



The Cross-Institutional Research Engagement Network (CI REN)

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EECS Lunch & Learn Series – August 30, 2024

Organization and Participants

Collaboration between the University of Tennessee, Knoxville and Arizona State University

- Lonnie D. Crosby – UTK CIREN Director, PI
- Gil Speyer – ASU CIREN Director, co-PI
- Marisa Brazil – ASU CIREN Director, co-PI

Cyberinfrastructure (CI) Facilitators

- Recruit, Train, and Mentor CI facilitators

Researchers

- Connect CI facilitators with researchers in collaborative research engagements.
- Opportunities to connect with national CI projects through NSF's ACCESS and the National AI Research Resource (NAIRR).

CIREN is a 5-year project: Jan. 2023 – Dec. 2027



Mission

“Our mission is to enable transformative research discoveries by connecting researchers with computational expertise.”

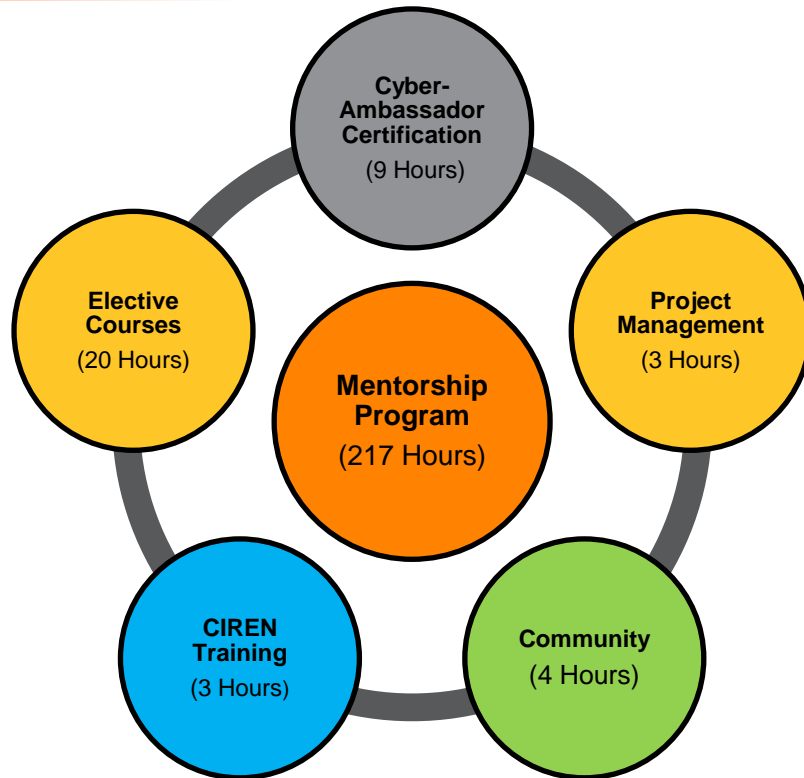
We are focused on:

- high-performance computing (HPC), machine learning (ML), and artificial intelligence (AI)

We fulfill our mission by:

- Recruiting CI facilitators and assessing their current facilitation and technical skills.
- Training CI facilitators in research facilitation skills.
- Providing CI facilitators opportunities and guidance for learning new technical skills.
- Mentoring CI facilitators through an initial research engagement project.
- Recruiting institutional and national research projects for potential CI facilitator research engagements.

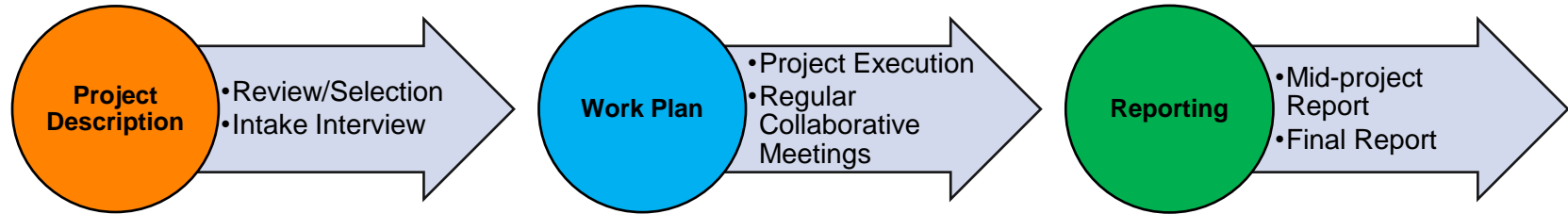
Training Curriculum



Includes 256 hours of training

- **CIREN Training (3 hours)**
 - Overview, Project Management, Continuous Training and Development.
- **CyberAmbassador Certificate (9 hours)**
 - Communication, Teamwork, and Leadership
 - <https://doi.org/10.1145/3332186.3332218>
- **Community (4 hours)**
 - Project Intake Interviews, Local ([ISAAC](#)) and National Resources ([ACCESS](#))
- **Project Management (3 hours)**
- **Mentorship Program (217 hours)**
 - Presentation on completed research engagement project
- **Elective Courses (20 hours)**
 - High-performance computing, machine learning, and artificial intelligence topics

