SciGaP Annual Report Metrics

Summary

The following table summarizes our team-wide efforts. Details are in separate sections below. Note figures are for the current project year only and not cumulative.

Science Metric	**Year 1**	**Year 2**	**Year 3**	**Year 4**	**Year 5**
Enabled Publications	558 (2014)	664 (2015)	817 (2016)	790 (2017)	1134 (2018)

Supported Allocations (#, SU)	7 awards, 16,990,000.00 SU	9 awards, 19,134,890 SU	19 awards, 27,861,384 SU	15 awards, 45,183,642 SU	24 awards, 42,833,364 SU
Collaborating Grants (#, $) awarded in project year	1 Grant, $263,000	4 Grants, > $2M	7 Grants, > $10.3 M	9 Grants, > $8M	12 Grants, > $10.6 M

Operational Metric	**Year 1**	**Year 2**	**Year 3**	**Year 4**	**Year 5**
Gateways Using one or more SciGaP services	2	6 (see XSEDE allocations table below)	10 (see XSEDE allocations table below)	> 25	30
Number of Users Supported	4205	7451	9351	11339	15617
Number of Experiments (Jobs Executed)	129,242	212,933	300,522	355,984	1,750,666
Resources Available to Users	6 clusters made available	13 XSEDE, Campus, and International Resources	> 10 XSEDE, Campus, and International Resources	> 20 XSEDE, campus, regional, and international resources.	> 35 XSEDE, campus, regional, and international resources.
Jira Tickets Created/Closed	515/288	370/148	272/151	413/254	361/184
New Apache Airavata Committers and PMC Members	8 committers, 0 PMC members	2 committers, 2 PMC members	1 PMC member	2 PMC members, 4 Committers	2 PMC members, 4 Committers

Science Metrics

Number of Publications Enabled for Year 5

We report publications for September 15, 2017-September 15, 2018.

Totals

We separate publications into those supported directly by the grant and those enabled by the grant. Totals for the year are below. For simplicity, we count enabled publications by calendar year rather than project year.

- SciGaP Team Publications, Year 5: 19 (includes peer reviewed papers, conference proceedings, and peer-reviewed posters)
- SciGaP Supported Science Publications, Year 5: 1134

Details are below.

Team Publications

Since the project began, team-authored publications about SciGaP cyberinfrastructure supported by this award have been cited 284 times (Google Scholar). Eight (8) of these citations have been cited at least eight (8) times, and five (5) papers have been cited more than ten (10) times (Google Scholar).

Team publications for Project Year 5 are below.

1. Wang, Y., Pamidighantam, S., Yaw, S., Abeysinghe, E., Marru, S., Christie, M., Ellett, K., Pierce, M. and Middleton, R., 2018, July. A New Science Gateway to Provide Decision Support on Carbon Capture and Storage Technologies. In *Proceedings of the Practice and Experience on Advanced Research Computing* (p. 76). ACM.
2. Wilson, N.M., Marru, S., Abeysinghe, E., Christie, M.A., Maher, G.D., Updegrove, A.R., Pierce, M. and Marsden, A.L., 2018, July. Using a Science Gateway to Deliver SimVascular Software as a Service for Classroom Instruction. In *Proceedings of the Practice and Experience on Advanced Research Computing* (p. 102). ACM.
3. Pierce, M., Marru, S., Abeysinghe, E., Pamidighantam, S., Christie, M. and Wannipurage, D., 2018, July. Supporting Science Gateways Using Apache Airavata and SciGaP Services. In *Proceedings of the Practice and Experience on Advanced Research Computing* (p. 99). ACM.
4. Wang, Z., Christie, M.A., Abeysinghe, E., Chu, T., Marru, S., Pierce, M. and Danko, C.G., 2018, July. Building a Science Gateway For Processing and Modeling Sequencing Data Via Apache Airavata. In *Proceedings of the Practice and Experience on Advanced Research Computing* (p. 39). ACM.
5. Phulwani, H., Thapa, M., Marru, S., Pierce, M., Pamidighantam, S. and Christie, M., 2018, July. Apache Airavata Resource Allocation System: A Tool for Allocating Resources in Science Gateways. In *Proceedings of the Practice and Experience on Advanced Research Computing*(p. 78). ACM.
6. Abeysinghe, E., Brylinski, M., Christie, M., Marru, S. and Pierce, M., 2018, July. The CSBG-LSU Gateway: Web based Hosted Gateway for Computational System Biology Application Tools from Louisiana State University. In *Proceedings of the Practice and Experience on Advanced*

