NSF OCI CAREER Workshop
ACCI Presentation

Workshop Co-Chairs:
Suzanne Shontz (Mississippi State University;
Formerly Penn State)
and Thomas Hacker (Purdue University)

December 12, 2012

Purpose of the Workshop

Goals:

- Networking to allow junior researchers to network with each other and with senior researchers.

- For NSF to give us an idea about OCI, and to provide feedback to NSF from CAREER awardees

Team:

- **Co-Chairs:** Suzanne Shontz (Penn State now Mississippi State) and Thomas Hacker (Purdue University)

- Discussed workshop ideas with Gabrielle Allen (former NSF OCI program director)

Purpose of the Workshop

Themes:

- **Grand Challenges in Computational- and Data-Enabled Science & Engineering (CDS&E) and Cyberinfrastructure**
- **Data-enabled Science and Engineering**
- **Visualization**
- **Computational-enabled Science and Engineering**
- **High Performance Computing**

Format:

- At Westin Arlington
- Continuous poster session
- Keynote talk followed by discussions
- One room, one track workshop

Workshop Attendees

- 26 attendees (from 24 institutions) and five keynote speakers attended the workshop

- Most attendees had CAREERS funded at least in part through OCI; several held awards partially funded through other directorates, including MPS, ENG, EHR, BIO, and CISE; seven attendees were funded entirely outside OCI
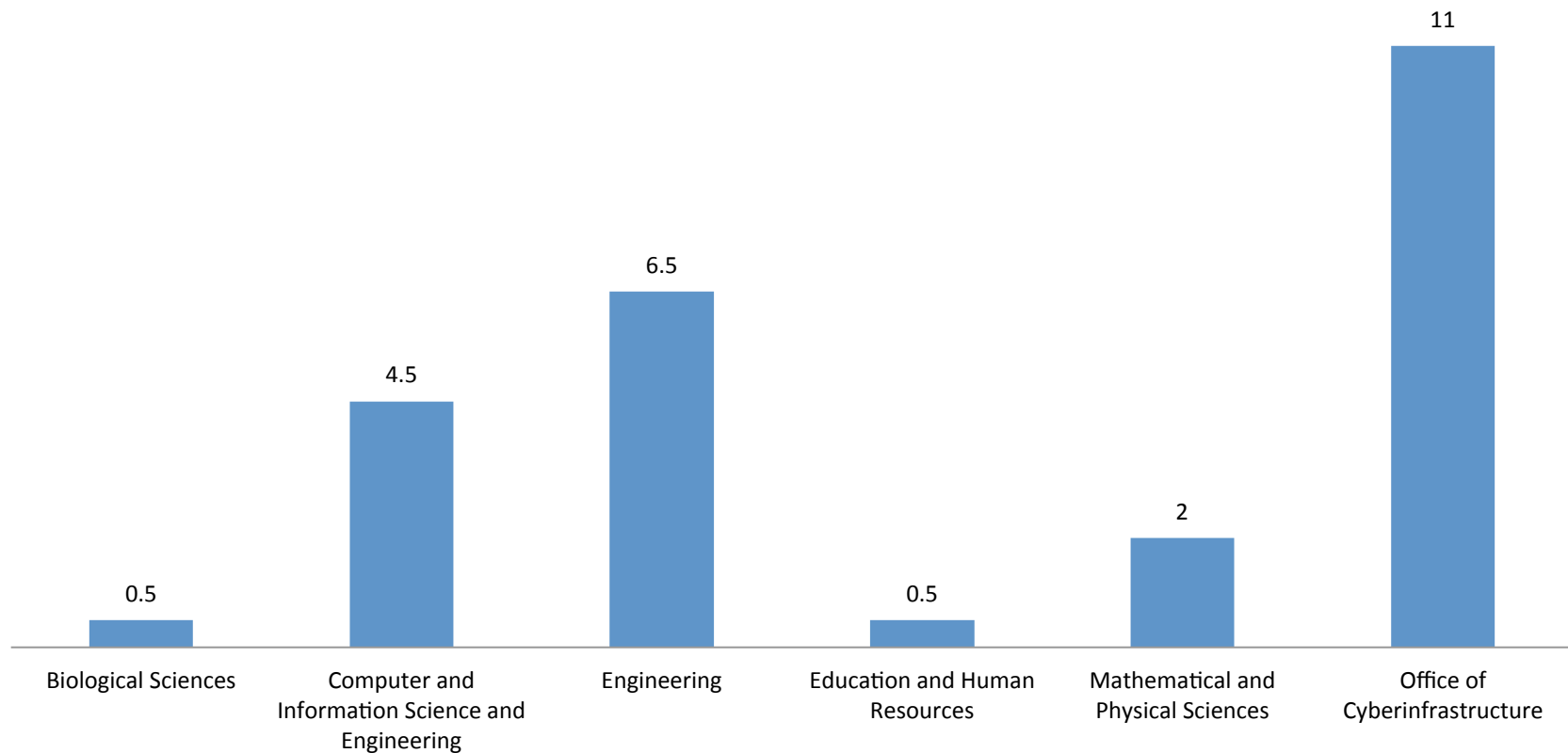
List of Attendees

