XSEDE EMPOWER

Led by the Shodor Education Foundation, EMPOWER (**E**xpert **M**entoring **P**roducing **O**pportunities for **W**ork, **E**ducation, and **R**esearch) is an undergraduate student program whose goal is to expand the community of advanced research computing by recruiting and enabling a diverse group of students who have the skills – or are interested in acquiring the skills – to participate in the work of the E **x**treme **S**cience and **E**ngineering **D**iscovery **E**nviro nment (XSEDE) project, funded by the U.S. National Science Foundation (NSF).

EMPOWER was honored by *HPCwire* with the **2021 Editors' Choice Award in Workforce Diversity and Inclusion Leadership.**

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- Program website
- Journal article about the program
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Participant Highlights

May 1 – July 31, 2022

- Four EMPOWER students participated in the PEARC22 Student Program and spoke during its Internship Spotlight event:
    - Sara El Houzaly, City College of New York
    - John Li, University of California San Diego
    - Davin Lin, Grinnell College
    - Arianna Martin, Southwestern Oklahoma State University
- Nirajan Acharya, Youngstown State University;
  Emma Liu, University of California, Los Angeles; and
  Alberto Lucas, California State University Monterey Bay:
    - **Acharya, N.**, **Liu, E.**, **Lucas, A.**, & Lazar, A. (2022, May 31). *Optimizing the Exa.TrkX Inference Pipeline for Manycore CPUs*. Poster presented at the 7th International Connecting the Dots Workshop, Princeton University.
- John Li, University of California San Diego:
    - First author in article submitted to International Computational and Mathematical Methods in Science and Engineering (CMMSE) conference and SC22 conference.
- Yilai Li (EMPOWER mentor), University of Michigan:
    - "With the EMPOWER students, I was able to initiate a software development project that will be very helpful in my field of study. I'm also planning to write a manuscript about the project, and I learned a lot myself from working with the students. EMPOWER connected me with students with software development skills which are very useful in our field, but not easy to find. I think from my perspective, the greatest part is to connect two groups of people that can benefit from each other, but are not familiar with each other otherwise." (written July 2022)
- Lisa Liang, University of Connecticut:
    - "I loved participating in the EMPOWER program -- it was truly an incredible learning experience, where I got to learn not just the basics of computational chemistry using VASP, but even more so how to grow as a whole researcher. The project has been integral to both my aspiration to continue incorporating computational chemistry into my future research career as well as my growth as a student. I hope that in the future I will be able to participate in a similar program." (written June 2022)
- Davin Lin, Grinnell College and
  Padma Prabagaran, Arizona State University:

- **Lin, D.**, **Prabagaran, P.**, & Colbry, D. (2022, July). Validating new Automated Computer Vision workflows to traditional Automated Machine Learning. *Proceedings of the Practice and Experience in Advanced Research Computing (PEARC '22)*. ACM, New York, NY, USA, Article 34, 5 pages. https://doi.org/10.1145/3491418.3535174
- Soknarith Sem, University of Rhode Island:
  - "recently presented a research poster in a department research forum that we hold each spring." (written May 2022)
- Josh Vermaas (EMPOWER mentor), Michigan State University:
  - "I have undergrads working in the laboratory that are actually paid for their time! Normalizing this through the program has made significant contributions to attracting undergraduates to computational science generally, since the unpaid alternatives don't make financial sense to many students working through college. It has given the lab a teaching focus beyond simply doing research on our own. In general, things go faster when the undergrads are there to run simulations and participate in the analysis. They also learn valuable coding skills. Our students will be presenting their research at an American Chemical Society meeting, and their postdoctoral mentors are working to get papers drafted for publication." (written July 2022)

February 1 – April 30, 2022

- Anonymous student feedback:
  - "XSEDE Empower has offered me throughout the last year early exposure to areas in the computational world such as machine learning, neural networks, etc that most students would be exposed to at a higher level in their academic career." (written spring semester 2022)
  - "Everything I have learned during the XSEDE EMPOWER program was towards my educational, research, and research development. I am able to conduct so much more computational science than I ever imagined. The conferences that I was able to attend with my research generated from the XSEDE EMPOWER program have granted me friendships, knowledge, public speaking skills, and more confidence. I feel more confident and assured after my year with XSEDE." (written spring semester 2022)
- Ermias Assefa, Bluffton University:
  - Accepted to summer 2022 internship at Lawrence Berkeley National Laboratory as part of Sustainable Horizons Institute Sustainable Research Pathways Program.
- Juan David Campolargo, University of Illinois at Urbana-Champaign:
  - 15-minute oral presentation at National Conference for McNair Scholars and Undergraduate Research, March 17, 2022.
- Qili (Samuel) Chen, Michigan State University:
  - "I learned so much from the project I am working on, such as the professional way of organizing a project, working on a Git project with group members, advanced machine learning concepts, and advanced coding skills. Those skill sets are typically not taught in my school. I am so glad I learned those skills. Now I am able to start my personal projects in a professional way." (written April 2022)
- Yingrong Chen, Emory University:
  - "I am preparing for the research symposium in my school at the end of the semester. I will host an oral presentation." (written April 2022)
- Dirk Colbry, EMPOWER mentor from Michigan State University:
  - "This program is amazing. I wish it was still going on as it has been a great source of connection and momentum for my research. The students and I are making good progress on our research. We have submitted papers and gotten the software to a level that will enable me to go after some funding and even hire a graduate student (or two). Working with students from schools other than my own is very helpful. It broadens the impact of my research and helps me set up connections. My students and I have submitted a publication to PEARC on the work with our SEE-Classify project." (written April 2022)
- Filipe Correia, EMPOWER mentor from University of Georgia:
  - "Participating in EMPOWER got me and students more acquainted with supercomputing and the XSEDE interface. Also, as someone in the social sciences, it is not very common for us to use this environment, but I think it has promising uses, and this realization would not be possible without EMPOWER and XSEDE. It has enabled me to manage large scale datasets in a manageable time frame and provide students with the opportunity to experience and learn about supercomputing, as it is outside my domain." (written April 2022)
- Hannah Crouse and Alyssa Van Fossen, Mount Vernon Nazarene University:
  - 20-minute presentation at SURC symposium at Mount Vernon Nazarene University.
- Stephanie DeCarvalho, University of Massachusetts-Dartmouth:
  - "I compiled my data into a powerpoint and a presentation for two different conferences where I will be presenting this project." (written April 2022)
  - "Under Dr. Jun Li, I was able to apply for the MA Space Grant through MIT. I am studying the computational investigations of additively manufactured polymer composites. This research has given me more knowledge about computational analysis. I have also been accepted into three different conferences: COExperience in New Orleans, ASEE Northeast 2022 Conference in Boston, and the Northeastern Regional Student Symposium of Society for Experimental Mechanics conference taking place at UMass Dartmouth." (source: https://www.umassd.edu/engineering/features/stephanie-decarvalho.html)
- Jessica Egleston, Michigan State University:
  - "Figures I created were highlighted in a poster presentation at the 2022 Biophysical Society annual meeting which was held in San Francisco, California." (written March 2022).
  - **Egleston, J.** (2022, April 8). *Structural Comparison Between Small Multi-drug Resistance (SMR) Transporter Family Members through Molecular Dynamics Simulations*. Poster presented at 2022 Michigan State University Undergraduate Research and Arts Forum. Winner of first-place honor. https://natsci.msu.edu/news/natsci-undergraduates-impress-at-2022-uuraf/
- Tim Hartman, University of South Dakota:
  - "Academically, I have been able to learn much more about available hardware and software related to biofilm image analysis. While assisting others in the lab I have been able to brainstorm new approaches to solving problems related to optics and data capture, transmission, analysis, and storage; and the performance requirements for all of these. Professionally, I have been exposed to a variety of tools made available to computational science researchers in the United States. The University of South Dakota's resources are small compared to many other institutions in the U.S., and simply knowing that these powerful resources exist helps me set the bar higher for what I want to achieve in my career. My EMPOWER work contributed to our bio-image analysis package which is currently under review for publication. I am the paper's first author. Our hardware limitations and software debugging hindered us from publishing earlier, but my EMPOWER work has taken us that much closer to being approved by a computational biology journal." (written April 2022)
- Devon Hood, San Diego State University:
  - "EMPOWER has allowed me to utilize powerful hardware to greatly improve the computation speed of my models which has directly aided in my ability to quickly iterate through experiments. It has also exposed me to a wonderful amount of resources, both with personnel and technical resources, which has improved my abilities as a successful computer scientist. EMPOWER has allowed me to focus more intently on my work which would have been difficult otherwise. The resources EMPOWER offers is an opportunity to not only increase my productivity, but also my focus." (written April 2022)
- Dorothy Najjuma Kamya, Swarthmore College:
  - "An important part of a career in research is understanding the work of others in your fields of interest, and the first part of my XSEDE project involved reading and understanding (at a high level at least) some research papers and related code, enough to edit it to run on

