

# Computing@Argonne


ALCF + CPS + DSL + MCS

**Michael E. Papka**

Division Director, Argonne Leadership Computing Facility

Deputy Associate Laboratory Director, Computing, Environment and Life Sciences, Argonne National Laboratory

Research Professor of Computer Science, Illinois Institute of Technology



MAN ACHIEVED HERE  
THE FIRST SELF-SUSTAINING CHAIN REACTION  
AND THEREBY INITIATED THE  
CONTROLLED RELEASE OF NUCLEAR ENERGY

## Argonne National Laboratory

The U.S. Department of Energy's Argonne National Laboratory delivers world-class research, technologies, and new knowledge that aim to make an impact — from the atomic to the human to the global scale.

# About Argonne

**Argonne is a multidisciplinary science and engineering research center located outside Chicago.**

- Born out of the University of Chicago's work on the Manhattan Project in the 1940s.
- **Managed by UChicago Argonne, LLC, for the U.S. Department of Energy's Office of Science.**
- Works with universities, industry, and other national labs on questions and experiments too large for any one institution to do by itself.

# Argonne's Research Directorates



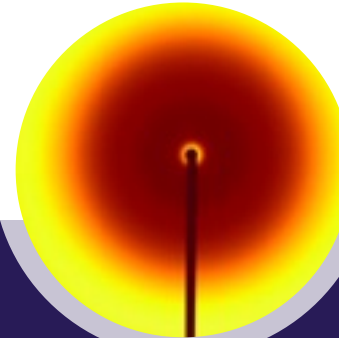
## Computing, Environment and Life Sciences

Couples computing-related activities with science domains whose futures are closely tied to progress in computing



## Energy and Global Security

Conducts applied R&D, creates tools that enable scientific and technological breakthroughs, and translates discoveries through engineering to the marketplace



## Photon Sciences

Provides the brightest X-ray beams in the Western Hemisphere and provides discoveries in nearly every scientific discipline



## Physical Sciences and Engineering

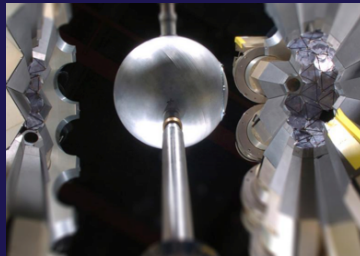
Creates new materials and chemistries and advances accelerator physics

# Our one-of-a-kind facilities enable science from the nanoscale to the exascale

Argonne's five flagship facilities support one of the largest user communities in the U.S. Department of Energy complex.



**Advanced Photon Source**



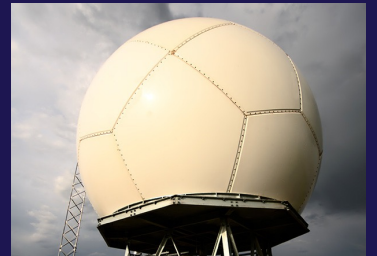
**Argonne Tandem Linear Accelerator System**



**Argonne Leadership Computing Facility**



**Center for Nanoscale Materials**



**Atmospheric Radiation Measurement – The Southern Great Plains**

# DOE Leadership Computing Facility

- Established in 2004 as a collaborative, multi-lab initiative funded by DOE's *Advanced Scientific Computing Research* program
- Operates as **one facility** with two centers, at Argonne and at Oak Ridge National Laboratory
- Deploys and operates at least two advanced architectures that are **10-100 times more powerful** than systems typically available for open scientific research
- **Fully dedicated** to open science to address the ever-growing needs of the scientific community



# Broad Engagement in HPC

## We enable and support science campaigns

- ALCF computational scientists assist science teams to ready their codes to efficiently use our resources
- Researchers are supported by performance engineers, user support staff, and data analysis and visualization services
- Each year, ALCF-supported research results in hundreds of refereed publications, in journals such as Proceedings of the National Academy of Sciences, Nature, and Physical Review Letters