- <u>Lorena Barba</u>, Assistant Professor in the Department of Mechanical Engineering at Boston University.
- <u>Luca Caracoglia</u>, Associate Professor in the Department of Civil and Environmental Engineering of Northeastern University
- <u>Diego Donzis</u>, Assistant Professor in the Department of Aerospace Engineering at Texas A&M University.
- <u>Gabriel Dos Reis</u>, Assistant Professor in the Department of Computer Science and Engineering at Texas A&M University.
- <u>Maria Emelianenko,</u> Associate Professor in the Department of Mathematical Sciences at George Mason University .
- <u>Baskar Ganapathysubramanian</u>, Assistant Professor of Mechanical Engineering and Electrical and Computer Engineering at Iowa State University.
- <u>Sophya Garashchuk</u>, Assistant Professor in the Department of Chemistry and Biochemistrya at the University of South Carolina.
- <u>Thomas Hacker</u>, Associate Professor in the Department of Computer and Information Technology at Purdue University.
- <u>Richard Hennig</u>, Assistant Professor in the Department of Materials Science and Engineering at Cornell University
- <u>Kapil Khandelwal</u>, Assistant Professor in the Department of Civil Engineering and Geological Sciences at Notre Dame University.
- <u>Xiaolin Li</u>, Associate Professor in the Department of Electrical and Computer Engineering at the University of Florida.
- <u>Laurence Loewe,</u> Assistant Professor in the Department of Genetics, University of Wisconsin-Madison
- <u>Alison Marsden</u>, Assistant Professor in the Department of Mechanical and Aerospace Engineering at UCSD.
- <u>Christian Ott</u>, Assistant Professor in the Department of Astronomy at Caltech

List of Attendees

- <u>Dario Pompili</u>, Assistant Professor in the Department of Electrical and Computer Engineering at Rutgers University

- <u>Ioan Raicu</u>, Assistant Professor in the Department of Computer Science at the Illinois Institute of Technology, as well as a guest research faculty in MCS at Argonne National Laboratory.

- <u>Pradeep Ravikumar</u>, Assistant Professor in the Department of Computer Science at the University of Texas at Austin. He is also affiliated with the Division of Statistics and Scientific Computation and the Institute for Computational Engineering and Sciences at UT Austin.

- <u>Pratim Sengupta</u>, Assistant Professor in the Department of Teaching and Learning at Vanderbilt University

- <u>Suzanne Shontz</u>, Assistant Professor in the Department of Computer Science and Engineering at The Pennsylvania State University.

- <u>Andres Tejada-Martinez</u>, Assistant Professor in the Department of Civil and Environmental Engineering at the University of South Florida.

- <u>Xavier Trioche</u>, Assistant Professor in the Department of Computer Science at Purdue University

- <u>Liqiang Wang</u>, Associate Professor in the Department of Computer Science at the University of Wyoming.

- <u>Clint Whaley</u>, Assistant Professor in the Department of Computer Science at the University of Texas at San Antonio

- <u>Xiong Yu</u>, Associate Professor in the Department of Civil Engineering at Case Western Reserve University, also holds a courtesy appointment in the Departments of Electrical Engineering, Computer Science, and Mechanical Engineering.

