

# Big Ideas

WITH MICHAEL E. PAPKA

DATA, DEVICES AND INTERACTION LABORATORY

March 29, 2022

## WHAT IS A BIG IDEAS CLASS?

- ▶ Lectures and discussions of current research and technical developments in computer science for beginning graduate research students. Topics will emphasize open problems and recent scientific advances. Content may vary to reflect research advances in areas such as data analytics, scientific computing, graphics and visualization.



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- **Who has active research projects?**
- **What are NIU CS faculty interests?**
- **Where do I get more information?**
- **How do I get involved?**



## BIT ABOUT ME (EDUCATION)

- ▶ Northern Illinois University - Physics (BS)
- ▶ University of Illinois @ Chicago - Computer Science (MS)
- ▶ University of Chicago - Computer Science (MS, PhD)
- ▶ Continuously learning in other areas
  - ▶ University of Chicago - Business School (SLLP)
  - ▶ Harvard University - Business School (GMP)
  - ▶ Stanford University - Hasso Plattner Institute of Design (Design Thinking)

## BIT ABOUT ME (CAREER)

- ▶ Fermi National Accelerator Laboratory (Undergraduate/Graduate)
- ▶ Argonne National Laboratory
- ▶ Northern Illinois University

## BIT ABOUT ME (RESEARCH)

- ▶ Advanced Display Environments and Collaboration Technology
- ▶ High Performance Computing (Systems and Environments)
- ▶ Internet of Things (Computing Continuum) [Edge Computing]
- ▶ Information and Scientific Visualization
- ▶ Data Analysis
- ▶ Augmented/Virtual Reality

## BIT ABOUT THE ddiLAB

- ▶ Joint with **School of Art and Design** and co-directed with Professor Joseph Insley (Time Arts)
- ▶ Focused on **visualization** and **data analysis** coupled to **high-performance computing** in the support of **science**, with side efforts involving the *Internet of Things* (edge computing) and interdisciplinary activities connected to computing
- ▶ Students
  - ▶ - 2 PhD (Information Visualization, machine learning/edge computing)
  - ▶ - 1 MS (HPC log analysis)
  - ▶ - 8 Undergraduates (IoT, VR, and HPC)

## BIT ABOUT ME (RESEARCH)

- ▶ Advanced Display Environments and Collaboration Technology
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- ▶ Data Analysis
- ▶ **Augmented/Virtual Reality**

# SUPERCOMPUTERS



Cray X-MP/4 supercomputer, 1985  
[www.computerhistory.org/revolution/supercomputers/10/25/23](http://www.computerhistory.org/revolution/supercomputers/10/25/23)

## SUPERCOMPUTERS



Argonne's Aurora Supercomputer, 2022/23

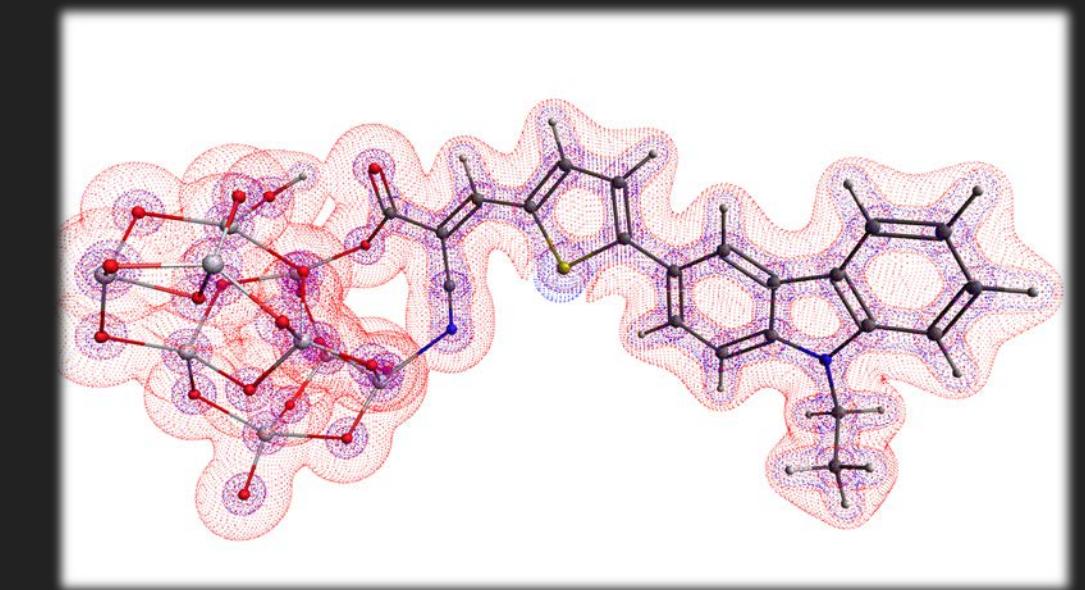
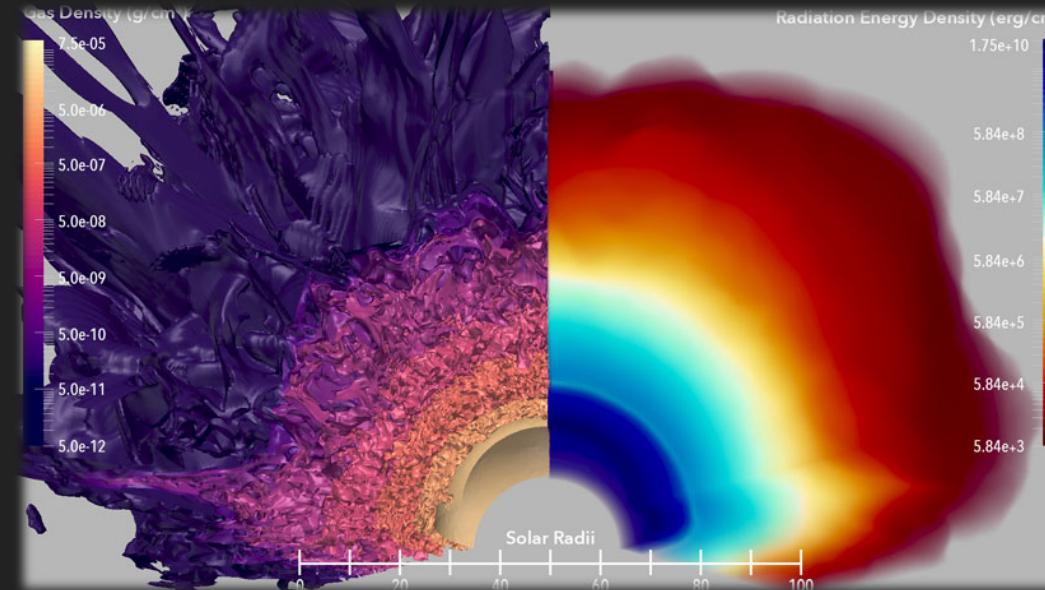
800 megaFLOPS to  $\sim$ 2 exaFLOPS