Research Computing (p. 100). ACM.
7. Pierce, M.E., Miller, M.A., Brookes, E.H., Wong, M., Afgan, E., Liu, Y., Gesing, S., Dahan, M., Marru, S. and Walker, T., 2018. Towards a Science Gateway Reference Architecture.
8. Adithela, S.P., Christie, M., Marru, S. and Pierce, M., 2018, July. Django Content Management System Evaluation and Integration with Apache Airavata. In *Proceedings of the Practice and Experience on Advanced Research Computing*(p. 86). ACM.
9. Madison, J.D., Abeysinghe, E., Pamidighantam, S., Marru, S., Christie, M., Jennewein, D.M. and Pierce, M., 2018, July. Science Gateway Implementation at the University of South Dakota: Applications in Research and Education. In *Proceedings of the Practice and Experience on Advanced Research Computing* (p. 97). ACM.
10. Christie, M.A., Bhandar, A., Nakandala, S., Marru, S., Abeysinghe, E., Pamidighantam, S. and Pierce, M.E., 2017. Using Keycloak for Gateway Authentication and Authorization.
11. Sunkara, S.S., Langin, C., Pierce, M., Abeysinghe, E., Pamidighantam, S. and Marru, S., 2018, July. Simplifying Access to Campus Resources at Southern Illinois University with a Science Gateway. In *Proceedings of the Practice and Experience on Advanced Research Computing* (p. 98). ACM.
12. Smith, C.W., Abeysinghe, E., Marru, S. and Jansen, K.E., 2018, July. PHASTA Science Gateway for High Performance Computational Fluid Dynamics. In *Proceedings of the Practice and Experience on Advanced Research Computing* (p. 94). ACM.
13. Levi, K., Rynge, M., Abeysinghe, E. and Edwards, R.A., 2018, July. Searching the Sequence Read Archive using Jetstream and Wrangler. In *Proceedings of the Practice and Experience on Advanced Research Computing* (p. 50). ACM.
14. Gleeson, P., Cantarelli, M., Marin, B., Quintana, A., Earnshaw, M., Piasini, E., Birgiolas, J., Cannon, R.C., Cayco-Gajic, N.A., Crook, S. and Davison, A.P., 2018. Open Source Brain: a collaborative resource for visualizing, analyzing, simulating and developing standardized models of neurons and circuits. *bioRxiv*, p.229484.
15. Sivagnanam, S., Yoshimoto, K., Carnevale, N.T. and Majumdar, A., 2018, July. The Neuroscience Gateway: Enabling Large Scale Modeling and Data Processing in Neuroscience. In *Proceedings of the Practice and Experience on Advanced Research Computing* (p. 52). ACM.
16. Williams, T.L., Gorbet, G.E. and Demeler, B., 2018. Multi-speed sedimentation velocity simulations with UltraScan-III. *European Biophysics Journal*, pp.1-9.
17. Kariyattin, S., Marru, S. and Pierce, M., 2018, July. Evaluating NextCloud as a File Storage for Apache Airavata. In *Proceedings of the Practice and Experience on Advanced Research Computing* (p. 87). ACM.
18. Gorbet, G.E., Mohapatra, S. and Demeler, B., 2018. Multi-speed sedimentation velocity implementation in UltraScan-III. *European Biophysics Journal*, pp.1-11.
19. Kim, H., Brookes, E., Cao, W. and Demeler, B., 2018. Two-dimensional grid optimization for sedimentation velocity analysis in the analytical ultracentrifuge. *European Biophysics Journal*, pp.1-8.

SciGaP-Supported Scientific Publications: 2018

These are scientific (rather than Cyberinfrastructure) publications and posters that were enabled by the SciGaP project. It is out of scope for our metric reporting, but it would be interesting to measure the impacts of these enabled publications.

UltraScan Enabled Publications: 2018

Total: 12

CIPRES-Enabled Science Publications, Year 5

Total (including In-Press): 852 (2018) with an additional 232 publications for Sept 30, 2017-December 31, 2017.