- <u>Jessica Zhang</u>, Associate Professor in the Department of Mechanical Engineering at Carnegie Mellon University with a courtesy appointment in the Department of Biomedical Engineering.

Keynote Talks/Areas/Formats

- **Ed Seidel:** *Paradigm Shifts in Science and Engineering*
  - *Introductory talk*
- **Miron Livny:** *Why Do I Build CI and What Did It Teach Me*
  - *Dr. Livny led a discussion among all attendees in a question/response format.*
- **Frederica Darema:** *From Big to New Capabilities*
  - *Dr. Darema posed several grand challenge questions, each of which were assigned to a discussion group to consider.*
    - *How do we create Comprehensive CyberInfrastructure Frameworks?*
    - *How do we foster "horizontal leverage" across CyberInfrastructures*
    - *What is the role and how to enable Academe-Industry Partnerships?*
    - *Education and Training within this terrain?*
- **Tinsley Oden:** *The Emergence of Predictive Computational Science: Tackling the Grand Challenges*
  - *Dr. Oden led a discussion among all attendees in a question/response format.*
- **Chris Johnson:** *Visual Computing: Making Sense of a Complex World*
  - *Dr. Johnson led a discussion among attendees in a question/response format.*

Workshop Outcomes – Potential Collaborations

- Collaborations were identified through collaboration cards and networking

- NSF CAREER attendees identified 55+ potential new collaborations at the workshop

- Examples of each to follow

Workshop Outcomes – Potential Collaborations

Example: Collaboration Cards

Researcher	Research Summary	Looking for Collaborations In:
Kapil Khandelwal	Multiscale methods for topology optimization	Optimization algorithms, distributed systems, sparse solvers
Sophya Garashchuk	Quantum molecular dynamics, modeling chemical reactions including quantum effects in complex molecular environments, enzymes, materials, solutions	Nonlocality in high (1000) dimension grids, meshes, interpolation, data clustering, random sparse matrix diagonalization
Dario Pompili	In-situ network data processing, supporting and running compute-intensive models in a distributed manner, extractive features online	Realtime medical apps, ocean modeling and observation. Data center management and cooling optimization
Diego Donzis	Massive simulations of turbulent flows. HPC, scalability, fundamental studies of turbulence and turbulent mixing	Sharing data, "community" codes and allocations, exascale simulations
Alison Marsden	Patient specific modeling for cardiovascular disease, optimization, UQ, multiscale modeling	Open source management, image segmentation, meshing.

Workshop Outcomes – Potential Collaborations

Example: Potential Collaborations Identified

Name: Baskar Ganapathysubramain

Dept/institution: ME
IOWA STATE UNIVERSITY

Did you make any new connections during the workshop that may lead to new collaboration?

Yes ✓   No _____

Please provide a list of people with whom you made new contact, and a **one sentence** summary of the nature of the collaboration.

Richard Henning : Linking scales
Suzanne shontz : adaptive meshing
Maria Emelianenko : energy minimization
Alison Marsden : UQ strategies
Pratim Sengupta : Learning strategies

Workshop Outcomes – Interdisciplinary Opportunities

- 1. **Interdisciplinary initiatives and universities:** Although no university structure is perfect, both graduate training and the tenure and promotion process can be more effective and efficiently structured when there is an interdisciplinary center or an institute in place.

- 2. **Interdisciplinary initiatives at NSF:** More interdisciplinary proposal initiatives are needed. Some existing multidisciplinary or interdisciplinary proposal ideas fall through the cracks. In addition, the interdisciplinary/multidisciplinary solicitations are always changing, so it is hard to be able to count on solicitations being in place. A more coherent approach across NSF directorates for soliciting and gathering feedback from program directors would help proposal teams to more effectively process and respond to program director comments.

- 3. **Academic-Industry Partnership:** We discussed the need to develop better linkages between academia and industry to encourage technology transfer to industry and to promote the development of sustainable cyberinfrastructure components.