800,000,000 to  
~2,000,000,000,000,000  
FLOPS

2,500,000,000x

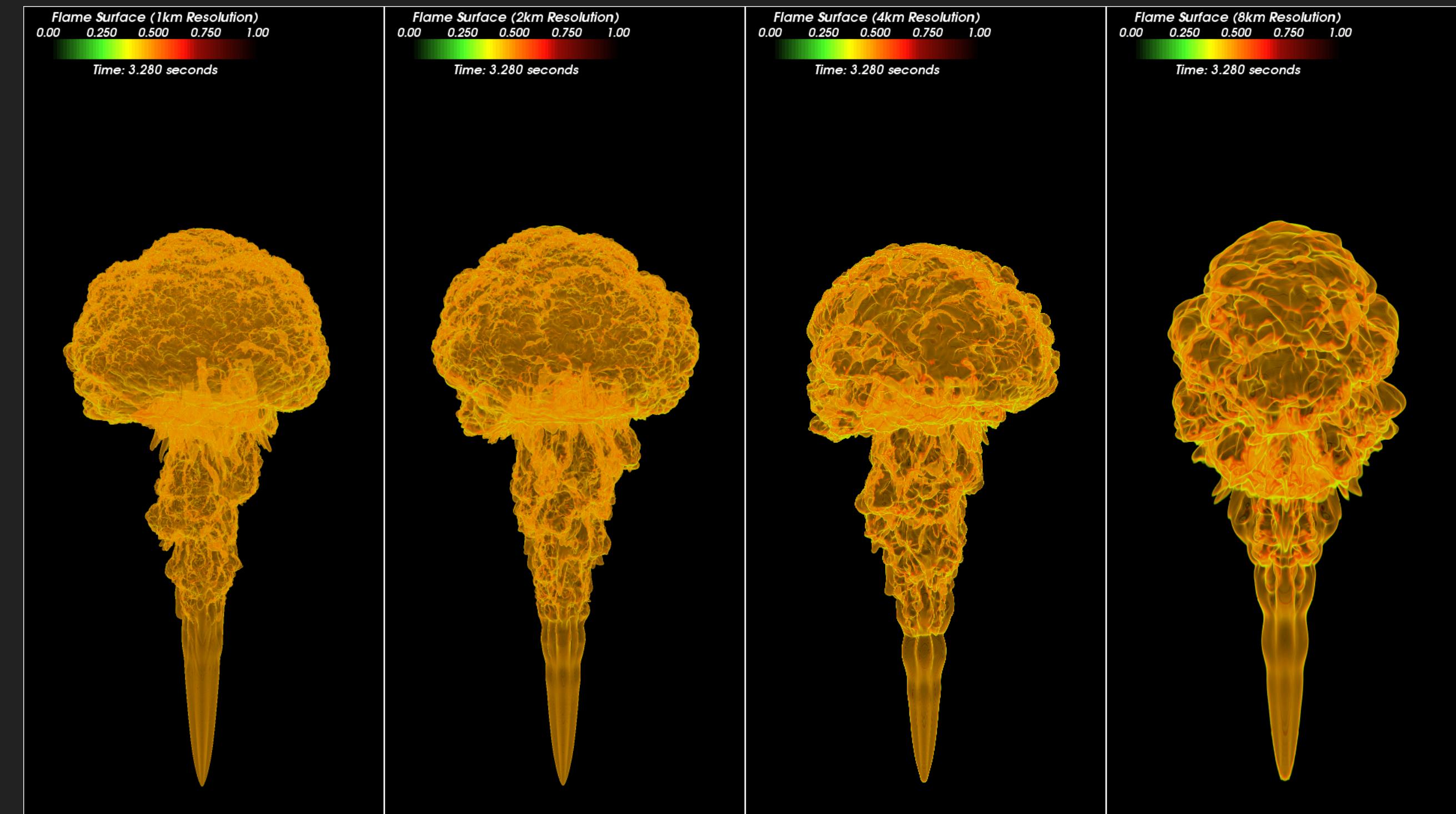
## SO WHAT DOES ALL THAT COMPUTE POWER ENABLE?

- ▶ Large-Scale Computing on the Connectomes of the Brain
- ▶ Global Radiation MHD Simulations of Massive Star Envelopes
- ▶ Molecular Design of Dye-Sensitized Solar Cells
- ▶ Real-time Computing in support of DIII-D National Fusion Facility



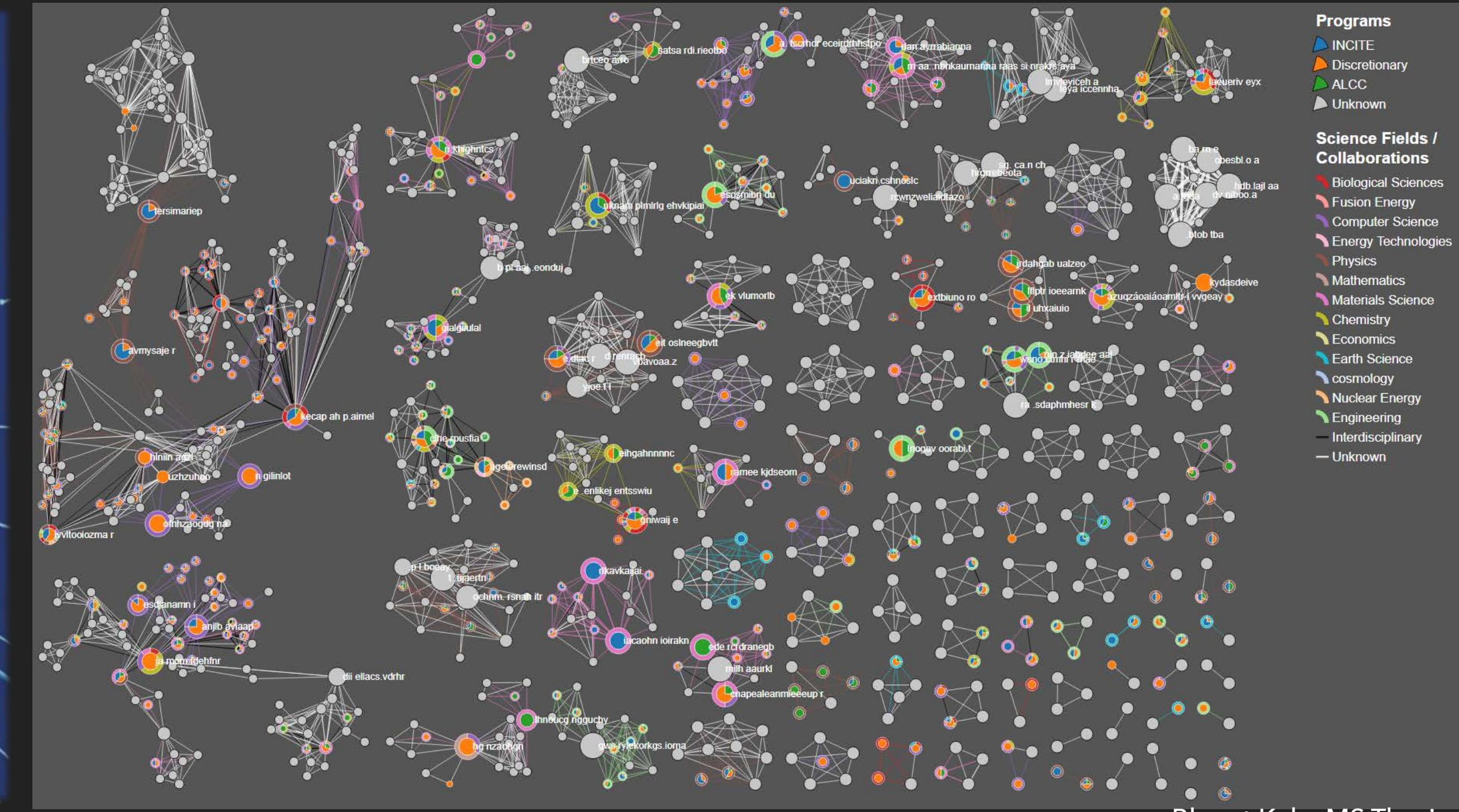
# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

- ▶ How do you translate theory into simulation?



