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14. ABSTRACT

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a. REPORT UU	b. ABSTRACT UU	c. THIS PAGE UU	19b. TELEPHONE NUMBER 609-737-1902

RPPR Final Report

as of 11-Feb-2019

Agency Code:

Proposal Number: 72270CHCF

Agreement Number: W911NF-17-1-0550

INVESTIGATOR(S):

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DUNS Number: 605799469

EIN: 916001537

Report Date: 14-Dec-2018

Date Received: 08-Feb-2019

Final Report for Period Beginning 15-Sep-2017 and Ending 14-Sep-2018

Title: Support for the ECS Data Sciences Hack Day

Begin Performance Period: 15-Sep-2017

End Performance Period: 14-Sep-2018

Report Term: 0-Other

Submitted By: Daniel Schwartz

Email: dts@uw.edu

Phone: (609) 737-1902ext

Distribution Statement: 1-Approved for public release; distribution is unlimited.

STEM Degrees:

STEM Participants:

Major Goals: ARO funding was used to partially support 20 participants, mostly early career scholars, at ECS Data Science Hack events at the 232nd and 233rd meetings of the electrochemical society. Research products include two papers accepted for publication, datasets and software. All research products are in long-lived archives and repositories with associated digital object identifiers.

Accomplishments:

Hack Day
<https://www.electrochem.org/232/hack-day/>

ARO funding was used to provide travel support for 14 participants (25 total attendees) in the inaugural ECS Hack Day in National Harbor, MD. The Hack Day participants traveled from around the globe and represented varying stages of careers in both academic and industry roles. The morning session consisted of a series of short tutorials covering the basics of open science tools (e.g. introductions to Python, Jupyter notebooks, and version control). During lunch, ideas for afternoon projects were pitched and teams for the afternoon session were formed around common interests. The remaining time was reserved for "hacking" on the projects.

The feedback from participants centered around several themes:

- * significant interest in continuing ECS Data Science Hack events
- * make future events longer to allow time for more learning, hacking, and interaction
- * provide introductory lesson material online, in advance for those who want to take their time learning before the event

Hack Week

<https://www.electrochem.org/233/hack-week>

Based off of this feedback, a week-long ECS Data Science Hack Week was organized at the ECS Meeting in Seattle, WA from May 14th to 19th, 2018. Remaining ARO funding was used to provide travel support for 6 of the participants (36 total). Based on the feedback from the Hack Day, a website (<https://ecshackweek.github.io/>) was created to provide the introductory information that was covered during the optional Monday and Tuesday afternoon Hack Week tutorials. Wednesday and Thursday morning offered participants a chance to learn about several advanced topics from outside experts (machine learning, Python packaging, cloud computing, and data visualization), while the afternoon was reserved for project "hacking" time. Friday was an opportunity for participants to make some last minute progress on their projects and then present to the group at an evening wrap-up event at the UW eScience studio.

RPPR Final Report

as of 11-Feb-2019

ECS provided hotel room space for both events, and featured Hack Events prominently.

The organizers and participants were delighted with the Hack Week format. It allowed for significant interaction between attendees, and significant training elements. Early tutorials were optional for more experienced software developers. The schedule for Hack Week was:

Monday, May 14

- 1300-1600h — (Optional Segment) Introduction to Data Science Tools #1 (using the shell/terminal, version control)
- 1930-2030h — Hack Week Kickoff Event

Tuesday, May 15

- 1300-1600h — (Optional Segment) Introduction to Data Science Tools #2 (introduction to Python using Conda and Jupyter)

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- 0830-1200h — Intermediate Python Topics (documentation and testing)
- 1200-1300h — Project Updates/Ideation and Team Formation (over lunch)
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- 0830-1200h — Project Hacking Time
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- 1330-1630h — Project Hacking Time
- 1700-1900h — Project Presentations and Wrap Up

Saturday, May 19 (Optional)

- 0900-1300h — (Optional) Social Event (clamming in the Puget Sound area)
- 1300-1700h — (Optional) Social Event Continues (cooking the catch and socializing)

Attendees were surveyed anonymously, and some of the comments related to open-software tools included:

- “Hack week provided me with the basis of tools and understanding to create accessible research that can be used by the community. I also found that my project, and others have very broad applications with only minor tweaks.”
- “I code in Python a lot, so the idea that a bit of effort combined with direction from a domain expert could make someone else’s research easier, faster, or more repeatable is really exciting.”

