XSEDE:
The Extreme Science and Engineering Discovery Environment

(OAC 15-48562)

Interim Project Report 13:

Report Year 5, Reporting Period 2

August 1, 2020 – October 31, 2020

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Reading this Report

This report is the result of an ongoing process of improving reporting on the progress in delivering on our mission and realizing our goals thus communicating the value XSEDE brings towards enhancing the productivity of a growing community of scholars, researchers, and engineers. For a large, complex, highly-distributed project such as XSEDE, this is a considerable undertaking. This process has helped XSEDE improve as an organization and as a provider and broker of services to the compute- and data-enabled science and engineering research and education community.

XSEDE reports on its activities and progress by using a metrics-based approach. Based on feedback from our review panels, advisory bodies, the NSF, and other stakeholders, we have defined KPIs (Key Performance Indicators) that measure progress toward our high-level strategic goals.

The key concept is not that the metrics [KPIs] themselves have a direct causal effect on eventual outcomes, but rather that the metrics are chosen so that actions and decisions which move the metrics in the desired direction also move the organization in the direction of the desired outcomes and goals.

KPIs at the project and Work Breakdown Structure Level 2 areas are intended to focus the attention of external stakeholders on what we believe to be the best (key) indicators of progress toward our long-term strategic goals.

The Executive Summary (§1) is intended to effectively and concisely communicate the status of the project toward delivery of the mission and realization of the vision by reaching three strategic goals. Stoplight indicators (§1.1) are used to visually provide a quick understanding of our assessment of overall project progress with respect to the strategic goals in light of our KPIs.

The Science, Engineering, & Program Highlights (§2) provide a small selection in a series of scientific and engineering research and education successes XSEDE has enabled. These successes are an ongoing testament to the importance of our services to the research community.

The Discussion of Strategic Goals and Key Performance Indicators (§3) provides the next level of detail in understanding project progress. It decomposes the strategic goals into subgoals and discusses progress toward each of the sub-goals using KPIs that, where possible, represent measures of impact to the communities XSEDE supports.

These first three sections take a project-wide view. A more detailed analysis of progress from the view of the areas responsible for supporting each of the sub-goals—and contributing toward the KPIs associated with those sub-goals—is provided by looking at each of the areas of the project in the remaining sections (§4, §5, §6, §7, §8, §9). These sections also contain area highlights and Key Performance Indicators (KPIs) that are deemed important, along with links to corresponding sections of the XSEDE KPIs & Metrics wiki page. The metric tables on the wiki page contain definitions, descriptions, and collection methodology information about each metric in the tables. When a new metric is added, table cells from previous reporting periods will contain an asterisk (*) to designate that data for that metric was not being collected or reported at that time. Prior to the RY2 Annual Report we have reported on metrics at the Work Breakdown Structure Level 3. Based on feedback from reviewers and discussion with the Cognizant Program Officer, we have discontinued this to reduce duplication and improve readability of the document.

Note that XSEDE Project Years (PY) run September-August and Report Years (RY) run May-April. The table below lists the schedule for Reporting Periods (RP) within each RY, including RY1 and RY6 which are slightly altered due to a shorter RY1 and a longer RY6.

	RP1	RP2	RP3	RP4 (Included in Annual Report)
Typical Schedule	May 1- July 31	Aug. 1- Oct. 31	Nov. 1- Jan. 31	Feb. 1- Apr. 30
RY1 **Sept. 2016-April 2017**	Period doesn't exist due to shortened first year.	Sept. 1- Oct. 31, 2016 (Abbreviated due to shortened year)	Nov. 1, 2016- Jan. 31, 2017	Feb. 1- Apr. 30, 2017 (Included in Annual Report)
RY2 **May 2017-April 2018**	May 1- July 31, 2017	Aug. 1- Oct. 31, 2017	Nov. 1, 2017- Jan. 31, 2018	Feb. 1- Apr. 30, 2018 (Included in Annual Report)
RY3 **May 2018-April 2019**	May 1- July 31, 2018	Aug. 1- Oct. 31, 2018	Nov. 1, 2018- Jan. 31, 2019	Feb. 1- Apr. 30, 2019 (Included in Annual Report)
RY4 **May 2019-April 2020**	May 1- July 31, 2019	Aug. 1- Oct. 31, 2019	Nov. 1, 2019- Jan. 31, 2020	Feb. 1- Apr. 30, 2020 (Included in Annual Report)
RY5 **May 2020-April 2021**	May 1- July 31, 2020	Aug. 1- Oct. 31, 2020	Nov. 1, 2020- Jan. 31, 2021	Feb. 1- Apr. 30, 2021 (Included in Annual Report)
RY6 **May 2021-August 2022**	May 1- July 31, 2021	Aug. 1- Oct. 31, 2021	Nov. 1, 2021- Jan. 31, 2022	Feb. 1- Aug. 31, 2022 (Longer period included in Final Report)

It is anticipated that this report is read in electronic form (PDF) using Adobe Reader®. There is extensive cross-linking to facilitate referencing content across the document. In general, all text that has blue underlining (e.g., §2) is clickable. Clicking on the underlined text will take you to the referenced section. These are set up to facilitate moving back and forth between the high level discussions in §1 and §3, to more detailed discussions regarding specific project areas and financial information in §4, §5, §6, §7, §8, §9.

As noted, this represents an ongoing effort at improvement, and we welcome comments on how to improve any and all aspects of our reporting process.

At the beginning of the XSEDE project, a Project Execution Plan (PEP) was submitted to and approved by NSF. Content in this and all preceding Interim Project and Annual Reports

supersede information submitted in the original PEP. The most recent version of the PEP can be viewed in Appendix 18 of this report and on the wiki.[1]

[1] https://confluence.xsede.org/display/XT/XSEDE+Project+Execution+Plan

1. Executive Summary

Computing across all fields of scholarship is becoming ubiquitous. Digital technologies underpin, accelerate, and enable new, even transformational, research in all domains. Researchers continue to integrate an increasingly diverse set of distributed resources and instruments directly into their research and educational pursuits. Access to an array of integrated and well-supported high-end digital services is critical for the advancement of knowledge. XSEDE (Extreme Science and Engineering Discovery Environment) is a socio-technical platform that integrates and coordinates advanced digital services within the national ecosystem to support contemporary science. This ecosystem involves a highly distributed, yet integrated and coordinated, assemblage of software, supercomputers, visualization systems, storage systems, networks, portals, gateways, collections of data, instruments, and personnel with specific expertise. XSEDE supports the need for an advanced digital services ecosystem distributed beyond the scope of a single institution and provides a long-term platform to empower modern science and engineering research and education. As a significant contributor to this ecosystem, driven by the needs of the open research community, XSEDE substantially enhances the productivity of a growing community of scholars, researchers, and engineers. XSEDE federates with other high-end facilities and campus-based resources, serving as the foundation for a national e-science infrastructure with tremendous potential for enabling new advancements in research and education. *Our vision is a world of digitally-enabled scholars, researchers, and engineers participating in multidisciplinary collaborations while seamlessly accessing computing resources and sharing data to tackle society's grand challenges*.

Researchers use advanced digital resources and services every day to expand their understanding of our world. More pointedly, research now requires more than just supercomputers, and XSEDE represents a step toward a more comprehensive and cohesive set of advanced digital services through our mission: *to substantially enhance the productivity of a growing community of scholars, researchers, and engineers through access to advanced digital services that support open research; and to coordinate and add significant value to the leading cyberinfrastructure resources funded by the NSF and other agencies*. XSEDE has developed its strategic goals in a manner consistent with NSF's strategic plan, *Building the Future: Investing in Discovery and Innovation - NSF Strategic Plan for Fiscal Years (FY) 2018 - 2022*[2], NSF's strategies stated broadly in the *Cyberinfrastructure Framework for 21st Century Science and Engineering*[3] vision document, and the more specifically relevant *Advanced Computing Infrastructure: Vision and Strategic Plan*[4] document. Though the latter two documents are now out of date for the NSF, in the absence of documents that supplant them, XSEDE continues to use them for general guidance until such time as successor documents are released. It should be noted here that three draft documents under the collective heading of *Transforming Science Through Cyberinfrastructure: NSF's Blueprint for a National Cyberinfrastructure Ecosystem for Science and Engineering in the 21st Century*, distributed by NSF's Office Director for the Office of Advanced Cyberinfrastructure, are currently available for public comment[5].

1.1. Strategic Goals

To support our mission and to guide the project's activities toward the realization of our vision, three strategic goals are defined:

[2] https://www.nsf.gov/pubs/2018/nsf18045/nsf18045.pdf
[3] https://www.nsf.gov/cise/oac/cif21/CIF21Vision2012current.pdf
[4] https://www.nsf.gov/publications/pub_summ.jsp?ods_key=nsf12051
[5] https://www.nsf.gov/cise/oac/vision/blueprint-2019/

Deepen and Extend Use: XSEDE will *deepen the use—make more effective use*—of the advanced digital services ecosystem by existing scholars, researchers, and engineers, and extend the use to new communities. We will contribute to preparation—workforce development—of the current and next generation of scholars, researchers, and engineers in the use of advanced digital services via training, education, and outreach; and we will *raise the general awareness of the value of advanced digital services*.

Advance the Ecosystem: Exploiting its internal efforts and drawing on those of others, XSEDE will advance the broader ecosystem of advanced digital services by *creating an open and evolving e-infrastructure*, and by *enhancing the array of technical expertise and support services* offered.

Sustain the Ecosystem: XSEDE will sustain the advanced digital services ecosystem by *ensuring and maintaining a reliable, efficient, and secure infrastructure*, and *providing excellent user support services*. XSEDE will further *operate an effective, productive, and innovative virtual organization*.

The strategic goals of XSEDE cover a considerable scope. To ensure XSEDE is delivering on its mission and to assess progress toward its vision, XSEDE has identified key metrics to measure its progress toward meeting sub-goals of each of the strategic goals. These Key Performance Indicators (KPIs) are a high-level encapsulation of XSEDE's project metrics that measure how well each sub-goal is met. Planning is driven by XSEDE's vision, mission, goals, and these metrics—which are in turn rooted in the needs and requirements of the communities served.

The key concept is not that the KPIs themselves must have a direct causal effect on eventual outcomes, or measure eventual outcomes or long-term impacts, but rather that the KPIs are chosen so that actions and decisions which move the metrics in the desired direction also move the organization in the direction of the desired outcomes and goals.

Table 1-1 below shows the project's progress toward the three strategic goals and associated sub-goals in RY4. Status icons are used in the table as follows:

A green status is defined as a strategic goal for which at least 90% of the targets for all KPIs are met.

A yellow status is defined as a strategic goal within which at least 60% of the targets for all KPIs are met.

A red status is a strategic goal with less than 60% of the KPI targets met.

A white status indicates there are currently no metrics tracked for this sub-goal or there is not complete data for any of the metrics tracked.

Multiple indicators represent a strategic goal that has sub-goals for which there is incomplete data or that have metrics not currently tracked. In these cases, the second indicator is a qualitative assessment of the status provided in lieu of sufficient data or a formal metric being in place.

Table 1-1: Summary of Key Performance Indicators (KPIs) for XSEDE.

Status	Sub-goals	KPIs
Strategic Goal: Deepen and Extend Use (§3.1)		
G	**Deepen use (existing communities)** (§3.1.1)	● Number of sustained users of XSEDE resources and services via the portal ● Number of sustained underrepresented individuals using XSEDE resources and services via the portal ● Percentage of sustained allocation users from non-traditional disciplines of XSEDE resources and service
Y	**Extend use (new communities)** (§3.1.2)	● Number of new users of XSEDE resources and services via the portal ● Number of new underrepresented individuals using XSEDE resources and services via the portal ● Percentage of new allocation users from non-traditional disciplines of XSEDE resources and services
G	**Prepare the current and next generation** (§3.1.3)	● Number of participant hours of live training delivered by XSEDE
G	**Raise awareness of the value of advanced digital services** (§3.1.4)	● Grand (aggregate) mean rating of XSEDE User Survey user awareness items regarding XSEDE resources and services ● Number of social media impressions over time
Strategic Goal: Advance the Ecosystem (§3.2)		
G	**Create an open and evolving e-infrastructure** (§3.2.1)	● Total number of capabilities in production
G	**Enhance the array of technical expertise and support services** (§3.2.2)	● Grand (aggregate) mean rating of XSEDE User Survey satisfaction items regarding XSEDE technical support services
Strategic Goal: Sustain the Ecosystem (§3.3)		
G	**Provide reliable, efficient, and secure infrastructure** (§3.3.1)	● Mean composite availability of core services (%)
Y	**Provide excellent user support** (§3.3.2)	● Mean time to ticket resolution (hours) ● Mean rating of user satisfaction with allocations process and support services ● Percentage of research requests successful (not rejected)
G	**Operate an effective and productive virtual organization** (§3.3.3)	● Mean rating of importance of XSEDE resources and services to researcher productivity ● Percentage of users who indicate the use of XSEDE-managed and/or XSEDE-associated resources in the creation of their work product
G	**Operate an innovative virtual organization** (§3.3.4)	● Percentage of Project Improvement Fund funded projects resulting in innovations in the XSEDE organization ● Mean rating of innovation within the organization by XSEDE staff

In grasping the scope of XSEDE's activities, it is perhaps useful to liken XSEDE's integrated set of efforts to that of a physical center supporting advanced digital services and research computing. In this case, research computing resources are operated and funded by separate NSF awards to Service Providers (SPs). XSEDE provides central services to complement and integrate those SP awards and resources into a common ecosystem and provides these services more efficiently and cost-effectively for NSF and the user community. XSEDE coordinates and supports education and outreach (CEE), front-line and advanced user support (CEE and ECSS), allocations review and processing (RAS), operation of shared enterprise services (Operations), and well-designed strategies for resource integration (XCI), all guided by common practices, communication, and administration (Program Office). XSEDE activities are logically organized across L2 (Work Breakdown Structure Level 2) areas to eliminate duplication of effort and allow effective management and focus; however, as with a physical center, each area depends on and supports the others in successfully completing XSEDE's mission and goals. And like a physical center, all parts of XSEDE are bound into a coherent and more effective whole by a shared set of values of the XSEDE project that bring synergy to the project:

- A focus on people: people are the most valuable resource in the pursuit of knowledge. XSEDE creates a strong sense of coherent community, connecting the research community and the technical expertise they partner with from XSEDE to harness a set of coherent services and infrastructure.
- Raising awareness of the value of advanced digital services: given that effective integration and coordination of advanced digital services within the national ecosystem to support contemporary science by nature makes that integration and coordination less visible, it is precisely the rich set of less visible cross-connections among the activities of XSEDE that make it much more than the sum of its parts and much more effective in the support of science and education.
- Integrating and helping expand effective use of the national cyberinfrastructure across disciplines and across campuses: XSEDE is driven to bring the capabilities of the advanced digital services ecosystem to scholars, researchers, and engineers across all domains. XSEDE aids academic institutions across the US by providing resources and enabling more effective use and integration of local resources as part of the national cyberinfrastructure, better leveraging local investments in CI.
- A significant, persistent, secure, and reliable environment for conduct of research: the highly integrated nature of XSEDE enables a coherent approach to creating a trusted and protected environment that provides a long-term platform to empower modern science and engineering research and education. The long-term lifespan of XSEDE means that researchers can plan activities and count on years of use of resources and support from XSEDE.
- Accountability and transparency: while XSEDE has organized in alignment with its strategic goals that provide primary focus for each of the organizational units of the project, it is only through the unified management of the project that full accountability and transparency can be realized given the underlying cross-dependencies and synergies of the organizational units.

Shared values are a social construct that XSEDE has developed over many years working with all its stakeholders. These values, in conjunction with the effective cross-organizational management techniques developed by XSEDE, enables XSEDE not only to articulate a vision of the future, but to demonstrate the trusted and dependable leadership necessary to make that vision a reality for the community.

1.2. Summary & Project Highlights

The XSEDE project continues to provide significant value to the national research community by enabling high-impact scientific advances across a broad range of disciplines. In XSEDE's continuing documentation of science success, a few key examples of efforts that have been enabled by XSEDE in

conjunction with our Service Provider (SP) partners have been selected. These are highlighted in §2 of this report and span a range of domains including: astrophysics, biological immunity, plasma physics, environmental science, genome sequencing, and COVID-19 antibodies. A continually updated collection of these successes is documented on the XSEDE website[6].

Adding value and expanding the value of NSF's investment in advanced computing for the research community, nationally and internationally, is the focus of the portion of the XSEDE mission statement which reads, "coordinate and add significant value to the leading cyberinfrastructure resources funded by the NSF and other agencies." This reporting period includes many examples of the project's efforts to advance this mission.

This reporting period, the XSEDE project had multiple contributions to the research community. In their continuing effort to modernize the XSEDE accounting infrastructure, Resource Allocation Service (RAS) completed and deployed the new RESTful API (application programming interface) version of the Account Management Information Exchange (AMIE) protocol. The legacy AMIE packet-exchange system has been converted to a modern JSON (JavaScript Object Notation) and REST (REpresentational State Transfer) system making onboarding easier for the many new Service Providers. See §8 for more details on this API and a new usage reporting API. XSEDE Cyberinfrastructure Integration (XCI) introduced a significant, new, and comprehensive XSEDE Software Discovery service that was integrated into the Research Software Portal to enhance the ability to find and use software and applications on XSEDE resources. See §6 for more details on this new resource. XSEDE allocations activity continued at high levels despite the continued pandemic. The XSEDE Resource Allocation Committee (XRAC) met virtually for the second time and reviewed requests for compute resources that were just over twice the amount available. The result of the XRAC was that 84% of Research requests received some allocation.

Multiple evaluation activities took place during this reporting period. The longitudinal tracking data for the Advanced Computing for Social Change student program was updated. Of the total 108 participants served since 2016, 65% are women and 63% are underrepresented minorities, with a majority of these students having been recruited from institutions with limited research opportunities. Data also shows effective engagement of students from non-STEM (science, technology, engineering, and math) disciplines and increased participation across XSEDE programs. Additional details can be found in §4. Community Engagement & Enrichment (CEE) is leading a project-wide Terminology Task Force in support of XSEDE's diversity and inclusion goals. The task force is reviewing all XSEDE materials for language that provides barriers to diversity, equity, and inclusion. Many people both inside the XSEDE project and within the XSEDE user community have contributed by reporting problematic terms. In addition, the Evaluation team completed evaluations for the 2020 Staff Climate Survey, the Practice & Experience in Advanced Research Computing 2020 conference (PEARC20), and an internal COVID-19 staff survey.

1.3. COVID-19 Contributions

XSEDE continues to play a key role in the nation's (and the world's) response to the COVID-19 pandemic.

COVID-19 HPC Consortium:[7] The Consortium continues to provide support to research addressing the COVID-19 pandemic. PI Towns and RAS Allocations Process & Policies (APP) L3 Manager Ken Hackworth continue in their respective roles as previously described in the XSEDE RY4 Annual Report. During this Reporting Period the number of allocations made via the Consortium has continued to decline, but requests continue to be submitted. As previously expected, as allocations made early in the

[6] https://www.xsede.org/science-successes
[7] https://covid19-hpc-consortium.org/

process expire, new/supplemental requests are being submitted by the PIs. Also, as noted in IPR12, the Consortium is currently transitioning to a "Phase II" which reflects guidance from the COVID-19 HPC Consortium Executive Board to more actively manage the portfolio of projects accepted by the Consortium. The Consortium is particularly, though not exclusively, interested in projects focused on:

- Understanding and modeling patient response to the virus using large clinical datasets
- Learning and validating vaccine response models from multiple clinical trials
- Evaluating combination therapies using repurposed molecules
- Epidemiological models driven by large multi-modal datasets

Details are provided in a series of weekly reports submitted by Towns to NSF aggregating much of the information regarding not only efforts related to the Consortium, but also allocations made by other means. These should all be available in the record of the project at NSF and will not be repeated here.

In total, as of October 31, 2020, the Consortium has received 177 requests through the XSEDE Resource Allocations System (XRAS) (19 new since the XSEDE IPR12). Of these, 93 (10 new since IPR12) projects were provided access to resources with 36 (7 new since IPR12) of these being allocated on NSF resources. A complete list of active projects provided access via the Consortium is available on the Consortium's Active Projects page. All projects allocated via the Consortium on resources typically allocated via XSEDE are also offered ECSS support to expedite their work.

CEE and ECSS staff have continued to support the COVID-19 consortium at the University of Texas at Austin, particularly developing spatially explicit visualizations of case counts and hospitalizations. More details can be found on the UT COVID-19 Modeling Consortium website[8] and in §5.

[8] https://covid-19.tacc.utexas.edu/

2. Science, Engineering, & Program Highlights

This section provides a select set of science and engineering highlights as well as program highlights from the community of researchers with whom we collaborate. These are drawn from the most recent reporting period (RP2 of RY5). A complete collection of highlights can be found on the XSEDE website.[9]

2.1. Galactic Archeology

The first stars are hypothesized to have formed about 100 million years after the Big Bang out of universal darkness from the primordial gases of hydrogen, helium, and trace light metals.

These gases cooled, collapsed, and ignited into stars up to 1,000 times more massive than our sun. The bigger the star, the faster they burn out. The first stars probably only lived a few million years, a drop in the bucket of the age of the universe, at about 13.8 billion years. They're unlikely to ever be observed, lost to the mists of time.

However, thanks to allocations from XSEDE, these first stars are being simulated by supercomputers at the Texas Advanced Computing Center (TACC) and the San Diego Supercomputer Center (SDSC) (see Figure 1).

As the metal-free first stars collapsed and exploded into supernovae, they forged heavier elements such as carbon that seeded the next generation of stars. One type of these second stars is called a carbon-enhanced metal-poor star. They're like fossils to astrophysicists. Their composition reflects the nucleosynthesis, or fusion, of heavier elements from the first stars.

"We can get results from indirect measurements to get the mass distribution of metal-free stars from the elemental abundances of metal-poor stars," said Gen Chiaki, a post-doctoral researcher in the Center for Relativistic Astrophysics, School of Physics, Georgia Institute of Technology.

Chiaki is the lead author of a study published in the September 2020 issue of the *Monthly Notices* of the Royal Astronomical Society. The study modeled for the first time faint supernovae of metal-free first stars, which yielded carbon-enhanced abundance patterns through the mixing and fallback of the ejected bits.

Their simulations also showed the carbonaceous grains seeding the fragmentation of the gas cloud produced, leading to formation of low-mass 'giga-metal-poor' stars that can survive to the present day and possibly be found in future observations.

The investigations of Wise and Chiaki are a part of a field called 'galactic archaeology.' They liken it to searching for artifacts underground that tell about the character of societies long gone. To astrophysicists, the character of long-gone stars can be revealed from their fossilized remains.

"We can't see the very first generations of stars," said study co-author John Wise, an associate professor also at the Center for Relativistic Astrophysics, School of Physics, Georgia Tech. "Therefore, it's important to actually look at these living fossils from the early universe, because they have the fingerprints of the first stars all over them through the chemicals that were produced in the supernova from the first stars."

"That's where our simulations come into play to see this happening. After you run the simulation, you can watch a short movie of it to see where the metals come from and how the first stars and their supernovae actually affect these fossils that live until the present day," Wise said.

The majority of the simulations ran on the Georgia Tech *PACE* cluster, while *Stampede2* at TACC and *Comet* at SDSC ran some of the main sequence radiative transfer simulations through XSEDE allocations.

[9] https://www.xsede.org/science-successes

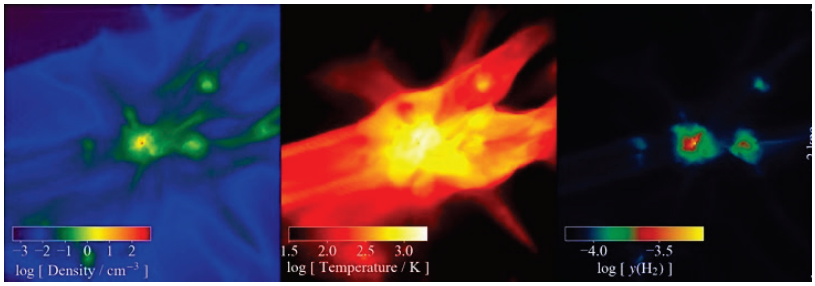


Figure 1: Formation cycle shown of a first star, or Pop III star, the main source of carbon, oxygen and iron in the early universe. Density, temperature, and H2 abundance of the dark matter minihalo star-forming region just before Pop III start formation (redshift z = 12.1) in a box with a side 1 kpc centered on the density maximum. Credit: Chiaki, et al.

"The XSEDE systems *Comet* at SDSC and *Stampede2* at TACC are very fast and have a large storage system. They were very suitable to conduct our huge numerical simulations," Chiaki said.

Wise has been using XSEDE system allocations for over a decade, starting when he was a postdoc. "I couldn't have done my research without XSEDE."

XSEDE also provided expertise for the researchers to take full advantage of their supercomputer allocations through the Extended Collaborative Support Services (ECSS) program. "Through ECSS, I worked with Lars Koesterke at TACC, and I found out that he used to work in astrophysics. He worked with me to improve the performance by about 50 percent of the radiation transport solver. He helped me profile the code to pinpoint which loops were taking the most time, and how to speed it up by reordering some loops. I don't think I would have identified that change without his help," Wise said.

Said Chiaki: "The aim of this study is to know the origin of elements, such as carbon, oxygen, and calcium. These elements are concentrated through the repetitive matter cycles between the interstellar medium and stars. Our bodies and our planet are made of carbon and oxygen, nitrogen, and calcium. Our study is very important to help understand the origin of these elements that we human beings are made of."

The study, "Seeding the second star — II. CEMP star formation enriched from faint supernovae," was published in the September 2020 issue of the *Monthly Notices* of the Royal Astronomical Society. The authors are Gen Chiaki and John H. Wise, Georgia Institute of Technology; Stefania Marassi and Raffaella Schneider, Universita`di Roma; Marco Limongi, Osservatorio Astronomico di Roma; Alessandro Chieffi, Istituto Nazionale di Fisica Nucleare - Sezione di Perugia. GC is supported by Research Fellowships of the Japan Society for the Promotion of Science (JSPS). JHW is supported by National Science Foundation grants AST-1614333 and OAC-1835213, and NASA grants NNX17AG23G and 80NSSC20K0520. The simulation was performed with NSF's XSEDE allocation AST120046 on the *Comet* and *Stampede2* resources and also on the Georgia Tech *PACE* compute system.

2.2. *Comet* Supercomputer Calculations Boost Understanding of Immune System

While researchers around the world race to develop an effective and safe COVID-19 vaccine, a team from the San Diego Supercomputer Center (SDSC) at UC San Diego contributed to a study led by Vanderbilt Vaccine Center of Vanderbilt University Medical Center (VUMC) on T cell receptors, which play a vital role in alerting the adaptive immune system to mount an attack on invading foreign pathogens including the Coronavirus SARS-CoV-2.

Thanks to an XSEDE allocation, SDSC's *Comet* was recently used to perform complex calculations on the receptor sequence data from sorted human T cells to allow scientists to better understand the size and diversity receptor repertoire in healthy individuals (see Figure 2). The team's findings were published

last month in *Cell Reports*[10] as a follow-up study to earlier findings about B cells published in the journal *Nature*[11] last year.

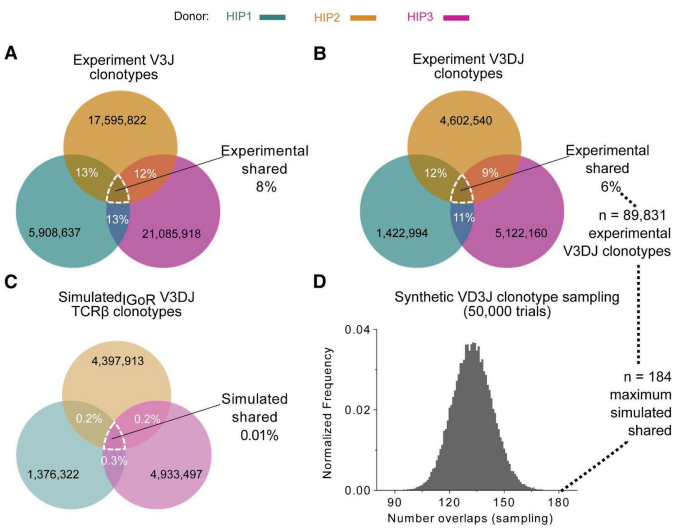


Figure 2: Overview of T cell receptor clonotype sharing between three healthy Caucasian subjects. Comparison to simulated data shows that the degree of overlap is more than two orders of magnitude greater than what would be expected by chance. Credit: San Diego Supercomputer Center and Vanderbilt University.

Both B cells and T cells are constituents of the adaptive immune system and form the second line of defense against viruses, bacteria, cancer, and other toxic pathogens that slip past the innate immune response. The adaptive immune system remembers the invading pathogen after first encounter and forms the basis of effective vaccines. To advance our understanding, the researchers sequenced receptors from the transcriptome of billions of cells to assess the somatic recombination of different gene segments that comprise the circulating B and T cell receptors from healthy Caucasian individuals. They found that T cell receptors, like B cell receptors, exhibit significantly higher overlap in different individuals than expected by chance.

In addition, the unprecedented scale of this sequencing project reveals that the size and diversity of immune repertoire are at least an order of magnitude larger than the estimation made from previous studies. This work is part of a broader effort supported by the Human Vaccines Project to decipher the components of the immune system, with the ultimate goal of understanding how to generate life-long protective immunity.

"Our most recent study puts us one step closer to truly understanding the extreme and beneficial diversity in the immune system, and identifying features of immunity that are shared by most people," said James E. Crowe, Jr., director of the Vanderbilt Vaccine Center of Vanderbilt University Medical Center. "Now we continue to identify T cell receptors and antibodies that can be targets for vaccines and treatments that work more universally across populations."

A primary aspect of the team's ongoing research is focused on integrating the findings of these two studies toward the development of an effective vaccine against emerging and evolving threats. Crowe explained, "We are getting closer to being able to use these large databases of human immune molecules to rapidly discover natural molecules that can be used as biological drugs."

Madhusudan Gujral, a senior bioinformatician at SDSC; Robert Sinkovits, SDSC's director of scientific computing applications; and Cinque Soto, a Vanderbilt computational biologist and lead author of the study, share Crowe's enthusiasm over the implications of this research and recognize the importance of access to high-performance computing resources, such as *Comet*, to make it possible.

"Being able to access *Comet* through an XSEDE allocation made us much more productive," said Sinkovits. "The larger memory nodes were also essential for some of the clustering calculations that could not have been completed on standard hardware.

[10] https://www.sciencedirect.com/science/article/pii/S2211124720308639

[11] https://www.nature.com/articles/s41586-019-0934-8

This work was supported by a grant from the Human Vaccines Project and institutional funding from Vanderbilt University Medical Center. The authors acknowledge support from TN-CFAR grant (P30 AI110527). This work also used XSEDE, which is supported by NSF grant (ACI-1548562), and *Comet* supercomputer at SDSC, supported by NSF grant (ACI-1341698). Computational support comes from XSEDE grant MCB170022.

2.3. Sipping from the Fire Hose

Fast radio bursts (FRBs) puzzle astronomers. They're so brief—lasting only a few thousandths of a second—that scientists haven't quite been able to identify their points of origin or how they are generated. Using the GPU nodes of the XSEDE-allocated *Bridges* supercomputing platform, a team from West Virginia University created a package of artificial intelligence (AI) programs that can sift through the thousands of FRB candidates expected to be detected in upcoming surveys quickly enough for astronomers to figure out where to point their telescopes to learn more.

One of the most difficult challenges in astronomy is figuring out the origin of FRBs (see Figure 3). Incredibly quick and unpredictable, these events flash out for only a few thousandths of a second before disappearing without any lingering trace—at least, not that scientists have yet detected. Despite that brevity, astronomers have used radio-frequency telescopes to detect more than 100 of them since they were discovered by researchers at West Virginia University (WVU) in 2007[12].

Scientists do know one thing about FRBs. They're coming from incredibly far away, outside our Milky Way galaxy. Though their signals are relatively weak when they get to Earth, they have to be pretty powerful at their distant points of origin. But that's it. Scientists have some educated guesses as to what might be causing FRBs—flaring neutron stars with powerful magnetic fields, interacting pairs of neutron stars and black holes are all possible sources. We just don't know. One big problem has been that, because FRBs are so brief, they don't give astronomers any warning time to redirect visible-light or X-ray telescopes to their location to check if there are lingering signals in those frequencies that could help them decide between the candidate causes.

Upcoming surveys will discover many more of these events by monitoring broad swaths of the sky. Researchers expect them to detect about a dozen FRBs every day, which would be great for the science. The problem is they'll also detect many thousands of false signals—similar but distinct astronomical signals, interfering radio signals from Earth-bound sources like mobile phones and satellites, as well as random noise. It's a "sipping from the fire hose" problem. Human experts can tell FRBs from these other signals, but with many thousands coming daily they simply can't sort them fast enough to re-aim other telescopes to look for non-radio signals. That's why Devansh Agarwal and Kshitij Aggarwal, graduate students working with advisors Duncan Lorimer and Sara Burke-Spolaor of WVU, respectively, wanted to use AI to make an automated "first cut" that reduced the number of candidates to a number manageable by humans.

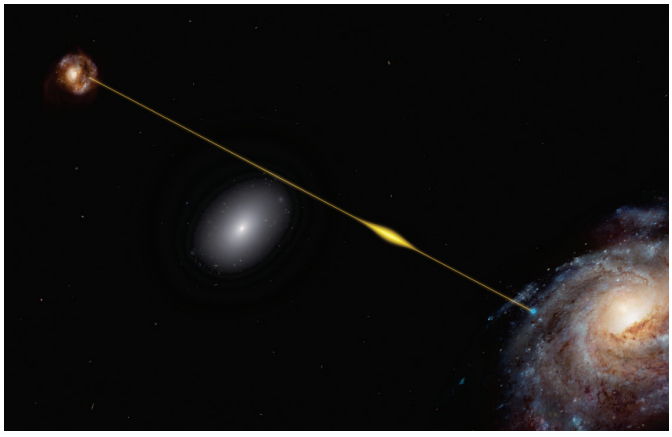


Figure 3: This artist's impression represents the path of the fast radio burst FRB 181112 traveling from a distant host galaxy to reach the Earth. Credit: European Southern Observatory/M. Kornmesser

[12] https://www.scientificamerican.com/article/flashes-in-the-night-the-mystery-of-fast-radio-bursts/

The type of AI that Agarwal and Aggarwal used is called a convolutional neural network (CNN). In CNNs, the computer creates several layers that represent different characteristics of an image. It also creates a network of connections between the data in each layer. It then trains itself on images that have been identified by humans. Somewhat like a developing biological brain, it removes faulty connections until the network succeeds in correctly identifying those images. Next scientists test it on data that have not been labeled, going back and forth between training and testing until it's got a high success rate. Then, the CNN can be used on real data.

The WVU scientists faced several challenges in their plan. First, whatever they came up with had to be fast. If it couldn't create a smaller list of candidates fast enough for humans to spot the real FRBs and then redirect telescopes to search for non-radio signals that followed the radio burst, it wouldn't improve the situation. Second, they decided to speed the development time by using pre-existing, freely available image-classifying CNNs. By training thousands of them, they could winnow it down to a small set that were really good at FRB classification. The end result would be a package of CNNs that are openly available to researchers.

Lastly, CNN works best when carried out on graphics processing units, or GPUs. Originally developed to create realistic images in video games, GPUs turned out to have huge scientific applications in processing image data and in AI. But training thousands of CNNs would require many more GPUs than the team had available through local resources at WVU.

The solution to all three problems came in the form of an XSEDE workshop offered at WVU. There the WVU scientists learned about *Bridges*, an XSEDE-allocated supercomputing platform at the Pittsburgh Supercomputing Center (PSC) that possesses a total of 58 powerful, late-model GPU nodes. *Bridges* offered them the GPU power they needed to scale up their testing.

Thanks to the XSEDE Resource Allocation System and an allocation on *Bridges-GPU*, the ease of getting a startup allocation as student researchers proved critical for getting their work started quickly and effectively.

Using *Bridges-GPU*, the team winnowed down thousands of candidate CNNs to a list of 11 that was over 99.5-percent accurate in classifying FRBs. A task that would have taken months using other resources available could now be done in a week. Their package of CNNs, available for free to scientists, is called FETCH, for Fast Extragalactic Transient Candidate Hunter. They reported their results and offered FETCH to astronomers carrying out upcoming FRB surveys in a report in the journal Monthly Notices of the Royal Astronomical Society online in June 2020.

You can read their paper here[13]. Computational support for this research was provided via XSEDE grant AST180069.

2.4. Machine Learning Helps Plasma Physics Researchers understand Turbulence Transport

As far as societal benefits go, fusion energy is viewed as a longer-term solution to meeting the world's overall energy needs. Fusion has the capability to provide large-scale, emissions-free energy wherever needed, while being a viable complement to intermittent renewables and battery storage. Although fusion energy shows great potential, some obstacles remain, one of them being how to manage plasma turbulence which drives the transport of heat and particles toward the wall of the fusion device, preventing adequate confinement.

For more than four decades, University of California, San Diego, Professor of Physics Patrick H. Diamond and his research group have been advancing our understanding of fundamental concepts in plasma physics, which has many applications, including fusion energy. When light nuclei fuse together, the

[13] https://doi.org/10.1093/mnras/staa1856

mass of the products is less than that of the reactants, and the missing mass becomes energy—hence Albert Einstein's famous $E=mc^2$ equation.

Most recently, Diamond worked with graduate student Robin Heinonen on a model reduction study that used the Extreme Science and Engineering Discovery Environment (XSEDE)-allocated *Comet* supercomputer at the San Diego Supercomputer Center (SDSC) at UC San Diego to showcase how machine learning produced a new model for plasma turbulence.

"Turbulence and its transport is chaotic in a sense, but this chaos is ordered and constrained," said Heinonen, who co-authored Turbulence Model Reduction by Deep Learning[14] with Diamond in the *Physical Review E* journal. "Moreover, in certain turbulent systems, the chaos conspires to spontaneously form large, long-lived coherent structures and, in many cases, we only have a tenuous understanding of why and how now. There are definitely aspects of structure formation and self-organization which we do understand, but it's still an active area of research."

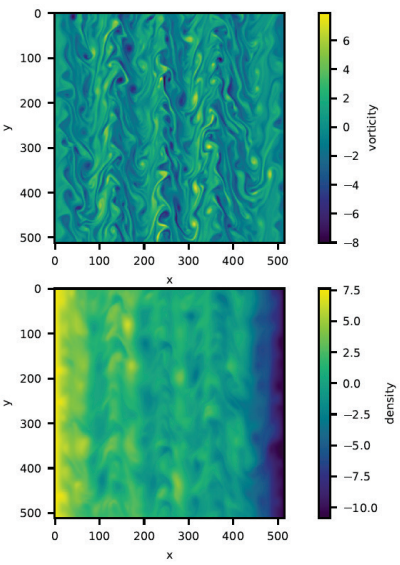


Figure 4: This snapshot of vorticity and turbulence density from a simulation using the XSEDE-allocated *Comet* supercomputer at the San Diego Supercomputer Center illustrates a notable physics concept: the formation of zonal (i.e. y-direction) structures, which have important consequences for magnetic confinement devices. Credit: Robin Heinonen, University of California San Diego Center for Energy Research.

The authors say that advances in machine learning (ML), notably deep learning techniques, have provided them with the tools they needed to develop their new model for turbulent transport. The power of ML lies in the ability to learn patterns from the data instead of being explicitly programmed and the 'deep' in deep learning refers to the many layers of interconnected processing units in the model.

