

COLORADO

Higher Education Competitive Research Authority



March 1, 2022

Honorable Members of the House and Senate Education Committees State Capitol 200 East Colfax Denver, Colorado 80203

Re: Annual Report of the Colorado Higher Education Competitive Research Authority (CHECRA)

Dear Representatives and Senators:

Colorado Revised Statutes §23-19.7-103(3) requires the Colorado Higher Education Competitive Research Authority (CHECRA), housed at the Colorado Department of Higher Education, to report annually to the Education Committees of the Colorado House of Representatives and Senate on research projects funded by CHECRA in the previous calendar year. This letter reports on activities and projects funded in the calendar year 2021. This includes multi-year projects that received continued funding in 2021, and new initiatives funded for the first time in 2021.

CHECRA was created to provide a source of matching funds for National Science Foundation (NSF), U.S. Department of Energy, and other competitive federal grants that require or benefit from a state match. CHECRA funding has helped to bring significant research dollars to Colorado. Funding is used both to support multi-year research initiatives, including Engineering Research Centers and Science and Technology Centers, and to purchase large, expensive research instruments housed by one institution but used by faculty and staff from multiple colleges and universities.

CHECRA spent almost \$1.75 million in 2021 to support seven multi-year research grants, and support the purchase of three Major Research Instruments, that collectively have brought over \$50 million in federal research dollars to the state. Following is a list of the multi-year research grants that received CHECRA funding in 2021:

University of Colorado (CU)

- In 2016, with CU Boulder as the lead awardee, the NSF awarded a \$24 million, 5-year grant for the Science and Technology Center on Real-Time Functional Imaging (STROBE). STROBE brings together universities, national laboratories, industry, and international partners to create a powerful new set of real-time imaging modalities. CHECRA has pledged \$400,000 for a renewal of five years; 2021 was the first year of funding for the second renewal.
- 2. The NSF Quantum Leap Challenge Institute, led by the University of Colorado Boulder, includes extensive collaborations with leaders from other academic institutions in the US and Europe, NIST, National Laboratories, and industry to make broad, fundamental advances in quantum science and engineering. The aim is to demonstrate and leverage quantum advantages in state-of-the-art quantum sensing across the field. The Institute is designed for core integration of research with education and workforce development. CHECRA has pledged \$400,000 annually for five years; 2021 was the second year of funding.
- 3. DOE Desalination Hub: NAWI Road mapping project, led by University of Colorado Boulder, the project engaged in the baseline evaluation and roadmap development of water reuse practices supporting NREL and the NAWI team in the areas of industrial reuse, agricultural reuse, oil and gas wastewater reuse and mining wastewater reuse. The CHECRA board has authorized a contribution of \$40,000.00.

Colorado School of Mines (CSM)

4. The National Alliance for Water Innovation (NAWI) is a research consortium that was formed in 2017 to partner with the U.S. Department of Energy to create the Energy-Water Desalination Hub. In 2019 the DOE announced that NAWI will manage the new Desalination Hub. NAWI vision is to support the develop affordable, energy-efficient, and resilient water supplies from unconventional resources (e.g., oil and gas, mining, agriculture, seawater/brackish water, power industry, and general industries). Research under NAWI focused on enhancing the U.S. economy through decentralized, small-scale, fit-for-purpose desalination. The CHECRA board has authorized a contribution of \$123,188.00.

Colorado State University (CSU)

- 5. Colorado State University's Industrial Assessment Center (CSU IAC), funded by the U.S. Department of Energy, provides industrial energy audits by engineering students to small and medium sized manufacturing facilities. The CHECRA has committed to providing a total of \$131,634 to the IAC over three years. CHECRA made the final of three payments in 2021 for \$43,878.00.
- 6. A Novel Electro-dialytic Crystallizer (EDC) for Energy Efficient Zero-liquid Discharge led by Colorado State University. This project investigates a new brine management

process called electro-dialytic crystallization (EDC). The core innovation of EDC is the use of the electrodialysis phenomenon to maintain a saturated brine stream for continuous salt precipitation. The CHERCA board authorized a contribution of \$89,275.00.

In addition to the payments listed above, CHECRA provided \$346,800 as a cost share for the following Major Research Instrumentation (MRI) grants received from NSF in 2021. These one-time grants provide higher education institutions with major instrumentation that supports the research and research training goals of the institution and are also used by other researchers regionally or nationally.

- CU MRI Consortium: Development of Fiber-coupled stimulated emission depletion microscopy (STED). With this grant, CU is developing a unique miniature optical fiber-coupled microscope that will enable flexible imaging at unprecedented spatial resolution. Developed with a diverse team that includes engineers, physicists, and neuroscientists, this cutting-edge microscope will yield far-reaching impacts through intellectual property development and future commercialization and deployment in industry. The research team will use the new instrument to expand ongoing efforts to mentor and inspire young students from groups underrepresented in Science Technology Engineering and Mathematics (STEM) fields.
- CU MRI: Acquisition of a High-Performance Computing Cluster for Next-Generation Computational Science in Southern Colorado. This project will enable the acquisition, deployment, and maintenance of a high-performance computing (HPC) cluster (to be called INCLINE). This instrument will provide much-needed computational resources to the UCCS campus and the Southern Colorado scientific and academic communities.
- CSU MRI: Acquisition of an Open Access Shared-Use MALDI-TOF/TOF Mass Spectrometer. This project provides partial cost share support for a National Science Foundation Major Research Instrumentation Grant awarded to Colorado State University in August 2021, to fund the acquisition of a high-resolution Matrix Assisted Laser Desorption/Ionization Tandem Time-of-Flight Mass Spectrometer (MALDI-TOF/TOF). This will serve as a shared resource for CSU faculty and students with open access to users from the surrounding Rocky Mountain region.

Appendices to this report include detailed information on each of the projects listed above. In addition to the millions of dollars in federal funding coming into the institutions and the state— and the impressive scientific results achieved under the projects—the research centers funded by CHECRA positively impact Colorado. These benefits include support for graduate and undergraduate students, outreach to K-12 students and teachers, and economic development benefits from spin-off technologies and companies.

Following are some highlights of these benefits to Colorado.

• CHECRA programs include industry partners and often drive new venture creation in the state. Many of the CHECRA supported programs have a triple helix ecosystem of

partners (research universities, industry, and government). A most recent example is support for projects at Mine and at CSU through NAWI (National Alliance for Water Innovation), which is led by a U.S. Department of Energy national lab (Lawrence Berkeley), has multiple participating companies in the sector, and includes open opportunities to all of Colorado's public research institutions.

- The future is bright for CHECRA and includes opportunities to amplify our impacts to contribute to the science and technology infrastructure of the Front Range and beyond across several areas. These include new investments in a hydrogen hub, in climate resilience, and general investments in our state science and technology infrastructure.
- These opportunities will remain linked to large federal investments that will enable our state to remain competitive and collaborative in generating important science and technology solutions to our most pressing problems.

Due to the State budget impacts of the pandemic, the annual distribution of Limited Gaming Funds in the amount of \$2.1 million to the Authority was suspended for two years, so CHECRA did not receive that revenue in 2021. Interest earnings on the Authority's funds totaled \$21,672 in 2021. Expenses totaled \$1,752,463.00. The CHECRA board recommends that the distribution from Limited Gaming Revenue be reinstated in FY22.

Thank you for your support of this ongoing research. We welcome any questions.

Sincerely,

Dr. Angie Paccione

Dr. Angie Paccione Executive Director, Colorado Department of Higher Education

 Cc: Dr. Alan Rudolph, Vice President for Research, Colorado State University, and Chair, CHECRA
 Dr. Jeri-Ann Lyons, Associate Vice President for Research, University of Northern Colorado, and Vice Chair, CHECRA
 Dr. Walter Copan, Vice President for Research and Technology, Colorado School of Mines
 Dr. Terri Fiez, Vice Chancellor for Research, University of Colorado Boulder

Attachments:

Appendix A: University of Colorado, Boulder- Science and Technology Center on Real-Time Functional Imaging (STROBE)

Appendix B:	University of Colorado, Boulder- QLCI - CI: NSF Quantum Leap Challenge
	Institute for Enhanced Sensing and Distribution Using Correlated Quantum
	States
Appendix C:	University of Colorado, Boulder- MRI Consortium: Development of Fiber-
	coupled stimulated emission depletion microscopy (STED)
Appendix D:	University of Colorado, Boulder- DOE Desalination Hub: NAWI Road mapping
Appendix E:	University of Colorado, Colorado Springs- MRI: Acquisition of a High-
	Performance Computing Cluster for Next-Generation Computational Science in
	Southern Colorado
Appendix F:	Colorado School of Mines Re-inventing the Nation's Urban Water Infrastructure
Appendix G:	Colorado State University- MRI: Acquisition of an Open Access Shared-Use
	MALDI-TOF/TOF Mass Spectrometer
Appendix H:	Colorado State University-A Novel Electro-dialytic Crystallizer (EDC) for
	Energy Efficient Zero-liquid Discharge
Appendix I:	Colorado State University Extension Industrial Assessment Center

Appendix A: University of Colorado Science and Technology Center on Real-Time Functional Imaging (STROBE)

NSF award to University of Colorado, Boulder (UCB) NSF Award: 1548924 Title: Science and Technology Center on Real-Time Functional Imaging (STROBE) Period of Performance: 10/01/2016 – 09/30/2026 (~\$48M over 10 years, renewed) Total 2021 CHECRA Funding: \$400,000 Award PI's: Margaret Murnane (Director), Jianwei Miao, Markus Raschke, Naomi Ginsberg

Abstract:

Microscopy is critical for discovery and innovation in science and technology, accelerating advances in materials, bio, nano and energy sciences, as well as nanoelectronics, data storage and medicine. Although electron, X-ray and optical nano imaging methods are all undergoing revolutionary advances, no single imaging modality can address critical questions underlying much of science and technology in the 21st century. These grand challenges include: How to capture high-resolution images of functioning nano, energy and quantum systems to guide design? What is the 3D atomic structure of glasses and how do the atoms rearrange themselves during the glass transition? How to rapidly image viruses and vaccines, with molecular-scale information? How to image nanoscale living matter without freezing or labeling? Addressing these major scientific challenges requires the development of the microscopes of tomorrow by integrating state-of-the-art microscopes, new methods, novel sample preparation, fast detectors, big data, advanced algorithms and machine learning - which could not be accomplished without a center.

