints. Tapis managed the key functionality of the gateways, including managing user and data security.

Tapis is also accessible using an enhanced command line interface (CLI) (https://github.com/TACC-Cloud/tapis-cli). Tapis CLI supports more naturally typed commands and automatically generates and submits the matching curl-based commands that are used by Tapis. This CLI includes command lists, command help, table-formatted outputs, and user-friendly authentication. It provides researchers a direct path toward automating any definable computational or analytical workflow.

Because of its open standards and flexible design, the infrastructure supports integration of numerous external tools to facilitate rapid engagement and collaboration across all teams. An example of this is the Synthetic Biology Open Language (SBOL) [9] which was requested during the SD2 project and supported by TA4 on SD2E resources. Other examples of integration include third-party services such as Illumina's BaseSpace, Google Drive, and Slack.

VI. Documentation

Both 3DEM.org and SD2E.org include information beneficial to users of the respective gateways. Both include tutorials and guides on accessing and using the gateways. Both offer tutorials at project meetings and provide support by email, slack, and scheduled videoconferences. Both include links to presentations at topic-related workshops. All project hardware systems have detailed documentation on specifications, usage, and best practices made available through the TACC Portal (https://tacc.utexas.edu).

SD2E.org included an online Learning Center with training materials for using TA4 resources and developing workflows. In addition to the documentation, the SD2E Learning Center included a searchable tutorial interface for Data and Compute, as well as a Program Information interface for scientific domain specific information and challenge-problem updates. This searchable format supported tag-based searches as well as difficult level descriptors, thus supporting users new to the project or new to the resources, as well as advanced users, and all users in-between. TA4 developed and provided sample applications, workflows, and notebooks along with detailed presentations and tutorials on how to construct and customize these. Sample applications and workflows were shared in the SD2E Gitlab, allowing team members to readily clone and modify for their own needs. A custom Jupyter notebook sharing application was created to allow for cloning, modification, and sharing.

This work was funded by DARPA contract HR001117C0094 and NSF grants DBI-1707356 and DBI-2014862.

VII. Deployment

The gateways are deployed on a virtual machine on Rodeo, TACC's in-house VMware cluster. The frontend is a web application using the React framework, proving users an interface for managing data and submitting HPC jobs. The backend is built with the Django web framework, providing API endpoints to primarily structure calls to Tapis apps, jobs, and systems and format the results for display on the front end. A PostgreSQL cluster is used for the database layer, which stores user profiles and project metadata. Searches for files, projects, and web content are managed by an Elasticsearch [10] cluster running on a dedicated virtual machine. Search indexing and other long-running tasks are handled by an asynchronous Celery worker with RabbitMQ as the message broker [11]. An Nginx server is placed in front of the rest of the services to route user requests and serve static web content [12].

The portal itself is completely Dockerized, with each service broken out into containers [13], with deployments managed by Jenkins, docker-compose, and an in-house customizable deploy-management suite called Camino. The content management system (CMS) also exists as its own image and container, allowing for seamless upgrades and deployments targeting specific services, maximizing uptime.

VIII. Hardware

TACC supports hierarchical, high-performance POSIX storage [14] on the Stockyard and Corral filesystems, backed by TACC's Ranch tape archive for disaster recovery support. This storage is accessible to users on all TACC HPC and cloud computing platforms and used for data storage and analysis. For SD2, object storage was provided via Amazon Web Services [15] and was used primarily for backups or in support of cloud-deployed applications and services.

TACC supports CPU and GPU compute capacity over the course of these programs collectively on the Frontera, Longhorn, Stampede2, Lonestar5, Lonestar6, Jetstream, Jetstream2, Maverick2, Hikari, and Wrangler HPC systems [16-20]. This complement of systems allows users to run on a wide array of processor architectures including Intel, AMD, and NVIDIA. Cloud computing capacity is delivered via a combination of on-premises OpenStack [21] and VMware [22] clusters as well as virtual machines operated by Amazon Web Services.

TACC provides high-performance networking and data ingress services that demonstrably supports inbound data transfer rates of >1 TB/day. This is accomplished by operating a dedicated MinIO S3 server on an access node with 100GB/sec external networking to the public Internet. In addition, high-speed SSH, SFTP, and HTTPS access are provided. For SD2E, integration with Illumina's BaseSpace service allowed experimentation facilities to connect with SD2E using their preferred protocol.

Data storage, compute, network, and data transfer services operate at an availability of over 99%.

