HUBzero's Variations of Sustainability: From Simulation/Modeling Tools to Communities

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ABSTRACT

Sustainability of science gateways and continuous funding for their developer teams is a major concern that many projects face. The HUBzero® project and its science gateway framework have evolved to be self-sustained via diversifying funding resources, extending outreach measures to further communities and targeting sustainability from different angles in concrete instances. nanoHUB, PURR and OneSciencePlace are examples of how the HUBzero® team and platform build science gateways and take their specific services into account to address sustainability beyond securing funding and outreach activities. They have been integrating additional procedures and concepts for sustainability: nanoHUB invests into reliability of the over 500 simulation tools and high quality lecture and tutorial content to keep the trust of the large community with over 1.5 million users; PURR developed policies and methods for preserving research output in a sensible and sustainable way and OneSciencePlace addresses the concern of projects that have a lack of continuous funding for maintaining a science gateway by offering a solution to keep science gateways available to their communities. The paper goes into detail for measures for sustainability for HUBzero® and especially for nanoHUB, PURR and OneSciencePlace.

Keywords—HUBzero®; nanoHUB; PURR; OneSciencePlace; science gateways; sustainability; research content; research frameworks

INTRODUCTION

The importance of sustainability of research software in general and thus of science gateways as subgroup has been recognized by various researchers, funding bodies and organizations evident in funded projects such as the Science Gateways Community Institute (SGCI) [1] and the UK Software Sustainability Institute (SSI) [2] as well as initiatives such as the Research Software Engineer (RSE) Association in the UK [3] and the RSE Communities in Germany and in the US [4]. There are many definitions for sustainability of software available, i.e. SSI states in their manifesto "Sustainability means that the software you use today will be available - and continue to be improved and supported - in the future." [5]. C.C. Venters et al. [6] define software sustainability as a composite, non-functional requirement which is "a measure of a systems extensibility, interoperability, maintainability, portability, reusability, scalability, and usability". Most definitions consider maintainability, fulfilling its purpose over time and surviving uncertainty as essential characteristics for sustainable software. Achieving sustainability based on these three characteristics requires continuous effort and a variety of actions by a project and/or group developing software or a science gateway, respectively. In the remainder of the paper we focus on science gateways and the science gateway landscape to define the variations of actionable items.

Science gateways are created for specific communities and are embedded in the science gateway landscape with similar and/or competing science gateways. Existing mature frameworks and APIs such as HUBzero® [7], Galaxy [8] and the Agave Platform [9] allow for creating science gateways more efficiently and support developers on focusing on a specific gateway while offering features such as connecting to distributed computing out of the box. The services of science gateways vary from offering simulations tools to data collections to computational workflows with different requirements on the user interface and the underlying research infrastructure.

The services and the target communities of various science gateways might be very different from each other, but actionable items can be determined in a similar way. We distinguish four key variations for actionable items: 1. a technical area, 2. a community area, 3. a science gateway landscape area and 4. a stakeholder or funding area.

Examples for action items for the areas include

1. Use of well-defined software engineering practices to support extensibility, interoperability, maintainability, portability, reusability, scalability, usability, reliability and security
2. Support measures and extension of features and/or technologies in a science gateway driven by the needs of a community
3. Outreach and expansion to new communities
4. Diversifying funding

The areas are not isolated from each other but influence and overlap with each other. For example, after analyzing the science gateway landscape and reaching out to a new promising community, the development of a novel science gateway necessitates the technical implementation based on gathering requirements from the community. The definition of concrete actionable items is a mixture of performing analyses and tasks in all four areas.

The HUBzero® project has been achieving sustainability for its science gateway framework and the team via multiple measures. The science gateway framework started in 1996 as online platform PUNCH [10] for nanoelectronic research and teaching. It was horizontally expanded for more simulation tools to nanoHUB [11] and vertically to HUBzero® to serve as generic science gateway framework for a variety of communities. These expansions led to novel developments on technical side. Reaching out to communities includes the participation in conferences and workshops as presenters and/or sponsor, social media such as Twitter and a yearly event that offers the opportunity to clients to interact with the HUBzero® team face-to-face. The financial independence of the developer team from funding provided by the Purdue University was a major step. It has been attained by diversifying funding resources with participation in grants, offering hosting services and offering memberships in the HUBzero® foundation, which allow supporting instances with a limited number of development time and consultancy for usability and community outreach measures specifically for the instance.