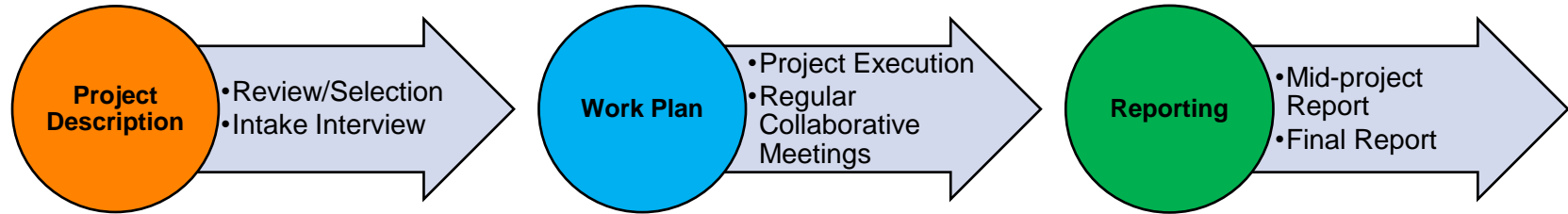
CIREN Project Timelines



Projects are expected to be 6-month engagements.

- Projects will be solicited from the institutions via the submission of a proposal including a “Project Description”.
- “Project Descriptions” are reviewed by facilitators and mentors. Facilitators will be able to indicate preferences and interests in projects.
- Projects are assigned to facilitators. Facilitator conducts an intake interview with the project’s PI.
- Facilitator creates a project “Work Plan” for the project and reviews with project’s PI. Due prior to project’s start date.

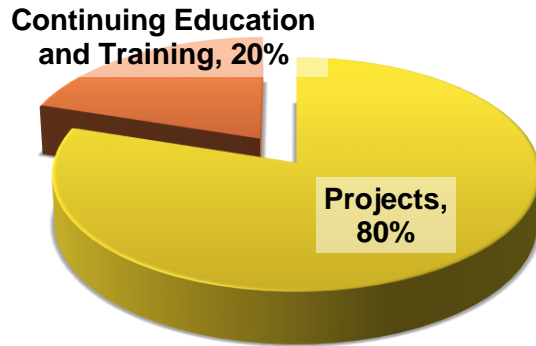
Mentorship Program



Mentorship Program (217 hours):

- New CIREN CI facilitators are assigned a mentor during their first research engagement project
- Mentor guides the CI facilitator through the project timeline
 - Review of project requests and Conducting intake interviews
 - Development of the project workplan
 - Regular collaborative meetings with project group
 - Submission of mid-project and final project reports
- Mentor meets with CI facilitators weekly to discuss project and training progress
- CI facilitators attend monthly CIREN community meetings
- CI facilitators present on the completed project and its results during a CIREN community meeting.

Facilitator Time Commitments



CIREN CI Facilitators (per 25% effort)

- Assigned one research engagement project every 6-months (80% of project effort)
- Take about 40 hours of continuing education and training per year.
- Contribute 20% of their overall project and training effort toward NSF's ACCESS Computational Science Support Network.

CIREN CI Facilitators

Od Odbadrakh

Bio: Od Odbadrakh has over twenty years of experience in computational materials research, scientific software development, high-performance computing, and managing scientific software packages. He has had extensive experience working on various leadership class supercomputers.

Expertise: Deep Learning; HPC application scalability; and Materials Science (compositionally complex alloys (CCA), metallic glasses, and alloys with extended defects and disorder)

Reed Sarasua Tucker

Bio: Reed Sarasua Tucker is an application developer and software engineer. Reed has experience writing highly performant code in Python and C/C++. His interests include GPU programming, machine learning, and artificial intelligence.

