Extended Collaborative Support Service (ECSS): Impact and Lessons Learned

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XSEDE

Extreme Science and Engineering Discovery Environment

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Impact and Lessons Learned

This is an abbreviated version of the talk that will (hopefully) be presented at PEARC20 (assuming paper was accepted)

XSEDE Extended Collaborative Support Service (ECSS): Impact and Lessons Learned

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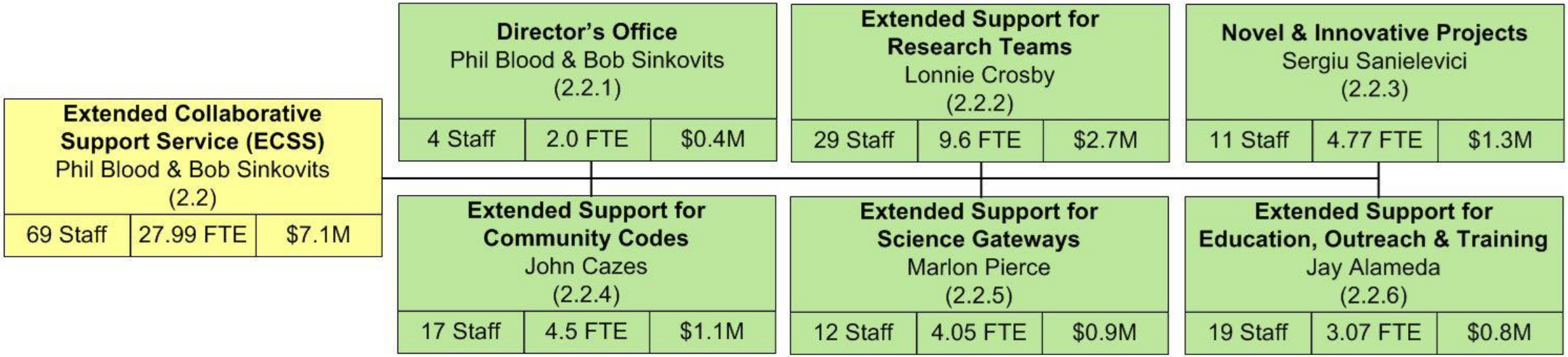
Extended Collaborative Support Services (ECSS)

The Extended Collaborative Support Service **improves the productivity** of the XSEDE user community through successful, **meaningful collaborations** to optimize their applications, improve their work and data flows, and **increase their effective use** of the XSEDE digital infrastructure and broadly expands the XSEDE user base by engaging **members of underrepresented communities and domain areas**



Impact (start of record keeping in parentheses)

- 184 ECSS projects (September 2016)
- 80 ECSS Symposia (Nov 2011)
- 2,098 Symposium attendees (July 2014)
- 37 Campus Champion Fellows (August 2012)
- 2,237 Adaptive reviews (December 2014)
- 841 Educational proposals reviewed (July 2014)
- 190 NIP engagements (September 2016)
- 391 Training Events (July 2011)

Lesson 1: Start with a work plan

A well thought out work plan ensures that ECSS experts address the correct problems and avoids mission creep

	Milestone (JIRA Issue)	Success Metric	Effort	Timeline
1	Develop an efficient numerical algorithm and corresponding multigrid solver for diffusive interface approximation for 3D graphene model. ECSS3-2675 OPEN	Simulation match the expectation of model proposed in NSF FRG.	intensive	Estimated completion: Completed Nov 2016.
2	Convert the parallel multigrid solver tested in TG-DMR140030 to MPI-OpenMP hybrid structure and Implement P3DFFT. ECSS3-2676 OPEN	The refactored application is deployed on Comet or Stampede and tested for various grid sizes. The results match those of previous versions.	intensive effort on converting the code to MPI-OpenMP hybrid structure and implement P3DFFT	Estimated completion: Completed Dec 15, 2016.
3	Implement efficient parallel input/output. ECSS3-2677 OPEN	The new output is consistent with previous output. It is easy to post process and improve the performance of the code. Some work related to parallel3DFFT is completed but other paprallel IO optimizations would be looked at during the extension.	Moderate	Estimated completion: Mar, 31, 2017

Lesson 2: End with a PI interview

The PI exit interview is an opportunity to collect valuable feedback and determine effectiveness of ECSS. Also allows closure for the project.