Examples for action items in nanoHUB, PURR, and OneSciencePlace are described in detail in the sections III – V after presenting the background for activities to reach sustainability for science gateways.

II BACKGROUND

While sustainability of software and science gateways has gained increased attention in the last decade, it is an emerging area with many aspects to analyze and explore such as software citation, metrics for success and defining actions to improve sustainability. SSI defines four key areas for sustainability in their manifesto:

- Recognition of software as research output
- Software skills
- Recognition of the role of Research Software Engineers in research
- Reproducible research

Concrete measures offered by SSI include software peer-review, best practices for software development and working on improving software citations. SSI collaborates on the latter with FORCE11 [12], a community of scholars, librarians, archivists, publishers and research funders with over 2,700 members organized in 36 working groups. One of the goals of FORCE11 is to change modern scholarly communications through the effective use of information technology. The FORCE11-RDA FAIRsharing Working Group, for example, maps the landscape of community-developed standards and aims at putting recommendations into practice.

SGCI offers a 5-day sustainability bootcamp [13] that provides hands-on training for different aspects of sustainability. Cohorts with up to 20 people work through exercises for their science gateways and projects, e.g. mapping the landscape of users, collaborators, stakeholders and competitors, defining a value proposition and user-centered design. The bootcamp elucidates through the training concrete actionable items for the participants and they create 3-months goals and 6-months goals for their science gateways.

Galaxy and the Globus Data Portal [14] are examples for solutions to set up science gateways out of the box that have achieved software sustainability and the sustainability of their developer teams over years. Apache Airavata [15] and the Agave Platform achieved the same as widely used frameworks applying RESTful APIs and supporting multiple programming languages. Despite the differences in technologies and their target user communities, the lessons learned for achieving sustainability from such examples is that approaches should be technology agnostic, using APIs and standard web technologies or deliver a complete solution. Another key factor is the community engagement and outreach.

In the sustainability of on-campus teams for creating science gateways is analyzed and a crucial factor is that successful sustained teams have an evangelist guiding the team and being enthusiastic about the science gateway [16]. The report "Recognising the Importance of Software in Research -

Research Software Engineers (RSEs), a UK Example" just published by the European Commission [17] analyses the drivers and barriers for software sustainability in research with focus on RSEs and their career paths in academia. The authors identified as one barrier that there is still a general lack of awareness of the importance of software in research despite the on-going initiatives and projects targeting sustainability of software. Thus, an important factor contributing to sustainability of software is to raise the awareness for the importance of software to reach a critical mass to achieve a cultural change in academia [18].

III NANOHUB AND SIMULATION/MODELING TOOL SUSTAINABILITY

nanoHUB is a cyber-community for nanotechnology theory, modeling, and simulation for researchers, educators, students, and professionals in the nanotechnology community. nanoHUB hosts more than 500 simulation/modeling tools and nearly 6,000 other resources for the 1.4 million users that visit nanoHUB each year from around the world (Figure 1).

nanoHUB is managed by the Network for Computational Nanotechnology (NCN), which was established in 2002 with funding from the National Science Foundation (NSF), and continued to sustain the community through additional NSF grants that will provide support for the community until 2023 [19].

nanoHUB's mission is to accelerate innovation through user-centric science and engineering, with an end-goal to make science and engineering products usable, discoverable, reproducible, and easy to create for the nanotechnology community [19]. Published tools on nanoHUB can be accessed and run by anyone with a free nanoHUB account. Each tool comes with a question and answer forum, overview page, author listing, citation, digital object identifier (DOI) that is minted through DataCite wish list for improvements, problem reporting area, and additional materials shared by the tool authors such as documentation or walk-through videos. All tools are indexed by the Web-Of- Science, Google scholar and other services.