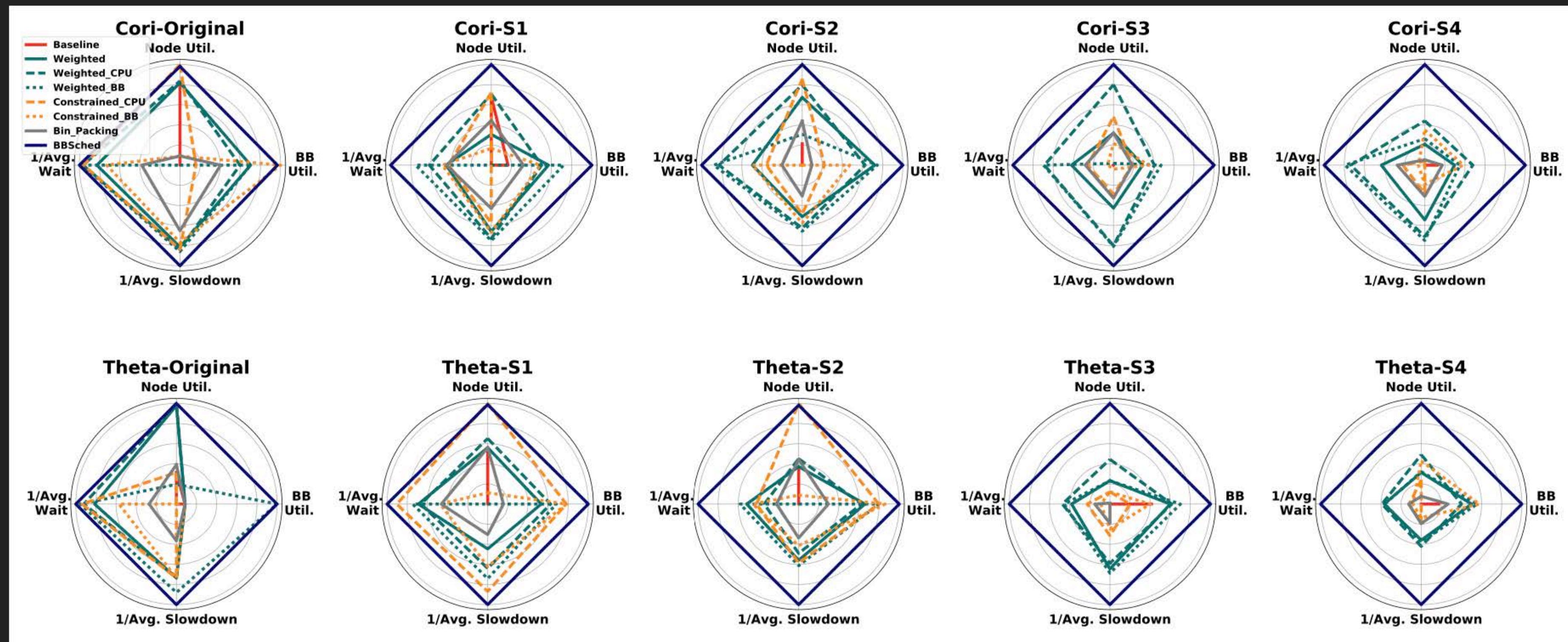
# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

- ▶ How do you more efficiently operate a facility?



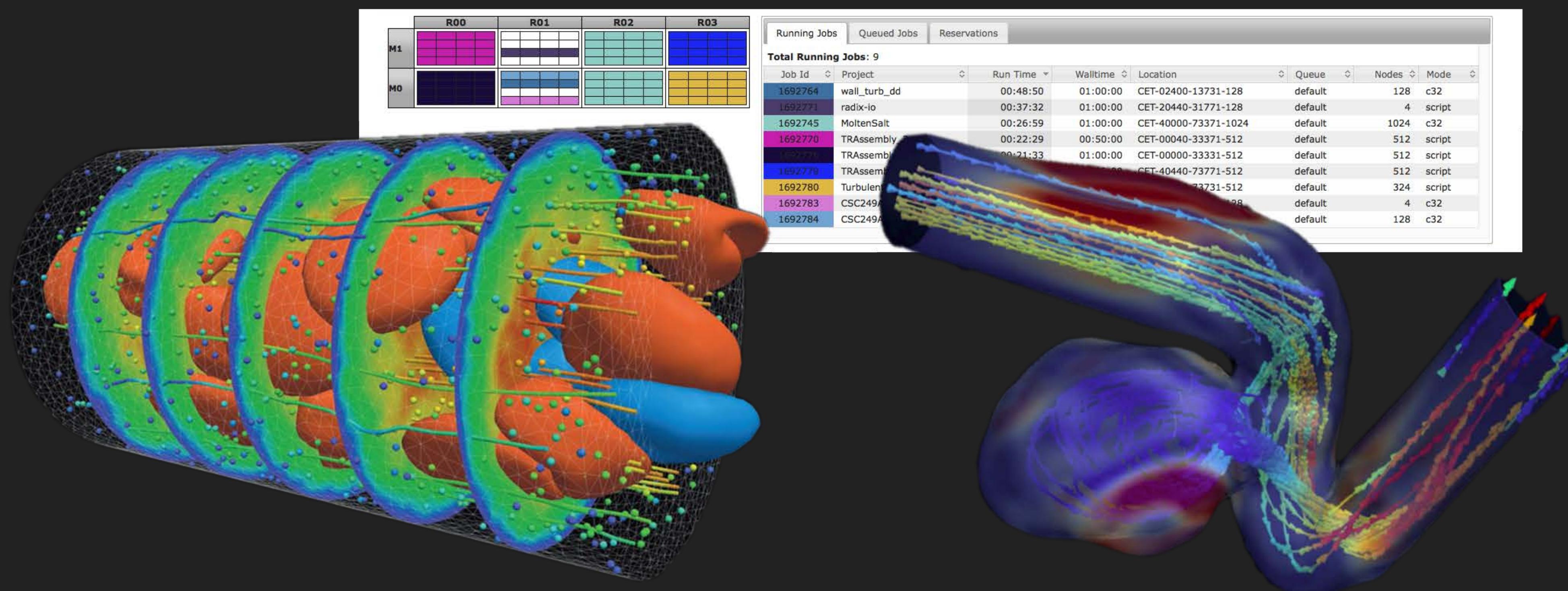
# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

- ▶ How do you effectively schedule and operate a resource?



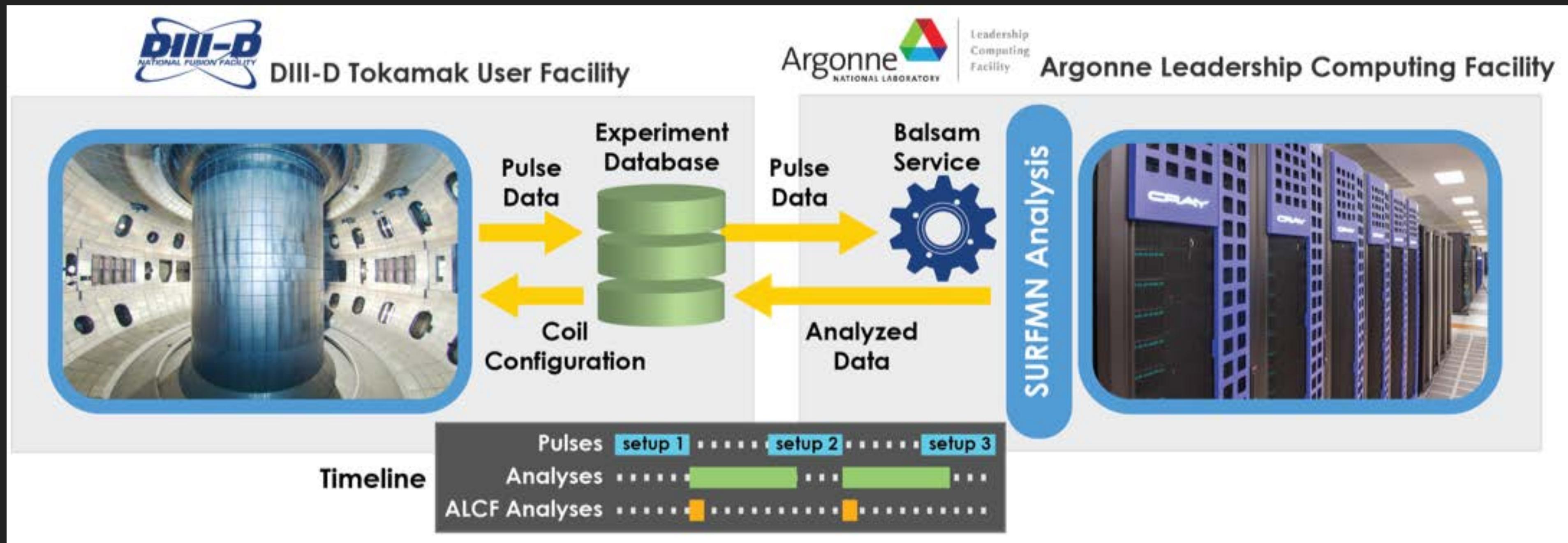
# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

- ▶ How do you evolve traditional HPC environment?