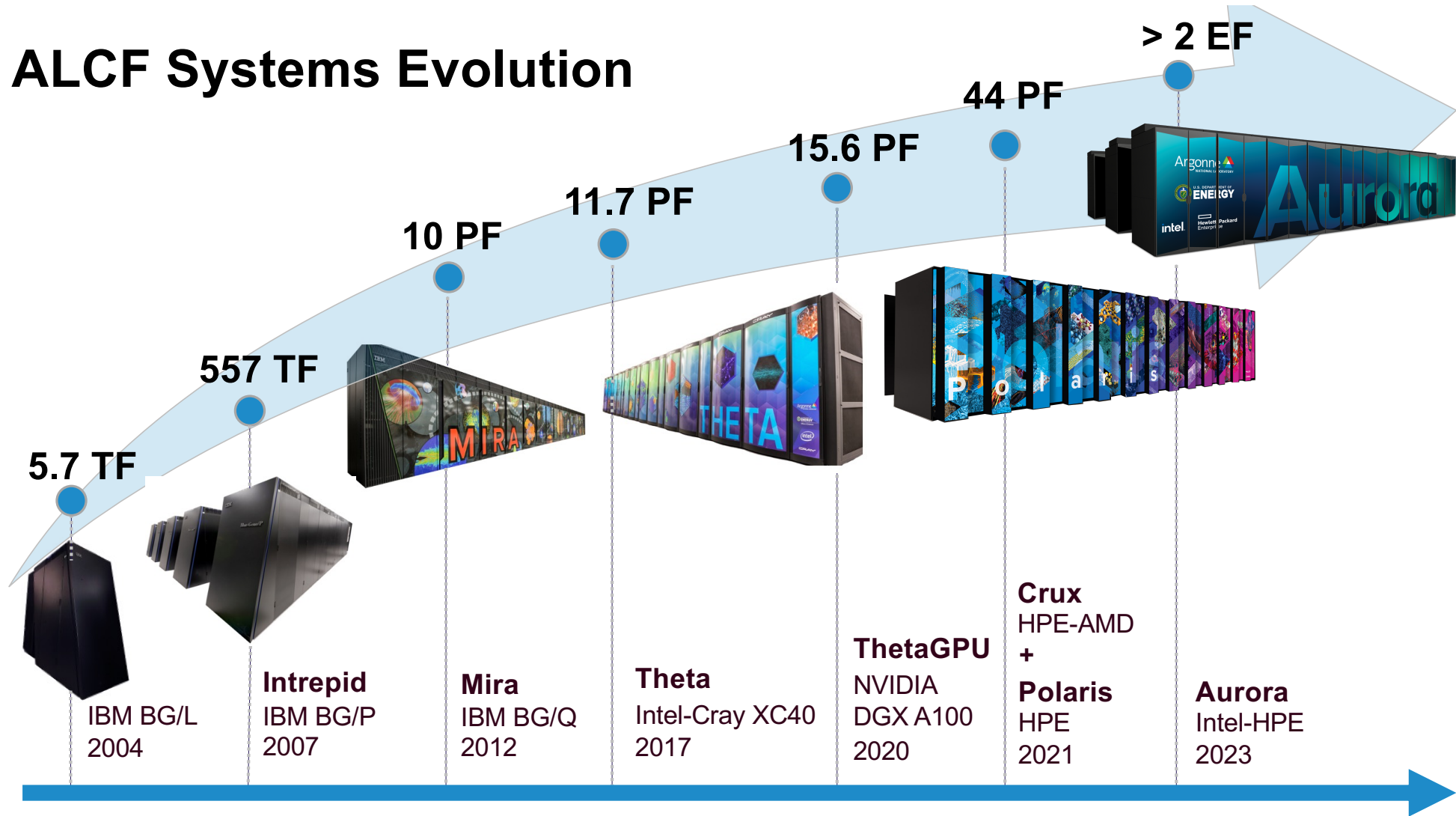
## We deliver cycles to computational scientists

- Delivers millions of node hours of compute time
- Scheduled availability for the resource exceeds 99%

## We partner with community on R&D in hardware and software



# ALCF Systems Evolution





# Aurora

Argonne's upcoming exascale supercomputer will leverage several technological innovations to support machine learning and data science workloads alongside traditional modeling and simulation runs.