Expertise: Python, Software Development, and Web Development

Scott Emert

Bio: Scott Emert has over thirteen years' experience in radiological protection safety, laboratory and machine shop management and supervision, and robotic development. He also has several inventions registered with UTK's Office of Research, Innovation, and Economic Development

Expertise: Radiation Safety, Laboratories (supervision, research, inventory, etc.)

CIREN CI Facilitators

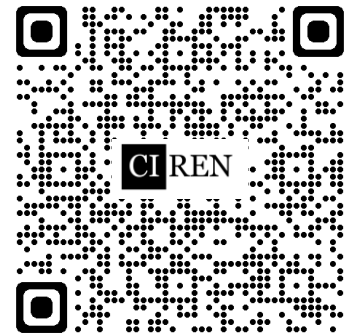
Micholas Smith

Bio: Micholas Smith is a Computational Biophysicist and Research Assistant Professor in the Department of Biochemistry and Cellular and Molecular Biophysics with nearly ten year of experience using both traditional HPC and leadership class supercomputers (ORNL: TITAN, SUMMIT & FRONTIER; NERSC: HOPPER, CORI, and PERLMUTTER). He has generated molecular models on systems ranging from plant cell walls to biomembranes.

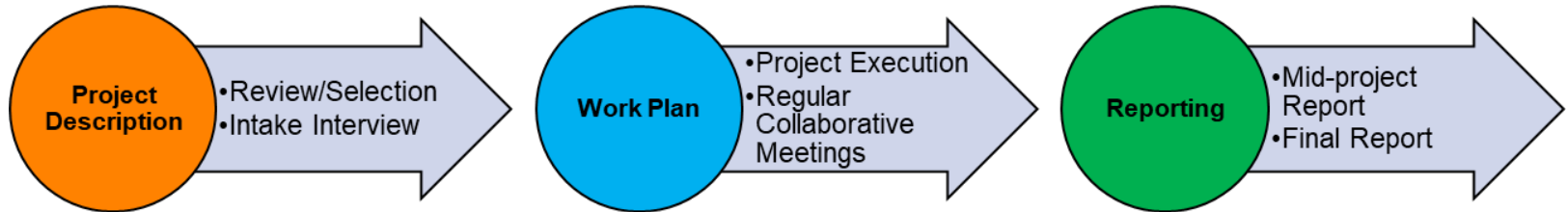
Expertise: Molecular dynamics simulations on HPC; “Shallow” machine learning; Molecular modeling of biological soft-matter such as biopolymers (including proteins, lignin, and carbohydrates), biomembranes, protein-ligand complexes, modeling of organic solvents and solvent property prediction.

Recruiting for CIREN CI Facilitators

CIREN is now recruiting for new CI Facilitators! Facilitators are supported for at least 25% of their time while engaged in training, mentorship, and research engagements. If you are interested in learning more about being a CIREN CI facilitator, please contact Lonnie Crosby (lcrosby1@utk.edu) or complete the following [Google web form](#).



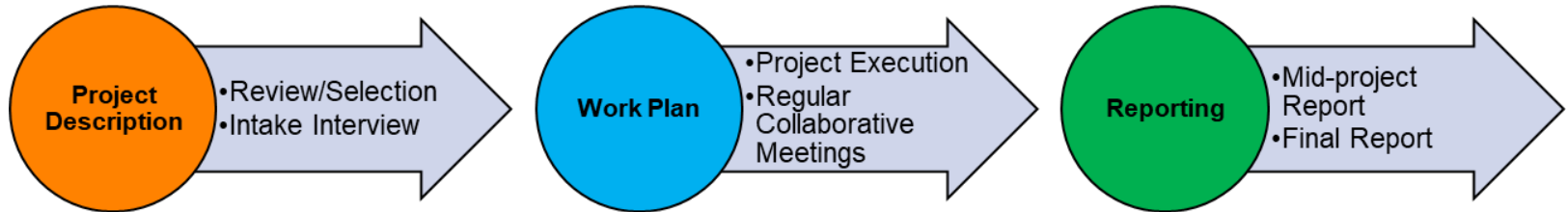
Research Engagement



Research Engagement Requests

- Researchers or principal investigators (PI) propose CIREN research engagements via the submission of a project description (about 2 pages).
 - **HPC:** Scaling, parallelizing, or performance optimizations of existing applications to take advantage of new computational resources, deal with increased data volume, or undertake larger target problems.
 - **ML:** Inclusion of ML or AI methodologies within existing analysis pipelines.
 - **AI:** Proof-of-Concept development and feasibility studies with respect to the incorporation of ML or AI technologies within a research program.