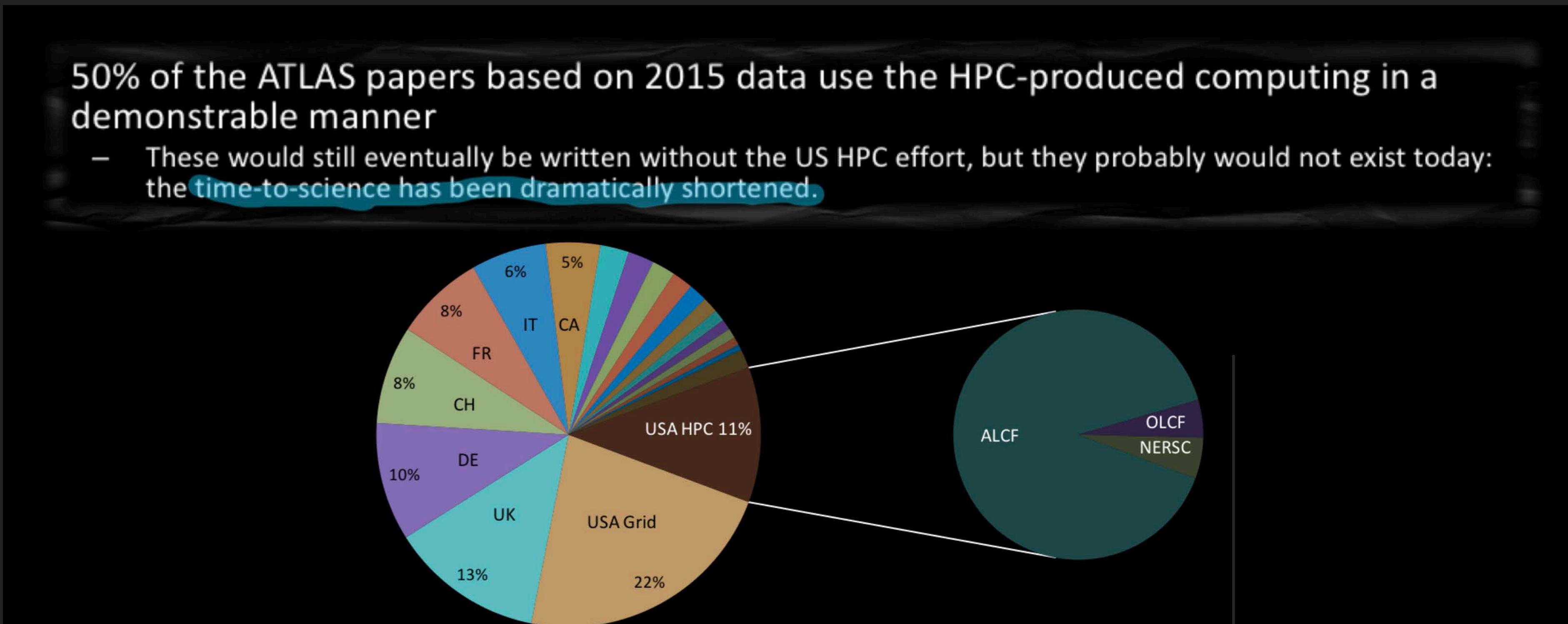
# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

- ▶ How do you evolve traditional HPC environment to address real-time needs?



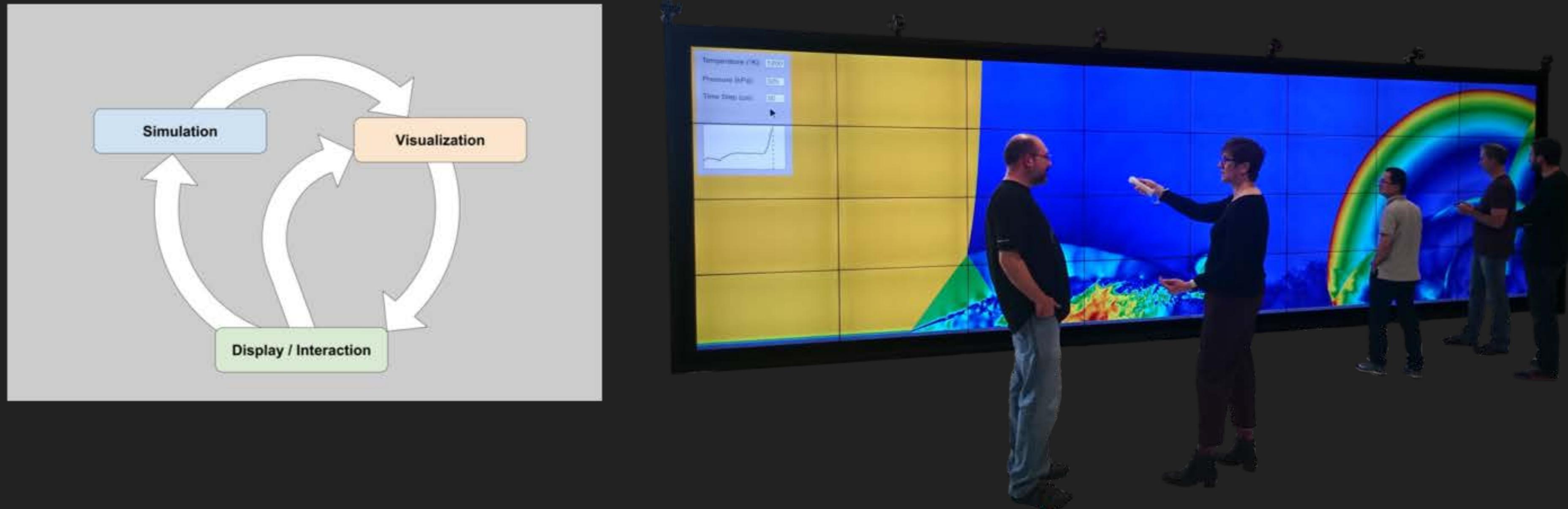
# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