"This deep learning approach allowed us to run many simulations and then train a neural network," explained Heinonen. "The neural network then outputs the average turbulence-driven fluxes as a function of a handful of physical variables of interest, which reduces the dimensionality of the model from two-dimensional to one-dimensional, making it more tractable and easier to understand."

The researchers used a particularly simple ML model and applied it to a simplified, yet physically rich, model of plasma turbulence. This approach sacrifices some predictive power for the sake of interpretability, which can lead to new insights. Previously unreported results include a non-diffusive flux driven by the flow and higher-order corrections to the fluxes that are difficult to calculate or understand (see Figure 4).

Heinonen first learned about XSEDE through Kevin Smith, who works with the information technology program within the UC San Diego Physics Department. Heinonen said that Smith helped him with the start-up program proposal and within a few days he was granted an XSEDE allocation on SDSC's *Comet* supercomputer, which is part of XSEDE's portfolio of available resources.

"After we received our *Comet* allocation, the XSEDE tech support team was extremely helpful from beginning to end," said Heinonen. "Installing and running software on a supercomputer can be a major challenge, and I am grateful for the XSEDE support team."

[14] https://journals.aps.org/pre/abstract/10.1103/PhysRevE.101.061201

The work on *Comet* was supported by XSEDE allocation (PHY190014), which is supported by the National Science Foundation (ACI1548562). The research was supported by the U.S. Department of Energy, Office of Science, Office of Fusion Energy Sciences (DE-FG02-04ER54738).

2.5. *Comet* Supercomputer Used to Simulate Environmental Changes in Chesapeake Bay

Encompassing more than 4,000 square miles, the Chesapeake Bay is the largest estuary in the continental U.S., providing an excellent testbed for scientists to better understand long-term changes occurring in coastal waters by using high-performance computing (HPC) resources to create detailed simulations.

The National Science Foundation-funded XSEDE project recently allocated time on *Comet* at the San Diego Supercomputer Center (SDSC) at UC San Diego for Virginia Institute of Marine Science (VIMS) Research Scientist Pierre St-Laurent and colleagues to examine impacts of both regional and global changes affecting the Chesapeake Bay. They discovered that historical increases in fertilizers and atmospheric carbon dioxide concentrations have forced the bay to behave increasingly like a small sea on a continental shelf rather than a traditional estuary.

"Upon using this XSEDE allocation to study (see Figure 5) what happened during the last 100 years, we determined that the bay now absorbs slightly more carbon dioxide than it releases into the atmosphere," said St-Laurent. "This result exemplifies the particularity of the continental U.S.'s largest estuary, but also may be indicative of the magnitude of the changes that are ongoing in coastal waters throughout the world."

St-Laurent and his colleagues published their detailed findings[15] in Volume 17 (issue 14) of the *Biogeosciences* journal.

"Our study provides valuable perspective to watershed managers as it compares the long-term impact of fertilizer usage with other global changes," said St-Laurent. "Not only is the health of the Chesapeake Bay important for ecological reasons, but also for economic purposes as the seafood industry driven by these waters is estimated to contribute around two billion dollars in sales each year and approximately 40,000 jobs, according to the Chesapeake Bay Foundation."

Additionally, the bay has long been a popular tourist destination with its variety of sandy beaches, wetlands, and open waters.

"Without our XSEDE allocation on *Comet*, we would have had to scale down our experiments drastically, affecting the scientific scope of the study and leaving important questions unanswered," added St-Laurent. "Because our research spanned two periods of time covering the early 1900s to the early 2000s, our computational requirement vastly exceeded the resources available at our local research center, but they were well within the computing capacities at SDSC."

In addition to these long-term overview comparison models, the researchers are also interested in specifics regarding the bay's health; specifically, they're studying hypoxia, or lack of oxygen, within the waters. Their Chesapeake Bay Hypoxia Forecast[16], which was developed by the study's second author and VIMS Research Professor Marjy Friedrichs, simulates present-day levels of dissolved oxygen and pH in the Chesapeake Bay, levels of dissolved oxygen and pH in the bay two days from now, and the percentage difference during that short time span.

[15] https://bg.copernicus.org/articles/17/3779/2020/bg-17-3779-2020.html

[16] https://www.vims.edu/research/topics/dead_zones/forecasts/cbay/index.php

Using this modeling system, the researchers also assess how the low-oxygen waters have changed over the past 35 years. Historically, the duration of low-oxygen waters in the bay has ranged between 93-143 days. Despite a general downward trend in hypoxic duration due to management actions reducing nutrient inputs to the bay, the past two years have had relatively severe hypoxia lasting 123 days in 2018 and 136 days in 2019.

"These unusually long durations of hypoxia are due to the high precipitation levels we've seen over the past two years," said Friedrichs. "One of our goals with this work is to help decision makers put recent data into a long-term context so that they can better understand how their clean-up efforts are improving the health of the bay."

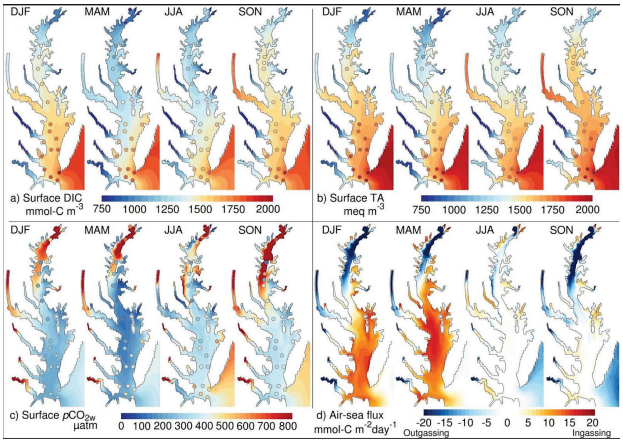


Figure 5: Seasonal changes taking place in Chesapeake Bay according to computer simulations conducted at SDSC via an XSEDE allocation. DJF is December-February, MAM is March-May, JJA is June-August, and SON is September-November. The figure shows exchanges of carbon dioxide with the atmosphere (air-sea flux, bottom right) and other related fields. (Dissolved inorganic carbon (DIC), Total alkalinity (TA), and CO2 partial pressure) Credit: St-Laurent et al (2020).

As Friedrichs and St-Laurent work to refine these simulations by increasing the horizontal resolution of their model grid, resources such as *Comet* will be needed to continue running these long-term (35+ years) simulations.

St-Laurent and Friedrichs were funded by grants from the NSF (OCE-1537013), NASA (NNX14AF93G), and the National Oceanic and Atmospheric Administration's National Centers for Coastal Ocean Science (NA16NOS4780207). Access to *Comet* was via XSEDE (OCE160013). William & Mary Research Computing also provided computational resources and technical support.

2.6. Damaged DNA

All life depends upon DNA repair and replication.

In every human cell the essential ability to replicate and repair genomes depends upon the coordinated actions of the genome sequence. Flaws or mistakes in repair and cell cycle regulation can lead to defects in the structure of the DNA and can prevent the replication from functioning properly.

Defects in DNA replication and repair processes contribute to the onset, progression, and prognosis of cancer. Bacolla and other researchers are using data and advanced computing to examine relevant responses in cells.

Today, Albino Bacolla studies cancer as a research investigator at The University of Texas MD Anderson Cancer Center. His recent research, published in *Progress in Biophysics and Molecular Biology* in October 2019[17], focuses on genome instability and uses a computational approach to uncover mechanisms underlying cancer.

Bacolla has dedicated his life to exploring the biological laws that govern how cells function within the body. His scientific work has ranged from detecting thyroid deficiencies in children, to the identification of one of the earliest non-canonical DNA structures, to the genetic engineering of an inhibitor of HIV,

[17] https://www.sciencedirect.com/science/article/pii/S0079610719301993

which is used to treat HIV/AIDS patients. Now, he has set his sights on a disease that affects millions: cancer.

"There is an enormous amount of data available in the public domain concerning cancer patients," Bacolla said. "What is lacking is the ability to analyze and mine the data. Advanced computing resources allow me to query a large number of data to probe its meaning."

Bacolla uses supercomputing resources allocated through XSEDE, a single virtual system funded by the National Science Foundation used by scientists to interactively share computing resources, data, and expertise. Specifically, Bacolla uses the XSEDE-allocated *Stampede2* supercomputer at the Texas Advanced Computing Center (TACC).

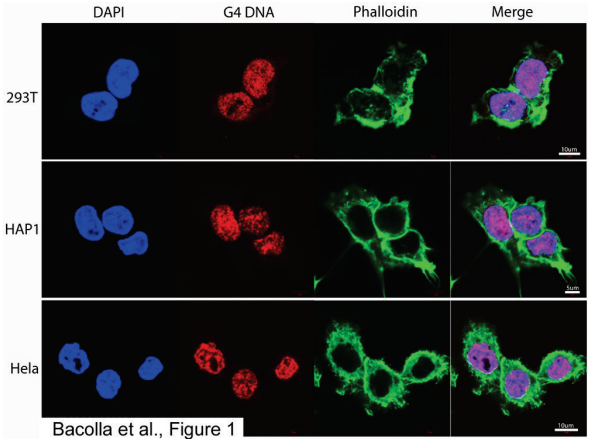


Figure 6: G4 DNA structures are readily detected in cell nuclei. Confocal microscopy of 293T, HAP1, and Hela cells stained with DAPI (blue) for nuclear DNA; a G4 DNA-structure specific antibody (red); and with Phalloidin for cytoplasmic cytoskeleton (green) display nuclear colocalization of G4 DNA structural foci with chromosomal DNA. Credit: Albino Bacolla, MD Anderson.

Exposure to radiation and chemotherapy is one way to damage DNA. It can also be damaged by oxidants normally produced by the body. In every cell, the genome experiences about 70,000 lesions every day. If left unrepaired, this damage can result in mutations within the cell, which results in unusual and dangerous rearrangements of chromosomes.

"These breaks in the double strand helix are extremely damaging and can cause the cell to die," Bacolla said. "And tumors use these breaks to rearrange the genome to their advantage."

His research started at sites where the DNA breaks into sequences that form a quadruplex DNA structure (see Figure 6). He found that many of these sequences are inside pieces of DNA called transposons that jump from one place to another in the genome, inserting themselves inside the gene and causing disruption.

"We found that one family of transposons was much more frequent near where the chromosomes break in the cancer genomes," Bacolla said. Transposons are known to cause rearrangements in cancer; however, it was not known that some do so using their quadruplex DNA structure. This discovery means that scientists can potentially stabilize these structures and induce cancer cell death by overwhelming it with DNA damage, as it is done with other anti-cancer treatments such as cisplatin.

Scientists know that tumors have mutations, and mutated genes allow the tumor cells to grow. What's not understood, however, is how tumors grow with the help of additional genes that promote mutations.

Bacolla set out to learn about these supplemental, mutation-promoting genes. He used public data sets to make correlations from 11,000 patients, such as the number of mutations the patient had and the degree to which each gene in the human body was expressed in that patient.

It became evident to Bacolla that tumors use these supplemental genes to grow very fast. "We found that it's the tumor cell that's pushed to replicate that causes many mutations—it's called replication stress."

Most of the cancer literature today focuses on what kind of mutations are in tumors and how they arise.

Instead, Bacolla's question centered on the iteration of mutated tumor cells, or the extent to which a tumor cell expresses one gene compared to its adjacent normal tissue. For genes used by the tumor to grow, such as one called CENPA, these genes are expressed up to 10 times more than in normal tissues.

"I suspect that these genes are protected by the tumor—they are the tumor's friends," Bacolla said. "These friends are upregulated genes in the tumor cell and cause mutations that support disease. There are about 190 of these genes and the tumor relies on them—it needs the machinery that takes the chromosomes apart and distributes them to the dividing cells. Best friends for the tumor, but the worst enemies for us."

The paper is called "Cancer mutational burden is shaped by G4 DNA, replication stress and mitochondrial dysfunction."[18] It appeared in *Progress in Biophysics and Molecular Biology*, October 2019. Authors: Albino Bacolla, Zu Ye, Zamal Ahmed and John A. Tainer, Department of Molecular and Cellular Oncology, The University of Texas MD Anderson Cancer Center. The researchers are grateful for funding by the National Institutes of Health and the Cancer Prevention and Research Institute of Texas for their efforts to understand DNA damage. Computational allocations provided through XSEDE via grant MCB170053.

2.7. Re-Engineering Antibodies to Find Relief for COVID-19

With millions of COVID-19 cases reported across the globe, people are turning to antibody tests to find out whether they have been exposed to the coronavirus that causes the disease.

But what are antibodies? Why are they important? If we have them, are we immune to COVID-19? And if not, why not?

"Antibodies are important because they prevent infection and heal patients affected by diseases," said Victor Padilla-Sanchez, a researcher at The Catholic University of America in Washington D.C. "If we have antibodies, we are immune to disease, as long as they are in your system, you are protected. If you don't have antibodies, then infection proceeds and the pandemic continues."

This form of foreign-antibody-based protection is called passive immunity—short-term immunity provided when a person is given antibodies to a disease rather than producing these antibodies through their own immune system.

"We're at the initial steps of this now, and this is where I'm hoping my work might help," Padilla-Sanchez said. Padilla-Sanchez specializes in viruses. Specifically, he uses computer models to understand the structure of viruses on the molecular level and uses this information to try to figure out how the virus functions.

For his research, Padilla-Sanchez relied on supercomputing resources allocated through the Extreme Science and Engineering Discovery Environment (XSEDE). XSEDE is a single virtual system funded by the National Science Foundation used by scientists to interactively share computing resources, data, and expertise. These particular allocations were provided through the COVID-19 HPC Consortium[19], a private/government academic partnership from The White House's Office of Science and Technology Policy[20] that seeks to expedite applications for advanced computing research to combat the COVID-19 pandemic.

Severe acute respiratory syndrome (SARS) was the first new infectious disease identified in the 21st century, and as the world learned more about it, The World Health Organization identified this new coronavirus (SARS-CoV) as the agent that caused the outbreak.

[18] doi.org/10.1016/j.pbiomolbio.2019.03.004

[19] https://covid19-hpc-consortium.org/

[20] https://www.whitehouse.gov/briefings-statements/white-house-announces-new-partnership-unleash-u-s-supercomputing-resources-fight-covid-19/

SARS-CoV-2 Infection Structural Model

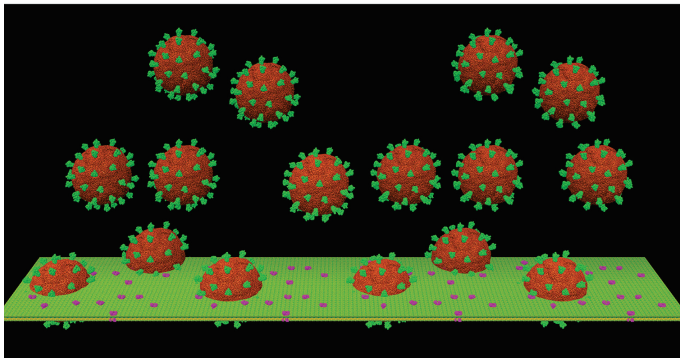


Figure 7: Structural model of SARS-CoV-2 infection. This structural model was built with UCSF Chimera using high-performance computers (*Bridges Large* and *Frontera*). The model shows 16 viruses, with the spike proteins shown in green (PDB ID: 6VSB) and an actual lipid bilayer membrane, with ACE2 dimers shown in magenta. All these structures are at atomic resolution. The length of the membrane is approximately 1 micrometer. Credit: Victor Padilla-Sanchez, The Catholic University of America

Now we're in the middle of yet another new coronavirus (SARS-CoV-2). COVID-19, the disease caused by SARS-CoV-2, has become a rapidly spreading pandemic that has reached most countries in the world. To date, there are not any vaccines or therapeutics to fight the illness.

Since both illnesses (SARS-CoV and SARS-CoV-2) share the same spike protein, the entry key that allows the virus into the human cells, Padilla-Sanchez's idea was to take the antibodies found in the first outbreak in 2002—80R and m396—and reengineer them to fit the current COVID-19 virus.

A June 2020 study[21] in the online journal, *Research Ideas and Outcomes*, describes efforts by Padilla-Sanchez to unravel this problem using computer simulation. He discovered that sequence differences prevent 80R and m396 from binding to COVID-19.

"Understanding why 80R and m396 did not bind to the SARS-CoV-2 spike protein could pave the way to engineering new antibodies that are effective," Padilla-Sanchez said. "Mutated versions of the 80R and m396 antibodies can be produced and administered as a therapeutic to fight the disease and prevent infection."

His docking experiments showed that amino acid substitutions in 80R and m396 should increase binding interactions between the antibodies and SARS-CoV-2, providing new antibodies to neutralize the virus (see Figure 7).

"Now, I need to prove it in the lab," he said.

The XSEDE-allocated *Stampede2* and *Bridges* systems at the Texas Advanced Computing Center (TACC) and Pittsburgh Supercomputer Center (PSC) supported the docking experiments, macromolecular assemblies, and large-scale analysis and visualization.

"XSEDE resources were essential to this research," Padilla-Sanchez said.

He ran the docking experiments on *Stampede2* using the Rosetta software suite[22], which includes algorithms for computational modeling and analysis of protein structures.

TACC's *Frontera* supercomputer, the 8th most powerful supercomputer in the world and the fastest supercomputer on a university campus, also provided vital help to Padilla-Sanchez. He used the Chimera software[23] on *Frontera* to generate extremely high-resolution visualizations. From there, he transferred the work to *Bridges* because of its large memory nodes.

"*Frontera* has great performance when importing a lot of big data. We're usually able to look at just protein interactions, but with *Frontera* and *Bridges*, we were able to study full infection processes in the computer," he said.

[21] https://riojournal.com/article/55281/

[22] https://www.rosettacommons.org/software

[23] https://www.cgl.ucsf.edu/chimera/

Padilla-Sanchez's findings will be tested in a wet lab. Upon successful completion of that stage, his work can proceed to human trials.

Currently, various labs across the world are already testing vaccines.

"If we don't find a vaccine in the near term we still have passive immunity, which can prevent infection for several months as long as you have the antibodies," Padilla-Sanchez said. "Of course, a vaccine is the best outcome. However, passive immunity may be a fast track in providing relief for the pandemic."

Molecular graphics and analyses were performed with UCSF *Chimera*, developed by the Resource for Biocomputing, Visualization, and Informatics at the University of California, San Francisco, with support from NIH P41-GM103311. Computational support from XSEDE was provided via Grant MCB200052.

2.8. NSF Awards 12-Month Extension for XSEDE 2.0 Project

The National Science Foundation's Office of Advanced Cyberinfrastructure has awarded XSEDE 2.0 an additional year in funding that will provide support for ongoing project operations until August 31, 2022. The $21.8M, 12-month extension enables XSEDE to continue its mission of accelerating open science discovery, enhancing user productivity, broadening participation in science and engineering, and engaging a new diverse generation of computational researchers.

"We are very pleased to have been awarded this extension of the XEDE project by the NSF. It is a testament to the success XSEDE has exhibited in supporting the national research community spanning a wide range of domains, and we look forward to continuing to enable researchers to discover more with XSEDE," says John Towns, XSEDE principal investigator and project director, and executive director of science and technology at NCSA.

In keeping with the existing project scope, the XSEDE team will continue with many activities that have been pursued in the first five years of the project, using the supplemental year to build on existing successes. While this additional year (the 11th year of XSEDE as a resource to the community supported by two rounds of funding) is expected to be a year of transition, the project remains fully committed to providing the best services and adapting them to meet the evolving needs of the advanced research community.

As in previous years, the project expects to produce many lay-friendly and technical publications that benefit both the general and technical communities continuing to document the high-impact scientific advances enabled by XSEDE. Stories from a broad range of disciplines will continue to be published regularly and added to XSEDE's expansive collection of successes. In conjunction with our Service Provider (SP) partners, documentation and success stories are accessible on the XSEDE website.

2.9. NSF Funds Five New XSEDE-Allocated Systems

This summer, five new National Science Foundation (NSF)-funded advanced computing systems have been awarded to partner institutions across the country, all with their own unique specialties and applications. Once deployed, all of these systems will be primarily allocated through XSEDE to help connect researchers, regardless of physical location in the United States, to the system that best suits their research needs.

"The recent announcements of awards by the NSF is a clear indicator of the NSF's re-commitment to providing critical advanced research computing capabilities to enable research in the United States and beyond," said John Towns, principal investigator and project director

of XSEDE. "These resources will enable research across all fields of scholarly pursuit and XSEDE stands ready to engage researchers in harnessing these resources."

These new machines continue XSEDE's robust demonstrated tradition of world-class, cutting-edge research, including a commitment to emerging domains like Artificial Intelligence, Big Data, Machine Learning, and more.

Read more about each system here, and click the system name to read the full press release:

Jetstream 2[24] (Indiana University — Lead / Texas Advanced Computing Center / University of Arizona / Johns Hopkins University, University Corporation for Atmospheric Research / Cornell University / University of Hawaii)

The NSF has awarded a $10 million grant to deploy *Jetstream 2*[25], a distributed cloud computing system to support on-demand research, artificial intelligence, and enhanced large-scale data analyses for the nation. The project is led by the Pervasive Technology Institute[26] at Indiana University. *Jetstream 2* is a follow-on project to *Jetstream*, which was funded in 2014 as the NSF's first production science and engineering research cloud system for the nation.

Delta[27] (National Center for Supercomputing Applications)

NCSA will integrate *Delta* into the national cyberinfrastructure ecosystem through XSEDE. Integration into XSEDE allows Delta to leverage the substantial portfolio of services and support offered therein and together deliver unprecedented advances in researcher productivity. This collaboration will promote synergy among multi-site workflows that include campus, national, and commercial cloud resources.

Anvil[28] (Purdue University)

Anvil, which is funded by a $10 million award from the NSF, will significantly increase the capacity available to XSEDE, which Purdue has been a partner for the past nine years. *Anvil* will enter production in 2021 and will serve researchers for five years. Additional funding from the NSF will support *Anvil*'s operations and user support.

Neocortex[29] (Pittsburgh Supercomputing Center)

A $5 million NSF award[30] will allow PSC to deploy a unique high-performance artificial intelligence (AI) system. Neocortex will introduce fundamentally new hardware to greatly speed AI research. PSC, a joint research organization of Carnegie Mellon University and the University of Pittsburgh,

[24] https://news.iu.edu/stories/2020/06/iub/releases/01-jetstream-cloud-computing-awarded-nsf-grant.html

[25] https://nsf.gov/awardsearch/showAward?AWD_ID=2005506&HistoricalAwards=false

[26] https://pti.iu.edu

[27] http://www.ncsa.illinois.edu/news/story/nsf_awards_ncsa_10_million_for_deployment_of_delta

[28] https://www.purdue.edu/newsroom/releases/2020/Q2/purdue-receives-10-million-from-national-science-foundation-for-anvil-supercomputer.html

[29] https://www.psc.edu/3206-nsf-funds-neocortex-a-groundbreaking-ai-supercomputer-at-psc-2

[30] https://www.nsf.gov/awardsearch/showAward?AWD_ID=2005597&HistoricalAwards=false

will build the new supercomputer in partnership with Cerebras Systems[31] and Hewlett Packard Enterprise[32].

Voyager[33] (San Diego Supercomputing Center)

The NSF has awarded SDSC at UC San Diego a $5 million grant to develop a high-performance resource for conducting artificial intelligence research across a wide swath of science and engineering domains. Called Voyager, the system will be the first-of-its-kind available in the NSF resource portfolio. In addition to the $5 million acquisition award, an equivalent amount of funding is expected to support community engagement and operation of the resource.

[31] https://www.cerebras.net
[32] https://www.hpe.com/us/en/home.html
[33] https://www.sdsc.edu/News%20Items/PR20200701_voyager.html

3. Discussion of Strategic Goals and Key Performance Indicators

The strategic goals of XSEDE (§1.1) cover a considerable scope. Additionally, the specific activities within XSEDE's scope are often very detailed; therefore, to ensure that this significant and detailed scope will ultimately deliver and realize the project's mission and vision, the three strategic goals are decomposed into components or sub-goals to be considered individually.

In determining the best measures of progress toward each of the sub-goals, KPIs that correlate to impact on the scientific community are used. These often pair measurements of outcome with an assessment of quality or impact to provide both a sense of scope and significance of the supporting activities.

3.1. Deepen and Extend Use

XSEDE will 1) *deepen the use—make more effective use*—of the advanced digital services ecosystem by existing scholars, researchers, and engineers and 2) *extend the use* to new communities. XSEDE will 3) *contribute to preparation—workforce development*—of scholars, researchers, and engineers in the use of advanced digital technologies via training, education, and outreach; and XSEDE will 4) *raise the general awareness of the value of advanced digital research services*.

3.1.1. Deepening Use to Existing Communities

XSEDE engages in a range of activities that serve to deepen use including identifying new technologies and new service providers, evolving the e-infrastructure, and enhancing the research prowess of current and future researchers. However, the ongoing use of resources and services available via XSEDE is the key indicator of this deepening use. As a result, the project has chosen three KPIs (Table 3-1) that together measure the ongoing engagement with the community with an emphasis on exposing the diversity of those consuming these services: 1) number of sustained users of XSEDE resources and services via the portal, 2) number of sustained underrepresented individuals using XSEDE resources and services via the portal, and 3) percentage of sustained allocation users from non-traditional disciplines of XSEDE resources and services.

Table 3–1: KPIs for the sub-goal of deepen use (existing communities).

KPI	Report Year	Target	RP1	RP2	RP3	RP4	Total	Owner
Number of sustained users of XSEDE resources and services via the portal[1]	RY5	4,500/ qtr	4,644	4,489				CEE (§4)
	RY4	3,500/ qtr	4,137	4,728	4,070	4,615	6,578	
	RY3	3,500/ qtr	4,196	4,089	3,099	4,864	6,851	
	RY2	3,000/ qtr	3,962	3,754	2,488	3,020	4,527	
	RY1	>5,000/ qtr	*	4,755	4,446	4,924	6,186	
Number of sustained under-represented individuals using XSEDE resources and	RY5	1,750/ yr	831	805				CEE (§4)
	RY4	1,750/ yr	625	809	564	705	1,014	
	RY3	1,500/ yr	529	509[1]	343	636	1,818	

KPI	Report Year	Target	RP1	RP2	RP3	RP4	Total	Owner
services via the portal[1]	RY2	1,500/ yr	490	408	296	402	1,053[1]	
	RY1	>1,000/ yr	*	322	238	535	649[1]	
Percentage of sustained allocation users from non-traditional disciplines of XSEDE resources and services	RY5	33%/yr	23.2	23.8				ECSS (§5)
	RY4	22%/yr	21.1	22.7	23.0	23.5	30.4	
	RY3	20%/qtr	22.1	20.7	25.8	22.7	22.8	
	RY2	*	21.5	20.4	21.1	21.0	21.0	
	RY1	*	*	18.2	19.9	18.6	18.9	

[1] The totals of these KPIs do not equal the sum of the data from each reporting period because one person could be counted as a sustained user/individual in more than one reporting period if they continue to log in for multiple reporting periods; however, they will only be counted once in the total.

The number of sustained users of XSEDE resources and services is slightly under the target but not of particular alarm this reporting period. The number of sustained users of XSEDE resources and services identifying as underrepresented minorities (URM) is strong for this current reporting period and is in line with the number that came in last year during this reporting period. Those who are aware of XSEDE resources and have previously used XSEDE resources are continuing usage.

The percentage of sustained allocation users from non-traditional disciplines is an annual metric. Intermediate reporting period results show a slightly increasing trend.

3.1.2. Extending Use to New Communities

New communities are defined as fields of science, industry, and underrepresented communities that represent less than one percent of XSEDE Resource Allocation Committee (XRAC) allocations. The Novel & Innovative Projects (NIP) team and the Broadening Participation team both work to bring advanced digital services to new communities. XSEDE measures both the number of new users and the number of new users on research projects from underrepresented communities and non-traditional disciplines of XSEDE resources and services as the indicators of progress (Table 3–2)

Table 3–2: KPIs for the sub-goal of extend use (new communities).

KPI	Report Year	Target	RP1	RP2	RP3	RP4	Total	Owner
Number of new users of XSEDE resources and services via the portal	RY5	2,500/qtr	2,157	2,612				CEE (§4)
	RY4	3,000/qtr	2,415	3,209	2,365	3,089	11,078	
	RY3	3,000/qtr	1,905	2,763	2,527[1]	2,757	9,952	
	RY2	2,000/qtr	2,305	2,813	2,346	2,917	10,381	
	RY1	>1,000/qtr	*	1,973	1,849	2,359	6,181	
	RY5	250/qtr	301	159				CEE (§4)

KPI	Report Year	Target	RP1	RP2	RP3	RP4	Total	Owner
Number of new underrepresented individuals using XSEDE resources and services via the portal	RY4	175/qtr	380	332	214	400	1,326	
	RY3	200/qtr	134	155	129	238	656	
	RY2	150/qtr	251	175	222	234	882	
	RY1	100/qtr	*	150	135	240	525	
Percentage of new allocation users from non-traditional disciplines of XSEDE resources and services	RY5	35%/yr	30.1	35.0				ECSS (§5)
	RY4	35%/yr	26.4	37.1	33.4	38.4	34.8	
	RY3	30%/yr	33.1	26.0	38.7	32.5	32.8	
	RY2	*	24.8	26.0	26.6	33.9	27.8	
	RY1	*	*	21.8	24.9	31.0	25.7	

The number of new users exceeded the target this reporting period, but the number of new users identifying as URM is significantly lower than the target. Pre-COVID outreach to researchers from URM groups relied on campus visits and in-person interaction at conferences such as the ACM Richard Tapia Celebration of Diversity in Computing and Society for Advancement of Chicanos/Hispanics and Native Americans in Science (SACNAS). Most campuses are operating with restrictions due to COVID-19. Fall conferences are virtual and visits to the virtual exhibits floor are low and have had minimal interaction. Alternative ways to interact with and contact potential new users are being investigated as COVID restrictions continue.

The percentage of new allocation users from non-traditional disciplines is an annual metric.

3.1.3. Prepare the Current and Next Generation

Part of XSEDE's mission is to provide a broad community of existing and future researchers with access and training to use advanced digital services via the sub-goal of preparing the current and next generation of computationally-savvy researchers. While many activities support this sub-goal, such as the various Champion (§4.6), Student Engagement (§4.4), and Education (§4.2) programs, the training offered through Community Engagement & Enrichment (CEE) impacts the most people directly. Therefore, the key indicator (Table 3-3) of performance toward this goal, which is reflective of industry standards, is the number of participant hours of live training delivered by XSEDE.

Table 3–3: KPI for the sub-goal of preparing the current and next generation.

KPI	Report Year	Target	RP1	RP2	RP3	RP4	Total	Owner
Number of participant hours of live training delivered by XSEDE[1]	RY5	40,000 hrs/yr	19,751	16,111				CEE (§4)
	RY4	40,000 hrs/yr	15,461	16,135	6,380	12,667	50,643	
	RY3	40,000 hrs/yr	14,140	8,274	7,259	12,352	42,025	
	RY2	NA	12,787	8,876	6,004	14,753	42,421	
	RY1	NA	5,994	3,770	5,180	9,199	24,143	

[1]This was a new KPI in RY3. Data provided for RY1 and RY2 was reported retroactively.

The number of training hours is on track to meet or exceed the annual target. The training team pivoted all synchronous trainings to online formats shortly after COVID travel and in-person gathering restrictions were put in place.

3.1.4. Raising Awareness

While many activities led by teams throughout the XSEDE organization, such as Workforce Development (§4.2), User Engagement (§4.3), Broadening Participation (§4.4), and Campus Engagement (§4.6) contribute to the ability to raise the general awareness of the value of advanced digital research services, the project has chosen to focus on measures in two areas (Table 3-4): user input and social media. Desirable trends in these key outcomes can be correlated to success for this sub-goal.

Table 3–4: KPIs for the sub-goal of raise awareness of the value of advanced digital research.

KPI	Report Year	Target	RP1	RP2	RP3	RP4	Total	Owner
Grand (aggregate) mean rating of XSEDE User Survey awareness items regarding XSEDE resources and services (1-5 Likert scale)	RY5	3.7 of 5/ yr	3.8	-				PgO (§9)
	RY4	3.7 of 5/ yr	3.8	-	-	-	3.8	
	RY3	3.5 of 5/ yr	3.7	-	-	-	3.7	
	RY2	*	3.6	-	-	-	3.6	
	RY1	*	*	-	-	-	NA	
Number of social media impressions over time[1]	RY5	430,000/yr	86,046	101,394				PgO (§9)
	RY4	426,198/yr	87,482	75,164	84,185	110,904	357,735	
	RY3	359,714/yr	112,806	63,269	93,803	85,287	355,165	
	RY2	NA	69,607	55,506	59,490	128,180	312,783	
	RY1	NA	*	52,200	128,675	88,332	269,207	

- Data reported annually

[1] This was the new KPI in RY3. Data provided for RY1 and RY2 was reported retroactively. Beginning in RY5, this KPI is calculated as the number of social media impressions with the annual target calculated based on a 20% increase over the previous year.

"Grand (aggregate) mean of XSEDE User Survey awareness items regarding XSEDE resources and services" is reported annually in RP1 based on XSEDE User Survey results, so there is no data to report during this reporting period.

In the second reporting period of this year, social media impressions are steadily increasing after a low first quarter, and were above average compared to past individual reporting periods. The External Relations (ER) team is encouraged by this growth and believes it to be an indication of a growing preference for XSEDE's original content due to consistent posting, as well as new targeted promotions by partner sites' social media accounts, coordinated through the ER team. There will be more increase required to meet the annual goal—the remaining two quarters must average ~120,000 impressions

each, which the ER team believes is an attainable goal given SC20's virtual format and a full editorial calendar to round out the year. Historically, RP3 and RP4 generate more impressions than RP1 and RP2, but the ER team is unclear if that will change due to external factors induced by the COVID-19 pandemic, including an all-virtual SC20. To maintain progress, the ER team will monitor social impressions very closely throughout November. If it becomes clear that an SC20 campaign generates markedly less engagement compared to years previous, ER will make recommendations around a social media campaign with the potential of promoted content across social platforms. This can be used to increase our follower base, promote a specific story, or share a lighter, more informal Q+A campaign.

3.2. Advance the Ecosystem

Exploiting its internal efforts and drawing on those of others, XSEDE will advance the broader ecosystem of advanced digital services by 1) *creating an open and evolving e-infrastructure*, and by 2) *enhancing the array of technical expertise and support services* offered.

3.2.1. Create an Open and Evolving e-Infrastructure

There are a variety of factors that affect the evolution of the e-infrastructure. These range from external factors, such as the number of XSEDE Federation members and the variety of services they provide, to internal factors, like Operations (§7) of critical infrastructure and services and the evaluation and integration of new capabilities. While XSEDE actively seeks new Federation members and Service Providers, as well as partnerships with national and international cyberinfrastructure projects, the group views their role as connectors of these elements to have the most impact. Thus, XSEDE focuses on the number of new capabilities in production as an indicator of performance with respect to this sub-goal (Table 3-5).

Table 3–5: KPI for the sub-goal of create an open and evolving e-infrastructure.

KPI	Report Year	Target	RP1	RP2	RP3	RP4	Total	Owner
Total number of capabilities in production[1]	RY5	110	102	104				XCI (§6)
	RY4	100	88	88	91	102	102	
	RY3	81	76	85	87	87	87	
	RY2	NA	72	74	74	75	75	
	RY1	NA	*	63	63	69	69	

[1] This was a new KPI in RY3. Data provided for RY1 and RY2 was reported retroactively.

Although the team has delivered slightly less than half the capabilities planned for the year (4 of 10), it is on track to reach the yearly target for "Total number of capabilities in production." There are several capabilities in progress that are close to delivery and several more that could be delivered by the end of the reporting year.

3.2.2. Enhance the Array of Technical Expertise and Support Services

To enhance the technical expertise of XSEDE's staff to offer an evolving set of support services, the project will continue many activities including workshops, symposia, and training events hosted by Extended Collaborative Support Services (ECSS) and Service Providers (§5.6). The KPI for this is feedback provided from the XSEDE user-base through the annual user survey (Table 3-6).

Table 3–6: KPI for the sub-goal of enhance the array of technical expertise and support services.

KPI	Report Year	Target	RP1	RP2	RP3	RP4	Total	Owner
Grand (aggregate) mean rating of XSEDE User Survey satisfaction items regarding XSEDE technical support services[1] (1-5 Likert scale)	RY5	3.5 of 5/ yr	4.4	-				PgO (§9)
	RY4	3.5 of 5/ yr	3.9	-	-	-	3.9	
	RY3	3.5 of 5/ yr	3.6	-	-	-	3.6	
	RY2	NA	3.4	-	-	-	3.4	
	RY1	*	*	*	*	*	*	

- Data reported annually.
[1] This is a new KPI in RY3. Data provided for RY2 was reported retroactively.

"Grand (aggregate) mean of XSEDE User Survey satisfaction items regarding XSEDE technical support services" is reported annually in RP1 based on XSEDE User Survey results, so there is no data to report during this reporting period.

3.3. Sustain the Ecosystem

XSEDE will sustain the advanced digital services ecosystem by 1) *ensuring and maintaining a reliable, efficient, and secure infrastructure*, and 2) *providing excellent user support services*. Furthermore, XSEDE will operate an 3) *effective*, 4) *productive*, and 5) *innovative virtual organization*.

3.3.1. Provide Reliable, Efficient, and Secure Infrastructure

Many activities support the provisioning and support of reliable, efficient and secure infrastructure—such as User Interfaces & Online Information (§4.5), Security (§7.2), Data Transfer Services (§7.3), Systems Operations and Support (§7.5), support for Allocations (§8.2), and Allocations, Accounting & Account Management (§8.3)—but perhaps the truest measure of an infrastructure's reliability is its robustness as reflected by sustained availability. Thus, the KPI for this sub-goal is the mean composite availability of core services, shown as a percentage (Table 3-7), measured as a geometric mean. This is a composite measure of the availability of critical enterprise services and the XRAS allocations request management service.

Table 3–7: KPI for the sub-goal of provide reliable, efficient, and secure infrastructure.

KPI	Report Year	Target	RP1	RP2	RP3	RP4	Total	Owner
Mean composite availability of core services (%)	RY5	99.9%/qtr	99.9	99.9				Ops (§7)
	RY4	99.9%/qtr	99.9	99.9	99.9	99.9	99.9	
	RY3	99.9%/qtr	99.9	99.9	99.9	99.9	99.9	
	RY2	99.9%/qtr	99.8	99.9	99.9	99.9	99.9	
	RY1	99.0%/qtr	*	99.9	99.9	99.9	99.9	

The "Mean composite availability of core services" remained high for the eleventh consecutive reporting period, yet again meeting the target of 99.9 percent.

3.3.2. Provide Excellent User Support

Although nearly every group in the organization has some support function, XSEDE has chosen to focus on metrics with respect to two primary support interfaces to the community: the XSEDE Operations Center (XOC) and the Resource Allocation Services (RAS) team. The XOC is the frontline centralized support group that either resolves or escalates tickets to the appropriate resolution center depending on the request. RAS is responsible for the allocations process and the allocation request system. These two support interfaces are the focus for gauging the progress towards achieving the sub-goal of providing excellent user support, specifically: 1) the mean time to resolution on support tickets that are resolved by the XOC or routed to, and resolved by, other XSEDE areas, 2) the aggregate mean rating of user satisfaction with allocations process and support services measured via a quarterly survey of users who have interacted with the allocations request system and the allocations process more generally, and 3) the percentage of research requests successful (not rejected) determined following the quarterly allocations session (Table 3-8).