1. How did you hear about the ECSS program?

Learned about ECSS on XSEDE website

2. How was your working relationship with ECSS staff? Was the staff member knowledgeable? courteous? Were there any difficulties (attitude, language, anything else)?

Amanda was a pleasure to work with. Her knowledge of parallel programming was outstanding and she helped us through a bottleneck we had struggled with for many years. No serious difficulties once we were able to understand the scientific goals and we got up to speed on computing.

3. Was the effort in developing the workplan worthwhile? Did it set expectations appropriately?

Absolutely! The scope of the project is rather ambitious and the work plan helped us to focus on the most critical elements of our computing.

4. Can you quantify the contribution of the ECSS support- e.g. by saying by how much the code was improved, or any other measure you have?

Lesson 3: Projects must be true collaborations

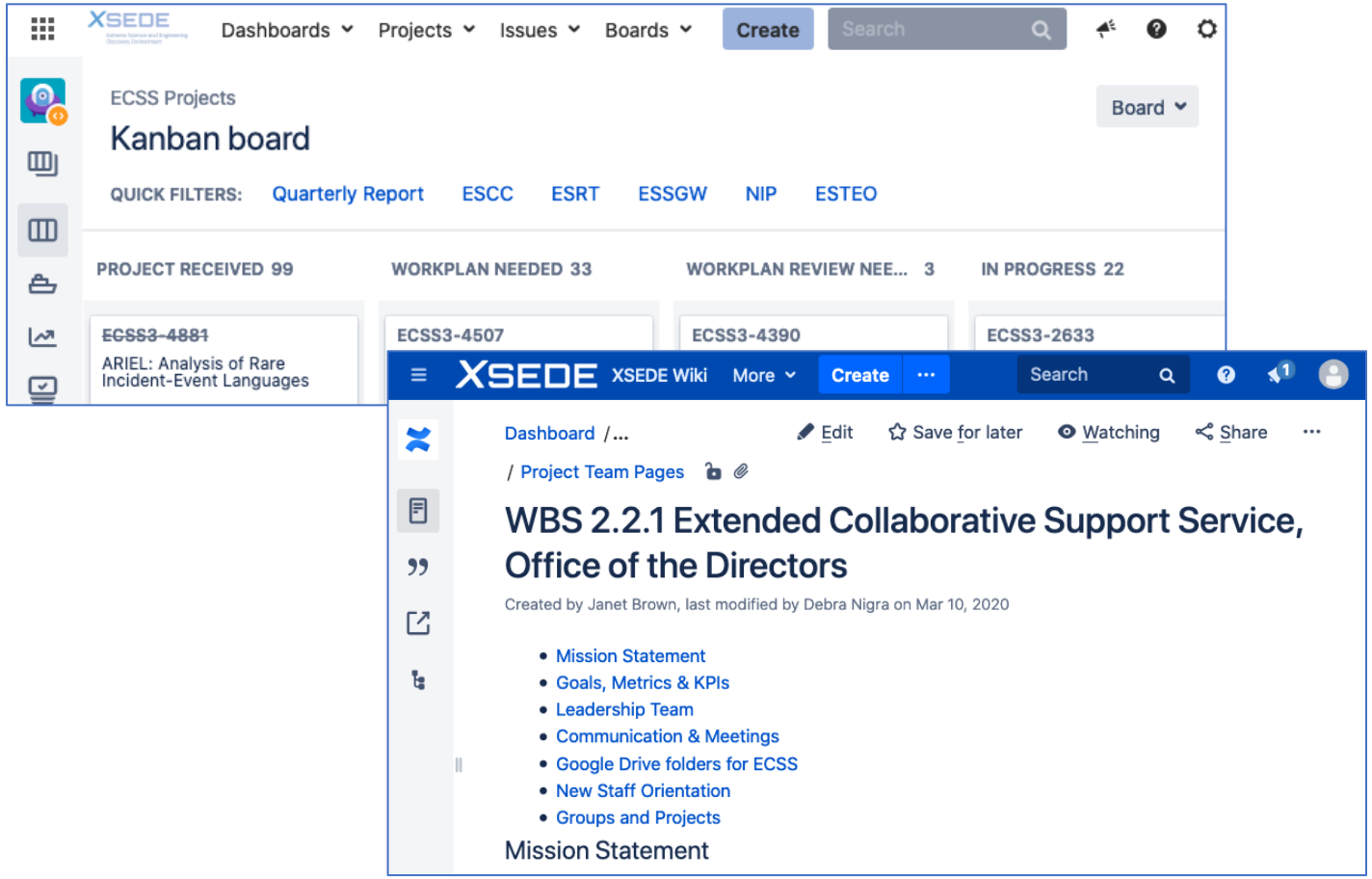
- The ECSS projects are most effective when they are true collaborations between the PI's lab and the ECSS experts
- Only the PI's team has the necessary expertise to set priorities, provide appropriate test problems and data sets, answer questions about reproducibility (e.g. for floating point codes, how close is good enough)
- Ultimate goal of any collaboration is knowledge transfer, which is impossible if the PI's team is not engaged.