## ► How do you evolve traditional HPC environment handle complex workloads?



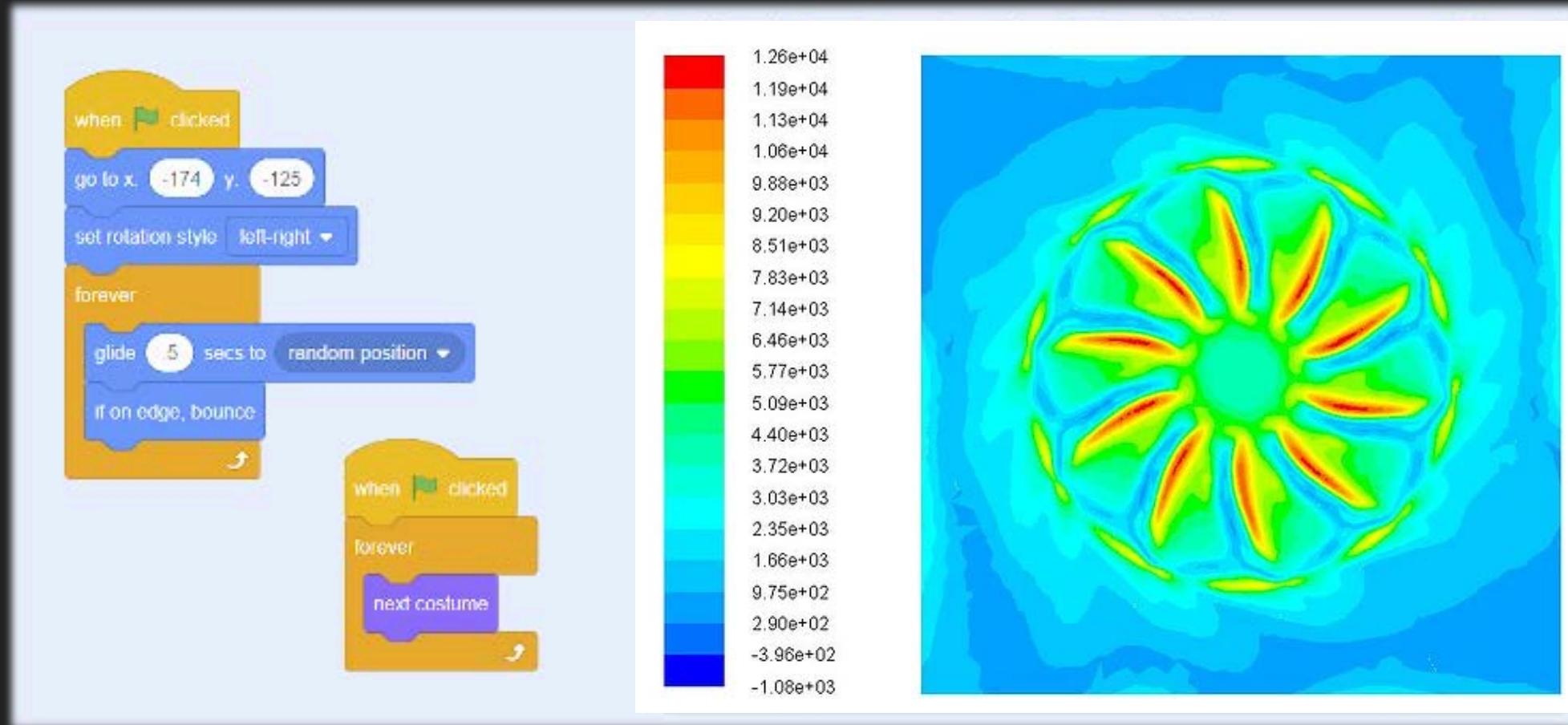
# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

- ▶ How do you evolve traditional HPC environment to increase engagement?



# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

- ▶ How do we **enable** scientists to be the most **productive** from **start to finish**?
- ▶ How do we improve **usability**?
- ▶ How do we **simplify** supercomputing?

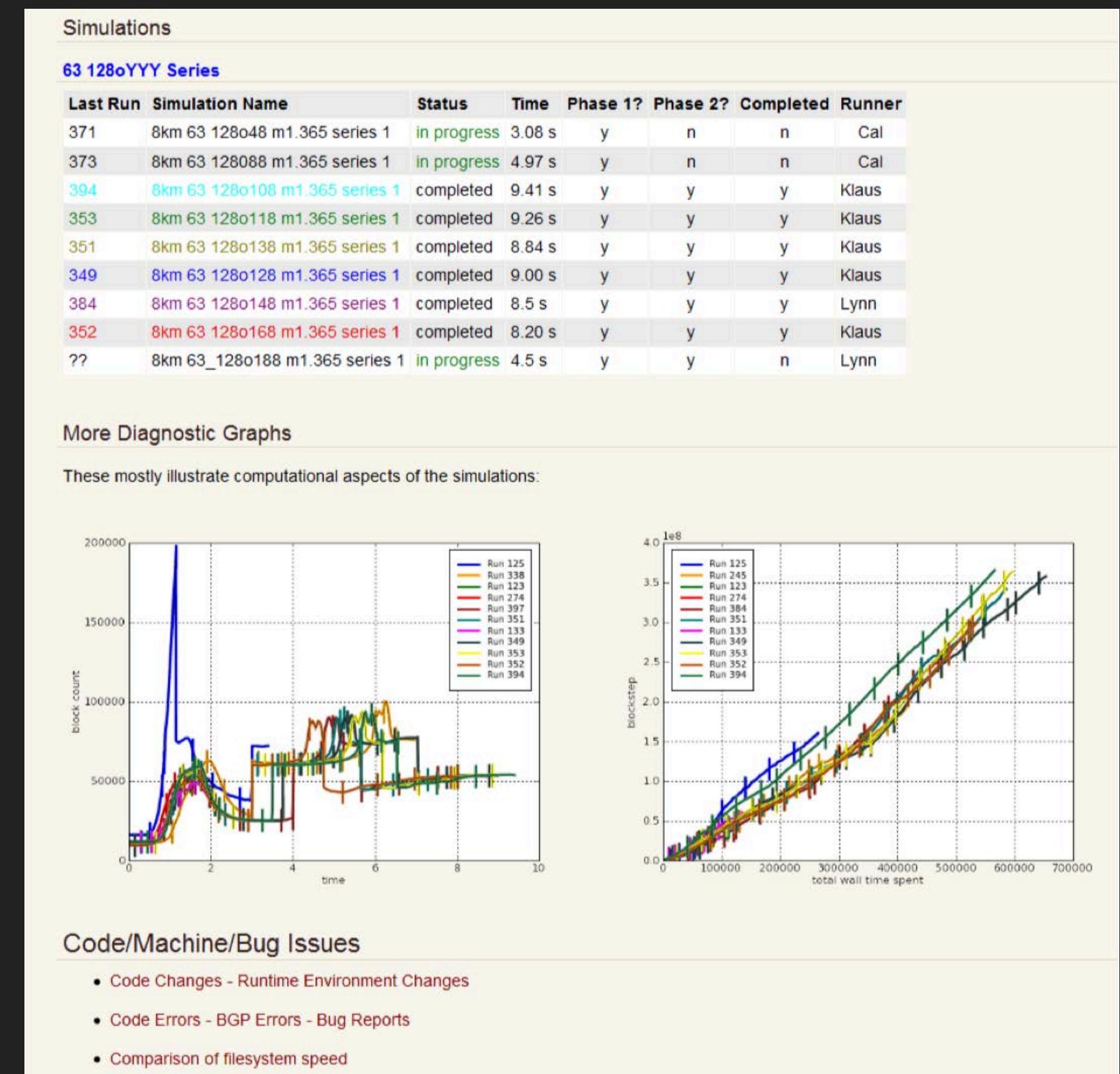


## HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

- ▶ How do we enable scientists to be the most productive from start to finish?
- ▶ Problems with science management:
  - ▶ Tracking simulations and output: **burdensome**
  - ▶ Finding and reproducing old simulations: **difficult**
  - ▶ Monitoring live simulations: **inconvenient, idiosyncratic**
  - ▶ Post-processing, analysis and archival of results: **haphazard**
  - ▶ Assessing simulation behavior/performance: **challenging**

# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

- ▶ How do we enable scientists to be the most productive from start to finish?
- ▶ Simulation management and analysis system for Flash (Smaash)
  - ▶ Tracking and coordination of data (simulation and meta)
  - ▶ Run-time monitoring of simulations and automated analysis of simulation output
  - ▶ Method for managing / executing common workflows



# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

- ▶ How do we enable scientists to be the most productive from start to finish?

