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Summary

The following table summarizes our team-wide efforts. Details are in separate sections below. Note figures are for the current 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)	
Supported Allocations (#, SU)	7 awards, 16,990,000.00 SU	9 awards, 19,134,890 SU	19 awards, 27,861,384 SU (includes both gateway community and power user accounts)	15 awards, 45,183,642 SU	
Collaborating Grants (#, \$) awarded in project year	1 Grant, \$263,000	4 Grants, > \$2M	7 Grants, > \$10.3 M	9 Grants, > \$8M	

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	
Number of Users Supported	4205	7451	9351	11339	
Number of Experiments (Jobs Executed)	129,242	212,933	300,522	355,984	
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.	
Jira Tickets Created/Closed	515/288	370/148	272/151	413/254	

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	
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Science Metrics

Number of Publications Enabled: 2017 to Date

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 for 2017: 5 (Year to Date)
- SciGaP Supported Science Publications for 2017: 790 (Year to Date)

Details are below.

Team Publications

Since the project began, team-authored publications on SciGaP cyberinfrastructure supported by this award have been cited 191 times (Google Scholar). Seven of these citations have been cited at least seven times, and five have been cited more than 12 times (Google Scholar).

Team publications for Project Year 4 are below.

1. Nakandala, Supun, Hasini Gunasinghe, Suresh Marru, and Marlon Pierce. "Apache Airavata security manager: Authentication and authorization implementations for a multi-tenant escience framework." In e-Science (e-Science), 2016 IEEE 12th International Conference on, pp. 287-292. IEEE, 2016.
2. Smith, Cameron W., and Eroma Abeysinghe. "The PHASTA Science Gateway: Web-based Execution of Adaptive Computational Fluid Dynamics Simulations." In Proceedings of the Practice and Experience in Advanced Research Computing 2017 on Sustainability, Success and Impact, p. 70. ACM, 2017.
3. Nakandala, Supun, Suresh Marru, Marlon Piece, Sudhakar Pamidighantam, Kenneth Yoshimoto, Terri Schwartz, Subhashini Sivagnanam, Amit Majumdar, and Mark A. Miller. "Apache Airavata Sharing Service: A Tool for Enabling User Collaboration in Science Gateways." In Proceedings of the Practice and Experience in Advanced Research Computing 2017 on Sustainability, Success and Impact, p. 20. ACM, 2017.
4. Gesing, Sandra, Rion Dooley, Marlon Pierce, Jens Krüger, Richard Grunzke, Sonja Herres-Pawlis, and Alexander Hoffmann. "Gathering requirements for advancing simulations in HPC infrastructures via science gateways." Future Generation Computer

Systems (2017).

5. Dura-Bernal S, Neymotin S.A., Kerr C.C., Sivagnanam S., Majumdar A., Francis J.T., Lytton W.W., "Evolutionary algorithm optimization of biological parameters in a biomimetic neuroprosthesis," IBM Journal of Research and Development, Vol. 61; Issue 2/3, March-May, 2017.