Additionally, the introductory and advanced tutorials throughout the week provided a chance for Hack Week attendees to learn and practice data science and computational skills that were transferable to their own fields/research.

Attendee comments related to educational training included

- “learned more in five days than I thought was possible”
- “Very good initiative, you get to learn a lot of new stuff and refresh old stuff”
- “ECS Hack week was one of the best things I could have done to compliment my PhD research. I only wish I could have done this years ago!”

Attendee comments related to community building included:

- “More possible collaborations can happen because of its openness”
- “ECS Hackweek was a really great experience for me to learn more about what other members are doing, and I had the opportunity to collaborate with some other really great scientists who are passionate about open science too.”

RPPR Final Report as of 11-Feb-2019

Overall, the success in creating open-software tools, providing educational training, and building an electrochemical data science community was reflected by the responses related to future events:

- 100% of participants in Hack Week would participate in a future ECS Data Science Hack event
- 100% would recommend a future ECS Data Science Hack event to a colleague

ECS Hack Event cycle

Iterating through the first two ECS Data Science events and taking into account the feedback from attendees has evolved into an ECS-approved plan for an annual cycle of events:

Spring meeting – a week-long Hack Week style event focused on education, bringing new individuals into the community, and providing an opportunity for attendees to learn about new techniques, best practices, and tools for reproducible and open data and software.

Fall meeting – a symposium style Showcase focused on reaching out to the wider ECS community through traditional research presentations, and a two-day Community Sprint focused on making significant short-term progress to open-software tools.

Ultimately, one could imagine a four part track for bringing in a new individual into a strong and collaborative electrochemical data science community:

1. Introduction to data science techniques and computational skills at Hack Week
2. Participation as a contributor to a new or existing open data or software project at the Hack Sprints
3. Participation as an instructor/helper at their second Hack Week
4. Presenting a talk at the Showcase on an open software or data project they've contributed to over the past year

Training Opportunities: Both Hack Day and Hack Week had an education and training element that sought to teach how to develop open, reproducible software tools. Training provided attendees an opportunity to learn best practices in code sharing and version control. However, single-day training in Hack Day proved problematic for neophytes, and whereas a week-long ECS event was well received by experienced and neophyte electrochemical data scientists.

An anonymous survey of Hack Week participants probed their skill level and use of public repositories for data and software products before and after the Hack Week event. The majority (60%) of Hack Week participants Disagreed or Strongly Disagreed with the statement “Before ECS Hack Week, most of my code and data was already on GitHub, OSF, or another public repository.” In contrast, the vast majority (90%) Agreed or Strongly Agreed with the statement, “I put code and/or data I created at ECS Hack Week up on GitHub, and OSF page, or another public repository.” This is one example of the learning promoted at the Hack events.

RPPR Final Report as of 11-Feb-2019

Results Dissemination: Hack Day and Hack Week education and research products are primarily disseminated as via the Center for Open Science's Open Science Framework (OSF) repository, with individual project component repositories. Research products include the following software and datasets.

Hack Day, National Harbor, MD

Outputs from the one-day inaugural Hack Day is archived on the Open Science Framework (OSF) project page. Because of the short time frame, many small projects were seeded into the effort.

The archived Hack Day OSF webpage is:

Murbach, M. D., Hendricks, C., Beckner, W. A., Chen, J., Yess, M., Schwartz, D. T., ... Dixit, M. ECS Data Science Hack Day 2017. <https://doi.org/10.17605/OSF.IO/Z4XKN>

Within this OSF page are the following project components

Murbach, M. D. (2018, May 16). Project: NASA Battery Prognostics Data. Retrieved from osf.io/swp9b

Chen, J., & Murbach, M. D. (2017, October 4). Project: Machine learning for battery degradation. Retrieved from osf.io/mkz7p

Murbach, M. D., Dixit, M., Karuppaiah, C., DeCaluwe, S. C., & Das, T. (2017, October 4). Project: Software tools for analyzing rotating disk electrode data. Retrieved from osf.io/qrhcw

Murbach, M. D. (2017, September 29). Project: Software tools for fitting open-circuit potential data. Retrieved from osf.io/vebdq

Hendricks, C., Stanley, P., Kononova, O., Haeberle, M., & Saxena, S. (2017, October 4). XPS Data from Li-Ion Battery Anodes. Retrieved from osf.io/58mw9

Beckner, W. A., Murbach, M. D., & Beck, D. (2017, October 4). Project: Genetic Algorithms with RDKit for Molecular Structure Search. Retrieved from osf.io/h3zuc

Hack Week, Seattle, WA

An OSF project page was created to gather the outputs from the ECS Hack Week effort. Each of these projects are more substantial, and have had follow-on work.

