# Peer comparison of XSEDE and NCAR publication data

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#### **ABSTRACT**

We present a framework that compares the publication impact based on a comprehensive peer analysis conducted by papers produced by scientists using XSEDE and NCAR resources. The analysis is based on a percentile ranking of citations of the papers while comparing them between to peer publication in the same journal not using the resources. This analysis is unique in that it is a comprehensive study involving thousands of published papers while associating them to a comparable peer group based on the journals issues. While analyzing the number of citations we can see that citations of papers that utilize XSEDE and NCAR resources are positive. Hence we find that XSEDE and NCAR reported publications achieve a higher score versus their peers from the same journal issue not using these resources while using our comparative journal peer comparison metric.

## **Categories and Subject Descriptors**

H.4 [Information Systems Applications]: Miscellaneous; D.2.8 [Software Engineering]: Metrics—complexity measures, performance measures

# **General Terms**

Theory, Measurement

## Keywords

Scientific impact, bibliometric, h-index, Technology Audit Service, XDMoD, XSEDE

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### 1. INTRODUCTION

To identify the impact on scientific advancements enabled by enhanced cyberinfrastructure it is important to conduct a comprehensive analysis of achievements that can be attributed to the use of such an advanced infrastructure as provided by XSEDE. Many recent science and engineering innovations and discoveries are increasingly dependent on access to high performance computing resources [13]. The demand for high end resources is met by large-scale compute resources that cannot typically be supported by any single research group. Accordingly, dedicated large-scale computing facilities play an important role in scientific research, in which resources are shared among groups of researchers, while the facilities themselves are managed by dedicated staff. The National Science Foundation and the Department of Energy have supported such facilities for many years. One such facility is the Extreme Science and Discovery Environment (XSEDE) [3, 12]. XSEDE allocates resources to approved projects, which represent a substantial financial investment by NSF. Thus, justification for their use is warranted and questions regarding the scientific impact of these resources naturally arise. In our previous work we have [13] focused on the creation of an framework that collects bibliometric data and analyzes them in regards to a number of metrics. However, this work did not yet include a mechanism to compare them with peers not using such resources.

In this paper we significantly enhance our previous work by comparing publication impact based on a comprehensive peer analysis conducted by papers produced by scientists using XSEDE and National Center for Atmospheric Research (NCAR) resources. The analysis is based on a percentile ranking of citations of the papers while comparing them to peer publications in the same journal not using the resources. This analysis is unique in that it is a comprehensive study involving thousands of published papers while associating them to a comparable peer group based on the journals issues. While analyzing the number of citations we can see that citations of papers that utilize XSEDE and NCAR resources are positive. Hence we find that XSEDE and NCAR reported publications achieve a higher score versus their peers from the same journal issue not using these resources.

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The paper is structured as follows. First we review some portions of our previous work and relate it to the work reported in this paper. Next we introduce a journal based peer metric that allows us to compare any resource providers related publications with non publications not using the resources. To demonstrate general applicability of this method we introduce in the next section a peer analysis of XSEDE and NCAR data. We present important statistics about this metric for both XSEDE and NCAR. Finally, we present our conclusions.

#### 2. RELATED WORK

Although a number of related work has been conducted [11, 5, 7, 6, 4] our work is unique as it provides a *comprehensive* analysis superior in data volume to other studies and is focused on the analysis of XSEDE and NCAR data. More information about related work can be found in [13]. We are happy to engage in collaborate efforts to enhance this work or to integrate other related work by contacting us.

# 3. BIBLIOMETRIC DATA ANALYSIS FRAMEWORK FOR RESOURCE PROVIDERS

The work described in this paper has been motivated by analyzing data related to XSEDE. However, as many other resource providers may have similar needs to analyze their data this framework can be applied is general enough that it could be adapted for utilization by resource providers. In case this is desired, a custom integration can be performed and the analysis can be adapted by the team from Indiana University. Hence, our framework is general enough that it can be applied to other resource providers.

## 3.1 Requirements

The motivation of the framework is focusing on three main objectives. First, we like our framework to be able to compare the impact the use of resources have on the users using them. Second we have to define suitable metrics that allow such a comparison. Third, we need to provide a framework that provides an integrated set of data services that these metrics can be applied upon to conduct a comparative impact analysis. This is depicted in Figure 1 on the left-hand side.