IX. Users Management

TACC has a robust, facile process for user enrollment into 3DEM.org and SD2E.org using the TACC User Portal combined with novel automation developed for these projects. This process was used to enable hundreds of distinct users in over 50 access control groups to access and collaborate on TACC systems to generate and analyze their respective program datasets. For SD2, the enrollment and management system was extended to support users from external programs as part of a data sharing exercise. Per-user quotas are not enforced, though user usage is tracked to ensure utilization efficiency.

Every user job, whether running on HPC or Cloud infrastructure, can be monitored for resource use efficiency. Metrics tracked included memory footprint, storage I/O, idle CPU, idle GPU, and network traffic. Historical records of each job are available for users to consult. In addition, TACC staff routinely survey the jobs database looking for usage that was less than optimally efficient. Staff members consult as needed with job owners to improve their computations, ensuring efficient use of federally-supported resources.

X. Data Management

Integral to the success of these projects is the capability to access and generate data and metadata from interactive environments and HPC resources. 3DEM.org uses the Corral filesystem as the central repository to facilitate public sharing, and the Stockyard filesystem for each user's private data area for active analysis. In contrast, SD2E used the Stockyard filesystem as its centralized repository due to the more compute intense mission and the less immediate need for public sharing. In addition to project-wide data, users can also create private directories and manage access with collaborators (using fine-grained access control lists behind the scenes). For SD2 metadata, a Data Dictionary was developed against a Mongo database to hold provenance information, data relationships, and categorical and secondary computed information. The Data Dictionary was not static but rather evolved as new data and metadata terms were discovered through the ETL process. Schemas were developed collaboratively, and the choice of a NoSQL document store enabled the SD2 program to iterate and adapt to changing requirements over time.

The nature of the SD2 project involved numerous hand-offs between teams and users, and each one represented a risk of mismatched expectations between the team generating the data and the team consuming the data for downstream analysis. Using an actor-based computing paradigm, the platform treated data-uploads as triggers for initiating ETL actors. Each actor could then call other actors based on its own results. Using this system, teams generating data were able to receive near-instant feedback if information was missing or otherwise did not match expectations. Similarly, teams conducting downstream analyses were able to automate their processes with the confidence that previous ETL steps would catch most data reliability issues and spend less time writing defensive code. Over time, the number and sophistication of automated ETL and data processing steps snowballed, allowing the time spent on interactive data exploration to always shift toward higher-value, novel analyses.

Rapid iteration of the scientific discovery process is a key goal of these science gateways. To facilitate this, we have supported, demonstrated, and encouraged best practices in software development and reproducible analysis. Use of GitLab and GitHub are encouraged, allowing users to individually or collaboratively develop and share their data processing workflows and analysis pipelines. Provenance of software versions is tracked in this way, and usage is tracked by Tapis, allowing specific reproducibility and interactive development applicability.

XI. Discussion

We have described the capabilities for two of the many science gateways that have in recent years been deployed from the CEP and Tapis. The success of these gateways in serving their research communities demonstrates in part the value of the template gateway approach. In both cases, initial deployment was rapid, with each gateway along with initial customization made available in less than a month. Collaboration was enabled (*e.g.*, over 20 publications reference the use of the SD2E). Importantly, using a common gateway template is a key part of a long-term sustainability plan, as it allows for future CEP and Tapis updates to be shared quickly across all gateways.

Acknowledgment

We acknowledge and thank the teams of users from the associated SD2 and NeuroNex projects for their usage of these gateways and feedback applied to their design. We acknowledge and thank all TACC staff as they provide the support and resources which make these projects possible.

References

[1] Wilkinson, Mark D., et al. "The FAIR Guiding Principles for scientific data management and stewardship." *Scientific Data* 3.1 (2016): 1-9.

[2] Stubbs, Joe, et al. “Tapis: An API Platform for Reproducible, Distributed Computational Research.” *Advances in Intelligent Systems and Computing* (2021): 878-900.

[3] Synergistic Discovery and Design (SD2), website accessed June 30, 2023 https://www.darpa.mil/program/synergistic-discovery-and-design

[4] Vaughn, Matt, et al. “Synergistic Discovery and Design Environment Final Technical Report” (2022)

[5] Broad Agency Announcement, Synergistic Discovery and Design (SD2) HR001117S0003, posted November 22, 2016

[6] Litvina, Elizabeth, et al. "BRAIN initiative: cutting-edge tools and resources for the community." *Journal of Neuroscience* 39.42 (2019): 8275-8284.

[7] Harris, Kristen M., et al. "A resource from 3D eletron microscopy of hippocampal neuropil for user tgraining and tool development." *Scientific Data* 2 (2015): a150046.

