Science Gateways, Virtual Labs and Virtual Research Environments

Nancy Wilkins-Diehr[1], Michelle Barker[2], Sandra Gesing[3]

[1] San Diego Supercomputing Centre, USA, wilkinsn@sdsc.edu
[2] Nectar, Australia, michelle.barker@nectar.org.au
[3] University of Notre Dame, USA, sandra.gesing@nd.edu

EXTENDED ABSTRACT

Science gateways, virtual laboratories and virtual research environments are enabling significant contributions to many research domains, with national and international initiative further evidencing their importance and impact. This presentation explores the impact of these international programs, highlighting their successes challenges, and future focus.

Science gateways, virtual laboratories and virtual research environments all refer to community-developed digital interfaces to advanced technologies that support research. Frequently implemented as web and mobile applications, these provide integrated access to research community resources such including software, data, collaboration tools, instrumentation, and high-performance computing. The community is substantial; an American-based online survey to nearly 29,000 principal investigators, senior administrators, and people with interest in science gateways provided nearly 5,000 respondents representing diverse expertise and geography [1].

This presentation begins by highlighting the impact of significance of science gateways, virtual laboratories and virtual research environments. This can be evidenced through both case studies of successful science gateways and detailing of the range of national/international programs that facilitate their development, including:

- Science Gateways Community Institute, funded by USA's National Science Foundation, to act as a focal point to facilitate the development of a sustainable software ecosystem for science gateways,

- National eResearch Collaborative Tools and Resources (Nectar), funded by the Australian Government to facilitate the development of virtual laboratories that provide highly collaborative, research-domain oriented, integrative research software infrastructure to meet researcher-defined needs.

- VRE4EIC, a Horizon 2020 research project, provides a Europe-wide interoperable virtual research environment to empower multidisciplinary research communities through the development of enhanced virtual research environments. Sci-GaIA, another Horizon 2020 project, promotes the uptake of science gateways and e-infrastructures in Africa and beyond.

- CANARIE, a non-profit corporation, with the major investment in its programs and activities provided by the Government of Canada, leads the development in Canada of research software tools that enable researchers to more quickly and easily access research data, tools, and peers, including 32 research platforms.

Development of science gateways is increasingly complex, and communities of practice have also formed across international initiatives through global consortiums, journals and conferences. The International Coalition on Science Gateways is an international forum that brings together national initiatives to provide leadership on future directions for science gateways. The Virtual Research Environment Interest Group within the Research Data

Alliance brings together those initiatives actively developing virtual research environments, virtual laboratories and science gateways, along with representatives of common infrastructure services and the researchers seeking to make use of these technologies in an effort to identify the necessary technical aspects, governance issues and best practice required to support a more coordinated approaches to their development. Workshops focusing on science gateways have been highly successful for over ten years in USA and eight years in Europe, and the International Workshop on Science Gateways - Australia is being held for the second year in Australia. A number of conferences also now include science gateways stream, including the Hawaii International Conference on System Sciences. Initiated through the yearly workshops, yearly special issues on science gateways are organized in journals including *Concurrency and Computation* [2,3] and *Journal of Grid Computing* (current issue in print).

This presentation will then explore the challenges shared by the science gateway community. While most science gateways are developed for a specific research domain, common issues emerge in integrating tools, applications, and data collections through a tailored web-based environment. Web technologies such as HTML5, WebGL and JavaScript libraries have been never so agile and fast developing than in the last five years, leveraging possibilities to utilise applications more efficiently and more effectively with increased positive user experience on the user interface level. With diverse and constantly changing technologies available also on the backend with cloud and distributed computing and data management capabilities, development of communities of practice is essential to share best practice and avoid reinventing the wheel where possible, and aid developers to easily develop science gateways for specific user communities. Sharing of best practice enhances science on issues including reproducibility, sustainability, interfaces to cloud computing, workflows, integration of scientific instruments, success metrics, usability studies, scaling of gateways, mobile applications and security. There are an increasing number of international organisations that address some of the issues, such as the Software Sustainability Institute and Centre for Open Science, to identify best practice solutions.