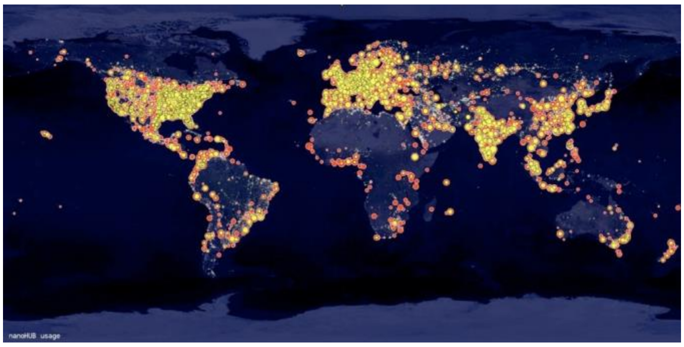

Figure 1: View of annual nanoHUB users. Yellow dots indicate simulation users (>17,000) and red dots indicate lecture and tutorial users (>1.5 million).

nanoHUB currently has simulation tools from a variety of nanotechnology disciplines, such as, nanoelectronics, nanomechanics, nanobiology, nanophotonics, and nanomaterials [20]. nanoHUB is designed to automate processes around tracking issues, answering questions, and improvement requests, but the contributor and team are expected to maintain their tool and provide supplemental materials to encourage usage by the community.

nanoHUB has been on the forefront of many science gateway aspects such as the first community accounts on TeraGrid and OSG where nanoHUB executes simulation runs on behalf of nanoHUB users, who do not have individual grid computing accounts [21] ultimately testing the reliability of such grid submissions [22]. Annual NSF site visits answered critical questions as to whether nanoHUB can be used for education or research. nanoHUB proved that research-based simulation tools can be used in formalized education settings (over 35,000 students used nanoHUB in over 1,800 classes at over 180 institutions). The median time between tool publication and first-time adoption has been documented to be less than 6 months [11]. Over 2,200 literature citations to nanoHUB with nearly 31,000 secondary citations (h-index 82) document use in research.

Under the initial two NSF awards from 2002-2007 and 2007-2012 (EEC-0228390 and EEC-0634750), the nanoHUB project encompassed not only cyber-infrastructure but also content development. During the second part of this funding cycle, nanoHUB administrators and tool managers from the HUBzero® team created a system to curate a set of published tools that were heavily used by the nanotechnology community. The Network for Computational Nanotechnology (NCN) consisted of teams from six different universities that were funded on the project to create content, and the Purdue team developing and operating nanoHUB.

Participants in NCN in this time period included Northwestern University, University of Illinois at Urbana-Champaign, and University of California at Berkeley, Norfolk State University and University of Texas at El Paso. These institutions committed to actively supporting a selection of tools they had developed. A badge icon was added to published tools to identify the support commitment. The remaining tools on nanoHUB are contributed and managed by the tool contributor and did not have such a badge next to the title.

For the tools developed by these funded partners, we negotiated and agreed on response expectations to community questions, requests, and bug reports:

1. One business day response time for support tickets, questions, and wish lists
2. Fix simple issues within a week of submission
3. Migration of long-term projects and tool improvement requests to a public wish list from private support tickets

With the end of the original 10-year awards in 2012 the Network for Computational Nanotechnology (NCN) was formally re-competed and split into multiple awards. The development and operation of the nanoHUB cyberplatform (NCN-CP) was separated from two independent content node awards. As such NCN-CP no longer had content development funds available and focused on garnering content contributions from the new node awards (nanoBIO and Nanoelectronics – NEEDS) as well as outside partners.

Some of the original tool authors from the funded teams continued to actively support their tools, while others did not. As a result, the supported tools badges have been retired and the commitment to maintain the tools is the decision of the original tool authors, as it is with tools submitted by the community at large. Moving forward, the current award focuses on continued development and operation of the nanoHUB infrastructure and exploring sustainability solutions for the entire community. Though the concept of NCN supported tools has been retired, through this effort a significant number of popular tools on nanoHUB were exemplars of a quality standard that encouraged adoption and use of the tools. By sustaining these tools, the community was encouraged to use these tools in college curriculum. This example of sustainability provides a model to encourage published materials on a gateway to be utilized and trusted.

IV PURR AND RESEARCH DATA SUSTAINABILITY

The Purdue University Research Repository (PURR) is an online, collaborative working space, and data-sharing platform to support Purdue University researchers and their collaborators [23]. PURR provides online solutions for project planning to publication. PURR meets data requirements by providing Purdue University researchers with digital project spaces to collaborate with teams by sharing research files and updating team members through collaborative features. Once the project has completed a milestone in their research, they can publish the data on PURR using the publication feature where datasets receive a minted DOI from DataCite. There are 3,604 registered researchers on PURR. Since the beginning of PURR, the researchers and their teams have submitted over 3434 data management plans, created 1,349 digital projects, and been awarded 341 grants.

