

SGX3: Novel Concepts to Enhance Knowledge and Extend the Community Around Science Gateways

Sandra Gesing
Discovery Partner Institute
University of Illinois Chicago
Chicago, Illinois, USA
sgesing@uillinois.edu

Claire Stirm
San Diego Supercomputer Center
University of California, San Diego
La Jolla, California, USA
cstirm@ucsd.edu

Michael Zentner
San Diego Supercomputer Center
University of California, San Diego
La Jolla, California, USA
mzentner@ucsd.edu

Maytal Dahan
Texas Advanced Computing Center
University of Texas, Austin
Austin, Texas, USA
maytal@tacc.utexas.edu

Linda Hayden
Elizabeth City State University
Elizabeth City, North Carolina, USA
haydenl@mindspring.com

Abstract—SGX3 is an NSF-funded Center of Excellence for Science Gateways complementing the mission of the Science Gateways Community Institute (SGCI) to serve the community of users, developers and providers of science gateways. The experiences and lessons learned via the over six years of SGCI has informed, which novel areas SGX3 offers, which areas are enhanced, which areas are continued in SGCI via community-funded opportunities and which areas are taken out. While SGCI has been successful in growing the community, there is still a lower uptake in different research domains such as social sciences. Computational sciences and engineering present the domains that are mostly covered by members. SGX3 focuses especially on growing the community for different sciences and research domains and growing a diverse workforce. This paper compares the SGX3 and SGCI offerings and goes into detail for the novel services of SGX3 and the expected impact.

Index Terms—SGX3, SGCI, community growth

I. INTRODUCTION

Science gateway projects combining access to data with software tools and underlying compute resources, access to lab instruments and data infrastructures straddle the line between computer science and hard sciences, as they bring together these two worlds to provide digital access to cutting-edge research models, educational software, or a central interactive data repository. Due to their blended nature, they need a team that has computer science and engineering, system administration, and research skills. They also have a continued need for software and hardware to enable consistent access for their audiences, while incorporating additional resources as needed when growth occurs. Thus, the community for science gateways include domain researchers, computational scientists, science gateways creators and science gateway providers.

The mission of the Science Gateways Community Institute (SGCI) is to support the community in their tasks: from using to developing to providing science gateways [1]. SGCI was funded in 2016 as part of the software sustainability institute

program of NSF and the funding ended in July 2023 while it will continue to offer services paid from clients. SGX3 as its successor is part of the NSF Center of Excellence program and was funded in August 2022. SGCI as well as SGX3 consider especially usability, reusability and sustainability of science gateways and to grow the community in all research areas. It has become evident in the last six years though that the growth of the community around SGCI from computer science and engineering was much larger than in research domains and that the user community needs more attention for a continued growth. Thus, SGX3 services has been partially differently structured than the SGCI services from lessons learned. These lessons learned are gathered via characteristics of involvements with SGX3 activities such as demographics of attendees at the annual conference and client engagements as well as surveys after events and metrics about the SGX3 website. Furthermore, we restructured services to fit the concept of the NSF Center of Excellence and the funding that is for five years the half sum than the project received via the NSF sustainability institute program before.

Successful services that could be still funded under Center of Excellence program has been taken over as is, some are adapted and some are not offered any more. Below is the list of SGX3 services:

- 1) UX evaluation and design engagements lasting up to 3 calendar months
- 2) Technology evaluation and gap analysis
- 3) Science Gateway architecture design
- 4) Once annually Science Gateways Focus Week sustainability sessions
- 5) Focus Week follow-on sustainability coaching
- 6) Summer Coding Institutes
- 7) Rising Stars program
- 8) Summer faculty and student internships

- 9) Science Gateway Hackathons
- 10) Gateways conference series
- 11) Gateways Central site for gateway listing, software listing, and partnership formation
- 12) SGX3 On the Road outreach to scientific communities where they meet
- 13) Blueprint Factory sessions to develop the future roadmap for Science Gateways serving new domain science needs

The first eight services are mostly continuation from SGCI services, always adapted to feedback from participants such as the successful Focus Week (renamed from bootcamp) [2]. The SGCI Young Professional Program is renamed to the Rising Star Program to emphasize that the age is not important in this program but the role of awardees for science gateways. The student internships and hackathons have been extended by faculty internships and Facultyhack so that faculty contribute to the outreach about science gateways and being multipliers of the concept via teaching and advising. The Gateway conference series has moved from an SGCI organized conference to a community-driven conference with the first time in 2023 the general chair being selected by a newly established advisory board for the conference and who is not part of the SGCI/SGX3 team. The goal is to attract additional research domains and tap into the chair's networks that are not already in contact with SGCI/SGX3. Gateways Central, SGX3 On the Road and the Blueprint Factories are novel services established in SGX3.