[8] Banker, Kyle, et al. *MongoDB in action: covers MongoDB version 3.0*. Simon and Schuster, 2016.

[9] Galdzicki, Michal, et al. "The Synthetic Biology Open Language (SBOL) provides a community standard for communicating designs in synthetic biology." *Nature biotechnology* 32.6 (2014): 545-550.

[10] Gormley, Clinton, and Zachary Tong. *Elasticsearch: the definitive guide: a distributed real-time search and analytics engine*. " O'Reilly Media, Inc.", 2015.

[11] Dossot, David. *RabbitMQ essentials*. Packt Publishing Ltd, 2014.

[12] Reese, Will. "Nginx: the high-performance web server and reverse proxy." *Linux Journal* 2008.173 (2008): 2.

[13] Merkel, Dirk. "Docker: lightweight linux containers for consistent development and deployment." *Linux j* 239.2 (2014): 2.

[14] Nichols, Bradford, Dick Buttlar, and Jacqueline Farrell. *Pthreads programming: A POSIX standard for better multiprocessing*. " O'Reilly Media, Inc.", 1996.

[15] Mathew, Sajee, and J. Varia. "Overview of amazon web services." *Amazon Whitepapers* 105 (2014): 1-22.

[16] Gaffney, Niall, et al. "Building wrangler: A transformational data intensive resource for the open science community." *2014 IEEE International Conference on Big Data (Big Data)*. IEEE, 2014.

[17] Stewart, Craig A., et al. "Jetstream: a self-provisioned, scalable science and engineering cloud environment." *Proceedings of the 2015 XSEDE Conference: Scientific Advancements Enabled by Enhanced Cyberinfrastructure*. 2015.

[18] Stanzione, Dan, et al. "Stampede 2: The evolution of an XSEDE supercomputer." *Proceedings of the Practice and Experience in Advanced Research Computing 2017 on Sustainability, Success and Impact*. 2017. 1-8.

[19] Stanzione, Dan, et al. "Frontera: The evolution of leadership computing at the National Science Foundation." *Practice and Experience in Advanced Research Computing*. 2020. 106-111.

[20] Hancock, David Y., et al. "Jetstream2: Accelerating cloud computing via Jetstream." *Practice and Experience in Advanced Research Computing*. 2021. 1-8.

[21] Sefraoui, Omar, Mohammed Aissaoui, and Mohsine Eleuldj. "OpenStack: toward an open-source solution for cloud computing." *International Journal of Computer Applications* 55.3 (2012): 38-42.

[22] Gulati, Ajay, et al. "VMware distributed resource management: Design, implementation, and lessons learned." *VMware Technical Journal* 1.1 (2012): 45-64.

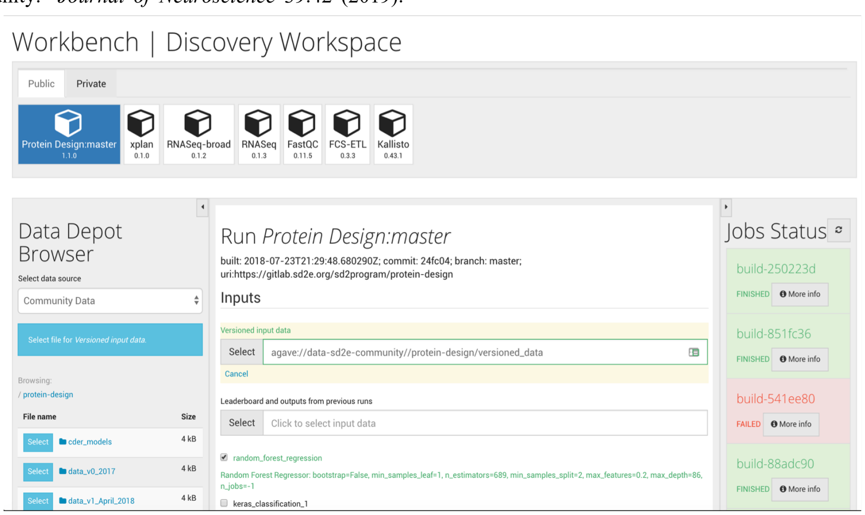

Figure 1. The Discovery Workspace is a GUI granting users browser-based access on their local computer or phone the community applications, any private applications they developed, and applications shared with them by others. All these applications run on HPC resources. Project raw data and data products are browsable and selectable as inputs for applications. Provenance for input datasets, application versions, applications parameters, and outputs are all tracked and stored for reproducibility.