UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

IBM-Illinois Discovery Accelerator Institute

AT THE GRAINGER COLLEGE OF ENGINEERING

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The Grainger College of Engineering
UNIVERSITY OF ILLINOIS URBANA-CHAMPAIGN

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Introduction

The IBM-Illinois Discovery Accelerator Institute (IIDAI) is a new model of academic-industry partnership designed to increase access to technology education and skill development to spur breakthroughs in emerging areas of technology, referred to in this document as research thrusts, which include Hybrid Cloud & AI, Quantum Computing, Materials Discovery, and Sustainability to accelerate the discovery of solutions to complex global challenges. At its inception in Fall 2021, the Institute's goal was to guide and support relevant projects within these thrusts.

In 2023, the Institute entered a new phase by refocusing its activities on the development of an open high-performance computing platform to support AI-infused applications. This platform will link classical and quantum computing at the infrastructure layer while providing optimized AI model training and inferencing. It will enable the community to better cope with the Gen AI explosion that we are all witnessing while providing end-to-end security; it will also provide leverage for various strategic downstream activities within the Institute's thrusts, including AI for code, sustainability, and accelerated materials discovery. While the development of the platform remains an aspirational goal, it has steered the selection of projects that are funded by the Institute. The following is a summary of activities that took place from August 2022 through August 2023. We conclude with a short preview of strategic goals for 2024 and beyond.

Hybrid Cloud & AI

Mission and Goals

The Hybrid Cloud & AI thrust is focused primarily on hybrid cloud technologies across the entire stack, spanning hardware, infrastructure and systems, operating systems, platform, middleware, software tools, and applications. Hybrid cloud technologies are at the core of all computing today, and the thrust therefore has strong synergies with other thrusts in the Institute, including those on sustainability, materials discovery, and quantum, as both a key platform enabler and a context provider. For example, sustainable computing is at the intersection of hybrid cloud and sustainability. Artificial intelligence (AI) is another computing discipline that is omnipresent today, again both as an important emerging workload and as a key enabling technology that promises innovative approaches to improve computing within the platform.

As more and more workloads move to the cloud, new applications and workloads emerge. The cloud is becoming more distributed, and new challenges are arising in programmability, management, security, compliance, cost, performance, and power efficiency. Within and across almost every layer of the stack, there is a need to examine and re-architect fundamental aspects of hardware and software to address these challenges. The Hybrid Cloud & AI thrust has pursued a top-down approach by prioritizing the needs of strategic emerging workloads and domains like edge computing in addition to focusing on the needs of enterprise workloads to accelerate their move to the cloud. As a result, three areas have emerged in which we anticipate opportunities to have a significant impact on the evolution of cloud computing:

- Emerging cloud applications, workloads, and environments, which entails development of a deep understanding of emerging needs to drive the evolution of hybrid cloud technologies.

- Intelligent, safe, and resilient automation for the hybrid cloud platform to simplify management and operations while providing the desired performance, scale, efficiency, and availability (we call this the “self-driving cloud” vision and believe it could push forward the state of the art).

- Secure, efficient, and performant hardware, systems, and infrastructure encompassing specialized hardware like accelerators, SmartNICs, programmable software-defined infrastructure, novel approaches to systems design, and virtualization.

The goal of the Hybrid Cloud & AI thrust is to generate tangible impact for the community at large while also influencing the technical strategy at IBM and the education agenda at UIUC. In setting goals for the thrust, we have considered two critical aspects. The first is significant research outcomes. These are measurable through publications, including academic papers in high-quality conferences and journals, blog articles, open-source contributions to strategic projects, and, where effective, creation of joint intellectual property through patents. The second is a culture of innovation enabled by open exchange of ideas and a high level of engagement and collaboration among faculty members, students, and IBM researchers. Activities we track to gauge progress on this goal include joint publications, number of graduate student theses based on work supported by the Institute, number of high-bandwidth collaborations enabled through mechanisms like externships and postdoctoral and sabbatical assignments at IBM, and information on IBM researchers who have presented invited lectures, taught classes, or influenced the curriculum. Joint pursuit of relevant external funding opportunities (like NSF grants) by collaborators within the Institute is another example of effective collaboration.

