

A black and white silhouette of a city skyline, likely New York City, with a body of water in the foreground. The skyline includes several prominent skyscrapers, with the tallest one on the left. The water is dark, and the sky is light.

# Big Ideas

WITH MICHAEL E. PAPKA

DATA, DEVICES AND INTERACTION LABORATORY

April 15, 2021

## 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 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)





# 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

**800megaFLOPS to ~2exaFLOPS**

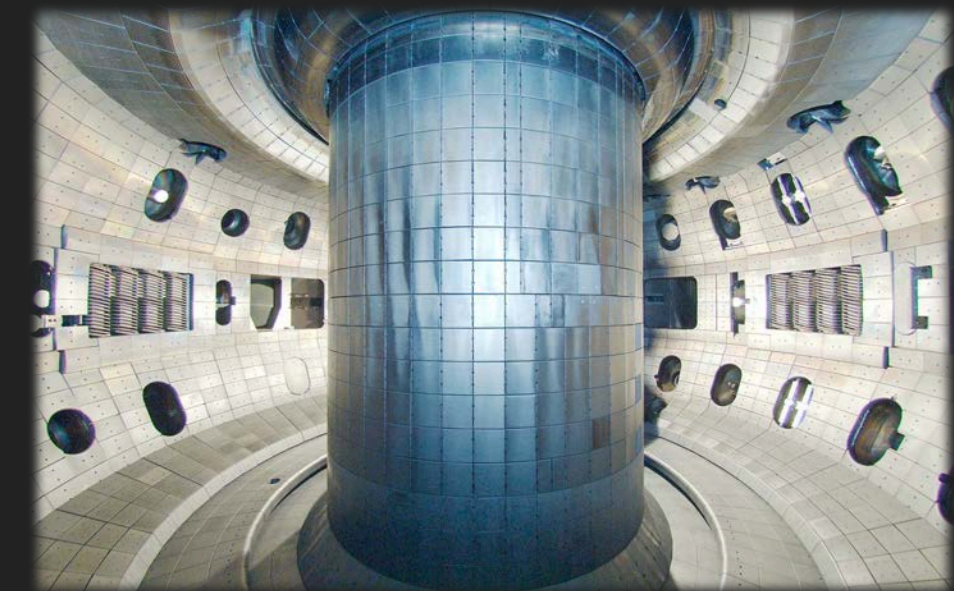
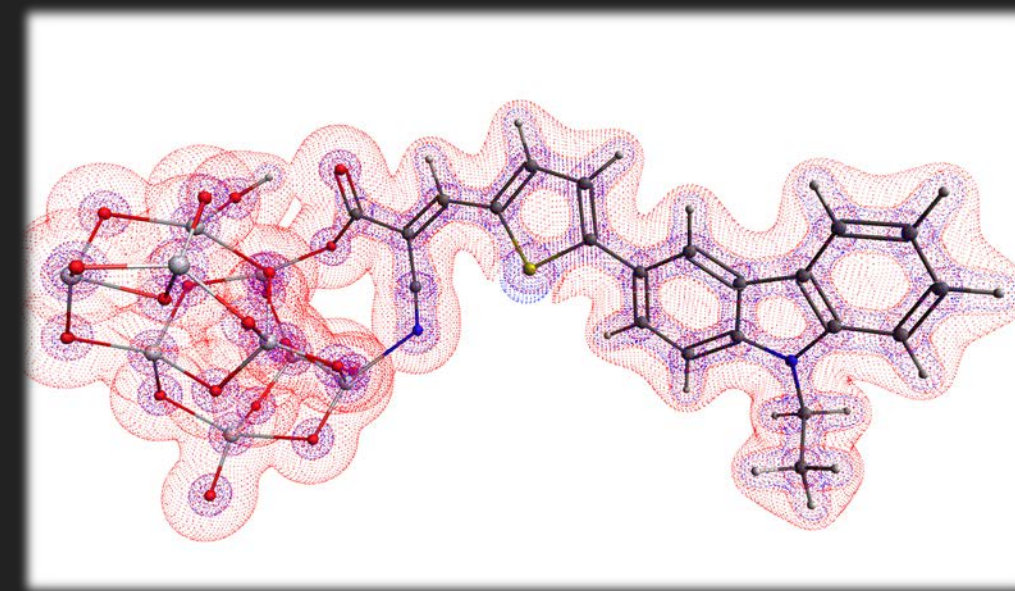
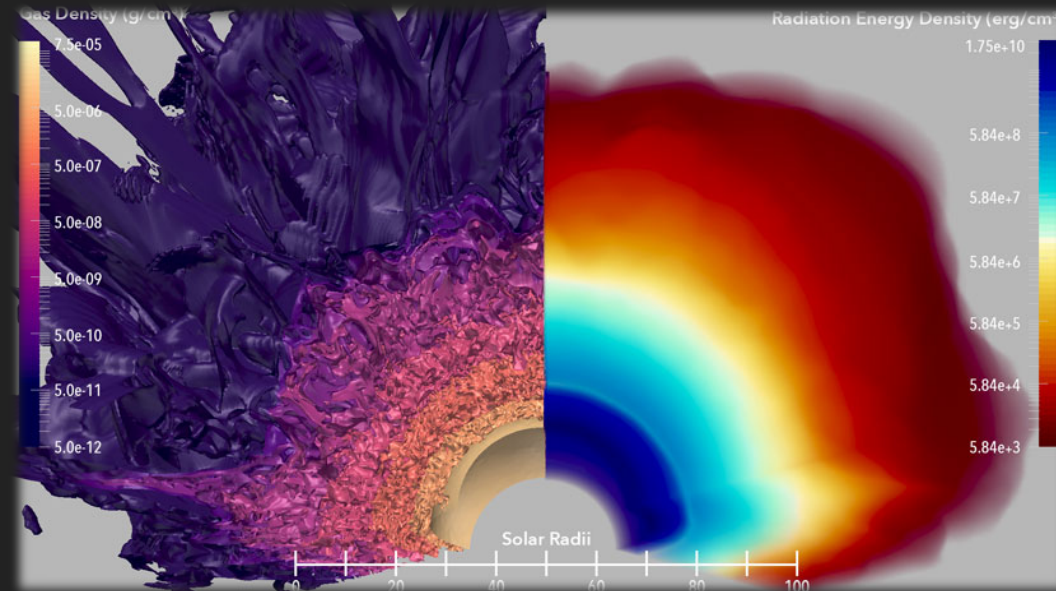
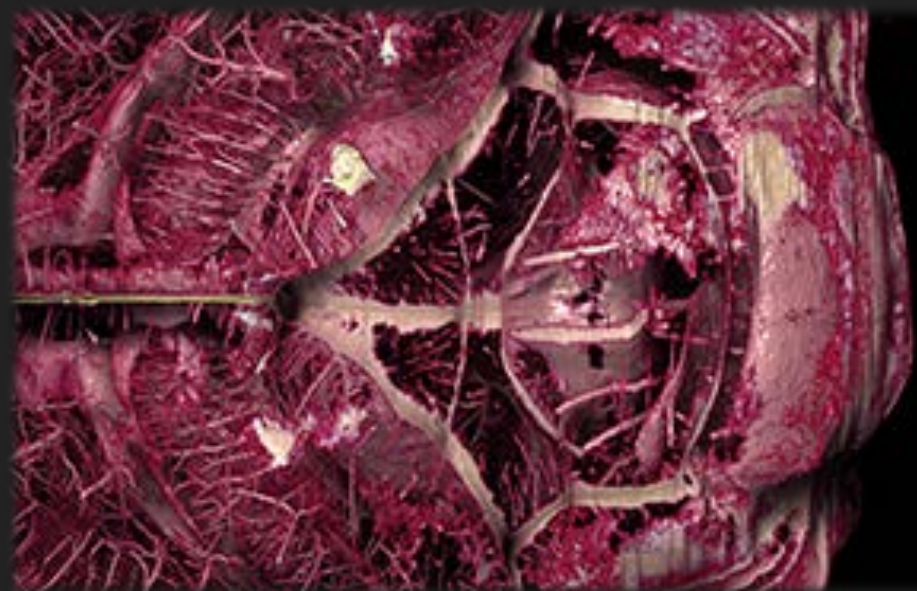
800,000,000 to  
~2,000,000,000,000,000,000  
FLOPS