Table 3–8: KPIs for the sub-goal of provide excellent user support.

KPI	Report Year	Target	RP1	RP2	RP3	RP4	Total	Owner
Mean time to ticket resolution (hours)	RY5	< 16 hrs/qtr	15.3	23.2				Ops (§7)
	RY4	< 16 hrs/qtr	14.0	14.6	21.0	14.3	16.0	
	RY3	< 16 hrs/qtr	12.3	18.5	23.2	17.5	17.9	
	RY2	< 24 hrs/qtr	26.0	20.1	22.8	15.0	21.0	
	RY1	< 24 hrs/qtr	*	24.0	28.2	23.1	25.1	
Mean rating of user satisfaction with allocations process and support services[1] (1-5 Likert scale)	RY5	4 of 5/yr	4.4	4.3				RAS (§8)
	RY4	4 of 5/yr	4.2	4.3	4.4	4.2	4.3	
	RY3	4 of 5/yr	4.1	4.2	4.1	4.4	4.2	
	RY2	4 of 5/yr	4.1	4.0	4.1	3.9	4.0	
	RY1	4 of 5/yr	*	4.0	4.0	4.0	4.0	
Percentage of research requests successful (not rejected)	RY5	85.0%/qtr	80.0	84.0				RAS (§8)
	RY4	85.0%/qtr	81.0	80.0	78.0	87.0	82.0	
	RY3	85.0%/qtr	65.0	70.0	72.0	75.0	70.5	
	RY2	85.0%/qtr	70.0	69.0	72.0	68.0	69.8	
	RY1	85.0%/qtr	*	76.0	75.0	74.0	75.0	

[1] KPI name updated in RY4.

The "Mean time to ticket resolution (MTTR)" this reporting period was a disappointing 23.2 hours, exceeding the target goal of less than 16 hours. Though the XSEDE Operations Center (XOC) continues to resolve tickets expeditiously with an MTTR of less than 30 minutes, tickets in some of the WBS

queues had unusually lengthy resolution times, pushing the overall average above the target. Operations will hold a ticket handling session during the December Quarterly Staff Meeting with the goal of improving ticket handling practices across all WBSs.

Resource Allocation Service (RAS) continues to receive satisfaction ratings above the target of 4.0 (out of 5) for both the allocations process as whole, as well as the XSEDE Resource Allocations System (XRAS), despite continuing high request levels for the quarterly Research opportunity. The target of 4.0 will remain given the uncertain and qualitative nature of this metric, as well as the regular reductions to recommended amounts for Research allocations.

3.3.3. Effective and Productive Virtual Organization

During the first five years of XSEDE, in conjunction with developing a methodology for driving and assessing performance excellence, XSEDE adopted the Baldrige Criteria[34] and has assessed and applied criteria from all seven criteria by that methodology. These include annual reviews of the vision, mission, strategic goals, project-wide processes and standards (KPIs); user and staff surveys (§4.3, §9.5); stakeholder communications (§9.2); advisory boards (§9.1); community engagement (§4); workforce development (§4.2); and the analysis of organizational data that leads to organizational learning, strategic improvement, and innovation. With this foundation, it is now appropriate to look to the XSEDE users to give an indication of the project's effectiveness by rating the importance of the resources and services provided by XSEDE (Table 3-9).

Table 3–9: KPIs for the sub-goal of operate an effective and productive virtual organization.

KPI	Report Year	Target	RP1	RP2	RP3	RP4	Total	Owner
Mean rating of importance of XSEDE resources and services to researcher productivity z(1-5 Likert scale)	RY5	4.4 of 5/yr	4.2	-				PgO (§9)
	RY4	4.4 of 5/yr	4.2	-	-	-	4.2	
	RY3	4.2 of 5/yr	4.4	-	-	-	4.4	
	RY2	NA	4.4[2]	-	-	-	4.4	
	RY1	NA	4.3[2]	-	-	-	4.3	
Percentage of users who indicate the use of XSEDE-managed and/or XSEDE-associated resources in the creation of their work product[1]	RY5	80%/yr	83	-				PgO (§9)
	RY4	80%/yr	79	-	-	-	79	
	RY3	79%/yr	79	-	-	-	79	
	RY2	*	*	*	*	*	*	
	RY1	*	*	*	*	*	*	

[1] New KPI added in RY3 RP2.
[2] These historical numbers are based on other survey data that was vaguely related to this KPI. We created a new survey item in RY3 to address it directly.
- Data reported annually.

Both of these KPIs are reported annually in RP1 based on XSEDE User Survey results, so there is no data to report during this reporting period.

[34] https://www.nist.gov/baldrige/

3.3.4. Innovative Virtual Organization

Measuring innovation for an organization like XSEDE (or for organizations in general) is difficult and represents an area of open research. After much thought and discussion both internally and with external stakeholders and advisors, XSEDE has identified two indicators that correlate to innovation within the project: 1) percentage of Project Improvement Fund proposals resulting in innovations in the XSEDE organization and 2) mean rating of innovation within the organization by XSEDE staff (Table 3-10). The first indicator is a measurement of XSEDE's ability to fund smaller innovative improvements within the project; the second measures how staff rate the level of innovation within the project. These KPIs will continue to be the subject of an open conversation within the organization and with stakeholders and advisors as XSEDE assesses these measurements and how to best quantify innovation.

Table 3–10: KPIs for the sub-goal of operate an innovative virtual organization.

KPI	Report Year	Target	RP1	RP2	RP3	RP4	Total	Owner
Percentage of Project Improvement Fund funded projects resulting in innovations in the XSEDE organization	RY5	70%/yr	-	-				PgO (§9)
	RY4	70%/yr	-	-	-	66.7	66.7	
	RY3	60%/yr	-	-	-	71.4	71.4	
	RY2	*	*	*	*	*	*	
	RY1	*	*	*	*	*	*	
Mean rating of innovation within the organization by XSEDE staff (1-5 Likert scale)	RY5	4 of 5/yr	-	4.2				PgO (§9)
	RY4	4 of 5/yr	-	4.0	-	-	4.0	
	RY3	3.5 of 5/yr	-	4.0	-	-	4.0	
	RY2	*	*	*	*	*	*	
	RY1	*	*	*	*	*	*	

- Data reported annually.

"Percentage of Project Improvement Fund funded projects resulting in innovations in the XSEDE organization" is reported annually in RP4, so there is no data to report at this time.

"Mean rating of innovation within the organization by XSEDE staff" exceeded its goal this year.

4. Community Engagement & Enrichment (WBS 2.1)

Community Engagement & Enrichment (CEE) sits at the front lines of XSEDE and is tasked with balancing support for a large and diverse portfolio of existing users and the broader population of potential users and future leaders in cyberinfrastructure. While maintaining high quality support for existing users engaged in science at all levels, CEE is concerned with training and educating future generations and trying to creatively address what has been widely accepted as a leaky pipeline of potential users, leaders, practitioners, and researchers.

At the core of Community Engagement & Enrichment (CEE) is the researcher, broadly defined to include anyone who uses or may potentially use the array of resources and services offered by XSEDE. The CEE team is dedicated to actively engaging a broad and diverse cross-section of the open science community, bringing together those interested in using, integrating with, enabling, and enhancing the national cyberinfrastructure. Vital to the CEE mission is the persistent relationship with existing and future users, including allocated users, training participants, XSEDE collaborators, and campus personnel. CEE will unify public offerings to provide a more consistent, clear, and concise message about XSEDE resources and services, and bring together those aspects of XSEDE that have as their mission teaching, informing, and engaging those interested in advanced cyberinfrastructure.

The five components of CEE are Workforce Development (§4.2), which includes Training, Education and Student Preparation, User Engagement (§4.3), Broadening Participation (§4.4), User Interfaces & Online Information (§4.5), and Campus Engagement (§4.6). These five teams ensure routine collection and reporting of XSEDE's actions to address user requirements. They provide a consistent suite of web-based information and documentation and engage with a broad range of campus personnel to ensure that XSEDE's resources and services complement those offered by campuses. Additionally, CEE teams expand workforce development efforts to enable many more researchers, faculty, staff, and students to make effective use of local, regional, and national advanced digital resources. CEE expands efforts to broaden the diversity of the community utilizing advanced digital resources.

The success of the CEE team depends on effective collaboration across all L2 areas of the project. Specifically, User Engagement works closely with RAS and ECSS to establish a dialogue with XSEDE's User Community in order to better understand their needs and desires. Workforce Development and Broadening Participation partner with ECSS to develop impactful training and education opportunities for the community, especially underrepresented students, researchers, and faculty. The User Interfaces & Online Information team relies heavily on all areas of the project to ensure that the website remains accurate and informative. The Campus Engagement team likewise depends on all parts of the project to facilitate the effective participation of a diverse national community of campuses in the application of advanced digital resources and services to accelerate discovery, enhance education, and foster scholarly achievement.

CEE is focused on personal interactions, ensuring that existing users, potential users, and the general public have sufficient access to materials and have a positive and effective experience with XSEDE public offerings and frontline user support. As such, the CEE Key Performance Indicators are designed to broadly assess this performance. CEE focuses on metrics that quantify how many users in aggregate are benefiting from XSEDE resources and services. Additionally, CEE focuses on how well the user base is sustained over time and how well training offerings evolve with changing user community needs.

Key Performance Indicators for CEE are listed in the table below. Additional information about these KPIs can be found on the XSEDE KPIs & Metrics wiki page.

For other metrics with respect to this WBS, see Appendix §12.2.2.1.

Table 4–1: KPIs for Community Engagement & Enrichment.

Area Metric	Report Year	Target	RP1	RP2	RP3	RP4	Total	Sub-goal Supported
Number of students benefiting from XSEDE resources and services through training, XSEDE projects, or conference attendance	RY5	2,000/ qtr	2,277	2,043				Deepen/ Extend — Prepare the current and next generation (§3.1.3)
	RY4	1,500/ qtr	2,210	2,634	1,649	2,252	6,196	
	RY3	1,250/ qtr	1,613	1,666	1,145	2,104	2,323	
	RY2	950/qtr	1,722	1,478	1,170	1,522	1,802	
	RY1	50/qtr	*	997	815	2,679	3,122	
Number of under-represented students benefiting from XSEDE resources and services through training, XSEDE projects, or conference attendance	RY5	650/qtr	741	632				Deepen/ Extend — Prepare the current and next generation (§3.1.3)
	RY4	500/qtr	674	974	492	753	2,072	
	RY3	625/qtr	449	438	307	436	1,630	
	RY2	475/qtr	488	399	347	423	1,104	
	RY1	50 / qtr	*	34	33	19	28	
Grand (aggregate) mean rating of Post Training Event Survey items related to training impact for attendees registered through the portal (1-5 Likert scale)	RY5	4.4 of 5 /qtr	4.6	4.5				Deepen/ Extend — Prepare the current and next generation (§3.1.3)
	RY4	4.4 of 5 /qtr	4.5	4.3	4.3	4.6	4.4	
	RY3	4.4 of 5 /qtr	4.5	4.4	4.5	4.3	4.4	
	RY2	4 of 5 /qtr	4.3	4.3	4.6	4.5	4.4	
	RY1	4 of 5 /qtr	*	4.5	4.4	4.3	4.4	
Number of institutions with a Champion	RY5	340	327	332				Deepen/ Extend — Deepen use to existing communities (§3.1.1)
	RY4	300	304	305	315	325	325	
	RY3	250	259	266	277	284	284	
	RY2	240	218	238	239	246	246	
	RY1	225	*	224	231	234	234	
Percentage of user requirements	RY5	98%/qtr	100 (16/16)	100 (20/20)				Sustain — Provide excellent user
	RY4	98%/qtr	100 (34/34)	96 (23/24)	100 (26/26)	97 (36/37)	98 (119/121)	

Area Metric	Report Year	Target	RP1	RP2	RP3	RP4	Total	Sub-goal Supported
addressed within 30 days	RY3	100%/ qtr	89 (40/45)	90 (47/52)	100 (36/36)	100 (27/27)	94 (150/160)	support (§3.3.2)
	RY2	100%/ qtr	78 (36/44)	102 (47/46)	86 (32/37)	93 (41/44)	91 (156/157)	
	RY1	100%/ qtr	*	50 (16/32)	89 (40/45)	75 (40/53)	74 (96/130)	

Despite Zoom fatigue and the demands of many institutions transitioning to online and remote delivery of their fall 2020 and (potentially spring 2021) semesters in response to COVID-19, the numbers of students benefiting from XSEDE resources and services continues to be strong. The number of students benefiting from XSEDE resources and services that identify as underrepresented minorities (URM) is slightly below the target for this reporting period and may be a reflection of the greater impact of COVID-19 on communities of color. Specifically, limited access to technology required for participation in virtual and remote activities has been a barrier to participation for communities of color. The primary barrier to participation that is beyond XSEDE's control is internet access and quality.

The grand (aggregate) mean rating of training impact is consistent with prior reporting periods.

The number of institutions with a Campus Champion continues to meet or exceed targets.

User Engagement (UE) connects with all active PIs every reporting period to ensure their projects are progressing and any issues their teams may be encountering are identified and addressed. UE relies on Service Providers (SPs) and other areas within XSEDE to engage on most issues, but, even so, the metric for the current reporting period remains consistent and has met the desired target for the reporting period. UE will continue to monitor this to determine if further action is warranted.

CEE Highlights

In support of XSEDE's diversity and inclusion goals, CEE is leading the XSEDE Terminology Task Force that is reviewing all XSEDE materials for language that creates barriers to diversity, equity, and inclusion. The taskforce has compiled a list of terms and has identified which ones XSEDE has jurisdiction or control over and those that require interaction with other organizations. All XSEDE L2 areas are participating in the effort. Additionally, many people both inside the XSEDE project and within the XSEDE user community have contributed by reporting terms.

Beau Christ (Wofford) recently obtained approval for a data science minor program, a result of mentoring from Kate Cahill (OSC) during Christ's 2019–2020 Campus Champion fellowship.

XSEDE recently updated longitudinal tracking data for the Advanced Computing for Social Change student program. Of the 108 total participants served since 2016, 65% are women, 63% are underrepresented minorities, and a majority of students have been recruited from institutions with limited research opportunities, including California State University, Los Angeles, and Chaminade University of Honolulu where XSEDE has delivered training. Data also shows effective engagement of students from non-STEM (science, technology, engineering, and math) disciplines and increased participation across XSEDE programs (e.g., Expert Mentoring Producing Opportunities for Work, Education, and Research (EMPOWER) and Student Champions). Collaboration in support of continued student engagement is referenced in shared positive student experiences:

> *Having participated in the XSEDE Advanced Computing for Social Change Institute and utilizing XSEDE resources for an independent data analysis project, I have learned so much and appreciate the community. . . . Prior to 2020, I was mostly involved with wet-lab science, but have been fascinated with applying computational skills and uniting bioinformatics with my foundation in wet-lab science.*

This has led me to be involved with XSEDE on my university campus as a Student Champion. – XSEDE EMPOWER applicant.

Of note, and directly due to XSEDE co-sponsoring the SPICE (Supporting Pacific Indigenous Computing Excellence) immersive program for Native Hawaiian and other Pacific Islander students, two staff members from the American Samoa Department of Health participated in mentored 10-week data science projects this past reporting period. Noelle Mageo studied factors contributing to the spread of COVID-19, particularly the effectiveness of keeping American Samoa's borders closed during the pandemic. Ruta Ropeti, a Maternal and Child Health Epidemiologist Tech, conducted a data driven investigation of Rheumatic Heart Disease in American Samoa. The studies were guided by both the SPICE faculty and liaisons at the American Samoa Department of Health. This engagement expanded XSEDE's student, faculty, and staff programs to American Samoa, with current persistent participation from Guam and the Hawaiian Islands.

4.1. CEE Director's Office (WBS 2.1.1)

The CEE Director's Office has been established to provide the necessary oversight to ensure the greatest efficiency and effectiveness of the CEE area. This oversight includes providing direction to the L3 management team, coordination of, and participation in, CEE planning activities and reports through the area's Project Manager, and monitoring compliance with budgets, and retarget effort if necessary. The Director's Office also attends and supports the preparation of project level reviews and activities.

The CEE Director's Office will continue to manage and set the direction for CEE activities and responsibilities. They will contribute to and attend bi-weekly Senior Management Team calls; contribute to the project level plan, schedule, and budget; contribute to XSEDE quarterly, annual, and other reports as required by the NSF; and attend XSEDE quarterly and annual meetings. Lastly, the Director's Office will advise the XSEDE PI on many issues, especially those relevant to this WBS area.

4.2. Workforce Development (WBS 2.1.2)

The Workforce Development mission is to provide a continuum of learning resources and services designed to address the needs and requirements of researchers, educators, developers, integrators, and students utilizing advanced digital resources. This includes providing professional development for XSEDE team members.

Workforce Development fulfills its mission through an integrated suite of training, education, and student preparation activities to address formal and informal learning about advanced digital resources. Workforce Development provides business and industry with access to XSEDE's workforce development efforts including training services and student internships that have historically proven beneficial to industry.

Workforce Development is comprised of three areas: Training, Education, and Student Preparation. The Training team develops and delivers training programs to enhance the skills of the national open science community and ensure productive use of XSEDE's cyberinfrastructure. The Education team works closely with Training and Student Preparation to support faculty in all fields of study with their incorporation of advanced digital technology capabilities within the undergraduate and graduate curriculum. The Student Preparation program actively recruits students to use the aforementioned training and education offerings to enable the use of XSEDE resources by undergraduate and graduate students to motivate and prepare them to pursue advanced studies and careers to advance discovery and scholarly studies.

Bob Panoff (Shodor) co-authored an article in the *Bulletin of Mathematical Biology*: "Agent-Based Modeling and Simulation in Mathematics and Biology Education." He has also continued to work with Wofford College faculty on incorporating computational thinking in courses. Beau Christ (Wofford)

recently obtained approval for a data science minor program, a result of mentoring from Kate Cahill (OSC) during Christ's 2019–2020 Campus Champion fellowship.

Twenty undergraduate students from 18 institutions were accepted for participation in the fall 2020 XSEDE EMPOWER program and began working on projects in a variety of research areas in computational science and HPC hardware support. Seven of the students are female, and seven are underrepresented minorities. The Campus Champions community, External Relations team, and Broadening Participation team remained instrumental in recruiting well-qualified students and mentors to the program as well as assisting with the application review process. One of students who has been participating in 2020 wrote,

> *The EMPOWER program kept me in school. I was considering taking a gap year due to the COVID-19 Pandemic, but my interest in research was strong enough to make me want to stay in school.*

Umairullah Khan (Portland State University), 2020 participant, said,

> *My work in [my mentor's lab], supported by the EMPOWER program, is actually the primary driver of my intent to pursue a computational research career in the life sciences. I have been exposed to a discipline and a community of scientists that I hope to contribute to and be a productive member of throughout my career. Moreover, the connections I've made so far will be invaluable in driving my future plans, into graduate school and beyond.*

Tanya Nesterova (University of Delaware) capped off a year of participation in EMPOWER by co-authoring an article in the *Journal of Chemical Physics*. Nicholas Grabill (Michigan State University) presented a poster about his summer 2020 EMPOWER work at a research symposium hosted by his university. Adith Srivatsa (Georgia Institute of Technology) prepared two posters about his EMPOWER work to be presented at the Biophysical Society Annual Meeting.

The training team continues to deliver synchronous training events with high user satisfaction and several training events introduced the new resources being deployed over the next several months.

- Monthly HPC workshops:
  - Aug 2020: XSEDE HPC Workshop: Big Data
  - Sep 2020: XSEDE HPC Workshop: MPI
  - Oct 2020: XSEDE HPC Workshop: Big Data
- Webinars:
  - *Comet* to *Expanse* Transition Tutorial
  - Writing a Successful XSEDE Allocation Proposal (offered twice)
  - XSEDE New User Training
  - XSEDE Code Performance and Scaling Training
  - *Expanse* 101: Accessing and Running Jobs on *Expanse*
  - Technical Overview of the Cerebras CS-1, the AI Compute Engine for *Neocortex*

Asynchronous training content additions and changes included:

- August 2020: CVW topic MATLAB Programming[35] Updated
- August 2020: Two outdated CVW topics were removed: VisIt and PerfExpert
- September 2020: CVW topic Python for Data Science Part 2[36] added

[35] https://cvw.cac.cornell.edu/matlab/
[36] https://cvw.cac.cornell.edu/pydatasci2/

The newest training roadmap, "Science Gateways: How-tos" was published and a new training Badge was issued this reporting period: XSEDE MPI Intermediate Badge. In addition, 25 badges were awarded (primarily the badge for XSEDE HPC Big Data Beginner).

For other metrics with respect to this WBS, see Appendix §12.2.2.1.1

4.3. User Engagement (WBS 2.1.3)

The mission of the User Engagement (UE) team is to capture community needs, requirements, and recommendations for improvements to XSEDE's resources and services, and to report to the national community how their feedback is being addressed. XSEDE places an emphasis on maintaining consistent user contact, traceability in tracking user issues, and closing the feedback loop.

UE continues to connect with all active PIs quarterly to ensure their projects are progressing and any issues their teams encounter are identified and addressed. In the current reporting period, inquiries were sent to 996 unique PIs: 88 responses were received, 20 issues were identified, and all 20 (100%) of these issues were addressed within 30 days. The goal is to completely address all issues within the reporting period, but UE relies on SPs and other areas within XSEDE to engage most issues. This KPI metric value for the current reporting period is consistent and has met the desired target for the reporting period.

For other metrics with respect to this WBS, see Appendix §12.2.2.1.2.

4.4. Broadening Participation (WBS 2.1.4)

Broadening Participation's mission is to engage underrepresented minority researchers from domains that are not traditional users of HPC and from Minority Serving Institutions. This target audience ranges from potential users with no computational experience to computationally savvy researchers, educators, Champions, and administrators who will promote change at their institutions for increased use of advanced digital services for research and teaching.

Broadening Participation will continue the most effective recruitment activities - conference exhibiting, campus visits, and regional workshops - while increasing national impact through new partnerships and the utilization of lower cost awareness strategies to continue the growth in new users from underrepresented communities. The Diversity Forum and the Minority Research Community listservs and community calls focus on user persistence in their use of XSEDE services and their deepening engagement through participation in committees such as the User Advisory Committee (UAC) and XSEDE Resource Allocations Committee (XRAC), and participation in Champions, Campus Bridging, and other programs. Persistent institutional engagement is enabled by curriculum reform and larger numbers of researchers adopting the use of advanced digital resources as a standard research method.

XSEDE recently updated longitudinal tracking data for the Advanced Computing for Social Change student program. Of the total 108 participants served since 2016, 65% are women, 63% are underrepresented minorities, and a majority of the students have been recruited from institutions with limited research opportunities, including California State University, Los Angeles, and Chaminade University of Honolulu where XSEDE has delivered training. Data also show effective engagement of students from non-STEM disciplines and increased participation across XSEDE programs (e.g., EMPOWER and Student Champions). Collaboration in support of continued student engagement is referenced in shared positive student experiences:

> *Having participated in the XSEDE Advanced Computing for Social Change Institute and utilizing XSEDE resources for an independent data analysis project, I have learned so much and appreciate the community. . . . Prior to 2020, I was mostly involved with wet-lab science, but have been fascinated with applying computational skills and uniting bioinformatics with my foundation in wet-lab science. This has led me to be involved with XSEDE on my university campus as a Student Champion.* – XSEDE EMPOWER applicant.

Broadening Participation exhibited at the ACM Tapia Celebration of Diversity in Computing and the Society for Advancement of Chicanos/Hispanics and Native Americans in Science (SACNAS). Both conferences were virtual, which resulted in conference attendees not being released from other responsibilities during the conference. Thus, attendees spent little time in general networking, which occurs more naturally in-person. Recruitment strategies for upcoming student programs will need to include inviting past participant peer referrals and less targeted, but more widely distributed, announcements of XSEDE student programs to larger mailing lists.

Campus visits have been restricted since March, and contact is mainly through email. Many faculty at smaller and minority-serving institutions (MSI) are facing challenges teaching in the online environment with significantly shortened semesters. We anticipate impact to recruitment of new users from URM groups and are working to identify strategies that can be used to mitigate impacts of the travel restrictions, limited access to campuses, and virtualization of conferences.

Linda Akli participated as a panelist on an American Association for the Advancement of Science (AAAS) panel, "Back to School and Out of School" in a New Paradigm of Teaching, Learning, and Conducting Research, that was attended by more than 100 faculty and students. Broadening Participation will be seeking similar opportunities to continue promotion of XSEDE resources and services to new communities; however, it will be more difficult to assess their success because analytics from these events and conferences are summarized.

For other metrics with respect to this WBS, see Appendix §12.2.2.1.3.

4.5. User Interfaces & Online Information (WBS 2.1.5)

User Interfaces & Online Information (UII) is committed to enabling the discovery, understanding, and effective utilization of XSEDE's powerful capabilities and services. Through UII's ongoing effort to improve and engage a variety of audiences via the XSEDE website and User Portal, UII has an immediate impact on a variety of stakeholders including the general public, potential and current users, educators, service providers, campus affiliates, and funding agencies. These stakeholders will gain valuable information about XSEDE through an information-rich website, the XSEDE User Portal, and a uniform set of user documentation.

The User Interfaces and Online Information team continued regular improvements and maintenance on the website and User Portal. This includes regular user guide updates and user documentation improvements. The team is actively completing development and testing of ORCID integration for publications and improving the account creation flow. The team also continues to support changes and improvements to the COVID-19 Consortium pages and process.

For other metrics with respect to this WBS, see Appendix §12.2.2.1.4.

4.6. Campus Engagement (WBS 2.1.6)

The Campus Engagement program promotes and facilitates the effective participation of a diverse national community of campuses in the application of advanced digital resources and services to accelerate discovery, enhance education, and foster scholarly achievement.

Campus Engagement, via the Campus Champions, works directly with institutions across the U.S. both to facilitate computing and data-intensive research and education, nationally and with collaborators worldwide, and to expand the scale, scope, ambition, and impact of these endeavors. This is done by increasing scalable, sustainable institutional uptake of advanced digital services from providers at all levels (workgroup, institutional, regional, national, and international), fostering a broader, deeper, more agile, more sustainable and more diverse nationwide cyberinfrastructure ecosystem across all levels, and cultivating inter-institutional interchange of resources, expertise, and support. Campus Engagement also aims to assist with the establishment and expansion of consortia (e.g., intra-state,

regional, domain-specific) that collaborate to better serve the needs of their advanced computing stakeholders.

While the pandemic restricted in-person meetings, it opened up the possibility to more people participating in virtual meetings. The virtual meetings included the usual Campus Champions, Campus Research Computing Consortium (CaRCC), and EDUCAUSE Research Computing and Data (RCD) Community Calls as well as new virtual meetings including, but not limited to, the Trusted CI Cybersecurity Summit, the CI CoE (Cyberinfrastructure Center of Excellence)/Cybersecurity workshop, the NSF CI workforce workshop (mentioned below), the Quilt Fall member meeting, Internet2's TechExtra Kickoff, the Eastern Regional Network's All-hands, and Open Science Grid's All-hands. Champions, who normally would not be able to travel to many of these events, were now able to participate and contribute on a scale not seen before, increasing the visibility not only of the Campus Champions, but of cyberinfrastructure professionals in general.

Campus Engagement co-manager Brunson served as co-PI for an NSF funded Cyberinfrastructure Workforce workshop that was held over three days in August and September. She also gave a keynote talk at the workshop highlighting the role that the Campus Champions program has played over the last decade as a community of practice for CI professionals who enable researchers to advance their computational and data intensive research. Many Campus Champions, including most of the elected leaders, were invited to participate and contribute to the workshop.

One of the outcomes from the workshop was the creation of a "Community of Communities" working group that is meeting biweekly and includes several Champions leadership team members: Julie Ma, Douglas Jennewein, Thomas Cheatham, and Dana Brunson. Brunson, Cheatham, Jennewein, and Ma are also involved in various CaRCC activities and other community groups. One of the goals of this new working group is to develop ways that the various CI communities can better coordinate to benefit research and new CI professionals learning about the ecosystem.

A long-standing cornerstone of the over 700 member Campus Champions community is the convivial discussion on the Campus Champions mailing list. Notably, this reporting period saw a vibrant discussion about the emerging and evolving role of commercial cloud providers in the research computing and data space. This topic is foremost on the minds of campus CI professionals and NSF program officers alike. The fact that this community looked to and was comfortable engaging with the Champions mailing list for this discussion speaks to the level of trust and esteem it has earned.

Campus Engagement continues to exceed its targets in all metrics: number of Champion institutions, number of unique contributors to the email list, and number of activities related to workforce development of cyberinfrastructure professionals. The targets for these metrics will be monitored and raised if deemed appropriate.

For other metrics with respect to this WBS, see Appendix §12.2.2.1.5.

5. Extended Collaborative Support Service (WBS 2.2)

The Extended Collaborative Support Service (ECSS) improves the productivity of the XSEDE user community through meaningful collaborations and well-planned training activities. The objective is to optimize applications, improve work and data flows, increase effective use of the XSEDE digital infrastructure, and broadly expand the XSEDE user base by engaging members of underrepresented communities and domain areas. The ECSS program provides professionals who can be part of a collaborative team—dedicated staff who develop deep, collaborative relationships with XSEDE users—helping them make the best use of XSEDE resources to advance their work. These professionals possess combined expertise in many fields of computational science and engineering. They have a deep knowledge of underlying computer systems and of the design and implementation principles for optimally mapping scientific problems, codes, and middleware to these resources. ECSS includes experts in not just the traditional use of advanced computing systems but also in data-intensive work, workflow engineering, and the enhancement of scientific gateways.

ECSS projects fall into five categories: Extended Support for Research Teams (ESRT), Novel and Innovative Projects (NIP), Extended Support for Community Codes (ESCC), Extended Support for Science Gateways (ESSGW), and Extended Support for Training, Education and Outreach (ESTEO). Project-based ECSS support is requested by researchers via the XSEDE peer-review allocation process, or, in some cases, suggested by reviewers as something that would benefit the researchers. If reviewers recommend support and if staff resources are available, projects progress through three activities. First, the project is assigned to an ECSS expert. Second, the project is quantified with the formation of a work plan through collaboration with the research group. The work plan includes concrete quarterly goals and staffing commitments from both the PI team and ECSS. Third, when the project is completed, the ECSS expert produces a final report with input from the research group. A successful project is the completion of all three phases. Each state of the progression is measured to provide an assessment of progress. Submission of work plans within 45 days of initial contact, 90% of projects with work plans completed, and 85% of completed projects with final reports within three months are additional criteria for success. The ECSS managers review work plans and also track progress via Interim Project Reports.

The success of the ECSS team depends on effective collaboration across all L2 areas of the project. Specifically, ECSS works closely with XCI to expand software capabilities; External Relations within PgO to communicate the science successes enabled by ECSS assistance; RAS to review allocations requests; and CEE to develop and deliver training in HPC, data intensive computing, effective use of XSEDE resources and other topics. In addition, ECSS partners with CEE to manage the Campus Champions Fellows program, which can involve mentors from any L2 area.

Key Performance Indicators for Extended Collaborative Support Service are listed in the table below. Additional information about these KPIs can be found on the XSEDE KPIs & Metrics wiki page.

For other metrics with respect to this WBS, see Appendix §12.2.2.2.

Table 5–1: KPIs for Extended Collaborative Support Service.

KPI	Report Year	Target	RP1	RP2	RP3	RP4	Total	Owner
Number of completed ECSS projects	RY5	45/yr	17	10				Deepen/Extend — Deepen use to existing communities (§3.1.1)
	RY4	45/yr	15	11	16	10	52	
	RY3	45/yr	17	10	12	8	47	
	RY2	50/yr	16	9	10	12	47	

KPI	Report Year	Target	RP1	RP2	RP3	RP4	Total	Owner
	RY1	50/yr	*	10	13	25	48	
Grand (aggregate) mean rating of ECSS impact by PIs measured by ECSS Project Exit Survey items (1-5 Likert scale)	RY5	4 of 5/yr	4.1	4.2				Deepen/Extend — Deepen use to existing communities (§3.1.1)
	RY4	4 of 5/yr	3.0	4.7	4.3	4.7	4.5	
	RY3	4 of 5/yr	NA	3.9	4.4	4.3	4.2	
	RY2	4 of 5/yr	4.1	4.0	3.8	4.3	4.0	
	RY1	4 of 5 /qtr	*	4.6	4.6	3.3	4.1	
Grand (aggregate) mean rating of PI satisfaction with ECSS support measured by ECSS Project Exit Survey items (1-5 Likert scale)	RY5	4.5 of 5/ yr	4.8	4.9				Deepen/Extend — Deepen use to existing communities (§3.1.1)
	RY4	4.5 of 5/ yr	3.0	5.0	5.0	4.7	4.8	
	RY3	4.5 of 5/ yr	NA	4.3	4.8	4.5	4.6	
	RY2	4.5 of 5/ yr	4.7	4.6	4.2	4.8	4.5	
	RY1	4.5 of 5/ qtr	*	4.9	4.7	4.6	4.5	

NA – Interviews were not conducted during this reporting period so no Impact and Satisfaction ratings were collected.

ECSS is still on track to complete 45 projects in RY5. Although the number of projects finished in RP2 is just shy of the average needed to reach this goal, this is compensated for by the large number of completions in RP1. This is consistent with the trends observed in RY2, RY3, and RY4. Mean ratings of ECSS impact (4.2) and satisfaction (4.9) continue to exceed the already ambitious goals of 4.0 and 4.5, respectively. The fact that impact lags satisfaction is often due to factors beyond ECSS's control, such as the PIs not having sufficient time to follow up on ECSS recommendations or ECSS staff determining that there are no viable paths to improving software performance and scalability.

ECSS Highlights

Supporting the UT Austin COVID-19 Modeling Consortium

PI Lauren Ancel Meyers, UT Austin; NIP member Kelly Pierce (TACC)

ECSS NIP expert Dr. Kelly Pierce is a key member of the UT Austin COVID-19 Modeling Consortium[37] helping to design and execute HPC workflows for their modeling efforts. Figure 9 illustrates the projections she helped make to understand the potential impact of social distancing in Houston, Beaumont, and Austin, TX. This work will appear in an invited manuscript for the *Computing in Science and Engineering* second special issue on COVID-19 to be published shortly. Currently, Dr. Pierce is helping the Consortium to develop a meta-population model that can describe disease transmission at the sub-city level. She is helping them to turn their scientific questions into software specifications and to come up with meaningful summaries of input data and model outputs. One in-progress aspect of what is a very large undertaking is developing spatially explicit visualizations of case counts and hospitalizations.

[37] https://covid-19.tacc.utexas.edu/

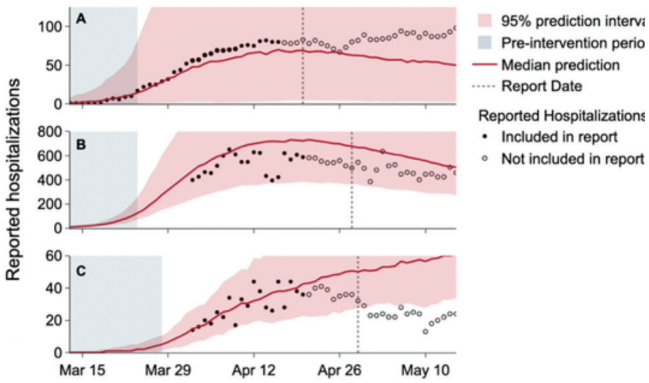


Figure 8**: Observed and projected COVID-19 hospitalization in the (A) Austin, (B) Houston, and (C) Beaumont area from March 13-May 15, 2020.** Filled points indicate reported hospital census data included in parameter estimation for our reports; empty circles indicate hospital census data reported after parameter estimation was complete; red lines and shading indicate median prediction and 95% prediction intervals; grey shading indicates the period prior to local stay-home orders; solid vertical lines mark the dates when reports were released.

Further highlights can be found in the sections for each of the ECSS L3 areas.

5.1. ECSS Director's Office (WBS 2.2.1)

The ECSS Director's Office has been established to provide the necessary oversight to ensure the greatest efficiency and effectiveness of the ECSS area. This oversight includes providing direction to the L3 management team, coordination of and participation in ECSS planning activities and reports through the area's Project Manager, monitoring compliance with budgets, and retargeting effort, if necessary. The Director's Office also attends and supports the preparation of project-level reviews and activities. The ECSS Director's Office will continue to manage and set direction for ECSS activities and responsibilities. They will contribute to and attend bi-weekly Senior Management Team calls; contribute to the project level plan, schedule, and budget; contribute to XSEDE quarterly, annual, and other reports as required by the NSF; and attend XSEDE quarterly and annual meetings. The Director's Office will advise the XSEDE PI on many issues, especially those relevant to this WBS area. The office consists of two Level 2 Co-Directors, Philip Blood, who manages ESRT and NIP activities, and Bob Sinkovits, who manages ESCC, ESSGW, and ESTEO activities. The office also has three project managers (Marques Bland, Sonia Nayak, and Leslie Morsek).

Blood and Sinkovits carry out the post-project interviews with all project PIs who have received ECSS support, both to get their assessment of how the project went, and to hear and act on any concerns they may express. Sinkovits also organizes the monthly symposium series, serves as one of the contributors to staff training, and runs the Campus Champions Fellows program (§4.6). Blood convenes User Advisory Committee meetings and supports the User Advisory Committee Chair.

The project managers aid in the management of the day-to-day activities of ECSS, which includes the management of project requests (XRAC and startups), active projects, project assignments, and staffing. They continuously refine the ECSS project lifecycle, further defining processes to aid in the management of over 100 active projects. They also administer Jira for the management and tracking of projects, both for the managers and directors of ECSS and for ECSS staff.

5.2. Extended Support for Research Teams (WBS 2.2.2)

Extended Support for Research Teams (ESRT) accelerates scientific discovery by collaborating with researchers, engineers, and scholars to optimize their application codes, improve their work and data flows, and increase the effectiveness of their use of XSEDE digital infrastructure.

ESRT projects are initiated as a result of support requests or recommendations obtained during the allocation process. Most projects focus on research codes associated with specific research teams, as community codes fall under ESCC (§5.4), but are not exclusively restricted to this classification. The primary mandate of ESRT is the support of individual research teams within the context of their research goals.

ESRT is on track to meet its metric of 27 projects per year. During this reporting period, six projects have been completed, which is within the average of six to seven projects needed each reporting period to meet the annual metric target. Although, ESRT will need to complete 16 projects over the next two reporting periods to meet the 27 projects per year metric target. ESRT has completed five PI interviews this reporting period, resulting in average satisfaction (4.8) and impact (4.0) scores that meet or exceed current targets. However, the average months of effort saved in these projects fell short of the 12 month target with six months of effort saved. Two respondents gave responses of two and six months, which brought down the average. However, in these cases, the respondents were very satisfied with ESRT effort (5.0 satisfaction). These projects did not require a large investment of ESRT effort, but still reaped large relative returns. In each case, the invested ESRT effort was about ten-percent of the effort saved.