SUSTAINED PERFORMANCE

**≥1 Exaflop DP**

X<sup>e</sup> ARCHITECTURE-BASED GPU

**Ponte Vecchio**

INTEL XEON SCALABLE PROCESSOR

**Sapphire Rapids**

PLATFORM

**HPE Cray EX**

## Compute Node

2 Intel Xeon scalable "Sapphire Rapids" processors; 6 X<sup>e</sup> arch-based GPUs; Unified Memory Architecture; 8 fabric endpoints; RAMBO

## GPU Architecture

X<sup>e</sup> arch-based "Ponte Vecchio" GPU; Tile-based chiplets, HBM stack, Foveros 3D integration, 7nm

## CPU-GPU Interconnect

CPU-GPU: PCIe  
GPU-GPU: X<sup>e</sup> Link

## System Interconnect

HPE Slingshot 11; Dragonfly topology with adaptive routing

## Network Switch

25.6 Tb/s per switch, from 64–200 Gbs ports (25 GB/s per direction)

## High-Performance Storage

≥230 PB, ≥25 TB/s (DAOS)

## Programming Models

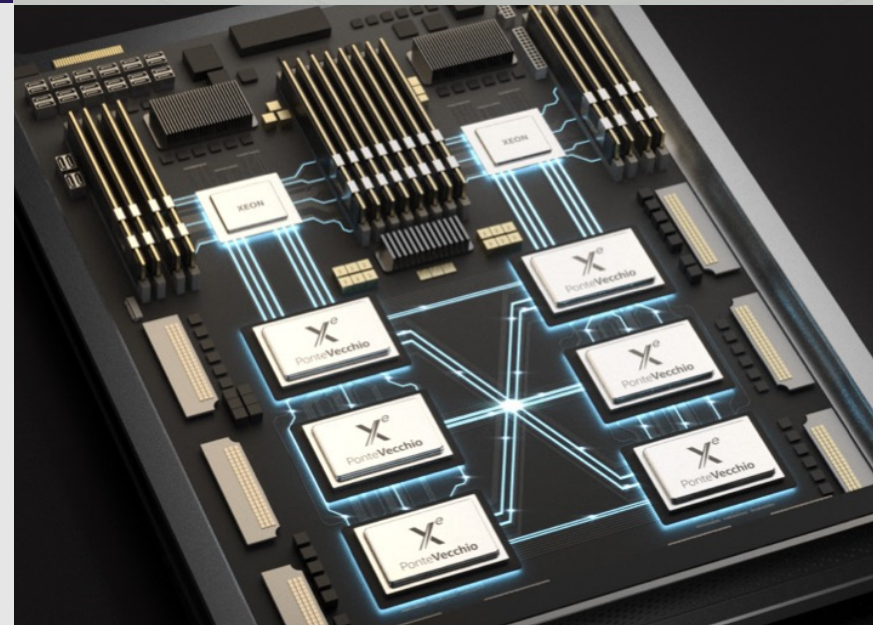
Intel oneAPI, MPI, OpenMP, C/C++, Fortran, SYCL/DPC++

## Node Performance

>130 TF

## System Size

>9,000 nodes





# Computing Resources

## Polaris

- HPE Apollo Gen10+
- AMD processors/NVIDIA GPUs
- 44 petaflops (double precision)
- NVIDIA GPU A100; HBM stack
- AMD EPYC Processor Milan
- 560 nodes

## Theta

### KNL NODES

- Intel-Cray XC40
- 11.7 petaflops
- 4,392 nodes
- 281,088 cores
- 843 TB (DDR4); 70 TB (HBM) of memory

### GPU NODES

- NVIDIA DGX A100
- 3.9 petaflops
- AMD EPYC 7742
- 24 nodes
- 24 TB of DDR4; 7.7 TB (HBM) of memory

## Cooley

- Cray/NVIDIA
- 126 nodes
- 1512 Intel Haswell CPU cores
- 126 NVIDIA Tesla K80 GPUs
- 48 TB RAM / 3 TB GPU

## Iota

- Intel/Cray XC40 architecture
- 117 teraflops
- 44 nodes
- 2,816 cores
- 12.3 TB of memory