XSEDE's servers. As an aspiring graduate student, I believe this has prepared me for engagement with others' research, an essential element of graduate school. EMPOWER introduced me to researchers working on very relevant cutting-edge work which I would not have been exposed to otherwise. Being able to make a contribution to a project that predicts the severity of COVID-19 strains without being a bioscientist was a significant achievement for me." (written April 2022)

- Lisa Liang, University of Connecticut:
  - "Thank you so much for this amazing opportunity to learn about computational chemistry and participate in research on it as a first-year undergraduate. I am so lucky to have been able to be part of the XSEDE program this past academic year!" (written April 2022)
- Abdullah Al Maruf, South Dakota State University:
  - "XSEDE EMPOWER has enabled me to pursue my passion in computational materials science research, where I was able to computationally design novel energy materials for solid-state electrolytes (SSE) and study/tune their properties (using DFT) for Li-ion batteries application. I also studied electrode materials for Li-ion batteries to optimize the condition for suppressing the dendrite growth (needle-like-structure) which is detrimental for such energy storage device performance. Finally, this research experience allowed me to start pursuing my graduate studies at Dartmouth College in computational geophysics in the upcoming Fall-2022 semester, where I aim to investigate magnetic properties of Fe-S based ancient earth and mars minerals, as well as hydrite formation at extreme conditions, which cannot be studied experimentally (with current technology). Participating in XSEDE EMPOWER has enabled me to gain valuable research experience utilizing XSEDE resources and mentorship (at my university). I gained hands-on experience in high performance computing and parallel programming, and learned to run and debug full scale simulation for research. I presented my research at the Sustainable Energy Materials and Device group at the Electrical Engineering Department of South Dakota State University, and plan to present it at upcoming ACS national conference in Fall. There's a manuscript currently in its final stage of preparation for submissions as well." (written April 2022)
- Sudha Vaishnavi Nannur, Wayne State University:
  - **Nannur, S.V.**, Crivelli, S., & Liu, X. (2022, April 22). *Geospatial Inspired Community Characterization with High Dimensional Data*. Poster presented at the Georgia Tech Women in HPC Poster Competition. https://cpn-us-w2.wpmucdn.com/sites.gatech.edu/dist/8/1779 /files/2021/03/poster-7-edited.png
- Dayna Olson, Michigan State University:
  - "My participation in EMPOWER has catalyzed me falling in love with computational sciences. Without EMPOWER, I would not have had as much time or resources to continue exploring my interest in the Vermaas lab, where I was able to learn about molecular dynamics simulation and other forms of computational biology. Since participation in the program, I have added a minor in Computational Mathematics, Science, and Engineering and plan to pursue this path in grad school. I have presented my work from this semester at my colleges undergraduate research symposium. We are in the process of writing up last semester's project, which I will be a co-author on." (written April 2022)
  - Presentation at 2022 Michigan State University Undergraduate Research and Arts Forum.
- Maria Pantoja (EMPOWER mentor), Cal Poly Pomona:
  - "I was able to work with one student at UCSD on Distributed HyperParameter Optimization and based on this research, I did submit a visiting scholar proposal to Argonne National Lab that was accepted and I will start this July working there. I was able to work for a longer period of time with an undergraduate student to do research. I do work for a teaching institution with a very small master program so most of the time we need to do research with undergraduates. Undergraduates are very busy with school work and smaller stuff , so what xsede allowed me to do is to work with a student that is supported by this grant (so doesn't need to look for extra work) and did also allow a continuity. Plus Xsede Empower did the main job of searching for students interested and super motivated in HPC."
- Tyler Prine, University of Alabama:
  - "I have submitted my first conference abstract on the topic of the fully compressible Rayleigh-Taylor Instability to the International Workshop on the Physics of Compressible Turbulent Mixing (IWPCTM). The workshop will be held in Atlanta, Georgia in July 2022." (written April 2022)
- Ciara Richardson and Madison Winkeler, Murray State University:
  - **Richardson, C. & Winkeler, M.** (2022, April 11–15). *Structures and Properties of Palladium Doped Silicon Clusters*. Poster presented at Murray State University Spring 2022 Scholars Week. https://digitalcommons.murraystate.edu/scholarsweek/Spring2022/SigmaXi/17/
- Briana Sobecks, University of Illinois at Urbana-Champaign:
  - "Participating in EMPOWER helped me discover a passion for computational research, specifically for applications in chemical engineering and biophysics. As I have gone through my undergraduate career, I continue using the computational skills I developed during my time in EMPOWER. This experience inspired me to pursue a doctoral degree in chemical engineering." (written April 2022)
  - **Sobecks, B.**, Chen, J., & Shukla, D. (2022). Dual Role of Strigolactone Receptor Signaling Partner in Inhibiting Substrate Hydrolysis. *Journal of Physical Chemistry B, 126*(11), 2188–2195. https://doi.org/10.1021/acs.jpcb.1c10663
- Wenhuan Tan, Bellevue College:
  - **Tan, W.** & Wang, X. (2022, April 22). *Association Between Different Air-Quality Index with Suicide Deaths on Geospatial Level*. Poster presented at the Georgia Tech Women in HPC Poster Competition. https://cpn-us-w2.wpmucdn.com/sites.gatech.edu/dist/8/1779/files /2021/03/poster-5-edited.png
  - Accepted for a Department of Energy summer internship through the Sustainable Horizons Institute Sustainable Research Pathways program.