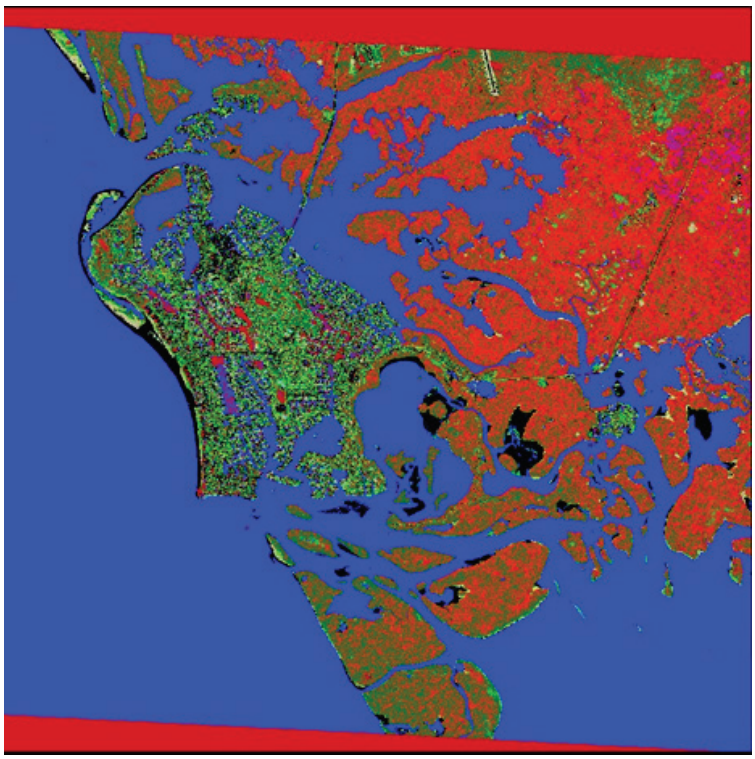


Figure 9: A color classification map obtained from the newly converted Python code.

Mapping of Coastal Southern US for Habitat and Flood Hazard Assessments

A project led by Dr. Tylar Murray of the University of South Florida is protecting communities in low-lying coastal regions by providing more accurate topographic and land cover maps. An ESRT consultant, Dr. DJ Choi from the San Diego Supercomputer Center (SDSC), worked with Dr. Murray to improve the portability, performance, and efficiency of the satellite image classification pipeline utilized to produce these maps. A metadata database was created with SQLite to manage the large amounts of input images and provide them to a newly developed MPI C code to perform classifications in parallel. Additionally, the original MATLAB classification code was converted into Python for improved portability (see Figure 10). This more portable pipeline can be utilized on most XSEDE parallel systems including clusters, large memory nodes, or cloud systems (i.e., *Jetstream*)

For other metrics with respect to this WBS, see Appendix §12.2.2.2.1.

5.3. Novel & Innovative Projects (WBS 2.2.3)

Novel and Innovative Projects (NIP) accelerates research, scholarship, and education provided by new communities that can strongly benefit from the use of XSEDE's ecosystem of advanced digital services. Working closely with the XSEDE Outreach team, the NIP team identifies a subset of scientists, scholars, and educators from *new communities,* i.e., from disciplines or demographics that have not yet made significant use of advanced computing infrastructure, who are now committed to projects that appear to require XSEDE services, and are in a good position to use them efficiently. NIP staff then provide personal mentoring to these projects, helping them to obtain XSEDE allocations and use them successfully.

XSEDE projects generated by, and mentored by, the personal efforts of the NIP experts should stimulate additional practitioners in their field to become interested in XSEDE. Strategies used include building and promoting science gateways serving communities of end-users and the enhancement of the Domain Champions program by which successful practitioners spread the word about the benefits of XSEDE to their colleagues.

NIP lightweight consulting helped to initiate the project "Data Processing System for Generating Predictions of Cognitive Outcome," by PI Brad Mahon of the Carnegie Mellon University (CMU) Psychology Department. Now supported by an ECSS project, the research team gathers data and performs spatial and temporal co-registration of electroencephalogram (EEG), functional magnetic resonance imaging (fMRI), brain-mapping, and behavioral data from awake patients who have different brain lesions. The goal is to build a predictive analytics model by using various machine learning and statistical models to minimize the risk to cognitive functions associated with brain tissue removal. NIP expert, Amit Chourasia (San Diego Supercomputer Center (SDSC)), helps the research group to design the platform architecture for managing data, processing, computing, and user management. The project has adopted the SeedMeLab[38] data framework as a data repository and user management environment for the project. A sandbox environment is being used to develop and test integration. The research group extended the SeedMeLab client and created a wrapper for Python. Current work is focusing on development of user authorization via JSON (JavaScript Object Notation) Web Tokens with SeedMeLab that will enable the project to easily integrate various components. NIP expert Roberto Gomez (Pittsburgh Supercomputing Center (PSC)) is providing consulting on software tools and computation on *Bridges*.

For other metrics with respect to this WBS, see Appendix §12.2.2.2.2

5.4. Extended Support for Community Codes (WBS 2.2.4)

Extended Support for Community Codes (ESCC) extends the use of XSEDE resources by collaborating with researchers and community code developers to deploy, harden, and optimize software systems necessary for research communities to create new knowledge.

ESCC supports users via requested projects and XSEDE-initiated projects. ESCC projects may be created in two different ways. Most ESCC projects are initiated as a result of requests for assistance during the allocation process. These projects are similar in nature to ESRT projects but involve community codes rather than codes developed for and by individual research groups. ESCC projects may also be initiated by staff to support a community's needs.

ESCC is on target to meet its goal for the number of completed projects. No satisfaction score was collected as no interviews were conducted during the last reporting period. This is due to the small total number of projects and is within the expected margins.

ESCC Consultant Dr. Manu Shantaram (SDSC) completed work on the project "Numerical study of supersonic turbulent boundary layer drag control and vortex reconnection cascade at high Reynolds numbers" with PI Dr. Fazle Hussain (Texas Tech University). The code was profiled with TAU and VTune and I/O hotspots were detected and performance was improved by adapting the number of stripes on the scratch Lustre file system on *Stampede2*. This successful project is to be extended (pending request from the PI and approval by the review committee) to address technical issues that limit the analysis to moderate problem sizes. The project falls into the category "traditional HPC" where a standard HPC bottleneck, here I/O, is diagnosed and alleviated with the help of a consultant.

For other metrics with respect to this WBS, see Appendix §12.2.2.2.3.

[38] https://seedmelab.org/

5.5. Extended Support for Science Gateways (WBS 2.2.5)

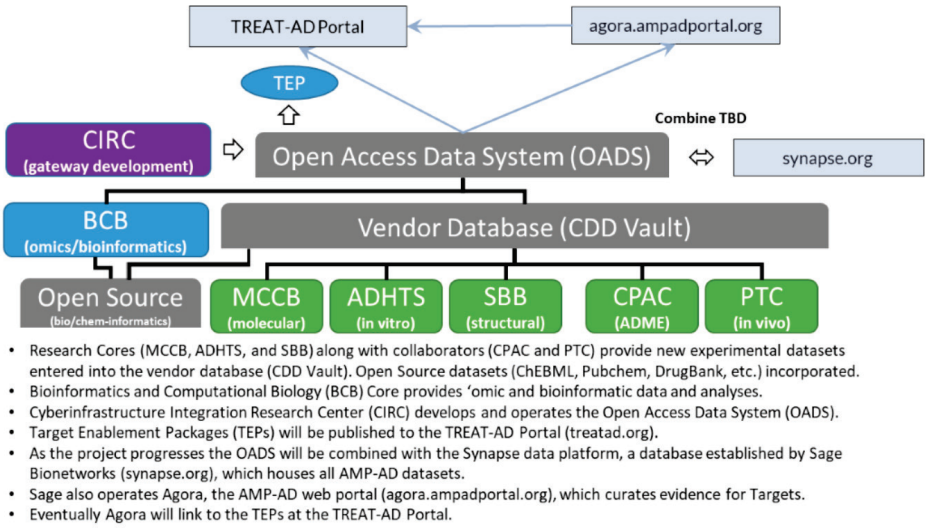
Extended Support for Science Gateways (ESSGW) broadens science impact and accelerates scientific discovery by collaborating in the development and enhancement of science-centric gateway interfaces and by fostering a science gateway community ecosystem.

ESSGW completed one project during this period. This is an expected correction to vastly overachieving in the previous reporting period. Even with this, ESSGW has already exceeded the target of nine total projects completed for the year. With four PI interviews done during the reporting period, ESSGW maintained a 4.5 Impact Rating and a 5.0 satisfaction score. During this period, ESSGW started reporting a new metric: Registered Production Gateways, which for this reporting period is 49. This will be regularly tracked for the remainder of the project to show the number of active Science Gateways using XSEDE resources. There were also five new ESSGW projects submitted this period, bringing the number of active projects to 22. This number is slightly higher than the normal capacity of ESSGW.

Alzheimer's Disease Drug Discovery Center (AD3C)

The ESSGW team of Eroma Abeysinghe, Surresh Marru, and Rob Quick began working with Antiviral Drug Discovery and Development Center (AD3C) researchers and administrators to create a Science Gateway environment that will allow Alzheimer's researchers to create an environment that allows them to do both common and custom drug discovery tasks (see Figure 11). This portal will combine traditional computational gateway components with additional open data sharing capabilities. Early activities in this project have included help with creation of a Data Management Plan, instantiation of Apache Airavata gateways for mass spectrometry data analysis and network analysis, and a security review for commercial software purchase.

Now that several of the core components have been implemented, the design and deployment of an Open Access Data Sharing (OADS) portal is underway. This component will publish the results in the form of Target Enablement Packages (TEP) to other Alzheimer's disease (AD) repositories including Sage Bionetworks and the AMP-AD portal as well as having a direct public interface for researchers to access the TEPs.



- Research Cores (MCCB, ADHTS, and SBB) along with collaborators (CPAC and PTC) provide new experimental datasets entered into the vendor database (CDD Vault). Open Source datasets (ChEBML, Pubchem, DrugBank, etc.) incorporated.
- Bioinformatics and Computational Biology (BCB) Core provides 'omic and bioinformatic data and analyses.
- Cyberinfrastructure Integration Research Center (CIRC) develops and operates the Open Access Data System (OADS).
- Target Enablement Packages (TEPs) will be published to the TREAT-AD Portal (treatad.org).
- As the project progresses the OADS will be combined with the Synapse data platform, a database established by Sage Bionetworks (synapse.org), which houses all AMP-AD datasets.
- Sage also operates Agora, the AMP-AD web portal (agora.ampadportal.org), which curates evidence for Targets.
- Eventually Agora will link to the TEPs at the TREAT-AD Portal.

Figure 10: Conceptual diagram and explanation of components for the AD3C infrastructure. ESSGW will assist in the design and development of the BCB, CIRC, and OADS portions of the infrastructure.

For other metrics with respect to this WBS, see Appendix §12.2.2.2.4.

5.6. Extended Support for Training, Education, & Outreach (WBS 2.2.6)

Extended Support for Training, Education & Outreach (ESTEO) prepares the current and next generation of researchers, engineers, and scholars in the use of advanced digital technologies by providing the technical support for Training, Education, and Outreach planned activities.

Typical events include train-the-trainers events, on-site classes requested by Campus Champions, regional workshops, conferences, and summer schools (including the International HPC Summer School). Staff also create and review online documentation and training modules. This on-demand training is increasingly popular with the user community when both time and travel budgets are limited.

ESTEO is on track to meet its targets for all of its metrics, including the staff training with the addition of new Service Providers, *Expanse* and *Bridges-2,* through staff training for the AMD processor-based architectures of *Expanse* and *Bridges-2* planned for December, along with in-depth *Jetstream* Openstack training in anticipation of the deployment of *Jetstream2*.

ESTEO finalized the assignment of mentors for the new cohort of six 2020-21 Campus Champion Fellows, all of whom chose to work with ECSS this year. Two of the Fellows' first choice ECSS projects expired around the start of the fellowship period and were not renewed. One was converted to a Fellows-designed project focused on the development of highly scalable computational chemistry software that will be executed on XSEDE resources. For the other Fellow, ESTEO recruited a new ECSS staff member who will provide mentorship in the application of machine learning techniques to materials science.

For other metrics with respect to this WBS, see Appendix §12.2.2.2.5.

6. XSEDE Cyberinfrastructure Integration (WBS 2.3)

The mission of XSEDE Cyberinfrastructure Integration (XCI) is to facilitate interaction, sharing, interoperability, and compatibility of all relevant software and related services across the national CI community, building and improving upon the foundational efforts of XSEDE.

XCI envisions a national cyberinfrastructure that is consistent, straightforward to understand, and practical for use by researchers and students. Service to XSEDE Service Providers (SPs) is a particularly important aspect of XCI's activities. XCI strives to make it possible for researchers and students to effortlessly use computational and data analysis resources ranging from those allocated by XSEDE to campus-based CI facilities, an individual's workstation, and commercial cloud providers, and to interact with these resources via CI software services such as science gateways and Globus Online. XCI provides two essential integrating services: XCI provides the software glue that ties XSEDE together; particularly, it enables the interoperability of advanced computing resources supported by XSEDE with each other and with the XSEDE portal and other underlying infrastructure (e.g., accounting information), and XCI also improves the capabilities of campus cyberinfrastructure administrators anywhere in the US to manage local facilities in ways that are easily interoperable with the evolving national CI fabric while simultaneously leveraging training and educational materials created and disseminated by XSEDE.

The success of the XCI team depends on effective collaboration across all L2 areas of the project. Specifically, the Requirements Analysis & Capability Delivery (RACD) team relies on Ops to integrate new capabilities as well as CEE, RAS, and the PgO's External Relations (ER) team to help improve XSEDE services and inform the user community of their existence. The Cyberinfrastructure Resource Integration (CRI) team also collaborates with ER to communicate the tools and services which XSEDE makes available to the national CI community.

Key Performance Indicators for XSEDE Cyberinfrastructure Integration are listed in the table below. Additional information about these KPIs can be found on the XSEDE KPIs & Metrics wiki page.

For other metrics with respect to this WBS, see Appendix §12.2.2.3.

Table 6–1: KPIs for XSEDE Cyberinfrastructure Integration (XCI).

KPI	Report Year	Target	RP1	RP2	RP3	RP4	Total	Owner
Grand (aggregate) mean rating of XSEDE User Survey user satisfaction items regarding XCI software and technical services, capabilities, and resources (1-5 Likert scale)	RY5	4 of 5/yr	4.4	-				Advance — Create an open and evolving e-infrastructure (§3.2.1)
	RY4	*	*	*	*	*	*	
	RY3	*	*	*	*	*	*	
	RY2	*	*	*	*	*	*	
	RY1	*	*	*	*	*	*	
Grand (aggregate) mean rating of XSEDE User Survey Service Provider satisfaction items regarding XCI software and technical services, capabilities, and resources (1-5 Likert scale)	RY5	4 of 5/yr	4.5	-				Advance — Create an open and evolving e-infrastructure (§3.2.1)
	RY4	*	*	*	*	*	*	
	RY3	*	*	*	*	*	*	
	RY2	*	*	*	*	*	*	
	RY1	*	*	*	*	*	*	
	RY5	18/yr	14	15				

KPI	Report Year	Target	RP1	RP2	RP3	RP4	Total	Owner
Number of non-XSEDE partnerships with XCI[2]	RY4	12/yr	9	10	11	21	21	Advance — Create an open and evolving e-infrastructure (§3.2.1)
	RY3	8/yr	13	12	11	12	20[1]	
	RY2	NA	-	-	-	-	8	
	RY1	NA	*	-	-	-	8	
Mean time to issue resolution (days)	RY5	<10 days/qtr	4.2	6.0				Sustain — Provide excellent user support (§3.3.2)
	RY4	<10 days/qtr	5.4	4.5	8.8	35.8	13.7	
	RY3	<14 days/qtr	22.3	7.3	2.9	2.9	8.8	
	RY2	<30 days	4.0	7.0	8.0	5.0	6.1	
	RY1	<45 days	*	7.0	4.0	16.0	9.0	

- Data reported annually.
[1] Engagements often continue over multiple reporting periods and get counted in each period they are active. The annual total is calculated by the number of unique engagements across all reporting periods.
[2] Number of non-XSEDE partnerships with XCI was a new KPI in RY3 so there were no targets set for RY1 or RY2. Annual totals were calculated retroactively.

"Grand (aggregate) mean rating of XSEDE User Survey user satisfaction items regarding XCI software and technical services, capabilities, and resources" and "Grand (aggregate) mean rating of XSEDE Survey Service Provider satisfaction items regarding XCI software and technical services, capabilities, and resources," are reported annually in RP1 so there is nothing to report. One new partnership was added this reporting period by CRI, so "Number of non-XSEDE partnerships with XCI" is on-track to meet the annual goal. The target for "Mean time to issue resolution (days)" was met.

XCI Highlights

In this reporting period, XCI delivered a significant new Comprehensive XSEDE Software Discovery service integrated into the Research Software Portal which enhances the ability to find and use: software and applications on XSEDE resources supported by HPC operators or by the community, hosted services provided by XSEDE or other members of the community, cloud images on *Jetstream*, cluster toolkits for campuses, packaged software provided by XSEDE, and public container registries. This service is available at https://software.xsede.org/xsede-software-discovery.

6.1. XCI Director's Office (WBS 2.3.1)

The XCI Director's Office has been established to provide necessary oversight to ensure the greatest efficiency and effectiveness of the XCI area. This oversight includes providing direction to the L3 management team, coordination of and participation in XCI planning activities and reports through the area's project manager, and monitoring compliance with budgets, retargeting effort, if necessary. The Director's Office also attends and supports the preparation of project-level reviews and activities.

The XCI Director's Office will continue to manage and set direction for XCI activities and responsibilities. They will contribute to and attend bi-weekly Senior Management Team calls; contribute to the project level plan, schedule, and budget; contribute to XSEDE IPRs, annual reports, and

other reports as required by the NSF; and attend XSEDE quarterly and annual meetings. Lastly, the Director's Office will advise the XSEDE PI on many issues, especially those relevant to this WBS area.

6.2. Requirements Analysis & Capability Delivery (WBS 2.3.2)

The Requirements Analysis & Capability Delivery (RACD) team facilitates the integration, maintenance, and support of cyberinfrastructure capabilities addressing user technical requirements. The process begins by preparing Capability Delivery Plans (CDPs) that describe the technical gaps in XSEDE's prioritized Use Cases. To fill the gaps, RACD evaluates and/or tests existing software solutions, engages with software providers, and facilitates software and service integration. To ensure software and service adoption and ROI, RACD involves users, Service Providers (SPs), and operators in an integration process that uses engineering best practices and instruments components to measure usage. Once components are integrated, RACD facilitates software maintenance and enhancements in response to evolving user needs and an evolving infrastructure environment.

At the September XSEDE Quarterly Meeting, RACD hosted one of its regular user requirements gathering sessions and invited Campus Champion members in addition to XSEDE staff. This resulted in five new Use Cases and some revisions to existing Use Cases. A few of these Use Cases will be prepared for prioritization by the UREP next reporting period. With these and other new Use Cases, RACD is on track to reach its RY5 goal by the end of November. The team also delivered two new capabilities in production: emergency account suspension and the ability to register availability of an application or service for use.

During this reporting period, RACD delivered 16 significant fixes and enhancements to production components. The most significant new capability, the new Comprehensive Software Discovery service, is detailed in the XCI Highlight above. This new service was made possible by a major upgrade to the Information Services Cross-Institutional Resource Catalog design to be more flexible, accommodate more types of resources, easier to search, maintain links to original sources, and track relationships between resources.

Other updates this past reporting period included: new Grid Community Toolkit versions of GridFTP, GSI OpenSSH, and GCT client tools for XSEDE Service Providers; improved Community Software Areas support; new public documentation about XSEDE supported YUM/RPM repositories; new XSEDE software copyright and licensing documentation; new software and digital services registration interface in the Research Software Portal; and a new Information Services Fields of Science catalog that enables public viewing and application programming interface (API) access to the fields of science used by XRAS and other XSEDE program areas.

This reporting period, RACD met its defect and support request response metric by addressing 36 issues in an average of 5.7 calendar days.

RACD instrumented Globus Auth usage this reporting period and is on track to complete three more components in the following reporting periods.

For other metrics with respect to this WBS, see Appendix §12.2.2.3.1.

6.3. Cyberinfrastructure Resource Integration (WBS 2.3.3)

The mission of the Cyberinfrastructure Resource Integration (CRI) team is to work with SPs, CI providers, and campuses to maximize the aggregate utility of national cyberinfrastructure. CRI facilitates the incorporation of XSEDE software at SPs and encourages SPs to publish their information in the RDR. CRI's activities are reflected in the uptake of CRI-integrated toolkits, such as the XSEDE Campus Bridging Cluster toolkit and XSEDE National Integration Toolkit, but also Globus Transfer clients and other toolkits as developed. Through XCI, XSEDE serves an aligning function within the nation by assembling a technical infrastructure that facilitates interaction and interoperability across the national CI ecosystem. In turn, this infrastructure is adopted by campus, regional, and national CI

providers because it makes their task of delivering services easier and the delivered services better. The suite of interoperable and compatible software tools that XSEDE makes available to the CI community is based on those already in use, and services are added that address emerging needs including data and computational services. Because the XSEDE Cyberinfrastructure Resource Integration team (CRI) deals primarily with Level 1, 2, and 3 SPs, along with campus cyberinfrastructure administrators and support experts, the SP Forum and Campus Champions are XCI's primary sources of direction regarding prioritization of efforts.

During this reporting period, CRI provided multiple simultaneous engagements over an extended period with University of Central Oklahoma, Langston University, and George Mason University. At the end of the period, the team initiated an ongoing dialog with University of Texas Dallas on their cluster strategy. While the previous reporting period required a shift in activities from in-person site visits to ongoing engagements, in this reporting period, the team found that multiple, longer-term remote engagements could be supported, with more flexibility for the on-site staff and an opportunity to engage multiple times over the period. The resulting engagements tended to be longer and result in additional follow-ups to ensure desired results were obtained. In the case of the Langston University engagement, activities there resulted in the incorporation of developments into an XCAT-enabled cluster toolkit. The aggregate total TeraFLOPS in cluster builds reached 1,091 thanks to these engagements. The engagement with George Mason University will include consulting on implementing both OpenStack and OpenHPC environments.

This reporting period, CRI was able to promote the virtual cluster toolkit (scalable cluster computing on OpenStack clouds including *Jetstream*) and Container Template Library (reproducible application containers) at the IEEE HPEC workshop in September. Cornell is in the process of adopting the virtual cluster toolkit to scale analyses on its on-premise OpenStack cloud.

From the beginning of the project, CRI has tracked the total number of systems that use one or more CRI provided toolkits and aggregate number of TeraFLOPS of cluster systems using CRI toolkits (see Appendix 12.2.2.3.2). The targets originally set for both at the beginning of the project have been surpassed, so the team will continue to monitor progress and determine if the targets should be adjusted.

With a considerable number of SPs entering the XSEDE Federation, and a change in staffing from Victor Hazlewood to Tabitha Samuel, SP coordination saw a significant uptick in activity. A total of 14 resources have stated intent to integrate with XSEDE as allocated resources. Eight of these are from NSF Category 1 or 2 awards, with the remainder coming from MRI awards or initiatives. The new coordination of activities has required considerable attention and collaboration with other XSEDE areas responsible for integrating new SPs.

For other metrics with respect to this WBS, see Appendix §12.2.2.3.2.

7. XSEDE Operations (WBS 2.4)

The mission of XSEDE Operations is to install, connect, maintain, secure, and evolve an integrated cyberinfrastructure that incorporates a wide range of digital capabilities to support national scientific, engineering, and scholarly research efforts.

In addition to the Operations Director's Office (§7.1), Operations staff is subdivided into four teams based on the work breakdown structure: Cybersecurity (SecOps) (§7.2), Data Transfer Services (DTS) (§7.3), XSEDE Operations Center (XOC) (§7.4), and Systems Operational Support (SysOps) (§7.5). The Operations management team meets weekly and individual Operations groups meet approximately bi-weekly with all meeting minutes posted to the XSEDE wiki.

The success of the Operations (Ops) team depends on effective collaboration across all L2 areas of the project. In particular, Ops relies on XCI to support new capabilities and services (e.g., security or networking technologies) and RAS to create and deploy solutions to improve help ticket response or the central database. In addition, Ops relies on all WBS teams and the Service Providers to respond to help tickets for their areas that are submitted by users.

Key Performance Indicators for Operations are listed in the table below. Additional information about these KPIs can be found on the XSEDE KPIs & Metrics wiki page.

For other metrics with respect to this WBS, see Appendix §12.2.2.4.

Table 7–1: KPIs for Operations.

Area Metric	Report Year	Target	RP1	RP2	RP3	RP4	Total	Sub-goal Supported
Mean rating of user satisfaction with tickets closed by the XOC (1-5 Likert scale)	RY5	4.5 of 5/ qtr	4.7	4.7				Sustain — Provide excellent user support (§3.3.2)
	RY4	4.5 of 5/ qtr	4.8	4.7	4.7	4.7	4.7	
	RY3	4.5 of 5 / qtr	4.5	4.9	4.6	4.7	4.7	
	RY2	4.5 of 5 / qtr	4.5	4.8	4.8	4.4	4.6	
	RY1	4 of 5 / qtr	*	4.8	4.2	5.0	4.7	
Hours of downtime with direct user impacts from an XSEDE security incident	RY5	0 hrs/qtr	0	0				Sustain — Provide reliable, efficient, and secure infrastructure (§3.3.1)
	RY4	0 hrs/qtr	0	0	22	0	22	
	RY3	0 hrs/qtr	0	0	0	0	0	
	RY2	0 hrs/qtr	0	0	0	0	0	
	RY1	< 24 hrs/qtr	*	0	146	0	146	

User satisfaction with tickets closed by the XOC once again remains very high, scoring a 4.7, and continues the streak of meeting the target goal for ten consecutive reporting periods.

Because there were no security incidents this reporting period, there was no downtime with user impact, thus the 0 hours target was met.

Operations Highlights

SecOps, in collaboration with SysOps, is in the process of auditing access to XSEDE's AWS service console to ensure that least privilege is enforced for those administrators who do have access. The group is also investigating the proper use of multi-factor authentication (MFA) for access to the service console. While MFA is enforced, the group is reviewing how it is implemented in AWS and how XSEDE is making use of it to provide access to the service console. These issues would affect any large IT enterprise organization using AWS and would be a good "lessons learned" or Birds of a Feather (BoF) for the Practice & Experience in Advanced Research Computing conference (PEARC), EDUCAUSE, or the NSF Cyber Summit. To this end, the National Center for Supercomputing Applications (NCSA) is in the process of hiring a security engineer to work specifically on security and auditing of XSEDE's enterprise computing within AWS.

SysOps migrated services to the XSEDE Duo platform for staff-level MFA. This will reduce the number of tokens (both hardware and software) that XSEDE staff need to maintain in order to access privileged services and hosts.

7.1. Operations Director's Office (WBS 2.4.1)

The Operations Director's Office has been established to provide the necessary oversight to ensure the greatest efficiency and effectiveness of the Operations area. This oversight includes providing direction to the L3 management team, coordination of and participation in Operations planning activities and reports through the area's Project Manager, and monitoring compliance with budgets, retargeting effort if necessary. The Director's Office also attends and supports the preparation of project-level reviews and activities.

The Operations Director's Office will continue to manage and set direction for Operations activities and responsibilities. The Office will contribute to and attend bi-weekly Senior Management Team calls; contribute to the project-level plan, schedule, and budget; contribute to XSEDE IPR, annual, and other reports as required by the NSF; and attend XSEDE quarterly and annual meetings. Lastly, the Director's Office will advise the XSEDE PI on many issues, especially those relevant to this WBS area.

7.2. Cybersecurity (WBS 2.4.2)

The Cybersecurity Security (SecOps) group protects the confidentiality, integrity and availability of XSEDE resources and services. Users expect XSEDE resources to be reliable and secure, thus the security team's goal is to minimize any interruption of services related to a security event.

As part of a goal to update XSEDE's security documents, the SecOps group has updated the project's Acceptable Use Policy (AUP) to include clarifying language concerning the requirement for SPs to adhere to XSEDE's security policies. Additionally, SecOps is drafting a new Identity and Access Management Policy, which has completed several rounds of comments and feedback from various XSEDE stakeholders.

The SecOps group also continues collaborations with SysOps to improve and update XSEDE's critical infrastructure. High impact examples include two activities. First, the group is deploying new Kerberos Key Distribution Centers (KDCs) for authentication and allowing XSEDE to securely scale authentication services. Second, both groups are working with the User Interfaces and Online Information (UII) group to upgrade the software used to operate the XSEDE User Portal services.

Also during this reporting period, SecOps expanded its student involvement in XSEDE's cybersecurity efforts. NCSA now has one undergraduate and one graduate student working on cybersecurity related activities. An undergraduate, Anthony Kwok, is helping manage XSEDE's vulnerability management program. A graduate student, Phuong Cao, is currently working on novel intrusion detection techniques for his research. Specifically, Cao is working on an analysis of authentication failures in global environments connecting Security Assertion Markup Language (SAML) identity providers with OpenID

Connect (OIDC) relying parties. This work is being done directly within the context of CILogon, a service that XSEDE relies on for its security operations.

For other metrics with respect to this WBS, see Appendix §12.2.2.4.1.

7.3. Data Transfer Services (WBS 2.4.3)

The Data Transfer Services (DTS) group facilitates data movement and management for the community by maintaining and continuously evolving XSEDE data services and resources.

The DTS group continues its efforts to engage directly with the advanced research community by investigating how to effectively interact with Campus Champions and, by extension, the universities and institutions they represent. In fact, the group is offering one-to-one consultation services based on feedback from users who responded to the data transfer section of the recent XSEDE User Survey. Of the ~600 respondents, 24 indicated they would like to be contacted by DTS staff to follow up on issues they have had with data transfers. DTS staff have contacted these users and are still collecting feedback in order to better understand their needs. The survey also revealed, as expected, that the most common endpoints used in the XSEDE CI were from Level 1 Service provider resources such as *Stampede*, *Comet*, *Wrangler,* and *Jetstream*. Tools most frequently used to transfer data were scp and Globus.

DTS also collaborates with new service provider sites when they request to add new resources to the XSEDE Federation. DTS then engages with these SPs in order to accommodate their networking and data transfer needs, with a special focus on getting the resources connected to XSEDENet. Many of these resources are then integrated into the XSEDE ecosystem when they are ready to go into production. This reporting period, there were a significant number of new resources who indicated interest in joining the XSEDE Federation. Among these were the following:

- *Anvil* system at Purdue
- *Disco* system at John Hopkins University
- *FASTER* system at Texas A&M
- *KyRIC* system at the university of Kentucky
- *Darwin* system at University of Delaware
- OSN project

For other metrics with respect to this WBS, see Appendix §12.2.2.4.2.

7.4. XSEDE Operations Center (WBS 2.4.4)

The XSEDE Operations Center (XOC) staff serve as user advocates, providing timely and accurate assistance to the XSEDE community, while simultaneously monitoring and troubleshooting user-facing systems and services.

For this reporting period, the XOC exceeded the user satisfaction target by scoring 4.7 in its quarterly survey, indicating that the users continue to be very satisfied with the services provided by the help desk. Also, the XOC was able to meet the goal of resolving tickets in less than an hour with a mean time to ticket resolution of 17 minutes for the reporting period.

For other metrics with respect to this WBS, see Appendix §12.2.2.4.3.

7.5. System Operations Support (WBS 2.4.5)

Systems Operational Support (SysOps) provides enterprise-level support and system administration for all XSEDE central services.

This reporting period, SysOps continued exploring new technologies and software to maintain a high level of enterprise service availability. This effort is important for ensuring that the group continues to meet the target goal of 99.9% availability.

In accordance with the hybrid cloud plan, the Identity Provider (IdP) service was migrated to AWS to help with maintainability of the service moving forward. The new deployment will now use a container to provide the service within AWS. This container image is provided and maintained by Internet2.

Finally, SysOps continued to work closely with SecOps in continuation of security patches and audits, including audits within AWS services and offerings. This will increase XSEDE's security posture for XSEDE's hybrid cloud implementation.

For other metrics with respect to this WBS, see Appendix §12.2.2.4.4.

8. Resource Allocation Service (WBS 2.5)

The Resource Allocation Service (RAS) is building on XSEDE's current allocation processes and evolving to meet the challenges presented by new types of resources to be allocated via XSEDE, new computing and data modalities to support increasingly diverse research needs, and large-scale demands from the user community for limited XSEDE-allocated resources. RAS is pursuing these objectives through three activities: managing the XSEDE allocations process in coordination with the XD Service Providers (§8.2), enhancing and maintaining the RAS infrastructure and services (§8.3), and anticipating changing community needs.

The success of the RAS team depends on effective collaboration across all L2 areas of the project. Specifically, RAS collaborates closely with Ops to ensure capabilities are available, secure, and up-to-date; with External Relations (ER) within the Program Office to promote allocations periods and services; with XCI for continual product improvement and optimization; with CEE's User Interfaces and Online Information (UII) for user optimization of services and processes; and with ECSS for efficient review of quarterly allocation requests.

Key Performance Indicators for the Resource Allocation Service are listed in the table below. Additional information about these KPIs can be found on the XSEDE KPIs & Metrics wiki page.

For other metrics with respect to this WBS, see Appendix §12.2.2.5.

Table 8–1: KPIs for Resource Allocation Service.

Area Metric	Report Year	Target	RP1	RP2	RP3	RP4	Total	Sub-goal Supported
Mean rating of user satisfaction with allocations process (1-5 Likert scale)	RY5	4 of 5/ qtr	4.4	4.3				Sustain — Provide excellent user support (§3.3.2)
	RY4	4 of 5/ qtr	4.2	4.3	4.3	4.3	4.3	
	RY3	4 of 5/ qtr	4.1	4.1	4.2	4.4	4.2	
	RY2	4 of 5/ qtr	4.1	4.0	4.1	3.9	4.0	
	RY1	4 of 5/ qtr	*	4.0	4.0	4.0	4.0	
Mean rating of user satisfaction with XRAS (1-5 Likert scale)	RY5	4 of 5/ qtr	4.3	4.3				Sustain — Provide reliable, efficient, and secure infrastructure (§3.3.1)
	RY4	4 of 5/ qtr	4.3	4.3	4.4	4.2	4.3	
	RY3	4 of 5/ qtr	4.0	4.2	4.1	4.3	4.2	
	RY2	4 of 5/ qtr	4.0	4.0	4.1	3.9	4.0	
	RY1	4 of 5/ qtr	*	4.0	4.0	4.0	4.0	

RAS continues to receive satisfaction ratings above the target of 4.0 (out of 5) for both the allocations process as whole, as well as the XSEDE Resource Allocation System (XRAS), despite continuing high request levels for the quarterly Research opportunity. The target of 4.0 will remain given the uncertain and qualitative nature of this metric, as well as the regular reductions to recommended amounts for Research allocations. The success rate, at 84% for Research requests, approached the 85% target and

efforts continue to pursue improvements to the users' ability to prepare successful requests. The 84% measure continues the increasing trend for this KPI, with values at or above 80% for five of the last six reporting periods.

RAS Highlights

RAS achieved several milestones during the reporting period. Most notably, the team completed and deployed the new RESTful API (application programming interface) version of the Account Management Information Exchange (AMIE) protocol. As part of modernizing the XSEDE accounting infrastructure, the A3M group has converted the legacy AMIE packet-exchange system to a modern JSON (JavaScript Object Notation) and REST (REpresentational State Transfer) system. The resulting change will make onboarding easier for the many new Service Providers on XSEDE's horizon and will simplify support of the AMIE protocol in the future. Alongside this deployment, the team has released a Python-based client library for the new API to further simplify implementation efforts for Service Providers. As part of this effort, the team has provided workshops, tutorials, documentation, and other assistance, to help Service Providers integrate with this new system.

Alongside the new AMIE API, A3M has also developed a new usage reporting API, taking advantage of AWS Lambda technology. (Usage reporting is technically also part of the AMIE protocol, but has been implemented via a separate API.) The new system is more than 10 times as efficient as the legacy implementation and able to ingest 40 jobs per second. These improvements position the accounting infrastructure to support significantly larger job volumes as new generations of resources come online, including the very high volume of jobs from Open Science Grid and other high-throughput computing systems.

XSEDE allocations activity continued at high levels despite the continued pandemic. The XSEDE Resource Allocation Committee (XRAC) met virtually for the second time, and 84% of Research requests received some allocation. For the meeting, requests for compute resources were just over two times the amount available. Even with the high success rate, the panel recommended 280M Service Units (SUs) (96B Normalized Units (NUs)), and essentially the recommended amounts were awarded in full, with some moving of allocations across resources.

8.1. RAS Director's Office (WBS 2.5.1)

The RAS Director's Office has been established to provide the necessary oversight to ensure the greatest efficiency and effectiveness of the RAS area. This oversight includes providing direction to the L3 management team, coordination of and participation in RAS planning activities and reports through the area's Project Manager, monitoring compliance with budgets, and retargeting effort if necessary. The Director's Office also attends and supports the preparation of project-level reviews and activities. The RAS Director's Office also contributes to an analytics effort to support NSF, Service Providers, and XSEDE in understanding and projecting the stewardship of, demand for, and impact of CI resources and services.

The RAS Director's Office will continue to manage and set direction for RAS activities and responsibilities. They will contribute to and attend bi-weekly Senior Management Team calls; contribute to the project-level plan, schedule, and budget; contribute to XSEDE IPR, annual, and other reports as required by the NSF; and attend XSEDE quarterly and annual meetings. Lastly, the Director's Office will advise the XSEDE PI on many issues, especially those relevant to this WBS area.

8.2. XSEDE Allocations Process & Policies (WBS 2.5.2)

Allocations enable the national open science community to easily gain access to XSEDE's advanced digital resources, allowing them to achieve their research and education goals.

For the August 2020 XRAC meeting, held virtually via Zoom, 226 proposals were submitted for XSEDE resources, of which 190 were recommended for award—a success rate of 84%. To continue addressing the success rate KPI, the team also continued to collaborate with ECSS/ESTEO (Extended Support for Training, Education, & Outreach) to produce user-oriented training for the preparation of Code Performance and Scaling documents; these documents are often the cause of Research requests being rejected by the XRAC.

For the meeting, requests for compute resources were just over two times the amount available; approximately 374M SUs (189B NUs) were requested with 280M SUs (96B NUs) recommended and 349M SUs (95B NUs) awarded. Note that SU values are impacted by both *Stampede2* being allocated in node-hours, GPU resources in GPU-hours, and allocations being moved among these and resources allocated in core-hours. In terms of agency support, 122 requests (54%) were either entirely or partially supported by NSF awards; 69 requests (31%) had support only from non-NSF sources, and 35 (15%) listed no supporting grants.

During the August Research opportunity, 131 different PI institutions were represented, 12 from minority-serving institutions (MSIs) and 27 from Established Program to Stimulate Competitive Research (EPSCoR) states. A total of 524 reviews were contributed by 107 individuals from both the XRAC panel and the scientific specialists from the XSEDE ECSS area. Materials Research led all fields of sciences with 18.2% of the approved SUs, followed by Biochemistry and Molecular Structure and Function with 10.6% of approved SUs. Engineering Systems led all fields of sciences with 18.2% of the approved SUs, followed by Biological Instrumentation and Resources with 10.6% of approved SUs.

Along with the New and Renewal submissions for the June Research opportunity, the RAS APP team managed the usual steady stream of requests for other allocation types and management actions for active projects in the May-July reporting period. The team processed 184 Startup New and Renewal requests, 51 Educational New and Renewal requests, and 30 Campus Champions New and Renewal requests. For management actions across all allocation types, the team also processed requests for 287 Extensions, 118 Supplements, 95 Transfers, 88 Early Access Period approvals, 31 Advances, and 16 Adjustments.

Also during this reporting period, the APP team worked with the A3M team to define and complete a number of activities, including replacing the old Fields of Science list, establishing an Early Access Period action to support the onboarding of new resources and Service Providers, and completing the first version of the XRAS Client Administrator's Guide.