#### 3.2 Design

For XSEDE we have identified specific design criteria that we are integrating into our architecture. Many of these design decisions will overlap with other resource providers. Certainly our design needs to be able to provide a comparative impact study for peers and also the funding agencies of the peers in conjunction with meaningful metrics. The metrics must be not only targeting the resource provider but also the community. Specifically for XSEDE interested parties in this analysis are not only the users, but also the Resource Allocation Committee (RAC) and the XSEDE leadership. The bibliometric data services and the data mashup are largely hidden from these groups. The groups benefit form a number of preconfigured analysis that may be further customized or enhanced. To show generality of this approach we have taken an analysis and applied it not only to XSEDE as a resource provider, but also to National Center for Atmospheric Research (NCAR) as a resource provider [2].

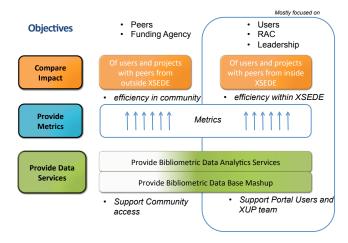


Figure 1: High level Objectives impacting the design of our framework

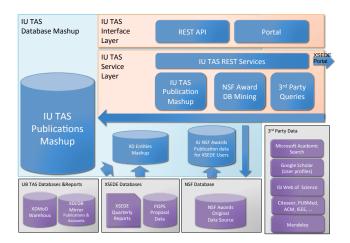


Figure 2: Architecture with the Interface, Service, Database Mashup, and Database Resources Layers

#### 3.3 Architecture

The requirements for XSEDE and our user community have resulted in a layered architecture as depicted in 2. The framework is based on distributed set of services. The service-oriented system consists of components for (a) publication and citation data retrieval (e.g., from NSF award database, Google Scholar, and ISI Web of Science), (b) parsing and processing while correlating data from various databases and services, such as the XSEDE central database (XDcDB), which stores all usage data for jobs run on XSEDE resources, and (c) the Partnerships Online Proposal System (POPS) database (currently been replaced by XSEDE), which stores publication and grant funding information for PI's applying for XSEDE allocations. The system also includes components for metrics generation and an analysis system for different aggregation levels (users, projects, organization, Field of Science), as well as a presentation layer using a lightweight portal in addition to exposing some data via RESTful API. [13]. The main layers include (a) Interface Layer – containing easy to use interfaces for various community, including an API, RST, and a Web GUI interface; (b) Service Layer – containing advanced services to bridge to a data base mashup via sophisticated services and queries to the underlying database layer; (c) Database Mashup Service

Layer – a sophisticated database mashup that contains the integration of data from a variety of data resources; and (d) the Database Resources that provide the underlying information for our service.

Due to this approach our framework is expandable as we are able to not only integrate resources relevant for XSEDE, but also other resource providers such as NCAR. However we need to customize this integration and allow relevant services to be exposed to the framework. In some cases it could be as simple as replacing the database with minor adaption in the service layer.

Our current framework for XSEDE include specialized services and curated focusing on XSEDE user specific publication data as well as, user, project, and Field of Science (FOS) views. The publication mashup component aggregates the publication data mined from the previous component, in addition to those from XDcDB, and from other available external services. It also retrieves citation data for each publication from external services. Another essential task of this framework is to generate metrics for users, projects, and FOS in which the POPS database is involved to get proposal and project data. This data will be stored into the mashup database which can then be integrated into the XDMoD [9] system at our partner site at University of Buffalo.

To conduct the analysis the general workflow includes obtaining the publication data for each XSEDE user, and then retrieving the citation data for each publication. Hence, the data is originally collected per user and per publication basis. As part of processing the data we are aggregating it based on organization, XSEDE project/account, and FOS. By correlating the data (for example the Service Units (SU) awarded by XSEDE) our intention is to identify if the analysis may reveal patterns and trends of how XSEDE can impact the sciences and possibly helps to achieve a better measure of return on investment (ROI) for NSF. Naturally the same is applied to NCAR data as to demonstrate generality of our methods.