PURR originated in 2011 from a collaboration between the Purdue Libraries and School of Information Studies, Information Technology at Purdue (ITaP), and the Office of the Executive Vice President for Research and Partnerships (EVPRP) around the need for a solution for campus researchers to share, publish, manage, and preserve date. An interdisciplinary working group comprised of members from the Libraries, ITaP and EVPRP identified the repository requirements, service model and digital preservation policy [24].

The Digital Preservation Policy documents how Purdue University will support sustainable access to, and long-term preservation of digital content deposited into PURR. The objectives of PURR as outlined in the digital preservation policy, are:

1. To collect, publish and preserve the digital data sets and associated documentation generated by researchers affiliated with Purdue or associated with Purdue's research projects.
2. To enable researchers at Purdue to satisfy the requirements of funding agencies in managing, sharing and preserving research data.
3. To provide the means for researchers, policy makers, and others to discover and access data sets generated through research done at or in conjunction with Purdue for the long term.
4. To provide a sustainable preservation environment where deposited research data are available to support the historical record of research, and accessible for use for contemporary scholarship.

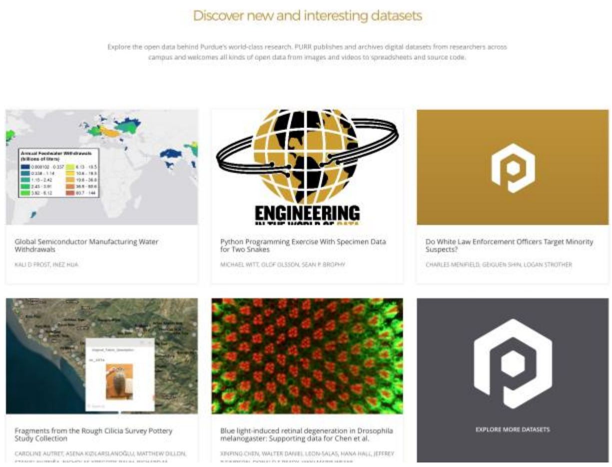

Figure 2: Examples of datasets in PURR for a variety of research domains.

PURR's Digital Preservation Policy clearly states that not all content deposited into PURR will be maintained indefinitely but rather, after ten years content will be subject to archival appraisal and Libraries' selection criteria. Content selected will be maintained as part of the Libraries existing collections. To this end, PURR identifies preservation priorities and associated levels of preservation commitment. The highest priorities are data associated with existing journal or scholarly publications followed by stand-alone data publications and data with high research or teaching value. Any preservation prioritization is contingent on sufficient funding and appropriate staffing Additional strategies and policies will be developed to support the digital preservation policy. Due to rapidly changing technical and research environments, these polices are expected to change to comply with evolving digital preservation standards and best practices.

PURR's commitment to policy-driven preservation decisions demonstrate PURR's credibility as a reliable data management and preservation program. The continued collaboration of the Libraries, Information Technology at Purdue, and Office of the Executive Vice President for Research and Partnerships demonstrate the University's commitment to creating a sustainable and stable solution for the long-term preservation and access to data. PURR acknowledges that technology, cost, custodianship, and accommodations are challenges the gateway will always face, which makes sustainability difficult. Yet, PURR is a part of the university and there are incentives to continue sustaining PURR and working towards the mission of providing the platform for Purdue University researchers to demonstrate the research taking place at the university. One incentive is that many funding agencies require data management plans, which is a service PURR provides.

PURR's preservation support policy outlines the specific preservation actions that adhere to the goals identified in PURR's Preservation Strategic Plan. PURR commits to preserving all materials at a bit-level. Bit-level preservation includes the creation of robust preservation metadata, redundant and geographically distributed backups, and normalization of files to access-friendly formats. Additionally, formats are monitored for obsolescence and some may be migrated to a more preservation-friendly or successive format, depending on environmental variables. PURR accepts all file formats, however, acknowledges that some formats are more sustainable for long-term preservation. The file format recommendations and preservation support policy identify sustainable formats and the characteristics of sustainable formats for the purpose of educating data producers and clarifying many of the challenges inherent with digital preservation [25]. These policies and procedures are currently be used and maintained by the PURR administrators.