The figure displays three screenshots of the Smaash/HACC web interface, showing different aspects of the simulation process:

- Model: MiraU / M019 / L2100**: A log-log plot of the primordial power spectrum  $P(k)$  versus wavenumber  $k$ . The y-axis ranges from  $10^{-1}$  to  $10^5$ , and the x-axis ranges from  $10^{-2}$  to  $10^1$ . Multiple curves represent different power spectrum models, labeled on the right.
- Run: MiraU / M019 / run001 / L2100**: A table of simulation timesteps. The table includes columns for Timestep, Run, Model, Simulation, Date, and Size. The data shows 210 entries, all from run001, dated 1 day, 16 hours ago, with sizes ranging from 1 to 1 MB.
- Run: MiraU / M019 / run000 / L2100**: A table of files. The table includes columns for Path, Date, Size, and Type. It lists three files: `/homes/turam/dev/smaash/data/606/hacc_gpu_m019.log` (1.0 MB, txt), `/homes/turam/dev/smaash/data/607/hacc_gpu_m019.err` (119.6 KB, txt), and `/homes/turam/dev/smaash/data/608/indat.params` (7.4 KB, txt).
- Parameter File Content**: A detailed view of the `indat.params` file. The file contains numerous comments and parameters related to cosmological simulations, including:
  - Header version information: HACC\_HEADER\_VERSION 1.0.0
  - Cosmological Parameters: OMEGA\_CDM, OMEGA\_NU, DEUT, Hubble constant, SSB, NS index, and W\_DE.
  - Simulation parameters: OMEGA\_CDM 0.145084, DEUT 0.02217382692, OMEGA\_NU 0.00686393, Hubble 0.825136069, SSB 0.854654384, NS 1.026482126, W\_DE -0.981272302, WA\_DE -0.39335368548398, T\_CMB 2.726, N\_EFF\_MASSLESS 0.0, and N\_EFF\_MASSIVE 3.04.
  - Initializer Set-up and read-ins: ZIN, USE\_WHITE\_NOISE\_INIT, and INIT parameters.
  - Distribution type: ROUND\_ROBIN, ALL\_TO\_ALL, ONE\_TO\_ONE, and TRANS.
  - Processor management: ALL\_TO\_ALL, ONE\_TO\_ONE, and improved ROUND\_ROBIN.
  - Restart: Z\_IN\_200.0, USE\_WHITE\_NOISE\_INIT, and TRANS functions.
  - Input files: INPUT\_BASE\_NAME cmbM019.tf, INPUT\_TYPE INIT, and DISTRIBUTION\_TYPE LAST.

# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

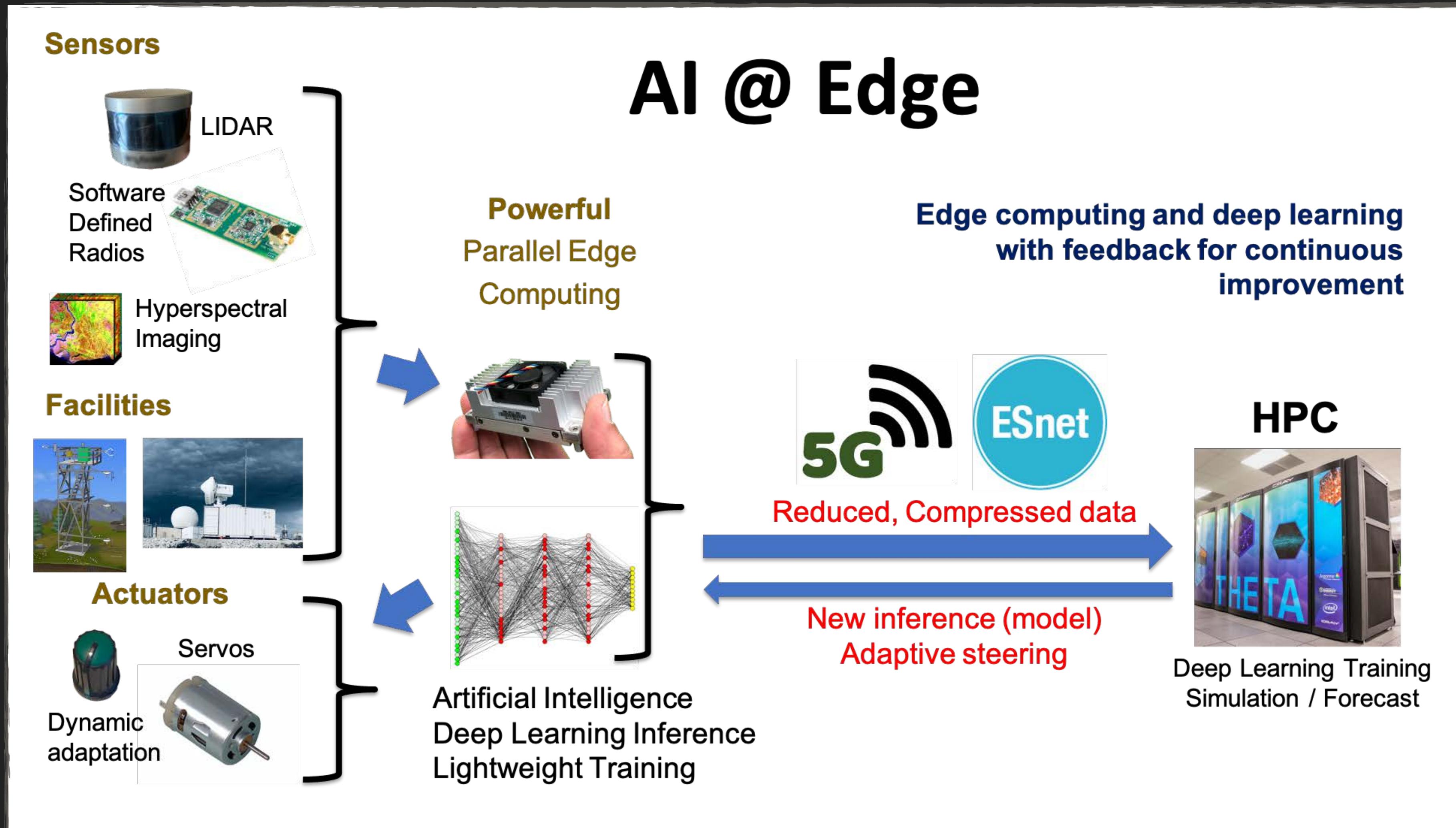
- ▶ How do we enable scientists to be the most productive from start to finish?

The collage illustrates the user interface for managing and visualizing high-performance computing research opportunities. It includes:

- A dashboard for generating visualizations: **Basic Overview**, **Feature-Based**, **Fly-Through**, and **Time-Varying Data**.
- A grid of job status cards:
  - APS Basic Job (Jan. 15, 2016, 11:47 a.m., In Progress)
  - APS Basic Job (Jan. 15, 2016, 11:41 a.m., In Progress)
  - APS Basic Job (Jan. 15, 2016, 11:11 a.m., In Progress)
  - HA\_tube5\_test2 Basic Job (Dec. 8, 2015, 6:14 p.m., Complete)
  - HA\_tube5\_test2 Basic Job (Dec. 8, 2015, 6:04 p.m., In Progress)
  - HA\_tube5\_test2 Basic Job (Dec. 8, 2015, 5:23 p.m., In Progress)
  - hacc\_160x160x160\_float.little\_endian.bin Basic Job (Dec. 4, 2015, 5:39 p.m., In Progress)
  - hacc\_160x160x160\_float.little\_endian.bin Basic Job (Dec. 4, 2015, 10:06 a.m., In Progress)
- A grid of thumbnail images for a video job.
- A detailed view of a job card for HA\_tube5, test2, showing:

job_id	1449620045101408
job_data	HA_tube5_test2
job_type	Basic
job_creator	oculus
time_received	Dec. 8, 2015, 6:14 p.m.
time_modified	Dec. 9, 2015, 10:04 a.m.
Snapshots	60
Comments	None