SciGaP-Supported Scientific Publications: 2017

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: 2017

Total: 29

1. G Plascencia-Villa, B Demeler, RL Whetten, WP Griffith, M Alvarez, DM Black, and M José-Yacamán. Analytical Characterization of Size-Dependent Properties of Larger Aqueous Gold Nanoclusters J. Phys. Chem. C, DOI: 10.1021/acs.jpcc.6b00448
2. Karabudak E, Brookes E, Lesnyak V, Gaponik N, Eychmüller A, Walter J, Segets D, Peukert W, Wohlleben W, Demeler B, H Cölfen. Simultaneous Identification of Spectral Properties and Sizes of multiple Particles in Solution with sub-nm Size Resolution. Angewandte Chemie 2016 Jul 27. doi: 10.1002/anie.201603844.
3. Wong SJ, Gearhart MD, Taylor AB, Nanyes DR, Ha DJ, Robinson AK, Artigas JA, Lee OJ, Demeler B, Hart PJ, Bardwell VJ, and CA Kim. KDM2B recruitment of the Polycomb group complex, PRC1.1, requires cooperation between PCGF1 and BCORL1. Structure, 2016 Aug 23. pii: S0969-2126(16)30222-2. doi: 10.1016/j.str.2016.07.011.
4. Bhattacharya A, Wang Z, White T, Buffone C, Nguyen L, Shepard C, Kim B, Demeler B, Diaz-Griffero F, and D Ivanov. Effects of T592 phosphomimetic mutations on tetramer stability and dNTPase activity of SAMHD1 can not explain the retroviral restriction defect. Sci Rep. 2016 Aug 11;6:31353. doi: 10.1038/srep31353.
5. Alvarez MM, Chen J, Plascencia-Villa G, Black DM, Griffith WP, Garzon IL, José-Yacamán M, Demeler B, Whetten RL. Hidden Components in Aqueous Gold-144 Fractionated by PAGE: High-Resolution Orbitrap ESI-MS Identifies the Gold-102 and Higher All-Aromatic Au-pMBA Cluster Compounds. J Phys Chem B. 2016 Jun 8. PMID: 27275518
6. G Plascencia-Villa, B Demeler, RL Whetten, WP Griffith, M Alvarez, DM Black, and M José-Yacamán. Analytical Characterization of Size-Dependent Properties of Larger Aqueous Gold Nanoclusters J. Phys. Chem. C, DOI: 10.1021/acs.jpcc.6b00448
7. Demeler B., and G. Gorbet. Analytical Ultracentrifugation Data Analysis with UltraScan-III. Ch. 8, In Analytical Ultracentrifugation: Instrumentation, Software, and Applications. Eds: Uchiyama S., Stafford W. F. and T. Laue. Springer, 119-143 (2016)
8. Villarreal OD, LY Chen, RL Whetten, B. Demeler. Aspheric Solute Ions Modulate Gold Nanoparticle Interactions in an Aqueous Solution: An Optimal Way to Reversibly Concentrate Functionalized Nanoparticles. J. Phys. Chem. B 11/2015;