## JLSE Experimental Testbeds

- 150 nodes
- Intel/AMD/IBM/Marvell/GPGPU
- EDR/100GbE/OPA
- Lustre/GPFS/DAOS

## Grand and Eagle (Storage)

Each system has:

- HPE ClusterStor E1000
- 100 petabytes of usable capacity
- 8,480 disk drives
- Lustre filesystem
  - 160 Object Storage Targets
  - 40 Metadata Targets
- HDR InfiniBand network
- 650 GB/s rate on data transfers

# ALCF AI-TESTBED

## Next-Generation AI-Accelerator Systems

- Infrastructure of next-generation machines with hardware accelerators customized for artificial intelligence (AI) applications with a goal to integrate AI accelerators in existing and upcoming supercomputers
- Provides a platform to evaluate usability and performance of machine learning-based HPC science applications running on these accelerators.
- Promising results for diverse spectrum of science ranging from cancer , covid19, high-energy physics, biosciences, climate, among others.
- Close collaboration with AI accelerator vendors on their product developments and roadmaps



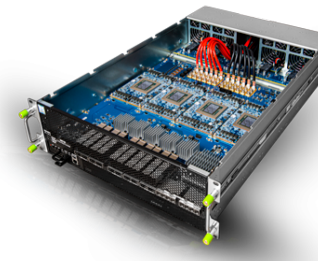
Cerebras (CS-2)



SambaNova



Graphcore



Habana



Groq

<https://www.alcf.anl.gov/alcf-ai-testbed>



## Getting Started: Director's Discretionary (DD)

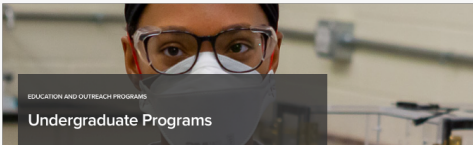
Director's Discretionary (DD) awards support various project objectives from scaling code to preparing for future computing competition to production scientific computing in support of strategic partnerships.

- **Award Cycle:** Ongoing (available year round)
- **Award size:** Up to several million compute-hours
- **Duration:** 3–6 months; renewable
- **Total percent of ALCF** resources allocated for DD projects: 20%

<https://www.alcf.anl.gov/science/directors-discretionary-allocation-program>

# Opportunities at Argonne

## Undergraduate



### Undergraduate Programs

Here at Argonne, we work to make the world a better place through science and innovation, and we want to help empower undergraduates as they start their journey into the world of science and engineering.

We pursue discovery by pushing boundaries, challenging ourselves and each other, and stretching our abilities. This makes Argonne an excellent place for undergrads to explore and test their own ideas in science and technology.

Argonne can help undergrads grow, choose, and hone their areas of interest with programs that immerse them in cutting-edge research and discovery in all areas of the Lab. Over 300 students each year participate in the various fellowship opportunities Argonne offers. We also hire undergraduate students for part-time and temporary assignments to provide technical support to our scientists and engineers.

**NOTE: The laboratory is tentatively planning for student programs to be fully onsite during Summer 2022. However, a student's workplace may shift to a hybrid or virtual status contingent upon local COVID infection rates. Student candidates will be notified of changes in the lab's operational status at the time of offer and/or during their appointment.**

- STEM Outreach
- Learning Center
- Undergraduate Programs
  - Undergraduate Internship
  - Undergraduate Temporary Employment
  - Visiting Student Program for Undergraduate Students
- Graduate Programs
- Faculty Programs

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Temporary Employment

Internship Opportunities

Visiting Students

Communicating Science

From writing reports to presenting an oral presentation, our fellowship programs offer numerous opportunities for you to exercise your communication skills, and the Communicating Science resource is here to help.

LEARN MORE

Educational Programs and Outreach Mailing List

Educational Programs and Outreach uses immersive and engaging programs to create STEM pathways for students throughout their journeys. We offer many opportunities for students, families, education professionals, and others to help students learn and grow. Stay up-to-date on our latest science competitions, summer camps, undergraduate and graduate internships, and more by subscribing to our email list.


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email address

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<https://www.anl.gov/education/undergraduate-programs>

## Graduate



### Graduate Programs

Argonne offers a variety of research appointments, cooperative education opportunities, and specialized schools to fit the needs – and schedules – of any graduate student. We encourage students pursuing a Master's degree as well as Ph.D. candidates to check out the many opportunities we offer. Come to Argonne, expand and create new knowledge – and change your world.