Research Engagement



Once a project is selected and a CI facilitator is assigned

- The CI facilitator conducts an intake interview and creates a project work plan with the PI.
- CI facilitators hold frequent (at least every 2 weeks) team meetings with the project PI and their team.
- The CI facilitator in collaboration with the PI completes mid-project (3-months) and final project reports.
- If the CI facilitator is in CIREN's mentorship program, they will be required to give a final presentation on the project and its results during a monthly CIREN community meeting.

CIREN Projects (2023)



The Absorption of Metropolitan Immigrants: Techniques for Analyzing Data Clustering across Time and Place

PI: Dr. Stephanie Bohon, Department of Sociology

Facilitator: Reed Tucker

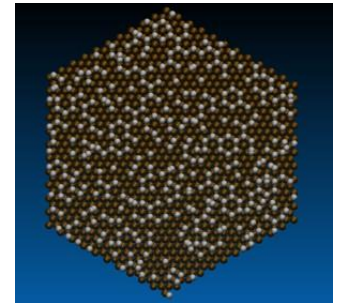
Image Credit: “[Cityscape Skyline](https://stocksnap.io/photo/cityscape-skyline-KDOIQSH4ZW)” (<https://stocksnap.io/photo/cityscape-skyline-KDOIQSH4ZW>) by [Verne Ho](#)/ [CC0 1.0](#)

Using Deep Neural Networks to Predict the Adsorption Energy of Atomic Oxygen on Silver Surfaces

PI: Dr. Sharani Roy, Department of Chemistry

Facilitator: Od Odbadrakh

Image Credit: “Atomic Oxygen Adsorbed on a Silver (111) Surface” created using [VMD](https://doi.org/10.1016/0263-7855(96)00018-5) ([https://doi.org/10.1016/0263-7855\(96\)00018-5](https://doi.org/10.1016/0263-7855(96)00018-5))



CIREN Projects (2024)

Quantum Monte Carlo Optimization via High Performance I/O with the Hierarchical Data Format

PI: Dr. Adrian Del Maestro, Department of Physics & Astronomy

Facilitator: Reed Tucker

Advancing Research Capabilities via new AI and ML methodologies to identify and treat misclassification of youth firearm mortality

PI: Dr. Lisa Lindley, College of Nursing

Facilitator: Reed Tucker

High-Performance Computing for Data-Driven Coupled-Cluster

PI: Dr. Konstantinos Vogiatzis, Department of Chemistry

Facilitator: Od Odbadrakh

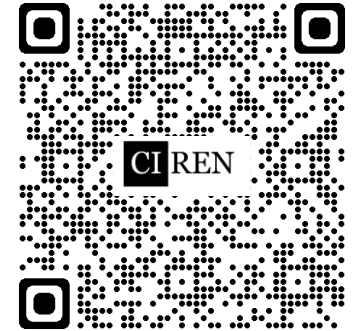
Developing ML/AI-based tools to analyze the multi-dimensional spectroscopic data of scanning tunneling microscopy

PI: Dr. Wonhee Ko and Dr. Ruixing Zhang, Department of Physics & Astronomy; Dr. Bing Yao, Department of Industrial and Systems Engineering

Facilitator: Od Odbadrakh

CIREN Research Engagement Requests

CIREN is accepting requests for research engagements! The next round of projects are expected to be reviewed in February 2025. Researchers interested in submitting a research engagement request should complete the following [Google web form](#).



CIREN is recruiting faculty for an Institutional Research Advisory Committee at UTK !

The purpose of this UTK Institutional Research Advisory Committee is to help provide community input and feedback to the CIREN project. We are interested in efforts to increase Research Engagement, Facilitator Recruitment, and CIREN program longevity at UTK. Meetings will be quarterly to begin with but may move a 6-month cadence. These meetings are expected to be virtual (Zoom) and will contain a briefing of the current state of the project, an opportunity for committee members to ask questions, and charges for the committee to provide recommendations to the project in these main areas. Please contact Lonnie Crosby (lcrosby1@utk.edu) for more information and if interested.

More information on CIREN

UTK CIREN Website: <https://ciren.utk.edu>

– Facilitation, Research Engagement, and News

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CIREN News will continue to post updated open calls for research engagements and announcements!

CIREN is recruiting faculty for an Institutional Research Advisory Committee at UTK !

Please contact Lonnie Crosby (lcrosby1@utk.edu) for more information and if interested.

Acknowledgements



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Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the National Science Foundation.