We go into detail for the novel programs Blueprint Factories, Rising Stars and Faculty Program, Gateways Central and SGX3 On the Road in the following sections.

II. BACKGROUND

SGCI was organized in the following way to deliver services, training, and community engagement opportunities:

- Incubator - training and consulting services with regard to financial and technological sustainability, cybersecurity, and user experience.
- Extended Developer Support (EDS) - placement of a 0.25 full-time equivalent technologist from SGCI staff into projects needing to solve difficult technical problems and instill best practices.
- Workforce Development - training developers in Science Gateway development skills, training faculty in incorporating Science Gateway development in curricula, student hackathons, and summer- and semester-long internship programs, all with a special focus on diversity.
- Scientific Software Collaborative - gathering of a comprehensive inventory of existing science gateways, software used in science gateways, and Tech Summit activities¹ that bring together Science Gateway stakeholders to develop software elements for the community. In addition, during its sixth year the SGCI has undertaken and is still in the process of developing a Science Gateway offering

for housing multiple science gateways under a common operation called OneSciencePlace.

- Community Engagement and Exchange - outwardly focusing on dissemination of SGCI results through an annual conference, a vibrant website, webinars, blogs, success stories, and a variety of other publications and postings for public dissemination.

To date, the SGCI has served over 200 clients with a variety of services, had over 3,400 attendees to its community building events, supported 1,200 students and faculty, and produced 195 research products.

In 2022, the team applied for an NSF Center of Excellence to further catalyze the science gateways community by incorporating more participants from research domains, and to formalize community-driven, forward-looking blueprints for next-generation emerging needs for future science gateways.

SGX3's high-level goal is to have activities result in extending access to computing resources to diverse audiences with varying levels of skill; in so doing, to expand the community of Science Gateway practitioners and users; and to encourage the community to do this with good practices that result in more sustainable outcomes for science gateways. Off of this foundation, there are four main work thrusts:

- Growing a Diverse Community
- Developing the Workforce
- Serving as Community Experts
- Envisioning the Future

To deliver on these four thrust goals, the following activities will happen under SGX3:

- Blueprint Factories - an avenue where we work with collaborators to better understand the CI needs of entire research communities and national-scale cyberinfrastructure providers.
- Workforce Development - to build a supportive HPC/Gateways community for the teaching faculty while providing them the training and support needed to succeed; opportunities for students to grow their HPC/science gateway skills through coding institutes, hackathons, and internships.
- Consulting - working with science gateway teams to provide expert advice on project lifecycle sustainability through workshop and consulting; advice on user interface and design improvements; and help define actionable technical roadmaps for projects entering into the next phase of their science gateway infrastructure.
- Gateways Central - a reimagining of the science gateways catalog that serves as a central point for stakeholders in science gateways to interact.
- Science Gateway Outreach - engaging science gateways and domain scientists/scholars using science gateways where they present ("On the Road"); collecting community knowledge through community surveys, focus groups, and interviews; community celebration through the annual Gateways conference series; and information

¹<https://sciencegateways.org/our-services/sgci-tech-summit>

sharing through the Science Gateways Community website and mailing list.

SGCI will reach in July 2023 the end of its funded period and will continue as an entity focused on its own sustainability through paid services. SGX3 will be a funded activity operating under the umbrella of the SGCI. For community members served by SGX3 who desire more intense engagements, such engagements can be undertaken as SGCI activities funded by the community members desiring those services.

III. BLUEPRINT FACTORIES

The concept of Blueprint Factories is the keystone of SGX3's work thrust on Envisioning the Future. A Blueprint Factory is a concentrated activity that takes place over an approximately 18-month period. Its purpose is to develop a forward looking blueprint of technical capabilities that science gateways will need to provide to support the future needs of a given scientific domain or computing resource.