A complete list can be found here: http://www.phylo.org/index.php/portal/enabled_publications.

NSG-Enabled Science Publications, Year 5

Total: 20 publications from Sept 2017 till September, 2018

A complete list is available from http://www.nsgportal.org/citation.html.

SEAGrid-Enabled Publications, Year 5

Total: 18

A complete list is available from https://seagrid.org/pages/publications.

SciGaP-Enabled XSEDE Allocations

XSEDE science gateways use community allocations obtained by the PI. CIPRES and SEAGrid encourage power users who will use significant allocation time to obtain personal allocations that can be used through the gateway. These personal allocations are included in the listing below. We report total allocations across all resources. Note this does not include other resources that the gateway accesses, such as campus resources.

Allocation	**Allocation Size (SU)**	**Comments**
SciGaP	200,000	Startup renewal/development award
UltraScan	425,000 275,600	XRAC award (2017) TACC award (2017)
NSG	9,582,277	XRAC award (2018) for Comet, Stampede2, Bridges, Jetstream
CIPRES	22,204,151	XRAC award (2018)
Evolution of Photosynthesis and the Nitrogen Cycle	50,000	CIPRES allocation for Lewis Ward, Harvard University
Phylogenetics of various marine invertebrate clades using targeted exon-capture	2,500	CIPRES allocation for Greg Rouse, UC San Diego

GenApp Framework Development and Support for Produced Science Gateways	751,125	GenApp and Airavata based gateways to support the NSF-funded CCP-SAS gateway. PI: Emre Brookes (UTHSCSA)
The Science and Engineering Grid (SEAGrid) Gateway: Sudhakar Pamidighantam	6,391,001	XRAC Allocation (2017)
Prashant Jain, UIUC TG-CHE160056 (Chemistry)	204,625	SEAGrid User's XSEDE Allocation
Dana Brunson, Oklahoma State U, TG-CCR090027	50,000	Campus Champion Allocation; OSU SEAGrid Users charge to this allocation
Alison Marsden, Stanford, TG-CDA170009	150,000	Educational allocation for SimVascular gateway
Charles Danko, Cornell, TG-BIO160048,	28,776	dREG Science Gateway
Michael Cianfranco, University of Michigan, TG-MCB170058	127,400	COSMIC2 Gateway (using CIPRES/NSG Workbench Framework)
Meghna Babbar-Sebens, TG-ENG170037	100,000	InterACTWEL science gateway using Apache Airavata
Robert Edwards, TG-BIO170108	750,000	Searching the SRA science gateway built with Apache Airavata
Barry Schnieder, TG-PHY180023	57,202	Gateway to support atomic physics software as a service, being built with Apache Airavata
Chen Zhu, TG-EAR180013	50,000	NextGen Thermodynamics Database Gateway
Yinzhi (Ian) Wang, TG-GEO180001	93,500	SimCCS Gateway for US-China bilateral carbon capture and storage

		infrastructure design
Suresh Marru, Marlon Pierce TG-CCR180043	800,000	Science Gateway Architecture Course at IU
Kristina Plazonic TG-TRA180026	364,100	The science gateway is https://gemr.scigap.org/ with SciGaP to use her personal allocation in the future.
Cameron Smith TG-CTS170006	75,107	PHASTA gateway
Yaqun Wang, TG-BIO170061	101,000	Longitudinal GWAS gateway
Doug Jennewein TG-TRA150003	50, 000	USD Campus gateway uses comet for computations

Grants Awarded to Collaborating Gateway Providers

The following list awards with start dates between 9/1/2017 to 9/1/2018. Award amounts are total for the award and not the awarded amount to date.