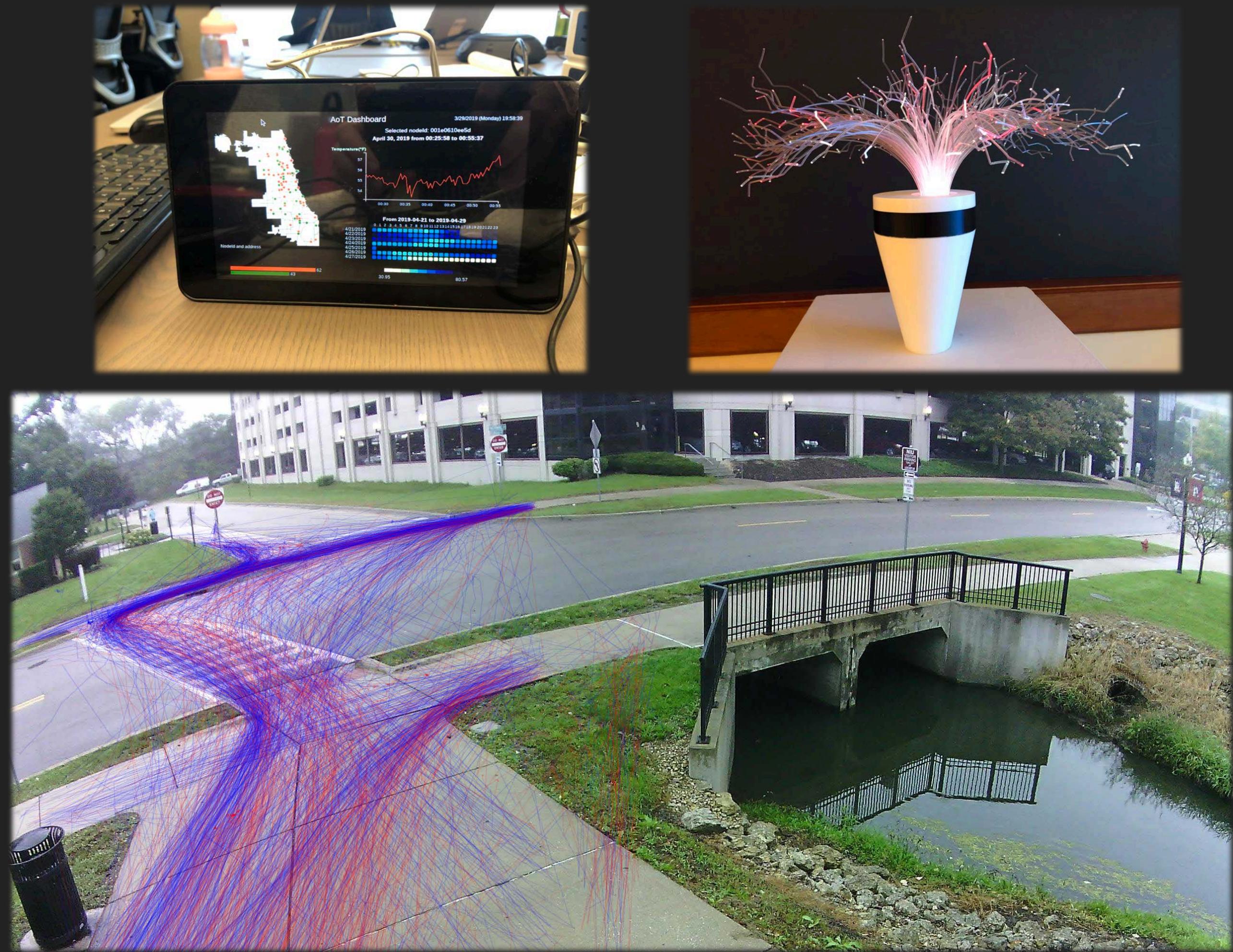
# INTERNET OF THINGS (COMPUTING CONTINUUM) [EDGE COMPUTING]