**2,500,000,000x**



## SO WHAT DOES ALL THAT COMPUTE POWER ENABLE?

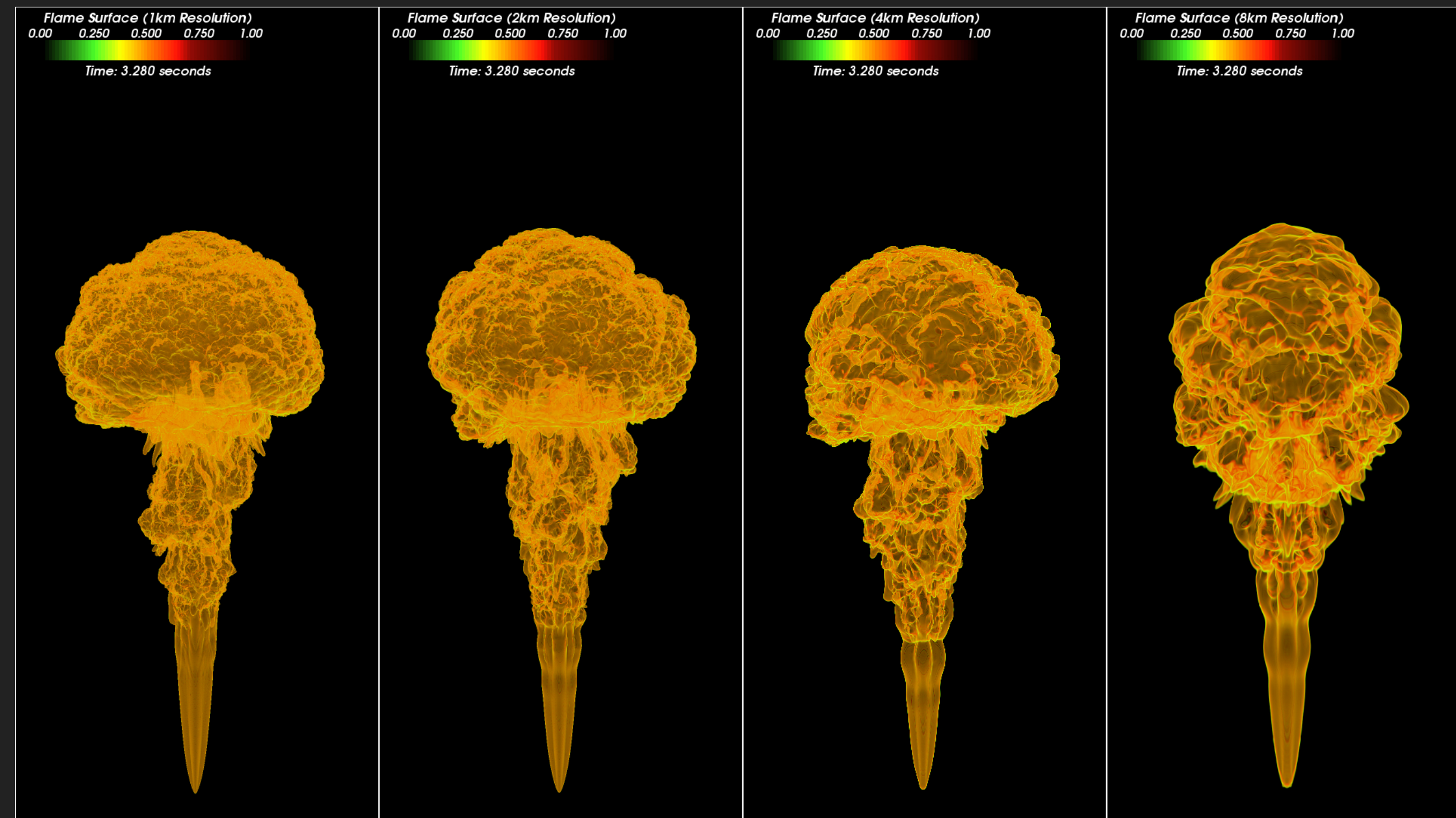
- ▶ Large-Scale Computing on the Connectomes of the Brain
- ▶ Global Radiation MHD Simulations of Massive Star Envelopes
- ▶ Molecular Design of Dye-Sensitized Solar Cells
- ▶ Real-time Computing in support of DIII-D National Fusion Facility





# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

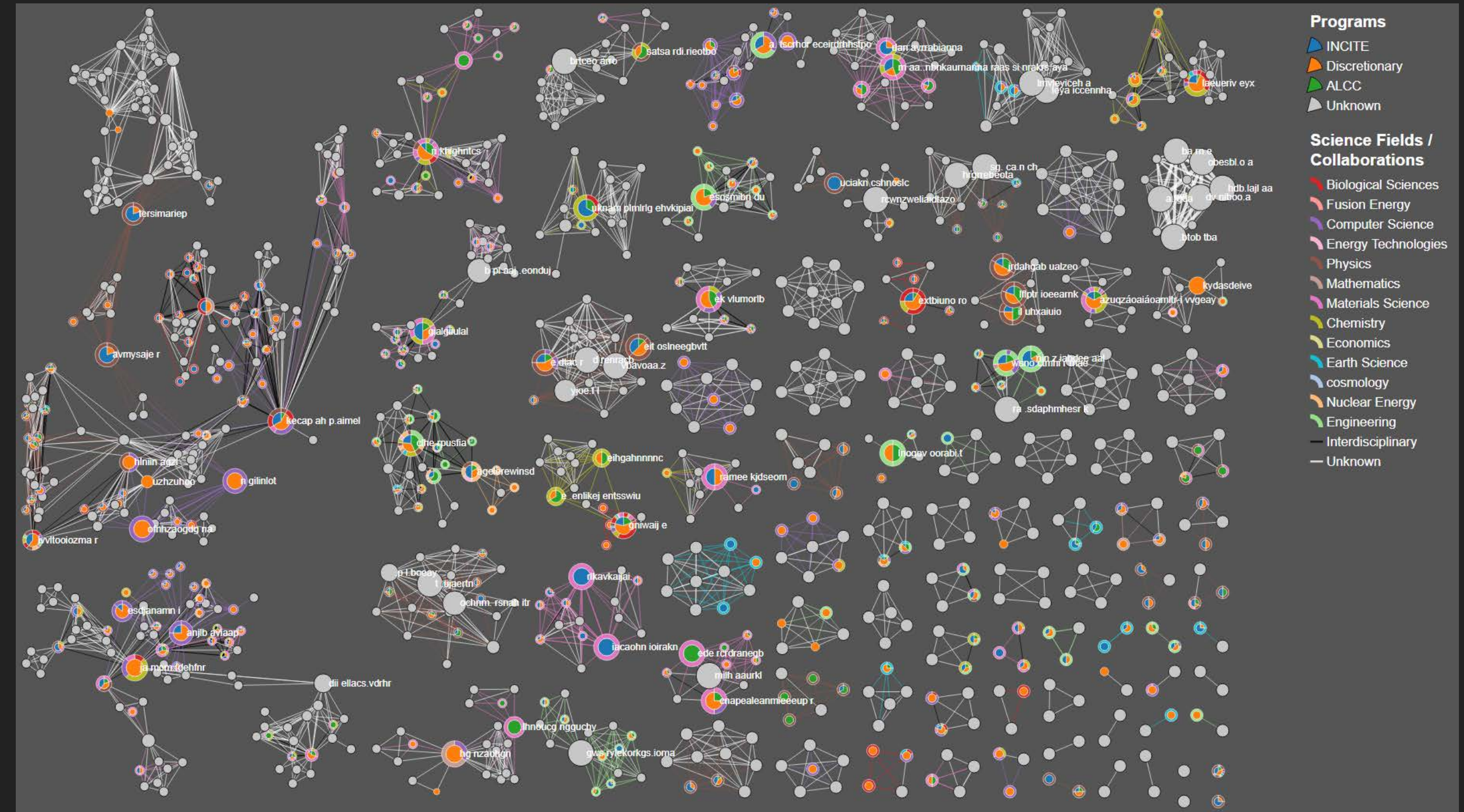
- ▶ How do you translate theory into simulation?





# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

► How do you more efficiently operate a facility?