**NOTE: The laboratory is tentatively planning for student programs to be fully onsite during Summer 2022. However, a student's workplace may shift to a hybrid or virtual status contingent upon local COVID infection rates. Student candidates will be notified of changes in the lab's operational status at the time of offer and/or during their appointment.**

- STEM Outreach
- Learning Center
- Undergraduate Programs
- Graduate Programs
  - Graduate Internship
  - Graduate Research
  - Graduate Temporary Employment
  - Graduate Training Programs
  - Visiting Student Program for Graduate Students
- Faculty Programs

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Guest Associates Program

Graduate Research

Graduate Internships

Graduate Temporary Employment

Graduate Training Programs


Visiting Student Program

Faculty Programs

Educational Programs and Outreach Mailing List

<https://www.anl.gov/education/graduate-programs>

## Faculty



### Faculty Programs

Argonne offers a number of programs that provide faculty with opportunities to conduct research, network with Argonne experts and enhance their understanding of our mission and science through conferences and workshops.

Argonne is a place where scientists, engineers, and researchers immerse themselves in the grand challenges of our society. We strive to find solutions and make discoveries that provide an enduring value to our nation and to the future of the American scientific enterprise. We believe that bringing together the brightest minds and ideas from across disciplines helps answer the grand challenges of today. Through partnerships and collaboration, we push the boundaries of what seems possible. This is a great place for university faculty to connect, collaborate, and reinvestigate their passion for scientific research.

As a faculty researcher at Argonne, you can discover new ideas to take back to your students, shaping the next generation of scientists. Everyone benefits from the leading edge at Argonne.

- STEM Outreach
- Learning Center
- Undergraduate Programs
- Graduate Programs
- Faculty Programs
  - Faculty Research
  - Faculty Sabbatical
  - Guest Faculty Research
  - DOE Visiting Faculty Program

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Faculty Sabbatical

Guest Faculty Research

DOE Visiting Faculty Program

Argonne National Laboratory  
9700 S. Cass Avenue  
Lemont, IL 60439  
+1630.252.2000

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<https://www.anl.gov/education/faculty-programs>

# Computing@Argonne: Research

ALCF + CPS + DSL + MCS

**Valerie Taylor**  
Division Director, Mathematics and Computer Science Division  
Argonne Distinguished Fellow  
Argonne National Laboratory

# Computing@Argonne



**Valerie Taylor**  
Director, Mathematics  
and Computer Science  
Division (**MCS**)



**Ian Foster**  
Director, Data  
Science and Learning  
Division (**DSL**)



**Salman Habib**  
Director, Computational  
Science Division (**CPS**)



**Mike Papka**  
Director, Argonne  
Leadership Computing  
Facility Division (**ALCF**)

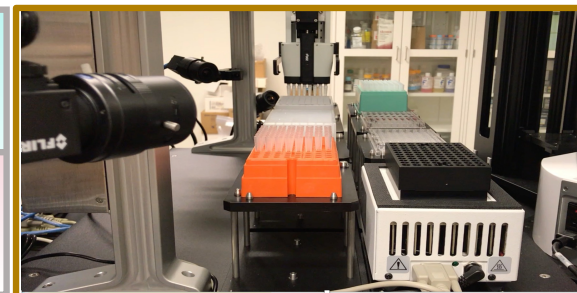
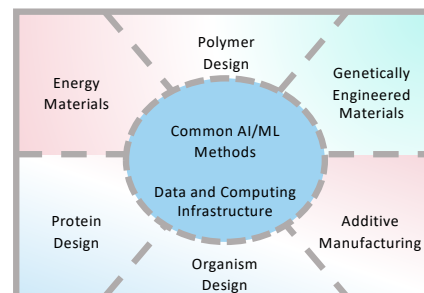
# Future Drivers