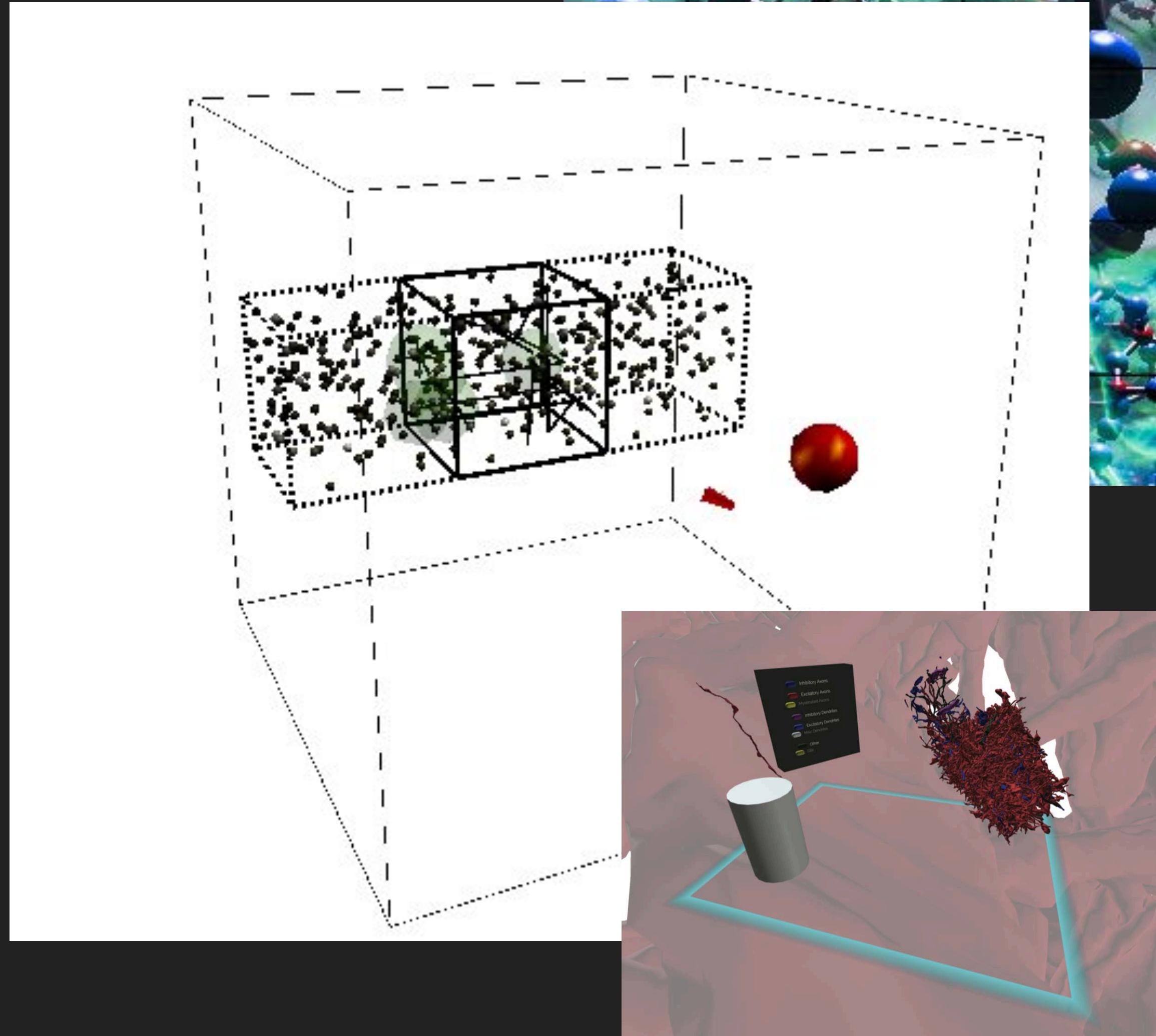
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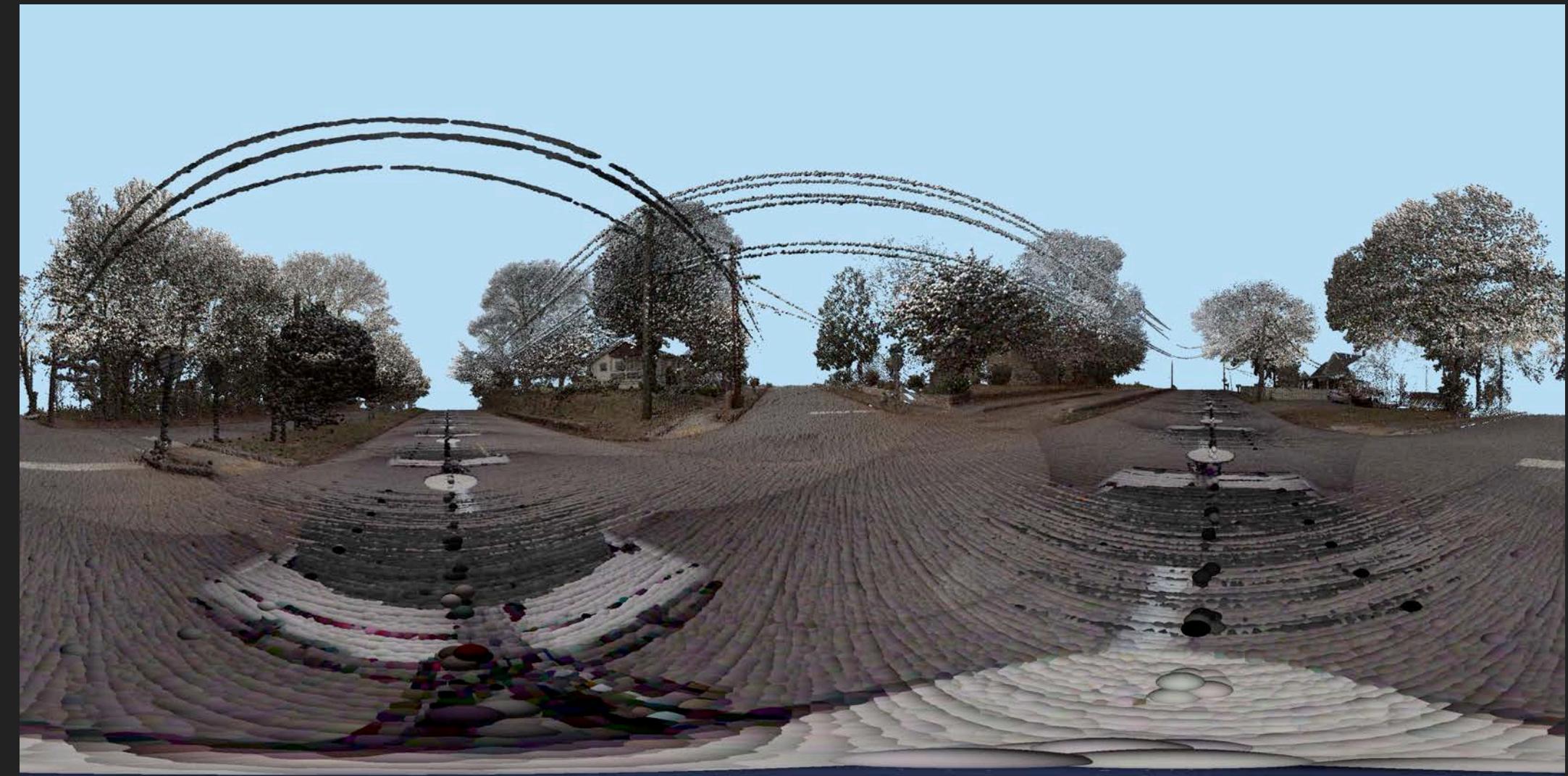
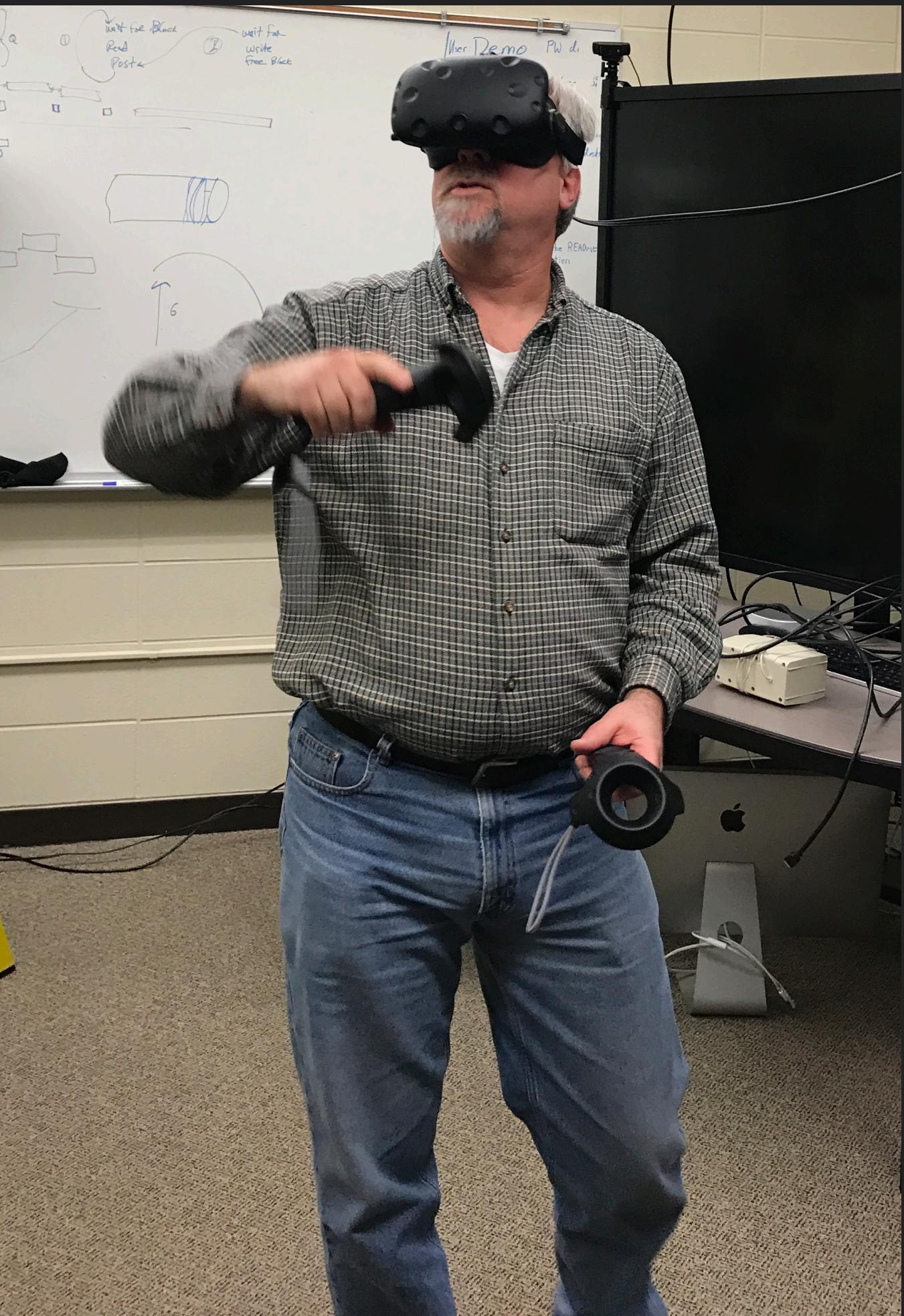
# VIRTUAL REALITY



## Use of **Virtual Reality** in Science

- ▶ Usability, virtual interactions
- ▶ Rendering, realistic data in VR time

# VIRTUAL REALITY



## SUMMER RESEARCH OPPORTUNITIES (IN PERSON NORMALLY, CURRENTLY VIRTUAL)



## ACKNOWLEDGMENTS

- ▶ Current funding is provided by the *Argonne Leadership Computing Facility*, a DOE Office of Science User Facility supported under contract DE-AC02-06CH11357 with additional support from the National Science Foundation grant OAC-1935984.
- ▶ Thanks to all the students of the ddiLab and my colleagues at NIU and ANL.



Spring 2019 ddiLab

If I have seen further it is by standing on the shoulders of giants.

35

Sir Isaac Newton