Progress made over the last year: (focusing on key objectives or milestone reached, challenges encountered, and/or other particularly noteworthy highlights (limit answer to 1/2 page).

STROBE brings together academia (CU Boulder, UCLA, UC Berkeley, UC Irvine, Florida International University and Fort Lewis College), national laboratories (LBNL, ORNL, NIST) and several US industries to develop and advance microscopy tools and techniques. Major achievements in 2021 include enhanced collaborations with partners who come to STROBE as a resource – Moderna, 3M, Moore Foundation, MRS, DOE LBNL, PPNL, PPPL, NIST, Imec, NSF IPAM, Penn State NSF MRSEC and elsewhere. STROBE curricula, training and best practices being adopted broadly. A diverse group of >100 graduate student and postdoctoral scientists are impacting workforce (from the first 5 years of STROBE). Most notably, STROBE technologies are now either used, or are impacting, several national laboratory facilities at NIST Boulder Labs, Lawrence Berkeley Labs, industry and elsewhere. Finally, UCLA STROBE scientist Hong Zhou continued to work with Moderna in 2021, to provide high resolution images of their vaccines.

Outcomes/benefits of this project over the past year, including both scientific advancements as well as other benefits:

- 1. STROBE is attracting many new collaborations from national labs, academe and industry please see slide below.
- 2. >100 STROBE diverse graduates are now impacting the US workforce. Of these trainees, ~30% were women and 10% URM, well above the national averages in STROBE fields.
- 3. UCLA STROBE scientist Hong Zhou continued to provide images of their vaccine to Moderna, as a service spanning two years. For bio-materials, sub-2Å resolution is required to obtain the chemical structure. Only the best electron imaging labs, like Zhou's, have the specialized setups to manage the immense amounts of data required to reach this resolution.

STROBE research into advanced algorithms that can extract structural information with less data is key for reaching molecular-level imaging and will have large future impact.

- 4. STROBE research advances have resulted in >260 papers that are highly cited (please see https://strobe.colorado.edu/ for Publications, News and Awards). The large majority of the papers are collaborative, involving joint university/national lab/industry work.
- 5. Trainees received multiple awards, including National Research Council Postdoctoral Fellowships to work at NIST, graduate fellowships, best papers (see https://strobe.colorado.edu/news-events/awards/)
- 6. STROBE technologies have been integral to ~8 joint university-industry grants with small and large businesses, and 2 SRC fellowships/grants in the first 5 years.
- 7. STROBE-enhanced IR sources are now available to a broad user community at the Department of Energy Synchrotron Source at UC Berkeley.
- 8. STROBE-enhanced advanced algorithms for X-ray imaging are now available to a broad user community at the Department of Energy Synchrotron Source at UC Berkeley.
- 9. STROBE-enhanced tabletop X-ray sources are now used by NIST Boulder Labs for advanced materials research.
- 10. STROBE hosted and mentored ~30 undergraduate students for remote/hybrid research experiences in the Summer of 2021.
- 11. Multiple outreach activities were implemented, including K-12 school visits and teacher kits development, as well as activities at the virtual Girls in Science Night at the WOW! Children's Museum.

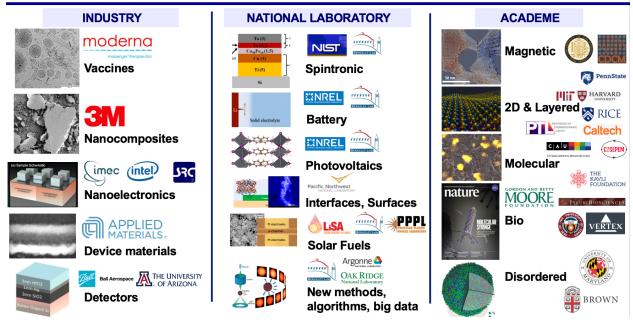


Additional documentation:

(Additional documentation may include additional artifacts, reports, or content that should be included as an appendix or addendum to the content supplied in this form.)

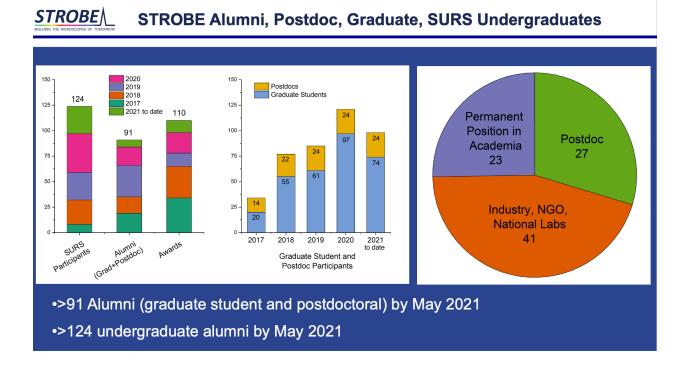
Please see the slides below.

STROBE Enhancing STROBE Research, Education, Knowledge Transfer, Impact – STROBE becoming a go-to place to address microscopy challenges!

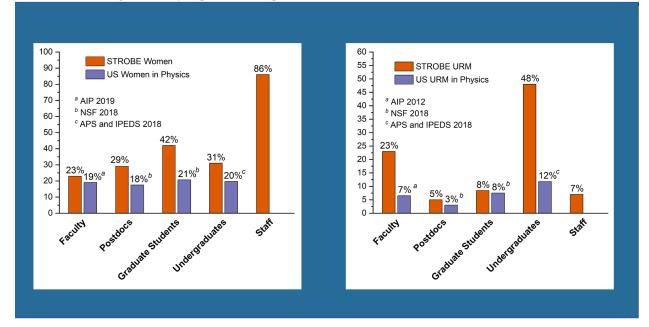


STROBE Knowledge Transfer Highlights from first 5 years (to May 2021)





STROBE Creates a rich, attractive, diverse and inclusive STEM environment by developing and using Best Practices



STROBE Education & Community during COVID-19

Multi-node/virtual Activities:

Project management short course Mentoring training Software Carpentries workshop STROBE science tutorials Emotional Intelligence Training Four Corners Outreach Physics PFC PREP with FIU

In-person Activities:

Community celebration events (UCLA, Berkeley, CU Boulder) Collaboration visit to Norfolk State University Collaboration visit to Fort Lewis College In-person research and visits during SURS 2021 Upcoming Software Carpentries Workshop at FIU Upcoming mentoring training in ECEE at CU Boulder

Appendix B: QLCI - CI: NSF Quantum Leap Challenge Institute for Enhanced Sensing and Distribution Using Correlated Quantum States

Full name of the funded project:

QLCI - CI: NSF Quantum Leap Challenge Institute for Enhanced Sensing and Distribution Using Correlated Quantum States

First and last name of the primary investigator (PI) for this project (or PI's):

Jun Ye (NIST and JILA, the University of Colorado Boulder)

Enter a short description or abstract of the project:

The Institute will design, build, and employ quantum sensors based on high-performance atomic, molecular, and optical systems. The Institute is designed around three ambitious Grand Challenges to significantly advance fundamental science, technology integration, and practical application of quantum-based technologies:

Grand Challenge 1: Perform basic research and enable technology to achieve "quantum advantage" in sensing and measurement: clear supremacy over classical or "Quantum 1.0" methods

Grand Challenge 2: Develop field-deployable quantum sensors and interconnections

Grand Challenge 3: Develop the experimental and technical tools to establish atomic strontium (Sr) as the industry standard in quantum sensing, thus facilitating more rapid advances by the wider academic and industry communities.

This ambitious research program has the potential for transformative extensions of quantum sensing for new basic physics (detection and characterization of dark matter, dark energy, and matter-antimatter asymmetry); for applications of quantum technologies to areas of practical importance (quantum communications and networking); and for establishing, and hastening use of, standards for quantum tools for academia and industry. We also seek strong impact of quantum technology on many different scientific fields, including some of which are yet to be imagined.