Awardee	**Award #**	**Amount**	**Comment**
Amit Majumdar (Co-PI, SDSC) with Gert Cauwenberghs (PI, UCSD), Emre Neftci (Co-PI, UCI), Subhashini Sivagnanam (Senior Personnel, SDSC)	NSF #1823366	$1,500,000	NSF CRI award to build a neuromorphic computing resource for the CISE community and provide access via NSG NSF abstract: https://www.nsf.gov/awardsearch/showAward?AWD_ID=1823366 8/1/18 - 07/31/21
Marlon Pierce (PI), Suresh Marru (Co-PI)	NSF #1827641	$200,000	NSF Partnerships for Innovation award, will industry collaborators and sustainability consultants; https://www.nsf.gov/awardsearch/showAward?AWD_ID=18276

			41
Marlon Pierce (PI), Suresh Marru (Co-PI), Jim Basney (NCSA, Co-PI), Enis Afgan (Johns Hopkins, Co-PI)	NSF #1840003	$997,672	NSF CICI award to extract and expand Apache Airavata security capabilities developed as part of SciGaP project as a standalone service/software. https://www.nsf.gov/awardsearch/showAward?AWD_ID=1840003
Robert Quick (PI), Marlon Pierce (Co-PI)	NSF #1839013	$300,000	Expands and operates a digital object architecture testbed that will be applied to science gateway data management and publication scenarios.
Google Summer of Code Students	NA	$22,000	Google pays $5,500 directly to mentored students. 4 total students were supported in GSOC 2018. See https://summerofcode.withgoogle.com/.
Borries Demeler	John R. Evans Leaders Fund, Canada Foundation for Infrastructure	$320,000	This grant funds the purchase of a Beckman Optima AUC instrument
Borries Demeler	Research Chairs Canada: Canada 150 Research Chair for Biophysics	$2,450,000	A 7 year endowed research position at the University of Lethbridge, Alberta
Borries Demeler	Alberta Research Capacity Program	$320,000	Matching funds for the purchase of an

			Optima AUC instrument
Mark Miller (PI)	NIH #1R01GM126463-01	$1,859,498	Expansion of CIPRES to support NIH research community. https://projectreporter.nih.gov/project_info_description.cfm?aid=9427252&icde=41217846
Mark Miller (PI)	NSF #1759844	$1,011,916	Sustainable ABI funding for the CIPRES science gateway. https://www.nsf.gov/awardsearch/showAward?AWD_ID=1759844
Yao Liang (PI) Sudhakar Pamidighantam (CoPI) Fengguang Song (Co-PI) plus linked collaborators	NSF #1835817	$1,076,859	Newly awarded CyberWater linked collaborative project will include a gateway for accessing data and software. https://www.nsf.gov/awardsearch/showAward?AWD_ID=1835817
Michael Cianfranco	NSF #1759826	$590,739	NSF ABI award to support the COSMIC2 CryoEM science gateway, based on the CIPRES Workbench Framework

Other Meritorious Activities

These include promotions, awards, recognition, etc given to team members and collaborators.

- HPC Wire 'Best Use of AI' Award November 2017 - NSG and SUNY Downstate

Operational Metrics

Gateways Using SciGaP Services: Number of Users:

The table below lists gateways using SciGaP services as well as numbers of users for the period 15 September 2017 to 15 September 2018. Gateways with no users (particularly InterACTWEL, NextGen Thermodynamics DB, and GEMR) are under development.

Gateway	**Gateway URL**	**# of Users**
UltraScan	http://ultrascan.aucsolutions.com/	387
CIPRES	www.phylo.org	12,988
NSG	https://www.nsgportal.org/	745
SEAGrid	https://seagrid.org/	966
PGA	https://testdrive.airavata.org/	136
Cornell dREG Gateway	https://dreg.dnasequence.org/	55
Phasta Gateway	https://phasta.scigap.org/	14
Computational Systems Biology Group LSU	https://sciencegateway.brylinski.org/	6
IGS Gateway	https://simccs.org/	13
SimVascular Gateway	https://gateway.simvascular.org/	40
IU Nano Confinement Gateway	https://nanoconfinement.sciencegateways.iu.edu/	76
Searching-SRA Gateway	https://www.searchsra.org/	28
Longitudinal GWAS gateway	http://js-156-155.jetstream-cloud.org/	6
NextGen ThermoDynamics DB Gateway	https://nexttdb.sciencegateway.scigap.org/	4