DOI:10.1021/acs.jpcc.5b09864

9. Boswell-Casteel RC, Johnson JM, Duggan KD, Tsutsui Y, Hays FA. Overproduction and biophysical characterization of human HSP70 proteins. (2015-02-01 Epub: 2014-09-27) *Protein Expr Purif* 106:57-65
10. Urbauer JL, Cowley AB, Broussard HP, Niedermaier HT, Bieber Urbauer RJ. Solution structure and properties of AlgH from *Pseudomonas aeruginosa*. (2015-06-01 Epub: 2015-04-29) *Proteins* 83:1137-50
11. Tsutsui Y, Johnson JM, Demeler B, Kinter MT, Hays FA. Conformation-Dependent Human p52Shc Phosphorylation by Human c-Src. (2015-06-09 Epub: 2015-05-26) *Biochemistry* 54:3469-82
12. Yudina Z, Roa A, Johnson R, Biris N, de Souza Aranha Vieira DA, Tshiperson V, Reszka N, Taylor AB, Hart PJ, Demeler B, Diaz-Griffero F, Ivanov DN. RING Dimerization Links Higher-Order Assembly of TRIM5 α to Synthesis of K63-Linked Polyubiquitin. (2015-08-04 Epub: 2015-07-23) *Cell Rep* 12:788-97
13. Zhang S, Hinck AP, Fitzpatrick PF. The Amino Acid Specificity for Activation of Phenylalanine Hydroxylase Matches the Specificity for Stabilization of Regulatory Domain Dimers. (2015-08-25 Epub: 2015-08-13) *Biochemistry* 54:5167-74
14. Ranaivoson FM, Liu Q, Martini F, Bergami F, von Daake S, Li S, Lee D, Demeler B, Hendrickson WA, Comoletti D. Structural and Mechanistic Insights into the Latrophilin3-FLRT3 Complex that Mediates Glutamatergic Synapse Development. (2015-09-01 Epub: 2015-07-30) *Structure* 23:1665-77
15. AbdulHalim LG, Bootharaju MS, Tang Q, Del Gobbo S, AbdulHalim RG, Eddaoudi M, Jiang DE, Bakr OM. Ag₂₉(BDT)₁₂(TPP)₄: A Tetravalent Nanocluster. (2015-09-23 Epub: 2015-07-07) *J Am Chem Soc* 137:11970-5
16. Aly SM, AbdulHalim LG, Besong TM, Soldan G, Bakr OM, Mohammed OF. Ultrafast static and diffusion-controlled electron transfer at Ag₂₉ nanocluster/molecular acceptor interfaces. (2015-11-09 Epub: 2015-11-09) *Nanoscale*
17. Klein BJ, Muthurajan UM, Lalonde ME, Gibson MD, Andrews FH, Hepler M, Machida S, Yan K, Kurumizaka H, Poirier MG, Côté J, Luger K, Kutateladze TG. Bivalent interaction of the PZP domain of BRPF1 with the nucleosome impacts chromatin dynamics and acetylation. (2015-11-30 Epub: 2015-11-30) *Nucleic Acids Res.*
18. Villarreal OD, Chen LY, Whetten RL, Demeler B. Aspheric Solute Ions Modulate Gold Nanoparticle Interactions in an Aqueous Solution: An Optimal Way To Reversibly Concentrate Functionalized Nanoparticles. (2015-12-17 Epub: 2015-12-03) *J Phys Chem B* 119:15502-8
19. Wang W, Damm C, Walter J, Nacken TJ, Peukert W. Photobleaching and stabilization of carbon nanodots produced by solvothermal synthesis. (2016-01-07 Epub: 2015-11-30) *Phys Chem Chem Phys* 18:466-7
20. Ballandras-Colas A, Brown M, Cook NJ, Dewdney TG, Demeler B, Cherepanov P, Lyumkis D, Engelman AN. Cryo-EM reveals a novel octameric integrase structure for betaretroviral intasome function. (2016-02-18 Epub: 0000-00-00) *Nature* 530:358-61
21. Rubio-Marrero EN, Vincelli G, Jeffries CM, Shaikh TR, Pakos IS, Ranaivoson FM, von Daake S, Demeler B, De Jaco A, Perkins G, Ellisman MH, Trehwella J, Comoletti D.

Structural Characterization of the Extracellular Domain of CASPR2 and Insights into Its Association with the Novel Ligand Contactin1. (2016-03-11 Epub: 2015-12-31) *J Biol Chem* 291:5788-802