We are implementing concrete ideas to train the next generation of the quantum workforce, spanning new undergraduate and postgraduate degrees, new educational modules for two-year colleges, and internships or summer schools with emphasis on introducing underserved minorities to the educational and professional opportunities in quantum science and engineering.

Summarize progress made over the last year, focusing on key objectives or milestone reached, challenges encountered, and/or other particularly noteworthy highlights (limit answer to 1/2 page).

During the Institute's first year (9/1/2020 - 8/31/2021), we focused on ramping up in four broad areas: Infrastructure, Education and Training, Research and Collaboration, and Communications (internal and public facing).

- Infrastructure accomplishments
 - Established the Institute's organizational structure. *See Org Chart in Attachment A.*

- Recruited a Director for Education and Workforce Development; identified and installed a Deputy for Science and Research Convergence; and confirmed and installed a Director for Operations
- Embedded the Institute in the broader campus-wide CUbit Quantum Initiative, with its newly recruited Executive Director supported for the first year by CHECRA funds
- Education and Training accomplishments
 - Recruited 6 postdoctoral fellows and 45 PhD level graduate students across the Institute's 12 partner organizations (*see Attachment B*) to conduct QLCI-related projects, and began the process of onboarding 4-6 undergraduate research students
 - Began development of a quantum education curricula including a Quantum PhD in Physics and Quantum Engineering master's degrees, and general quantum technology education in Undergraduate studies
 - Continued to foster integration of traditionally separate disciplines of Physics and Engineering, as will be necessary for success in meeting the Institute's ambitious technical goals
- Research and Collaboration accomplishments
 - Grouped Senior Investigators into our three Grand Challenge research groups and, for each Grand Challenge group, convened a "Crystallization Meeting" to build team communications and goals and identify paths and teams for specific research projects (*see Attachment E*)
 - Initiated a monthly "Research Convergence" seminar series to foster crossdisciplinary and multi-institution collaborations among the Institute's 37 (now 40) Senior Investigators and their graduate students and postdocs (*see Attachment C*)
- Communications: (Internal and Public facing) accomplishments
 - Developed a website¹ dedicated to sharing results and plans among the Senior Investigators, students, and more broadly to the public; established and populated a Dropbox folder hierarchy with access-controlled sub-folders for specific groups; established Slack channels for communications among Institute investigators and students
 - Convened our first Annual Meeting to highlight early scientific progress, reenforce collaborations, and give graduate students and postdocs an opportunity to present their projects and directly engage with the entire Institute community

¹ https://www.colorado.edu/research/qsense/

Provide outcomes/benefits of this project over the past year, including both scientific advancements as well as other benefits. Examples of the latter include contributing to graduate and undergraduate education; K-12 or other outreach; technology commercialization and/or spin-off companies; collaboration with others

Further examples of noteworthy outcomes in Year 1 include:

- Research and Collaboration
 - Produced multiple outstanding results including a systematic survey among quantum industry partners and ensuing data analysis/research on quantum education; setting the most stringent constraints on the ultralight dark matter with the use of a state-of-the-art optical atomic clock and example of precision metrology meeting cosmology; generating new molecule-based quantum systems and exploring quantum entanglement between molecules; and investigating the connection between quantum complexity and quantum information by studying quantum chaos in strongly-correlated many-body systems. *For details, see Attachment D.*
 - Established working groups within individual Grand Challenges or spanning several. Regular meetings of these working groups established several effective collaborative projects within the Institute.
 - Recruited an External Advisory Committee to suggest initiatives and modifications that would increase the Institute's impact on science, engineering, and the public: Alexander Gaeta (Columbia University), Elsa Garmire (Dartmouth College), Jack Harris (Yale University), Eugene Polzik (Niels Bohr Institute), Mark Saffman (University of Wisconsin), Kerry Vahala (Caltech), Benjamin Zwickl (Rochester Inst. of Technology), Jay Lowell (Boeing)
 - Used the successful NSF QLCI award to ignite interest in, and take initial steps toward establishing, a new Quantum Engineering Institute (QEI) at CU to better realize the benefits of Physics-Engineering deep collaborations in quantum
- Education and Training
 - Made initial steps to establish Quantum Forge as an education platform to provide hands-on training of undergraduate students to prepare them for quantum research and industry positions, and began process of establishing Quantum Forge as an official class at CU
 - Initiated design and preparation of a simulation module in the internationally recognized PhET² system at CU to translate the idea of quantum superposition and coherence in an intuitive way to pre-college students and the public
 - Began preparations for a Research Exchange program to provide undergraduate students with quantum-related laboratory experience; initiated contact with internship program directors at LANL, Sandia National Labs and Boeing.
- Communications: (Internal and Public-facing

² https://phet.colorado.edu

- Convened an Institute-wide annual meeting virtually (with a combination of Zoom and GatherTown); included all Senior Investigators, students and postdocs, other collaborators, and the External Advisory Board
- Infrastructure
 - Appointed an Executive Committee and set a standing meeting time for use as needed to discuss significant, Institute-wide policy matters and the evolution of its constituent initiatives
 - Drafted and led negotiation of an IP Management Plan and secured signature approval of all Partners: 8 universities, 2 National labs, NIST and an FFRDC

Additional documentation:

(Additional documentation may include additional artifacts, reports, or content that should be included as an appendix or addendum to the content supplied in this form.)

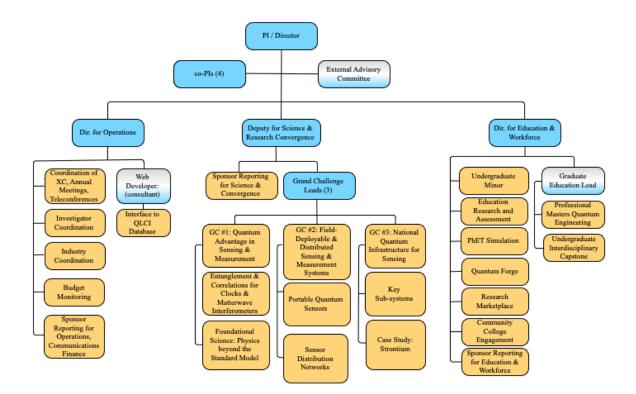
Attachment A: Organization Chart for our NSF Quantum Leap Challenge Institute (Q-SEnSE, for "Quantum Sensing through Entangled Science and Engineering")

Attachment B: Universities and laboratories partnering in the Institute

Attachment C (PDF): "Community" page of the Institute website, listing meetings, seminars that foster coherence and collaboration among the Institute's senior investigators and across its 12 participating organizations, and presentations of Institute work to a wider audience

Attachment D: (PDF): "Publications" of the Institute

Attachment E: Working Groups



Attachment A: Organizational Chart of NSF QLCI

Principle Investigator & Director:

• Jun Ye, NIST and JILA, University of Colorado Boulder

Co-PIs:

- Prof. Mark Kasevich, Stanford (Applied Physics)
- Prof. Svenja Knapp, University of Colorado (Engineering)
- Prof. Greg Rieker, University of Colorado (Engineering)
- Prof. Marianna Safronova, University of Delaware (Physics & Astronomy)

Deputy for Science & Research Convergence:

• Prof. Cindy Regal, JILA and University of Colorado (Physics)

Director for Education and Workforce Development:

• Michael Bennett, PhD

Director for Operations:

• Stephen ONeil, PhD, MBA

Attachment B: Universities and Laboratories Partnering in the Institute

- JILA and University of Colorado Boulder (lead)
- Harvard University
- Los Alamos National Laboratory
- Massachusetts Institute of Technology (MIT)
- MIT Lincoln Laboratory
- National Institute of Standards and Technology (NIST)
- Sandia National Laboratories
- Stanford University
- University of Delaware
- University of Innsbruck (Austria)
- University of New Mexico
- University of Oregon

Attachment C begins on following Page



Q-SEnSE: Quantum Systems through Entangled Science and Engineering

Community

From individual researchers and laboratories to departments, institutes, and organizations, **modern science and engineering are team efforts**. Communities large and small coordinate to expand our understanding of the world and apply that new understanding to **inform**, **involve** and **advise** colleagues and the public, and help develop novel products and services for the economy.

Q-SEnSE investigators are involved with the community in many ways, with recent examples included below.