# 4. METRIC FOR JOURNAL PUBLICATION-BASED PEER COMPARISON

While we have focused in our previous work more on the internal analysis of data within XSEDE in regards to FOS, h-index [10], g-index [1] and i-index [8], we extend in this work the scope of peer comparison to external peers and hence significantly expand our original analysis. We introduce the definition of a metric that allows us to analyses and compares journal publications amongst peers. To conduct an analysis we have to identify a suitable peer group to compare to, as well as introducing a metric that makes a comparison possible.

Hence we have considered for this work all publications that are uploaded through self identification by users into the XSEDE portal, as well as XSEDE reports. We have than identified from this set all all journal publications and identified from that subset all journals that had at least ten self identified publications from XSEDE. Although the number to meet this threshold is small, we found the restriction useful as it defines a peer group of scientists that publish repeatedly in these journals, thus making the comparison more meaningful. Once we identified such journals, we compared the citation count in each publication located in a

journal issue that had at least one XSEDE publication. Our comparison is between publications in such journals that we identified as XSEDE papers and those that were not.

Next we introduce a ranking metric allowing for a comparative analysis metric for Journal Publication-based Peer Comparison for each journal issue in which we find publications using the a percentile ranking. The percentile ranking is based on the sum of all citations in a paper while at the same time ranking that number in four uniform percentile categories. Thus the papers in the first percentile have the most citations, the ones in the second hev viewer, and so forth. We are summing up the weighted sums of these counts. Thus the performance score is defined as:

$$S = 1 * P_{Q_1} + 0.5 * P_{Q_2} + (-0.5) * P_{Q_3} + (-1) * P_{Q_4}$$

In which,  $P_{Q_i}$  is the percentage of pubs falling into the top i quarter.  $P_{Q_i}$  gets the value in [0,1] and  $\sum_i P_{Q_i} = 1$  for one FOS.

It is trivial to see that S has its value from [-1,1]. A Positive value implies more publications appear on upper half in ranking and negative means more on lower half.

To apply the percentile ranking to the field of science of TG/XD publications among the journal issues where each publication was published, we aggregate them based on Field of Science (FOS), according to the categories defined in XSEDE central database (XDcDB), and calculate the average and median percentile ranking for each field of science, as well as the resulting *performance score*. We include only those with at least ten<sup>1</sup> publications so the results are not statistically meaningless.

To identify the FOS for each publication, we followed this process:

- Find the FoS information out of the past TG/XD quarterly reports as this information may have explicitly been associated with them;
- Find the FOS information from the project data in the XDcDB. Unfortunately, it is possible that one project is associated with multiple FOS. In such cases we counted that publications of the project to all involved FOS.
  - (a) Some publications from TG/XD quarterly reports were identified only by the project proposal number. We mapped them to the project charge number and account id used internally within XSEDE central database;
  - (b) For user uploaded publications data via the XSEDE user portal, a project charge number was associated with the publications.

Through this data mashup we obtained enough data to conduct our analysis. We present our results in a number of graphs and tables. However we provide first some data related to identify the sample. Figure 3 shows the kernel density of the distributions of XSEDE publications' percentile ranking and that of peers'. It shows XSEDE publications tend to have higher percentile ranking. Table 1 listed the average and median rankings and citations received of the two groups to evaluate and compare. We can perform a

 $<sup>^1{\</sup>rm For}$  NCAR data we have chosen a value of five due to the smaller number of overall publications

T-test to show the statistic significance. The results show that XSEDE group has statistically higher ranking as well as absolute citation than the peers group does.

- 1. T-test for ranking (Welch Two sample t-test)
  - (a) T=21.4134, df=2412.99, p-value<2.2e-16
  - (b) 95% confidence interval: [10.80, 12.98]
- 2. T-test for citation count:
  - (a) T=7.057, df=2358.929, p-value=2.228e-12
  - (b) 95% confidence interval: [9.40, 16.63]

Table 1: Basic statistics of XSEDE publications group and peers group

	Number of	Rank		Citations		
	Publications	Average	Median	Average	Median	
XD	2349	61	65	26	11	
Peers	168422	49	48	13	5	

The results are depicted in Figuree 6, 7, 8, 4, and 5.

NSF and XSEDE define a hierarchy of FOS. In 5 we show the top level FOS as defined by NSF. When we look axpand the FOS to the next level in the hierarchy we find the results as depicted in 8. The next level is shown in 7. In each of these Figures shows the list of FOS in decreasing order by the performance score S.