22. Cockburn, Darrell W., Nicole I. Orlovsky, Matthew H. Foley, Kurt J. Kwiatkowski, Constance M. Bahr, Mallory Maynard, Borries Demeler, and Nicole M. Koropatkin. "Molecular details of a starch utilization pathway in the human gut symbiont *Eubacterium rectale*." *Molecular microbiology* 95, no. 2 (2015): 209-230.
23. Tsutsui, Yuko, Jennifer M. Johnson, Borries Demeler, Michael Kinter, and Franklin Alan Hays. "Conformation-Dependent Human p52Shc Phosphorylation by Human c-Src." *Biochemistry* (2015).
24. Ranaivoson, Fanomezana M., Qun Liu, Francesca Martini, Francesco Bergami, Sventja von Daake, Sheng Li, David Lee, Borries Demeler, Wayne A. Hendrickson, and Davide Comoletti. "Structural and Mechanistic Insights into the Latrophilin3-FLRT3 Complex that Mediates Glutamatergic Synapse Development." *Structure* 23, no. 9 (2015): 1665-1677.
25. Gorbet, Gary E., Joseph Z. Pearson, Aysha K. Demeler, Helmut Cölfen, and Borries Demeler. "Next-Generation AUC: Analysis of Multiwavelength Analytical Ultracentrifugation Data." *Methods in Enzymology* (2015).
26. Ivanov, Dmitri, Zinaida Yudina, Rory Johnson, Nikolaos Biris, Alexander Taylor, P. Hart, and Borries Demeler. "The Role of RING Dimerization in the E3 Ubiquitin Ligase Activity of the TRIM5 α Retroviral Restriction Factor." *The FASEB Journal* 29, no. 1 Supplement (2015): 888-9.
27. Kim, Haram, Emre H. Brookes, and Borries Demeler. "A performance predictor for UltraScan supercomputer calculations." In *Proceedings of the 2015 XSEDE Conference: Scientific Advancements Enabled by Enhanced Cyberinfrastructure*, p. 42. ACM, 2015.
28. Pearson, Joseph, Frank Krause, Dirk Haffke, Borries Demeler, Kristian Schilling, and Helmut Cölfen. "Next-Generation AUC Adds a Spectral Dimension: Development of Multiwavelength Detectors for the Analytical Ultracentrifuge." *Methods in Enzymology* (2015).
29. Yudina, Zinaida, Amanda Roa, Rory Johnson, Nikolaos Biris, Daniel A. de Souza Aranha Vieira, Vladislav Tshiperson, Natalia Reszka et al. "RING Dimerization Links Higher-Order Assembly of TRIM5 α to Synthesis of K63-Linked Polyubiquitin." *Cell reports* 12, no. 5 (2015): 788-797.

CIPRES-Enabled Science Publications 2017

Total (including In-Press): 726 (2017). 928 publications in 2016.

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

NSG-Enabled Science Publications 2017

Total: 20 publications

A complete lists is available from <http://www.nsgportal.org/citation.html>.

SEAGrid-Enabled Publications 2017

Total: 15

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

SciGaP-Enabled XSEDE and Related 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. Stampede2 allocations are awarded in nodes rather than cores, so we have multiplied Stampede2 SUs by 31.25 to normalize. Note this does not include other other resources that the gateway accesses.

Allocation	Allocation Size (SU)	Comments
SciGaP	200,000	Startup renewal/development award
UltraScan	398,750	XRAC award (2016)
NSG	9,040,452.5	XRAC award (2017)
CIPRES	25,014,286	XRAC award (2017)
VertLife Terrestrial: A complete, global assembly of phylogenetic, trait, spatial and environment characteristics for a model clade	8,000	CIPRES allocation for Project PI Nathan S Upham
Evolutionary relationships between sturgeon nucleocytoplasmic large DNA viruses (sNCLDVs) and members of the proposed Megavirales order	18,650	CIPRES Allocation for Project PI: Rachel Breyta.
Parallel Unstructured Mesh Infrastructure: Mark Shephard (RPI), Cameron Smith (RPI)	424,383	PHASTA gateway, https://phasta.scigap.org
Computational support for small angle scattering for advanced analyses of	817656	GenApp and Airavata based gateways to support the NSF-funded CCP-SAS

structural data in chemical biology and soft condensed matter: Emre Brookes (UTHSCSA)		gateway.
The Science and Engineering Grid (SEAGrid) Gateway: Sudhakar Pamidighantam	8,503,580.5	XRAC Allocation (2017)
Prashant Jain, UIUC TG-CHE160056 (Chemistry)	351129	SEAGrid User's XSEDE Allocation
Iwona Jasiuk, UIUC TG-DMR170049 (Mechanical and Structural Systems)	150,000	SEAGrid User's XSEDE Allocation
Zhen Guan, UC Irvine TG-DMR150113	190,125	XSEDE ECSS Collaboration
Dana Brunson, Oklahoma State U, TG-CCR090027	50000	Campus Champion Allocation; OSU SEAGrid Users charge to this allocation
Alison Marsden, Stanford, TG-CDA170009	150,000	Educational allocation for SimVascular gateway
Vikram Jadhao, Indiana University, TG-DMR170089	50,000	Startup allocation to support new NSF NCN award; Geoffrey Fox, PI
Charles Danko, Cornell, TG-BIO160048,	109,957	dREG Science Gateway
Benjamin Winjum, UCLA, TG-PHY170029	100,000	PICKSC Science Gateway
Mark Perri, Sonoma State, TG-CDA170003	200,000	ChemCompute Gateway
Michael Cianfranco, University of Michigan, TG-MCB170058	76400	COSMIC2 Gateway (using CIPRES/NSG Workbench Framework)