On a day-to-day basis, the RAS APP group fields user tickets and inquiries, processes Startup and Educational Requests within 11.4 days on average (less than the goal of 14 days), and handles allocation management requests (e.g., advances, transfers, supplements, and extensions). The team hosted two training webcasts to assist with Research request writing. Throughout the year, the APP team supported the XSEDE-wide reporting effort and ad hoc queries related to allocation information and other data in the XSEDE Central Database (XDCDB). The APP group also worked closely with the RAS A3M team of developers to test and recommend updates to the XRAS system.

For other metrics with respect to this WBS, see Appendix §12.2.2.5.1.

8.3. Allocations, Accounting, & Account Management CI (WBS 2.5.3)

The Allocations, Accounting and Account Management CI (A3M) group maintains and improves the interfaces, databases, and data transfer mechanisms for XSEDE-wide resource allocations, accounting of resource usage, and user account management.

During this reporting period, the team completed and deployed the new REST API version of the AMIE protocol. To make onboarding easier for new Service Providers, and to simplify support of the AMIE protocol in the future, A3M has converted the legacy AMIE communications system to a modern JSON and REST system. Alongside this deployment, the team has released a Python-based client library for

the new API to further simplify implementation efforts for Service Providers. As part of this effort, the team has been providing workshops, tutorials, documentation, and other assistance, to help Service Providers integrate with this new system.

Alongside the new AMIE API, A3M has also developed a new usage reporting API, taking advantage of AWS Lambda technology. The old usage reporting system was slow, able to process only 2-3 jobs per second, which could lead to backlogs or delays when systems uploaded their usage data to the XSEDE accounting system. The new system is more than 10 times as efficient, being able to handle 40 jobs per second. These improvements should significantly streamline the usage upload process and improve XSEDE accounting.

In addition to these changes, the team has begun implementation of the redesign of the rest of the XSEDE Accounting Service (XACCT). Building on the design plan that was created in the previous reporting period, the actual development efforts have begun to implement the new XACCT. It is planned that this effort will take a significant portion of the year to complete.

During this time, the team also continued to support and make User Interface (UI) improvements to XRAS to support the handling of XSEDE allocations and client processes.

For other metrics with respect to this WBS, see Appendix §12.2.2.5.2.

9. Program Office (WBS 2.6)

The purpose of the Program Office (PgO) is to ensure critical project level functions are in place and operating effectively and efficiently. The oversight provided via the Project Office is necessary to provide consistent guidance and leadership to the L3 managers across the project. A common and consistent approach to managing projects and risks is provided by the Project Management, Reporting, and Risk Management (PM&R) team (§9.3), while Business Operations (§9.4) manages all financial functions and sub-awards. The crucial aspect of communications to all stakeholders is the focus of the External Relations team (§9.2). Finally, Strategy, Planning, Policy, Evaluation & Organizational Improvement (SP&E) (§9.5) focuses attention in precisely those areas to ensure the best possible structure continues to exist within XSEDE to allow the support of all significant project activities and enable efficient and effective performance of all project responsibilities.

The success of the PgO depends on effective collaboration across all L2 areas of the project. The PgO conducts all administrative work for XSEDE, ensuring each project area is able to stay in operation and focused on the user-base. In addition, External Relations works with all L2 areas of the project to ensure that the user community is aware of the services offered by each area and to highlight project successes.

Key Performance Indicators for the Program Office are listed in the table below. Additional information about these KPIs can be found on the XSEDE KPIs & Metrics wiki page.

For other metrics with respect to this WBS, see Appendix §12.2.2.6.

Table 9–1: KPIs for Program Office.

Area Metric	Report Year	Target	RP1	RP2	RP3	RP4	Total	Sub-goal Supported
Variance between relevant report submission and due date (days)	RY5	0	0	0				Sustain — Operate an effective and productive virtual organization (§3.3.3)
	RY4	0	0	0	0	-1[4]	-1	
	RY3	0	0	0	0	0	0	
	RY2	0	0	0	0	0	0	
	RY1	0	*	NA	0	0	0	
Percentage of subaward invoices processed within target duration	RY5	90%/qtr	92.6	83.3				Sustain — Operate an effective and productive virtual organization (§3.3.3)
	RY4	95%/qtr	95.0	100.0	79.5	90.9	91.3	
	RY3	95%/qtr	82.4	77.8	94.4	92.9	86.9	
	RY2	95%/qtr	100.0	90.9	87.7	67.4	86.6[4]	
	RY1	90%/qtr	*	NA[1]	100.0	NA[2]	100.0	
Percentage of recommendations addressed by relevant project areas within 90 days	RY5	90%/yr	100	90				Sustain — Operate an effective and productive virtual organization (§3.3.3)
	RY4	90%/yr	47	48	0.1	0	24	
	RY3	90%/yr	46	74	0	62	45.5	
	RY2	90%/qtr	23	15	37	49	31	
	RY1	90%/qtr	*	NA[3]	100	57	78.5[4]	

Area Metric	Report Year	Target	RP1	RP2	RP3	RP4	Total	Sub-goal Supported
Grand (aggregate) mean of Staff Climate Study satisfaction items regarding content and accessibility of the XSEDE Staff Wiki (1-5 Likert scale)	RY5	3.9 of 5/ yr	-	3.9				Sustain — Operate an effective and productive virtual organization (§3.3.3)
	RY4	3.9 of 5/ yr	-	3.8	-	-	3.8	
	RY3	3.5 of 5/ yr	-	3.9	-	-	3.9	
	RY2		*	*	*	*	*	
	RY1		*	*	*	*	*	
Number of staff publications	RY5	50/yr	2	16				Sustain — Operate an innovative virtual organization (§3.3.4)
	RY4	32/yr	11	44	7	18	80	
	RY3	20/yr	19	16	7	6	48	
	RY2	20/yr	2	6	0	1	9	
	RY1	70/yr	*	5	0	13	18	
Grand (aggregate) mean of Staff Climate Study awareness items regarding inclusion in XSEDE (1-5 Likert scale)	RY5	4.1/yr	-	4.3				Sustain — Operate an innovative virtual organization (§3.3.4)
	RY4	4.1/yr	-	4.2	-	-	4.2	
	RY3	4.1/yr	-	4.1	-	-	4.1	
	RY2	5% improve-ment/yr	*	4.3	*	*	4.3	
	RY1		*	*	*	*	*	
Grand (aggregate) mean of Staff Climate Study awareness regarding equity in XSEDE (1-5 Likert scale)	RY5	4.0/yr	-	4.4				Sustain — Operate an innovative virtual organization (§3.3.4)
	RY4	4.0/yr	-	4.2	-	-	4.2	
	RY3	4.0/yr	-	4.1	-	-	4.1	
	RY2		*	*	*	*	*	
	RY1		*	*	*	*	*	
Number of XSEDE-related media hits	RY5	325/yr	624	467				Deepen/ Extend — Raise awareness of the value of advanced digital services (§3.1.4))
	RY4	165/yr	66	92	101	237	496	
	RY3	169/yr	23	29	54	60	166	
	RY2	169/yr	42	30	44	29	145	
	RY1	147/yr	*	32	30	18	80	

- Data reported annually.
[1] Subaward institutions did not have XSEDE2 contracts in place yet, so no invoices had been issued.
[2] No subaward invoices received during this reporting period.
[3] No recommendations received during this reporting period.

[4] -1 indicates that the report was submitted one day early in this reporting period.

The last Interim Project Report was submitted on time, so the target for "Variance between relevant report submission and due date" was met.

"Percentage of subaward invoices processed within target duration" fell short of the target this reporting period. The trend suggests that further analysis is needed to understand the root cause of the trend and determine if corrective action is needed. Business Operations has started the in-depth analysis of the last 12 months of invoice processing to determine the source of the delays for the invoices that were not processed within the identified timeframe. Results of the analysis and recommended actions will be provided to the L1 and Deputy L1 for review. The analysis results are expected to be provided by the end of November 2020.

"Percentage of recommendations addressed by relevant project areas within 90 days" achieved the goal of 90% addressed within 90 days with nine out of ten recommendations being addressed within 90 days.

Staff satisfaction with the XSEDE staff wiki met its yearly target.

The "Number of staff publications" improved this reporting period but remains behind the number that was submitted by this time last year. The target was increased after the high number of staff publications the project had last year. Project leadership will continue to encourage staff to publish and to be sure those publications are uploaded to the User Portal and tagged as staff publications, and if it determines that the high number that was published last year was an anomaly, the target will be adjusted down.

This year XSEDE staff rated inclusion and equity both very high. Both KPIs exceeded their annual targets.

"Number of XSEDE-related media hits" continued to exceed the annual goal in a single reporting period during RP2. This increase is due in part to the increased listening ability of the Cision software, which allows the XSEDE External Relations team to monitor newswires and every news source that picks up a press release mentioning XSEDE. The other reason for the increase compared to previous years is XSEDE's role in the COVID-19 HPC Consortium, which has resulted in many science stories that are shared nationwide via a variety of media. Though this has slowed down some from RP1, it still contributes to a significant amount of media coverage mentioning XSEDE. The ER team would expect to see this level off during RP3 and RP4, which will give us a more realistic goal of where to set our target for RY6.

PgO Highlights

The project is beginning to see the positive results expected from External Relation's social media impressions improvement plan. This impact is expected to increase the project's follower base. ER will continue to keep XSEDE visible within and outside the community with targeted campaigns for the Supercomputing 2020 conference (SC20) and science highlight stories.

Business Operations is kicking off an in-depth analysis of invoice processing to determine the sources of delays that have caused a trend of missing the quarterly KPI target.

Evaluations have been completed for 2020 Staff Climate, the Practice & Experience in Advanced Research Computing 2020 conference (PEARC20), and an internal COVID-19 survey.

9.1. Project Office (WBS 2.6.1)

The Project Office has been established to provide the necessary oversight to ensure the greatest efficiency and effectiveness of the Program Office area and to establish responsibility for assuring advisory activities of the project occur. This oversight includes providing direction to the L3 management team and coordination of and participation in Program Office planning activities and reports through the area's Project Manager. The Project Office also attends and supports the preparation of project-level reviews and activities. Importantly, the Project Office is responsible for ensuring that the XSEDE Advisory Board, the User Advisory Committee, and the SP Forum are functioning. The Project Office is responsible for coordination of project-level meetings such as the bi-weekly Senior Management Team (SMT) teleconference calls and the project quarterly meetings. Lastly, the Project Office will advise the XSEDE PI on many issues, especially those relevant to this WBS area.

9.2. External Relations (WBS 2.6.2)

External Relations' (ER) mission is to communicate the value and importance of XSEDE to all stakeholders (including the internal audience) through creative and strategic communications.

The External Relations team is starting to see growth in social media impressions across all combined platforms as RY5 progresses, as well as continued high levels for media coverage. The team hopes to continue this trend on social media, with an eye toward expanding XSEDE's follower base, something that will be vital to meet increasing social media impression goals. In order to achieve the annual goal, External Relations will need to gain 120,000 impressions across platforms in each of the remaining reporting periods of RY5. ER believes this is attainable via campaigns surrounding SC20 and year-end recap activities, which typically bring a bump to impression totals as the team highlights the best science stories of the year. In addition to this, ER will also track impressions on a weekly basis through November and, if impressions are sub-optimal, will make limited recommendations for digital advertising of social media platforms.

XSEDE sponsored the Gateways Conference again this year. The Gateways community is a fast-growing user base within XSEDE, which makes this a valuable event to support. The ER team provided a variety of content for XSEDE's virtual exhibitor booth and promoted the event via social media. The Gateways Conference tagged XSEDE in their social media posts which provided XSEDE with great exposure.

A large activity for ER each year is staffing the SC20 conference, which is going to an all-digital format this year. While this format could be a positive (more attendees interacting on social media), it could also be a negative (less total attention paid to SC20 due to virtual attendance). ER will keep a close eye on the social analytics around SC and plan accordingly. Pre-promotion is already underway and has been performing well.

For other metrics with respect to this WBS, see Appendix §12.2.2.6.1.

9.3. Project Management, Reporting, & Risk Management (WBS 2.6.3)

The Project Management, Reporting & Risk Management (PM&R) team enables an effective virtual organization through the application of project management principles; provides visibility to project progress, successes, and challenges; brings new ideas and management practices into the project; and disseminates lessons learned in XSEDE to other virtual organizations. Communication is critical to success in this highly distributed virtual organization.

During this reporting period, the PM&R team worked with project leadership to ensure the on-time submission of the Annual Report and Program Plan in August. The team also worked with project leadership to ensure that 100% of project risks were again reviewed during this reporting period and that ten open recommendations were addressed (nine of these, or 90%, were addressed within the 90 day target). PM&R coordinated project change requests (PCRs) for a number of KPI changes during this reporting period and ensured that revisions were made to all affected project documents.

For other metrics with respect to this WBS, see Appendix §12.2.2.6.2.

9.4. Business Operations (WBS 2.6.4)

The Business Operations (BusOps) group, working closely with staff at the University of Illinois's Grants and Contracts Office (GCO) and National Center for Supercomputing Applications' (NCSA) Business Office, manages budgetary issues and sub-awards, and ensures timely processing of sub-award amendments and invoices.

During this reporting period, BusOps worked to finalize collection and submission of all subaward PY10 funding amendments. The team also began work with all of the subaward partners to gather spend plans for PY10 and PY11 to ensure that the project is on track with projections for project spending through the end of the award. There seems to be a trend of invoice processing missing the KPI target. As such, Business Operations will be completing a detailed analysis of the last 12 months of invoice processing to understand the source(s) of the delay in processing and recommending corrective actions. The analysis results and recommended action(s) will be provided to the L1 and Deputy L1 for review. The recommended next steps are expected to be provided by the end of November, 2020.

For other metrics with respect to this WBS, see Appendix §12.2.2.6.3.

9.5. Strategy, Planning, Policy, Evaluation & Organizational Improvement (WBS 2.6.5)

XSEDE dedicates effort to project-wide strategic planning, policy development, evaluation and assessment, and organizational improvement in support of sustaining an effective and productive virtual organization.

XSEDE has engaged an independent Evaluation Team designed to provide XSEDE with information to guide program improvement and assess the impact of XSEDE services. Evaluations are based on five primary data sources: (1) an Annual User Survey that is part of the XSEDE annual report and program plan; (2) an Enhanced Longitudinal Study, encompassing additional target groups (e.g., faculty, institutions, disciplines, etc.) and additional measures (e.g., publications, citations, research funding, promotion and tenure, etc.); (3) an Annual XSEDE Staff Climate Study; (4) XSEDE KPIs, Area Metrics, and Organizational Improvement efforts, including ensuring that procedures are in place to assess these data; and (5) Specialized Studies as contracted by Level 2 directors and the Program Office.

During this reporting period, the Evaluation team finalized reporting on the XSEDE Staff Climate Study and distributed focused reports to each of the L2 Directors with results from their program area. Each of the L2 Directors will share plans for responding to results from their staff at the December XSEDE Quarterly Meeting. The team also finalized the PEARC20 evaluation report and submitted it to PEARC leadership. It also deployed an internal staff survey regarding impacts of COVID-19 which provided project leadership with insights into how XSEDE staff are adjusting to the many challenges resulting from the pandemic. This survey formed the basis of a discussion about these concerns during an all-staff meeting that was well-received.

The team reviewed concerns about several KPIs during this reporting period and recommended a number of changes to provide clarification and better understanding of what is actually being reported with each KPI.

The Return on Investment (ROI) team submitted a paper to the Utility and Cloud Computing conference and began its next round of data collection.

The team continued work with the Institute for Research on Innovation and Science (IRIS) to understand the economic impact of XSEDE across the country. IRIS submitted a report with preliminary findings, and the team is determining next steps.

For other metrics with respect to this WBS, see Appendix §12.2.2.6.4.

10. Financial Information

The XSEDE Business Operations team (§9.4) tracks and manages the financial aspect of the XSEDE project. This section conveys the financial status at a project level. The focus is on spending against the approved budget.

Note that closing out any given reporting period could take up to nine months after the reporting period ends. The actual duration is dependent on the timeliness of invoice submissions by the partner institutions, plus the University of Illinois invoice processing, typically 30-45 days. The table below shows the status of reported and paid costs during the defined reporting period. The understood delay in receipt and processing of invoices results in the need to update data associated with prior reporting periods, upon the release of each IPR.

The tables below show the financial summary, at a project level and a partner institution level, as of the submission of this report.

Table 10–1: Project Level Financial Summary.

Reporting Period	Invoices (Paid/Expected)	Budgeted	Spent	Projected
RY1 RP2: Sept '16 – Oct '16	38 of 38	$3,504,153	$2,478,940	N/A
RY1 RP3: Nov '16 – Jan '17	57 of 57	$5,256,230	$4,238,946	N/A
RY1 RP4: Feb '17 – Apr '17	57 of 57	$5,256,230	$5,131,523	N/A
RY1 Total: Sept '16 – Apr '17	**152 of 152**	**$14,016,613**	**$11,813,504**	**N/A**
RY2 RP1: May '17 – Jul '17	57 of 57	$5,256,230	$5,455,524	N/A
RY2 RP2: Aug '17 – Oct '17	57 of 57	$5,325,759	$5,012,569	N/A
RY2 RP3: Nov '17 – Jan '18	57 of 57	$5,423,416	$4,909,549	N/A
RY2 RP4: Feb '18 – April '18	57 of 57	$5,423,416	$4,831,465	N/A
RY2 Total: Sept '17 – April '18	**228 of 228**	**$21,428,820**	**$20,179,942**	**N/A**
RY3 RP1: May '18 – Jul '18	56 of 56	$5,332,257	$5,918,791	N/A
RY3 RP2: Aug '18 – Oct '18*	57 of 57	$5,485,889	$5,204,824	N/A
RY3 RP3: Nov '18 – Jan '19*	57 of 57	$5,560,866	$5,012,275	N/A
RY3 RP4: Feb '19 – Apr '19*	58 of 58	$5,628,783	$5,343,120	N/A
RY3 Total: Sept '18 – April '19*	**228 of 228**	**$22,007,794**	**$21,479,009**	**N/A**
RY4 RP1: May '19 – Jul '19*	57 of 57	$5,662,741	$5,340,260	N/A
RY4 RP2: Aug '19 – Oct '19	53 of 53	$5,743,027	$5,338,504	N/A
RY4 RP3: Nov '19 – Jan '20	51 of 51	$5,783,170	$5,443,052	N/A
RY4 RP4: Feb '20 – Apr '20	51 of 51	$5,783,170	$5,146,415	N/A
RY4 Total: Sept '19 – April '20	**212 of 212**	**$22,972,109**	**$21,268,232**	**N/A**
RY5 RP1: May '20 – Jul '20	46 of 51*	$5,750,235	$4,924,769	$1,084,001
RY5 RP2: Aug '20 – Oct '20	26 of 51*	$5,773,499	$2,297,279	$4,729,702
RY5 RP3: Nov '20 – Jan '21				
RY5 RP4: Feb '21 – Apr '21				
RY5 Total: Sept '20 – Apr '21				
RY6 RP1: May '21 - Jul '21				

RY6 RP2: Aug '21 - Oct '21				
RY6 RP3: Nov '21 - Jan '22				
RY6 RP4: Feb '22 - Apr '22				
Extended RY6: May '22 - Aug '22				

* Partial information available; will be updated in future IPRs.

The following tables reflect received invoices and the breakdown distribution within the XSEDE Invoice Portal. The expenses reported may reflect back transfers, and we are reporting based on the month the expense posted to the grant/subaward account.

Table 10–2: Partner Institution Level Financial Summary.

	RY1 RP2: Sept '16 – Oct '16			RY1 RP3: Nov '16 – Jan '17		
Partner Institution	**Invoices Paid (of 2)**	**Budgeted**	**Spent**	**Invoices Paid (of 3)**	**Budgeted**	**Spent**
NCSA	2	$733,278	$179,527	3	$1,099,917	$623,728
TACC	2	$550,304	$31,027	3	$825,457	$55,141
PSC/MPC	2	$532,169	$487,486	3	$789,253	$738,316
SDSC/UCSD	2	$463,680	$471,304	3	$695,520	$681,232
NICS/UTK	2	$286,575	$263,222	3	$429,862	$397,643
U Chicago/ANL	2	$226,231	$188,387	3	$339,346	$221,649
Indiana University	2	$189,172	$122,602	3	$283,758	$293,470
Shodor	2	$107,262	$109,862	3	$160,893	$137,963
Cornell University	2	$105,112	$89,470	3	$157,668	$124,968
NCAR/UCAR	2	$66,215	$0	3	$99,323	$69,224
Purdue University	2	$52,897	$54,084	3	$79,345	$111,537
Georgia Tech	2	$55,357	$4,320	3	$83,035	$6,480
SURA	2	$38,333	$31,027	3	$57,500	$55,141
OK State (OSU)	2	$33,573	$8,574	3	$50,361	$16,321
Ohio State (OSC)	2	$18,367	$0	3	$27,550	$32,197
USC-ISI	2	$13,333	$31,027	3	$20,000	$55,141
U Oklahoma (OU)	2	$11,261	$10,578	3	$16,892	$15,866
U Georgia	2	$10,567	$2,788	3	$15,850	$4,182
U Arkansas	2	$10,467	$8,749	3	$15,700	$16,184
Project Level	38 of 38	$3,504,153	$2,094,031	57/57	$5,256,230	$3,656,383

	RY1 RP4: Feb '17 – Apr '17			RY1 Total: Sept '16 – May '17		
Partner Institution	**Invoices Paid (of 3)**	**Budgeted**	**Spent**	**Invoices Paid (of 8)**	**Budgeted**	**Spent**
NCSA	3	$1,099,917	$1,207,527	8	$2,933,112	$2,010,781
TACC	3	$825,457	$63,772	8	$2,201,218	$149,940
PSC/MPC	3	$798,253	$801,638	8	$2,128,675	$2,027,439
SDSC/UCSD	3	$695,520	$711,326	8	$1,854,720	$1,863,862
NICS/UTK	3	$429,862	$406,402	8	$1,146,299	$1,067,266
U Chicago/ANL	3	$339,346	$491,477	8	$904,923	$901,513
Indiana University	3	$283,758	$256,475	8	$756,688	$672,547
Shodor	3	$160,893	$117,830	8	$429,048	$365,655
Cornell University	3	$157,668	$107,949	8	$420,448	$322,387
NCAR/UCAR	3	$99,323	$90,254	8	$264,861	$159,478
Purdue University	3	$79,345	$58,688	8	$211,587	$224,308
Georgia Tech	3	$83,035	$6,480	8	$221,427	$17,281
SURA	3	$57,500	$63,772	8	$153,333	$149,940
OK State (OSU)	3	$50,361	$14,547	8	$134,295	$39,442
Ohio State (OSC)	3	$27,550	$32,471	8	$73,467	$64,667
USC-ISI	3	$20,000	$63,772	8	$53,333	$149,940
U Oklahoma (OU)	3	$16,892	$15,867	8	$45,045	$42,310
U Georgia	3	$15,850	$4,182	8	$42,267	$11,151
U Arkansas	3	$15,700	$13,123	8	$41,867	$38,056
Project Level	57 of 57	$5,256,230	$4,527,552	152 of 152	$14,016,613	$10,277,966

	RY2 RP1: May '17 – Jul '17			RY2 RP2: Aug '17 – Oct '17		
Partner Institution	**Invoices Paid (of 3)**	**Budgeted**	**Spent**	**Invoices Paid (of 3)**	**Budgeted**	**Spent**
NCSA	3	$1,099,917	$1,147,967	3	$1,098,678	$974,612
TACC	3	$825,457	$916,498	3	$816,652	$847,586
PSC/MPC	3	$798,253	$830,786	3	$807,749	$828,314
SDSC/UCSD	3	$695,520	$722,633	3	$705,544	$723,763
NICS/UTK	3	$429,862	$496,015	3	$459,812	$404,335
U Chicago/ANL	3	$339,346	$336,242	3	$350,002	$147,712
Indiana University	3	$283,758	$263,689	3	$277,231	$275,840
Shodor	3	$160,893	$164,529	3	$162,986	$134,506
Cornell University	3	$157,668	$152,928	3	$178,616	$125,746
NCAR/UCAR	3	$99,323	$83,082	3	$107,430	$98,807
Purdue University	3	$79,345	$68,088	3	$72,795	$70,039
Georgia Tech	3	$83,035	$62,090	3	$75,542	$107,992
SURA	3	$57,500	$59,371	3	$58,229	$62,519
OK State (OSU)	3	$50,361	$38,016	3	$54,250	$125,817
Ohio State (OSC)	3	$27,550	$33,963	3	$27,830	$25,220
USC-ISI	3	$20,000	$33,955	3	$20,300	$13,152
U Oklahoma (OU)	3	$16,892	$15,404	3	$20,455	$14,054
U Georgia	3	$15,850	$31,924	3	$15,888	$16,871
U Arkansas	3	$15,700	$17,975	3	$15,772	$15,682
Project Level	57 of 57	$5,256,230	$5,475,155	57 of 57	$5,325,759	$5,012,569

	RY2 RP3: Nov '17 – Jan '18			RY2 RP4: Feb '18 – Apr '18		
Partner Institution	**Invoices Paid (of 3)**	**Budgeted**	**Spent**	**Invoices Paid (of 3)**	**Budgeted**	**Spent**
NCSA	3	$1,154,307	$1,016,137	3	$1,154,307	$935,931
TACC	3	$812,249	$869,772	3	$812,249	$303,524
PSC/MPC	3	$812,496	$851,171	3	$812,496	$809,751
SDSC/UCSD	3	$710,556	$716,848	3	$710,556	$727,397
NICS/UTK	3	$474,787	$395,172	3	$474,787	$413,610
U Chicago/ANL	3	$355,330	$148,934	3	$355,330	$730,303
Indiana University	3	$273,968	$272,403	3	$273,968	$258,732
Shodor	3	$164,032	$127,160	3	$164,032	$128,962
Cornell University	3	$189,090	$144,466	3	$189,090	$141,914
NCAR/UCAR	3	$111,483	$101,823	3	$111,483	$136,090
Purdue University	3	$69,520	$74,499	3	$69,520	$66,940
Georgia Tech	3	$78,439	$42,557	3	$78,439	$24,414
SURA	3	$58,594	$42,633	3	$58,594	$55,266
OK State (OSU)	3	$56,195	$37,584	3	$56,195	$30,217
Ohio State (OSC)	3	$27,970	$22,023	3	$27,970	$22,727
USC-ISI	3	$20,450	$16,735	3	$20,450	$19,177
U Oklahoma (OU)	3	$22,237	$13,229	3	$22,237	$13,228
U Georgia	3	$15,907	$18,633	3	$15,907	$18,633
U Arkansas	3	$15,808	$16,404	3	$15,808	$13,283
Project Level	57 of 57	$5,423,416	$4,928,182	57 of 57	$5,423,416	$4,850,097

RY2 Total: May '17 – Apr '18			
Partner Institution	**Invoices Paid (of 12)**	**Budgeted**	**Spent**
NCSA	12	$4,507,209	$4,074,646
TACC	12	$3,266,607	$2,937,380
PSC/MPC	12	$3,230,994	$3,320,022
SDSC/UCSD	12	$2,822,175	$2,890,641
NICS/UTK	12	$1,839,249	$1,709,132
U Chicago/ANL	12	$1,400,007	$1,363,192
Indiana University	12	$1,108,925	$1,070,664
Shodor	12	$651,942	$555,158
Cornell University	12	$714,463	$565,054
NCAR/UCAR	12	$429,719	$419,801
Purdue University	12	$291,179	$279,566
Georgia Tech	12	$315,454	$237,053
SURA	12	$232,917	$219,789
OK State (OSU)	12	$217,001	$231,634
Ohio State (OSC)	12	$111,320	$103,934
USC-ISI	12	$81,200	$83,018
U Oklahoma (OU)	12	$81,822	$55,914
U Georgia	12	$63,553	$86,060
U Arkansas	12	$63,087	$63,345
Project Level	228 of 228	$21,428,820	$20,266,003

† Subawardee transitioned institutions during this period, thus, there was only one invoice from each of those institutions during this period.

Partner Institution	RY3 RP1: May '18 – July '18			RY3 RP2: Aug '18 – Oct '18		
	Invoices Paid (of 3)	Budgeted	Spent	Invoices Paid (of 3)	Budgeted	Spent
NCSA	3	$1,079,267	$1,061,000	3	$1,196,029	$1,134,369
TACC	3	$799,010	$1,371,895	3	$793,074	$839,725
PSC/MPC	3	$813,725	$822,138	3	$841,714	$825,881
SDSC/UCSD	3	$710,556	$709,180	3	$721,408	$696,515
NICS/UTK	3	$474,787	$543,968	3	$461,707	$410,580
U Chicago/ANL	3	$355,446	$278,271	3	$353,810	$282,262
Indiana University	3	$273,968	$280,742	3	$269,780	$251,812
Shodor	3	$164,132	$187,195	3	$173,967	$128,270
Cornell University	3	$189,090	$156,765	3	$191,982	$171,593
NCAR/UCAR	3	$111,483	$107,236	3	$106,323	$77,394
Purdue University	3	$69,520	$64,669	3	$70,595	$72,138
Georgia Tech	3	$78,439	$146,226	3	$86,559	$65,189
SURA	3	$58,594	$70,674	3	$64,542	$62,935
OK State (OSU)	3	$56,195	$34,666	3	$24,427	$102,256
Ohio State (OSC)	3	$27,970	$21,567	3	$33,257	$26,865
USC-ISI	3	$20,450	$27,463	3	$20,757	$29,259
U Oklahoma (OU)	3	$22,238	$14,601	3	$22,563	$14,276
U Georgia	1†	$6,363	$6,211	0	$0	$0
Notre Dame	1†	$5,219	$0	3	$15,656	$0
U Arkansas	3	$15,808	$14,326	3	$15,940	$13,506
Project Level	56 of 56	$5,332,257	$5,918,791	57 of 57	$5,485,889	$5,204,824

† Subawardee transitioned institutions during this period, thus, there was only one invoice from each of those institutions during this period.

Partner Institution	RY3 RP3: Nov '18 – Jan '19			RY3 RP4: Feb '19 – Apr '19		
	Invoices Paid (of 3)	Budgeted	Spent	Invoices Paid (of 3)	Budgeted	Spent
NCSA	3	$1,254,410	$1,029,286	3	$1,254,410	$1,067,177
TACC	3	$790,106	$678,184	3	$790,106	$961,363
PSC/MPC	3	$855,709	$883,438	3	$855,709	$826,496
SDSC/UCSD	3	$726,834	$682,790	3	$726,834	$685,154
NICS/UTK	3	$455,168	$345,594	3	$455,168	$427,196
U Chicago/ANL	3	$352,992	$423,139	3	$352,992	$317,198
Indiana University	3	$300,386	$261,815	3	$300,386	$280,099
Shodor	3	$178,884	$144,815	3	$178,884	$153,524
Cornell University	3	$193,428	$198,933	3	$193,428	$266,505
NCAR/UCAR	3	$103,743	$97,268	3	$103,743	$103,775
Purdue University	3	$71,133	$72,890	3	$71,133	$47,359
Georgia Tech	3	$90,619	$49,657	3	$90,619	$46,103
SURA	3	$67,517	$46,680	3	$67,517	$86,153
OK State (OSU)	3	$8,543	$26,391	1†	$2,848	$8,878
Internet2				3†	$73,612	$0
Ohio State (OSC)	3	$35,901	$22,952	3	$35,901	$27,291
USC-ISI	3	$20,910	$7,402	3	$20,910	$7,837
U Oklahoma (OU)	3	$22,726	$27,441	3	$22,726	$17,411
U Georgia	0	$0	$0	0	$0	$0
Notre Dame	3	$15,656	$0	3	$15,656	$0
U Arkansas	3	$16,204	$13,601	3	$16,204	$13,601
Project Level	57 of 57	$5,560,866	$5,012,275	58 of 58	$5,628,783	$5,343,120

† Subawardee transitioned between institutions during this period resulting in net one additional invoice due to transition timing and billing periods.

RY3 Total: May '18 – Apr '19				
Partner Institution	**Invoices Paid (of 12)**	**Budgeted**	**Spent**	**Projected**
NCSA	12	$4,784,116	$4,291,832	$0
TACC	12	$3,172,295	$3,851,167	$0
PSC/MPC	12	$3,366,857	$3,357,953	$0
SDSC/UCSD	12	$2,885,632	$2,773,638	$0
NICS/UTK	12	$1,846,830	$1,727,338	$0
U Chicago/ANL	12	$1,415,239	$1,300,869	$0
Indiana University	12	$1,166,320	$1,074,468	$0
Shodor	12	$695,866	$613,804	$0
Cornell University	12	$767,927	$793,797	$0
NCAR/UCAR	12	$425,293	$385,673	$0
Purdue University	12	$282,381	$257,055	$0
Georgia Tech	12	$346,235	$307,175	$0
SURA	12	$258,170	$266,441	$0
OK State (OSU)	10	$92,012	$172,191	$0
Internet2	3	$73,612	$0	$0
Ohio State (OSC)	12	$133,028	$98,674	$0
USC-ISI	12	$83,027	$71,960	$0
U Oklahoma (OU)	12	$90,253	$73,728	$0
U Georgia	1	$6,363	$6,211	$0
Notre Dame	10	$52,185	$0	$0
U Arkansas	12	$64,154	$55,034	$0
Project Level	228 of 228	$22,007,794	$21,479,009	$0

	RY4 RP1: May '19 – Jul '19			RY4 RP2: Aug '19 – Oct '19		
Partner Institution	**Invoices Paid (of 3)**	**Budgeted**	**Spent**	**Invoices Paid (of 3)**	**Budgeted**	**Spent**
NCSA	3	$1,254,410	$987,332	3	$1,221,496	$1,040,514
TACC	3	$790,106	$776,066	3	$809,638	$549,787
PSC/MPC	3	$855,709	$835,783	3	$857,989	$894,619
SDSC/UCSD	3	$726,834	$711,843	3	$788,548	$692,240
NICS/UTK	3	$455,168	$452,047	3	$469,599	$422,264
U Chicago/ANL	3	$352,992	$347,184	3	$364,621	$353,438
Indiana University	3	$300,386	$247,478	3	$331,570	$390,765
Shodor	3	$178,884	$188,947	3	$160,243	$213,694
Cornell University	3	$193,428	$213,863	3	$195,934	$206,135
NCAR/UCAR	3	$103,743	$161,398	3	$105,301	$141,144
Purdue University	3	$71,133	$84,844	3	$72,163	$74,618
Georgia Tech	3	$90,619	$98,865	3	$88,560	$73,146
SURA	3	$67,517	$48,937	3	$87,176	$72,419
OK State (OSU)	0	$0	$0	0	$0	$0
Internet2	3	$110,418	$53,879	3	$77,222	$133,036
Ohio State (OSC)	3	$35,901	$27,115	3	$36,174	$30,494
USC-ISI	3	$20,910	$7,297	3	$21,224	$18,376
U Oklahoma (OU)	3	$22,726	$18,357	3	$22,991	$18,137
U Georgia	0	$0	$0	0	$0	$0
Notre Dame	3	$15,656	$63,645	1	$16,101	$7,317
U Arkansas	3	$16,204	$15,382	2	$16,476	$6,361
Project Level	57 of 57	$5,662,741	$5,340,260	53	$5,743,027	$5,338,504

	RY4 RP3: Nov '19 – Jan '20			RY4 RP4: Feb '20 – Apr '20		
Partner Institution	**Invoices Paid (of 3)**	**Budgeted**	**Spent**	**Invoices Paid (of 3)**	**Budgeted**	**Spent**
NCSA	3	$1,205,039	$1,091,031	3	$1,205,039	$1,055,366
TACC	3	$819,405	$966,294	3	$819,405	$730,304
PSC/MPC	3	$859,130	$837,147	3	$859,130	$857,841
SDSC/UCSD	3	$819,405	$730,210	3	$819,405	$712,713
NICS/UTK	3	$476,815	$473,779	3	$476,815	$500,998
U Chicago/ANL	3	$370,436	$357,562	3	$370,436	$179,802
Indiana University	3	$347,163	$316,887	3	$347,163	$410,438
Shodor	3	$150,923	$94,127	3	$150,923	$124,724
Cornell University	3	$197,188	$143,999	3	$197,188	$137,333
NCAR/UCAR	3	$106,080	$114,560	3	$106,080	$127,488
Purdue University	3	$72,678	$78,428	3	$72,678	$45,525
Georgia Tech	3	$87,531	$58,608	3	$87,531	$48,373
SURA	3	$61,369	$77,099	3	$97,006	$97,126
OK State (OSU)	0	$0	$0	0	$0	$0
Internet2	3	$60,624	$42,958	3	$60,624	$40,031
Ohio State (OSC)	3	$36,311	$31,142	3	$36,311	$32,066
USC-ISI	3	$21,381	$19,135	3	$21,381	$31,160
U Oklahoma (OU)	3	$23,123	$10,086	3	$23,123	$15,129
U Georgia	0	$0	$0	0	$0	$0
Notre Dame	0	$16,324	$0	0	$16,324	$0
U Arkansas	0	$16,612	$0	0	$16,612	$0
Project Level	51	$5,747,533	$5,443,052	51	$5,783,170	$5,146,415

RY4 Total: May '19 – Apr '20				
Partner Institution	**Invoices Paid (of 12)**	**Budgeted**	**Spent**	**Projected**
NCSA	12	$4,885,984	$4,174,243	$0
TACC	12	$3,238,553	$3,022,452	$0
PSC/MPC	12	$3,431,957	$3,425,390	$0
SDSC/UCSD	12	$3,154,191	$2,847,006	$0
NICS/UTK	12	$1,878,397	$1,849,088	$0
U Chicago/ANL	12	$1,458,484	$1,237,987	$0
Indiana University	12	$1,326,282	$1,365,567	$0
Shodor	12	$640,973	$621,492	$0
Cornell University	12	$783,737	$701,329	$0
NCAR/UCAR	12	$421,204	$544,589	$0
Purdue University	12	$288,653	$283,415	$0
Georgia Tech	12	$354,242	$278,992	$0
SURA	12	$348,706	$295,581	$0
OK State (OSU)	0	$0	$0	$0
Internet2	12	$308,887	$269,904	$0
Ohio State (OSC)	12	$144,697	$120,816	$0
USC-ISI	12	$84,895	$75,967	$0
U Oklahoma (OU)	12	$91,963	$61,708	$0
U Georgia	0	$0	$0	$0
Notre Dame	4	$64,404	$70,962	$0
U Arkansas	4	$65,903	$21,743	$0
Project Level	212	$22,972,109	$21,268,232	$0

RY5 RP1: May '20 – July '20				
Partner Institution	**Invoices Paid (of 3)**	**Budgeted**	**Spent**	**Projected**
NCSA	3	$1,205,039	$1,060,364	$0
TACC	3	$819,405	$983,225	$0
PSC/MPC	3	$859,130	$810,950	$0
SDSC/UCSD	3	$819,405	$737,176	$0
NICS/UTK	3	$476,815	$586,305	$0
U Chicago/ANL	3	$370,436	$534,409	$0
Indiana University	3	$347,163	$370,990	$0
Shodor	3	$150,923	$220,991	$0
Cornell University	3	$197,188	$205,975	$0
NCAR/UCAR	3	$106,080	$90,259	$0
Purdue University	3	$72,678	$45,531	$0
Georgia Tech	3	$87,531	$97,821	$0
SURA	3	$97,006	$131,719	$0
OK State (OSU)	0	0	0	0
Internet2	3	$60,624	$42,050	$0
Ohio State (OSC)	3	$36,311	$71,917	$0
USC-ISI	3	$21,381	$47,115	$0
U Oklahoma (OU)	2	$23,123	$18,126	$6,382
U Georgia	0	0	0	0
Notre Dame	0	0	0	0
U Arkansas	0	0	0	0
Project Level	50	$5,750,235	$6,054,924	$6,382

RY5 RP2: August '20 – October '20				
Partner Institution	**Invoices Paid (of 3)**	**Budgeted**	**Spent**	**Projected**
NCSA	2	$1,226,682	$777,042	$333,058
TACC	2	$835,704	$411,332	$23,137
PSC/MPC	3	$869,377	$768,675	$0
SDSC/UCSD	1	$779,726	$182,421	$472,006
NICS/UTK	2	$468,032	$401,299	$151,609
U Chicago/ANL	3	$372,110	$344,411	$0
Indiana University	2	$349,102	$218,792	$92,045
Shodor	3	$153,001	$157,448	$0
Cornell University	2	$202,079	$143,579	$78,444
NCAR/UCAR	2	$107,672	$53,131	$49,984
Purdue University	2	$73,731	$28,239	$24,165
Georgia Tech	3	$88,620	$44,111	$0
SURA	2	$98,588	$65,644	$23,137
OK State (OSU)	0	0	0	0
Internet2	2	$71,873	$55,401	$27,256
Ohio State (OSC)	3	$32,107	$35,252	$0
USC-ISI	3	$21,701	$30,606	$0
U Oklahoma (OU)	0	$23,394	$0	$19,147
U Georgia	0	0	0	0
Notre Dame	0	0	0	0
U Arkansas	0	0	0	0
Project Level	37	$5,773,499	$3,717,385	$1,293,990

11.Project Improvement Fund

The XSEDE Project Improvement Fund (PIF) is an extension of the XSEDE PY7-PY9 annual planning and budget review process to strategically invest approximately 2% of the annual budget ($465k annually) towards short-term project improvements specific to the XSEDE project. A lightweight Phase-Gate process is used to facilitate the review and prioritization of proposed project improvements by the XSEDE Senior Management Team (SMT). Funding is allocated based on this prioritization. The details of the process can be found on the XSEDE wiki PIF page. It is important to note that the annual budget for project improvement funds, while expected to be used during a specific project year, are not intended to be fully allocated during the project year planning period. The funds are allocated prior to and throughout the first half of the project year via a review process for the project to fund important ideas that bring value to the project and, in particular, to the community we support.