From 7 we can identify that for most Field of Science the TeraGrid/XSEDE publications performed better compared to their peers. The average and median score higher than 50 and the sore is positive performance. When looking at individual results, we see that astronomy and physics benefit most from using TeraGrid/XSEDE. When looking at the fields that perform worst, we find fields such as Experimental and Theoretical Geochemistry, Geometric Analysis and Mechanical and Structural systems. Such fields are typically not dominated by simulation science, and less computational resources. Other fields such as Training include also many other areas of training outside of supercomputing usage. We even find field such as Computer and Computation Research to be less impacted. We certainly have to acknowledge in this case that many theoretical papers and papers not using super computers are published.

To show the percentile distribution in more detail for each journal we present in Figure 6 a stacked barchart. Also here we see as expected from our previous results that for most of the journals we see a positive impact in the percentile citation count. This is made obvious by looking at Figure 4. Here we also have included the average of the top 66 journals in which we found 10 or more XSEDE publications and find that the number is positive with a value of 0.284. Thus we can conclude that papers that use XSEDE resources based on self identification in reports and bibliographic upload to the XSEDE portal is beneficial while being more cited on average than their peers from the same journal.

#### 5. NCAR

We have replicated the analysis with data we have obtained from NCAR. The data we obtained from NCAR was

#### Percentile ranking distribution of TG/XD publications vs peers

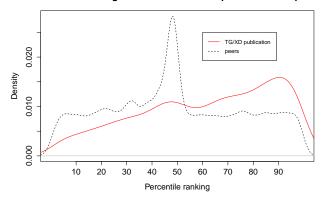


Figure 3: Kernel density of distributions for XSEDE publication percentile ranking versus peers.

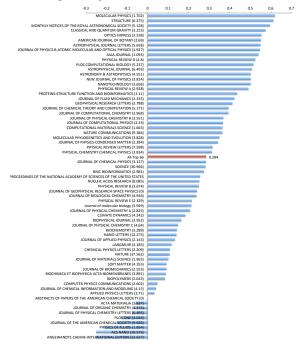


Figure 4: The socre of our peer comparision metric for XSEDE publications by journal.

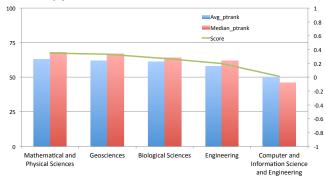


Figure 5: Peers Comparison based on the top most Field of Science category as defined by NSF.

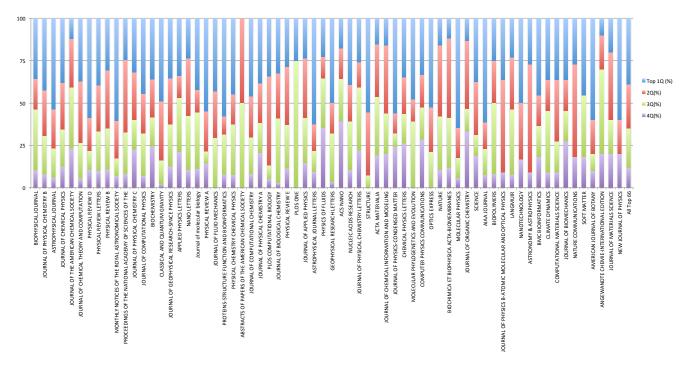


Figure 6: Percentile ranging by FOS in a stacked barchart of XSEDE publications.

smaller than the one we obtained from XSEDE. Thus instead of looking at all journals that have at least ten publications, we have reduced the value to five. This will give a large enough journal number to conduct our analysis in this case. To conduct the analusis we have taken the following steps.

A text file with 880 publications curated by NCAR. Processing:

- 1. We parsed the text file containing 880 publications into structured database while identifying titles, and doi's.
- With our framework we queried ISI Web of Knowledge to get detailed information of the publications – journal name, issue, citation data and other identifying information. We were able to verify and obtain data for 813 publications.
- 3. Through our framework we identified and obtained peer data based on journal issue information. In total 130 different publication venues have been identified. To ensure the results are statistically meaningful, we eliminated those with less than 5 publications appeared on them. This leads to 35 different journals that cover 653 identical publications. Out of the 35 journals, we had peers data for 12 of them (based on what we had for XSEDE peers comparison). For the other 23 journals, we obtained additionally 39k peer publication data.
- 4. For each NCAR publication we computed the percentile ranking among peers within the same journal issue against all publication entries as obtained from ISI Web of Knowledge.
- 5. We grouped the percentile ranking scores based on each journal, and divided the scores into each rank-

ing quarters ( $Q_1$ : top 25%; top  $Q_2$ : 25% 50%; bottom  $Q_3$ : 50%-75%, bottom  $Q_4$ : 75%-100%). Compute the percentile for those that fall into each ranking quarter.