Grants Awarded to Gateway Users and Collaborators

The following list awards with start dates between 9/1/2016 to 9/1/2017. Award amounts are total for the award and not the awarded amount to date.

Awardee	Award #	Amount	Comment
Amit Majumdar PI, SDSC, with PIs Scott Makeig (lead) and Arnaud Delorme, UCSD; Subhashini Sivagnanam Senior Personnel, UCSD	NIH 1R01EB023297-01A 1	\$2,400,000	New NIH award in August 2017 https://projectreporter.nih.gov/project_info_description.cfm?aid=9384412&icde=35945345 9/1/17 - 06/30/21
Amit Majumdar, Co-PI SDSC; Satish Nair lead PI U. Missouri; other Co-PIs Prasad Calyam, David Bergin; Subhashini Sivagnanam Senior Personnel, UCSD	NSF CyberTraining award	\$494,651	https://nsf.gov/awardsearch/showAward?AWD_ID=1730655&HistoricalAwards=false 9/1/17- 8/31/20
Google Summer of Code Students	NA	\$11,000	Google pays \$5,500 directly to mentored students. 2 total students were supported in GSOC 2016. See https://summerofcode.withgoogle.com/ .
Borries Demeler	Voelcker Biomedical Research Academy	\$5,000/year	The VBRA funded two new high school students to work for 3 summers in Dr. Demeler's laboratory to learn about biophysics and hydrodynamics
Borries Demeler	Fulbright Organization	\$50,000 (approx)	3 year Fulbright Specialist Grant. Funds travel to foreign countries to promote UltraScan

			and collaborate on AUC Science projects. Grant covers travel expenses and does not have a specific amount.
Borries Demeler	Erskine Endowment	\$50,000 (approx)	Travel Grant for visiting professorship at the University of Canterbury, New Zealand. Visiting Professor to teach biophysics to undergraduate students and present UltraScan workshops. Award covers travel expenses and is not a specific amount.
Borries Demeler	Beckman Coulter: New Optima AUC Instrument	\$500,000	Beckman installed a new Optima AUC in Dr. Demeler's laboratory to advance UltraScan integration for the latest instrumentation.
Emre Brookes	NSF SSE Award for GenApp	\$500,000	NSF SSE award; GenApp integration with Apache Airavata is a deliverable
Geoffrey Fox	NSF Award #1720625 Network for Computational Nanotechnology - Engineered nanoBIO Node	\$4,000,0000	Suresh Marru, Sudhakar Pamidighantam, and Marlon Pierce are Senior Personnel

Other Meritorious Activities

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

- IU PTI Science Gateways Research Center: Marlon Pierce has been promoted to be the director of the newly created Science Gateways Research Center, part of the Pervasive Technology Institute. Co-PI Suresh Marru is promoted to be the deputy director of the Science Gateways Research Center at Indiana University.
- Dr. Borries Demeler promoted to full professor with tenure.

Operational Metrics

Gateways Using SciGaP Services

SciGaP services are hosted on IU's Quarry Gateway Hosting Service (<https://portal.xsede.org/iu-quarry>). This list includes only the Gateways using or developing with one or more SciGaP services and does not include gateways using Airavata software elsewhere.