## AI-Driven Modes of Discovery

- **Learned Models Begin to Replace Data**
  - Queryable, portable, pluggable, chainable, secure
- **Experimental Discovery Processes Dramatically Refactored**
  - ML models drive processes; experiments improve ML models
- **Many Questions Pursued Semi-Autonomously at Scale**
  - Searching for materials, molecules and pathways
- **Simulation and AI Approaches Merge**
  - Deep integration of ML, numerical simulation and UQ
- **Theory Becomes Data for Next Generation AI**
  - AI begins to contribute to explaining the how and why of phenomena
- **AI Becomes Common Part of DOE Laboratory Activities**
  - Infuses scientific, engineering and operations

## Self-Driving Laboratories

- Are emerging as the **next-generation facilities** for an accelerated scientific discovery process.
- They augment automated experimentation platforms with artificial intelligence to enable autonomous experimentation.

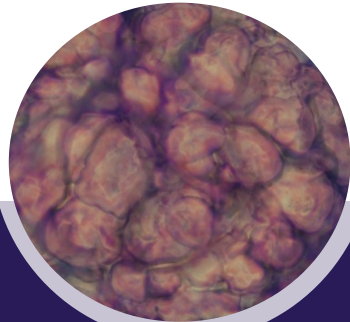


## Computing Continuum



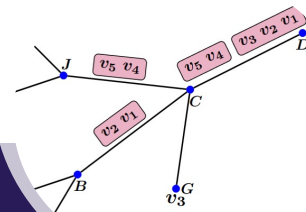


# Research Capabilities: Applied Math



## PDEs and PDE Solvers

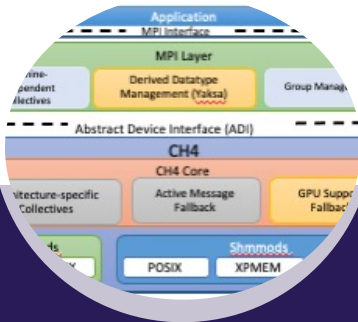
Develops, analyzes, and implements algorithms and software for obtaining numerical solutions to science problems that can be modeled as PDEs



## Mathematical Optimization

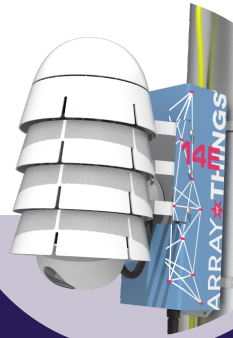
Develops the theory, algorithms, and software for minimizing some function subject to a set of constraints.

# Research Capabilities: CS, Visualization and Data



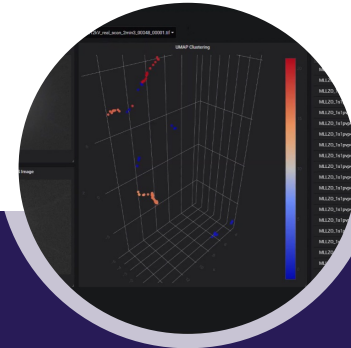
## Operating Systems, Programming Models, and Compilers

Develop software that makes computational approaches to DOE science possible



## Advanced Architectures

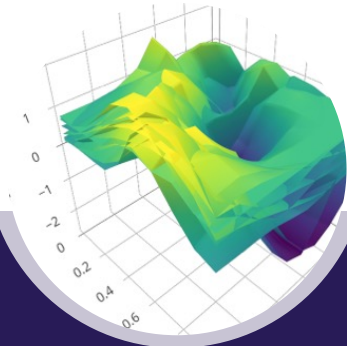
Accelerate the adoption of advanced architectures and lay foundations for Post-Moore opportunities, include edge computing, clouds, quantum information science



## Data Management, Storage Systems, Visualization

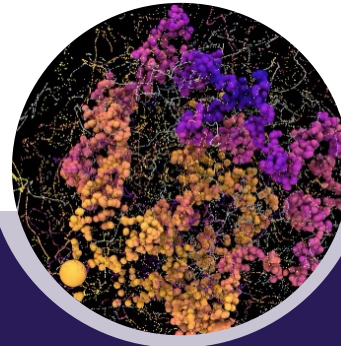
Enable the storing, organizing, transport, and transformation of scientific research data to be readily available and actionable