INTERNAL COMMUNITY

Q-SEnSE Convergence Seminar Series

1:00 - 1:15pm Mountain Time reserved for Senior Investigators; 1:15 - 2:30pm Mountain Time open to all Q-SEnSE investigators, collaborators, students, and postdocs

- Wednesday, May 25, 2022: All Q-SEnSE Convergence Seminar (Regal & Huang)
- Wednesday, Apr 27, 2022: All Q-SEnSE Convergence Seminar (Jau & Hollberg)
- Wednesday, Mar 2, 2022: All Q-SEnSE Convergence Seminar (*Education & Workforce Special Edition*)

 Next up! Wednesday, Feb 23, 2022: All Q-SEnSE Convergence Seminar (<u>Gopinath</u> & <u>Diddams</u>)

- Wednesday, Jan 19, 2022: All Q-SEnSE Convergence Seminar (<u>Hogan</u> & <u>Allcock</u>); 23 Q-SEnSE Investigators; 32 collaborators, students & postdocs
- Tuesday, Dec 14, 2021: All Q-SEnSE Convergence Seminar (<u>Martin</u> & <u>Combes</u>); 18 Q-SEnSE Investigators; 8 collaborators, students & postdocs
- Tuesday, Nov 30, 2021: All Q-SEnSE Convergence Seminar (Axelrad); 21 Q-SEnSE

Investigators; 11 collaborators, students & postdocs

- Tuesday, Oct 19, 2021: All Q-SEnSE Convergence Seminar (<u>Stick & Yelin</u>); 23 Q-SEnSE Investigators; 45 collaborators, students & postdocs
- Tuesday, Sep 21, 2021: All Q-SEnSE Convergence Seminar (<u>Doyle</u> & <u>Rieker</u>); 16 Q-SEnSE Investigators; 18 collaborators, students & postdocs
- Tuesday, Jun 8, 2021: All Q-SEnSE Convergence Seminar (<u>Deutch & Rey</u>); 18 Q-SEnSE Investigators; 21 collaborators, students & postdocs
- Tuesday, May 4, 2021: All Q-SEnSE Convergence Seminar (<u>Chiaverini</u> & <u>Nam</u>; 22 Q-SEnSE Investigators; 22 collaborators, students & postdocs
- Tuesday, Apr 20, 2021: All Q-SEnSE Convergence Seminar (<u>Kasevich</u> & <u>Kaufman</u>; 22 Q-SEnSE Investigators; 28 collaborators, students & postdocs
- Tuesday, Mar 23, 2021: All Q-SEnSE Convergence Seminar (<u>Papp</u> & <u>Newbury</u>; 17 Q-SEnSE Investigators; 20 collaborators, students & postdocs
- Tuesday, Feb 23, 2021: All Q-SEnSE Convergence Seminar (<u>Monteleoni</u> & <u>Lehnert</u>; 21 Q-SEnSE Investigators; 21 collaborators, students & postdocs

Collaboration Builders for Grand Challenges 2 & 3

Informal lunches to spark novel pair-wise collaborations among Investigators in Grand Challenges 2 & 3. Currently scheduled for noon in Boulder, with highlights presented in the next Convergence Seminar chat session.

- Tuesday, May 24, 2022, Noon Mountain Time
- Monday, Apr 11, 2022, Noon Mountain Time
- Next up!
 Wednesday, Mar 2, 2022, Noon Mountain Time
- Thursday, Jan 27, 2022, Noon Mountain Time -- CANCELLED for Covid Restrictions
- Thursday, Nov 18, 2021, 12:30pm Mountain Time

Grand Challenge Crystallization (Team-building) Meetings

- Feb 23, 2021: Grand Challenge 2 Crystallization Workshop II (Axelrad, Knappe, & Rieker organizers; 20 Q-SEnSE Investigators)
- Oct 23, 2020: Grand Challenge 3 "Crystallization Workshop" (14 Q-SEnSE Investigators)
- Oct 22, 2020: Grand Challenge 2 "Crystallization Workshop" (25 Q-SEnSE Investigators)
- Oct 13, 2020: Grand Challenge 1 "Crystallization Workshop" (26 Q-SEnSE Investigators)

Governance and Annual Meetings

- Aug 11-12, 2021: NSF Year 1 Site Visit (Investigators, Collaborators, Students, Postdocs, Staff)
- Jul 20-21, 2021: NSF Q-SEnSE Annual Meeting (Investigators, Collaborators, Students, Postdocs, External Advisory Board)
- Dec 18, 2020: Social Intelligence Workshop for Q-SEnSE Leadership (attendees Ye, Regal, Thompson, Lehnert, ONeil et al.)
- Nov 5, 2020: Q-SEnSE Executive Committee Meeting (9 XC Members)
- Oct 8, 2020: Q-SEnSE Executive Committee Meeting (9 XC Members)
- Sep 10, 2020: Q-SEnSE Executive Committee Meeting (9 XC Members)

EXTERNAL COMMUNITY

- Dec, 2021, "How Does Laser Cooling of Molecules Work?", lab presentation to high school students by graduate students Justin Burau, Kameron Mehling, and Parul Aggarwal in Ye group.
- Oct 2020 onwards: National Quantum Initiative Advisory Committee, organized by the White House Office of Science and Technology Policy (OSTP) and the U.S. Department of Energy (Ye)
- Oct 2021: "Preparing to enter the quantum workforce," Southwest Quantum Information and Technology Workshop, (virtual) (Lewandowski)
- Sep 2021: "Preparing to enter the quantum workforce," Co-design Center for Quantum Advantage: Quantum Career Fair, (virtual) (**Lewandowski**)
- Aug 2021: "Hiring Challenges in Quantum Information Science", Keynote address, Quantum Workforce Recruitment in Government Workshop, (virtual) Laboratory for Physical Sciences (**Lewandowski**)
- Jun 2021: "Preparing for the Quantum Revolution: What Is the Role of Higher Education?" Software-Tailored Architectures for Quantum Codesign (STAQ) Virtual Summer School, Duke University (virtual) (Lewandowski)
- Jun 2021: "Preparing for the Quantum Revolution: What Is the Role of Higher Education?" QUEST: Quantum Undergraduate Education & Scientific Training Workshop, Cal State San Marcos (virtual) (Lewandowski)
- Apr 2021: "Preparing for the Quantum Revolution: What Is the Role of Higher Education?" Physics Colloquium, University of Utah, Salt Lake City, Utah (virtual) (**Lewandowski**)
- Mar 2021: "Preparing for the Quantum Revolution: What Is the Role of Higher Education?" DOE Office of Science's Quantum Information Science Education Working Group, (virtual) (Lewandowski)

- Mar 2021: QED-C Quantum Industry Workforce Needs Survey: Preliminary Results", 2021 QED-C Plenary (virtual) (Lewandowski) (Lewandowski)
- Feb 2021: "Preparing for the Quantum Revolution: What Is the Role of Higher Education?" NSF Workshop on Quantum Engineering Education, (virtual) (Lewandowski)
- Aug 18, 2021: "QED-C Workforce TAC Webinar: NSF Quantum Centers and their engagement with industry" (**Regal**)
- Jan 26, 2021: Aerospace Corporation Distinguished Speaker Series (Ye)
- Dec, 2020: USAF Virtual Quantum Collider 2.0, panel member (Lewandowski)
- Dec, 2020: NSF Project Scoping Workshop: "Does the QISE Community Need a Goal-Oriented Distributed User Facility?" (Ye)
- Dec, 2020: NQI Community Meeting: NSF, NIST, DOE (Ye, Lewandowski)
- Dec, 2020: Overview of Q-SEnSE, CUbit, and JILA for the Missile Defense Agency Advanced Technology Directorate (**Regal**)
- Nov 19, 2020: Overview of CUbit and Quantum for CO-Labs and U.S. Congressman Joe Neguse (**Ye**)
- Nov 17, 2020: OSA High Brightness Virtual Conference (Ye)
- Nov 11, 2020: 2020 Chicago Quantum Summit, hosted by the Chicago Quantum Exchange (Ye)
- Oct 21, 2020: Quantum 2020, hosted by IOP Publishing, Chinese Physical Society and the University of Science and Technology of China (**Ye**)
- Oct 20, 2020: ColdQuanta announces public availability of Albert, a remote acess platform for students anywhere to form, manipulate, and study Bose-Einstein Condensates (Anderson)
- Oct 2020: IEEE Quantum Week, Quantum Workforce Track, Chair (Lewandowski)
- Sep 29, 2020: NSF QLCI Grantees' Meeting (Ye)
- Sep 16, 2020: DOE OSA Quantum 2.0 Conference (Ye)
- Aug 6, 2020, Virtual Photonics for Quantum 2 Workshop, hosted by Rochester Institute of Technology (Regal)

Archived Entries

2019 Community Outreach & Engagement

November 2019

- Kavli Futures Symposium: Achieving a Quantum Smart Workforce (Lewandowski)
- IEEE Quantum Initiative Sessions at IEEE Rebooting Computing Week 2019 (Lewandowski)

University of Colorado Boulder

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Attachment D, Publications

(Senior Investigators of the Institute are in **boldface**)

M. F. J. Fox, B. M. Zwickl, and H. J. **Lewandowski**, "Preparing for the quantum revolution: What is the role of higher education?", Physical Review Physics Education Research 16, 020131 (2020), DOI: 10.1103/PhysRevPhysEducRes.16.02013

C. J. Kennedy, E. Oelker, J. M. Robinson, T. Bothwell, D. Kedar, W. R. Milner, G. E. Marti, A. Derevianko, and J. **Ye**, "Precision Metrology Meets Cosmology: Improved Constraints on on Ultralight Dark Matter from Atom-Cavity Frequency Comparisons", Phys. Rev. Lett. 125, 201302 (2020), DOI 10.1103/PhysRevLett.125.201302

K. Matsuda, L. De Marco, J-R. Li, W.G. Tobias, G. Valtolina, G. Quéméner, J. Ye, "Resonant collisional shielding of reactive molecules using electric fields", Science, Vol. 370, Issue 6522, pp. 1324-1327 DOI 10.1126/science.abe737

S. Kelly, A. M. **Rey**, and J. Marino, "Effect of active photons on dynamical frustration in cavity QED", Physical Review Letters 126, 133603 (2021), 10.1103/PhysRevLett.126.133603