With increasing acknowledgment of the critical role of software in research, the development of science gateways is crucial. A recent survey showed that 84 percent of researchers view the development as software as "important or very important for their own research" [4]. The USA's National Science Foundation's research software vision identifies software as "an integral enabler of computation, experiment and theory and a central component of the new computational infrastructure … Software is also directly responsible for increased scientific productivity and significant enhancement of researchers' capabilities" [5]. Providing platforms that enable researchers to collaborate is essential, with platforms needed at national, international and discipline levels. A world-wide collaboration can overcome such boundaries in best practices and allow for a broader view with less siloisation of solutions.

REFERENCES

1.   Lawrence, K.A., M. Zentner, N. Wilkins-Diehr, J.A Wernert, M. Pierce and S.M. Marru, Science gateways today and tomorrow: Positive perspectives of nearly 5,000 members of the research community. Concurrency and Computation: Practice and Experience, 2015, 27(16): p 4252-5268. DOI: 10.1002/cpe.3526.

2. Gesing, S. and Wilkins-Diehr, N., Science gateway workshops 2014 special issue conference publications. Concurrency and Computation: Practice and Experience, 2015, 27: p 4247–4251. DOI: 10.1002/cpe.3615.

3. Wilkins-Diehr N., S. Gesing and T. Kiss, Science gateway workshops 2013 special issue conference publications, Concurrency and Computation: Practice and Experience, 2014: p 253–257. DOI: 10.1002/cpe.3362.

4.   J.E. Hannay, J.E., C. MacLeod, J. Singer, H.P. Langtangen, D. Pfahl and G. Wilson, How Do Scientists Develop and Use Scientific Software. Proceedings of 2009 ICSE Workshop on Software Engineering for Computational Science and Engineering, IEEE CS, 2009, p. 1–8. DOI: 10.1109/SECSE.2009.5069155.

5. National Science Foundation, Implementation of NSF CIF21 Software Vision. http://www.nsf.gov/funding/pgm_summ.jsp?pims_id=504817.

ABOUT THE AUTHOR(S)

Nancy Wilkins-Diehr is Associate Director at San Diego Supercomputer Centre and co-director of XSEDE's Extended Collaborative Support program. She has been involved in science gateways and their interfaces to high-performance computing since 2005 and is the Principal Investigator on the NSF-funded Science Gateways Community Institute. Nancy received her Bachelor's degree from Boston College in Mathematics and Philosophy and her Master's degree in Aerospace Engineering from San Diego State University.

Michelle Barker is Deputy Director (Research Software Infrastructure) at National eResearch Collaborative Tools and Resources (Nectar), a National Collaborative Research Infrastructure Strategy (NCRIS) funded program. She is one of the convenors of the annual International Workshop on Science Gateways - Australia, and the International Coalition on Science Gateways. As Deputy Director at Nectar, Michelle directs the virtual laboratory program, which has facilitated the development of twelve virtual laboratories in diverse disciplines, with over 10,000 users. In this role she also facilitates national conversations around common challenges such as research reproducibility, software sustainability and impact metrics. She was previously Program Director of a science gateway for the malaria community, based at James Cook University. She has a Ph.D in sociology and a Masters of Business Administration..

Sandra Gesing is a research assistant professor at the University of Notre Dame, USA. Her research interests include science gateways, especially for bioinformatics applications, workflows and distributed and parallel computing. In this context, she also works on analysis frameworks for modeling and simulations. She is heavily involved in the US Science Gateway Community Institute, where her role focuses on outreach and community engagement. Sandra is also founder of the successful European workshop series IWSG (International Workshop on Science Gateways). The significance of science gateways has been also recognized by IEEE and she chairs and coordinates the IEEE technical area on science gateways. Prior to her current position at Notre Dame, Sandra was a research associate in the Data-Intensive Research Group at the University of Edinburgh, UK, and in the Applied Bioinformatics Group at the University of Tübingen, Germany. Additionally, she has perennial experience as a project manager and system developer in industry. As head of a system programmer group, she has led long-term software projects (e.g. infrastructure on web-based applications). She received her German diploma in computer science from extramural studies at the FernUniversität Hagen and her PhD in computer science from the University of Tübingen, Germany.