# Research Capabilities: AI/ML



## Foundations of ML, Data Analysis & Statistics

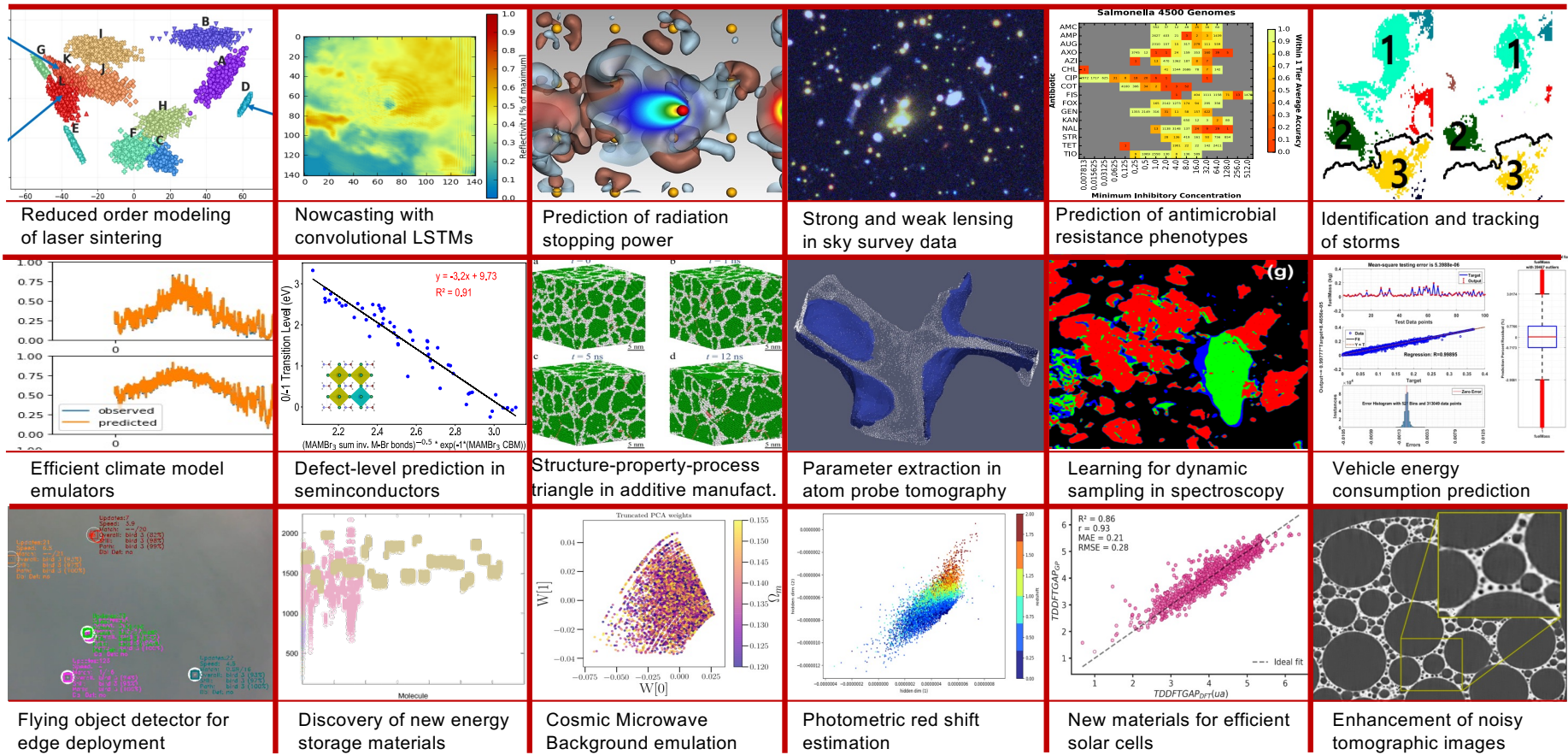
Leverage expertise in automatic differentiation, modeling, optimization and uncertainty quantification



## Application of AI/ML

Explore the application of AI/ML to problems in science and engineering; application to many different areas including design of new materials, additive manufacturing, climate models, weather prediction, COVID therapeutics