Murbach, M. D., Juhasz, G., Yess, M., Chavan, K., Baroody, H., Teo, L., ... Parke, C. D., 2018 ECS Hack Week Seattle. <https://osf.io/hefmb>

The longer format of the Hack Week provided additional time for deeper project "hacking" focused on:

Mirabal, A., Murbach, M. D., Daramola, D., & Gibson, L. (2018, September 29). NanoParticle Image Analysis. Retrieved from osf.io/5nhf9

Bonezzi, J., Murbach, M. D., Feng, Z., Pang, Q., Dawson-Elli, N., Timbillah, S., & sarfo. (2018, November 29). [impedance.py](https://osf.io/cpxgj). Retrieved from osf.io/cpxgj

Chavan, K., Budanovic, M., Schwartz, D. T., & Beck, D. (2018, May 17). Redox potential prediction based on molecular properties. Retrieved from osf.io/x95kw

Baroody, H., & Muzaffar, T. (2018, May 20). Platinum cyclic voltammetry scan facet detection through image classification. Retrieved from osf.io/5pw6c

Cohen, T., Senju, A., & DEVKOTA, J. (2018, May 19). Peak Shoulder Finder. Retrieved from osf.io/87zkh

Hu, V., Murbach, M. D., Teo, L., Zhao, M., Masse, R., & Kimura, K. (2018, June 6). GITT-Toolkit. Retrieved from

RPPR Final Report as of 11-Feb-2019

osf.io/ny28q

Beckner, W. A. (2018, May 22). python package creation demo. Retrieved from osf.io/ny28q

ECS will feature data science in the Spring 2019 Electrochemical Society Interface issue, co-edited by Daniel T. Schwartz, Matthew D. Murbach, and David A.C. Beck, the co-founders of ARO funded ECS Data Science Events. Two papers accepted for publication cite ARO support:

D.T. Schwartz, M.D. Murbach, and D.A.C. Beck, "ECS in the Era of Data Science", ECS Interface, DOI: 10.1149/2.F03191if Accepted (2019).

M.D. Murbach and D.T. Schwartz, "Open Software and Datasets for the Analysis of Electrochemical Impedance Spectra", ECS Interface, DOI: 10.1149/2.F05191if Accepted (2019).

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Chen, J., & Murbach, M. D. (2017, October 4). Project: Machine learning for battery degradation. Retrieved from osf.io/mkz7p

Murbach, M. D., Dixit, M., Karuppaiah, C., DeCaluwe, S. C., & Das, T. (2017, October 4). Project: Software tools for analyzing rotating disk electrode data. Retrieved from osf.io/qrhcw

Murbach, M. D. (2017, September 29). Project: Software tools for fitting open-circuit potential data. Retrieved from osf.io/vebdq

Hendricks, C., Stanley, P., Kononova, O., Haeberle, M., & Saxena, S. (2017, October 4). XPS Data from Li-Ion Battery Anodes. Retrieved from osf.io/58mw9

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RPPR Final Report as of 11-Feb-2019

Bonezzi, J., Murbach, M. D., Feng, Z., Pang, Q., Dawson-Elli, N., Timbillah, S., & sarfo. (2018, November 29). impedance.py. Retrieved from osf.io/cpxgj

Chavan, K., Budanovic, M., Schwartz, D. T., & Beck, D. (2018, May 17). Redox potential prediction based on molecular properties. Retrieved from osf.io/x95kw

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Hu, V., Murbach, M. D., Teo, L., Zhao, M., Masse, R., & Kimura, K. (2018, June 6). GITT-Toolkit. Retrieved from osf.io/ny28q

Beckner, W. A. (2018, May 22). python package creation demo. Retrieved from osf.io/yu25g

Honors and Awards: The organizers have been invited to create a special issue of ECS Interface focused on electrochemical and solid state data science for Spring, 2019. The special issue will be edited by Professor Schwartz, Professor Beck, and Dr. Murbach from the University of Washington.

Protocol Activity Status:

Technology Transfer: All software and datasets associated with Hack Events at ECS are licensed under open access copywriting standards via Creative Commons or MIT licensing. Hack Event research is freely available for reuse by researchers worldwide.