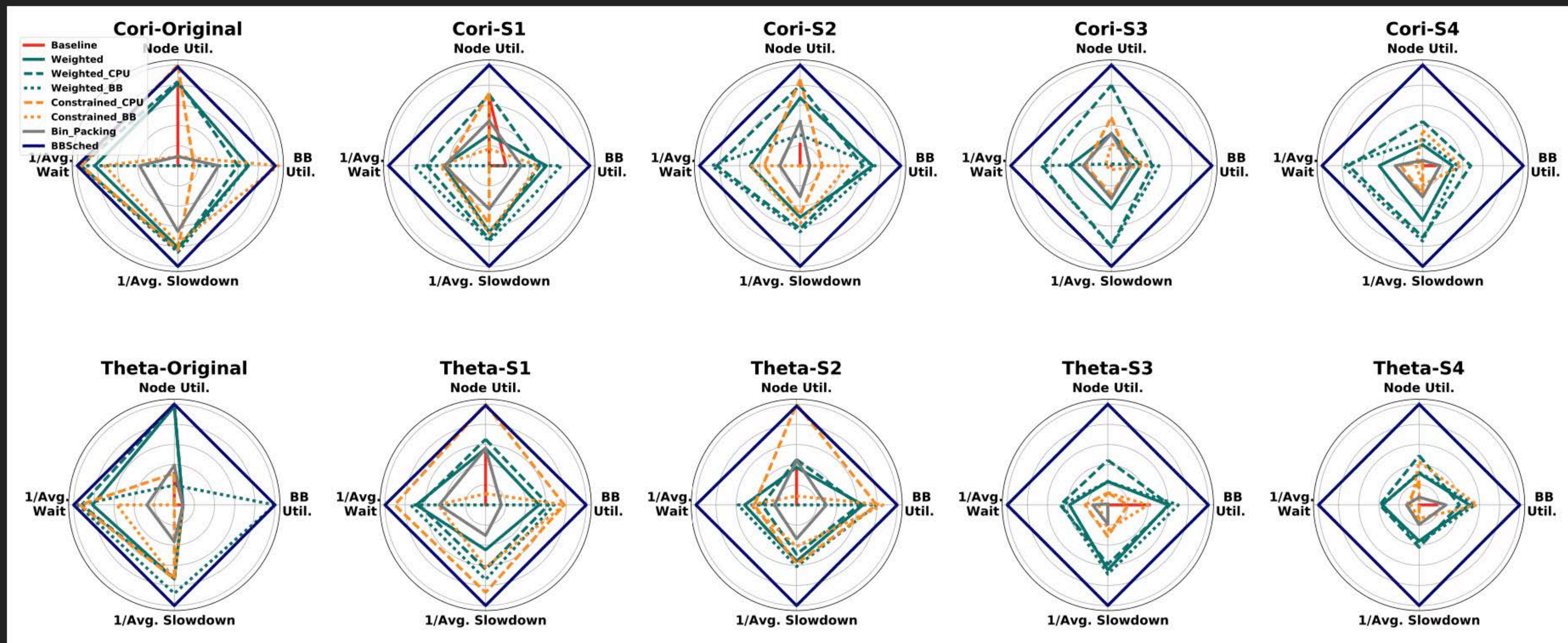


Bharat Kale, MS Thesis



# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

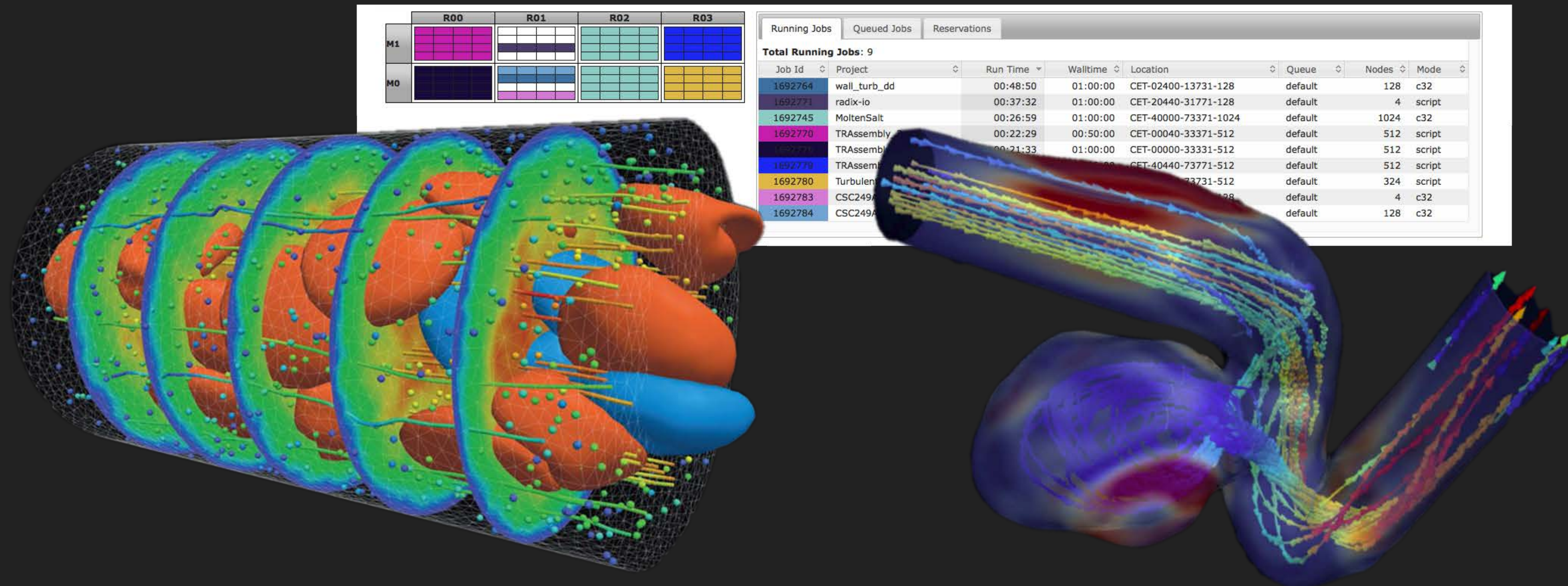
- ▶ How do you effectively schedule and operate a resource?





# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

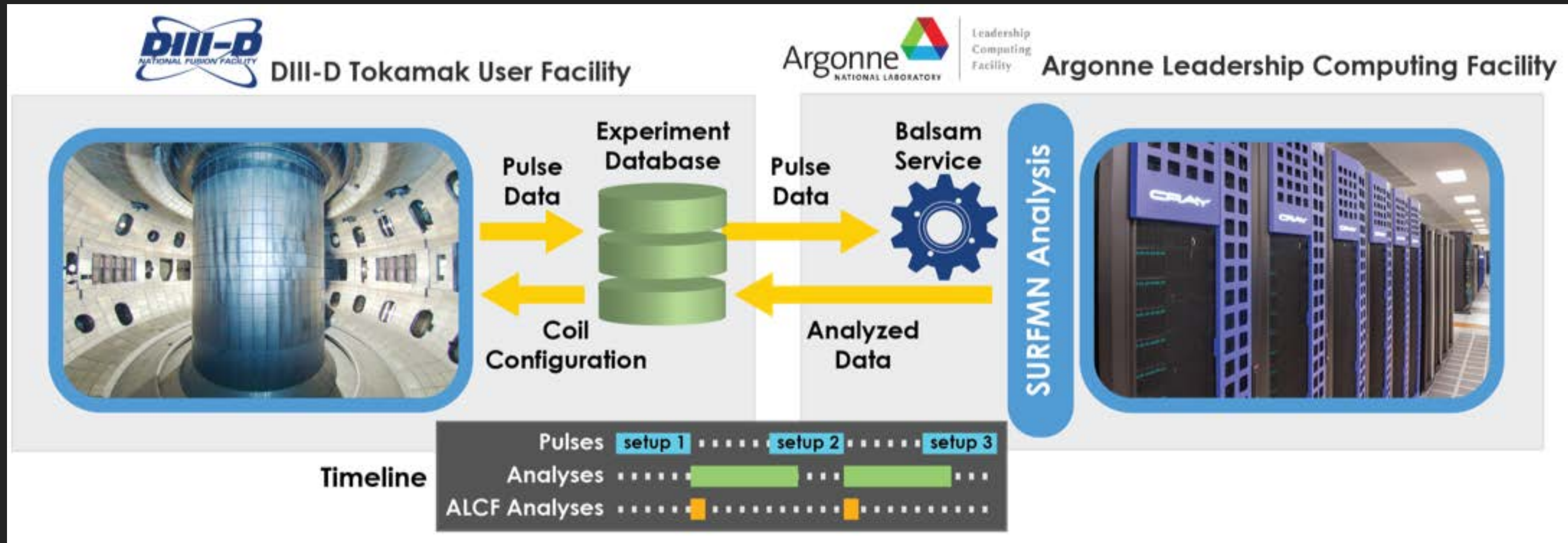
- ▶ How do you evolve traditional HPC environment?





# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

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

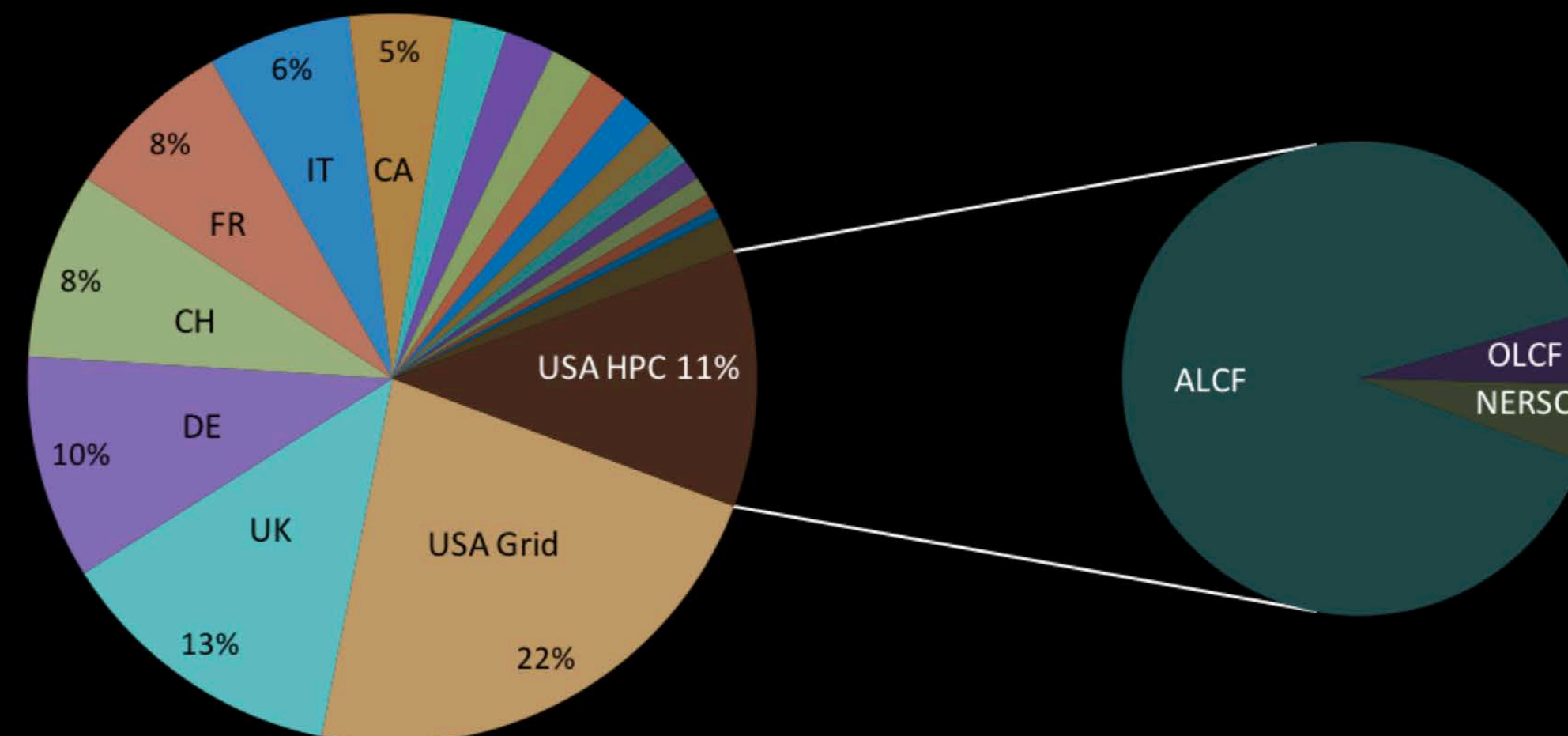


# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

- ▶ How do you evolve traditional HPC environment handle complex workloads?

50% of the ATLAS papers based on 2015 data use the HPC-produced computing in a demonstrable manner

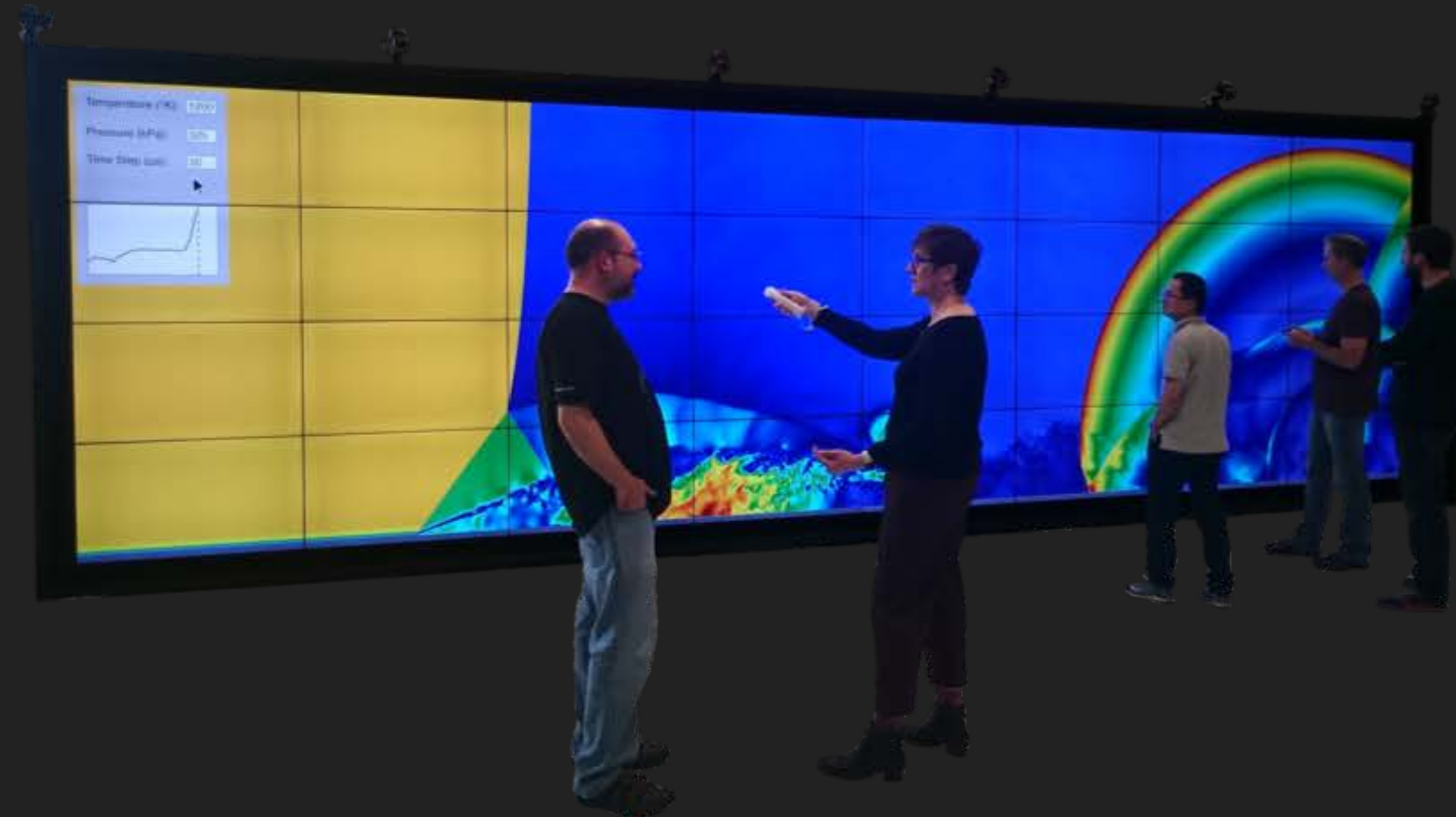
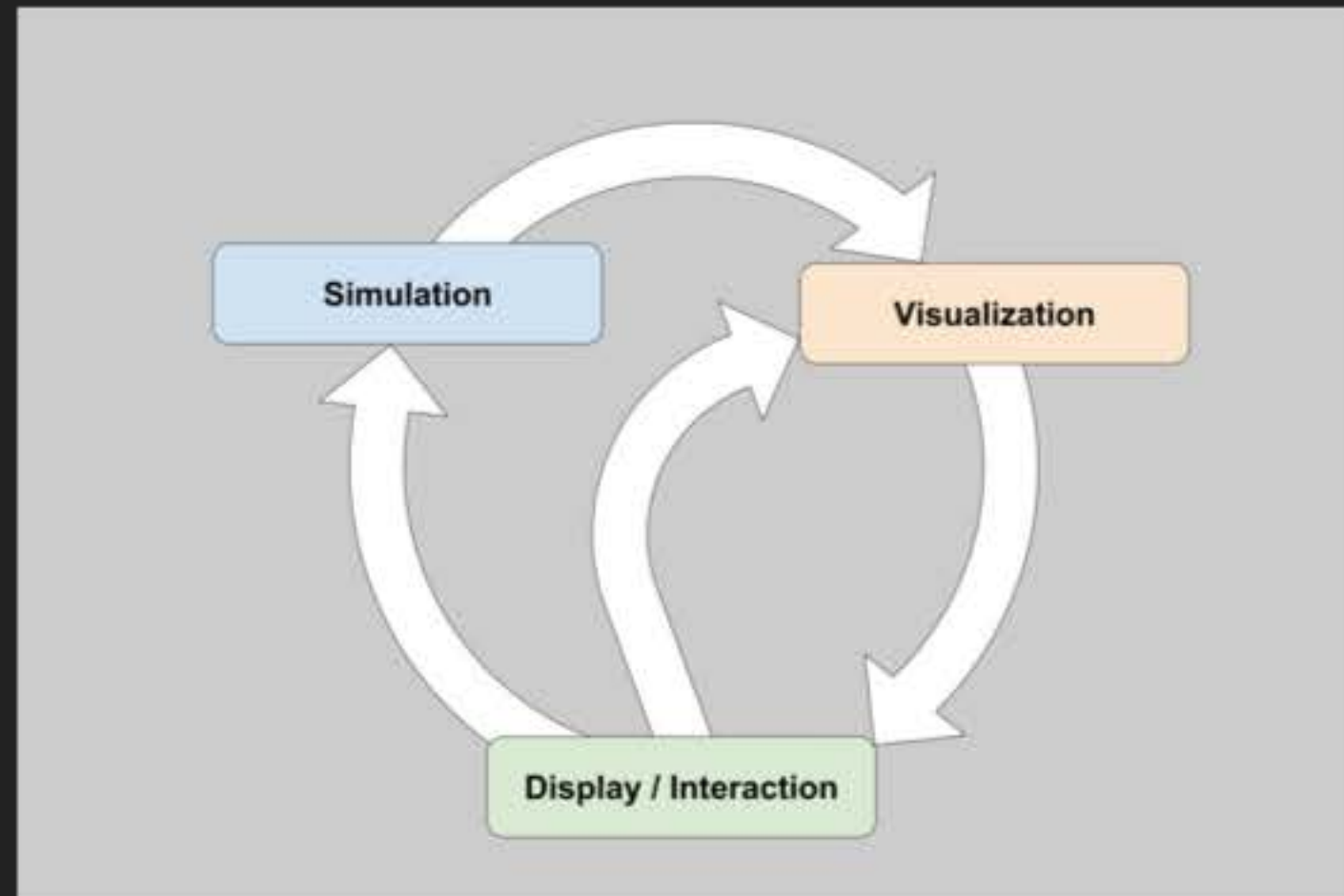
- These would still eventually be written without the US HPC effort, but they probably would not exist today: the **time-to-science has been dramatically shortened.**





# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

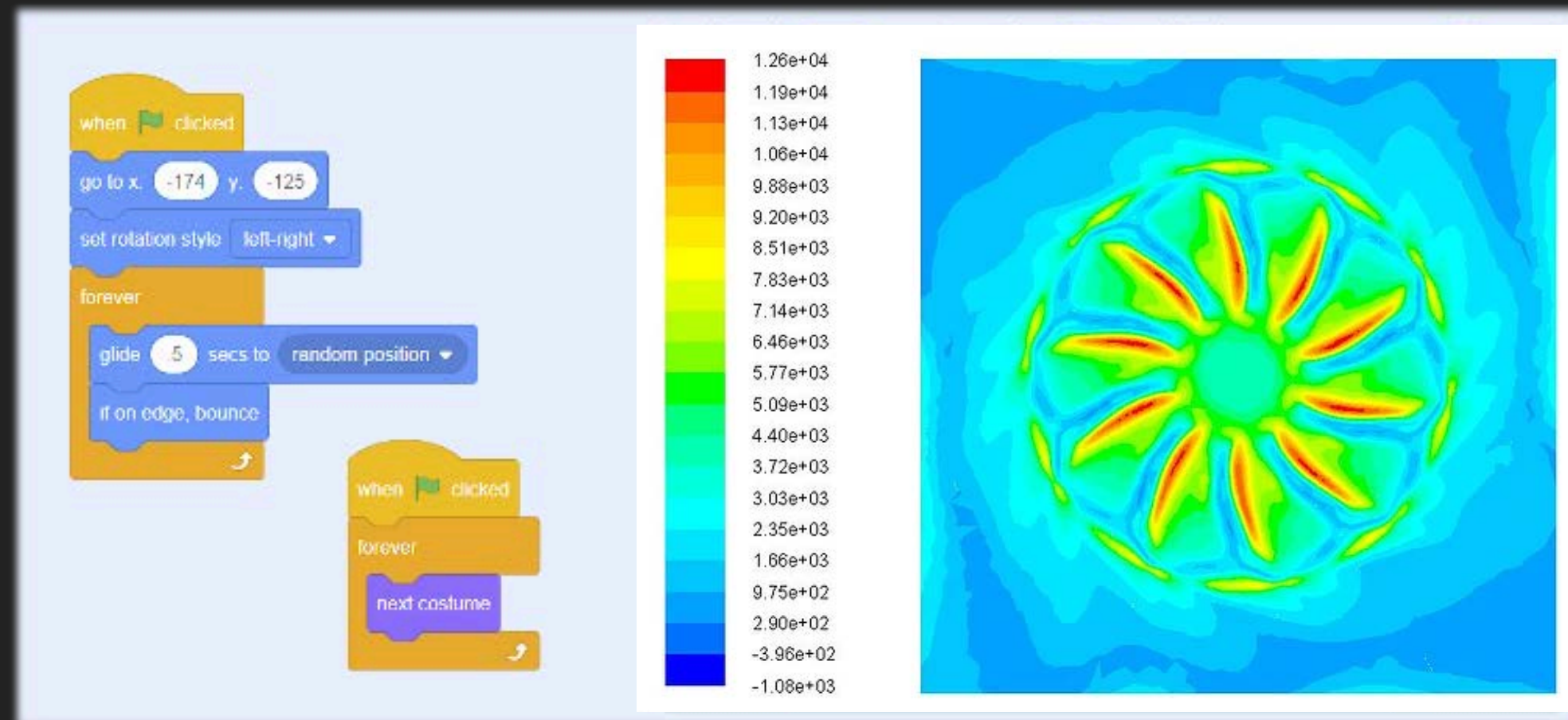
- ▶ How do you evolve traditional HPC environment to increase engagement?





# 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 **simplify** supercomputing?

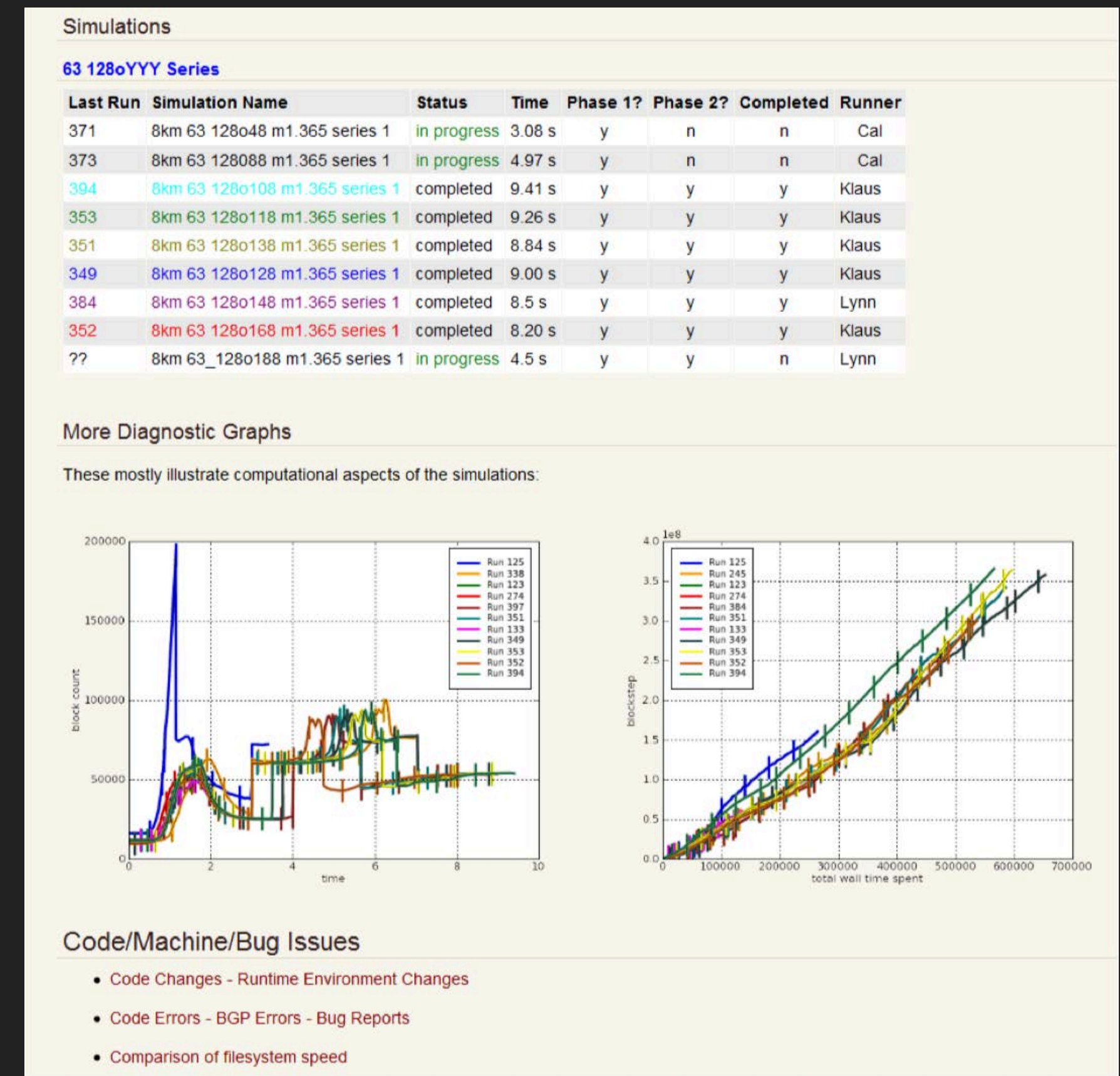






# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

- ▶ How do we enable scientists to be the most productive from start to finish?
  - ▶ **S**imulation **m**anagement and **a**nalysis system for **F**lash (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 image displays four screenshots of the Smaash/HACC web interface, illustrating the workflow for managing and analyzing cosmological simulations.