PURR is committed to complying with the Open Archival Information System (OAIS) model and other standards and practices as they and the digital preservation community evolve. PURR is invested in the maintenance of hardware, software, and storage media that contains archival content and as such, regularly checks for vulnerabilities and file corruption. Purdue University Libraries and School of Information Studies is a member of the MetaArchive Cooperative, a peer-to-peer private Lots Of Copies Keep Stuff Safe (LOCKSS) network [26]. PURR content is replicated on distributed servers that use a system of voting and polling to ensure content does not change due to corruption.

While PURR is only a platform and service for Purdue researchers and affiliated projects, the PURR platform is managed by the HUBzero® team. Through this relationship, development requests from PURR impact the larger HUBzero® community by being added to the core HUBzero® instance.

V OneSciencePlace and Research Community Sustainability

Where nanoHUB focuses on simulations and PURR on research data products, other key aspects of science gateways that should be preserved include all of the activities undertaken by community members as they use various features of the gateway and the vibrant community of users itself. Often gateways are funded by a limited duration grant and, at the end of funding, face a difficult conundrum regarding how to continue operations or to shut down. Left alone, many gateways will not have sufficient user bases to monetize in a way significant enough to maintain robust operations (continuous security monitoring, upgrading, patching, and continuing to make the gateway on par with current technologies), and may not have third parties seeing sufficient value in a small community of users to help sustain the effort.

A significant opportunity exists, however, to facilitate the banding together of multiple small gateway projects into a larger effort that may have its own sustainability solution. Key attributes that will allow this to happen involve interoperability of the frameworks on which those gateways are constructed and continued ability to maintain those frameworks as underlying operating systems, libraries, and other supporting aspects of the compute infrastructure on which the gateways run continues to evolve. Such properties ensure that economies of scale in running multiple gateways can be exploited, and that the individual communities can be combined together into a larger community of sub-communities. The latter is of particular importance when seeking funds from parties other than the direct users of the gateways, such as university libraries, engineering departments, and philanthropists.

Since its creation, HUBzero® has operated in excess of 35 science gateways serving a wide variety of disciplines. In addition, many more gateway efforts have downloaded and used HUBzero®'s open source release. After observing many such gateways experience difficulties in sustaining operations, the HUBzero® team has undergone a code restructuring effort that affords housing multiple communities in a single operating gateway, OneSciencePlace. This gateway takes advantage of sharing resources by virtue of its implementation as a set of composable services, each of which may be scaled dynamically in a cloud environment as needed. Gateways wishing to make OneSciencePlace their sustainability plan can operate their gateway during its funded project life with the HUBzero® organization. At the end of the funding period, the gateway's branding is modified to be a sub-branded member of OneSciencePlace, and its users and content merged into OneSciencePlace.

While OneSciencePlace is not a solution for all gateways, such as those with significant audiences that can be self-sustaining, those containing confidential data, those serving private communities, and those connected to specific institutional needs, it is a model that provides the starting point of a new model of open, sustainable science where code and data are not just preserved, but continue to be live entities with which the world can interact. It also can be a second step where communities that have been incubated during their grant funded period can experience significant growth with the assurance that their online presence will not cease operation.

VI Conclusion

Achieving sustainability for a science gateway framework and its supporting team is a challenging task and successful approaches require effort on different levels from technical extensions to outreach to analyzing the needs in the science gateway landscape. We presented in this paper diverse actions taken in the HUBzero® project regarding expanding functionality of the science gateway framework, intensifying community engagement and diversifying funding. Such actions are applicable for science gateways in general. The described activities in nanoHUB, PURR, and OneSciencePlace consider specific aspects of each instance or in the community, which might be applicable for other science gateways such as checking the reliability of integrated tools. Such activities can serve as inspiration for further instances or other science gateway frameworks. We will continue to use established measures such as expanding HUBzero® on technical level and aiming at different funding sources as well as analyzing specifics of instances and commonalities in the science gateway community to extend the portfolio of actionable items for sustainability.

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