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Preview of Award 1440677 - Annual Project Report

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Cover

Federal Agency and Organization Element to Which Report is Submitted:	4900
Federal Grant or Other Identifying Number Assigned by Agency:	1440677
Project Title:	SI2-SSE: RADICAL Cybertools: Scalable, Interoperable and Sustainable Tools for Science
PD/PI Name:	Shantenu Jha, Principal Investigator
Recipient Organization:	Rutgers University New Brunswick
Project/Grant Period:	01/01/2015 - 12/31/2017
Reporting Period:	01/01/2015 - 12/31/2015
Submitting Official (if other than PD\PI):	Shantenu Jha Principal Investigator
Submission Date:	01/11/2016
Signature of Submitting Official (signature shall be submitted in accordance with agency specific instructions)	Shantenu Jha

Accomplishments

* What are the major goals of the project?

The computing infrastructure for science and engineering has historically been a necessary adjunct to the core domain science goals. This has resulted in computing infrastructure that is characterized by singular, inflexible and arguably inefficient solutions. There are many reasons for this state-of-play. One important reason is the way we develop our tools, middleware and software and hardware infrastructure that in turn defines the "platforms" on which computational aspects of science and engineering is conducted.

It can be argued that current approaches to developing the platform as a whole, but definitely the tools are devoid of

satisfactory and suitable abstractions and design principles. Most software development for tools and middleware represents local solutions (which conflates "correct solution" for working solution"), does not conform to or promote the many *ity (scalability, extensibility, interoperability etc.) and are often with implemented with careful systems engineering principles. As such much of the software development underpinning the platforms is not sustainable.

Against this backdrop, we proposed RADICAL-Cybertools --- a set of building blocks each of which captures well-defined requirements and abstractions and adhere to systems and software engineering principles alike. Where meaningful, RADICAL-Cybertools also conforms to community standards (such as the Open Grid Forum). RADICAL-Cybertools also attempts to foster informal community consensus where suitable forums do not exist. SAGA and Pilot-Jobs are examples of the former and latter respectively.

The goals of this project are to implement, enhance and sustain RADICAL-Cybertools, as both an enabler of science and engineering on NSF's production computing platforms, as well as an exemplar of abstractions-driven and standards-based tools. Specifically, RADICAL-Cybertools will bring new users to XSEDE and OGF, as well improve the usability of these platforms.

*** What was accomplished under these goals (you must provide information for at least one of the 4 categories below)?**

- Major Activities:
- In the first year of the RADICAL-Cybertools project, we focussed on improving software development process, enhancing implementaion and new functionality, and reaching out to new/existing users to capture requirements.
 - As the github project page for RADICAL-Pilot shows (<https://github.com/radical-cybertools/radical.pilot>) there have been 770 tickets opened for RADICAL Pilot. Of these 600 tickets have been closed and 170 approximately remain in progress.
 - As the github project page for RADICAL-SAGA shows (<https://github.com/radical-cybertools/saga-python/issues>) there have been approximately 440 tickets open for RADICAL-SAGA. Of the 360 have been closed and 80 remain open.
 - RADICAL-Cybertools was instrumental in running a tutorial at SC'15 (Austin). Details of the tutorail can be found at: <http://sc15.radical-cybertools.org>
 - RADICAL-Cybertools was also central to a two day workshop on "High Performance and Distributed Computing" as part of a larger two week workshop on "Macromolecular simulation software workshop" (Please see: <http://www.cecarn.org/workshop-0-1214.html>).
- Specific Objectives:
- Significant Results:
- Whereas the primary products of this project is community software, we also wrote three papers on RADICAL-Cybertools to help capture the design principles, systems engineering and abstractions underlying RADICAL-Cybertools.
 - "SAGA - A standardized access layer to heterogeneous Distributed Computing Infrastructure"([doi:10.1016/j.softx.2015.03.001](https://doi.org/10.1016/j.softx.2015.03.001)) was published in the inaugural issue of the software journal -- "Software X" has been downloaded several thousands times (5100 and counting) in under 6 months! Please see: <http://www.sciencedirect.com/science/article/pii/S2352711015000023>
 - We strongly believe that software publications and tracking needs improvement as much as software development. Thus, of the many possible venues where we could have published, we chose Software X as the right venue given its adoption of good software evaluation metrics.
 - Very advanced draft of two papers. One a review paper of Pilot Systems and the other a preliminary paper on the design and some implementation of RADICAL-pilot have also been written.