There have been a wide range of PIFs approved, including: updates and improvements to tools, staff training, new offerings to the community, and analysis efforts of the project's tools and services.

To date, 25 idea submissions have been received and reviewed. The following is a summary of the current status:

PY7 Project Improvement Fund Status

Total PIF funds allocated: $389K of $389K

State/Phase	Submissions	Comments
Complete	6	Projects officially closed • ECSS cloud support specialist • XDCDB improvements • Jira bootcamp • ECSS: Ease transition to *Stampede2* • 2K Duo licenses • 2017 IHPCSS
Not Funded	4	Other recent efforts were similar or the submission requested annually recurring funding
Withdrawn	1	Withdrawn due to significant overlap with another submission

Notes:

PY7 PIF funds have been reduced by $76K, as per PCR #14, to fund the 2018 International HPC Summer School. The NSF proposal to cover the funding of the summer school was not approved by NSF, resulting in PCR #14 being triggered to ensure sufficient funding for the summer school.

PY8 Project Improvement Fund Status

Total PIF funds allocated: $356K of $356K

State/Phase	Submissions	Comments

Complete	3	Activity was completed during PY8: • ER Market Analysis • ORCID Membership Fee • 2019 IHPCSS
Funded/Execute	4	No PY8 PIFs moved to Funded this reporting period. PY8 PIF proposals that were funded and continue to be executed: • Update Applications of Parallel Computing online course (PY8 & PY9) • ROI analysis of CI systems (PY8-10) • Longitudinal studies (PY8-10) • Equity & Belonging (PY8-10)
In Process/Planning	2	Proposals received in PY8 that are still in review: • OpenStack Toolkit • ECSS staff training
Withdrawn	2	Two proposals withdrawn due to lack of available funds

Notes:

The PY8 PIF funds have been reduced by approximately $108K to fund the 2019 International HPC Summer School. This is due to the lack of NSF funding for the Summer School event.

Two PIF submissions that were received during PY8 continue to be reviewed by the SMT. Although all budgeted PIF funds have been fully allocated, the PIF submission window will remain open to collect and prioritize valuable ideas to prepare for possible future unspent funds being reallocated for high impact ideas.

PY9 Project Improvement Fund Status

Total PIF funds allocated: $465K of $465K

State/Phase	Submissions	Comments
Complete	1	Funded activities to be completed during PY9 • Duo licenses
Funded/Execute	4	No PIFs moved to Funded this reporting period. Four PIF activities continued from PY8: • Update Applications of Parallel Computing online course (PY8 & PY9) • ROI analysis of CI systems (PY8-10) • Longitudinal studies (PY8-10)

		• Equity & Belonging (PY8-10)
In Process/Planning	1	Proposals received in PY9 that are still in review: • Integrate online textbook exercises with CCRS toolkit
Withdrawn	2	One proposal withdrawn due to lack of available funds. One proposal was withdrawn because funds were allocated from another area of the project to cover the cost.

One PIF submission that was received during PY9 continues to be reviewed by the SMT. Although all budgeted PIF funds have been fully allocated, the PIF submission window will remain open to collect and prioritize valuable ideas to prepare for possible future unspent funds being reallocated for high impact ideas.

PY10 Project Improvement Fund Status

While there are no PIF funds budgeted for PY10, there are multi-year PIF funded activities that were funded in PY8 and 9 and will be continued in PY10 using unspent non-PIF project funds from PY6-8.

State/Phase	Submissions	Comments
Complete	0	
Funded/Execute	3	Three activities continue from previous year: • ROI analysis of CI systems (PY8-10) • Longitudinal studies (PY8-10) • Equity & Belonging (PY8-10)
In Process/Planning	0	

12. Appendices

12.1. Glossary and List of Acronyms

ACRONYM	DESCRIPTION	Notes
A3M	Allocations, Accounting & Account Management	
A&AM	Accounting & Account Management	
A&D	Architecture & Design	
ADR	Architecture Design Review	
AL2S	Advanced Layer 2 Service	Enables Internet2 users to create point-to-point VLANs
AMIE	Account Management Information Exchange	
API	Application Programming Interface	
Area Metric	A quantifiable measure that is used to track and assess the status of a specific process. Area Metrics can measure performance or operational status. Area Metrics relating to performance can be used alone or in combinations as a key performance indicator (KPI) for the project.	
AWS	Amazon Web Services	
BoF	Birds of a Feather	Group of community members who informally gather to discuss best practices and/or plans
C4C	Computing4Change	
CaRCC	Campus Research Computing Consortium	
CB	Campus Bridging	Infrastructure to make XSEDE resources appear to be proximal to the researcher's desktop
CC	Campus Champion	
CDPs	Capability Delivery Plans	
CEE	Community Enhancement & Engagement	
CERN	Organisation Européenne pour la Recherche Nucléaire	
co-Pi	Co-Principal Investigator	
CRI	Cyberinfrastructure Resource Integration	
CRM	Customer Relationship Management	
CS&E	Computational Science & Engineering	
CSR	Community Software Repository	
CTSC	Center for Trustworthy Scientific Infrastructure	
DNS	Domain Name Service	
DNSKEY	Domain Name Service Key	
DNSSEC	DNS Security	

DTS	Data Transfer Services	
E&O	Education and Outreach	
ECSS	Extended Collaborative Service	
e-infrastructure	The integration of networks, grids, data centers and collaborative environments, and are intended to include supporting operation centers, service registries, and credential delegation services.	
ER	External Relations	
ESRT	Extended Support for Research Teams	
ESSGW	Extended Collaborative Support for Science Gateways	
ESTEO	Extended Support for Training, Education, & Outreach	
FTE	Full Technical Equivalent	
GAAMP	General Automated Atomic Model Parameterization	
GFFS	Globus Federated File System	
GridFTP	Grid File Transfer Protocol	
HBCUs	Historically Black Colleges and Universities	
HPC	High Performance Computing	
HPCU	HPC University	
HSI	Hispanic Service Institution	
HSM	Hardware Security Models	
I2	Internet2	
IC	Industry Challenge	
IdM	Identity Management	
IGTF	Interoperable Global Trust Federation	
INCA/Nagios	A service monitoring tool	
IPR	Interim Project Report	
IR	Incident Reports	
JIRA	an activity tracking tool	
KB	KB documents	
KPI	Key Performance Indicators - A metric or combination of metrics meant to measure performance in key areas of the program so that actions and decisions which move the metrics in the desired direction also move the program in the direction of the desired outcomes and goals.	
L2	WBS Level 2	
L3	WBS Level 3	
MFC	Minority Faculty Council	
MS	Microsoft	
MSI	Minority Serving Institution	
MTTR	Mean Time To Resolution	
NCAR	National Center for Atmospheric Research	
NCSA	National Center for Supercomputing Applications	

NICS	National Institute of Computational Science	
NIP	Novel & Innovative Projects	
OSG	Open Science Grid	
OTP	One Time Password	
PEARC	Practice & Experience in Advanced Research Computing Conference Series (www.pearc.org)	
PEP	Program Execution Plan	
perfSONAR	PERFormance Service Oriented Network monitoring Architecture	
PI	Principal Investigator	
PM	Project Management/Project Manager	
PM&R	Project Management, Reporting & Risk Management	
POPS	PACI Online Proposal System	this is no longer an acronym and POPS is just the name for the allocation submission system; being supplanted by XRAS
PRACE	Partnership for Advanced Computing in Europe	
PSC	Pittsburgh Supercomputing Center	
PY	Program Year	
RAS	Resource Allocations Service	
RACD	Requirements Analysis & Capability Delivery	
RDR	Resource Description Repository	
RESTful	Representational state transfer	
rocks roll	An open source cluster distribution solution that simplifies the processes of deploying, managing, upgrading, and scaling high-performance parallel computing clusters.	
RT	Request Tracker Ticketing System	
SACNAS	Society for Advancement of Chicanos and Native Americans	
SCxy	Supercomputing Conference (e.g. SC16)	
SD&I	Software Development & Integration	
SDIACT	Software Development & Integration Activity	
SDSC	San Diego Supercomputer Center	
SecOps	Operations - Cybersecurity	
SH2	SH2 Security	
Shodor	A National Resource for Computational Science Education	
SP	Service Provider	
SP&E	Strategy, Planning, Policy, Evaluation & Organizational Improvement	
STEM	Science Technology Engineering Mathematics	
SURA	Southeastern Universities Research Association	
SysOps	Systems Operations	

TACC	Texas Advanced Computing Center	
TAGPMA	The Americas Grid Policy Management Authority	
TEOS	Training, Education and Outreach Service	
TAS	Technology Audit Service	
TeraGrid	An e-Science grid computing infrastructure combining resources at eleven partner sites.	
TTX	Table Top Exercise	
UCCAN	Canonical Use Case	
UCCB	Campus Bridging Use Case	
UCDA	Data Analytics Use Case	
UCDM	Data Management Use Case	
UCF	Federation & Interoperation Use Case	
UCFC	First Connecting Instrumentation Use Case	
UCHPC	High Performance Computing Use Case	
UCHTC	High Throughput Computing Use Case	
UCSGW	Science Gateway Use Case	
UCSW	Scientific Workflow Use Case	
UCVIS	Visualization Use Case	
UE	User Engagement	
UII	User Interfaces & Information	
URC	Under-represented communities	
URCE	Under-Represented Community Engagement	
UREP	User Requirement Evaluation & Prioritization	
URM	Under-Represented Minority	
US	United States	
WBS	Work Breakdown Structure	Numerical code for each group within XSEDE
WISE	Wise Information Security for E-infrastructure	
WLCG	Worldwide LHC Computing Grid	
XCBC	XSEDE Compatible Basic Cluster	Enables campus resource administrators to build a local cluster operating on open source software and compatible with XSEDE supported resources from scratch.
XCI	XSEDE Cyberinfrastructure Integration	

XDCDB	XSEDE Central Database	The XDCDB contains 24 schemas, notably the accounting, resource repository, portal, and AMIE databases.
XDMoD	XSEDE Metrics on Demand	Comprehensive HPC system management tool
XES	XSEDE Enterprise Services	
XMS	XD Net Metrics Services	
XNIT	XSEDE National Integration Toolkit	A suite of software modules intended for extant clusters so they are easily interoperable with XSEDE-supported resources.
XOC	XSEDE Operation Center	
XRAC	XSEDE Resource Allocation Committee	
XRAS	XSEDE Resource Allocations System	
XSEDE	eXtreme Science and Engineering Discovery Environment	
XSEDE CA	XSEDE Certificate Authorities	Entity responsible for certifying encryption keys for identity management
XSEDE KDC	XSEDE Kerberos	
XSEDE14	XSEDE Conference in 2014	
XSEDEnet	an XSEDE-only network	
XSO	XSEDE Security Officer	
XSP	XSEDE Scholars Program	
XSWoG	XSEDE Working Group	
XTED	XSEDE Technology Evaluation Database	
XUP	XSEDE User Portal	The XSEDE web pages at http://xsede.org
XWFS	XSEDE Wide File System	

12.2. Metrics

12.2.1. SP Resource and Service Usage Metrics

To demonstrate its success and help focus management attention on areas in need of improvement, XSEDE monitors a wide range of metrics in support of different aspects of "success" for the program. The metrics presented in this section provides a view into XSEDE's user community, including XSEDE's success at expanding that community, the projects and allocations through which XSEDE manages access to resources, and the subsequent use of the resources by the community.

Table 12-1 summarizes a few key measures of the user community, the projects and allocations, and resource utilization. Expanded information and five-year historical trends are shown in three corresponding subsections.

In Q3 2020, XSEDE user community metrics were mixed. For traditional users, the number of open HPC user accounts climbed back over 11,000, while the number of active users dipped slightly to 4,200, and

the number of institutions represented among the users running jobs climbed to 532. The number of gateway dropped substantially to nearly 12,000. Gateways have seen usage dips during this quarter in the last four years, though this year's drop was particularly steep; the typical decline may be related to the start of the academic year, and the pandemic may have exacerbated the drop this year. More details are in §12.2.1.1. Project and allocation activity held strong, with resource requests about 1.9 times what was available; and the XRAC recommended support for 1.06 times what was available. More details are in §12.2.1.2.

Total XSEDE-allocated resource capacity held steady at 18.4 Pflops (peak); however, the XRAC considered the first requests for and recommended allocations for the forthcoming *Expanse* system at SDSC and *Bridges-2* system at PSC. The central accounting system showed 9 compute resources reporting activity. Altogether, SP resources reported 52.0 billion NUs of computing delivered, comparable. More details are in §12.2.1.3.

Table 12–1: Quarterly activity summary.

User Community	Q4 2019	Q1 2020	Q2 2020	Q3 2020
Open user accounts	10,915	11,110	10,975	11,178
Active individuals	4,386	4,535	4,646	4,229
Gateway users	18,922	16,599	21,941	12,148
New user accounts	1,690	2,511	1,914	1,779
Active fields of science	40	40	40	67
Active institutions	472	474	515	532
Projects and Allocations				
NUs available at XRAC	53.5B	67.6B	79.8B	100.8B
NUs requested at XRAC	143.7B	144.7B	197.9B	189.0B
NUs recommended by XRAC	70.3B	80.9B	84.5B	96.2B
NUs awarded at XRAC	50.6B	70.5B	77.8B	94.9B
Open projects	2,298	2,298	2,305	2,443
Active projects	1,422	1,432	1,343	1,492
Active gateways	19	19	16	22
New projects	242	201	326	269
Closed projects	295	287	265	233
Resources and Usage				
Resources open (all types)	19	23	23	30
Total peak petaflops	18.4	18.4	18.4	18.4
Resources reporting use	9	9	9	9
Jobs reported	3.30M	3.87M	3.36M	3.11M
NUs delivered	49.7B	50.6B	52.3B	52.0B

12.2.1.1. *User community metrics*

Figure 12-1 shows the five-year trend in the XSEDE user community, including open user accounts, total active XSEDE users, active individual accounts, active gateway users, the number of new HPC user

accounts, and the total number of new XUP accounts at the end of each quarter. The quarter had 11,178 open accounts and saw 4,229 traditional users charging jobs. The number of active gateway users declined sharply to 12,148. Q3 has shown a consistent drop in gateway users for the past four years, possibly due to the start of the fall semester; however, this drop is particularly steep. The pandemic may have played a role.

Figure 12-2 shows the activity on XSEDE resources according to field of science across program years, including the relative fraction of PIs, open accounts, active users, allocations, and NUs used according to discipline. The figure shows the fields of science that consume ~2% or more of delivered NUs per quarter. PIs and users are counted more than once if they are associated with projects in different fields of science. The quarterly data show that the percentages of PIs and accounts associated with the "other" disciplines represent almost 50% of all PIs, 60% of direct-access user accounts, and 50% of active users. Collectively the "other" fields of science represented 16% of total quarterly usage.

Note that XSEDE introduced an updated set of fields of science in Q3 2020, and with this report we are using XSEDE's new fields of science list. We have developed a mapping from the prior fields of science to the new ones so that we can report usage across the cutover date. This mapping likely explains the current prominence of "Other Physical Sciences" and "Other Chemical Sciences." As projects are renewed and have the chance to select a new field of science, we expect to see more projects get categorized in the more specific options.

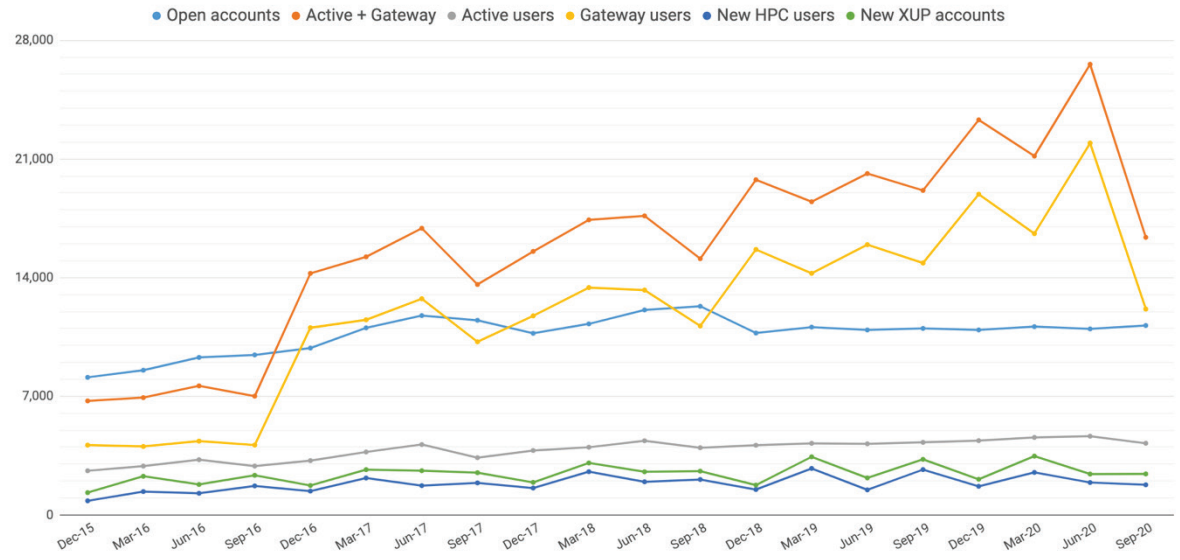


Figure 12-1: XSEDE user census, excluding XSEDE staff. The dramatic increases in gateway users starting in Q4 2016 are due to the I-TASSER gateway beginning to use XSEDE-allocated resources.

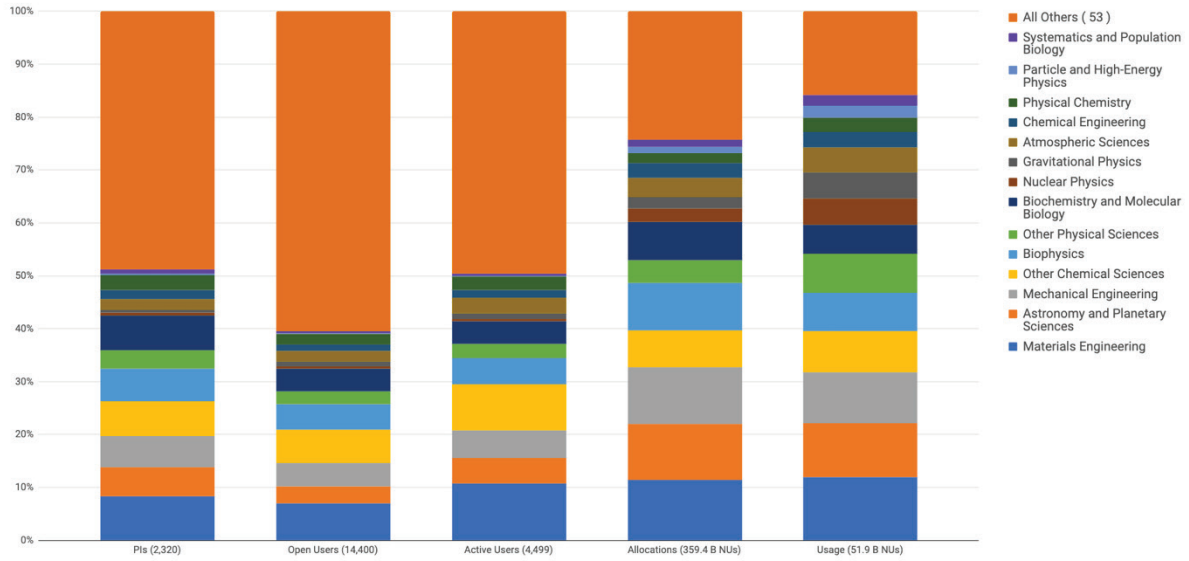


Figure 12-2: Quarterly XSEDE user, allocation, and usage summary by field of science, in order by usage, excluding staff projects. Note: PIs and users may appear under more than one field of science.

Table 12-2 and Table 12-3 highlight aspects of the broader impact of XSEDE. The former shows that graduate students, postdoctoral researchers, and undergraduates consistently make up two-thirds of the XSEDE user base. The latter table shows XSEDE's reach into targeted institutional communities, including a substantial increase in representation from MSIs and from EPSCoR state institutions. Institutions with Campus Champions represent a large portion of usage because this table shows all users at Campus Champion institutions, not just those on the champion's project. The table also shows XSEDE's reach into EPSCoR states, the MSI community, and countries outside the U.S.

Table 12–2: End of quarter XSEDE open user accounts by type, excluding XSEDE staff.

Category	Q4 2019	Q1 2020	Q2 2020	Q3 2020
Graduate Student	4,273	4,532	4,380	4,436
Faculty	2,051	2,033	2,056	2,091
Postdoctoral	1,261	1,202	1,182	1,208
Undergraduate Student	1,577	1,677	1,745	1,761
University Research Staff (excluding postdocs)	613	566	580	602
High school	153	164	82	95
Others	987	936	950	985
TOTALS	***10,915***	***11,110***	***10,975***	***11,178***

Table 12–3: Active institutions in selected categories. Institutions may be in more than one category.

Category		Q4 2019	Q1 20120	Q2 2020	Q3 2020
Campus Champions	Sites	122	123	106	124
	Users	2,342	2,192	2,671	2,131
	% total NUs	52%	51%	60%	54%
EPSCoR states	Sites	89	81	89	90
	Users	676	573	663	542
	% total NUs	13%	12%	11%	13%
MSIs	Sites	46	43	45	53
	Users	379	363	397	355
	% total NUs	2.9%	2.3%	3.1%	3.4%
International	Sites	64	65	97	80
	Users	87	82	73	117
	% total NUs	1%	2%	3%	4%
Total	**Sites**	***472***	***474***	***515***	***532***
	Users	***4,379***	***4,515***	***4,646***	***4,214***

12.2.1.2. *Project and allocation metrics*

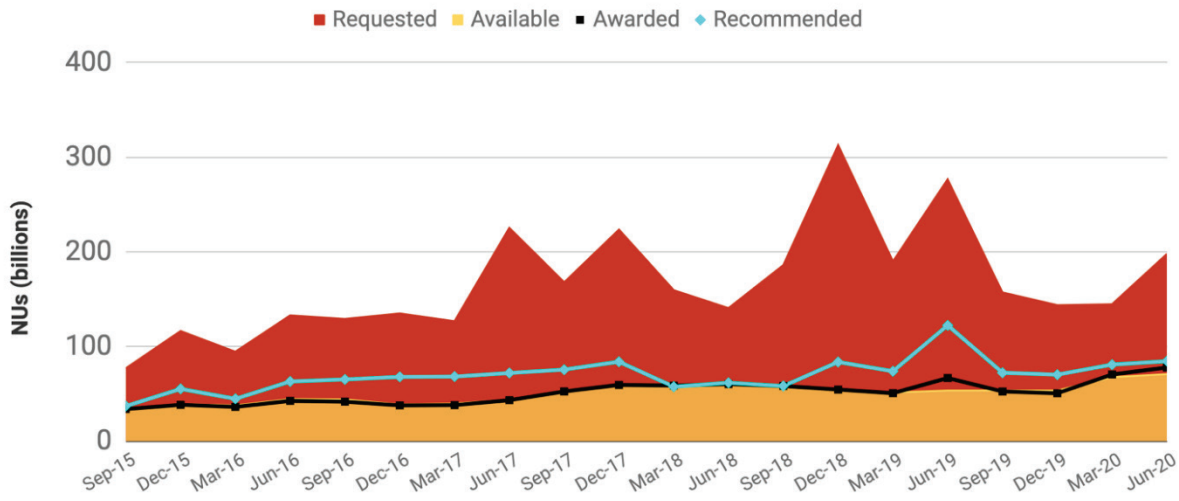


Figure 12-3 shows the five-year trend for requests and awards at XSEDE quarterly allocation meetings. NUs requested were 1.9x greater than NUs available, and the XRAC recommendations were approximately the same as the NUs available.

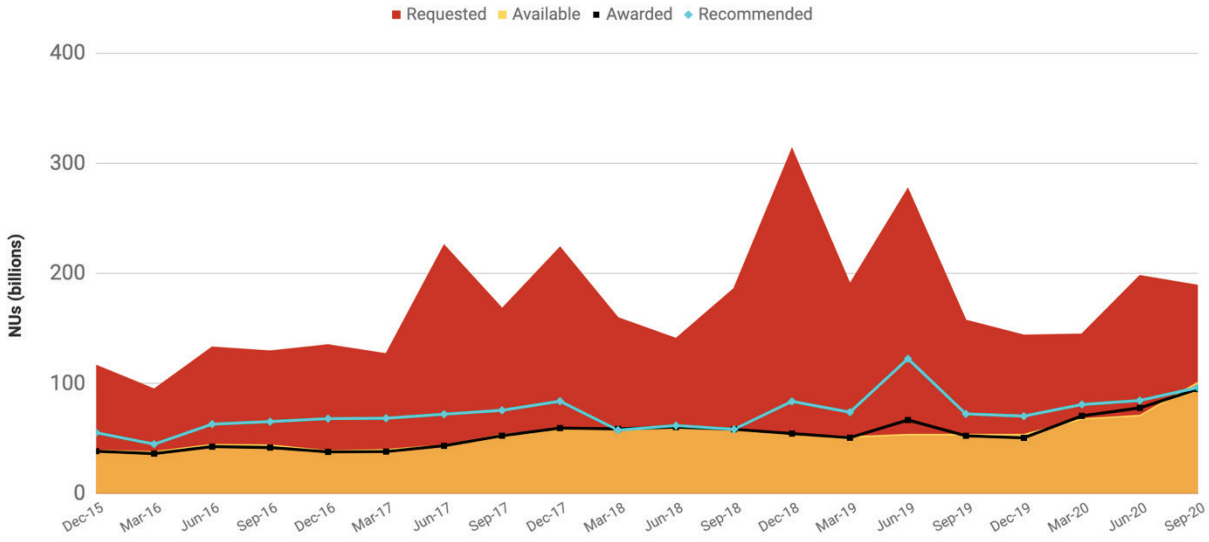


Figure 12-3: Five-year allocation history, showing NUs requested, awarded, available, and recommended.

Figure 12-4 showing continued high levels of usage and users from these projects.

Table 12-4 presents a summary of overall project activity, and Table 12–5 shows projects and activity in key project categories as reflected in allocation board type. Note that Science Gateways may appear under any board. The new Rapid Response project type identifies the projects awarded through the COVID-19 HPC Consortium. As a special class of projects, science gateway activity is detailed in Figure 12-4 showing continued high levels of usage and users from these projects.

Table 12–4: Project summary metrics.

Project metric	Q4 2019	Q1 2020	Q2 2020	Q3 2020
XRAC requests	219	206	197	226
XRAC request success	78%	87%	80%	84%
XRAC new awards	45	46	50	57
Startups requested	195	198	198	186
Startups approved	197	185	178	183
Projects new	242	201	326	269
Projects closed	295	287	265	233

Table 12–5: Project activity by allocation board type.

	Q4 2019			Q1 2020			Q2 2020			Q3 2020		
	Open projects	Active projects	% NUs	Open projects	Active projects	% NUs	Open projects	Active projects	% NUs	Open projects	Active projects	% NUs
Campus Champions	151	64	0.3%	149	61	0.2%	154	70	0.2%	150	55	0.2%
Discretionary	6	4	0.0%	6	5	0.1%	10	4	0.1%	11	6	0.1%
Educational	173	100	0.8%	196	88	0.7%	181	101	1.0%	205	93	0.5%
Staff	13	11	0.1%	13	11	0.1%	13	12	0.1%	12	10	0.1%
Startup	1065	462	2.3%	1049	479	3.0%	1070	512	3.2%	1,077	504	2.4%
XRAC	890	781	96.5%	885	788	95.9%	877	783	90.9%	894	801	92.0%
Rapid Response							78	4	4%	93	23	4.8%
Totals	2,298	1,422	100%	2,298	1,432	100%	2,305	1,482	100%	2,442	1,492	100%

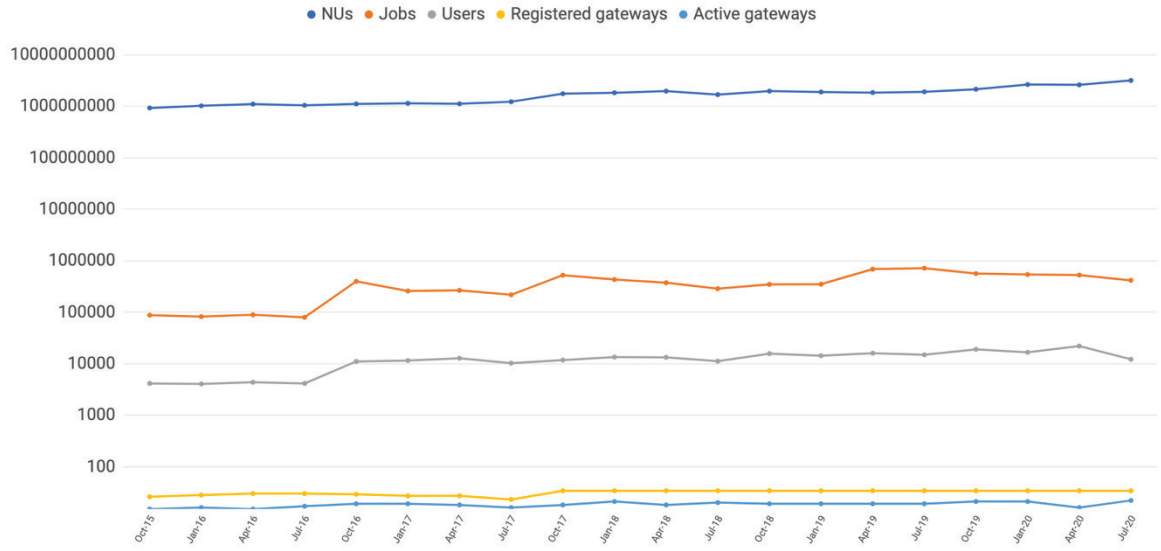


Figure 12-4: Quarterly gateway usage (NUs), jobs submitted, users (reported by ECSS), registered gateways, and active gateways.

12.2.1.3. *Resource and usage metrics*

SP systems delivered 52.3 billion NUs in Q3 2020, up from the previous quarter. Table 12–6 breaks out the resource activity according to different resource types. Figure 12-5 shows the total NUs delivered by XSEDE-allocated SP computing systems, as reported to the central accounting system over the past five years. Usage reported for "cloud systems" (i.e., *Jetstream*) is low for Q3 2020 due to technical difficulties with sending accounting data from TACC; we expect the information to be corrected in the next reporting period.

Table 12–6: Resource activity, by type of resource, excluding staff projects.

		Q4 2019	Q1 2020	Q2 2020	Q3 2020
High-performance computing	Resources	7	6	6	6
	Jobs	2,583,846	2,527,396	3,294,211	2,594,153
	Users	3,742	4,018	4,166	3,774
	Nus	46,542,293,315	47,240,372,890	49,504,998,604	49,898,177,007
Data-intensive computing	Resources	2	1	1	1
	Jobs	131,491	69,876	58,661	51,958
	Users	139	130	129	146
	Nus	247,993,769	283,724,864	306,401,481	355,199,316
High-throughput computing	Resources	1	1	1	1
	Jobs	19,129	17,542	8,252	20,338
	Users	8	8	4	5
	Nus	860,022,066	733,073,988	402,999,559	843,067,586
Cloud system	Resources	1	1	1	1
	Jobs	1,980,268	1,231,300	1,330,618	420,768
	Users	533	492	471	445
	Nus	3,122,149,022	2,274,951,447	2,113,752,137	838,975,969

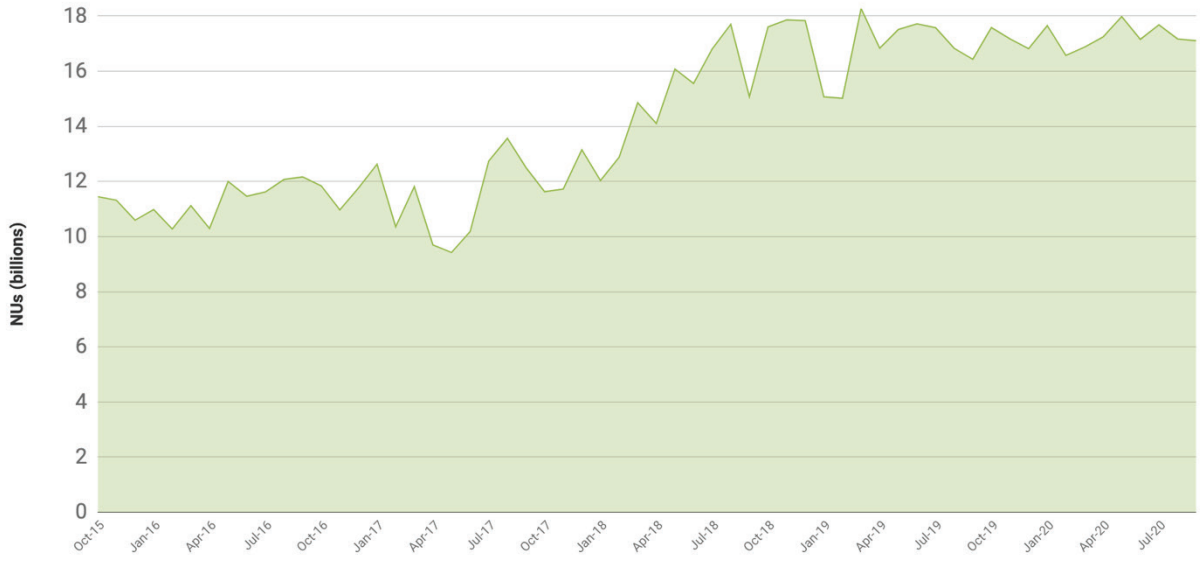


Figure 12-5: Total XSEDE resource usage in NUs.

12.2.1.4. *Data Services*

XSEDE supports monitoring for the Globus data transfer service for connecting XSEDE service providers and external sites. Table 12–7 shows summary metrics and increasing Globus adoption over the past five years. Figure 12-6 shows the trends in Globus data transfer activity and user adoption over five years.

Table 12–7: Globus data transfer activity to and from XSEDE endpoints, excluding XSEDE speed page user.

		RY4 RP3	RY4 RP4	RY5 RP1	RY5 RP2
To/from XSEDE endpoint	Files to XSEDE (millions)	37	33	61	69
	TB to XSEDE	2,392	1,825	2,640	2,161
	Files from XSEDE (millions)	159	58	31	44
	TB from XSEDE	3,040	2,714	2,761	2,850
	Users	623	719	658	639
To/from XSEDE via Globus Connect	Files to XSEDE (millions)	2	7	10	3
	TB to XSEDE	48	64	45	148
	Files from XSEDE (millions)	54	11	7	15
	TB from XSEDE	203	76	164	157
	Users	427	519	458	433
To/from XSEDE from/to Campuses	TB to XSEDE	913	561	751	473
	TB from XSEDE	1,050	800	935	1,248
	Campuses	55	50	57	60
	Campus endpoints	81	83	89	97
To/from Campus	TB to Campuses	38,516	30,163	25,565	23,410
	TB from Campuses	39,420	31,339	25,235	26,462
	Campuses	133	131	135	133
	Campus endpoints	404	437	427	415

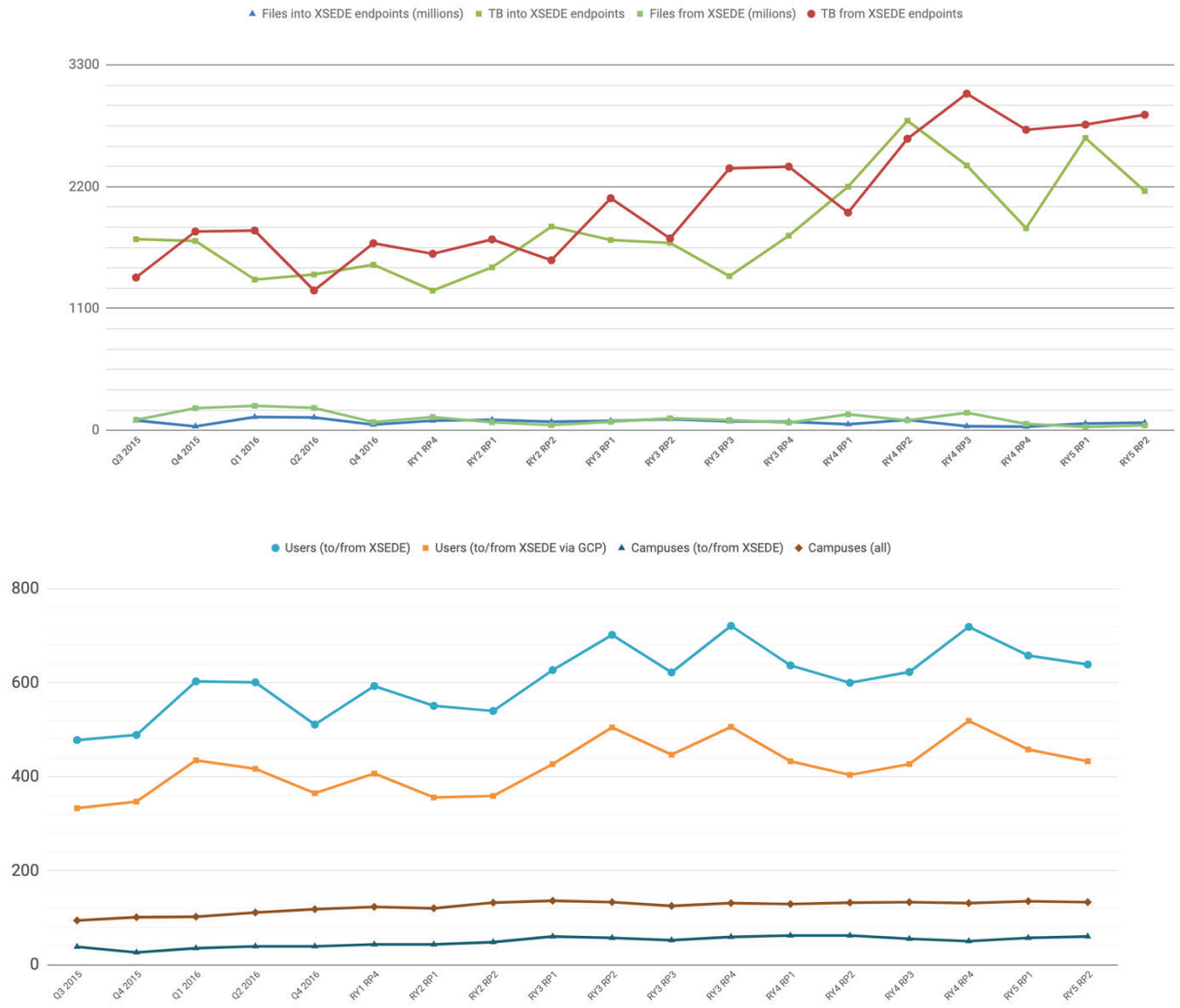


Figure 12-6: Top: Aggregate Globus file and data transfer activity to and from XSEDE endpoints. Bottom: Numbers of active Globus users and campuses moving data to and from XSEDE endpoints.