R. J. Lewis-Swan, D. Barberena, J. R. K. Cline, D. Young, J.K. **Thompson**, and A. M. **Rey**, "Cavity-QED quantum simulator of dynamical phases of a BCS superconductor", Phys. Rev. Lett. 126, 173601 (2021), DOI 10.1103/PhysRevLett.126.173601

T. Bilitewski, L. De Marco, J. Li, K. Matsuda, W. Tobias, G. Valtolina, J. Ye, and A. M. Rey, "Dynamical generation of spin squeezing in ultra-cold dipolar molecules", Phys. Rev. Lett. 126, 113401 (2021). DOI 10.1103/PhysRevLett.126.113401

M. Mamaev, I. Kimchi, R. Nandkishore, and A.M. **Rey**, "Tunable spin model generation in spinorbital coupled fermions in optical lattices", Physical Review Research 3, 013178 (2021). DOI 10.1103/PhysRevResearch.3.013178

A. Chu, J. Will, J. Arlt, C. Klempt, and A. M. **Rey**, "Simulation of XXZ Spin Models using Sideband Transitions in Trapped Bosonic Gases", Physical Review Letters 125, 240504 (2020). DOI 10.1103/PhysRevLett.125.240504

R. J. Lewis-Swan, S.R. Muleady, and A. M. **Rey**, "Detecting out-of-time-order correlations via quasiadiabatic echoes as a tool to reveal quantum coherence in equilibrium quantum phase transitions", Physical Review Letters 125, 240605 (2020). DOI 10.1103/PhysRevLett.125.240605

M. H. Muñoz-Arias, P. Poggi, and I. **Deustch**, "Nonlinear dynamics and quantum chaos of a family of kicked p-spin models", Phys. Rev. E 103, 052212 (2021). DOI 10.1103/PhysRevE.103.052212

R.J. Fasano, Y.J. Chen, W.F. McGrew, W.J. Brand, R.W. Fox, and A.D. Ludlow, "Characterization and Suppression of Background Light Shifts in an Optical Lattice Clock", Phys. Rev. Applied 15, 044016, DOI 10.1103/PhysRevApplied.15.044016

R. Lewis-Swan, S. R. Muleady, D. Barberena, J. J. Bollinger, and A. M. **Rey**, "Characterizing the dynamical phase diagram of the Dicke model via classical and quantum probes", Phys. Rev. Res. 3, L022020 (2021), DOI 10.1103/PhysRevResearch.3.L022020

A. Cidrim, P. Orioli, C. Sanner, R. B. Hutson, J. Ye, R. Bachelard, and A. M. **Rey**, "Dipoledipole frequency shifts in multilevel atoms", Phys. Rev. Lett 127, 013401 (2021), DOI 10.1103/PhysRevLett.127.013401

C. D. Marciniak, T. Feldker, I. Pogorelov, R. Kaubruegger, D. V. Vasilyev, R. van Bijnen, P. Schindler, P. **Zoller**, R. Blatt, T. Monz, "Optimal metrology with variational quantum circuits on trapped ions", Preprint: https://arxiv.org/abs/2107.01860

C. Hughes, D. Finke, D.-A. German, C. Merzbacher, P. M. Vora, and H. J. **Lewandowski**, "Assessing the Needs of the Quantum Industry", Preprint: arxiv.org/abs/2109.03601

B. Li, J. Bartos, Y. Xie, and S-W **Huang**, "Time-magnified photon counting with 550-fs resolution", Optica 8, 1109 (2021) DOI 10.1364/OPTICA.420816

D. T. C. **Allcock**, W. C. Campbell, J. **Chiaverini**, I. L. Chuang, E. R. Hudson, I. D. Moore, A. Ransford, C. Roman, J. M. Sage, and D. J. **Wineland**, "Blueprint for trapped ion quantum computing with metastable states", arxiv.org/abs/2109.01272

K. W. Lehnert, "Quantum enhanced metrology in the search for fundamental physical phenomena", to appear in "Quantum Information Machines; Lecture Notes of the Les Houches Summer School 2019", M. Devoret, B. Huard, and I. Pop editors, arXiv:2110.04912

K. Wurtz, B. M. Brubaker, Y. Jiang, E. P. Ruddy, D. A. Palken, and K. W. **Lehnert**, "A cavity entanglement and state swapping method to accelerate the search for axion dark matter", arXiv:2107.04147

K. Gilmore, M. Affolter, R. J. Lewis-Swan, D. Barberena, E. Jordan, A. M. **Rey**, and J. J. **Bollinger**, "Quantum-enhanced sensing of displacements and electric fields with twodimensional trapped-ion crystals", Science 373(6555), 673–678. (2021), DOI 10.1126/science.abi5226

R. Kaubruegger, P. Silvi, C. Kokail, R. van Bijnen, A. M. **Rey**, J. **Ye**, A. M. **Kaufman**, and P. **Zoller**, "Variational spin-squeezing algorithms on programmable quantum sensors", Phys. Rev. Lett., 123, 260505 (2019), DOI 10.1103/PhysRevLett.123.260505

M. A. Perlin, D. Barberena, M. Mamaev, B. Sundar, R. J. Lewis-Swan, and A. M. **Rey**, "Engineering infinite-range SU(n) interactions with spin-orbit-coupled fermions in an optical lattice", arxiv.org/abs/2109.11019 (2021)

T. Bilitewski, A. Pineiro Orioli, C. Sanner, L. Sonderhouse, R. B. Hutson, L. Yan, W. R. Milner, J. Ye, and A. M. Rey, "Disentangling Pauli blocking of atomic decay from cooperative radiation and atomic motion in a 2D Fermi gas", arxiv.org/abs/2108.02819 (2021)

A. Pineiro Orioli, J. K. **Thompson**, A. M. **Rey**, "Emergent dark states from superradiant dynamics in multilevel atoms in a cavity", arxiv.org/abs/2106.00019 (2021)

J. Huber, A. M. **Rey**, P. Rabi, "Realistic simulations of spin squeezing and cooperative coupling effects in large ensembles of interacting two-level systems", arxiv.org/abs/2105.00004 (2021)

A. Chu, P. He, J. K. **Thompson**, A. M. **Rey**, "Quantum enhanced cavity QED interferometer with partially delocalized atoms in lattices", arxiv.org/abs/2104.04204 (2021).

C. Sanner, L. Sonderhouse, R. B. Hutson, L. Yan, W R. Milner, and J. Ye, "Pauli blocking of atom-light scattering", Science Vol 374, Issue 6570, pp. 979-983, DOI: 10.1126/science.abh348

S. Omanakuttan, A. Mitra, M. J. Martin, and I. H. **Deutsch**, "Quantum optimal control of tenlevel nuclear spin qudits in 87Sr", Phys. Rev. A 104, L060401, DOI: 10.1103/PhysRevA.104.L060401

Attachment E, Workgroups within the Grand Challenges

Working groups within individual Grand Challenges or spanning several. Regular meetings of these working groups established several effective collaborative projects within the center.

- Spin squeezing collaboration between The University of Colorado (CU), MIT, and Stanford
- Tweezer collaboration between CU, The University of New Mexico (UNM), and Los Alamos National Laboratory (LANL)
- Integrated photonics and trapped ion collaboration between CU/NIST, MIT Lincoln Lab, Sandia National Lab, and University of Oregon
- A portal for atomic structure calculation that is relevant for fundamental physics search has been established, along with effective collaboration between U. Delaware, CU/NIST
- A cross-center collaboration on the connection between quantum information science, quantum sensing, and machine learning between CU, UNM, Harvard, U. Innsbruck
- Phase-stabilized fiber network collaboration between CU and NIST
- Magnetometer-based quantum sensing collaboration within CU
- Portable atomic clocks and integrated photonics collaboration between CU, NIST, and external partners such as U. California Santa Barbara
- Sr quantum information infrastructure collaboration between Stanford and CU
- Cold molecule-based quantum sensing platform between Harvard and CU

Appendix C: MRI Consortium: Development of Fiber-coupled stimulated emission depletion microscopy (STED)

Full name of the funded project: MRI: Development of a Mobile High-speed Dual Frequency Comb Spectroscopy User Facility

First and last name of the primary investigator (PI) for this project (or PI's): Gregory B. Rieker

Enter a short description or abstract of the project:

Laser light has long been a preferred tool for watching chemical processes evolve in systems ranging from combustion engines to the atmosphere to biology. Molecules in these systems absorb light in a specific pattern of wavelengths, and thus can be detected without perturbing the process by illuminating the sample with different wavelengths of light and quantifying the absorption.