InterACTWEL Gateway	http://interactwel.scigap.org/	8
AMP Gateway	http://ampgateway.scigap.org/	3
R-HPC Gateway	http://r-hpc.scigap.org/	3
Prostate Cancer Prediction Gateway	https://gemr.scigap.org/	3
University of South Dakota Gateway	https://sciencegateway.usd.edu/	14
Indiana University Gateway	https://cybergateway.iu.edu/	28
University of Kentucky Science Gateway	https://hpcgateway.uky.edu/	8
Oklahoma University	https://sciencegateway.oscer.ou.edu/	8
Georgia State University	https://hpcgateway.gsu.edu/	21
University of Southern Illinois	https://sciencegateway.siu.edu/	17
University of Alabama Birmingham	https://torana.rc.uab.edu/	9
New Mexico State University	https://sciencegateway.nmsu.edu/	11
Virginia ACCORD Gateway	https://accord.hpc.virginia.edu/	8
West Virginia State University	https://sciencegateway.wvstateu.edu/	4
NCSA Industry Gateway	http://ncsaindustry.scigap.org/	8

Number of Computational Experiments

The follows totals are for the period September 15, 2017-September 14, 2018

Gateway	**# of Experiments**

UltraScan	1,345,526
CIPRES	319,371
NSG	63,536
SEAGrid	19498
All others	2735

Resources Used

Gateway	**Resources**
UltraScan	Alamo (UTHSCSA), Comet (SDSC), Jureca (Juelich), Juwel (Juelich), Stampede2 (XSEDE), Lonestar5 (TACC), Jetstream (TACC, IU), Taito (University of Helsinki, Finland)
SEAGrid	Karst (IU), Big Red 2 (IU), Comet, Stampede, Stampede2, Bridges, Jetstream
NSG	Comet (regular nodes and GPU nodes) , Stampede2 (KNL and Skylake nodes), Bridges, Jetstream
CIPRES	Comet, Comet GPU, TSCC
PGA	Comet, Jetstream, Stampede, Stampede2, BigRed2 (IU), Karst (IU)
Cornell dREG Gateway	Comet, Bridges
Phasta Gateway	Stampede, Stampede2
Computational Systems Biology Group LSU	SuperMIC (LSU)
IGS Gateway	BigRed2 (IU), Karst (IU)
SimVascular Gateway	Comet
IU Nano Confinement Gateway	BigRed2 (IU), Comet
Searching-SRA Gateway	Jetstream
South Dakota Gateway	Comet, HPC (USD), Lawrence (USD)

Indiana University Gateway	BigRed2 (IU), Karst (IU), Jetstream, Carbonate (IU)
Longitudinal GWAS	Jetstream
Oklahoma University	Schooner
NextGen ThermoDynamics DB Gateway	BigRed2 (IU), Karst (IU)
InterACTWEL Gateway	Jetstream
AMP Gateway	Comet
Prostate Cancer Prediction Gateway	Comet
University of Kentucky Science Gateway	DLX2/3 (UK)
Georgia State University	HPC (GSU)
University of Southern Illinois	BigDog (SIU), LittleDog (SIU), BigDawg (SIU)
University of Alabama Birmingham	Cheaha (UAB)
New Mexico State University	Joker (NMSU)
West Virginia State University	Stinger (WVSU)
NCSA Industry Gateway	IForge (NCSA)

Airavata Jira Tickets

JIRA Tickets between 15 September 2017 - 14 September 2018.

Type	**Created**	**Closed**
All	361	184
Bugs	177	107
Improvements	31	12
New Features	31	14

Epic/Story/Task/Subtask	119	49
Other	3	2

New Committers and Project Management Committee Members

Committers are contributors who have been granted full access to the Airavata code base. PMC members are committers of merit who have been granted full (binding) voting writes in the project. The following additions were made between September 2017 and September 2018

1. Committers: Eldho Mathulla, Sneha Tilak, Stephen Paul Adithela, Sachin Kariyattin
2. PMC Members: Marcus Christie, Dimuthu Wannipurage

Number of Downloads of Airavata Software

This information is available from https://repository.apache.org/index.html (login required, Apache ID required, more information available on request). During the period of September 2017-September 2018, Airavata software had over 2200 IP-unique downloads of all software artifacts.

Additional available statistics:

- All public Airavata mailing lists: http://airavata.markmail.org/
- Airavata Developer mailing list: http://airavata.markmail.org/search/?q=#query:%20list%3Aorg.apache.incubator.airavata-dev+page:1+state:facets
- Apache Airavata GitHub mirrors:
    - https://github.com/apache/airavata
    - https://github.com/apache/airavata-php-gateway