12.2.2. Other Metrics

For previous year's metrics, please refer to the XSEDE Project-wide KPIs & Metrics wiki page.

12.2.2.1. *Community Engagement & Enrichment (WBS 2.1) (Gaither)*

RY5 Metrics		RP1	RP2	RP3	RP4	Total
Number of sustained users of XSEDE resources and services via the portal (Project KPI)	4,500/qtr	4,644	4,489			
Number of sustained underrepresented individuals using XSEDE resources and services via the portal (Project KPI)	1,750/yr	831	805			
Number of new users of XSEDE resources and services via the portal (Project KPI)	2,500/qtr	2,157	2,612			
Number of new underrepresented individuals using XSEDE resources and services via the portal (Project KPI)	250/qtr	301	159			

Number of participant hours of live training delivered by XSEDE (Project KPI)	40,000/yr	19,751	16.111			
Number of students benefiting from XSEDE resources and services through training, XSEDE projects, or conference attendance (Area KPI)	2,000/qtr	2,277	2,043			
Number of underrepresented students benefiting from XSEDE resources and services through training, XSEDE projects, or conference attendance (Area KPI)[1]	650/qtr	741	632			
Grand (aggregate) mean rating of Post Training Event Survey items related to training impact for attendees registered through the portal (1-5 Likert scale) (Area KPI)	4.4 of 5/qtr	4.6	4.5			
Number of institutions with a Champion (Area KPI)	340	327	332			
Percentage of user requirements addressed within 30 days (Area KPI)	98%/qtr	100 (16/16)	100 (20/20)			

[1] The reporting of underrepresented students is no longer being reported as a percentage, but instead as a number as of RP4. The use of percentages does not provide the appropriate lens for understanding our progress in engaging underrepresented students.

12.2.2.1.1. Workforce Development (WBS 2.1.2) (Akli)

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
Number of unique attendees, synchronous training	1,200/yr	1,010	791			
Number of total attendees, synchronous training (One person can take several classes)	1,400/yr	1,270	939			
Number of unique attendees, asynchronous training	1,200/yr	144	112			
Number of total attendees, asynchronous training (One person can take several classes)	4,000/yr	403	261			
Grand (aggregate) mean rating of Post Training Event Survey items related to training impact for attendees registered through the portal (1-5 Likert scale) (Area KPI)	4.4 of 5	4.6	4.5			
Number of formal degree, minor, and certificate programs added to the curricula	3/yr	0	1			
Number of materials contributed to public repository	50/yr	5	0			
Number of materials downloaded from the repository	62,000/ yr	16,895	17,992			
Number of computational science modules added to courses	40/yr	0	0			

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
Number of students benefiting from XSEDE resources and services through training, XSEDE projects, or conference attendance (Area KPI)	1,500/ qtr	2,277	2,043			
Number of underrepresented students benefiting from XSEDE resources and services through training, XSEDE projects, or conference attendance (Area KPI)[1]	500/qtr	741	632			

[1] The reporting of underrepresented students is no longer being reported as a percentage, but instead as a number as of RP4. The use of percentages does not provide the appropriate lens for understanding our progress in engaging underrepresented students.

12.2.2.1.2. User Engagement (WBS 2.1.3) (Snead)

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
Percentage of active and new PIs contacted quarterly	100%	100 (1,217)	100 (996)			
Percentage of user requirements addressed within 30 days (Area KPI)	98/qtr	100 (16/16)	100 (20/20)			
Number of responses to PI emails each quarter		62	88			
Number of responses to each microsurvey		NA[1]	NA[1]			
Number of annual user satisfaction survey respondents interviewed		NA[2]	NA[2]			
Number of XSEDE-wide tickets		28	11			
Number of XSEDE-wide tickets addressed		28	11			

[1] No microsurveys this reporting period.
[2] Survey report not yet available.

12.2.2.1.3. Broadening Participation (WBS 2.1.4) (Akli)

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
Number of new underrepresented individuals using XSEDE resources and services via the portal (Project KPI)	250/qtr	301	159			
Number of sustained underrepresented individuals using XSEDE resources and services via the portal (Project KPI)[1]	1,750/yr	831	805			

[1]The total for this KPI does not equal the sum of the data from each reporting period because one person could be counted as a sustained individual in more than one reporting period if they continue to log in for multiple reporting periods; however, they will only be counted once in the total.

12.2.2.1.4. User Interfaces & Online Information (WBS 2.1.5) (Dahan)

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
Number of new users of XSEDE resources and services via the portal (Project KPI)	2,500/ qtr	2,157	2,612			

Number of sustained users of XSEDE resources and services via the portal (Project KPI)[1]	4,500/ qtr	4,644	4,489			
Number of pageviews to the XSEDE website	80,000/ qtr	42,166	40,313			
Number of pageviews to the XSEDE User Portal	250,000/ qtr	255,184	246,124			
User satisfaction with website (1-5 Likert scale)	4 of 5	4.3	-			
User satisfaction with User Portal (1-5 Likert scale)	4 of 5	4.3	-			
User satisfaction with user documentation (1-5 Likert scale)	4 of 5	4.2	-			

[1] The total for this KPI does not equal the sum of the data from each reporting period because one person could be counted as a sustained user in more than one reporting period if they continue to log in for multiple reporting periods; however, they will only be counted once in the total.
-No data this reporting period

12.2.2.1.5. Campus Engagement (WBS 2.1.6) (Neeman, Brunson)

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
Number of Institutions with a Champion (Area KPI)	340	327	332			
Number of unique contributors to the Champion email list (campuschampions@xsede.org)	125/yr	110	130			
Number of activities that (i) expand the emerging CI workforce and/or (ii) improve the extant CI workforce, participated in by members of the Campus Engagement team	40/yr	64	90			

12.2.2.2. Extended Collaborative Support Services (WBS 2.2) (Blood, Sinkovits)

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
Percentage of sustained allocation users from non-traditional disciplines of XSEDE resources and services (Project KPI)	33%/yr	23.2	23.8			
Percentage of new allocation users from non-traditional disciplines of XSEDE resources and services (Project KPI)	35%/yr	30.1	35.0			
Number of completed ECSS projects (ESRT + ESCC + ESSGW) (Area KPI)	45/yr	17	10			
Grand (aggregate) mean rating of ECSS impact by PIs measured by ECSS Project Exit Survey items (1-5 Likert scale)(Area KPI)	4 of 5/yr	4.1	4.2			
Grand (aggregate) mean rating of PI satisfaction with ECSS support measured by ECSS Project Exit Survey items (1-5 Likert scale) (Area KPI)	4.5 of 5/yr	4.8	4.9			
Average estimated months saved due to ECSS support	12 mo/ project	11	13.5			

12.2.2.2.1. Extended Support for Research Teams (WBS 2.2.2) (Crosby)

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
Number of completed ESRT projects	27/yr	5	6			
Average ESRT impact rating (1-5 Likert scale)	4 of 5/yr	5.0	4.0			
Average satisfaction with ESRT support (1-5 Likert scale)	4.5 of 5/yr	4.5	4.8			
Number of projects initiated		10	5			
Number of projects discontinued		2	0			
Number of PI interviews		2	5			
Number of active projects		28	25			
Average estimated months saved due to ESRT support	12 mo/ project	12	6.0			

12.2.2.2.2. Novel & Innovative Projects (WBS 2.2.3) (Sanielevici)

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
Number of new users from non-traditional disciplines of XSEDE resources and services	500/yr	154	173			
Number of sustained users from non-traditional disciplines of XSEDE resources and services	1900/qtr	1,833	1,960			
Number of new XSEDE projects from target communities generated by NIP	30	31	25			
Number of successful XSEDE projects from target communities mentored by NIP	25	41	29			

12.2.2.2.3. Extended Support for Community Codes (WBS 2.2.4) (Koesterke)

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
Number of completed ESCC projects	9/yr	2	3			
Average ESCC impact rating (1-5 Likert scale)	4 of 5/yr	2.0	-			
Average satisfaction with ESCC support (1-5 Likert scale)	4.5 of 5/yr	5.0	-			
Number of projects initiated		0	1			
Number of projects discontinued		0	0			
Number of active projects		10	6			
Number of PI interviews		1	0			
Average estimated months saved due to ESCC support	12 mo/ project	0	-			

-There were no ESCC PI interviews conducted this reporting period to generate impact and satisfaction scores and an estimate of months saved.

12.2.2.2.4. Extended Support for Science Gateways (WBS 2.2.5) (Quick)

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
Number of completed ESSGW projects	9/yr	10	1			
Average ESSGW impact rating (1-5 Likert scale)	4 of 5/yr	4.5	4.5			
Average satisfaction with ESSGW support (1-5 Likert scale)	4.5 of 5/ yr	5.0	5.0			
Number of projects initiated		0	5			
Number of projects discontinued		0	0			
Number of active projects		17	22			
Number of PI interviews		1	4			
Currently Registered Production Gateways		-	49			
Average estimated months saved due to ESSGW support	12 mo/ project	21	21			

-New metric for RP2

12.2.2.2.5. Extended Support for Education Outreach, & Training (WBS 2.2.6) (Alameda)

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
Number of Campus Champions fellows	4	-	6			
Average score of fellows assessment (1-5 Likert scale)	4.5 of 5	-	-			
Number of live training events staffed	20	12	4			
Number of staff training events	2	0	0			
Attendees at staff training events	40	0	0			
Attendees at ECSS Symposia	300	143	143			
Live training event contact hours		26.5	7			
Live training event attendees		185	194			
Live training even attendee hours		676	424			
Requests for service		15	10			
Training modules reviewed		0	0			
Training modules produced		2	2			
Meetings and BoFs		8	10			
Mentoring		9	12			
Talks and presentations		10	4			
Education proposals reviewed		38	60			

- Data reported annually.

12.2.2.3. XSEDE Cyberinfrastructure Integration (WBS 2.3) (Lifka)

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
Total number of capabilities in production (Project KPI)	110	102	104			
Grand (aggregate) mean rating of XSEDE User Survey user satisfaction items regarding XCI software and technical services, capabilities, and resources (1-5 Likert scale)[8]	4/5	4.4	-			
Grand (aggregate) mean rating of XSEDE User Survey Service Provider satisfaction items regarding XCI software and technical services, capabilities, and resources (1-5 Likert scale)[8]	4/5	4.5	-			
Number of non-XSEDE partnerships with XCI (Area KPI)	14/yr	14	11			
Mean time to issue resolution (Area KPI)	10 days	4.2	6.0			
Number of new capabilities made available for production deployment	7	0[5]	2			
Total number of systems that use one or more CRI provided toolkit	1,500 by the end of RY5	2,196	2,373			
Percentage of Level 1 SPs that fully incorporate all of the recommended tools from the XSEDE Community Repository	100%	100[1]	100[1]			
Percentage of Level 2 SPs that allocate resources through XSEDE that fully incorporate all of the recommended tools from the XSEDE Community Repository	100%	33[2]	66[2]			
Percentage of Level 2 SPs that do not allocate resources through XSEDE that fully incorporate all of the recommended tools from the XSEDE Community Repository	100%	80[3]	75[3]			
Percentage of Level 3 SPs that fully incorporate all of the recommended tools from the XSEDE Community Repository	100%	73[4]	73[4]			

-Data reported annually.
[1]All Level 1 SPs are up to date.
[2]One out of three. One Level 2 SP added (University of Delaware) and not integrated yet; Open Storage Network not integrated yet — joined late Oct.; OSG fully integrated.
[3]4 of 5 have all the required tools installed: RDR entry and information publishing framework.
[4]19 out of 26 have the required RDR entry.
[5]Correcting last reporting period's number from total to number that reporting period.

12.2.2.3.1. Requirements Analysis & Capability Delivery (WBS 2.3.2) (Navarro)

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
Number of capability delivery plans (CDPs) prepared for UREP prioritization	8/yr	0	0			
Number of CI integration assistance engagements	6[1]	7	7			

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
Average time from support request to solution	10 days or less	3.8 (n=28)	5.7 (n=36)			
Number of new components instrumented and tracked for usage and ROI analysis	4/yr	0	1			
Number of significant fixes and enhancements to production components	40/yr[1]	12	16			
Number of maintenance releases and upgrades delivered of service provider software	4/yr	2	3			
Number of fixes and enhancements to centrally operated services	36/yr[1]	10	13			
Operator rating of components delivered for production deployment (1-5 Likert scale)	4 of 5/yr	-	-			
Software/Service Provider rating of our integration assistance (1-5 Likert scale)	4 of 5/yr	-	-			

- No components were delivered this period.
[1] Changes based on PY1-PY8 observed rates.

12.2.2.3.2. Cyberinfrastructure Resource Integration (WBS 2.3.3) (Knepper)

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
Total number of systems that use one or more CRI provided toolkits	1500 by end of RY5	2,196	2,373			
User satisfaction with CRI services[1] (1-5 Likert scale)	4 of 5/yr	4.5	n/a			
Number of repository subscribers to CRI cluster and laptop toolkits	150	114	117			
Aggregate number of TeraFLOPS of cluster systems using CRI toolkits	1,000 by end of RY5	1,020	1,091			
Number of partnership interactions between CRI and SPs, national CI organizations, and campus CI providers	12	7	4			
Toolkit updates	4/yr	3	3			
New Toolkits released	2/yr	1	0			
Average time from support request to solution	<14 days	10.5 (n=2)	12 (n=1)			

[1]This KPI was retired after RP1. Going forward satisfaction with XCI services will be measured at the L2 level only.

12.2.2.4. XSEDE Operations (WBS 2.4) (Peterson)

RY4 Metrics	Target	RP1	RP2	RP3	RP4	Total
Average composite availability of core services (geometric mean of critical services and XRAS) (Project KPI)	99.9%/qtr	99.9	99.9			
Hours of downtime with direct user impacts from an XSEDE security incident (Area KPI)	0 hrs/qtr	0	0			

Mean time to ticket resolution by XOC and WBS ticket queues (hrs) (Project KPI)	<16 hrs/qtr	15.3	23.2			
Mean rating of user satisfaction with tickets closed by the XOC (1-5 Likert scale) (Area KPI)	4.5 of 5/qtr	4.7	4.7			

12.2.2.4.1. Cybersecurity (WBS 2.4.2) (Withers, Simmel)

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
Hours of downtime with direct user impacts from an XSEDE security incident. (Area KPI)	0 hrs/qtr	0	0			
Hours of downtime WITHOUT direct user impacts from an XSEDE (affects central service or multiple SPs) security incident	< 24 hrs	0	0			
XSEDE account exposures	< 10	4	0			
Time, beyond 24 hours, to disable XSEDE accounts	0 hrs	0	0			

12.2.2.4.2. Data Transfer Services (WBS 2.4.3) (Wheeler)

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
Performance (Gbps) of instrumented, intra-XSEDE transfers > 1GB	3.0 Gbps	3.17	3.12			
New services added		0	0			
Services retired		0	0			
Total Globus Online users		658	639			
Total new Globus Online users		197	177			
Total transfers (Million) inbound		61	69			
Total transfers (Million) outbound		31	44			
Size of transfers (TBs) inbound		2,640	2,161			
Size of transfers (TBs) outbound		2,761	2,850			
Total number of days in which any Network Interface error occurred		0	0			
XSEDEnet maximum bandwidth used (Gbps)		146.5	60			

12.2.2.4.3. XSEDE Operations Center (WBS 2.4.4) (Hendricks)

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
Mean time to resolution in XOC queue (hrs)	< 1 hr	0.46	0.28			
Mean time to ticket resolution by XOC and WBS ticket queues (hrs) (Project KPI)	< 16 hrs	15.3	23.2			
User satisfaction with tickets closed by the XOC (1-5 Likert scale) (Area KPI)	4.5 of 5	4.7	4.7			

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
Mean time to resolution in WBS queue		36.6	55.6			
Number of Support tickets opened for WBS queues		304	333			
Number of Support tickets closed by WBS queues		265	302			
Number of Support tickets opened for XOC		381	426			
Number of Support tickets closed by XOC		381	426			
Mean time to first response by XOC (hrs)		0.44	0.27			

12.2.2.4.4. System Operations Support (WBS 2.4.5) (Rogers)

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
Average availability of critical enterprise services (%) [geometric mean] (Project KPI)	99.9%	99.9	99.9			
Average availability of core enterprise services (%)	99.9%	99.9	99.9			
Total enterprise services		47	47			
Core enterprise services		8	8			
Services added/subtracted		0	0			

12.2.2.5. Resource Allocation Service (WBS 2.5) (Hart)

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
Mean rating of user satisfaction with allocations process (1-5 Likert scale) (Area KPI)	4 of 5/qtr	4.4	4.3			
Mean rating of user satisfaction with XRAS (1-5 Likert scale)(Area KPI)[1]	4 of 5/qtr	4.3	4.3			
Mean rating of user satisfaction with allocations process and support services (1-5 Likert scale)(Project KPI)[1]	4 of 5/yr	4.4	4.3			
Percentage of research requests successful (not rejected) (Project KPI)	85%/qtr	80.0	84.0			

12.2.2.5.1. XSEDE Allocations Process & Policies (WBS 2.5.2.) (Hackworth)

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
User satisfaction with allocations process (1-5 Likert scale) (Area KPI)	4 of 5	4.4	4.3			
Average time to process Startup requests	14 calendar days or less/qtr	8.5	11.4			
Percentage of XRAC-recommended NUs allocated	100%	92	99			

Percentage of research requests successful (not rejected) (Project KPI)	85%/qtr	80.0	84.0			
Continuous allocation requests processed		780	912			
Research allocation requests processed		197	226			

12.2.2.5.2. Allocations, Accounting, & Account Management CI (WBS 2.5.3) (Tolbert)

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
User satisfaction with XRAS system (1-5 Likert scale) (Area KPI)	4 of 5	4.3	4.3			
Availability of the XRAS systems	99.9%	99.9	100.0			
Number of XRAC client organizations		8	8			

12.2.2.6. Program Office (WBS 2.6) (Payne)

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
Grand (aggregate) mean rating of XSEDE User Survey awareness items regarding XSEDE resources and services (1-5 Likert scale) (Project KPI)	3.7 of 5 / yr	3.8	-			
Number of social media impressions over time (Project KPI)	429,282 / yr	86,046	101,394			
Grand (aggregate) mean of XSEDE User Survey satisfaction items regarding XSEDE technical support services (1-5 Likert scale) (Project KPI)	3.5 of 5/yr	4.4	-			
Percentage of users who indicate the use of XSEDE-managed and/or XSEDE-associated resources in the creation of their work product (Project KPI)	80/yr	83	-			
Mean rating of importance of XSEDE resources and services to researcher productivity (1-5 Likert scale) (Project KPI)	4.4 of 5/yr	4.2	-			
Percentage of Project Improvement Fund funded projects resulting in innovations in the XSEDE organization (Project KPI)	70%/yr	-	-			
Mean rating of innovation within the organization by XSEDE staff (1-5 Likert scale) (Project KPI)	4 of 5/yr	-	4.2			
Variance between relevant report submission and due date (days) (Area KPI)	0 days	0	0			
Percentage of sub-award invoices processed within target duration (Area KPI)	90%/qtr	92.6	83.3			
Percentage of recommendations addressed by relevant project areas within 90 days (Area KPI)	90%	100	90			
Grand (aggregate) mean of Staff Climate Study satisfaction items regarding content and accessibility of the XSEDE Staff Wiki (1-5 Likert scale) (Area KPI)	3.9 of 5/yr	-	3.9			

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
Number of staff publications (Area KPI)	50/yr	2	16			
Grand (aggregate) mean of Staff Climate Study awareness items regarding inclusion in XSEDE (1-5 Likert scale) (Area KPI)	4.1/yr	-	4.3			
Grand (aggregate) mean of Staff Climate Study awareness items regarding equity in XSEDE (1-5 Likert scale) (Area KPI)	4.0/yr	-	4.4			
Number of XSEDE-related media hits (Area KPI)	325/yr	624	467			

- Data reported annually

12.2.2.6.1. External Relations (WBS 2.6.2) (Hutson)

RY4 Metrics	Target	RP1	RP2	RP3	RP4	Total
Number of social media impressions over time (Project KPI)	429,282/ yr	86,046	101,394			
Number of XSEDE-related media hits (Area KPI)	325/yr	718	467			
Monthly open rate of XSEDE's newsletter	32%	35%	24.3%			
Monthly click-through rate of XSEDE's newsletter	3%	1.3%	2%			

12.2.2.6.2. Project Management, Reporting, & Risk Management (WBS 2.6.3) (Froeschl)

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total
Variance, in days, between relevant report submission and due date (Area KPI)	0 days/report	0	0			
Grand (aggregate) mean rating of Staff Climate Study satisfaction items regarding content and accessibility of the XSEDE Staff Wiki (1-5 Likert scale) (Area KPI)	3.9 of 5/yr	-	3.9			
Percentage of risks reviewed	100%	100	100			
Number of total risks		174	174			
Number of active risks		140	142			
Number of new risks		1	0			
Number of risks triggered		4	5			
Number of risks retired		1	0			
Number of PCRs submitted		4	5			
KPI/Metrics		3	3			
Technical		0	0			
Scope		0	0			
Budget		0	1			
Staff		1	1			
Other		0	0			

- Data reported annually.

12.2.2.6.3. Business Operations (WBS 2.6.4) (Payne)

RY5 Metrics	Target	RP1	RP2	RP3	RP4	Total

Percentage of subaward invoices processed within target duration (Area KPI)	90%/qtr	92.6	83.3			

12.2.2.6.4. Strategic Planning, Policy, Evaluation & Organizational Improvement (WBS 2.6.5) (Payne)

RY5Metrics	Target	RP1	RP2	RP3	RP4	Total
Grand (aggregate) mean rating of XSEDE User Survey awareness items regarding XSEDE resources and services (1-5 Likert scale) (Project KPI)	3.7 of 5 / yr	3.8	-			
Grand (aggregate) mean rating of XSEDE User Survey satisfaction items regarding XSEDE technical support services (1-5 Likert scale) (Project KPI)	3.5 of 5/yr	4.4	-			
Percentage of users who indicate the use of XSEDE-managed and/or XSEDE-associated resources in the creation of their work product[1] (Project KPI)	80%/yr	83	-			
Mean rating of importance of XSEDE resources and services to researcher productivity (1-5 Likert scale) (Project KPI)	4.4 of 5/yr	4.2	-			
Percentage of Project Improvement Fund proposals resulting in innovations in the XSEDE organization (Project KPI)	70%/yr	-	-			
Mean rating of innovation within the organization by XSEDE staff (1-5 Likert scale) (Project KPI)	4 of 5/yr	-	4.2			
Percentage of recommendations addressed by relevant project areas within 90 days (Area KPI)	90%	100	90			
Number of staff publications (Area KPI)	50/yr	2	16			
Grand (aggregate) mean of Staff Climate Study awareness items regarding inclusion in XSEDE (1-5 Likert scale) (Area KPI)	4.1/yr	-	4.3			
Grand (aggregate) mean of Staff Climate Study awareness items regarding equity in XSEDE (1-5 Likert scale) (Area KPI)	4.0/yr	-	4.4			

- Data reported annually.

12.3. Scientific Impact Metrics (SIM) and Publications Listing

This appendix presents the current Scientific Impact Metrics data as of October 31 of year 2020. This is part of the *XD Metrics Service (**XMS**) (*formerly ***NSF Technology Audit Service (TAS)***) effort.

12.3.1. Summary Impact Metrics

Table SIM-1 shows the essential scientific summary impact metrics as of October 31 of year 2020. The increasing values for each metric are listed in the table indicating the changes during the last quarter. By calculating such metrics periodically we can show the trends, as depicted in Figure SIM-2 and Figure SIM-3. Both show steadily increasing trends.

Table SIM-1: Overall Scientific Impact Metrics Data

	Number of externally verified unique publications*	i10-index (Number of publications cited at least 10 times)	Overall citation count*	h-index	g-index
Since 2005 (TG+XD)	18,936	10,917	675,453	269	485
Since 2011 (XD)	16,377	8,871	469,166	217	378
Change since last quarter (TG+XD)	+547	+443	+34,575	+6	+12
Change since last quarter (XD)	+536	+432	+30,861	+8	+13
* Data updated as of October 31st, 2020.					

12.3.2. Historical Trend

Figure SIM-2 and SIM-3 show the increasing quarterly trend regarding publications, citations, and other impact metrics such as H-Index and G-Index. Both suggest the increasing impact of XSEDE during the past years, based on verified unique publication count; citation count; H-index and G-index.

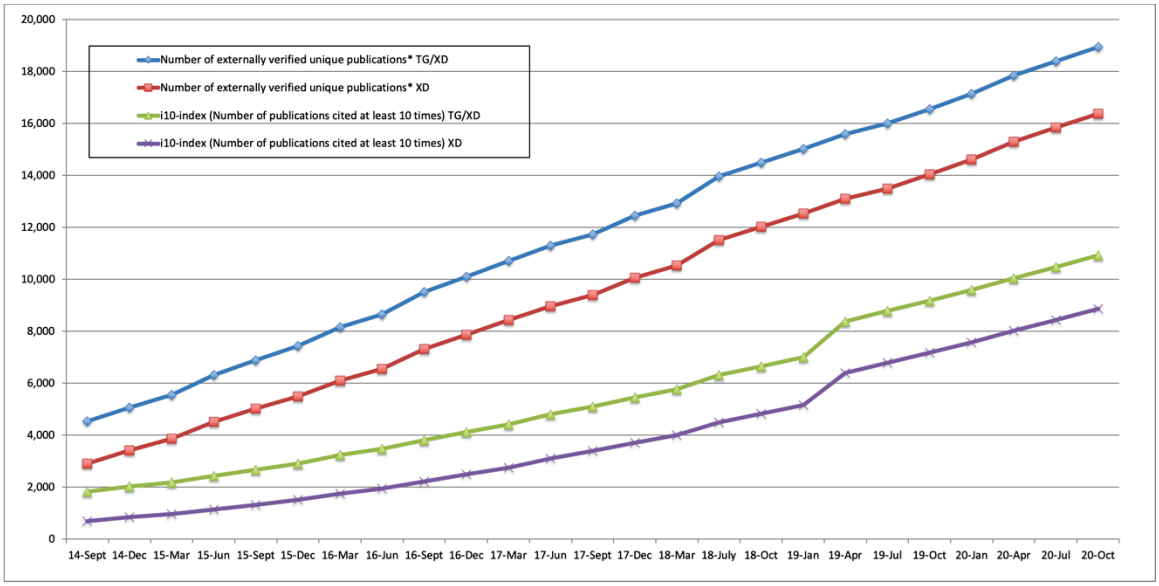


Figure SIM-2. Counts of all externally verified publications for TG/XD (since 2005) and XD (since 2011) and of those being cited at least 10 times (i10-index).

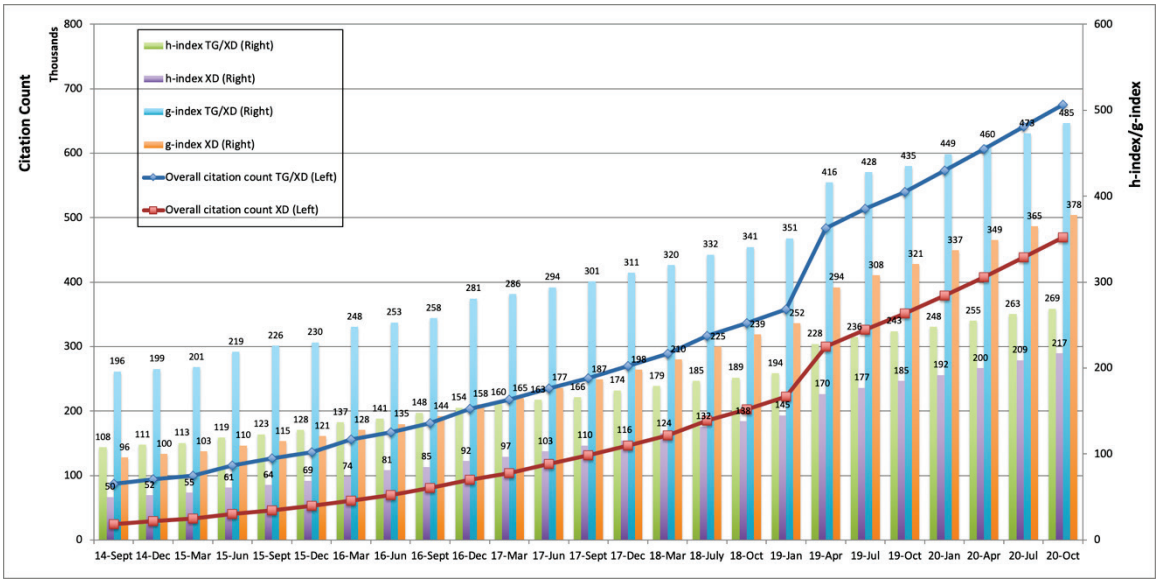


Figure SIM-3. Accumulated citation count (line, left axis) as well as h-index and g-index metrics (bar, right axis) for TG/XD (since 2005) and XD (since 2011).

12.3.3. Publications Listing

Figure 12-7 shows the number of publications, conference papers, and presentations reported by XSEDE users each quarter, including the 605 reported by 188 projects in Q3 2020; these publications are listed below according to allocated project. Starting with the December 2017 XRAC meeting, all submitters must add publications to their user profiles in the XSEDE User Portal, which may have contributed to the decline beginning at the end of 2017.

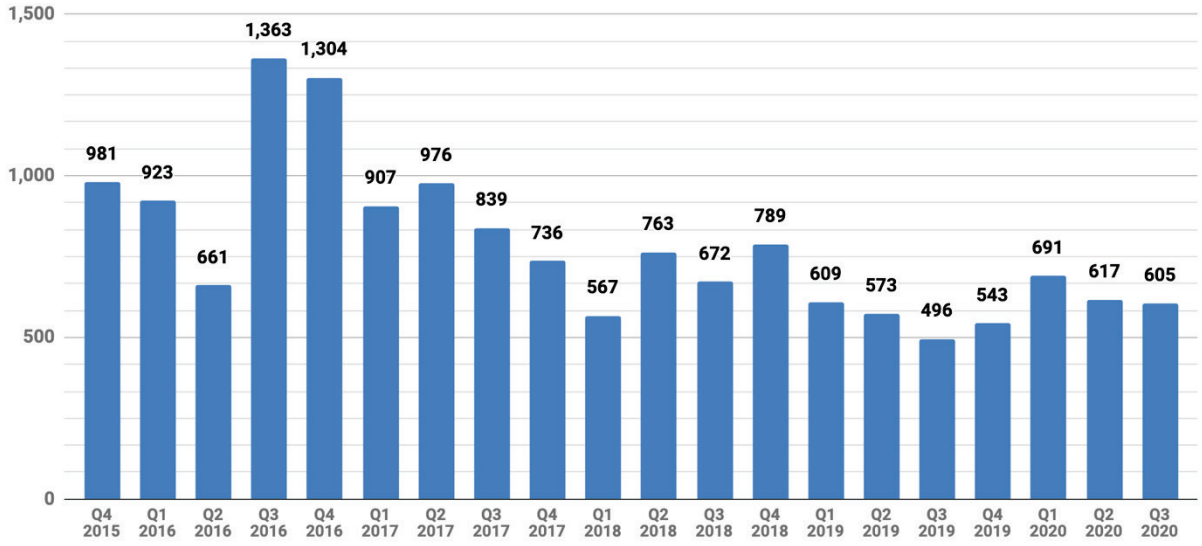


Figure 12-7: Publications, conference papers, and presentations reported by XSEDE users.

12.3.3.1. *XSEDE Staff Publications*

XSEDE staff reported 16 publications from August 2020 to October 2020. Twelve publications were reported via staff members' XSEDE User Portal user profiles, and four were published by staff in the XSEDE Digital Object Repository (XDOR).

1. Bodine, E. N., R. M. Panoff, E. O. Voit, and A. E. Weisstein (2020), Agent-Based Modeling and Simulation in Mathematics and Biology Education, Bulletin of Mathematical Biology, 82(8), doi:10.1007/s11538-020-00778-z. (*published*)
2. Broude Geva, S. et al. (2020), Fostering Collaboration Among Organizations in the Research Computing and Data Ecosystem, Practice and Experience in Advanced Research Computing, doi:10.1145/3311790.3396645. (*published*)
3. Christie, M., S. Marru, E. Abeysinghe, D. Upeksha, S. Pamidighantam, S. Paul Adithela, E. Mathulla, A. Bisht, S. Rastogi, and M. Pierce (2020), An extensible Django-based web portal for Apache Airavata, Practice and Experience in Advanced Research Computing, doi:10.1145/3311790.3396650. (*published*)
4. Froeschl, L., S. Wells, and M. Bland (2020), Best Practices in Project Management in a Large, Distributed Organization, Practice and Experience in Advanced Research Computing, doi:10.1145/3311790.3396632. (*published*)
5. Knepper, R., S. Mehringer, A. Brazier, B. Barker, and R. Reynolds (2019), Red Cloud and Aristotle, Proceedings of the Humans in the Loop: Enabling and Facilitating Research on Cloud Computing, doi:10.1145/3355738.3355755. (*published*)
6. Liming, L., J. Basney, J. P. Navarro, and S. Smallen (2020), Use Case Methodology in XSEDE System Integration, Practice and Experience in Advanced Research Computing, doi:10.1145/3311790.3399622. (*published*)
7. Mehringer, S., and B. Barker (2020), Using Containers to Create More Interactive Online Training and Education Materials, Practice and Experience in Advanced Research Computing, doi:10.1145/3311790.3396641. (*published*) [**Training**]
8. Miles, Tonya A.; Wernert, Julie A.; DeStefano, Lizanne; Rivera, Lorna I. 2020. Practice & Experience in Advanced Research Computing (PEARC20) Evaluation Report. Oct. 12, 2020. http://hdl.handle.net/2142/108892
9. Navarro, J.-P., E. Blau, and L. Liming (2020), Secure XSEDE Information APIs, Practice and Experience in Advanced Research Computing, doi:10.1145/3311790.3399623. (*published*) [**Blacklight, Bridges GPU, Bridges Large, Bridges Regular, Comet, Data Oasis, Data Supercell, FutureGrid, GaTech, Globus Online, Gordon, HPSS, IU, Jetstream, Keenland, Lonestar, LSU, Mason, Maverick, NICS, OSG, PSC, Pylon, Ranch, SDSC, Stampede, Stampede2, Stanford, SuperMIC, TACC, Trestles, Wrangler, XStream**]
10. Neeman, H. et al. (2020), Cyberinfrastructure Facilitation Skills Training via the Virtual Residency Program, Practice and Experience in Advanced Research Computing, doi:10.1145/3311790.3396629. (*published*)
11. Schmitz, P., C. Mizumoto, J. Hicks, D. Brunson, G. Krovitz, J. Bottum, J. Cutcher-Gershenfeld, K. Wetzel, and T. Cheatham (2020), A Research Computing and Data Capabilities Model for Strategic Decision-Making, Practice and Experience in Advanced Research Computing, doi:10.1145/3311790.3396643. (*published*)

12. Vaillancourt, P., B. Wineholt, B. Barker, P. Deliyannis, J. Zheng, A. Suresh, A. Brazier, R. Knepper, and R. Wolski (2020), Reproducible and Portable Workflows for Scientific Computing and HPC in the Cloud, Practice and Experience in Advanced Research Computing, doi:10.1145/3311790.3396659. (*published*)
13. XSEDE. 2020. XSEDE Service Provider Checklist Version 4.3. Oct. 29, 2020. http://hdl.handle.net/2142/108886
14. XSEDE. 2020. XSEDE Software and Services Table for Service Providers and Campus Bridging Version 2.2. Oct. 29, 2020. http://hdl.handle.net/2142/108887
15. XSEDE. 2020. XSEDE Project Execution Plan Version 2.4 . Aug. 21, 2020. http://hdl.handle.net/2142/107827.
16. Zonca, A., Signell, R., Chastang, J., Fisher, J., Lowe, J., et al. 2020. Deploy Kubernetes and JupyterHub on XSEDEJetstream. Gateways 2020 (Online). https://osf.io/zyhwt/. (*published*) [**ECSS, IU, Jetstream, Science Gateways, Training**]

12.3.3.2. Publications from XSEDE Users

The following publications were submitted by users to their XSEDE User Portal profiles in Q3 2020. Most publications are associated with submissions to the August 2020 meeting, while some may be from Startup or other projects. The publications are organized by the proposal with which they were associated.

This quarter, 188 projects identified 605 publications and other products that were published, in press, accepted, submitted, or in preparation. Because these publications are submitted by users and not manually verified by XSEDE staff, there is a small chance of data entry error.