Activities

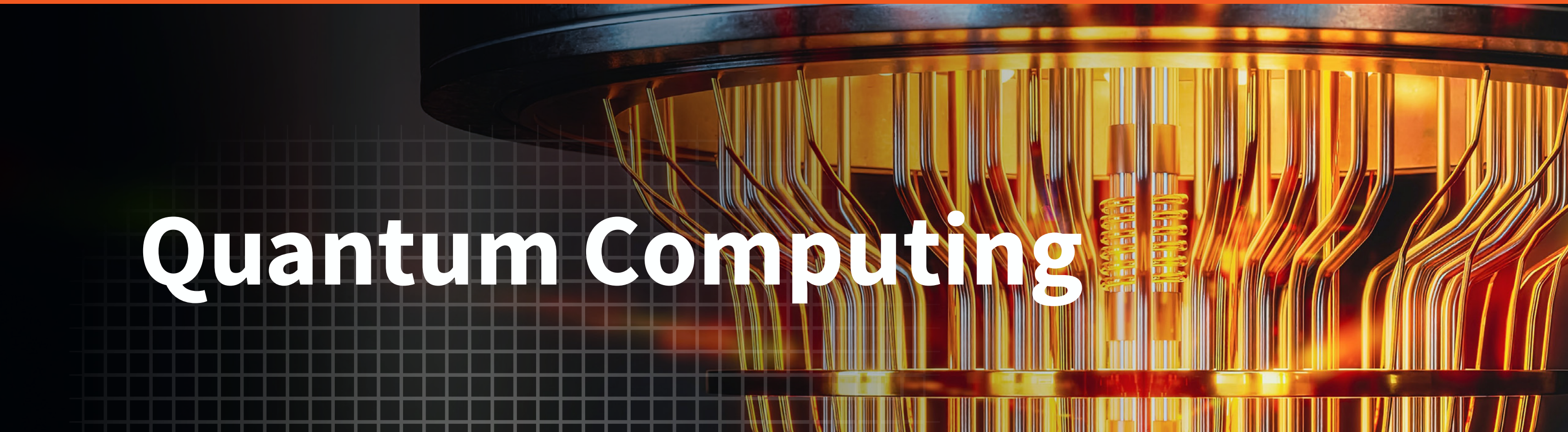
The Hybrid Cloud & AI thrust carried out collaborative efforts whose eventual goal will be end-to-end demonstration of a new open-source hybrid cloud system that incorporates research outcomes across different projects, including ones addressing data management, auto-scaling, software-defined infrastructure, AI-driven resource management for energy efficiency, hardware virtualization, and security.

Ten Hybrid Cloud & AI students visited IBM during Summer 2023 as externs. They worked closely with their IBM mentors, accessed IBM computing resources and data onsite, and made significant research progress through their externships.

Highlights of Accomplishments

The Hybrid Cloud & AI thrust made great progress towards the goals described above. We succeeded in establishing the culture we envisioned and in building a compelling vision together. In year 2, 54 papers were published (about 30 of which were jointly authored by UIUC and IBM researchers; the count of 54 does not include papers published from the seed-funding projects), and an additional 11 papers either were submitted or are being prepared for submission. There were also 5 invention/patent disclosures. Over 10 open-sourcing activities were completed, and opportunities for more were identified. Some successful student externships were completed in 2023 as well.

In addition to research publications, the joint projects produced media reports, datasets, and posters and presentations at esteemed forums and workshops.



Quantum Computing

Mission and Goals

The Quantum Computing thrust aims to advance the field of quantum information science (QIS), integrate quantum discoveries with related future technologies, and train a new generation of students to work in quantum-related fields. QIS is moving quickly and showing promise, but is still in its early stages, with many unknowns. Progress in QIS relies on the creativity and ingenuity of physicists, computer scientists, electrical engineers, chemists, mathematicians, materials scientists, and industry experts.

Therefore, the Quantum Computing thrust takes an agile approach with bold programs that will change the way industry and academia collaborate to advance quantum hardware and approaches. The Quantum Computing thrust is addressing the most pressing and complex challenges in the field and preparing students for careers in QIS.

The Quantum Computing thrust strives to work with and recruit the most talented researchers from the quantum computing industry. It prioritizes building diversity at all levels and an inclusive community that is equitable and welcoming to all.

The goals of the Quantum Computing thrust are to:

» Combine multiple academic disciplines and industrial research expertise to advance next-generation quantum hardware and software and pursue high-risk, high-reward research directions.

» Promote future quantum computing infrastructure by involving researchers from a wide range of engineering fields in developing the classical toolchain and integrating modern computing architectures.