The frequency comb is a CU/NIST invention that led to part of the 2005 Nobel Prize in Physics. It is a laser source that emits hundreds of thousands of distinct, narrowly spaced wavelengths of light. When interfered with a second frequency comb in a special process called dual frequency comb spectroscopy, the light source offers unparalleled potential to probe the evolution of chemical species and conditions in reacting systems with a combination of broad spectral bandwidth, high spectral resolution, and fast time resolution that is not available with any other instrument. In recent years, our groups have been at the forefront of developing fundamental and next generation frequency comb sources and detection techniques (Diddams), and engineering dual frequency comb systems for field application in real world combustion and atmospheric systems (Rieker and Hoghooghi). However, the true potential for frequency comb spectroscopy to proliferate and make an impact in more research fields and experiments has been hindered by three key limitations:

- 1) The complexity and immobility of traditional dual-comb systems has been a barrier to adoption by chemists, physicists, and engineers that are not experts in frequency comb spectroscopy.
- 2) The output for current portable dual-comb systems is not at the optimal mid- and longwaveinfrared wavelengths where most molecules absorb strongly.
- 3) The speed with which current broadband dual-comb systems can measure absorption spectra is fast (millisecond), but increasing the acquisition speed by two orders of magnitude to 10s of microseconds will open the door to a much larger range of chemically reacting systems.

Here, we address all three challenges by developing a new high-speed dual-comb spectrometer capable of acquiring broadband, high-resolution mid- and longwave-infrared spectra at microsecond rates. The system will become part of a new *mobile* user facility at CU, which will deploy the system for user experiments in chemistry, physics, and engineering across CU and the US.

Summarize progress made over the last year, focusing on key objectives or milestone reached, challenges encountered, and/or other particularly noteworthy highlights (limit answer to 1/2 page).

During the first year of the project, we developed two 1GHz mid-infrared (MIR) frequency combs with broad spectral coverage of 3-14 microns and several milliwatts of optical power. Specifically, in year 1 we successfully developed the following modules for each frequency comb system:

a) 1-GHz near-infrared (NIR) mode-locked lasers (commercial laser, purchased)

- b) Chirped pulse fiber amplifiers
- c) Nonlinear broadening and temporal compression

d) MIR generation through intra-pulse difference frequency generation

1-GHz NIR lasers At the core of the spectrometer are two robust NIR 1-GHz frequency combs with slightly offset pulse repetition rates. These lasers have only become commercially available within the last year and are one of the key enabling technologies for developing this spectrometer. The exact repetition rates of the lasers can be adjusted to achieve the required time resolution and spectral bandwidth of the dual-comb measurement at hand (sub-ms to microsecond time resolution). During year 1, we acquired the first pair of these lasers, and used them to seed light into the rest of the system described below.

Chirped pulse fiber amplifier module We take advantage of the chirped pulse amplification (CPA) technique (Nobel Prize in physics in 2018) in our amplifier design. CPA has enabled development of table-top amplifiers which can generate very high energy pulses. In this design, optical pulses after the pre-amplifier are chirped and temporally stretched before entering the high-power amplifier. This step happens in a dispersion compensating fiber (DCF). The length of the fiber needs to be precisely controlled for optimum performance of the amplifier. The chirped pulses then enter the amplifier. The high-power amplifier is an all-in-fiber cladding pumped amplifier. The gain fiber is a Er/Yb doped fiber which is pumped with a high power 18W multimode diode laser. The cladding pump technique allows for extracting higher gain. Optimization of the amplifier design is critical to achieve high gain and suppress amplified spontaneous emission. We have designed and implemented the all-fiber amplifier to achieve pulse energies of 5 nJ (5W average power).

Nonlinear broadening and temporal compression module High energy pulses generated in the chirped pulse amplifier module undergo nonlinear broadening in a highly nonlinear fiber (HNLF) to generate a bandwidth of ~600 nm. We investigated spectral broadening using normal dispersion HNLF (ND-HNLF) and anomalous dispersion HNLF (AD-HNLF). Positively chirped pulses generated using ND-HNLF are temporally compressed using a pair of fused silica wedges to generate 20 fs pulses. Spectral broadening in AD-HNLF generated few-cycle pulses (~8 fs) directly out of the fiber without a need for silica wedges.

MIR generation module We use the intrapulse difference frequency generation (DFG) technique to generate MIR light by focusing the high power few cycle pulses generated through self-compression in AD-HNLF into a PPLN nonlinear crystal. The various parts of the few cycle pulse spectrum mix within the nonlinear crystal. Intrapulse DFG happens between the comb

modes of the same pulse which simplifies the MIR generation, and critically, no delay control between pulses is required. In this manner, we generate broadband MIR light covering the entire 3- 5mm region (2000- 3400 cm⁻¹) containing up to 4.5 mW of power in a compact setup with the majority of the optical path in fiber.

Provide outcomes/benefits of this project over the past year, including both scientific advancements as well as other benefits. Examples of the latter include contributing to graduate and undergraduate education; K-12 or other outreach; technology commercialization and/or spin-off companies; collaboration with others.

In our work so far, we demonstrated generation of mid- and longwave infrared frequency combs through a robust approach (all-in-fiber short near-infrared pulse generation + intra-pulse difference frequency generation) at 1-GHz repetition rate. The wavelength and the 1-GHz repetition rate give the mid-infrared spectrometer an unparalleled combination of acquisition speed, bandwidth and resolution, providing impact across multiple fields including combustion science, fundamental chemical kinetics, materials science, atmospheric chemistry, near-field nanoscopy, and bio-medical microscopy and imaging.

The project has provided significant opportunities for training and professional development for a PhD student. He has learned a diverse sets of skills in nonlinear optics (experimental and simulation), as well as basic optics laboratory and collaboration skills.

Additional documentation:

(Additional documentation may include additional artifacts, reports, or content that should be included as an appendix or addendum to the content supplied in this form.)

Appendix D: University of Colorado, Boulder- DOE Desalination Hub: NAWI Road mapping

Full name of the funded project:

DOE Desalination Hub: NAWI Road mapping year 1

First and last name of the primary investigator (PI) for this project (or PI's):

Karl G. Linden

Enter a short description or abstract of the project:

Engage in the baseline evaluation and roadmap development of water reuse practices supporting NREL and the NAWI team in the areas of industrial reuse, agricultural reuse, oil and gas wastewater reuse and mining wastewater reuse.

Summarize progress made over the last year, focusing on key objectives or milestone reached, challenges encountered, and/or other particularly noteworthy highlights:

Provided literature review and expert analysis on information and data for the roadmap teams engaged in the water impact and reuse opportunities through treatment technology selection for steel industry, mining industry, oil and gas industry and agriculture industry. Support for development of a tool to allow selection of treatment technology for a given water quality objective.

Provide outcomes/benefits of this project over the past year, including both scientific advancements as well as other benefits. Examples of the latter include contributing to graduate and undergraduate education; K-12 or other outreach; technology commercialization and/or spin-off companies; collaboration with others.

This work engaged 2 graduate students, one post-doc, 2 undergraduate students and 3 faculty members from the Civil, Environmental, and Architectural Engineering Department at University of Colorado. Outcomes are 3 publications in peer-reviewed journals summarizing the roadmapping activities. This work will form the basis for future research proposals as part of the NAWI goal of advancing water reuse and technology.

Appendix E: University of Colorado, Colorado Springs- MRI: Acquisition of a High-Performance Computing Cluster for Next-Generation Computational Science in Southern Colorado

NSF Award to University of Colorado, Colorado Springs (UCCS)

NSF Award: 2017917

Title: MRI: Acquisition of a High-Performance Computing Cluster for Next-Generation Computational Science in Southern Colorado

PI: Brandon Runnels, Ph.D. Assistant Professor, Mechanical and Aerospace Engineering.

Total CHECRA Funding: \$112,500

Abstract:

This project will enable the acquisition, deployment, and maintenance of a high-performance computing (HPC) cluster (to be called INCLINE). This instrument will provide much-needed computational resources to the UCCS campus and the Southern Colorado scientific and academic communities. The size and power of the instrument will bridge the growing gap between workstation-level machines and Top 500 supercomputers, allowing researchers to test and leverage code scalability on an HPC platform, to expedite result processing, and to gain expertise on a local HPC environment. The work to be performed will yield insight into biomedical applications, such as microbubble drug delivery and bone fracture, military applications, such as additively manufactured energetics, and civil applications, including improved structural materials. In addition to research applications, INCLINE will be used as an educational platform for teaching the fundamentals of an HPC to undergraduate and graduate students and allow students to investigate classroom problems more deeply with the computational power provided by an HPC. It will also be used to supplement existing outreach programs to spark enthusiasm and interest in HPC in the Southern Colorado community, which is diverse in both population and the range of applications.

The instrument's state-of-the-art hardware is designed to support a broad range of highperformance scientific applications, ranging from compiler design to computational fluid dynamics. The instrument will contain both CPU compute (including standard and high memory), and GPU nodes. The compute nodes will enable standard massively parallel computations such as computational solid mechanics and fluid dynamics. The GPU nodes will allow acceleration on computational physics and machine learning projects and will be used in conjunction with CPU nodes to test optimal load balancing on heterogeneous architectures. All nodes will be connected using InfiniBand high speed interconnects to minimize latency for communication-intense applications, including CFD and computational solid mechanics. A high speed SCRATCH storage file system will minimize I/O latency for applications with large output file sizes and I/O requirements. The estimated peak performance of the instrument is approximately 90 TFLOPS. The Slurm queueing system will be used to manage accounts and allocations across the diverse user base. The robust design of this instrument will allow it to fill the growing need for a local HPC research facility at UCCS and in Southern Colorado and will facilitate the training of the next generation of computational scientists.