We depict the result in a stacked column chart as shown in Figure 6. In Figure 9 we show the distribution of the publications in the top 10 journals sorted by the number of publications. The top 10 journals (totaling 484 publications). They account for about 3 quarters of the 653 publications from the 35 journals with at least five publications appeared on them; or 60% of the 813 publications from the 130 journals we identified via ISI source (see Table 2).

Table 2: Top ten journals with the most publications ns of NCAR publication data  $\,$ 

Publication Venue	Publication Count
Journal of Climate	110
Journal of Geophysical Research-Atmospheres	72
Geophysical Research Letters	66
Atmospheric Chemistry and Physics	56
Monthly Weather Review	53
Journal of the Atmospheric Sciences	42
Climate Dynamics	35
Journal of Geophysical Research-Space Physics	19
Journal of Geophysical Research-Oceans	16
Journal of Hydrometeorology	15

We also computed and compared the *performance score* as defined earlier. The result is shown in Figure 11. Here we see that the average over all 35 entries is a positive value with about 0.35.

#### 6. CONCLUSION

We make the observation that the score is slightly higher than that of that of XSEDE. However we need to take into

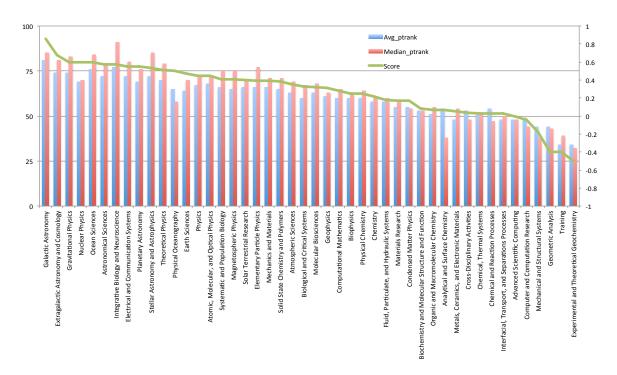
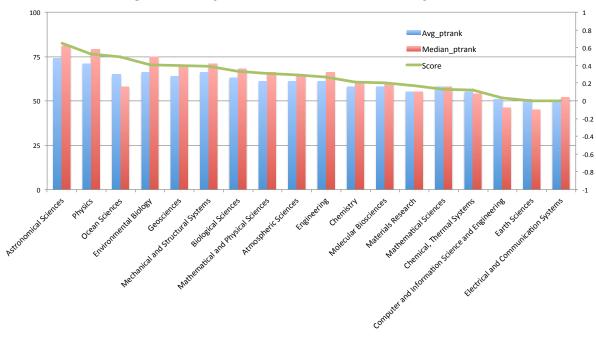


Figure 7: Peer comparison based on Field of Science of XSEDE publications.



 $Figure \ 8: \ Peer \ comparison \ based \ on \ Parent \ Field \ of \ Science \ from \ the \ original \ analysis \ of \ XSEDE \ data.$ 

account that XSEDE publications have a wider range of FOS than NCAR has that focusses on a much narrower FOS. Furthermore as we can see from XSEDE research in the atmospheric sciences while using XSEDE resources result in highest score values. Thus we can certainly expect that the value is higher for NCAR as they do not include the other disciplines that have lower values.

However, the most important conclusion we make for our

metric is that for both XSEDE and NCAR identified publications the impact measured by a percentile score is positive and higher than their peers that have not used such resources.

We will further expand upon our metric and can define such values also for other groups defined in XSEDE, or other resource providers. The important information we need to accomplish this is a reliable source that identifies publica-

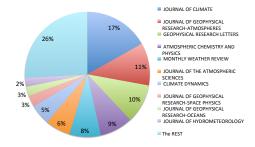


Figure 9: Distribution of the top most journals by publication count.