» Pioneer educational tools and programs that open QIS to all learners and develop inclusive academic programs in quantum information science and engineering.

» Create a new model for equitable cloud access to advanced quantum computing hardware, which will enable a diverse set of learners and experts to familiarize themselves with QIS and contribute their expertise to advancing this field.

» Expand the quantum workforce through focused internship and mentorship programs at the undergraduate, post-baccalaureate, graduate, and postdoctoral levels.

Activities

The Quantum Computing thrust supports four research projects:

» **"Modular Quantum Computing Architectures,"** *Matthias Steffen (IBM), Wolfgang Pfaff (UIUC)*

» **"Optimal Measurements in State Discrimination Problems and their Efficient Implementation,"** *Srinivasan Arunachalam (IBM), Eric Chitambar (UIUC), Felix Leditzky (UIUC)*

» **"First-Principles Defect Simulations and Quantum Embedding,"** *Barbara Jones (IBM), Andre Schleife (UIUC)*

» **"Superconducting Devices based on High Kinetic Inductances,"** *Matthias Steffen (IBM), Benjamin Wymore (IBM), Oliver Dial (IBM), Angela Kou (UIUC)*

The Quantum Computing thrust supports one education/outreach project:

» **"Quantum Education and Training,"** *Kayla Lee (IBM), Brian DeMarco (UIUC), Emily Edwards (UIUC)*

Highlights of Accomplishments

» A de-mateable cable connection between separated transmon qubits housed in a single dilution refrigerator was demonstrated. A fast (100 ns) and high-fidelity (95%) SWAP gate was achieved through the connection.

» Significant progress was made on making a new qubit platform involving high kinetic-inductance devices. Resonators with inductors greater than 100 nH were characterized, and phase slip rates in 100 nm-wide wires were made.

» A paper describing the discovery of a new duality between teleportation and dense coding was published, and a paper on exponential separation between quantum statistical query learning and quantum probability approximately correct learning was published.

» A novel error mitigation technique involving deep learning was developed and used to predict noiseless results for materials simulations.

There were also externships at IBM for the first time for the Quantum Computing thrust. Postdoc Vijaya Begum-Hudde spent several weeks working with Jones at IBM Almaden. Students Hanuel Kim and Louis Schatzki worked with Arunachalam at Yorktown Heights.

Materials Discovery

Mission and Goals

IBM and UIUC have a common interest in developing tools for the future of materials discovery, including tools for extracting materials information from the scientific literature, frameworks for efficient simulation or virtual screening of materials candidates, AI models for hypothesis generation and materials evaluation, tools for retrosynthesis planning, and automated laboratory systems for the synthesis and analysis of candidate materials. Along with these technologies, there is a parallel need to develop a technical workforce skilled in modern materials discovery.

Functional organic small molecules and polymers stand out as key areas of mutual interest. UIUC boasts the Molecule Maker Lab Institute, which emphasizes targeted reaction types (e.g., Suzuki couplings) and automated systems for complex chemical transformations. Meanwhile, IBM leverages its RXN framework for reaction prediction and retrosynthetic analysis, complemented by automated lab systems for small molecule and polymer synthesis. In both cases, a critical barrier to unlocking the full potential of automation lies in the need for more robust and extensive incorporation of AI tools and techniques, e.g., for tasks such as suggesting novel polymers or defining an optimal synthetic strategy. The goal of the Materials Discovery thrust is to accelerate the design and discovery of novel materials through the development of frontier AI/ML, high-throughput materials synthesis and characterization, and advanced laboratory automation tools. A secondary goal is to seed a new discovery-ready workforce through training of graduate students and development of deep relationships between IBM and UIUC.