Progress made over the last year:

The project team has successfully worked with the UCCS OIT and College of Engineering to create the needed HPC infrastructure to support deployment. This includes server space, installation of racks, creation of a support team and the acquisition of necessary software. The INCLINE web interface is now stood up, including the creation of an HPC account request system, creation of the HPC software request page, and finalization of the allocation policy. One important benefit is that project has also led to UCCS joining the Rocky Mountain Advanced Computing Consortium (RMACC) as a full member.

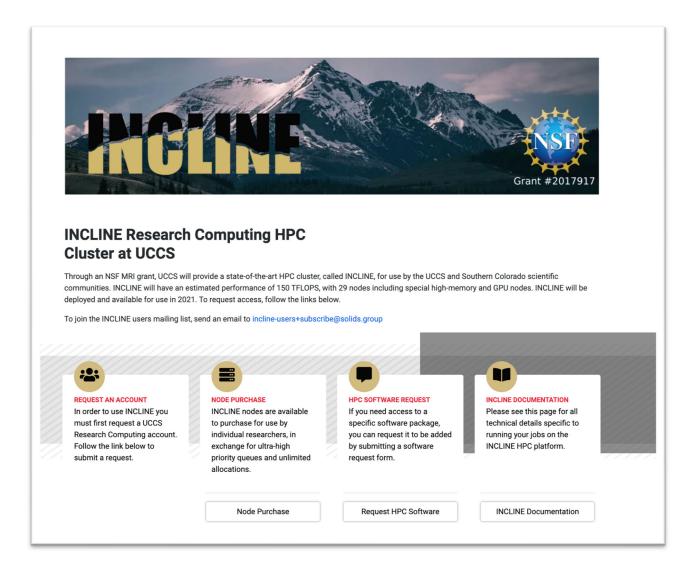
It is worthwhile to note that project progress was significantly impacted due to the global chip shortage. As a result the delivery of many of the instrument components have been delayed. Components were not complete until Fall of 2021. The vendor (Dell) negotiated with us to adjust the support of the project to align with the new finalized component delivery date. We are happy to report that INCLINE is now deployed and fully operational despite these delays.

A summary of recent achievements include:

- User account request process created
- User accounts created for key personnel
- Software request system put in place and some software has been installed and tested
- Primary documentation has been created and made available online
- Mailing list created
- Tested successfully with large-scale simulations.
- Results generated for several manuscripts, some currently under review and some in preparation.

Additional Documentation:

https://rc.uccs.edu/incline

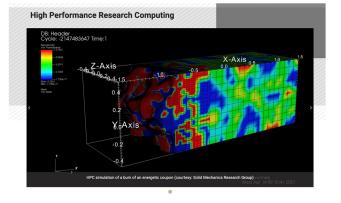




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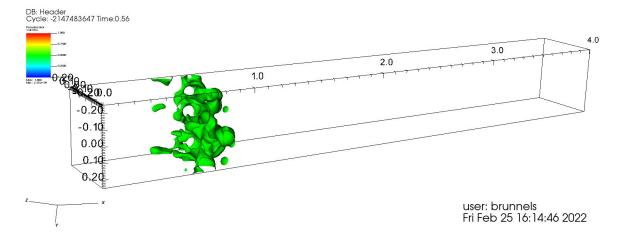
- Getting Started on INCLINE
- Preparing Your Code
- Running Jobs on INCLINE
- Data Transfer on INCLINE
- System Overview
- **INCLINE** Resources
- Tutorials



Welcome to Research Computing at UCCS

This is the home page for holp performance computing (HCP) resources to support research and training at UCCS. Scientific computing is the application of computers to simulate or predict the answers to complex problem. It allows researchers to find the answers the questions that are too expensive, dangraperu, and allow the impossible to determine experimentally or theoretically. Scientific computing has advanced rapidly in recent decades, and can legitimately be called a "hird branch" of the scientific methylac. Computational science public computer to behin limits in other too chain accuster, subplicateurs. May simulations can take months or years to run on a single decktop computer. The use of HPC allows researchers to run these simulations in a fraction of the tare the runner to the scientific methylaction of the custers.

Through an NSF MRI grant, UCCS will provide a state-of-the-art HPC cluster, called NCLINE, for use by the UCCS and Southern Colorado scientific communities, INCLINE will have an estimated performance of 100 TFLOPS, with 25 nodes including special high-memory and GPU nodes, INCLINE will be deployed and available for use in early 2021. To request access (finds the links before)



Example of results generated from INCLINE use:

"Deflagration of ammonium perchlorate (AP) and hydroxyl-terminated polybutadiene (HTPB) solid rocket propellant, from a simulation run on INCLINE." - from Kanagarajan, Quinlan, Runnels (under review).

Appendix F: Colorado School of Mines Re-inventing the Nation's Urban Water Infrastructure

DOE National Alliance for Water Innovation (NAWI) – Foundational Control

Reporting Period: July 15, 2020 - June 30, 2022

Summary: The National Alliance for Water Innovation (NAWI) is a research consortium that was formed in 2017 to partner with the U.S. Department of Energy to create the Energy-Water Desalination Hub. In 2019 the DOE announced that NAWI will manage the new Desalination Hub. NAWI vision is to support the develop affordable, energy-efficient, and resilient water supplies from unconventional resources (e.g., oil and gas, mining, agriculture, seawater/brackish water, power industry, and general industries). Research under NAWI focused on enhancing the U.S. economy through decentralized, small-scale, fit-for-purpose desalination.

NAWI is managed by Laurence Berkeley National Lab (LBNL), with support from the National Renewable Energy Lab (NREL), Oak Ridge National Lab (ORNL), and the National Energy Technology Lab (NETL). Colorado School of Mines was one of the first universities in the country to join NAWI, and shortly after CU Boulder and CSU have joined NAWI. Today there are more than 19 universities associated with NAWI, including Yale, UCONN, Rice, UCONN, UT Austin, Baylor, Texas A&M, UC Berkeley, Stanford, UCLA, UC Irvine, USC, University of Cincinnati, NMSU, and more.

Description of the project, the principal persons or entities involved in the project, and the amount of funding allocated to each principal person or entity

Mines was fortunate to have two faculty involved in two of the NAWI six (6) first-year projects. Prof. Cath (CEE) is involved in the Foundational Controls project (Project 5.3: integration of data science in water treatment and developing novel control systems for autonomous water treatment plants) and Prof. Tilton (ME) in involved in the Computational TestBed project (Project 5.4: development of computational fluid dynamics program to reduce process degradation and system integrity).

In project 5.3 we have developed unique computer models that run in parallel to a pilot desalination system, and in real time optimize the operation of the desalination system (digital twine). This system maximizes the productivity of the desalination system, minimize electricity use, and minimize brine production. This project was extremely successful and resulted in additional grant from NAWI for the next 3 years, totaling \$810,000. Furthermore, the new project build upon another project that was partially supported by CHECRA, the Pure Water Colorado Direct Potable Reuse Demonstration in which Mines constructed and operating a unique water research infrastructure (https://www.csu.org/Pages/DirectPotableReuse.aspx). The mobile demonstration lab will be a key component in the new NAWI project.

CHECRA funding supported the faculty, staff, and students at Mines that were involved in data collection and analysis, system construction, water quality analysis, and preparation of reports. The project is in its final stages and publications are under preparation.

DOE National Alliance for Water Innovation (NAWI) – Desalination Road mapping

Reporting Period: July 15, 2020 - June 30, 2022

Summary: The National Alliance for Water Innovation (NAWI) is a research consortium that was formed in 2017 to partner with the U.S. Department of Energy to create the Energy-Water Desalination Hub. In 2019 the DOE announced that NAWI will manage the new Desalination Hub. NAWI vision is to support the develop affordable, energy-efficient, and resilient water supplies from unconventional resources (e.g., oil and gas, mining, agriculture, seawater/brackish water, power industry, and general industries). Research under NAWI focused on enhancing the U.S. economy through decentralized, small-scale, fit-for-purpose desalination.

NAWI is managed by Laurence Berkeley National Lab (LBNL), with support from the National Renewable Energy Lab (NREL), Oak Ridge National Lab (ORNL), and the National Energy Technology Lab (NETL). Colorado School of Mines was one of the first universities in the country to join NAWI, and shortly after CU Boulder and CSU have joined NAWI. Today there are more than 19 universities associated with NAWI, including Yale, UCONN, Rice, UCONN, UT Austin, Baylor, Texas A&M, UC Berkeley, Stanford, UCLA, UC Irvine, USC, University of Cincinnati, NMSU, and more.

Description of the project, the principal persons or entities involved in the project, and the amount of funding allocated to each principal person or entity

Research under NAWI started in summer 2020. The main task of the first year was road mapping of the water industry to define the knowledge gaps that require research in the next 5-10 years to enable cost and energy reduction during production of clean water from unconventional sources. Professors from Mines (Cath and Seetharaman), CU Boulder (Linden), and CSU (Borch) were involved in the road mapping process, specifically as it is related to the oil and gas, mining, and agricultural industries.