November 1 – January 31, 2022

- Students attending the 2021 Sustainable Horizons Institute Sustainable Research Pathways Workshop:
  - Sudha Vaishnavi Nannur, Wayne State University
  - Wenhuan Tan, Bellevue College
- Nicole Avila, California State Polytechnic University-Pomona:
  - Inorganic Chemistry Undergraduate Poster Presentation Award at the 2021 Society for the Advancement of Chicanos/Hispanics and Native Americans in Science (SACNAS) National Diversity in STEM Conference.
  - "I completed and participated in the SACNAS conference using my XSEDE EMPOWER research. After I spent much time practicing presenting my research, I finally presented to two judges. I was able to answer questions about the science behind my project and even questions regarding the spectra I have generated. I am happy to announce that I won the Inorganic Chemistry award. I plan to present my XSEDE EMPOWER research with more judges at the SCCUR conference on November 20th. I have already begun writing a new outline considering questions I was asked at the SACNAS conference." (written November 2021)
- Spencer Bryngelson (EMPOWER mentor), Georgia Institute of Technology:
  - "It has been invaluable to work with students at different universities and from different backgrounds. At the same time, the students are selected such that the pool is filled with folks interested in my research. This makes things very convenient for me, and seems like a smart way to link up students and researchers. Having extra students available and their ability to interact with the group has been valuable for everyone involved." (written January 2022)
- Yingrong Chen, Emory Oxford College:

- Presented research at the 2021 Southeastern Regional Meeting of American Chemical Society (SERMACS) (LinkedIn post), Georgia Undergraduate Research Conference, and Oxford Research Scholars Spring Symposium.
- "I feel that computational tools can accelerate and open new perspectives for my scientific research, and I have decided to be a computational biochemist in the future. I have gotten to learn computational chemistry in a systematic way. This is a valuable opportunity since most colleges do not offer computational classes at the undergraduate level." (written January 2022)
- Damien Cooper, University of Southern Mississippi:
  - "At the beginning of November, I presented research based on this project at the Southeastern Regional Meeting of the American Chemical Society (SERMACS) in Birmingham, AL." (written December 2021)
- Luis Cueva Parra (EMPOWER mentor), University of North Georgia:
  - "My participation in the XSEDE EMPOWER program has impacted positively my academic career. My supervisor values this effort with our students, and it is reflected in my faculty evaluations. In addition, the Computer Science Department, which I am a faculty for, is recognized for these opportunities for the students. The XSEDE EMPOWER program provided the structure and financial support for students, who helped me to make progress in my research agenda. Without this support, it would be difficult to find students who devote time and effort to this extracurricular activity (learning HPC and contributing to a research project). Most students have a full schedule including part-time or full-time job that limit their availability. The support of XSEDE EMPOWER program is particularly important in non-research universities and predominantly teaching institutions with no Graduate programs." (written January 2022)
- Sudha Vaishnavi Nannur, Wayne State University:
  - "I have learned a lot throughout this semester at XSEDE. I am quite grateful for this program because it has given me such an incredible foundation in my machine learning and data science journey. Thank you so much for letting me be a part of this." (written December 2021)
- Tanya Nesterova, University of Delaware:
  - Ni, T., Zhu, Y., Yang, Z., Xu, C., Chaban, Y., **Nesterova, T.**, Ning, J., Böcking, T., Parker, M.W., Monnie, C., Ahn, J., Perilla, J.R., & Zhang, P. (2021, November). Structure of native HIV-1 cores and their interactions with IP6 and CypA. *Science Advances, 7*(47). https://doi.org/10.1126/sciadv.abj5715
- Bianca Ortega, Kean University:
  - "I have acquired such a generous amount of knowledge and skills in less than a year that I would not trade for anything. I am honored to be an intern for such an amazing program that has inspired me for the future." (written December 2021)
- Ciara Richardson and Madison Winkeler, Murray State University:
  - **Winkeler, M.** & **Richardson, C.** (2021, November). *Exploring the Geometric and Electronic Properties of Palladium Doped Silicon Clusters.* Poster presented at Murray State University Fall 2021 Scholars Week. https://digitalcommons.murraystate.edu/scholarsweek/Fall2021/GeneralPosters/2/
- Nitin Sukhija (EMPOWER mentor), Slippery Rock University:
  - "This project allowed me to further my research skills related to working in the data provenance, machine learning, cybersecurity, and high-performance computing areas. From the beginning of finding and reading academic papers, to how to develop and execute provenance workflows, how to utilize new tools such as Apache hop on HPC systems, and the overall provenance data framework, I have gained immense of experience in domain of cybersecurity and data lineage research field. Moreover, the research work has lead to collaboration with Lawrence Berkeley National Labs researchers and having diverse experience in multiple domains was extremely rewarding. Furthermore, the research work has also resulted in a potential paper which might be presented at PEARC22 or other peer reviewed ACM or IEEE conference. This project also facilitated the students to collaborate and network with research scientists from different domains from Lawrence Berkeley National Laboratory (LBNL) which will aid in achieving student's goal of attending a high research graduate school in coming years. The participation in EMPOWER program enabled me and my student to work with scalable provenance data analysis tools on XSEDE systems which was not possible at my current institution due to scalabilty challenges." (written January 2022)
- Wenhuan Tan, Bellevue College:
  - "EMPOWER gave me a chance to wake my dream and confidence up. I never thought I could get connected with science before I joined EMPOWER. I realized my passion for research and curiosity for the truth behind data and phenomenons. I decide to continue pursuing further education after finishing the undergraduate program. EMPOWER enabled me to participate in a research project, which was beyond my expectations. From EMPOWER, I found my potential talent in data science and machine learning, which also enhanced my interest and confidence in the IT field. I joined the SPR workshop and submitted a poster and a proposal for the summer internship with the help of my mentor." (written January 2022)
- Josh Vermaas (EMPOWER mentor), Michigan State University:
  - "The real power for the EMPOWER program has been in increasing accessibility of my computational research to new and emerging researchers. I'm a new assistant professor, with no grants but enough time to devote to meeting with a handful of undergraduates a few times a week to help them along in their first steps as computational scientists. Without the support the EMPOWER program provides, only the well-heeled students can access this tremendous undergraduate research experience, as they'd be doing the same work for college credit alone. Having the EMPOWER program offer this kind of hands on training democratizes the types of undergraduate researchers I can recruit. This means that my lab is bigger than it otherwise would be, and my postdocs have the opportunity to gain mentoring experience that a newly started lab would not be able to provide. Concretely, I think that the EMPOWER program has doubled the number of undergraduates working in the lab." (written January 2022)
- Benjamin Walls, Northeastern University:
  - From Michael Cianfrocco, Benjamin's EMPOWER mentor from University of Michigan:
    - "The EMPOWER program has helped us make critical steps towards developing an open source web platform for cryo-EM software. Prior to EMPOWER, we had several approaches but were unclear as to the best approach. Our EMPOWER student Ben Walls helped us create a plan and execute key steps towards creating a Java-based web platform. He brought significant expertise in Node.js and React to show us that the future of our web platform should use these tools for an intuitive software platform. We could not have done this without Ben." (written January 2022)
- Raquel Yupanqui, University of North Georgia:
  - **Yupanqui, R.** (2021, November). *Developing and Implementing Machine Learning Models to Analyze EEG Data Using MNE Libraries*. Poster presented at Georgia Undergraduate Research Conference (GURC) 2021. YouTube video