The former, "A Comprehensive Perspective on the Pilot-Job Systems", by Matteo Turilli, Mark Santcroos, Shantenu Jha can be found at <http://arxiv.org/abs/1508.04180>

The paper "RADICAL-Pilot: Scalable Execution of Heterogeneous and Dynamic Workloads on Supercomputers" is under review for the International Supercomputing Conference (ISC'2106) and can be found at: <http://arxiv.org/abs/1512.08194>

Key outcomes or

Other achievements:

Other achievements: In addition to the core development and improvement (of code base and process), the publications and training, we also engaged with XSEDE's ECSS team to help address the perpetual and recurring confusion/challenges associated with "Workflows" (and whatever that might mean in the context!). To this end, we collaborated with the XSEDE Workflows team to help develop tutorials and material to help users get their "workflows" kick-started on XSEDE. These efforts are documented at:

<https://sites.google.com/site/xsedeworkflows/>

<https://portal.xsede.org/user-news/-/news/item/7333>

*** What opportunities for training and professional development has the project provided?**

RADICAL-Cybertools are important community tools used by hundreds of scientists including students for their research.

RADICAL-Cybertools is also used by dozens of MS students (at Rutgers University, Edinburgh, ASU to name just a few) for their projects and thesis.

Thus, RADICAL-Cybertools is a vehicle for both research as well as training & teaching opportunities.

*** How have the results been disseminated to communities of interest?**

Through a mix of publications, tutorials and other outreach venues such as mailing lists. Please see details in subsequent sections.

*** What do you plan to do during the next reporting period to accomplish the goals?**

The internal project is designed around (i) functional improvements, (ii) performance and scalability issues, and (iii) Usability aspects.

Each of these three will be receiving attention in the next reporting period. In addition, we will continue to engage in community activity -- training and outreach, but also consolidation of software and development activity.

Products

Books

Book Chapters

Inventions

Journals or Juried Conference Papers

Andre Merzky, Ole Weidner, Shantenu Jha (2015). SAGA: A standardized access layer to heterogeneous Distributed Computing Infrastructure. *SoftwareX*. 1-2 (1), Page 3-8. Status = ACCEPTED; Acknowledgment of Federal Support = Yes ; Peer Reviewed = Yes ; DOI: 10.1016/j.softx.2015.03.001

Licenses

Other Conference Presentations / Papers

Andre Merzky, Mark Santcroos, Matteo Turilli and Shantenu Jha (2016). *RADICAL-Pilot: Scalable Execution of Heterogeneous and Dynamic Workloads on Supercomputers*. International Supercomputing Conference (ISC) 2016 Available at: <http://arxiv.org/abs/1512.08194>. Germany. Status = UNDER_REVIEW; Acknowledgement of Federal Support = Yes

Other Products

Software or Netware.

Please see: <https://github.com/radical-cybertools>

which consists of both production codes:

- RADICAL-SAGA <https://github.com/radical-cybertools/saga-python>

and

- RADICAL-Pilot <https://github.com/radical-cybertools/radical.pilot>

RADICAL-Cybertools also contains "experimental" ideas, which will either become new RADICAL-Cybertools, or parts of the existing cybertools.

Other Publications

Patents

Technologies or Techniques

Thesis/Dissertations

Websites

Participants/Organizations

What individuals have worked on the project?