- Leftmost screenshot:** Shows a plot of the matter power spectrum  $P(k)$  versus wavenumber  $k$  for the 'MiraU / M019 / L2100' model. The plot shows multiple curves for different particle counts (pk.50 to pk.499). Below the plot is a table of runs, a file list, and a search bar.
- Second screenshot:** Shows a table of simulation timesteps for 'Run: MiraU / M019 / run001 / L2100'. The table lists timestep numbers, run IDs, models, simulations, dates, and sizes.
- Third screenshot:** Shows a table of simulation files for 'Run: MiraU / M019 / run000 / L2100'. The table lists file paths, dates, sizes, and types.
- Rightmost screenshot:** Shows the content of an 'indat.params' file, which contains cosmological parameters such as  $\Omega_{CDM}$ ,  $\Omega_{B}$ ,  $H_0$ ,  $\sigma_8$ ,  $n_s$ ,  $w_{DE}$ ,  $T_{CMB}$ , and simulation-specific settings like  $Z_{IN}$  and  $N_{EFF\_MASSLESS}$ .



# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

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

Argonne HPC portal interface showing visualization options. The page includes a header with the Argonne logo and a 'Create a Job' button. Below the header, there are four columns of visualization options, each with a thumbnail image and a description:

- Basic Overview**: A general overview visualization.
- Feature-Based**: A single movie that provides an overview and highlights individual features.
- Fly-Through**: Generates a video with a general view around the data.
- Time-Varying Data**: Visualize the time-based evolution of your data.

Argonne HPC portal interface showing job status. The page includes a header with the Argonne logo and a 'Create a Job' button. Below the header, there are eight job cards arranged in a 2x4 grid. Each card shows a thumbnail image, the job name, the job type, the start time, and the status:

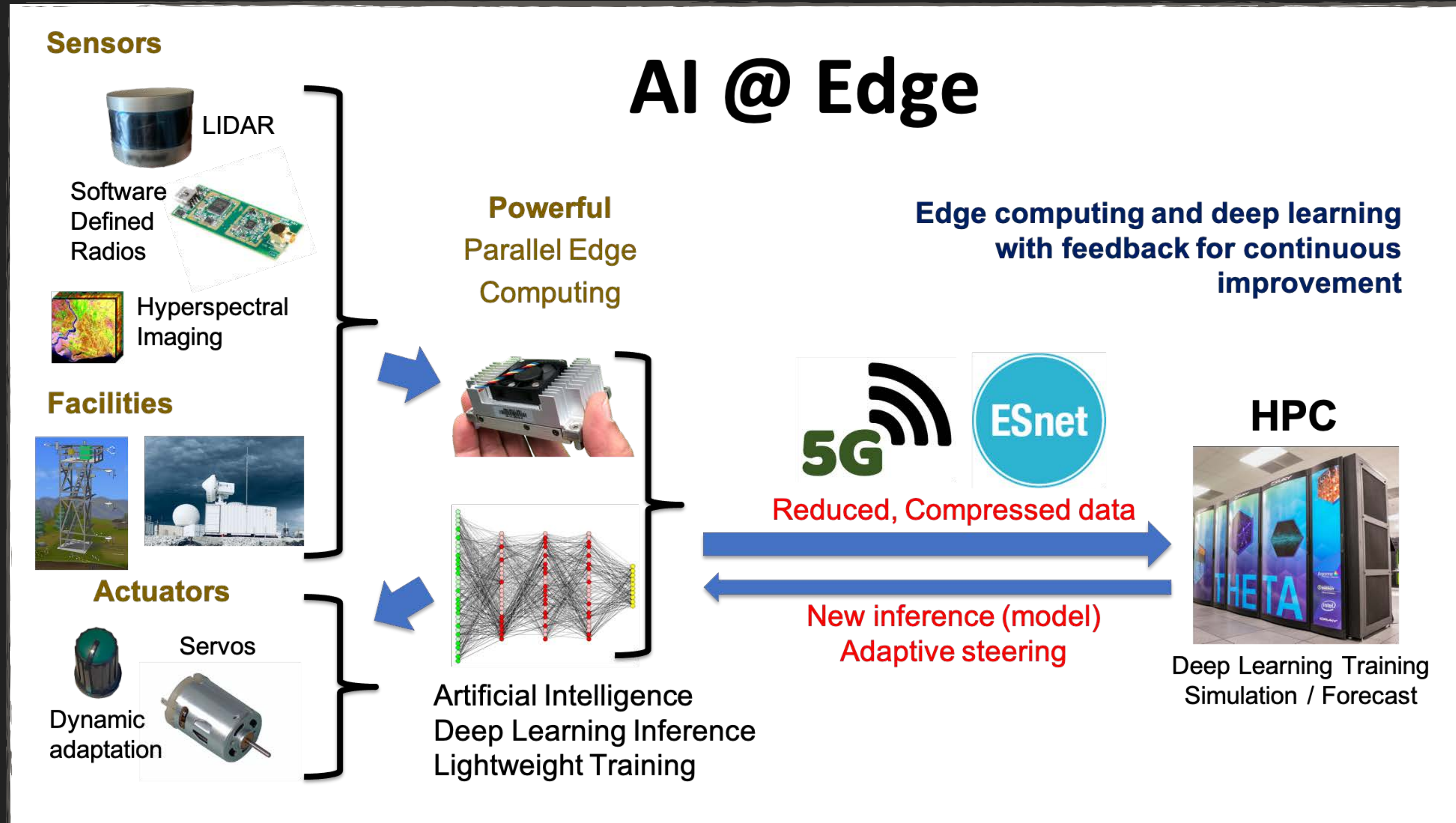
- Job 1: APS Basic Job, Jan. 15, 2016, 11:47 a.m., Complete.
- Job 2: APS Basic Job, Jan. 15, 2016, 11:41 a.m., In Progress (Processing...).
- Job 3: APS Basic Job, Jan. 15, 2016, 11:11 a.m., In Progress (Processing...).
- Job 4: HA\_tube5\_test2 Basic Job, Dec. 8, 2015, 6:14 p.m., Complete.
- Job 5: HA\_tube5\_test2 Basic Job, Dec. 8, 2015, 6:04 p.m., In Progress.
- Job 6: HA\_tube5\_test2 Basic Job, Dec. 8, 2015, 5:23 p.m., In Progress.
- Job 7: hacc\_160x160x160\_float\_little\_endian.bin Basic Job, Dec. 4, 2015, 3:39 p.m., In Progress.
- Job 8: hacc\_160x160x160\_float\_little\_endian.bin Basic Job, Dec. 4, 2015, 10:06 a.m., In Progress.

Argonne HPC portal interface showing job details and snapshots. The page includes a header with the Argonne logo and a 'Create a Job' button. Below the header, there are two sections: 'Videos' and 'Images'. The 'Videos' section shows a single video thumbnail. The 'Images' section shows a grid of 60 snapshots. On the right side, there is a sidebar with job details:

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
Download Files	

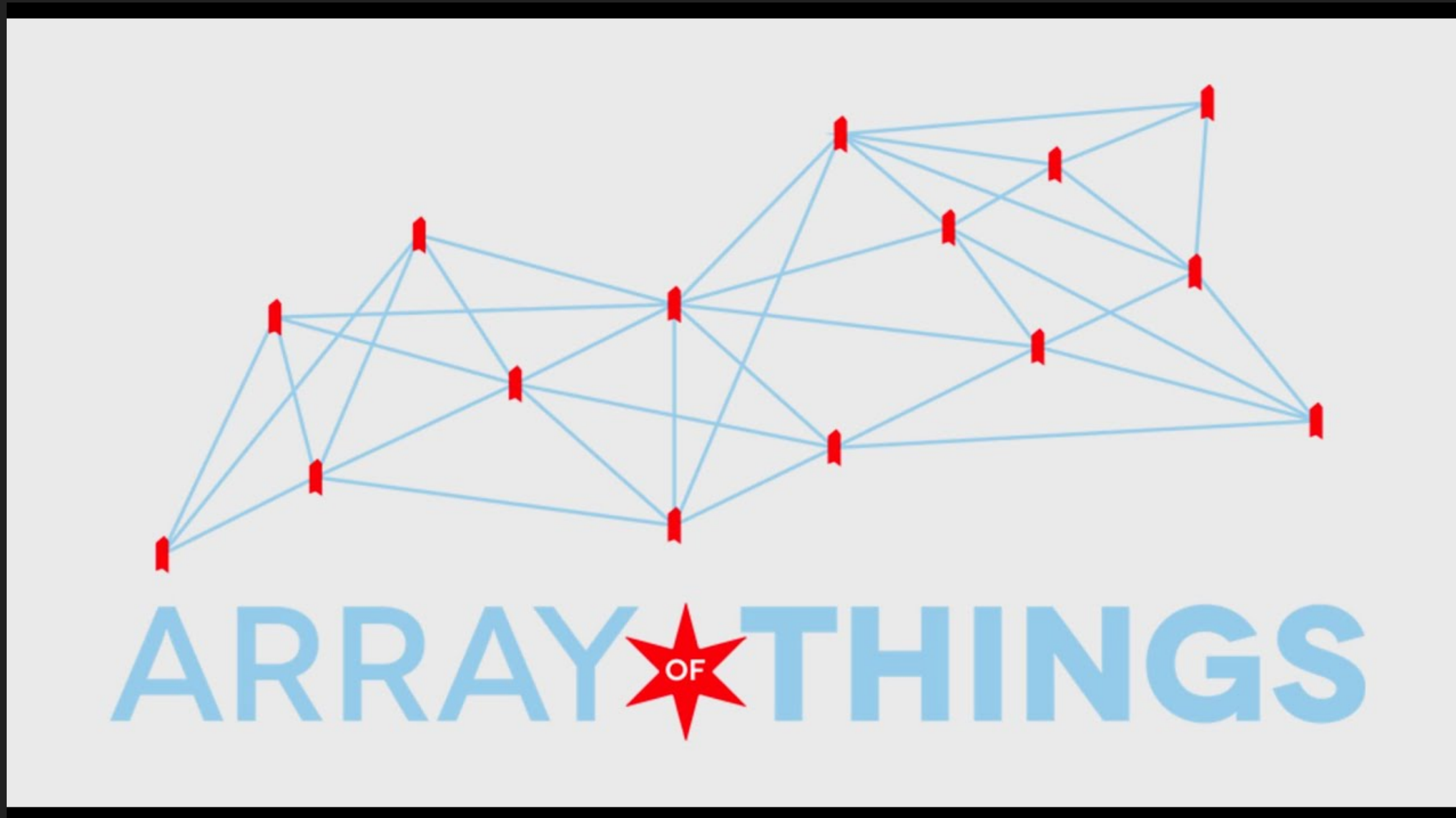


# INTERNET OF THINGS (COMPUTING CONTINUUM) [EDGE COMPUTING]



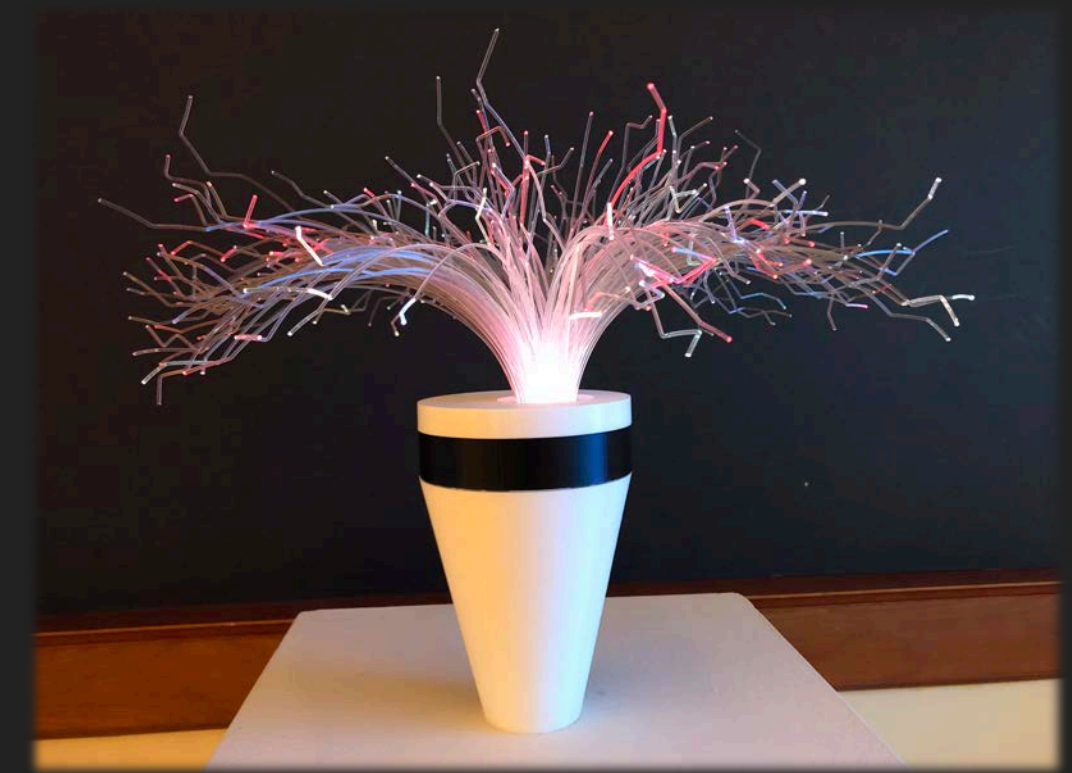
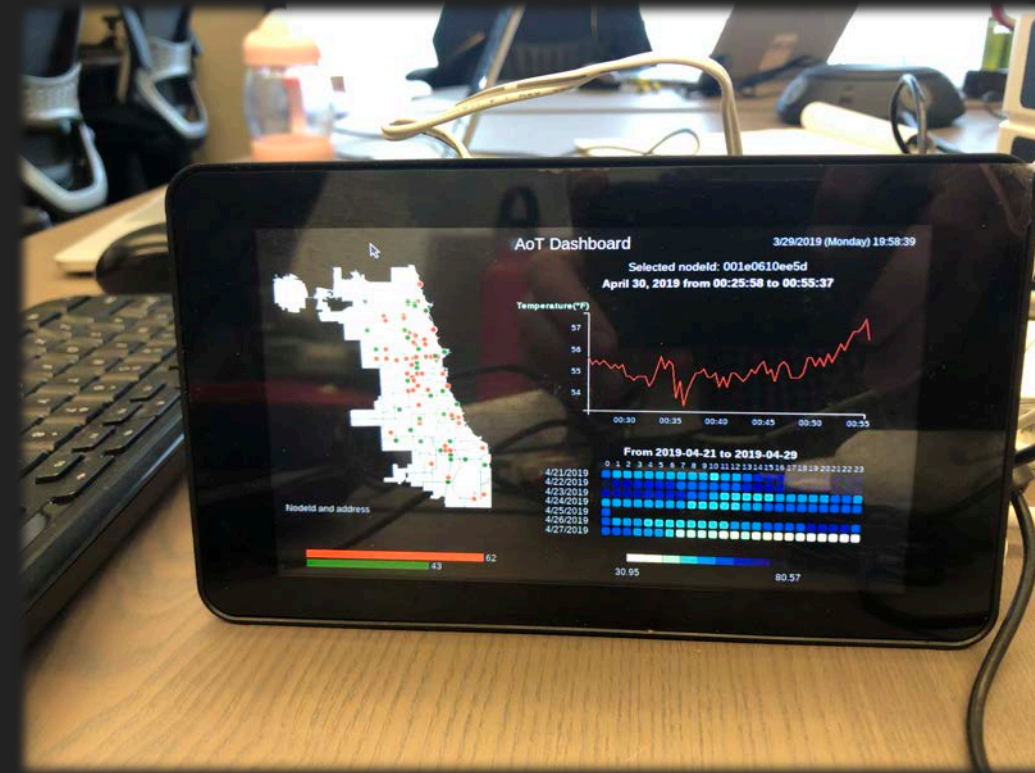