August 1 – October 31, 2021

- Daniel Adams, University of Mount Union:
  - "I wrote a scientific report as well as created a poster highlighting the main topics of my project that will be presented at the University of Mount Union during the fall semester in front of the Eastern Great Lakes Section of the American Physical Society." (written August 2021)
- Ermias Assefa, Bluffton University:
  - Accepted to the 2021 Sustainable Horizons Institute Sustainable Research Pathways program.
- Nicole Avila, California State Polytechnic University-Pomona:

- "I have truly grown as a scientist and am so proud of my progress due to the XSEDE EMPOWER program. I have been working on creating and editing my poster for the SACNAS conference and SCURR conference I will present at." (written September 2021)
- Spencer Brady and Kristopher Erlitz, California State Polytechnic University-Pomona:
  - Monaco, S., Baer, R.P., Giernacky, R.P., Villalba, M.E., Garcia, T.M., Mora-Perez, C., **Brady, S.E.**, **Erlitz, K.D.**, Kunkel, C., Jezowski, S.R., Oberhofer, H., Lange, C., & Schatschneider, B. (2021, September). Electronic property trends of single-component organic molecular crystals containing C, N, O, and H. *Computational Materials Science, 197*. https://doi.org/10.1016/j.commatsci.2021.110510
- Colin Campbell (EMPOWER mentor), University of Mount Union:
  - "The program allowed me to mentor an undergraduate student for a formative summer research experience. These kinds of experiences are fantastic for students looking to immerse themselves in a field of research and gain marketable skills. I am grateful that the EMPOWER program was able to fund my student and I hope the program will be able to support other students in the future. My student will be presenting his work during the Eastern Great Lakes Section of the American Physical Society (APS) this November." (written October 2021)
- Dirk Colbry (EMPOWER mentor), Michigan State University:
  - "The EMPOWER students are outstanding additions to our team. Our research has advanced greatly due to the program. Their work has significantly progressed the development of our SEE-Insight software and has resulted in at least one publication and authoring of multiple scientific software packages. My work is in the preliminary stages and working with the EMPOWER students has resulted in me being able to write one grant proposal and have two additional proposals to be submitted. This could not have been done without the help of my undergraduate students." (written October 2021)
- Matthew Donahue (EMPOWER mentor), University of Southern Mississippi:
  - "EMPOWER really has given me the opportunity to have a student focus on using computational methods for my synthetic organic work. Through regular discussions with my student, I as a PI have learned more about using computational chemistry as an asset to facilitate traditional wet bench research" (written October 2021)
- Precious Fadimiroye, University of Houston-Clear Lake:
  - "We worked to prepare a presentation for the Robotics for Risky Intervention and Environmental Surveillance Conference in October." (written October 2021)
  - "On October 8th, we attended a four-hour conference (TC-17 VRISE2021; virtual) where we presented research to a group of participants from around the globe and TC-17 members of IMEKO." (written October 2021)
- Nicholas Grabill, Michigan State University, and Kai Pinckard, Reed College:
  - **Pinckard, K.**, **Grabill, N.J.**, & Colbry D. (2021, September 21). *Scaling of Evolutionary Search of Algorithm Space to Speed-Up Scientific Image Understanding Workflows*. Poster presented at 2021 IEEE High Performance Extreme Computing Virtual Conference — HPEC.
- Stephen Harnish (EMPOWER mentor), Bluffton University:
  - "My experiences mentoring EMPOWER students in HPC research this past and recent years have led to several benefits: enlarging my lists of applications of concepts of mathematics or computer science for class room use; participation in the 2019 Sustainable Horizons Institute Sustainable Research Pathways program; participation in UC Berkeley's Applications of Parallel Computers offering for Bluffton students; several new lines of research for me and my students; strengthening my students' motivation for and success in pursuing graduate studies in data science, computer science, applied mathematics or physics; and multiple presentations of EMPOWER-supported research at the Joint Mathematics Meetings and at the Miami University and at Midwest Relativity Meetings. Thank you for offering XSEDE EMPOWER over recent years. It has really opened up new opportunities for my students and myself." (written October 2021)
- Hannah Johnson, Lane College:
  - "Our work has been prepared for submission to a conference in high-performance computing." (written August 2021)
- Umair Khan, Portland State University:
  - Tong, J.J., **Khan, U.**, Haddad, B.G., Minogue, P.J., Beyer, E.C., Berthoud, V.M., Reichow S.L., & Ebihara, L. (2021, August 19). Molecular mechanisms underlying enhanced hemichannel function of a cataract-associated Cx50 mutant. Manuscript submitted for publication. https://doi.org/10.1101/2021.08.18.456706
- Jonathan Lyon (EMPOWER mentor), Murray State University:
  - "The EMPOWER program has helped me professionally in several ways. First, it has helped me recruit talented undergraduate students into my research lab. Second, it has helped bring funding to support the science majors in my department, allowing them the financial security to spend a large amount of time learning and performing the research project rather than pursue work from other sources. Third, XSEDE has provided a collection of training resources to aid me in mentoring these students. EMPOWER has helped me considerably as I transitioned to a new institution. The EMPOWER program aided a former student at Kennesaw State University continue her research project with me remotely while I moved to Murray State University in the Fall 2020. The program has made it easier to recruit, train, and mentor talented students at Murray State University while transitioning my research laboratory at a primarily undergraduate institution." (written October 2021)
- Emily Maroni, University of Mount Union:
  - "We are working to submit an abstract to the ACS spring conference in San Diego." (written October 2021)
- David McDowell, University of Houston-Clear Lake:
  - "On October 8th, we attended a four-hour conference (TC-17 VRISE2021; virtual) where we presented research to a group of participants from around the globe and TC-17 members of IMEKO." (written October 2021)
- Phan Phu, California State Polytechnic University-Pomona:
  - "EMPOWER provided me an opportunity to learn computational chemistry and new skills that were not offered through coursework at my school. It allowed me to conduct chemistry research and gained research experiences that were valuable prior to my application to graduate school. With the findings I gained during this internship, I received the ACS COMP award and presented my research at the 255th American Chemistry Society National Meeting in 2018. At the meeting, I attended graduate school workshops and learned about the opportunities in chemistry. This really inspired me to attend graduate school where I am currently a third year graduate school at University of California, Irvine." (written October 2021)
- Steve Reichow (EMPOWER mentor), Portland State University:
  - "This has been a rewarding experience that provided excellent structure to undergraduate mentorship and research training. The provided research experience was a critical component to defining the students career trajectory, and is now applying their skills at a graduate program at UCSF."
- Ciara Richardson and Madison Winkeler, Murray State University:
  - **Winkeler, M.**, **Richardson, C.**, Carlin, R., & Lyon, J.T. (2021). *Structural evolution of SinPd2 (n = 1-17) clusters*. Manuscript in preparation.
- Bohdan Schatschneider (EMPOWER mentor), California State Polytechnic University-Pomona:
  - "EMPOWER has enabled me to employ 10 undergraduate researchers (UGRs) over the last 4-5 years. The large majority (8) of these researchers were from underrepresented minorities (URMs) in the sciences. The ability to put these UGRs to work and have them generate useful data has allowed me to generate 3 publications over the last 4-5 years that would not have been completed otherwise. It has also allowed for these URMs to complete senior projects that they would have otherwise opted out of because of a need to work. As

a result of performing research, 5 of these URMs are now in graduate programs or are preparing to partake in a graduate program. EMPOWER really does just that, it allows PI's to empower UGRs to explore research opportunities and other lines of employment." (written October 2021)