Each of the Blueprint Factories will involve core team members of approximately five cyberinfrastructure professionals and five domain experts. Over the lifespan of the Blueprint Factory the core team will define scope, engage their professional networks to build a group of approximately 30 stakeholders, conduct individual pain-point interviews, convene virtual focus groups, and ultimately produce an analyst-like report defining a technological roadmap for Science Gateways for the next 5-10 years to support the domain studied by the Blueprint Factory.

As proposed, SGX3 contemplates between seven and eight such Blueprint Factories over its 5-year funding. Four of these are as follows:

- PATH - The high throughput computing facilities collected under the umbrella of the PATH project² present an opportunity to expand the user base with the ease of access that a Science Gateway can provide.
- ACCESS - Similar to PATH, the new ACCESS program³ also presents an opportunity for an expanded user base facilitated by one or more Science Gateways. Unlike PATH, where service provider complexities are managed by PATH, ACCESS has no common means by which its various service providers are managed, with each resource potentially having its own unique considerations.
- The Materials Genome Initiative (MGI) - The MGI⁴ is a complex and significant initiative funded by multiple federal agencies with a goal of increasing United States innovation in materials. Under this umbrella are many different types of activities that are both experimental and computational. These activities involve significant demands for data management and sharing, model validation, simulation, and artificial intelligence. These demands occur at multiple scales, from atoms to manufactured parts. Science Gateway technology ideally would

support these multiple needs of the members of this community, and also increase participation by broadening access to data and compute resources for new researchers who today may not otherwise have such access.

- Sustainability for Science Gateways - The SGCI conducted many of its Focus Week workshops and subsequent consulting engagements to assist Science Gateway owners with sustaining their efforts. In the course of these activities, the SGCI consulting team was able to observe sustainability challenges across a spectrum of scientific disciplines, project longevity, and funding levels.

The additional Blueprint Factories not included in the first four will be decided as the teams become available following their involvement in the first four, and will align with a specific domain science that is most relevant at that time. Since the time of proposal, the Office of Science and Technology Policy has issued the National Artificial Intelligence Research Resource report⁵. This report has significant implications on Science Gateways and other cyberinfrastructure. Therefore, the ACCESS and PATH Blueprint Factories will be focused more closely on how research utilizing artificial intelligence can benefit from these national compute resources.

IV. RISING STARS AND FACULTY PROGRAM

Rising Stars is a program that has been adapted from the Young Professionals Program. The focus is to give recognition to students, faculty and/or science gateway creators who contribute with outstanding and/or novel activities to the growth of the community and spreading the word about science gateways. Examples for categories of Rising Stars include

- Students who are standing out during internships and hackathons
- Faculty integrating science gateways as novel concept in their classes
- Science gateway creators incorporating cutting-edge technologies in science gateway frameworks

Rising Stars receive their award at the Gateways conference.

The goal of Faculty Program is to build a supportive science gateways community for the faculty while providing them the training and support needed to succeed. The goal is to enable faculty to be a gateway user and/or enthusiast and be a multiplier to bring the concept of science gateways to students. SGX3 staff can assist faculty in establishing high-performance computing (HPC) accounts for their classes and consult with them through the implementation phase of their curriculum changes. Seminars will cover gateway tools with a focus on classroom usage. Faculty receive hackathon mentor training in preparation for service as mentors in upcoming hackathons. During the academic year, opportunities will be available for faculty to continue their preparation via support for the Gateways and Supercomputing Conference tutorials, sessions, and workshops. In particular, SGX3 plans

²https://www.nsf.gov/awardsearch/showAward?AWD_ID=2030508

³<https://new.nsf.gov/funding/opportunities/advanced-computing-systems-services-adapting-rapid>

⁴<https://www.mgi.gov/>

⁵<https://www.ai.gov/wp-content/uploads/2023/01/NAIRR-TF-Final-Report-2023.pdf>

a FacultyHack at the Gateways conference each year. For the FacultyHack@Gateways SGX3 will look for teams of two faculty from each participating university. We anticipate four to five teams for each such hackathon. The focus of FacultyHack@Gateways is on further development of HPC curriculum and use of HPC tools at Minority Serving Institutions (MSIs). During the hack, faculty will be challenged to identify existing curricula to modify and adapt for their classes.