PARTICIPANTS:

Participant Type: Graduate Student (research assistant)

Participant: Yoolhee Kim

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Daniel Parr

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Saurabh Saxena

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

RPPR Final Report
as of 11-Feb-2019

Participant Type: Staff Scientist (doctoral level)

Participant: Steven DeCaluwe

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Abhishek Sarkar

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Lynza Sprowl

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Olga Kononova

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Hamid Reza Seyf

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Yuanchao Liu

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

RPPR Final Report
as of 11-Feb-2019

Participant Type: Staff Scientist (doctoral level)

Participant: Min Zheng Haeberle

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Tridip Das

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Staff Scientist (doctoral level)

Participant: Lok-kun Tsui

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Staff Scientist (doctoral level)

Participant: Ross Fontenot

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Patrick Stanley

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Daniel L. Parr IV

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

RPPR Final Report
as of 11-Feb-2019

Other Collaborators:

Participant Type: Staff Scientist (doctoral level)

Participant: Damilola Daramola

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Alex Mirabal

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Kanchan Chavan

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Meng Zhao

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Participant Type: Graduate Student (research assistant)

Participant: Qin Pang

Person Months Worked: 1.00

Funding Support:

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

RPPR Final Report
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Report of ARO funds for ECS Hack Day

Summary of Events

Accomplished

Hack Day

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The feedback from participants centered around several themes:

- ❖ significant interest in continuing ECS Data Science Hack events
- ❖ make future events longer to allow time for more learning, hacking, and interaction
- ❖ provide introductory lesson material online, in advance for those who want to take their time learning before the event

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Attendees were surveyed anonymously, and some of the comments related to open-software tools included:

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Attendee comments related to educational training included

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- “Very good initiative, you get to learn a lot of new stuff and refresh old stuff”
- “ECS Hack week was one of the best things I could have done to compliment my PhD research. I only wish I could have done this years ago!”

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Ultimately, one could imagine a four part track for bringing in a new individual into a strong and collaborative electrochemical data science community:

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3. Participation as an instructor/helper at their second Hack Week

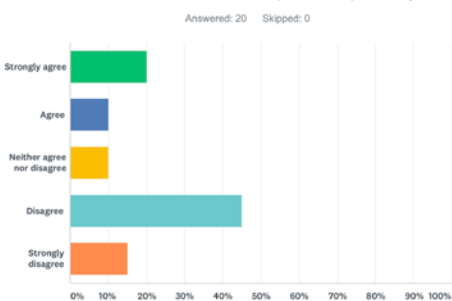
4. Presenting a talk at the Showcase on an open software or data project they've contributed to over the past year

Training

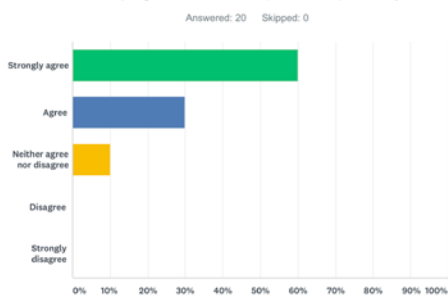
Both Hack Day and Hack Week had an education and training element that sought to teach how to develop open, reproducible software tools. Training provided attendees an opportunity to learn best practices in code sharing and version control. However, single-day training in Hack Day proved problematic for neophytes, and whereas a week-long ECS event was well received by experienced and neophyte electrochemical data scientists.

Below is an example from the anonymous survey of Hack Week participants regarding their skill level and use of public repositories for data and software products.

Before ECS Hack Week, most of my code & data was already on GitHub, OSF, or another public repository.



I put code and/or data I created at ECS Hack Week up on GitHub, an OSF page, or another public repository.



Dissemination

Hack Day and Hack Week education and research products are primarily disseminated as via the Center for Open Science's Open Science Framework (OSF) repository, with individual project component repositories. Research products include the following software and datasets.

Hack Day, National Harbor, MD

Outputs from the one-day inaugural Hack Day is archived on the Open Science Framework (OSF) project page. Because of the short time frame, many small projects were seeded into the effort.