- Wenhuan Tan, Bellevue College:
  - "From my previous understanding, I thought research was a tough and boring job but after one and half months of experience working within XSEDE, I found research is an amazing and super interesting job. When I found the trends and changes over the years from a mass of environment-related data, I couldn't be more excited; when I created a map with a few lines of code, I felt that I created an artist work; when I was told that the findings I got may be referenced by a research paper, I couldn't be more proud. This job brought too much amazing experience for me. From the experience working with XSEDE, I am more confident to be a software engineer or a data scientist in the future." (written October 2021)
- Dave Toth (EMPOWER mentor), Centre College:
  - "At a small liberal arts college, providing an experience like EMPOWER for students is looked upon extremely favorably. When it comes time for me to apply for promotion to full professor, this is something that will be helpful. Without support from EMPOWER, I couldn't have done the research with my students (there was no funding for them without that)." (written October 2021)
- Yigui Wang, Southern Connecticut State University:
  - "EMPOWER program provide me an opportunity to work with students to do research not only at SCSU but also across USA. The current public universities, especially primary undergraduate institutions put all resources on full-time teaching faculties. Without EMPOWER program, I will be limited to do research of others and without opportinties to teach students" (written October 2021)
- Madison Winkeler, Murray State University:
  - "EMPOWER has impacted me professionally by helping me to step out of my comfort zone and pursue participation in a virtual presentation that requires a professional abstract which I have not done previously. It has also impacted me academically by providing a real-life understanding of some topics I have learned throughout the last few years. For my major, coding classes are not something that is required and I am not one to add any more classes than I need. Without EMPOWER I wouldn't have been able to learn my first coding language through EXPANSE. I have also been introduced to other programs such as Inkscape and GaussView which has been a great experience as they are programs I could be using in the future. A labmate and I are currently co-authoring an abstract and presentation of our current research to do at a university-led event entitled Scholar's Week. Specifically, we will be doing a virtual poster presentation about our current research and what we hope to accomplish in the future." (written October 2021)
- Raquel Yupanqui, University of North Georgia:
  - "Being able to participate in the EMPOWER program has helped me realize my passion for research and the impact research can have on the world. I will be applying to PhD programs to continue exploring my field and hopefully add meaningful knowledge to it. Being able to work with my mentor has taught me a lot about doing research and what it entails. Being able to use the Expanse supercomputer has allowed me to process large amounts of data quickly and efficiently which is an important part of my work. I will be presenting my research from EMPOWER at the Georgia Undergraduate Research Conference (GURC) in November." (written October 2021)

May 1 – July 31, 2021

- Four students presented talks about their EMPOWER projects at the PEARC21 Internship Spotlight (https://pearc.acm.org/pearc21/student-program/pearc21-internship-spotlight/):
  - Christy Marchese, Pomona College
  - Arianna Martin, Southwestern Oklahoma State University
  - Tanya Nesterova, University of Delaware
  - Christopher Sherald, University of Kansas
- Christy Marchese, Pomona College:
  - **Marchese, C.** (2021, July 21). *Predicting Mental Health Outcomes with Deep Learning*. Poster presented at 2021 ACM Practice & Experience in Advanced Research Computing — PEARC21. Photo
  - "At PEARC21, I attended many presentations, workshops, Q&As, and exhibitor booths. I think PEARC is a really valuable experience for anyone interested in computing. I was able to learn so much in such a short time from workshops, presentations, and experts in the field of computing. I was able to meet people who I know aspire to be. I think especially when it comes to inspiring underrepresented students in HPC, PEARC is an amazing conference to go to. I met so many women in computing that I never knew existed, and I was incredibly inspired by them and their resilience working in the research computing field. I just want to thank you all so much for encouraging me to go to this conference and supporting me through it. I found the EMPOWER program to be an incredibly fulfilling experience in introducing me to research computing, and this conference was just the cherry to top it all off. I had a great time at this conference, and I hope future EMPOWER students will also be able to experience the same amazing opportunities." (written July 2021)
  - "I truly learned a lot from this experience [of participating in EMPOWER], and I am incredibly grateful that I was able to have this opportunity to receive mentorship and use XSEDE's computational resources." (written June 2021)
- Sudha Vaishnavi Nannur, Wayne State University:
  - "I am very happy to say that this internship is going really well! I have honed my modern computing skills and gained immense perspective on how they can be put to use. This project has provided me with the context to apply skills that I learned in college to produce real - world results. For that, I'd like to thank you for providing me the opportunity to work with [my mentor] and allowing me to explore the different spaces where computing skills can be put to use." (written July 2021)

February 1 – April 30, 2021

- Nicole Avila, California State Polytechnic University-Pomona:
  - "My participation in the EMPOWER program has given me opportunities beyond what I could have imagined. I felt supported and encouraged to do my best for the entirety of my spring apprenticeship. For example, my scientific academic writing has increased dramatically because of the monthly progress reports and publication that I am working on. Specifically, I have gained the ability to present my thoughts more professionally, clearly, and concisely. Professionally, I now have computational experience that I will take on to graduate school. I also have computations that will eventually be published, which has increased my resume. I now have research experience that I could not have attained without the program! The positive experience that I have had at XSEDE has encouraged me to continue onto graduate school for computations!" (written April 2021)
- Nicholas Grabill, Michigan State University:
  - "I believe the XSEDE EMPOWER program was a fantastic way to get introduced to computational research. I will be doing the Applied Mathematics REU (SUAMI) at Carnegie Mellon University this summer." (written April 2021)
- Umair Khan, Portland State University:
  - Yue, B., Haddad, B.G., **Khan, U.**, Chen, H., Atalla, M., Zhang, Z., Zuckerman, D.M., Reichow, S.L., & Bai, D. (2021, April 20). Connexin 46 and connexin 50 gap junction channel properties are shaped by structural and dynamic features of their N-terminal domains. *Journal of Physiology, 599*(13), 3313-3335. https://doi.org/10.1113/JP281339