Activities

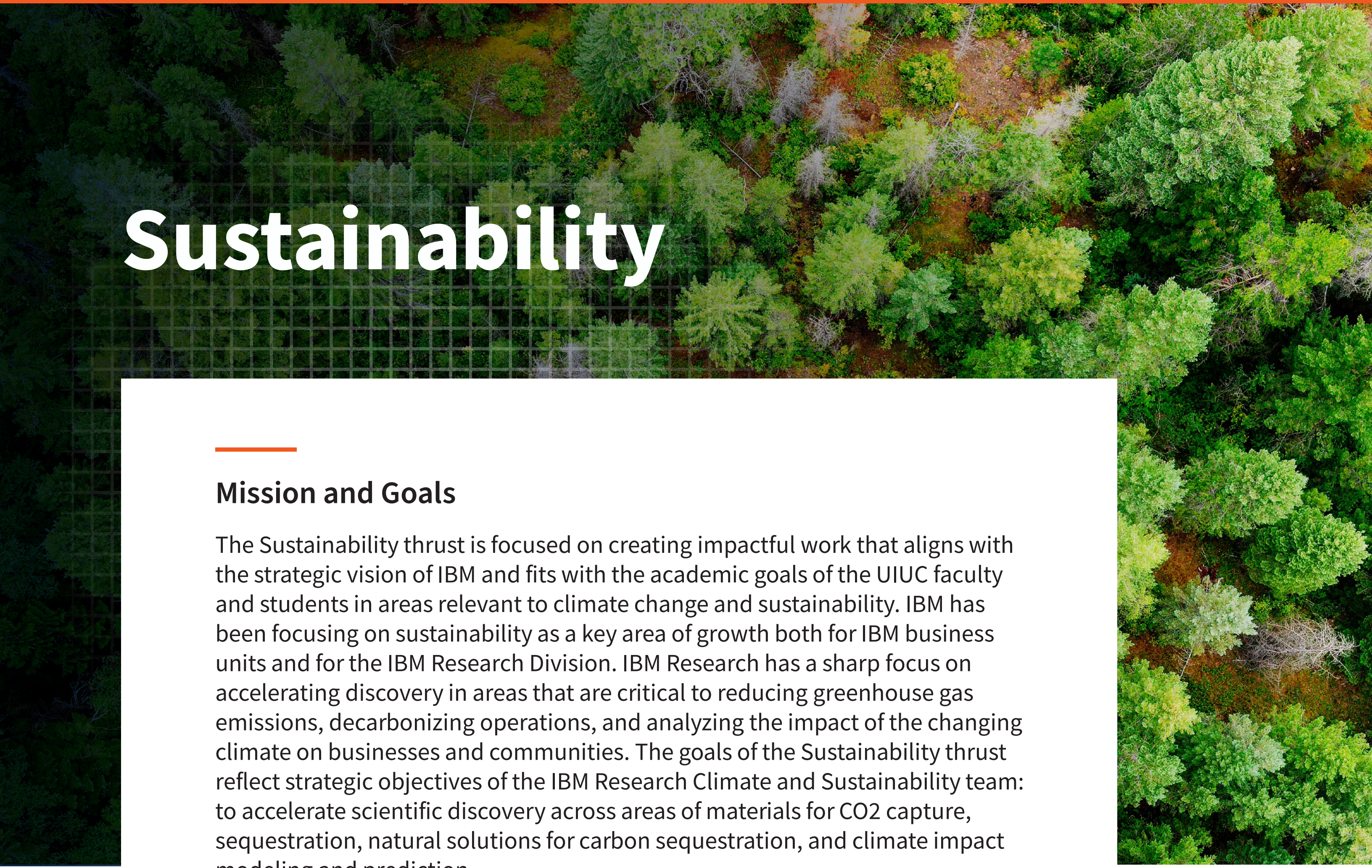
The joint UIUC and IBM team have been working on three distinct yet interconnected projects:

» Development of a synthetic field guided asynchronous chemoenzymatic retrosynthesis planning algorithm (ACERetro) by leveraging template-free chemical retrosynthesis tools and template-based enzymatic retrosynthesis tools. Chemoenzymatic synthesis integrates the advantages of chemocatalysis and biocatalysis to design efficient synthesis routes. ACERetro performs hybrid searches of molecules that are commercially available by prioritizing the exploration of the most promising synthetic field of molecules through a trained synthetic field score (SFScore). We also introduced a synthetic field guided synthesis route optimization algorithm. In the optimization algorithm, the SFScore can identify the crux steps that could potentially be optimized for a given synthesis route, and then ACERetro can be used to find bypasses. Overall, ACERetro represents a versatile and effective synthesis planning tool for chemoenzymatic synthesis, which opens a new avenue in catalysis.