The archived Hack Day OSF webpage is:

Murbach, M. D., Hendricks, C., Beckner, W. A., Chen, J., Yess, M., Schwartz, D. T., ... Dixit, M. ECS Data Science Hack Day 2017. <https://doi.org/10.17605/OSF.IO/Z4XKN>

Within this OSF page are the following project components

Murbach, M. D. (2018, May 16). Project: NASA Battery Prognostics Data. Retrieved from osf.io/swp9b

Chen, J., & Murbach, M. D. (2017, October 4). Project: Machine learning for battery degradation. Retrieved from osf.io/mkz7p

Murbach, M. D., Dixit, M., Karuppaiah, C., DeCaluwe, S. C., & Das, T. (2017, October 4). Project: Software tools for analyzing rotating disk electrode data. Retrieved from osf.io/qrhcw

Murbach, M. D. (2017, September 29). Project: Software tools for fitting open-circuit potential data. Retrieved from osf.io/vebdq

Hendricks, C., Stanley, P., Kononova, O., Haeberle, M., & Saxena, S. (2017, October 4). XPS Data from Li-Ion Battery Anodes. Retrieved from osf.io/58mw9

Beckner, W. A., Murbach, M. D., & Beck, D. (2017, October 4). Project: Genetic Algorithms with RDKit for Molecular Structure Search. Retrieved from osf.io/h3zuc

Hack Week, Seattle, WA

An OSF project page was created to gather the outputs from the ECS Hack Week effort. Each of these projects are more substantial, and have had follow-on work.

Murbach, M. D., Juhasz, G., Yess, M., Chavan, K., Baroody, H., Teo, L., ... Parke, C. D., 2018 ECS Hack Week Seattle. <https://osf.io/hefmb>

The longer format of the Hack Week provided additional time for deeper project “hacking” focused on:

Mirabal, A., Murbach, M. D., Daramola, D., & Gibson, L. (2018, September 29). NanoParticle Image Analysis. Retrieved from osf.io/5nhf9

Bonezzi, J., Murbach, M. D., Feng, Z., Pang, Q., Dawson-Elli, N., Timbillah, S., & sarfo. (2018, November 29). *impedance.py*. Retrieved from osf.io/cpxgj

Chavan, K., Budanovic, M., Schwartz, D. T., & Beck, D. (2018, May 17). Redox potential prediction based on molecular properties. Retrieved from osf.io/x95kw

Baroody, H., & Muzaffar, T. (2018, May 20). Platinum cyclic voltammetry scan facet detection through image classification. Retrieved from osf.io/5pw6c

Cohen, T., Senju, A., & DEVKOTA, J. (2018, May 19). Peak Shoulder Finder. Retrieved from osf.io/87zkh

Hu, V., Murbach, M. D., Teo, L., Zhao, M., Masse, R., & Kimura, K. (2018, June 6). GITT-Toolkit. Retrieved from osf.io/ny28q

Beckner, W. A. (2018, May 22). python package creation demo. Retrieved from osf.io/yy25g

Honors

The organizers have been invited to create a special issue of *ECS Interface* focused on electrochemical and solid state data science for Spring, 2019. The special issue will be edited by Professor Schwartz, Professor Beck, and Dr. Murbach from the University of Washington.

Tech Transfer

All software and datasets associated with Hack Events at ECS are licensed under open access copywriting standards via Creative Commons or MIT licensing. Hack Event research is freely available for reuse by researchers worldwide.

Participants

ARO funding under this award provided travel support to 14 participants for attending the inaugural ECS Data Science Hack Day in National Harbor, MD (October 4, 2017) and 6 participants at the ECS Data Science Hack Week in Seattle, WA (May 14-19, 2018).

ECS Hack Day (National Harbor, MD)

- Yoolhee Kim (Carnegie Mellon U)
- Daniel Parr (University of Iowa)
- Saurabh Saxena (University of Maryland)
- Dr. Steven DeCaluwe (Colorado School of Mines)
- Lynza Sprowl (Oregon State University)
- Olga Kononova (University of California, Berkeley)
- Hamid Reza Seyf (Georgia Tech)
- Yuanchao Liu (Michigan State University)
- Min Zheng Haeberle (TE Connect)
- Abhishek Sarkar (Iowa State University)

- Tridip Das (Michigan State University)
- Dr. Lok-kun Tsui (University of New Mexico)

- Ross Fontenot (Naval Underseas Warfare Center)
- Patrick Stanley (University of Maryland)

ECS Hack Week (Seattle, WA)

- Daniel L. Parr IV (University of Iowa)
- Damilola Daramola, Ph.D. (Ohio University)
- Alex Mirabal (Michigan State University)

- Kanchan Chavan (Michigan State University)
- Meng Zhao (Stanford)
- Qin Pang (Oregon State University)