- Tyler Kibler and Nicolas Null, West Virginia University Institute of Technology:
  - **Null. N., Kibler, T.**, & Lowe, E. (2021, April). *Using Machine Learning to Predict Classes of Astronomical Data.* Presentation at the West Virginia Academy of Science 95th Annual Meeting.
    - Abstract: http://pwvas.org/index.php/pwvas/article/view/798
    - Video: https://www.youtube.com/watch?v=3T-3EFF0tjU
- Nicolas Null, West Virginia University Institute of Technology:
  - "Participating in the EMPOWER program has not only helped me learn tons about machine learning, but also has given me a passion for data science and machine learning. I am now seriously considering a career in this field. I started this semester not knowing how to code in python and having very limited exposure to machine learning concepts to being fairly fluent in python and using tons of open source libraries for our project. I am also learning how to be a good team member as I work with a group of two other students on the same project. I would never have considered the machine learning field. It all seemed so complicated to me. After doing a deep dive this semester on machine learning basics, I now understand the core concepts and can apply them to everyday problems. My school does not even offer a machine learning class, so the EMPOWER program alone opened my eyes to this amazing field of study and work." (written April 2021)
  - "I also presented my work to the Artificial Intelligence class on campus and helped introduce the topics of machine learning to the class. With these presentations, we created a well commented Jupyter Notebook that could help others in getting started with machine learning. This included nice looking graphics to represent the results. We published this on my github account so people could use it as a template to start their own machine learning projects. Here is the link to the tutorial notebook we created: https://github.com/Nicolasnull /Machine-Learning-Using-Scikit-Learn" (written May 2021)
- Arianna Martin, Southwestern Oklahoma State University:
  - **Martin, A.**, & Evert, J. (2021, March). *Using OSG to Facilitate Research Computing at a Regional University.* Presentation at Oklahoma Research Day, Weatherford, Oklahoma. https://dc.swosu.edu/cpgs_edsbt_bcs_student/30/
  - "On April 10, I took my code and presentation to the Oklahoma High Performance Computing Competition and placed 1st in my division. I also helped coach a high school team at the same competition." (written April 2021)
  - **Martin, A.**, Evert, J., & Sleeper, C. (2021, April). *MPI4PY Implementation of Greedy Algorithm for the Shortest Path Problem*. Presentation at Southwestern Oklahoma State University Spring Research Fair.
- Billy Stone, University of Colorado Colorado Springs:
  - **Stone, W.B.**, Duster, A.W., Bennett, A.L., Ramsey, I.S., & Lin, H. (2021, February 12). Exploring the Proton-Transfer Mechanism in Hv1 by Multi-Scale Simulations. *Biophysical Journal, 120*(3). https://doi.org/10.1016/j.bpj.2020.11.590

November 1, 2020 – January 31, 2021

- Zachery Casey, Northeastern University:
  - **Casey, Z.,** & Shah, M. (2020, November 12). *Combating Run-time Performance Bugs with Performance Claim Annotations*. Presentation at the 11th Symposium on Software Performance 2020, Leipzig, Germany. https://www.performance-symposium.org /fileadmin/user_upload/palladio-conference/2020/Papers/SSP2020_paper_25.pdf
- Kobe Davis, Portland State University:
  - "The XSEDE EMPOWER program impacted me academically by introducing me to the world of HPC. I was able to learn about parallel programs over a variety of systems. This experience motivated me to register for courses on parallel computing, GPU programming, and performance analysis. After graduation, those experiences helped me prepare for, and obtain my current role as a Software Tools Infrastructure Architect at Nvidia. Without the XSEDE EMPOWER program I wouldn't have been exposed to as many topics in HPC or GPU architecture & programming especially. And without that exposure, I may not have been offered my current position. I feel very fortunate to have had access to the education provided by the XSEDE EMPOWER program. Additionally, XSEDE EMPOWER was the sole reason for my exposure to a research setting/environment. Without the program I would not have had the opportunity to contribute to research efforts at Portland State; that experience was invaluable." (written in January 2021)
- Ansa Malik, Kennesaw State University:
  - **Malik, A.**, & Lyon, J.T. (2021, January). *Investigating the Structures and Properties of Iridium Doped Silicon Clusters.* Presentation at Birla Carbon Symposium, Kennesaw, GA.
- Phan Phu and Carlos Gutierrez, California State Polytechnic University-Pomona:
  - **Phu, P.N.**, **Gutierrez, C.E.**, Kundu, S., Sokaras, D., Kroll, T., Warren, T.H., & Stieber, S.C.E. (2020, December 29). Quantification of Ni–N–O Bond Angles and NO Activation by X-ray Emission Spectroscopy. *Inorg. Chem. 60*(2), 736–744. https://doi.org/10.1021/acs. inorgchem.0c02724
- Tanya Nesterova, University of Delaware:

  - "Targeting the Deadly Coils of Ebola." https://www.xsede.org/-/targeting-the-deadly-coils-of-ebola. December 22, 2021.
  - "Using supercomputers to combat Ebola." https://www.newswise.com/articles/using-supercomputers-to-combat-ebola. October 20, 2020.

August 1 – October 31, 2020

- Anonymous participant: "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." (written in October 2020)
- Alan Andonian, University of Massachusetts Dartmouth:

  - "The Empower program has given me the opportunity to research and implement software for the conversion of tomographic images to 3D meshed volumes. The Goal being to take the 3D volume into Abaqus for FEA analysis. Participation in the EMPOWER program has helped me grow my capabilities with Finite Element Software and my ability to do computational research. The EMPOWER program has allowed me to learn about 3D visualization software and the process behind creating a CT to FEA workflow. For research projects I learned the important of creating a plan and documenting steps." (written October 2020)
- Nicholas Grabill, Michigan State University:

  - **Grabill, N.** (2020, August 4). *Analysis of Scaling Techniques in SEE Image Segmentation Software Utilizing Evolutionary Algorithms*. Poster presented at the 2020 MID-SURE Research Symposium, Michigan State University.
- Umair Khan, Portland State University:

  - "My work in the Reichow 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. In particular, the EMPOWER program has supported my long-term

participation in the lab, particularly over the summer months. Otherwise, I would be unable to dedicate extended and uninterrupted time towards the Reichow Lab's various research projects. Continued support from XSEDE is the reason I have co-authored recent publications." (written October 2020)

- Tanya Nesterova, University of Delaware:

  - Xu, C., Katyal, N., **Nesterova, T.**, & Perilla, J.R. (2020, October 20). Molecular determinants of Ebola nucleocapsid stability from molecular dynamics simulations. *The Journal of Chemical Physics, 153*(15). https://doi.org/10.1063/5.0021491
- Christopher Sherald, University of Kansas:

  - **Sherald, S.** (2020, November 6). *A first-principles investigation of V2O5 as a sensor.* Poster presented at the National Society of Black Physicists 2020 Conference. Won best poster award.
  - "As an aspiring physicist, the XSEDE EMPOWER program has helped me in realizing my career goals in a number of ways. The program is currently helping to familiarize me with programming and supercomputing, to learn more about data analysis, and providing computation resources that will help in speeding up sizeable simulations. My research with XSEDE and my current mentor is being used to create a presentation at the National Society of Black Physicists (NSBP) conference." (written October 2020)
- Adith Srivatsa, Georgia Institute of Technology:

  - "My participation with the EMPOWER program has given me a better understanding of ion channels, its mechanism, and its generalizability across all fields. Under the guidance of my mentor, I was able to critically analyze literature, develop novel protocols, and reach out to experts in the field for advice on my scripts. I believe that EMPOWER has allowed me to have a better vision for the direction of simulation research. I hope to continue getting hands-on experience in the future. Two abstracts for poster presentations were submitted to the Biophysical Society Annual Meeting as a result of the work performed under the EMPOWER program. I am the first author on the submission "Molecular dynamic simulations suggest novel PIP2 binding sites for SK2 channels regulation". I am second author on the submission "Utilizing umbrella MD sampling to assess contradictory PIP2 binding site in the membrane embedded SK2-CaM complex to help further understanding of sk2 activation"." (written October 2020)
- Billy Stone, University of Colorado Colorado Springs:

  - "I'm grateful for the program because it connected me to a professor that could teach me these techniques [in multiscale (quantum mechanical/ classical mechanical) chemical simulations]. I am presenting at the Biophysical Society annual meeting in Feb. 2021, and hopefully a publication will follow shortly after that." (written October 2020)

May 1 – July 31, 2020

- Alexandra Ballow, Youngstown State University:

  - Presentation at Scientific Computing with Python Virtual Conference (SciPy 2020): https://www.youtube.com/watch?v=Av5htgmVb3s
- Olivia Shaw, University of Delaware:
  - **Shaw, O.R.**, & Hadden-Perilla, J.A. (2020, July 23). TactViz: A VMD Plugin for Tactile Visualization of Protein Structures. *Journal of Science Education for Students with Disabilities, 23*(1). https://doi.org/10.14448/jsesd.12.0015
- Tori Zottarelli, University of Portland:

  - **Zottarelli, T.** & Taylor, B. (2020, July 29). *DFT Studies of the Transmetalation Mechanism in Stille Cross-Coupling Reactions.* Poster presented at the virtual MU3CCC Conference, Iowa State University.