Workshop Outcomes – Interdisciplinary Opportunities

- 4. **Collaborations:** Dr. Chris Johnson offered his model for developing successful collaborations. Prior to initiating new collaborations, both parties need to discuss the goals and expectations of the collaboration. In addition, both parties need to spend time on the collaboration and need to spend time learning about the other area. Also, both parties need to clearly understand the individual benefits to be gained from the collaboration. This is important for the buy-in for the collaboration as well as for career advancement.

- 5. **Education:** Dr. Tinsley Oden shared with workshop attendees a successful model of immersive interdisciplinary graduate education currently in place at the Institute for Computational Engineering and Sciences at the University of Texas at Austin. In particular, beginning graduate students in the program must take a specific set of courses spanning advanced mathematics and computer science, as well as physics, biology, etc. This introduces students to concepts in relevant disciplines. It also gives them a common language with which to discuss problems. Finally, it gives them a basic foundation on which to then pursue interdisciplinary, computational research.

Workshop Outcomes – Challenges in the Field

- 6. **Data:** There are many research challenges within the area of data. In particular, there are questions on storing, moving, interpreting, visualizing, and quantifying uncertainties in large data sets.

- 7. **People:** As Dr. Miron Livny posited, Cyberinfrastructure =Hardware +Software +People. The communities needs to shape and define the "data scientist" of the coming decade and to develop the educational programs focused on CDS&E.

- 8. **Engineering vs. Science:** We discussed how cyberinfrastructure is a science and engineering discipline, and how investments can help to fuel a virtuous cycle of science -> engineering -> application/use -> new discoveries.

- 9. **Sustainability:** We discussed the inherent problem of sustainability for software and data created as a part of NSF funded research, and the need to devise new models for sustainability that will uphold the academic values of open research and inquiry as well as the needs of the marketplace.

- 10. **Cyberinfrastructure Framework:** What common elements of cyberinfrastructure can we identify across the range of cyberinfrastructure systems that can lead to a definition of a common framework for cyberinfrastructure?

Workshop Outcomes –
NSF CAREER Attendee Feedback

Faculty appreciated the power and potential of interdisciplinary research.

• Faculty were inspired by the talks from the senior keynote speakers on interdisciplinary research topics.

• Faculty are very interested in open source software, dissemination of software and data produced, and gaining promotion and tenure credit for such efforts.

• Faculty noted many issues surrounding promotion and tenure for interdisciplinary activities. Many felt they did not fit cleanly within a single department. There is also concern as to which NSF division to submit a particular interdisciplinary proposal.

• Attendees indicated that, while it was helpful to learn more about NSF at the workshop, they would like to see program directors from NIH and other relevant agencies give presentations, as well.

• Faculty liked the single track workshop.

• Faculty liked the pacing of the workshop with time for discussion and networking

Observations from Workshop

- Workshop provided many opportunities for discussions among attendees and speakers
    - We distilled attendee comments into a set of observations

- ***Observation 1.*** The attendees felt that there is a lack in the number of interdisciplinary solicitations that bridge between the domain sciences, computer science, and cyberinfrastructure.

- ***Observation 2.*** The attendees suggested that the CAREER proposal review criteria could be expanded to encourage the development and dissemination of open source software and data as part of the proposed project.

- ***Observation 3.*** The attendees described a unmet need for a central cyberinfrastructure that could be used by CAREER awardees to disseminate open source software and data (an example of this type of system is the NEEShub)

Observations from Workshop

- ***Observation 4.*** To aid early-career researchers in developing their research program and seeking federal sponsorship for their research, many attendees described a need for clear guidelines to CAREER awardees on the science and engineering areas covered by NSF programs and solicitations, and when researchers should approach other agencies such as NIH, DOE, etc.

- ***Observation 5.*** The NSF CyberBridges Workshop provided a productive venue for CAREER awardees to meet, network, and explore integrative and joint research and education activities; and to allow senior researchers to provide career advice to young researchers.

Observations from Workshop

- ***Observation 6.*** There is a need to create more core solicitation programs with a well-defined submission schedule to allow researchers to better plan in advance to submit proposals to a specific program, rather than the need to respond more quickly to singular solicitations that are not part of a recurring program.

- **The recent move of OCI into CISE brings up several questions**
  - Need to communicate this ASAP to the community
  - Researchers working on OCI CAREER proposals will need guidance as soon as possible if there will be changes to the program