» Development of a multidisciplinary approach to further understand structure-property relationships of organic photovoltaics (OPVs) by integrating automated synthesis, machine learning, and closed-loop experimentation. Collaborating with the Molecule Maker Lab Institute, we explored oligomers using Suzuki-Miyaura cross-coupling chemistry, aiming to fill knowledge gaps in the field and achieve the "10-10" target (10% power conversion efficiency and 10 years of photostability). The closed-loop system, incorporating Bayesian optimization and solution-based testing, identifies thiophenes as optimal motifs for stable organic solar cells. The current study focuses on designing and synthesizing sequence-defined thiophene oligomers. Anticipated outcomes include advancing molecular design criteria, optimizing bandgap width, ultimately enhancing power conversion efficiency, and streamlining thiophene oligomer production for commercially viable OPVs, contributing to next-generation energy applications and climate change mitigation.

Highlights of Accomplishments

The major accomplishments of the thrust in this program year include (1) the development of a synthetic field guided asynchronous chemoenzymatic retrosynthesis planning algorithm (ACERetro) by leveraging template-free chemical retrosynthesis tools and template-based enzymatic retrosynthesis tools, and (2) the development of a multidisciplinary approach to further understand structure-property relationships of organic photovoltaics (OPVs) by integrating automated synthesis, machine learning, and closed-loop experimentation. Three manuscripts have been submitted. In addition, the thrust nucleated one seed project focusing on AI foundation models for materials, which led to the funding of a major project focusing on the development of AI foundation models for predicting materials properties in Year 3 and Year 4 and a minor project focusing on the development of foundation models for generating faithful retrosynthetic pathways and experimental procedures in Year 3.



Sustainability

Mission and Goals

The Sustainability thrust is focused on creating impactful work that aligns with the strategic vision of IBM and fits with the academic goals of the UIUC faculty and students in areas relevant to climate change and sustainability. IBM has been focusing on sustainability as a key area of growth both for IBM business units and for the IBM Research Division. IBM Research has a sharp focus on accelerating discovery in areas that are critical to reducing greenhouse gas emissions, decarbonizing operations, and analyzing the impact of the changing climate on businesses and communities. The goals of the Sustainability thrust reflect strategic objectives of the IBM Research Climate and Sustainability team: to accelerate scientific discovery across areas of materials for CO2 capture, sequestration, natural solutions for carbon sequestration, and climate impact modeling and prediction.

Highlights of Accomplishments

Accomplishments for the Sustainability thrust include:

- 13 papers were published by researchers working on projects within the Sustainability thrust.
- 15 tutorials have been presented at various conferences.
- 4 keynote/invited talks were presented by researchers working on projects within the Sustainability thrust.

Activities

Concluded projects

» "An AI-based Framework for Accelerated Discovery of Climate Impacts on Different Societal Sectors"
(PI: Atul K. Jain, Co-PIs: Lav Varshney, Donald Wuebbles, Ashish Sharma)

The team (1) applied new state-of-the-art climate change datasets for statistical and dynamical downscaling, and then analyzed the resulting climate impacts and developed high-resolution datasets for the community of interest; (2) studied the impacts of past extreme climate events and farm management practices on agricultural productivity; (3) developed machine learning models (MLMs) to estimate crop yield at regional and global scales; and (4) leveraged GAN for simulating synthetic climate scenarios and demonstrated the efficacy of the proposed method on two datasets (CHIRPS, WRF).

» "Knowledge Engine for Catalysts for Carbon Dioxide Conversion and Utilization" *(PI: Jiawei Han, Co-PIs: Chengxiang Zhai, Jaemin Kim, Chinmoy Baroi)*