Lesson 4: Establish a critical mass of ECSS staff

- ECSS is mandated to work with XSEDE users from all research domains
- At any given time, the XSEDE service providers deploy systems spanning multiple generations of CPUs, GPUs, networks and storage systems in addition to novel resources such as the *Jetstream* cloud resource
- Given the broad scope, ECSS can achieve it's mission only by having a large pool of talent to draw upon

Lesson 5 & 6: Rigorous project management is essential, Modern project management tools increase productivity

Given the scope of ECSS (full projects, short term engagements, training, mentoring, etc.) and large number of staff, rigorous project management is essential to keep things functioning smoothly

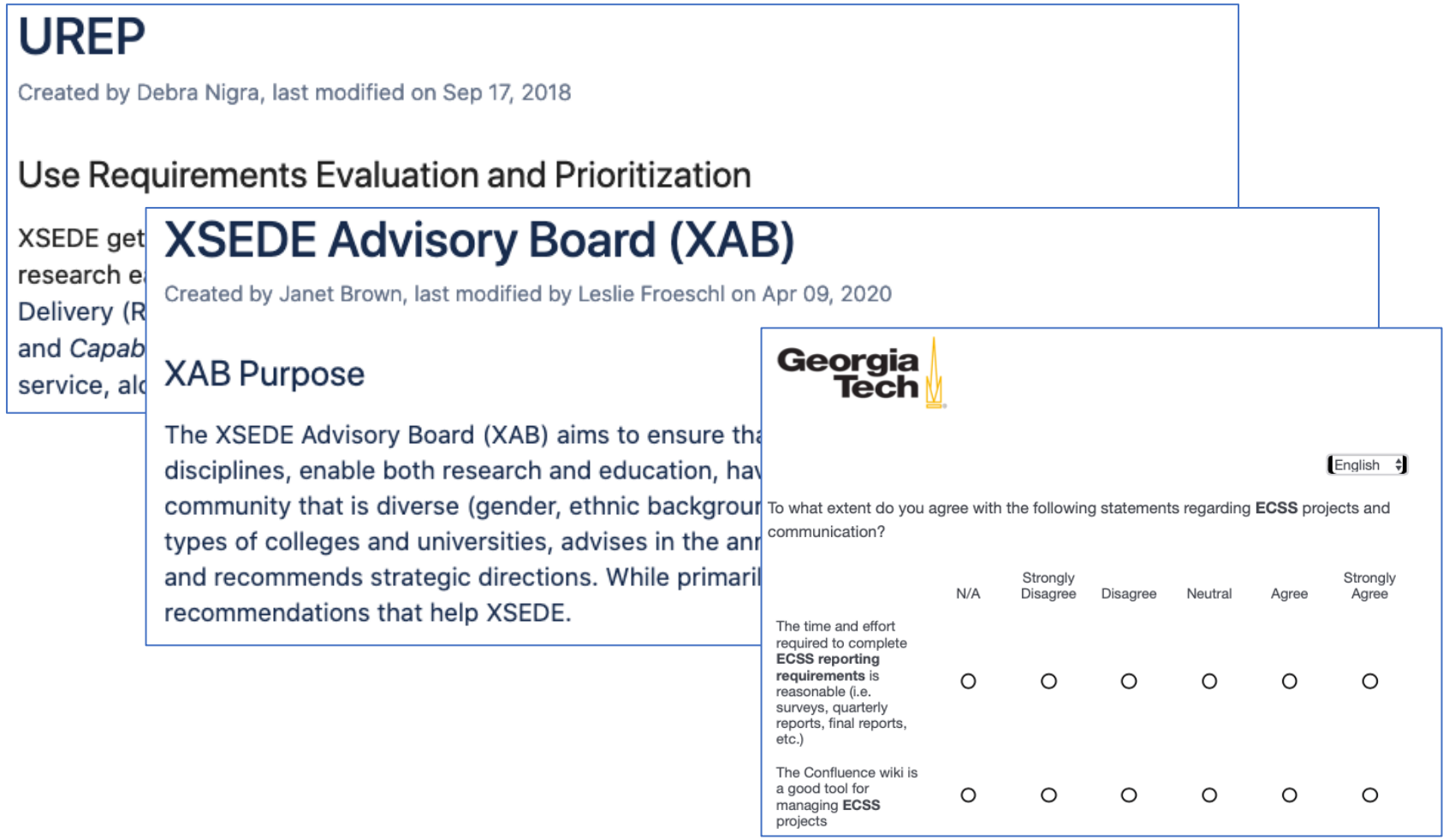


Lesson 7: Involve ECSS in allocations process

- ECSS provides a service to XSEDE by reviewing a subset of the allocations proposals submitted each quarter (recall that ECSS has completed > 2,000 reviews to date)
- Staff are ideally suited to identifying projects that can benefit from engagement with ECSS
- Staff can improve the allocations process and have recently developed training materials to help XSEDE PIs write better proposals

Lesson 8: Look for feedback from without and within

A significant risk for any project is that the participants may become so invested in the project or work so closely together that they fail to see what is obvious to outside observers



UREP

Created by Debra Nigra, last modified on Sep 17, 2018

Use Requirements Evaluation and Prioritization

XSEDE get
research e
Delivery (R
and *Capab*
service, alc

XSEDE Advisory Board (XAB)

Created by Janet Brown, last modified by Leslie Froeschl on Apr 09, 2020

XAB Purpose

The XSEDE Advisory Board (XAB) aims to ensure tha
disciplines, enable both research and education, hav
community that is diverse (gender, ethnic backgrour
types of colleges and universities, advises in the anr
and recommends strategic directions. While primaril
recommendations that help XSEDE.

Georgia Tech

English

To what extent do you agree with the following statements regarding **ECSS** projects and communication?

	N/A	Strongly Disagree	Disagree	Neutral	Agree	Strongly Agree
The time and effort required to complete **ECSS reporting requirements** is reasonable (i.e. surveys, quarterly reports, final reports, etc.)	○	○	○	○	○	○
The Confluence wiki is a good tool for managing **ECSS** projects	○	○	○	○	○	○

Lesson 9: Collaborate with organization facing similar challenges

ECSS is not alone in facing challenges associated with knowledge transfer, scalability, mission creep, project management and supporting a broad community of users. Working with others gives us the chance to see how they deal with issues