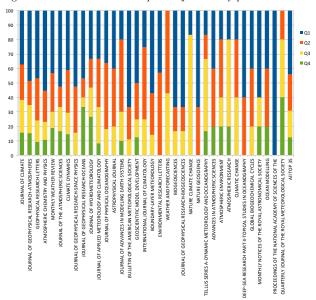


Figure 10: Percentile ranging by FOS in a stacked barchart of NCAR publications.

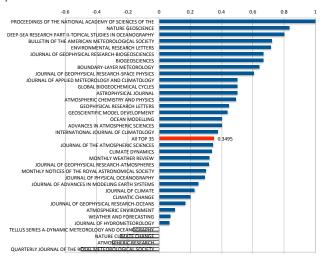


Figure 11: Peer comparison based on Parent Field of Science from the original analysis of XSEDE data.

tions that can be associated with the resource. While exploring not only XSEDE, but also NCAR data we have in principle shown that our approach is applicable to other resource providers.

#### 7. ACKNOWLEDGMENTS

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#### 8. REFERENCES

- [1] i-10 index | google scholar citations open to all. URL: http://googlescholar.blogspot.com/2011/11/google-scholar-citations-open-to-all.html.
- [2] NCAR. Web Page. URL: http://ncar.ucar.edu.
- [3] XSEDE. Web Page. URL: https://www.xsede.org/.
- [4] J. Bollen, G. Fox, and P. R. Singhal. How and where the TeraGrid supercomputing infrastructure benefits science. *Journal of Informetrics*, 5(1):114–121, 2011.
- [5] J. Bollen, M. A. Rodriguez, and H. Van de Sompel. MESUR: Usage-based Metrics of Scholarly Impact. In Proceedings of the 7th ACM/IEEE-CS Joint Conference on Digital Libraries, JCDL '07, pages 474-474, New York, NY, USA, 2007. ACM. URL: http://doi.acm.org/10.1145/1255175.1255273, doi:10.1145/1255175.1255273.
- [6] J. Bollen, H. Van de Sompel, A. Hagberg, and R. Chute. A principal component analysis of 39 scientific impact measures. *PloS one*, 4(6):e6022, 2009.
- [7] J. Bollen, H. Van de Sompel, and M. A. Rodriguez. Towards Usage-based Impact Metrics: First Results from the Mesur Project. In *Proceedings of the 8th ACM/IEEE-CS Joint Conference on Digital Libraries*, JCDL '08, pages 231–240, New York, NY, USA, 2008. ACM. URL:
  - http://doi.acm.org/10.1145/1378889.1378928, doi:10.1145/1378889.1378928.
- [8] L. Egghe. Theory and practise of the g-index. *Scientometrics*, 69(1):131–152, 2006.
- [9] T. R. Furlani, B. L. Schneider, M. D. Jones, J. Towns, D. L. Hart, S. M. Gallo, R. L. DeLeon, C.-D. Lu, A. Ghadersohi, R. J. Gentner, A. K. Patra, G. von Laszewski, F. Wang, J. T. Palmer, and N. Simakov. Using xdmod to facilitate xsede operations, planning and analysis. In Proceedings of the Conference on Extreme Science and Engineering Discovery Environment: Gateway to Discovery, XSEDE '13, pages 46:1–46:8, New York, NY, USA, 2013. ACM. URL:
  - http://doi.acm.org/10.1145/2484762.2484763, doi:10.1145/2484762.2484763.
- [10] J. E. Hirsch. An index to quantify an individual's scientific research output. Proceedings of the National academy of Sciences of the United States of America, 102(46):16569–16572, 2005.
- [11] P. Thomas and D. Watkins. Institutional research rankings via bibliometric analysis and direct peer review: A comparative case study with policy implications. *Scientometrics*, 41(3):335–355, 1998.
- [12] J. Towns, T. Cockerill, M. Dahan, I. Foster, K. Gaither, A. Grimshaw, V. Hazlewood, S. Lathrop, D. Lifka, G. Peterson, R. Roskies, J. Scott, and

Table 3: The top level Field of Sciences in XSEDE as defined by NSF

FOS	Avarage ptrank	Median ptrank	Score
Mathematical and Physical Sciences	63	68	0.35
Geosciences	62	67	0.33
Biological Sciences	61	64	0.27
Engineering	58	62	0.2
Computer and Information Science and Engineering	50	46	0.01

Table 4: Percentile ranking and score of XSEDE publication data grouped by parent field of science.