1. TG-ASC090080, TG-AST150057, TG-AST160021, TG-BCS100001, TG-PHY190047, TG-PHY200028, TG-SES170014

1. Zonca, A., Signell, R., Chastang, J., Fisher, J., Lowe, J., et al. 2020. Deploy Kubernetes and JupyterHub on XSEDEJetstream. Gateways 2020 (Online). https://osf.io/zyhwt/. (*published*) [**ECSS, IU, Jetstream, Science Gateways, Training**]

2. TG-ASC160018, TG-CCR190043

2. Javanmard, M. M., Z. Ahmad, M. Kong, L.-N. Pouchet, R. Chowdhury, and R. Harrison (2020), Deriving parametric multi-way recursive divide-and-conquer dynamic programming algorithms using polyhedral compilers, Proceedings of the 18th ACM/IEEE International Symposium on Code Generation and Optimization, doi:10.1145/3368826.3377916. (*published*) [**Stampede2, TACC**]

3. TG-ASC160018, TG-MCB140110

3. Ingber, L. (2020), Forecasting with Importance-Sampling and Path-Integrals: Applications to COVID-19, , doi:10.20944/preprints202009.0385.v3. (*published*) [**Comet, Data Oasis, SDSC**]

4. TG-ASC160048

4. Y. S. Kim, . 2020. Teaching Cyber Physical System Co-design: IoT on an FPGA Approach. 2020 IEEE International Conference on Electro Information Technology (EIT). 162-165. (*published*) [**Bridges Regular, PSC, Training**]
5. Kim, Y., Jadhav, S. 2020. An FPGA-Based Optimized Memory Controller for Accessing Multiple Memories. IEEE UEMCON 2020 (Virtual). (*accepted*) [**Bridges Regular, PSC**]

5. TG-ASC160068

6. Montlouis, W., R. Fauconier, and M. Ndoye (2020), Rapidly Moving Target Parameter Estimation Using Phased Array Radars, 2020 43rd International Conference on Telecommunications and Signal Processing (TSP), doi:10.1109/tsp49548.2020.9163492. (*published*) [**Stampede, TACC**]

6. TG-ASC170023

7. Vadala-Roth, B., S. Acharya, N. A. Patankar, S. Rossi, and B. E. Griffith (2020), Stabilization approaches for the hyperelastic immersed boundary method for problems of large-deformation incompressible elasticity, Computer Methods in Applied Mechanics and Engineering, 365, 112978, doi:10.1016/j.cma.2020.112978. (*published*) [**Comet, SDSC**]

7. TG-AST100038

8. Graur, O., K. Maguire, R. Ryan, M. Nicholl, A. Avelino, A. G. Riess, L. Shingles, I. R. Seitenzahl, and R. Fisher (2019), A year-long plateau in the late-time near-infrared light curves of type Ia supernovae, Nature Astronomy, 4(2), 188–195, doi:10.1038/s41550-019-0901-1. (published) [SDSC, Stampede, TACC]
9. Fisher, R., P. Mozumdar, and G. Casabona (2019), Carbon Detonation Initiation in Turbulent Electron-degenerate Matter, The Astrophysical Journal, 876(1), 64, doi:10.3847/1538-4357/ab15d8. (published) [Ranch, SDSC, Stampede, TACC]
10. Byrohl, C., R. Fisher, and D. Townsley (2019), The Intrinsic Stochasticity of the 56Ni Distribution of Single-degenerate Near-Chandrasekhar-mass SN Ia, The Astrophysical Journal, 878(1), 67, doi:10.3847/1538-4357/ab1f73. (published) [Ranch, SDSC, Stampede, TACC]
11. Zenati, Y., Fisher, R. 2020. Universality and Non-Universality in Distributed Nuclear Burning in Homogeneous Isotropic Turbulence. (*published*) [**Ranch, SDSC, Stampede, TACC**]

8. TG-AST140014

12. Castrejon, A., W. Lyra, A. J. W. Richert, and M. Kuchner (2019), Disentangling Planets from Photoelectric Instability in Gas-rich Optically Thin Dusty Disks, The Astrophysical Journal, 887(1), 6, doi:10.3847/1538-4357/ab3f3b. (*published*) [**Stampede2, TACC**]

9. TG-AST160063

13. Buie, E., W. J. Gray, E. Scannapieco, and M. Safarzadeh (2020), Modeling Photoionized Turbulent Material in the Circumgalactic Medium. II. Effect of Turbulence within a Stratified Medium, The Astrophysical Journal, 896(2), 136, doi:10.3847/1538-4357/ab9535. (*published*) [**Stampede2, TACC**]

10. TG-AST180007

14. La Plante, P., A. Lidz, J. Aguirre, and S. Kohn (2020), The 21 cm kSZ–kSZ Bispectrum during the Epoch of Reionization, The Astrophysical Journal, 899(1), 40, doi:10.3847/1538-4357/aba2ed. (*published*) [**Bridges Large, PSC**]

11. TG-AST180058

15. Fernandez, M., Bird, S., Upton Sanderbeck, P. 2020. Effect of Separate Initial Conditions on the Lyman-alpha Forest in Simulations. (*published*)

12. TG-AST180059

16. Zhai, Z., Chuang, C., Wang, Y., Benson, A., Yepes, G. 2020. Clustering in the Simulated Hα Galaxy Redshift Survey from Nancy Grace Roman Space Telescope. (*submitted*)

13. TG-AST180060

17. Teague, R., J. Bae, and E. A. Bergin (2019), Meridional flows in the disk around a young star, Nature, 574(7778), 378–381, doi:10.1038/s41586-019-1642-0. (*published*) [**Comet, SDSC**]

14. TG-AST180069

18. Agarwal, D., K. Aggarwal, S. Burke-Spolaor, D. R. Lorimer, and N. Garver-Daniels (2020), FETCH: A deep-learning based classifier for fast transient classification, Monthly Notices of the Royal Astronomical Society, 497(2), 1661–1674, doi:10.1093/mnras/staa1856. (*published*) [**Bridges GPU, PSC**]

15. TG-AST190035

19. Prem, P., D. M. Hurley, D. B. Goldstein, and P. L. Varghese (2020), The Evolution of a Spacecraft-Generated Lunar Exosphere, Journal of Geophysical Research: Planets, 125(8), doi:10.1029/2020je006464. (*published*) [**Stampede2, TACC**]

16. TG-ATM100026

20. Longley, W. J., P. J. Erickson, J. Vierinen, M. M. Oppenheim, F. D. Lind, and Y. S. Dimant (2020), Millstone Hill ISR Measurements of Small Aspect Angle Spectra, Journal of Geophysical Research: Space Physics, 125(6), doi:10.1029/2019ja027708. (*published*)
21. Longley, W. J., M. M. Oppenheim, N. M. Pedatella, and Y. S. Dimant (2020), The Photoelectron-Driven Upper Hybrid Instability as the Cause of 150-km Echoes, Geophysical Research Letters, 47(8), doi:10.1029/2020gl087391. (*published*) [**Stampede2, TACC**]

22. Young, M. A., M. M. Oppenheim, and Y. S. Dimant (2020), The Farley-Buneman Spectrum in 2-D and 3-D Particle-in-Cell Simulations, Journal of Geophysical Research: Space Physics, 125(1), doi:10.1029/2019ja027326. (*published*) [**Stampede2, TACC**]
23. Guttormsen, G., A. C. Fletcher, and M. M. Oppenheim (2020), Atomic-Scale Simulations of Meteor Ablation, Journal of Geophysical Research: Space Physics, 125(9), doi:10.1029/2020ja028229. (*published*) [**Stampede2, TACC**]

17. TG-ATM160014

24. Guo, J. et al. (2020), The Climatology of Lower Tropospheric Temperature Inversions in China from Radiosonde Measurements: Roles of Black Carbon, Local Meteorology, and Large-Scale Subsidence, Journal of Climate, 33(21), 9327–9350, doi:10.1175/jcli-d-19-0278.1. (published) [Comet, SDSC]
25. Wang, J., and X.-M. Hu (2020), Evaluating the performance of WRF urban schemes and PBL schemes over Dallas Fort Worth during a dry summer and a wet summer, Journal of Applied Meteorology and Climatology, 1–53, doi:10.1175/jamc-d-19-0195.1. (*published*) [**Comet, SDSC**]

18. TG-ATM170024

26. Barthelmie, R. J., T. J. Shepherd, J. A. Aird, and S. C. Pryor (2020), Power and Wind Shear Implications of Large Wind Turbine Scenarios in the US Central Plains, Energies, 13(16), 4269, doi:10.3390/en13164269. (published) [IU, Jetstream, TACC, Wrangler]
27. Pryor, S. C., R. J. Barthelmie, M. S. Bukovsky, L. R. Leung, and K. Sakaguchi (2020), Climate change impacts on wind power generation, Nature Reviews Earth & Environment, doi:10.1038/s43017-020-0101-7. (*published*) [IU, Jetstream, TACC, Wrangler]

19. TG-ATM170030

28. Dominguez, F., Chug, D., Pal, S. 2021. Tracking Moist Static Energy. (*in preparation*)
29. Chug, D., Dominguez, F., Grimm, A. 2021. Observed Influence of Root Zone Soil Moisture Variability on the Intraseasonal Hydroclimate Variability over South America in the Summer Season. (*in preparation*)

20. TG-BIO170011

30. Tiitto, M. V., and R. A. Lodder (2020), Working Memory and Impulsivity and Artificial Neural Networks, , doi:10.1101/2020.10.26.355990. (*published*) [ECSS, NIP, Science Gateways, SDSC, Stampede, Training]
31. Campbell, H., Lodder, R. 2020. Methods for Using NHANES for Exposure Estimates. (*published*) [ECSS, NIP, Science Gateways, SDSC, Stampede, Training]

21. TG-CCR190023

32. Chin, T., Chuang, P., Chandra, V., Marculescu, D. 2020. One Weight Bitwidth to Rule Them All. (published)
33. Ding, R., Chin, T., Liu, Z., Marculescu, D. 2019. Regularizing Activation Distribution for Training Binarized Deep Networks. (published)
34. Chin, T., Ding, R., Marculescu, D. 2019. AdaScale: Towards Real-time Video Object Detection Using Adaptive Scaling. (*published*)

22. TG-CCR190024

35. Pistorius, J., Martin, C., Sudarshan, S. 2020. Exosphere -- Bringing The Cloud Closer. (*published*) [**IU, Jetstream, TACC**]

23. TG-CCR190027

36. Mionis, S., Franchetti, F., Larkin, J. 2020. Quantum Circuit Optimization with SPIRAL: A First Look. (*published*) [**Bridges GPU, Bridges Large, Bridges Regular, PSC, Pylon**]

24. TG-CCR190043

37. Chelini, L., Gysi, T., Grosser, T., Kong, M., Corporaal, H. 2020. Automatic Generation of Multi-Objective Polyhedral Compiler Transformations. Proceedings of the 2020 International Conference on Parallel Architectures and Compilation Techniques (PACT '20) (Atlanta, GA, USA). 14. https://doi.org/10.1145/3410463.3414635. (*accepted*) [**ECSS, Ranch, Stampede, TACC, Training**]

25. TG-CCR190053

38. Wu, Y., Wang, Z., Jia, Z., Shi, Y., Hu, J. 2020. Intermittent Inference with Nonuniformly Compressed Multi-Exit Neural Network for Energy Harvesting Powered Devices. (published) [Bridges GPU, ECSS, NIP, PSC, Science Gateways, Training]

39. Wu, Y., Wang, Z., Shi, Y., Hu, J. 2020. Enabling On-Device CNN Training by Self-Supervised Instance Filtering and Error Map Pruning. (*published*) [**Bridges GPU, ECSS, NIP, PSC, Science Gateways, Training**]

26. TG-CCR200004

40. Li, B., Kong, Z., Zhang, T., Li, J., Li, Z., et al. 2020. Efficient Transformer-based Large Scale Language Representations using Hardware-friendly Block Structured Pruning. Findings of the ACL Empirical Methods in Natural Language Processing (EMNLP) (online). (*accepted*)

27. TG-CDA170003

41. Perri, M. J. (2020), Online Data Generation in Quantitative Analysis: Excel Spreadsheets and an Online HPLC Simulator Using a Jupyter Notebook on the Chem Compute Web site, Journal of Chemical Education, 97(9), 2950–2954, doi:10.1021/acs.jchemed.0c00565. (*published*) [**ECSS, IU, Jetstream, Science Gateways**]
42. Agnew-Francis, K. A., and C. M. Williams (2020), Squaramides as Bioisosteres in Contemporary Drug Design, Chemical Reviews, 120(20), 11616–11650, doi:10.1021/acs.chemrev.0c00416. (*published*) [**Bridges Regular, Comet, IU, Jetstream, PSC, Science Gateways, SDSC**]
43. Firme, C. 2019. Introductory Organic Chemistry and Hydrocarbons: A Physical Chemistry Approach. CRC Press. (*published*) [**Bridges Regular, Comet, IU, Jetstream, PSC, Science Gateways, SDSC**]
44. Semakin, A., Y. Nelyubina, S. Ioffe, and A. Sukhorukov (2020), 2,4,9-Triazaadamantanes with "Clickable" Groups: Synthesis, Structure and Applications as Tripodal Platforms, European Journal of Organic Chemistry, doi:10.1002/ejoc.202000832. (*published*) [**Bridges Regular, Comet, Jetstream, PSC, Science Gateways, SDSC**]
45. Lu, J., Z. Zhang, D. Yan, Z. Zhang, J. Guan, and J. Qiao (2020), Synthesis of 4-Chloro-1,3-Diazobenzene Bent-Cores Liquid Crystal and Characterizations of Its Mesogenic Behaviors and Photosensitivity, , doi:10.26434/chemrxiv.12115878.v3. (*published*) [**Bridges Regular, Comet, Jetstream, PSC, Science Gateways, SDSC**]

28. TG-CDA190007

46. Lee, B., Bartsch, S., Lin, M., Asti, L., Welling, J., et al. 2020. How Long-Term Acute Care Hospitals (LTACHs) Can Play an Important Role in Controlling Carbapenem-Resistant Enterobacteriaceae (CRE) in a Region: A Simulation Modeling Study. (*accepted*)

29. TG-CHE070030N, TG-CHE080068N

47. Savoo, N., J. Z. A. Laloo, L. Rhyman, P. Ramasami, F. M. Bickelhaupt, and J. Poater (2019), Activation Strain Analyses of Counterion and Solvent Effects on the Ion-Pair SN2 Reaction of and CH3Cl, Journal of Computational Chemistry, 41(4), 317–327, doi:10.1002/jcc.26104. (published) [Bridges GPU, Bridges Large, Bridges Regular, Comet, IU, Jetstream, PSC, Science Gateways, SDSC, Stampede, Stampede2, TACC, Wrangler]
48. Dumett Torres, D., S. Pamidighantam, and P. K. Jain (2020), Crystal Symmetry, Strain, and Facet-Dependent Nature of Topological Surface States in Mercury Selenide, The Journal of Physical Chemistry C, 124(19), 10344–10352, doi:10.1021/acs.jpcc.0c01663. (published) [Bridges GPU, Bridges Large, Bridges Regular, Comet, IU, Jetstream, PSC, Science Gateways, SDSC, Stampede, Stampede2, TACC, Wrangler]
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13. Collaborations

XSEDE considers collaboration within the research community to be essential to the advancement of all fields of research. It is XSEDE's policy and practice to encourage and engage in collaborations, where applicable.

In addition to the collaborations with Service Providers via the SP Forum (§14), XSEDE collaborates with NSF awardees and other domestic and international projects.

The following list represents the active collaborations with NSF awardees:

PI/Contact	NSF Proposal Title	Award Number
David Anderson	Mainstreaming Volunteer Computing	1105572
Ian Foster	SI2-SSI: SciDaaS -- Scientific data management as a service for small/medium labs	1148484
Abani Patra	Collaborative Research: Integrated HPC Systems Usage and Performance of Resources Monitoring and Modeling (SUPReMM- SUNY Buffalo)	1203560
Abani Patra	Collaborative Research: Integrated HPC Systems Usage and Performance of Resources Monitoring and Modeling (SUPReMM- UT-Austin)	1203604
Von Welch	Center for Trustworthy Scientific Cyberinfrastructure (CTSC)	1234408
Kevin Franklin	Latin America-US Institute 2013: Methods in Computational Discovery for Multidimensional Problem Solving	1242216
Nicholas Berente	EAGER proposal: Toward a Distributed Knowledge Environment for Research into Cyberinfrastructure: Data, Tools, Measures, and Models for Multidimensional Innovation Network Analysis	1348461
Jerzy Bernholc	Multiscale Software for Quantum Simulations in Materials Design, Nano Science and Technology	1339844
Seung-Jong Park	MRI: Acquisition of SuperMIC-- A Heterogeneous Computing Environment to Enable Transformation of Computational Research and Education in the State of Louisiana	1338051
Marlon Pierce	Open Gateway Computing Environments Science Gateways Platform as a Service (OGCE SciGaP)	1339774
Steven Tuecke	Sustaining Globus Toolkit for the NSF Community (Sustain-GT)	1339873
Kathy L. Benninger	CC-NIE Integration: Developing Applications with Networking Capabilities via End-to-End SDN (DANCES)	1341005
Renata Wentacovitch	Quantum Mechanical Modeling of Major Mantle Materials	0635990
Dr. Kate Keahey	A Large-Scale, Community-Driven Experimental Environment for Cloud Research	1419141

Shaowen Wang	MRI: Acquisition of a National CyberGIS Facility for Computing- and Data-Intensive Geospatial Research and Education	1429699
Todd Martinez	Acquisition of an Extreme GPU cluster for Interdisciplinary Research	1429830
Donna Cox	The Centrality of Advanced Digitally-ENabled Science: CADENS	1445176
Robert Ricci	CloudLab: Flexible Scientific Infrastructure to Support Fundamental Advances in Cloud Architectures and Applications	
Dr. Kerk F. Kee, Almadena Y. Chtchelkanova	RUI: CAREER Organizational Capacity and Capacity Building for Cyberinfrastructure Diffusion	1453864
Nicholas Berente	Fostering Successful Innovative Large-Scale, Distributed Science and Engineering Projects through Integrated Collaboration	1551609
Allen Pope	EarthCube RCN: Collaborative Research: Research Coordination Network for High Performance Distributed Computing in the Polar Sciences	1541620
Thomas Hauser	MRI Collaborative Consortium: Acquisition of a Shared Supercomputer by the Rocky Mountain Advanced Computing Consortium	1532236
Edward Seidel	BD Hubs: Midwest: “SEEDCorn: Sustainable Enabling Environment for Data Collaboration that you are proposing in response to the NSF Big Data Regional Innovation Hubs (BD Hubs): Accelerating the Big Data Innovation Ecosystem (NSF 15-562) solicitation	1550320
Alexander Withers	Secure Data Architecture: Shared Intelligence Platform for Protecting our National Cyberinfrastructure” that you are proposing in response to the NSF Cybersecurity Innovation for Cyberinfrastructure (NSF 15-549) solicitation	1547249
James Basney	CILogon 2.0 project that you are proposing in response to the NSF Cybersecurity Innovation for Cyberinfrastructure (NSF 15-549) solicitation	1547268
Bertram Ludaescher	DIBBs: Merging Science and Cyberinfrastructure Pathways: The Whole Tale	1541450
Philip J. Puxley	Associated Universities, Inc. (AUI) and the National Radio Astronomy Observatory (NRAO)	1519126
J. Bernholc	SI2-SSE: Multiscale Software for Quantum Simulations of Nanostructured Materials and Devices	1615114
David Anderson	Collaborative Research: SI2-SSI: Adding Volunteer Computing to the Research Cyberinfrastructure	1550601
Thomas Crawford	Molecular Sciences Software Institute (MolSSI) that you are proposing in response to the NSF Scientific Software Innovation Institutes (S2I2, NSF 15-553) solicitation	1547580

Nancy Wilkins-Diehr	Science Gateways Software Institute for NSF Scientific Software Innovation Institutes (S2I2, NSF 15-553) solicitation	1547611
Ron Hawkins	CC* Compute: BioBurst in response to the Campus Cyberinfrastructure (CC*) Program solicitation (NSF 16-567)	1659104
Farzad Mashayek	CC* Networking Infrastructure: Building HPRNet (High-Performance Research Network) for advancement of data intensive research and collaboration	1659255
Ewa Deelman	SI2-SSI: Pegasus: Automating compute and data intensive science	1664162
Doug Jennewein	MRI: Acquisition of the Lawrence Supercomputer to Advance Multidisciplinary Research in South Dakota	1626516
Dirk Colbry	Cybertraining:CIP – Professional Training for CyberAmbassadors	1730137
Eric Shook	Collaborative Research: CyberTraining: CIU: Hour of Cyberinfrastructure: Developing Cyber Literacy for Geographic Information Science	7/26/6909
Jennifer M. Schopf	CC* NPEO: A Sustainable Center for Engagement and Networks	1826994
Alex Szalay	Collaborative Research: Building the Community for the Open Storage Network	1747493
Von Welch	CICI: CSRC: Research Security Operations Center (ResearchSOC)	1840034
Larry Smarr	CC* NPEO: Towards the National Research Platform	1826967
Thomas Doak	Collaborative Research: ABI Sustaining: The National Center for Genome Analysis Support	1759906
Peter Kasson	SI2-SSI Collaborative Research: SCALE-MS-Scalable Adaptive Large Ensembles of Molecular Simulations	1835780
Mao Ye	A Workshop to Jumpstart High-Performance Computing in Finance/ BIGDATA: IA: Collaborative Research: Understanding the Financial Market Ecosystem	1838183
Dmitry Pekurovsky	Elements: Software: Multidimensional Fast Fourier Transforms on the Path to Exascale	1835885
Von Welch	CICI: CCoE: Trusted CI: Advancing Trustworthy Science	1920430
Rudolph Eigenmann	MRI: Acquisition of a Big Data and High Performance Computing System to Catalyze Delaware Research and Education	1919839
Timoty Menzies	Can Empirical Software Engineering be Adapted to Computational Science	1908762
William Gropp	Category I: Crossing the Divide Between Today's Practice and Tomorrow's Science	2005572

X. Carol Song	Category I: *Anvil* - A national advanced computational resource to meet the changing needs of the nation's research and education communities	2005632
David Y. Hancock	Category I – *Jetstream 2*: On-demand high performance computing	2005506
Honggao Liu	MRI: Acquisition of FASTER - Fostering Accelerated Sciences Transformation Education and Research	2019129
Elise D. Miller-Hooks	MRI: Acquisition of an Adaptive Computing Infrastructure to Support Compute- and Data-Intensive Multidisciplinary Research	2018631

The following list represents other active formal domestic and international collaborations:

Project	Collaboration Summary
Domestic Collaborations	
Marshall University - Campus Bridging Site (CRI)	Indiana University CRI staff visited Marshall University for server build and XSEDE software toolkit installation
Southern Illinois University - Campus Bridging Site (CRI)	Indiana University CRI staff visited Southern Illinois University for server build and XSEDE software toolkit installation
Bentley University - Campus Bridging Site (CRI)	Indiana University CRI staff visited Bentley University for server build and XSEDE software toolkit installation
University Texas El Paso - Campus Bridging Site (CRI)	Indiana University CRI staff visited University Texas El Paso for server build and XSEDE software toolkit installation
Brandeis University - Campus Bridging Site (CRI)	Indiana University CRI staff visited Brandeis University for server build and XSEDE software toolkit installation
Incorporated Research Institutions for Seismology (IRIS)	Indiana University partnering with IRIS to use the *Jetstream* system to disseminate data to the research community
CyVerse	Indiana University partnered with CyVerse projects to deploy and operate the *Jetstream* system as part of the XSEDE ecosystem
National Center for Genome Analysis Support (NCGAS)	Indiana University partnered with the National Center for Genome Analysis Support to use the *Jetstream* system for creation of virtual machine images for research and analysis of genome data
South Dakota State University - Campus Bridging Site	Indiana University CRI staff visited SDSU for cluster build and XSEDE software toolkit installation
Slippery Rock University - Campus Bridging Site	Indiana University CRI staff visited Slippery Rock University for server build and XSEDE software toolkit installation

Doane University - Campus Bridging Site	Indiana University CRI staff visited Doane University for cluster build and XSEDE software toolkit installation
UltraScan Science Gateway - Virtual Cluster	CRI staff worked with UltraScan to create a virtual cluster in *Jetstream*
3-D Quantitative Phenotyping Gateway - Virtual Cluster	CRI staff worked with A. Murat Maga in order to create a virtual cluster in *Jetstream* for the biological sciences
XSEDE Web SSO	RACD is helping XSEDE federated services providers (XDMoD, CI-Tutor, and Cornell Virtual Workshop) to integrate with the XSEDE Web SSO capability.
Use of XRAS by NCAR/CISL	Agreement to use XRAS for managing the NCAR allocations
Use of XRAS by NCAR/EOL	Agreement to use XRAS to manage EOL Lower Atmosphere Observing Facilities (LAOF) allocations
Use of XRAS by *Blue Waters*	Agreement to use XRAS for managing the *Blue Waters* allocations
Use of Information Services by UIUC	Agreement to use Information Services to enable resource discovery in the UIUC Research Portal (https://researchit.illinois.edu)
Delivering Kepler to XSEDE Users	XSEDE Providing Capability Integration Assistance to make Kepler available to XSEDE users
Open Storage Network CI integration collaboration	XCI is participating in OSN software working group to facilitate documenting requirements and use cases, support the engineering process, and provide other useful XSEDE services
Institute for Research on Innovation & Science (IRIS)	Agreement to use network science methods and administrative data maintained by the Institute for Research on Innovation & Science to develop preliminary models that examine the scientific effects of XSEDE usage by researchers on more than 30 U.S. university campuses.
International Collaborations	
International HPC Summer School	Partnership with PRACE (EU), RIKEN AICS (Japan), and Compute Canada (Canada) to familiarize the best students of the respective continents or countries in computational sciences with a strong bond to supercomputing with all major state-of-the-art aspects related to HPC for a broad range of scientific disciplines, catalyze the formation of networks, provide mentoring through faculty members and supercomputing experts from renowned HPC centers, and to facilitate international exchange and open further career options.
Open Grid Forum (www.ogf.org)	JP Navarro is GLUE working group chair. XSEDE leverages and influences infrastructure information management through this collaboration.
HPC Development and Summer Exchange Program for HPC visiting staff	Craig Stewart entered into a formal MOU of Collaboration with TU-Dresden

Membership in the Research Data Alliance (RDA) organization	Indiana University entered into a formal membership agreement with RDA to explore open data standards as part of the international scope of the organization
Distributed Organization for Scientific and Academic Research (DOSAR)	International grid computing research and education organization; Indiana University participates as a contributing partner to summer teaching in the African Grid School
International collaboration of regional research infrastructures (XSEDE, PRACE, and RIKEN)	XSEDE entered into an MOU jointly with PRACE and RIKEN committing to opening lines of communications and seeking more areas of collaboration. This occurred in May 2017.
Compute Canada Accounting Service	Exploring possible collaboration on re-design of Federated Accounting Service
WISE (Wise Information Security for Collaborating e-Infrastructures)	Support trusted global framework where security experts can share information on topics such as risk management, experiences about certification processes and threat intelligence
IGTF/TAGPMA	To establish common policies and guidelines that help establish interoperable, global trust relations between providers of e-Infrastructures and cyber-infrastructures, identity providers, and other qualified relying parties.
International Identity Federation	XCI-302: Participate in REFEDS Assurance Framework Pilot
Engagement Group for Infrastructures (AEGIS)	XCI-256: Participate in AARC Engagement Group for Infrastructures (AEGIS)
Technische Universitat Darmstadt: ROI on academic advanced cyberinfrastructure systems	Understanding ROI on university-owned advanced cyberinfrastructure systems, including cloud systems with Technische Universitat Darmstadt
RTWH Aachen University : ROI on academic advanced cyberinfrastructure systems	Understanding ROI on university-owned advanced cyberinfrastructure systems, including cloud systems with RTWH Aachen University

14. Service Provider Forum Report

Service Providers (SPs) are independently funded projects and/or organizations that provide cyberinfrastructure (CI) services to the science and engineering community. There is a rich diversity of SPs in the U.S. academic community, spanning centers that are funded by NSF to operate large-scale resources for the national research community to universities that provide resources and services to their campus researchers. The Service Provider Forum (SPF) is intended to facilitate this ecosystem of Service Providers, thereby advancing the science and engineering researchers that rely on these cyberinfrastructure services. The SPF has two primary elements of its charter:

1. An open forum for discussion of topics of interest to the SP community
2. A formal communication channel between the SPF members and the XSEDE project

The SPF conducts its business primarily through conference calls scheduled on a biweekly cadence on Thursdays at 4PM Eastern Time. We meet at least once a month; if there is no new business to discuss within two weeks of a 'held' meeting, then that interim biweekly meeting is cancelled. Agendas are distributed in advance of the meetings and minutes are maintained on the XSEDE SP wiki (https://confluence.xsede.org/display/XT/XSEDE+Federation). NSF Program Officers are invited and occasionally participate. Many people from the XSEDE program routinely participate in SPF meetings to facilitate direct interaction with the XSEDE program. For example, regular updates are provided by John Towns (XSEDE PI) and Tim Boerner (XSEDE Deputy Project Director), Victor Hazlewood (XSEDE SP Coordinator), and other XSEDE management and area leads. Additional contributors from XSEDE and other organizations are frequently invited to brief the SPF on XSEDE topics or seek the Forum's input in the development of program plans and activities.

This report is the quarterly summary of the SPF's activities covering the period of August 1, 2020 – October 31, 2020.

14.1. SP Forum administrative and membership activities during this reporting period

- Mostly monthly SPF meetings – attendance typically ranges from 18 to more than 25 participants
- SP Forum participation at the September XSEDE Remote Quarterly Meeting (Ruth Marinshaw)
- SP Forum participation at the October XAB virtual meeting (Ruth Marinshaw, Dave Hancock, Jon Anderson)
- SP Forum participation at the biweekly XSEDE Senior Management Team calls (Ruth Marinshaw)

The full membership of the SP Forum is maintained on the XSEDE website, https://www.xsede.org/ecosystem/service-providers.

Technical and programmatic discussions

Noteworthy SPF activities from this reporting period include:

- Regular attendance and updates by Tim Boerner on the XSEDE project.
- Regular attendance and updates by Victor Hazlewood XSEDE Engineering and Operations topics.
- Regular attendance and updates from Tabitha Samuel regarding SP Coordination activities.
- Key presentations and discussion topics:
    - JP Navarro and others from the XSEDE RACD team and the OSC Open OnDemand team – an initial discussion with the SP Forum regarding interest in and/or value of exploring OOD for XSEDE, followed two months later by a discussion of their joint recommended approach to providing Open OnDemand to SPs, through XSEDE
    - The XSEDE Cybersecurity team – discussion of recent rise in attacks on systems and mitigations available to address those.

- Dave Hart and the RAS team – presentation of and discussion with SPs around the new AMIE environment and capabilities. This was met with resounding appreciation and thanks from all of the service providers.

15. UAC

XSEDE User Advisory Committee Report
Reporting period: August 1, 2020 through October 31, 2020

The XSEDE User Advisory Committee (UAC) represents the "user's voice" to XSEDE management, presenting recommendations regarding emerging needs and services and act as a sounding board for plans and suggested developments. It meets two or three times a year via conference call. The UAC makes suggestions to improve XSEDE operations and helps identify areas where more support expertise is required. It reviews findings of XSEDE's Performance Evaluation Plan, Self-Assessment, and User Survey. Subsets of the UAC advise XSEDE's Extended Collaborative Support Service (ECSS) management on where to dedicate support effort on community codes. One member of the UAC serves on the User Requirements Evaluation and Prioritization Working Group (UREP). The chair of the UAC (elected by its members) participates in regular XSEDE senior management meetings (currently bi-weekly).

There were no meetings of the UAC during this reporting period, the prior meeting was held on 16 July 2020. The next meeting will be held in early December 2020. No other actions were made by or requested of the UAC over this period

16. XMS Summary

16.1. Executive Summary

During the current reporting period substantial progress was achieved in a number of areas. Open XDMoD version 9.0 was released. It includes a number of improvements, enhancements, new features and a number of "under the hood" improvements, as noted in the release notes. Of special note is the development work in the Cloud realm, the "groupby" refactoring and the addition of GPU tracking to the Jobs realm. The integration of XDMoD and OnDemand also made substantial progress with the release of the first fully functional version of Open XDMoD/OnDemand that displays user job information and job efficiency information within OnDemand and provides OnDemand users with single-click direct access to XDMoD data and the XDMoD job viewer. The Frontera Open XDMoD instance hosted by XMS is now fully functional with user credentials distributed to CCR, TACC and NSF. The XMS engagement with Trusted CI has produced a more secure version of Open XDMoD and a better procedure to deal with potential cyber-attacks.

17. XAB Executive Summaries

17.1. Executive Summary of XSEDE Advisory Board Meeting, August 28, 2020

Meeting Date: Friday, August 28, 2020
Meeting Place: Teleconference via Zoom
Preface: The main topic of this call was a recap of the NSF Review
Next Call: October 23, 2020

Approval of June Meeting Minutes

- Approved.

Recap of NSF June Review

Good June review. Our response to the report was accepted by NSF & funding for next project year was approved.

- Response doc will be circulated to the XAB.
- No major concerns presented by panel. Some good suggestions that we've addressed. Nothing to change our plans for the coming year.

Supplemental year to XSEDE2 was approved, so the new project end date is August 31, 2022 with $21.8M in funding.

No solicitation for what will follow XSEDE2 at this point. Hope to see that solicitation no later than the first quarter of next calendar year. If not, we will have a similar problem to what we had this year.

- John has noted to NSF that it is not productive to request us to submit a bridge proposal
- Believe XSEDE's response to the Blueprint doc may have made them revisit their thinking re. what will follow XSEDE
- NSF leadership hasn't said much other than that they are actively working on the issue. Hope that means they are writing the solicitation, but can't say for sure.

COVID-19 HPC Consortium Update

- In March, XSEDE was approached by OSTP to see if we can manage how the collective consortium resources can be allocated to the community. Quickly stood up an instance of XRAS to support the consortium and conducted reviews similar as we would in our XAC process. Have ~170 proposals submitted. ~20 returned because of incomplete submissions. ~150 reviewed with ~90 approved. About 1/3 are on XSEDE allocated resources. Others on resources contributed by other consortium members. Starting to see some results.
- Most proposals around molecular biophysics in various forms. Understanding structure & docking, some on small molecule design.
- Fewer proposals that look at drug design, therapeutics, patient care. Consortium leadership has a strong desire to see more work in that space to have more direct impact on the pandemic. This gets a bit sticky as NSF typically doesn't get involved in this kind of work. Have not received guidance from NSF on whether these changes would impact XSEDE's involvement.
    - Reluctance by NSF to go this route.
    - Incorporating into review more weighting for proposals of this nature.
- Providers come from throughout the community including NSF, DOE, Microsoft, AWS, and a variety of companies like BP. More recently includes some international partners.
    - Q: What NSF resources? All XSEDE Allocated resources that can be requested, Frontera, Cheyenne, Chameleon. Decisions are made on the PI's part about whether to participate.

    - Have helped with crises in the past. NSF is directly involved in making the decision to commit resources. There was high level NSF commitment before it came to XSEDE.
    - The Executive Board observes, manages bringing in major partners including OSTP. They are concerned about aspects of the pandemic that aren't being addressed by the consortium. Feel there should be a better balance of projects with more therapeutics, patient-oriented work. NSF is nervous but hasn't said we aren't going there. NASA is hesitant as well, but they aren't contributing resources.
- Question to XAB: How should XSEDE conduct itself if NSF pushes away from the consortium? Should we push back? How hard?
    - Q: what resources/effort is being given by XSEDE?
        - XRAS is the mechanism that allows proposals to be submitted/reviewed/allocated.
            - Receiving funding from the community for their use of XRAS (NCAR, PSC, Frontera, NCSA). Offering this at no cost to the consortium.
            - If NSF chooses to separate from consortium, could be treated as an XRAS usage that would need to be paid for in some way.
        - XSEDE allocated resources: *Stampede2, Comet, Bridges*. ECSS staff assigned as well
            - SP awards have some discretionary cycles they can allocate as they like
        - Q: If competition can help solve COVID problems, it is worth continuing to do so. Suggest pushing NSF to continue.
            - John & Ken's time towards this effort could become problematic.
            - NSF charter: The National Science Foundation (NSF) is an independent federal agency created by Congress in 1950 "to promote the progress of science; to advance the national health, prosperity, and welfare; to secure the national defense... Used this previously when they tried to limit participation.
        - Q: Has NSF said anything about their role?
            - Early press releases that recognized participation. Not a delineation of roles.
            - Possibility to get someone to go up through the chain to get an official statement about how they support this consortium, agencies working together for the good of the nation. John will ask Amy about this to see if she can push this.
        - Q: Would be surprised if NSF isn't having the same discussions. If they pull out, likely because they can't bend the rules.
        - Q: Is the governing committee thinking about completely pivoting focus or just emphasizing other areas more?
            - Won't exclude other work, but will be weighted higher for these healthcare areas
            - Good chunk of the proposals received are molecular dynamic simulations in one way or another. That is the community that is associated with those involved in the consortium, so not a surprise.
        - John: XRAS is the linchpin to everything running.
        - Q: Disease spread types of projects? Just a few.
            - Q: MD better prepared for parallel/HPC environment. Lauren Myers' lab: works with MatLab or R. Period of transitioning them to a large scale environment. Their use of machines is not sophisticated.

            - JT: not a significant use of these resources in that community. Many haven't had large enough data sets for it to matter, but have larger data sets now.
        - Q: Any evaluation of scientific efficacy of what has been done so far?
            - Not a lot yet. People are asking this. Asking PIs to provide biweekly updates & have been getting some good info. Just starting to see results from most of the projects. Consortium is trying to share highlights of results of time & effort that's gone into it. Interesting results thus far have not been articulated well on the website. Webinar this week with a researcher presenting their work. Hard to do an assessment quite yet.
        - Overall response from the board: Keep proceeding as you are. Push back at NSF if they try to curb XSEDE's participation.
        - John: concerns that other work is being impeded by COVID work, but feel addressing the pandemic is a priority issue. Worried about what will happen in the next couple of months with schools back in session. Could see a dramatic spike depending on how it is handled.
    - Q: how has this pandemic impacted the project?
        - Already distributed project.
        - Putting aside consortium work, the impact has been nominal. Have worked effectively as a distributed project for a long time. Not much of a change from an operational perspective.
        - Provide NSF with reports on financial impacts in terms of staff time spent on pandemic. Report weekly to NSF on consortium related work. Part of that is an accounting for time on systems used.
        - Q: Hidden impacts. Some people are well-suited to working at home, but others are dealing with a drop in productivity or personal problems. Not sure we've done a good job of thinking about the long term effects of this.
          RECOMMENDATION: XSEDE should consider long-term effects of this nature on people.
            - JT: we are trying to accommodate people homeschooling or with kids at home doing virtual learning. Groups of people with different tolerance levels. Hard to characterize well, but it is a concern. At institutional level trying to help staff work through issues.
        - Q: support John staying the course. Have a contingency plan in case NSF pulls out.
- Q: worried about what will come after XSEDE. Took a long time for XSEDE to become the well-oiled machine that it is. Community can expect several years (3-4?) of disruption if there is a cold turkey replacement.
    - Was difficult to get the project to where it is today.
    - Overlap on training new teams? Many discussions around continuity/overlap. John has repeatedly made the point that transition from TeraGrid to XSEDE was disruptive to the community. Feel that NSF has heard this & appreciates the need for overlap, but not clear how it will play out as time goes on. If we're going to do a detailed & careful transition, we will need overlap time. Too complex to just turn off and then turn back on. Hope that we'll see a solicitation by the end of the year.
    - Q: knowing the transition will be a problem, is there a mechanism to have XSEDE not get re-awarded from the ground up every 5 years? Persist as a living organism.
        - NSF has a mechanism such as this, but many are reluctant to go that route.

- The funds have a limit on award length. Incumbent may or may not win the next award. Makes sense in the research base, but much of what we do is infrastructure.
- MRSEC process doesn't exactly fit, but could be modified. How does NSF provide CI services to awardees in a more holistic way. Looking at it now more narrow. Difficult path for NSF as it would mean a lot of change for the way things are done.

18. XSEDE Project Execution Plan

At the beginning of the XSEDE project, a Project Execution Plan (PEP) was submitted to and approved by NSF. Content in this and all preceding Interim Project and Annual Reports supersede information submitted in the original PEP. The most recent version of the PEP (V. 2.4) can be viewed on the wiki[39]. Given that there were no changes to the PEP during this reporting period, a copy is not included in this report.

[39] https://confluence.xsede.org/display/XT/XSEDE+Project+Execution+Plan