V. GATEWAYS CENTRAL

The science gateways landscape can be overwhelming for users and developers. It is time-intensive to keep up with novel features in Science Gateway frameworks, new Science Gateway instances, beneficial software libraries, and cutting-edge resources. The SGCI catalog⁶ partially addressed this and, with over 600 entries, the catalog serves as a starting point for SGX3's Gateways Central. The new goal for Gateway Central is to reimagining the catalog that will service as a central point for stakeholders in science gateways to interact. In its first year of SGX3, it is gathering requirements from stakeholders and the community to facilitate the following types of navigation and interaction:

- Enable computational tool creators to find Science Gateway(s) where they can make their tools available for wide adoption and partner with Gateways to address sustainability.
- Enable educators to find computational tools and relevant content for instruction in specific domains.
- Provide users with personalized recommendation of content based on their user profile and activity.
- Listed gateway providers will be able to contribute new content such as information about their communities, success stories, contact points, and short videos as demos of the capabilities.

A forum to discuss topics related to gateways and related technologies or share information about upcoming events. The forum will also be seeded with features from two communities per month with news and novel developments in different formats - from blog posts to short videos - one tailored with information for users and one with information for developers. A mechanism to seek help with gateway development, sustainability, and other SGX3 related topics. These requests will be triaged, matched, and routed to appropriate experts and channels including SGX3 consultants, US Research Software Engineers Association (US-RSE) members, ACCESS awardees, and PATH experts. These extra layers will dramatically change the catalog from a solid inventory of the field into an interactive nexus for community members to learn from and interact with each other.

VI. SGX3 ON THE ROAD

The goal of SGX3 On the Road is to bring SGX3 and science gateways as a concept to domain researchers and

diversify and grow the community especially around sciences and research different from computer science and engineering. Computer science and engineering are areas, which are well presented by attendees in the Gateways conference series, for example, and by partners of SGX3 as well as providers and developers of science gateways. SGX3 on the Road is planned as bimonthly presentations at a variety of domain science webinar series or community meetings. One focus area is on community organizations that have broad reach and provide an opportunity for highlighting Science Gateways. The first months of this SGX3 service consisted of several webinars and participation in meetings. Two of SGX3 staff members attended at the AGU Fall meeting in Chicago⁷, where we reached out to universities and organizations such as NASA at the booths in the exhibition, elucidating our services and handing out the SGCI storybooks⁸. SGX3 staff members also were part of the RDA (Research Data Alliance) 10th anniversary series with two contributions⁹. One was a joint podcast with an Australian co-chair of the FAIR for Virtual Research Environment Interest Group and one an expert discussion about the vision for science gateways for the next 10 years. This expert discussion has been recorded and has been selected by RDA for a highlights summary reel. SGX3 also got invited to the Neuroscience Gateway conference¹⁰ at the University of Alabama that was attended by about 70 people who belong to the neuroscience community and included 90% neuroscientists and about 10% computational sciences. The participation led to several contacts interested in extending their portfolio on campus via science gateways and to students interested in participating in SGX3 internship programs. Another invitation gave SGX3 the opportunity to present science gateways and SGX3 to the advisory board of faculty at the University of Central Florida. Faculty requested as a follow-up a letter of collaboration for a proposal aiming at using the usability consultancy and attending Focus Week. SGX3 will continue to connect to more research domain organizations and community organizations such as ACCESS, which have the potential to accelerate SGX3's outreach.

VII. OUTLOOK

The combination of SGX3 and SGCI services provides the community with support that fills gaps for users bringing the concept of science gateways to them and for developers and providers the adaption of novel technologies and concepts. Flagships like the Focus Week and the Annual Conference will enhance the community growth on all levels and the novel services such as the Gateways Central, Facultyhack and SGX3 on the Road will give a more in depth outreach into research communities. The Blueprint Factories are the vehicles to understand the needs of the community for the next 5 to 10 years and plan for the sustainability of SGX3. SGX3 will adapt any aspects on each program to feedback and lessons

⁷<https://www.agu.org/Fall-Meeting-2022>

⁸<https://sciencegateways.org/about/storybook>

⁹<https://www.rd-alliance.org>

¹⁰<https://www.neurogateways.com/>

⁶<https://catalog.sciencegateways.org/>

learned to be able to continue to serve the community to accelerate their research and provide advice on technologies, sustainability and usability.

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