February 1 – April 30, 2020

- Umair Khan, Portland State University:
  - Yue, B., Haddad, B.G., **Khan, U.**, Atalla, M., Reichow, S.L., & Bai, D. (2020, February). *Functional Characterization of VJ-gating and Single Channel Conductance of Sheep Cx46 and Cx50 Gap Junctions.* Poster presented at the 64th Annual Meeting of The Biophysical Society, San Diego, CA. https://doi.org/10.1016/j.bpj.2019.11.1573
- Andrew Roberts, Southwestern Oklahoma State University, participant in spring 2020:

  - **Roberts, A.**, & Evert, J. (2020, March). *Using Supercomputers to Control Multiple Robots.* Poster presented at Oklahoma Research Day, Weatherford, OK.
- Vatsal Shah, New Jersey Institute of Technology:

  - Tong, A., Pham, Q.L., **Shah, V.**, Naik, A., Abatemarco, P., & Voronov, R. (2020, February 12). Automated Addressable Microfluidics Device for Minimally Disruptive Manipulation of Cells and Fluids within Living Cultures. *ACS Biomater. Sci. Eng., 6*(3), 1809-1820. https://doi.org/10.1021/acsbiomaterials.9b01969
- Olivia Shaw, University of Delaware:

  - "A Bright Future in Research." https://www.udel.edu/udaily/2020/april/blind-chemistry-student-research/. April 3, 2020.
- Lindsey Tam, Pomona College:

  - (email from mentor) "We released V2.0 of the app that was developed in part with the grant from Shodor/EMPOWER program which is mentioned in About section. Lindsey Tam, a Math major from Pomona College worked on the content last summer and led a group of 6 or so students to develop additional functionality using Pomona College's Hahn grant the rest of the year. https://apps.apple.com/us/app/hpc-pondr/id1486499863" (written March 2020)

November 1, 2019 – January 31, 2020

- Mackenzie Tygh, Haverford College:
  - "I will present my work at the 2020 meeting of the American Astronomical Society."

August 1 – October 31, 2019

- Hamid Abbasi, Rutgers University, and Christian Wagner, Hood College:

- "We co-authored a paper, generated a poster, and participated in a joint formal presentation of our work throughout the summer with our mentor and some of his other interns." (written August 2019)
- Braden Box, Southwestern Oklahoma State University:

  - "SWOSU Students Win Two Firsts at High Performance Computing Competition" https://www.swosu.edu/news/2019/2019-09-30b.php. September 30, 2019.
- Matthew Veter, Portland State University:

  - "I will presenting the preliminary data I have collected at a computational conference scheduled on August 22 for dissemination of my findings at the NSF-sponsored PacNOW symposium held in Portland, OR." (written August 2019)

May 1 – July 31, 2019

- Alfonso Guevara, University of Houston Clear Lake:

  - **Guevara, A.**, & Kindla, N. (2019, July). *Solving the Traveling Salesmen Problem with IBM Q Quantum Computers*. Poster presented at PEARC '19: Practice and Experience in Advanced Research Computing, Chicago, IL.
- David Hughes, California State Polytechnic University-Pomona:
  - "My major is Computer Science, so academically the program has given me exposure to modern subjects in the field. I had a chance to experience various topics like new programming languages, super-computers, advanced math, etc. that are not part of a normal curriculum. The amount of knowledge and experience I gained through the program directly exceeds what any lecture class could possibly give to a typical undergraduate student. Professionally, the program has greatly improved my public speaking skills and abilities to talk about Computer Science. Due to working with my mentor, I have taken part in giving guest lectures, going to research fairs, and talking to individuals and large groups about my research. In the past I dreaded public speaking, but now the XSEDE EMPOWER program has given me confidence in an area that is not directly related to what was written in the project summary. The XSEDE EMPOWER program was instrumental in helping me be chosen to be my University's College of Science Valediction; this year there happened to be four perfect GPAs vying for the honor, so student research made an enormous impact on the faculty's decision. Additionally, the aforementioned effects on public speaking skills made it easy for me to give my speech in front of hundreds of people at commencement." (written June 2019)
  - "College of Science to Honor Two Valedictorians." http://polycentric.cpp.edu/2019/05/college-of-science-to-honor-two-valedictorians/. May 17, 2019.
- Diego Losada Rubio, Wofford College:

  - "As first year student I had the opportunity to experience by first hand the world of High Performance Computing and so this was an experience that I will never forget and regret. Thanks to XSEDE EMPOWER Program, apart from learning, working and exploring with my mentor about parallel computing concepts using Little Fe on Physics, I was able to travel to the Petascale Institute and get to know with other students the main ideas of the concepts on parallel computing that I was going to learn right after during that summer and also I was able to go to the PEARC18 and meet lots of passionate and intelligent people that work on the world of High Performance Computing. The XSEDE EMPOWER Program helped me to understand and learn complicated concepts and challenges on parallel computing and simulations. And those challenges that I once overcame are going to help me now in a new summer research experience where I am going to be doing molecular dynamics simulations using a supercomputer." (written May 2019)
- Tanya Nesterova, University of Delaware:

  - "I attended a National Institutes of Health (NIH) meeting on the structural biology of HIV. I have also produced a poster for a chemistry /biochemistry conference in my university's department and the Summer Scholars conference. I presented this poster to colleagues in the chemistry and biology field. I also went to the data science symposium in my university and provided a lightning talk and presented my poster in front of other faculty and students who do research in mathematics and computational science. I networked and met people who also do work like mine in chemistry." (written July 2019)
- Daniel Norment, California State Polytechnic University, Pomona:

  - YouTube video summarizing project work: https://www.youtube.com/watch?v=K7fqzHzSpdI
- Ryan Oostland, Bluffton University. "Senior and professor collaborate on research." https://www.bluffton.edu/news/_beaversall /Beavers062019ryanoostland.aspx. June 20, 2019.
- Manuel E Santiago Rodríguez, University of Puerto Rico-Mayagüez:

  - **Santiago, M.**, Torres, G., & Araya, G. (2019). *High order statistics in Favorable Pressure Gradient (FPG) flows*. Unpublished manuscript.
  - "My participation in the XSEDE EMPOWER program had a positive impact on my academic and professional life. Participation helps me increase my knowledge and experience. Now I have a better knowledge of turbulent flow behavior and better programming skills. In my professional life, I would like to participate in future research like this. My participation in the XSEDE EMPOWER program helped me overcome the challenges. It helps me increase my confidence. In the research, we found reasonable results that can help predict the behavior of the turbulent flow population. The results have created an inclination in me for research and graduate school. The mentor I had was excellent." (written June 2019)
- Bimarsh Sharma, West Virginia University Institute of Technology:

  - **Sharma, B.**, Carter, T., & Rai, S. (2019, June 15). *Using NetLogo to Simulate Building Occupancy of a University Building Environment*. Presented at the 2019 ASEE Annual Conference & Exposition, Tampa, Florida.
- Rylee Sundermann, South Dakota State University:
  - **Sundermann, R.**, Stegmeier, N., McClanahan, N., Kimn, J.-H., & Doom, J. (2019, July). *3D Simulations of Biofilms using the Modified Cahn-Hilliard Equation*. Poster presented at PEARC '19: Practice and Experience in Advanced Research Computing, Chicago, IL.