CHECRA funding supported the faculty, staff, and students at Mines that were involved in data collection and analysis, interviews with industry stakeholders, and preparation of reports. Specifically, Mines faculty were involved in the oil and gas roadmap, and overseeing the master roadmap. The main product produced following this project is the master roadmap (<u>https://www.nawihub.org/knowledge/roadmap-publication-series/</u>) and a specific publication in a scientific journal related to the baseline technologies for treatment and reuse of produced water from the oil and gas industry (<u>https://pubs.acs.org/doi/10.1021/acsestengg.1c00248</u>

Appendix G: MRI: Acquisition of an Open Access Shared-Use MALDI-TOF/TOF Mass Spectrometer

CHECRA Annual Report #1

Submitter: Travis Bailey

Email: travis.bailey@colostate.edu

Date: February 15, 2022

Institution: Colorado State University

Project Name: MRI: Acquisition of an Open Access Shared-Use MALDI-TOF/TOF Mass Spectrometer

Primary Investigator: Travis Bailey

Project Abstract: This CHECRA project provides partial cost share support for a National Science Foundation Major Research Instrumentation Grant awarded to Colorado State University in August 2021, to fund the acquisition of a high-resolution Matrix Assisted Laser Desorption/Ionization Tandem Time-of-Flight Mass Spectrometer (MALDI-TOF/TOF) to serve as a shared resource for CSU faculty and students with open access to users from the surrounding Rocky Mountain region. The MALDI-TOF/TOF will provide state-of-the-art molecular mass and structural characterization for CSU research programs with foundations in synthetic polymers, nanomaterials, and biological macromolecules. This new instrument will bring transformative improvements in mass resolution, mass accuracy, sensitivity, and dynamic range over CSU's existing benchtop MALDI Biotyper, while adding currently non-existent capabilities for structural elucidation provided by tandem MS/MS technology. The instrument will be housed in the mass spectrometry laboratory of the established CSU Analytical Resources Core (ARC), and be managed by two dedicated, full-time, female staff scientists with over 25 years of experience with mass spectrometry operations and management. The ARC is an essential CSU resource for advanced analytical research, research training, and education services in support of chemical, biological and materials sciences, and thus a natural home for the proposed MALDI-TOF/TOF. The award is for a 36-month/3-year duration.

Project Progress: This project officially started on 8/1/2021, however, access to funding provided by the three funding sources (NSF, CHECRA, and CSU OVPR) were only made available to the PI and co-PIs in January 2022. Thus, the project is in its infancy at the time of this submission. Current progress has been limited to submission of the purchase order for procurement of the instrument (Bruker UltrafleXtreme MALDI TOF/TOF) which is scheduled for delivery and installation mid-April of 2022. In addition, a post-doctoral research associate dedicated to the training and development of training materials was successfully identified and hired through a competitive search and joined the ARC facility January 15th, 2022. We look forward to the installation and commissioning of the new instrument in the coming spring and the subsequent development of a new userbase of students anticipated to number in the 60s over the first year alone.

Appendix H: Colorado State University-A Novel Electro-dialytic Crystallizer (EDC) for Energy Efficient Zero-liquid Discharge

Annual report - CHECRA

Tiezheng Tong

Tiezheng.tong@colostate.edu

02/11/2022

Colorado State University

Project name: A Novel Electro-dialytic Crystallizer (EDC) for Energy Efficient Zero-liquid Discharge

PI: Tiezheng Tong

Description of the project: In this project, we aim to investigate a new brine management process called electro-dialytic crystallization (EDC). The EDC process integrates electrodialysis, which is a desalination technology driven by electricity, and crystallization into a single system to enable brine crystallization without evaporation or large temperature swing. The core innovation of EDC is the use of the electrodialysis phenomenon to maintain a saturated brine stream for continuous salt precipitation. We plan to perform experiments in order to prove the concept and acquire fundamental understanding of the system behavior. In addition, we will perform system-scale modeling to guide system design and optimization of EDC, which includes understanding the tradeoffs between system performance, longevity, scale, treatment cost (CAPEX and OPEX) through techno-economic analysis (TEA). Lastly, we will perform lifecycle assessment (LCA) and market analysis to evaluate the potential of the proposed technology for future practical adoption and the consequent environmental impacts. This is a collaboration with Vanderbilt University, and CSU is mainly responsible for understanding membrane scaling and fouling during brine treatment using EDC, performing system-scale modeling to guide system.

Project progress: This project started in October 2021. We focused on recruiting graduate students for this project and building the proof-of-concept EDC system. Two graduate students have been recruited by the Departments of Civil and Environmental Engineering and Mechanical Engineering of CSU. We have purchased all the elements and finished building the EDC system.

Outcomes/benefits of this project: This project is a collaboration with Vanderbilt University supported by Department of Energy Innovation Hub (National Alliance for Water Innovation). This project provides an opportunity to promote research on desalination and water treatment at CSU and has been supporting two PhD students. We aim to develop a novel technology that has the potential for revolutionizing hypersaline brine treatment. Multiple peer-reviewed journal articles and patents are expected from this project. As we just started this project in October 2021, more progresses will be reported in the annual report next year.

Appendix I: Colorado State University Extension Industrial Assessment Center

First and last name: Jason Quinn Email address: Jason.Quinn@colsotate.edu Date: 2/11/2022 Institution: Colorado State University Annual Report

Project Title: Colorado State University Extension Industrial Assessment Center

PI: Jason Quinn

Project Abstract:

The DOE sponsored CSU industrial assessment center (IAC) is a student led program that provides no cost, in-depth, energy assessments to small and medium sized manufactures. The program aims to reduce the energy and environmental impact of the manufactures, improve cost competitiveness, and train the next generation of energy engineers. The CSU IAC program has two major goals: (1) to provide engineering students with hands-on training and experience in the industrial and commercial energy systems field, and (2) to sponsor and promote assessments to stimulate more efficient operations and productivity enhancements at manufacturing facilities in Colorado and the Rocky Mountain West.

Project Progress:

The Global Pandemic has had a significant impact on the operation of the IAC. In person visits to manufactures were more challenging however with strong team commitment and the willingness of local manufacturers, we were able to conduct 5 in person assessments. The assessments generated 28 explicit energy related recommendations, with a total annual energy savings of over \$348,000. The program engaged 11 CSU students in 2021 and currently has 9 active students. As a result of the activity in 2021 and student accomplishments, two of the students were able to attain official DOE Student IAC Energy Certifications. In addition, 3 members of the team were trained in ISO 50001 Energy Management Systems.

In parallel with the in-person assessments, CSU continued to engage the broader educational community. In July, the team had a meeting with CSU's Impact MBA program director and student members to discuss collaboration opportunities. The Impact MBA program focuses on corporate sustainability practices and, as such, aligns with the goals of the CSU IAC program. The Impact MBA coordinates with the CSU IAC to provide backend support for the manufacturers that are assessed in order to encourage and support the implementation of recommendations. This meeting was also held with the project lead for Green Business Programs at the Colorado Department of Public Health and Environment (CDPHE). These three groups (CSU IAC, Impact MBA, and CDPHE) aim to work together to build a diverse engagement with manufacturers, as well as to support the assessment recommendation implementation process.

The collaboration between the IAC and these two other programs will greatly increase the number of assessment recommendation referrals and will greatly increase the potential for recommendations to be implemented. Presently, the CDPHE, CSU IAC, and CSU Impact MBA

programs are collaborating with contacts in a specific manufacturing sector to earn energy assessment opportunities as well as fellowship opportunities for Impact MBA students.

Project Outcomes:

The outcomes of the project are twofold: 1)training of an engineering workforce and 2) reduction in CO energy consumption in the manufacturing sector. In addition to the direct training of CSU students through the assessment process, CSU has integrated additional training opportunities during the weekly coordination meeting. Trainings occur biweekly or monthly. As part of this activity CSU has created a significant number of training and informational resources for our student team. Examples of the trainings provided as well as the expanded curriculum are given in the list below. Each of the topics outlined below has been documented by creating a resource on the subject. Each resource is designed to be used as a training module for new students and is available in CSU's training resource manual. Training resources are constantly being compiled for "how to be a center lead student", "new student training", "how to be an assessment lead", "how to assess various energy consuming system types", etc.

- The trainings and expanded curriculum are listed below:
- Training: "Understanding ISO50001" training completed by the lead student during Q4
- Training: "ISO50001 CP EnMS" training was completed by the lead student in late October; this training will be completed by a senior team member in the spring of 2022
- Training: Updated WWTP energy management resource
- Training: Calculating unit cost of demand when both coincident peak and peak demand exist on client billing
- Created a manual for compiling and submitting reports to the database
- Expanded the task sign-up sheet to include inputs for all fields required in IAC database
- Resources on emissions analysis, ISO 50001, and cybersecurity were created by the students and shared during a weekly training.
- Students were instructed to research and create a comprehensive resource on "High Global Warming Potential Refrigerants"
- Students created resources for estimating the total water savings due to curbed grid electricity and NG usage from our recommendations (similar to emissions analysis but for water)
- Training seminar with the CDPHE and CSU's Impact MBA: "Understanding Colorado's Green Business Programs and the Pollution Prevention (P2) Act"

This program is very much a hands-on educational program that trains our next generation energy professionals. The commitment of CO and our local manufacturing provides a hands-on opportunity that bridges the gap between in-class curriculum, and real world applied engineering.