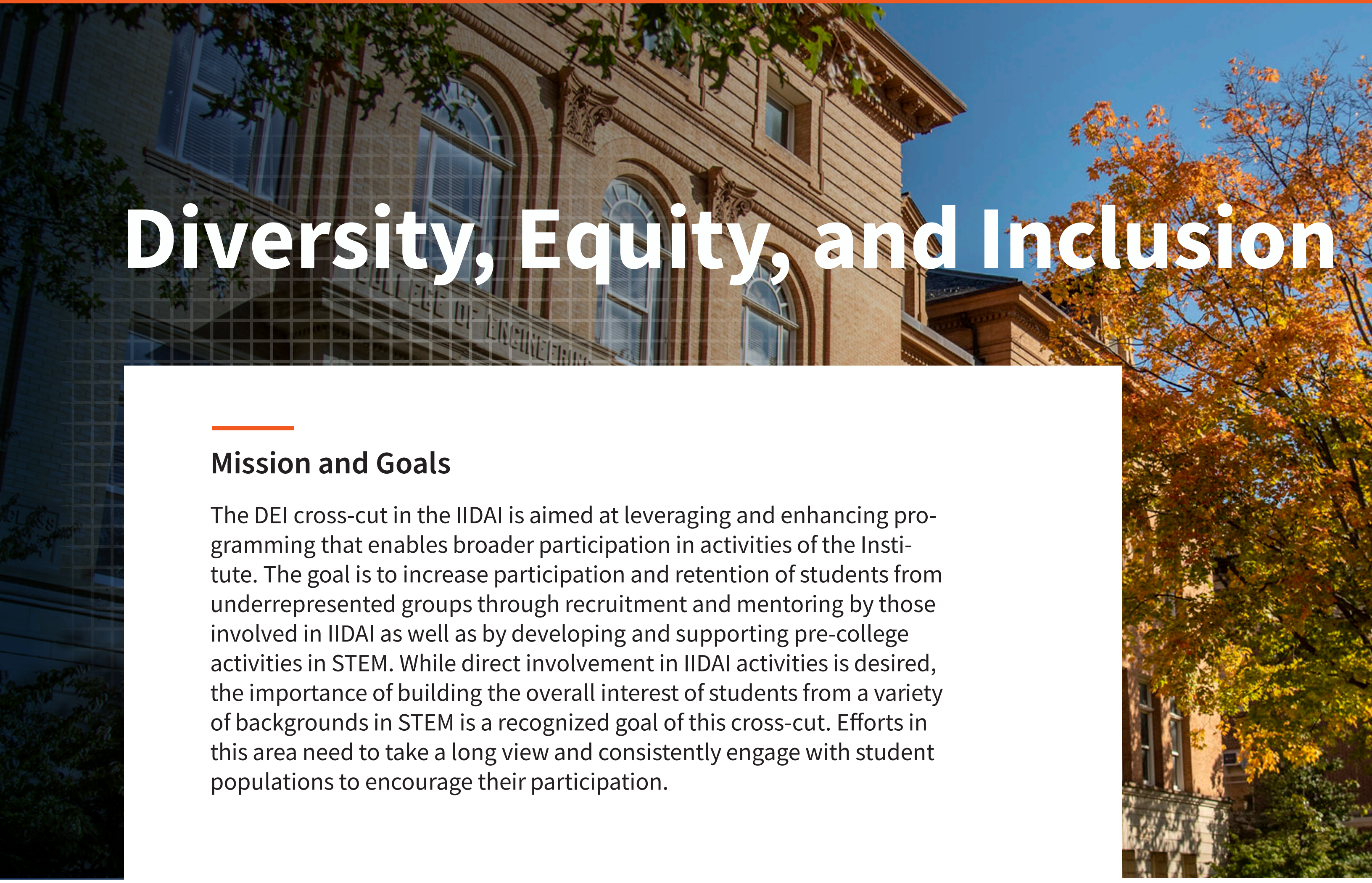
The team developed (1) a method for taxonomy-guided fine-grained entity set expansion that can generate new entities of similar nature based on a provided corpus and a very small number of similar entities provided by users; (2) a novel algorithm that leverages Wide and Deep Reasoning to more effectively support complex question answering; and (3) novel architectures for adapting foundation large language models (LLMs) to the materials discovery domain.

» Seed Project "Deep Climate Anomaly Modeling and Impact Analysis"
(PI: Jingrui He, Co-PI: Hanghang Tong)

The team (1) developed an end-to-end deep generative model that takes as input the historical tensor time series, outputs the future tensor time series, and detects possible anomalies; (2) developed a multi-view autoencoder-based clustering framework, augmented by a similarity-guided contrastive loss, tailored for detecting anomalous nodes within multi-view graphs; and (3) studied fairness-aware multi-view clustering.

» Seed Project "An Innovative Framework to Quantify the Compound Heat-Toxicity from Ambient PM2.5 based on satellite data, measurements, and modeling"
(PI: Vishal Verma, Co-PIs: Hannah Horowitz, Lei Zhao)

The team (1) performed high-resolution GEOS-Chem simulations of chemically resolved PM2.5 for a hindcast evaluation period for April to August 2021; (2) developed a dataset for oxidative potential from various chemical mixtures; and (3) tested several machine learning models of different capacities to predict oxidative potential from the chemical mixtures.