February 1 – April 30, 2019

- Maritza Anguiano Carrillo, California State University-San Marcos:
  - "My mentor and I have begun a tutorial session for new students wanting to participate in future research." (written February 2019)
- April Horton, Bluffton University:

- (email from mentor) "Last week April Horton received offers from two REU programs in Astronomy: The University of Hawaii, and The University of Wisconsin-Madison. Both had a computational slant—based on her EMPOWER project, a computational science course I taught and other programming courses at Bluffton. The University of Hawaii was her top choice for REU; she'll be headed there soon after spring semester." (written March 2019)
      - "I presented at Bluffton University's Research Fair for my XSEDE EMPOWER Program internship entitled "Sonification and Visualization of Scientific Data." This poster presentation session allowed me to share my research with other Bluffton students while encouraging them to pursue research opportunities they are interested in."
- David Hughes, California State Polytechnic University-Pomona:
      - **Hughes, D.**, & Ji, H. (2019, March 1). Novel Randomized Linear Algebra in Apache Spark. Poster presented at the 2019 Student RCSA Conference, Pomona, CA.
- Xinlian Liu (EMPOWER mentor), Hood College:

      - "Researchers Attempt To Predict & Prevent Suicide Using Deep Learning And Math." https://www.forbes.com/sites/robinseatonjefferson/2019/04/15/researchers-confident-deep-learning-and-math-can-help-end-veteran-suicide. April 15, 2019.
- Felix Quintana, participant in spring 2019:
      - **Quintana, F.**, Kodera A., Horan, B.G., Yamashiro, S., Mittal, J., Watanabe, N., & Vavylonis, D. (2019, March). *Mechanism of formin-mediated actin polymerization: alternate delivery of profilin-actin to the barbed end.* Poster presented at the 63rd Annual Meeting of the Biophysical Society, Baltimore, MD.
- Bimarsh Sharma, West Virginia University Institute of Technology:
      - **Sharma, B.**, Carter, T., & Rai, S. (2019, February 26). *Using NetLogo To Create Building Occupancy Simulation of University Building Environment.* Poster presented at the 16th Annual Undergraduate Research Day at the Capitol, Charleston, WV.

November 1, 2018 – January 31, 2019

- Phan Phu, California State Polytechnic University-Pomona:

      - Kundu, S., **Phu, P.N.**, Ghosh, P., Kozimor, S.A., Bertke, J.A., Stieber, S.C.E., & Warren, T.H. (2019, January 2) Nitrosyl Linkage Isomers: NO Coupling to N2O at a Mononuclear Site. *J. Am. Chem. Soc., 141*(4), 1415-1419. http://doi.org/10.1021/jacs.8b09769
- Jean Santiago, University of Puerto Rico-Mayagüez:
      - **Santiago, J.**, Araya, G., Marin, G., & Cucchietti, F. (2018, November). *Symbiosis of quasi-streamwise vortices and low-speed streaks in laminarescent boundary layers.* Visualization presented at the Gallery of Fluid Motion at the Annual Meeting of the American Physical Society Division of Fluid Dynamics, Atlanta, GA. https://gfm.aps.org/meetings/dfd-2018/5b97f004b8ac31610362f38b

August 1 – October 31, 2018

- David Hughes, California State Polytechnic University-Pomona:
      - "I created an XSEDE/Bridges user guide and gave a lecture about my project, XSEDE, Bridges, and Spark to the Big Data Analytics course on my campus." (written October 2018)
- Diego Losada Rubio and Taeyoung Shin, Wofford College:

      - "Paid to learn: Students delve into the world of high performance computing." http://wofford.edu/newsroom/2018/Paid-to-learn/. September 14, 2018.

May 1 – July 31, 2018

- Mark Hisle, Centre College, and Maxwell Meier, Earlham College:

      - **Hisle, M.S.**, **Meier, M.S.**, & Toth, D.M. (2018, July). Accelerating AutoDock Vina with Containerization. *Proceedings of the Practice and Experience in Advanced Research Computing (PEARC '18).* ACM, New York, NY, USA, Article 36, 5 pages. https://doi.org/10.1145/3219104.3219154
- Phan Phu, California State Polytechnic University-Pomona:
      - **Phu, P.N.**, & Stieber, S.C.E. (2018, July 27). *Understanding the Mechanism for Disproportionation of NO at Copper Center through DFT X-ray Emission Spectroscopy.* Presentation at UC Irvine SoCal Undergraduate Research Symposium, Irvine, CA.
- Jean Santiago, University of Puerto Rico-Mayagüez:
      - Araya, G. & **Santiago, J.** (2018, June 5). *Quasi laminarization process induced by Strong Favorable Pressure FPG gradient* [Video file]. Retrieved from https://www.youtube.com/watch?v=LaUYJ6NBKwE
- Brian O. Torres Torres, University of Puerto Rico-Mayagüez:
      - "I was part of the XSEDE EMPOWER program as a learner for one semester where I worked with my professor Ana Gonzalez on a parallel computing project. This opened up many doors for me since it was my first work experience out of my curriculum related to my major and recruiters seem to be very interested in what I did with my professor. By being part of the program I was able to secure a COOP with NAVSEA in Newport for the upcoming semester. In addition, before starting the program I was not sure if I wanted to pursue a graduate degree and now I have decided to do a Masters on Computer Science and I am considering applying for Georgia Tech's MS in machine learning. Honestly the program helped professionally and academically and it's something I will never regret doing." (written June 2018)
- Brandon Ubiera, Hood College:

      - (email from mentor) "First of all, we deeply appreciate this opportunity. This opportunity of the exposure to HPC and computational research means a lot for a small regional institution like Hood College. Our EMPOWER intern Brandon Ubiera was able to learn about parallel computing, deep learning, UNIX administration while helping me with system configuration and out-reaching. We have a student poster accepted by PEARC 18 [...]." (written June 2018)

February 1 – April 30, 2018

- Phan Phu, California State Polytechnic University-Pomona:
      - **Phu, P.N.**, (2018, March). *Quantifying Metal-Nitrosyl Coordination Modes and Oxidation States through X-ray Emission Spectroscopy and Density Functional Theory.* Presentation at COMP Undergraduate Workshop, 255th American Chemical Society National Meeting and Exposition, New Orleans, LA.

- "On January 13, 2018, I presented "Spectroscopic and Computational Studies of Metal Nitrosyl Complexes to Elucidate the Mechanism of Nitrite Reductase" at 30th Annual CSU Biotechnology Symposium in Santa Clara, California"

May 1 – July 31, 2017

- Adrian Rodriguez, Auburn University at Montgomery:
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