Name	Most Senior Project Role	Nearest Person Month Worked
Jha, Shantenu	PD/PI	2
Merzly, Andre	Other Professional	6
Santcroos, Mark	Other Professional	3
Turilli, Matteo	Staff Scientist (doctoral level)	1

Full details of individuals who have worked on the project:

Shantenu Jha

Email: shantenu.jha@rutgers.edu

Most Senior Project Role: PD/PI

Nearest Person Month Worked: 2

Contribution to the Project: Technical leadership, publications, outreach and engagement.

Funding Support: NSF and funding as Rutgers Faculty/Academic.

International Collaboration: No

International Travel: No

Andre Merzly

Email: andre@merzky.net

Most Senior Project Role: Other Professional

Nearest Person Month Worked: 6

Contribution to the Project: Core development, software engineering process.

Funding Support: NSF

International Collaboration: No

International Travel: No

Mark Santcroos

Email: mark.santcroos@rutgers.edu

Most Senior Project Role: Other Professional

Nearest Person Month Worked: 3

Contribution to the Project: Development, performance analysis and optimization and code review.

Funding Support: NSF and internal Rutgers (fellowship) awards.

International Collaboration: No

International Travel: No

Matteo Turilli

Email: matteo.turilli@gmail.com

Most Senior Project Role: Staff Scientist (doctoral level)

Nearest Person Month Worked: 1

Contribution to the Project: Design and analysis of RADICAL-Pilot

Funding Support: NSF, DOE and internal Rutgers project money.

International Collaboration: No

International Travel: No

What other organizations have been involved as partners?

Nothing to report.

What other collaborators or contacts have been involved?

RADICAL-Cybertools benefits from contributions from the "community". The community transcends the traditional definition of an institution, and includes projects, people (both in their individual and professional capacity). Some examples include, but are not limited to; (i) Jeremy Cohen (Imperial College London), (ii) Andrey Khmlevskiy and Anna Kostikova (Technical University, Vienna, Austria), and (iii) Mehdi Sadeghi (Germany), and (iv) Philip Fowler (Oxford University). A full listing can be found on the mailing lists:

(i) <https://groups.google.com/forum/#!forum/saga-users>

and

(ii) <https://groups.google.com/forum/#!forum/radical-pilot-users>

Impacts

What is the impact on the development of the principal discipline(s) of the project?

The ongoing validation of the systems and software engineering approach to building abstractions-driven and standards-based tools and middleware for distributed computing platforms.

What is the impact on other disciplines?

Some scientific domains that use RADICAL-Cybertools include, Climate Science, Molecular Science, Mathematics, Bioinformatics, High-energy physics.

What is the impact on the development of human resources?

Nothing to report.

What is the impact on physical resources that form infrastructure?

RADICAL-Cybertools is widely used on NSF production infrastructure such as XSEDE and OSG. They provide simple, scalable and sustainable approaches to the development of the software ecosystem on this infrastructure, as well as campus infrastructures.

What is the impact on institutional resources that form infrastructure?

Nothing to report.

What is the impact on information resources that form infrastructure?

Nothing to report.

What is the impact on technology transfer?

Nothing to report.

What is the impact on society beyond science and technology?

Nothing to report.

Changes/Problems

Changes in approach and reason for change

No fundamental changes. The project has been very vibrant and has benefited from significant community engagement and feedback, as well as synergy with ongoing projects. We have to be careful in direct engagement with end-users due to the time commitments.

Actual or Anticipated problems or delays and actions or plans to resolve them

Nothing to report.

Changes that have a significant impact on expenditures

Thanks to Mark Santcroos being awarded a fellowship (Rutgers), we have spent less than expected in PY1.

Significant changes in use or care of human subjects

Nothing to report.

Significant changes in use or care of vertebrate animals

Nothing to report.

Significant changes in use or care of biohazards

Nothing to report.