FOS	Number of Pubs	average ptrank	Score
Astronomical Sciences	74	81	0.65
Physics	71	79	0.53
Ocean Sciences	65	58	0.5
Environmental Biology	66	75	0.41
Geosciences	64	70	0.4
Mechanical and Structural Systems	66	71	0.39
Biological Sciences	63	68	0.33
Mathematical and Physical Sciences	61	66	0.31
Atmospheric Sciences	61	65	0.29
Engineering	61	66	0.27
Chemistry	58	60	0.21
Molecular Biosciences	58	60	0.2
Materials Research	55	55	0.17
Mathematical Sciences	58	58	0.13
Chemical, Thermal Systems	55	54	0.12
Computer and Information Science and	51	46	0.03
Engineering			
Earth Sciences	51	45	0
Electrical and Communication Systems	50	52	0

Table 5: Overview of the number of publications, average percentile ranking and performance score for XSEDE publication data based on Field of science.

FOS	Number of Pubs	average ptrank	Score
Galactic Astronomy	14	81	0.86
Extragalactic Astronomy and Cosmology	57	74	0.68
Gravitational Physics	104	74	0.60
Nuclear Physics	5	69	0.60
Ocean Sciences	5	76	0.60
Astronomical Sciences	187	72	0.57
Integrative Biology and Neuroscience	7	77	0.57
Electrical and Communication Systems	54	72	0.55
Planetary Astronomy	10	69	0.55
Stellar Astronomy and Astrophysics	31	72	0.53
Theoretical Physics	49	70	0.51
Physical Oceanography	5	65	0.50
Earth Sciences	19	64	0.47
Physics	147	67	0.45
Atomic, Molecular, and Optical Physics	55	68	0.45
Systematic and Population Biology	37	66	0.41
Magnetospheric Physics	11	65	0.41
Solar Terrestrial Research	10	66	0.40
Elementary Particle Physics	27	66	0.39
Mechanics and Materials	14	66	0.39
Solid State Chemistry and Polymers	8	65	0.38
Atmospheric Sciences	44	63	0.35
Biological and Critical Systems	6	60	0.33
Molecular Biosciences	494	63	0.32
Geophysics	8	61	0.31
Computational Mathematics	9	60	0.28
Biophysics	323	60	0.25
Physical Chemistry	168	60	0.25
Chemistry	259	58	0.23
Fluid, Particulate, and Hydraulic Systems	51	58	0.18
Materials Research	305	55	0.13
Condensed Matter Physics	61	55	0.17
Biochemistry and Molecular Structure and Func-	141	53	0.08
tion	1-11	00	0.00
Organic and Macromolecular Chemistry	44	51	0.07
Analytical and Surface Chemistry	7	54	0.07
Metals, Ceramics, and Electronic Materials	11	48	0.05
Cross-Disciplinary Activities	26	53	0.03
Chemical, Thermal Systems	38	51	0.04
Chemical and Reaction Processes	31	54	0.03
Interfacial, Transport, and Separations Pro-	17	48	0.03
cesses	11	40	0.03
Advanced Scientific Computing	18	48	0.00
Computer and Computation Research	14	49	-0.04
Mechanical and Structural Systems	14	44	-0.18
Geometric Analysis	5	44	-0.10
Training	5	34	-0.40
	5 5	34	-0.40
Experimental and Theoretical Geochemistry	O.	34	-0.50

N. Wilkins-Diehr. XSEDE: Accelerating Scientific Discovery. Computing in Science Engineering,

16(5):62-74, Sept 2014. doi:10.1109/MCSE.2014.80.

[13] F. Wang, G. von Laszewski, G. C. Fox, T. R. Furlani, R. L. DeLeon, and S. M. Gallo. Towards a scientific impact measuring framework for large computing facilities - a case study on xsede. In Proceedings of the 2014 Annual Conference on Extreme Science and Engineering Discovery Environment, XSEDE '14, pages 25:1–25:8, New York, NY, USA, 2014. ACM. URL:

http://doi.acm.org/10.1145/2616498.2616507, doi:10.1145/2616498.2616507.