CaRCC
Campus Research Computing Consortium

US RSE
US RESEARCH SOFTWARE ENGINEER ASSOCIATION

NSF XSEDE

Lesson 10: Prioritize knowledge capture and dissemination

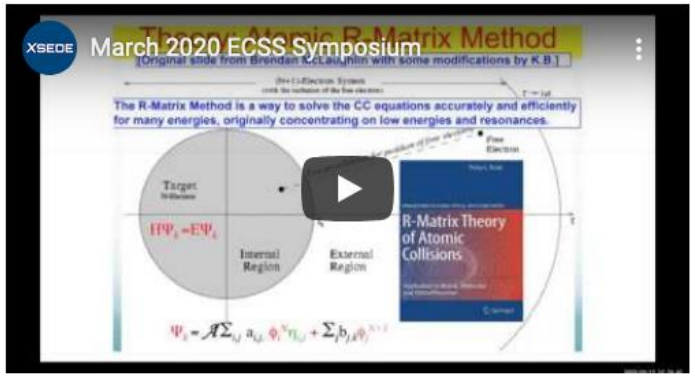
Knowledge lost can be gone forever. Make a concerted effort to capture through technical reports, symposia and other channels

March 17, 2020

AMP Gateway: An portal for atomic, molecular and optical physics simulations.

Presenter(s): Sudhakar Pamidighantam **(Indiana University)**

Presentation Slides



We describe the creation of a new Atomic and Molecular Physics science gateway (AMPGateway). The gateway is designed to bring together a subset of the AMP community to work collectively to make their software suites available and easier to use by the partners as well as others. By necessity, a project such as this requires the developers to work on issues of portability, documentation, ease of input, as well as making sure the codes can run on a variety of architectures. The gateway was built using Apache Airavata gate
the Airavata PHP client on the web but has since been redeploye
organization and facility of the Django deployment and how it ha

Bursting into the public Cloud – Sharing my experience doing

Presenter(s): Igor Sfiligoi **(SDSC)**

Presentation Slides

When compute workflow needs spike well in excess of the capac
temporarily provisioned from somewhere else to both meet dead
become an attractive option due to their ability to be provisioned
IceCube expand their resource pool by a few orders of magnitud
PFLOP32s for a whole workday. In the process we moved O(50 T

Optimization and parallelization of a time series classification algorithm

Robert S. Sinkovits

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Abstract **– This technical report describes the steps taken to optimize and parallelize a time series classification algorithm as part of an Extended Collaborative Support Services (ECSS) project with XSEDE researcher Ramon Huerta at the University of California, San Diego. Switching from the GNU compiler to the Intel compiler and enabling Advanced Vector Extensions (AVX) resulted in a 2x speedup, while linking to the Intel Math Kernel Library (MKL) instead of the default LAPACK**

For background and completeness, the PI statement for the ECSS project is reproduced below. This has been very lightly edited for clarity and can be skipped for readers who are only interested in the technical details of optimization and parallelization.

PI statement: We have developed classification calibrated algorithms that are faster to train than regular support vector machines. The trick that we discovered by exploring a

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Lesson 11: It's easy to fall behind

- Cyberinfrastructure was never easy, but in one sense it was easier 25 years ago since there was a more limited set of things you had to know. Could get by with knowledge of C, Fortran and MPI.
- There has since been an explosion of languages, libraries, accelerators, modes of computing, containerization, virtualization, etc.
- Providing staff with training and educational opportunities is essential along with hiring staff who bring new knowledge and perspective.

Acknowledgements

This work was supported by NSF award OAC 1548562 XSEDE 2.0: Integrating, Enabling and Enhancing National Cyberinfrastructure with Expanding Community Involvement. The authors thank the more than 100 ECSS staff who have made valuable contributions over the years. Without their hard work and expertise, ECSS could not have possibly been successful. We also express our gratitude to our XSEDE colleagues outside of ECSS. Special thanks to Ken Hackworth (PSC) for providing statistics on adaptive reviews. Finally, we thank everyone who served on our advisory boards, review panels and forums for your valuable input.