Diversity, Equity, and Inclusion

Mission and Goals

The DEI cross-cut in the IIDAI is aimed at leveraging and enhancing programming that enables broader participation in activities of the Institute. The goal is to increase participation and retention of students from underrepresented groups through recruitment and mentoring by those involved in IIDAI as well as by developing and supporting pre-college activities in STEM. While direct involvement in IIDAI activities is desired, the importance of building the overall interest of students from a variety of backgrounds in STEM is a recognized goal of this cross-cut. Efforts in this area need to take a long view and consistently engage with student populations to encourage their participation.

Highlights of Accomplishments

Two new GIANT projects were identified and supported (https://idea.illinois.edu/giant/giant-project-selections-2023) to augment the 5 selected in the previous year. The first cohort of 16 supported students successfully completed the ISUR undergraduate research program, and a second cohort of 20 students was recruited and identified. A new IIDAI-supported summer camp (Learning Electronics, AI, and Programming) was developed by faculty, staff, and graduate students and presented to 20 high school students. 2 high schoolers received support to participate in the Young Scholars research program and performed research with IIDAI faculty in the area of Quantum Computing. To support the GIANT program, a program coordinator (Bryana Rivera) was hired.

Activities

The DEI cross-cut is engaging with IIDAI research teams to:

» Identify and recruit IIDAI mentors and implement undergraduate research projects through the Illinois Scholars Undergraduate Research (ISUR) program.
https://isur.engineering.illinois.edu

» Support Grassroots Initiatives to Address Needs Together (GIANT) projects through the Institute for Inclusion, Diversity, Equity & Access IDEA.
https://idea.illinois.edu/

» Develop and implement Worldwide Youth in Science and Engineering summer camp programming relevant to IIDAI technical research areas of interest.
https://wyse.engineering.illinois.edu

» Identify and recruit IIDAI projects and mentors and integrate them into the Young Scholars research program.
https://wyse.engineering.illinois.edu/hs-summer-stem-research-programs/

ISUR Program

In collaboration with the ISUR program, the DEI cross-cut is supporting 20 undergraduate researchers involved in 13 Hybrid Cloud & AI, 1 Quantum Computing, 1 Materials Discovery, and 2 Sustainability projects. The 20 students were selected from 58 applicants to serve as IIDAI Research Scholars working on these projects. The demographic makeup of the selected scholars is as follows: 60% women, 20% first-generation college students, 15% Hispanic, 0% African-American. Students will continue their research through the Spring 2024 semester; they presented their work at the Illinois Scholars Undergraduate Research (ISUR) Expo on April 23, 2024.

GIANT Projects

Five projects co-funded by the DEI cross-cut and the IDEA Institute started in the Summer and Fall of 2022; two projects co-funded by IIDAI and the IDEA Institute started in Fall 2023. These projects are focused on pre-college family engagement (one project), skill development and career awareness for undergraduate students (three projects), building community and belonging for graduate students (two projects), and making lab courses more inclusive (one project).

Three GIANT projects are led by teams of graduate students. These students are developing project management and leadership skills by carrying out all aspects of their projects (e.g., writing the proposal, leading a team, designing the research survey and getting IRB approval, running the initiative, and managing the budget). The Graduate Diversity Ambassadors program has 7 ambassadors (5 sponsored by IIDAI and 2 sponsored by other sources). All five of the projects from 2022 were presented at the Spring 2023 IDEA conference.

Concluding Remarks

The first 2 years of IIDAI have seen the successful launch of the four technical thrusts described in this report, helping the Institute reach its initial objective of developing strong bonds between UIUC and IBM Research while driving technical agendas in strategic areas. As we approach the completion of the initial set of projects defined during the launch, the Institute is preparing itself to enter a new phase with a focus on a smaller set of larger research initiatives aiming at producing external impact and eminence. Areas under consideration include the development of a platform for accelerated discovery powered by state-of-the-art multi-cloud technologies, bringing together classical and quantum computing seamlessly to support sustainability and materials discovery research.

Appendix: Paper Published

Published in August 2022 – August 2023

Hybrid Cloud & AI Thrust

1. Arpandeep Khatua, Vikram Sharma Mailthody, Bhagyashree Taleka, Tengfei Ma, Xiang Song, and Wen-mei Hwu. 2023. IGB: Addressing the Gaps in Labeling, Features, Heterogeneity, and Size of Public Graph Datasets for Deep Learning Research. In Proceedings of the 29th ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD '23). Association for Computing Machinery, New York, NY, USA, 4284–4295. https://doi.org/10.1145/3580305.3599843

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