# Applications of AI/ML

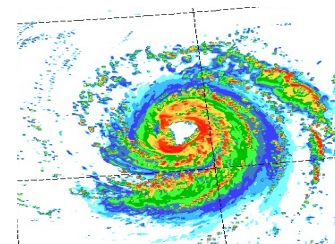


# Research Capabilities: Computational Science

Accelerate understanding of how the SARS-COV-2 virus binds to human cells

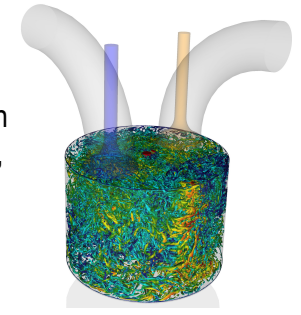


Predicting hurricane tracks to mitigate risks, hindcasting with earth system model data to gauge impact of global change

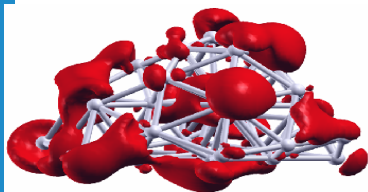


**Earth System Model**

Predictive simulation tools for nozzle flow, spray, combustion, and turbulence to understand cyclic variability

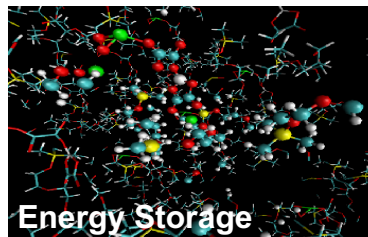


**Internal Combustion**



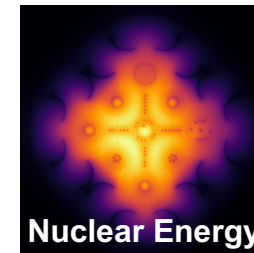
**Nano Catalysts**

Mapping out properties of nanoparticles to design catalysts for fuel cells and methane conversion



**Energy Storage**

Next generation battery technologies. Here, optimizing electrolyte stability in metal-air batteries



**Nuclear Energy**

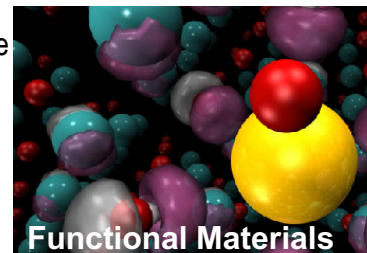
High-fidelity, Multiphysics simulations combining particle transport and fluid dynamics for modeling next-generation fission and fusion reactors

Extreme-scale multi-physics simulations for next-generation sky surveys investigating the "Dark Universe"



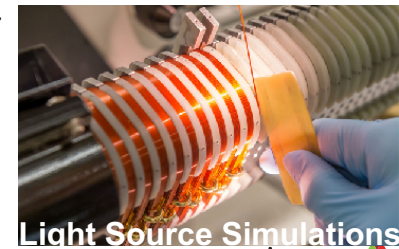
**Computational Cosmology**

Enhanced predictive capability for functional materials with ab initio quantum Monte Carlo methods



**Functional Materials**

Advanced accelerator simulation methods for next-generation light source design, and improved beam quality, as applied to APS-U



**Light Source Simulations**

# Initial IIT- CELS Seminar Series

## Goal: Facilitate collaborations

- March 9: AI/ML
  - IIT: Mustafa Bilgic (AI/ML), Yan Yan (computer vision)
  - ANL: Prasanna Balaprakash (AI/ML), Venkat Vishwanath (AI Testbed)
- March 23: HPC
  - IIT: Stefan Muller (programming languages), Ruja Wang (computer architecture)
  - ANL: Yanfei Guo (MPI), Katherine Riley (science of ALCF)
- March 30<sup>th</sup>: Edge Computing
  - IIT: Kyle Hale (virtualization), Nik Sultana (networking)
  - ANL: Nicola Ferrier (AI@edge, computer vision), Tekin Bicer (scientific workflows)
- April 6<sup>th</sup>: Data Science
  - IIT: Lulu Kang (data science), Maggie Cheng (data analytics and graph theory)
  - ANL: Julie Bessac (multidimensional statistics), Ryan Chard (on-demand data science)