1. UltraScan
2. Neuroscience Gateway
3. CIPRES
4. PGA: <http://test-drive.airavata.org>. This hosts the PHASTA code gateway as well as several demonstration applications.
5. PHASTA: this is an XSEDE ECSS project to support finite element simulations and uses the PGA. Cameron Smith at RPI is the contact.
6. SEAGrid Science Gateway is revamped from GridChem infrastructure to use Airavata based services: <https://seagrid.org>
7. University of South Dakota: <https://cybergateway.usd.edu/>
8. University of Oklahoma Cybergateway: <http://oscer.scigap.org/>

The PGA is a reference implementation in PHP of the Airavata API that is used for tutorials and interested gateways are encouraged to reuse. We run a persistent version at <https://testdrive.airavata.org>.

Number of Users: 15 September 2016 to 15 September 2017

Gateway	# of Users
UltraScan	387
CIPRES	10207
NSG	561
SEAGrid	934
PGA	127
Cornell dREG Gateway	18

Phasta Gateway	8
Computational Systems Biology Group LSU	4
IGS Gateway	7
SimVascular Gateway	18
IU Nano Confinement Gateway	6
IU Nano Shape Gateway	3
South Dakota Gateway	11
Indiana University Gateway	18
University of Utah	7
Oklahoma University	6
Oklahoma Innovation Institute	9
Georgia State University	5
University of Southern Illinois	12
University of Alabama Birmingham	6
New Mexico State University	6
Virginia ACCORD Gateway	6
West Virginia State University	4
PICSC Gateway	6
NCSA Industry Gateway	5

Number of Computational Experiments

The follows totals are for the period September 15, 2016-September 15, 2017

Gateway	# of Experiments
UltraScan	1,345,526
CIPRES	273,627

NSG	22,235
SEAGrid	30,607
All others	2355

Resources Used

Gateway	Resources
UltraScan	Alamo (UTHSCSA), Comet (SDSC), Jureca (Juelich), Lonestar (TACC), Stampede (XSEDE), Lonestar5 (TACC)
SEAGrid	Karst (IU), Big Red 2 (IU), Comet, Stampede, Bridges, Jetstream
NSG	Comet , Stampede, Bridges, Jetstream
CIPRES	Comet, TSCC
PGA	Comet, Jetstream, Stampede, BigRed2 (IU), Karst (IU)
Cornell dREG Gateway	Comet, Bridges
Phasta Gateway	Stampede, Stampede2
Computational Systems Biology Group LSU	SuperMike (LSU)
IGS Gateway	BigRed2 (IU), Karst (IU)
SimVascular Gateway	Comet
IU Nano Confinement Gateway	BigRed2, Comet
IU Nano Shape Gateway	BigRed2 (IU)
South Dakota Gateway	Comet, HPC (USD)
Indiana University Gateway	BigRed2 (IU), Karst (IU), Jetstream
University of Utah	Ember (Utah), Kingspeak (Utah)
Oklahoma University	Schooner
Oklahoma Innovation Institute	Tandy (OII)

Georgia State University	HPC (GSU)
University of Southern Illinois	BigDog (SIU), LittleDog (SIU)
University of Alabama Birmingham	Cheaha (UAB)
New Mexico State University	Comet
Virginia ACCORD Gateway	Pending local resources
West Virginia State University	Stinger (WVSU)
NCSA Industry Gateway	IForge
PICSC Gateway	Comet, Hoffman (UCLA)

Airavata Jira Tickets

JIRA Tickets between 15 September 2016 - 15 September 2017.

Type	Created	Closed
All	414	255
Bugs	289	198
Improvements	28	14
New Features	24	10
Epic/Story/Task/Subtask	70	31
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 2016 and September 2017

1. Committers: Gourav Shenoy, Ajinkya Dhamnaskar, Anuj Bhandar, Marcus Christie.

2. PMC Members: Eroma Abeysinghe

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 2016-September 2017, Airavata had over 3500 downloads.

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>