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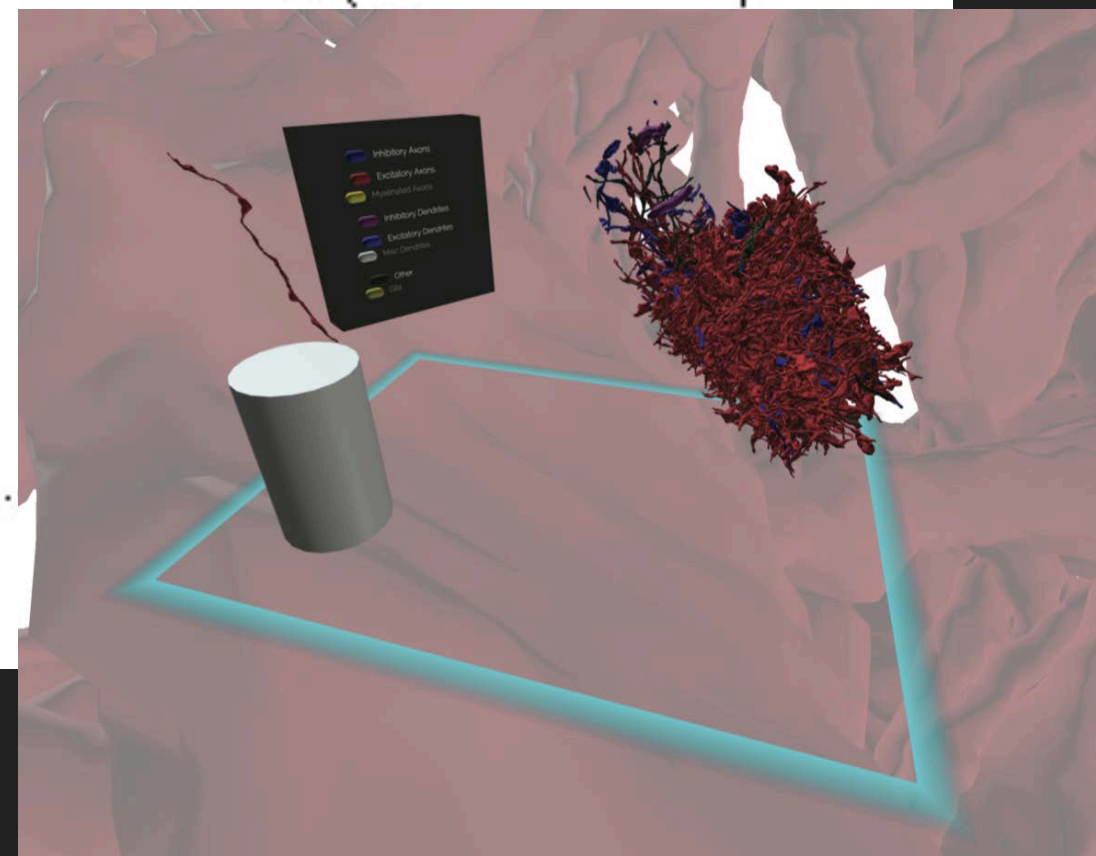
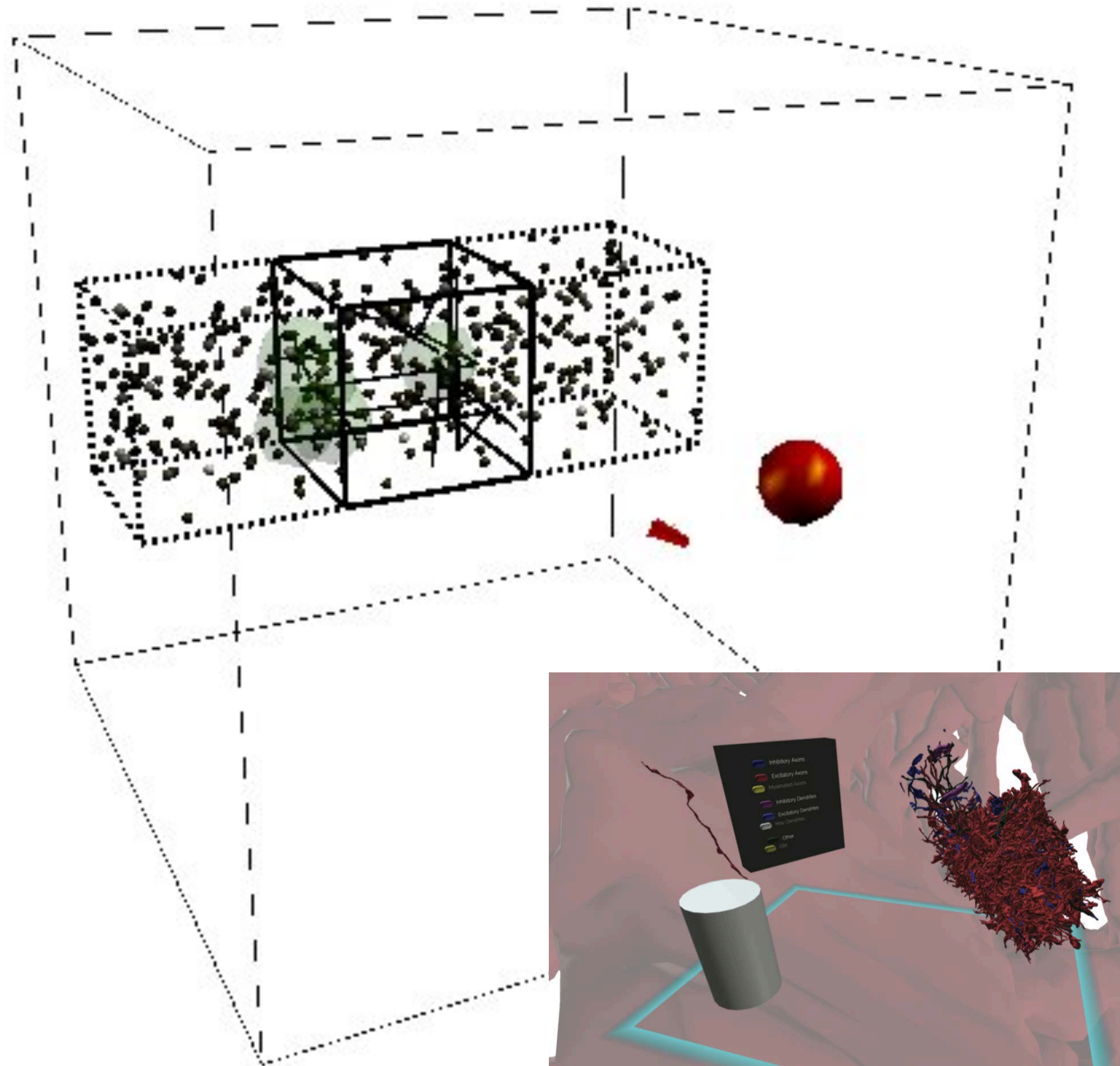


# INTERNET OF THINGS (COMPUTING CONTINUUM) [EDGE COMPUTING]





# VIRTUAL REALITY

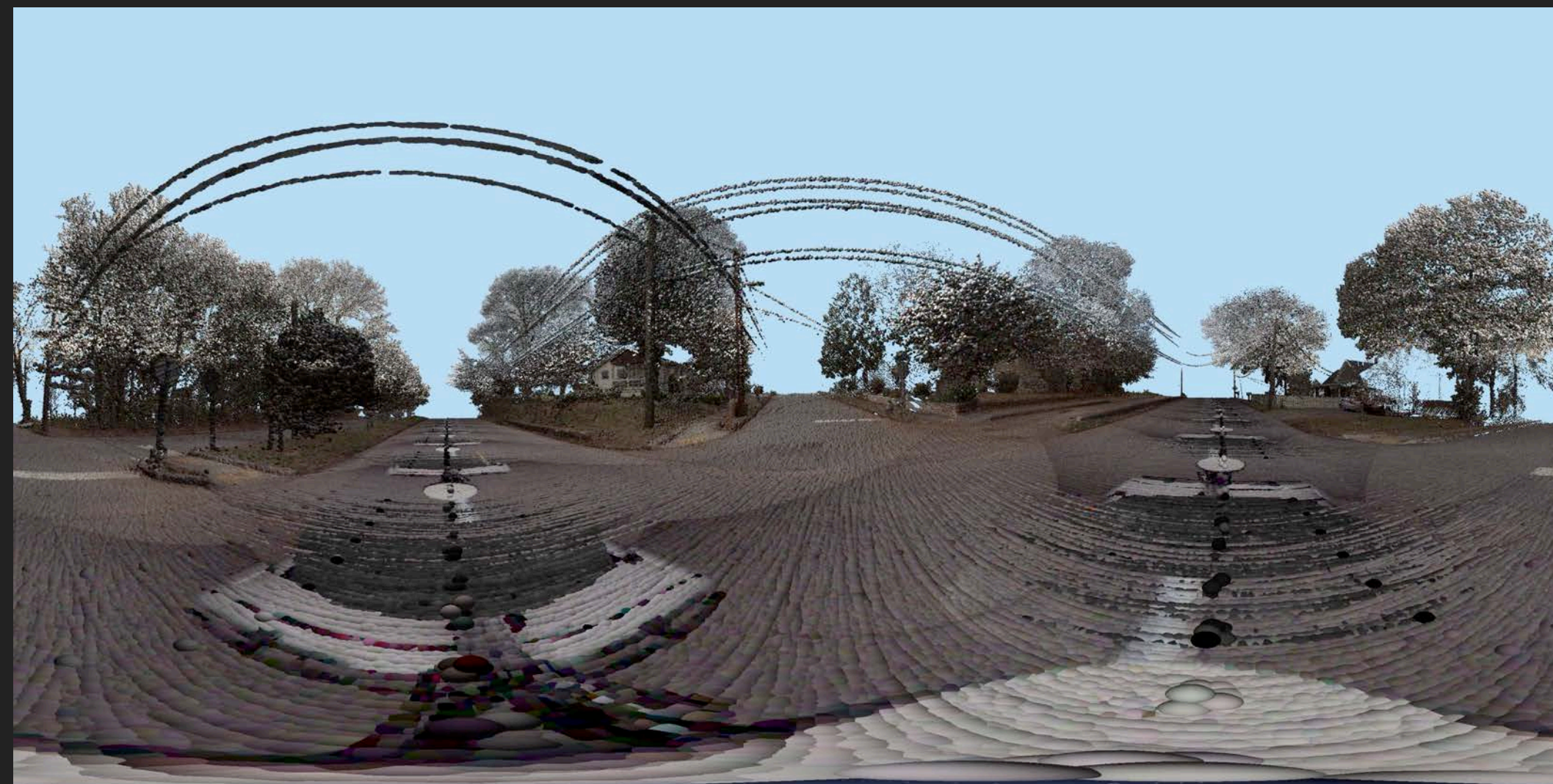
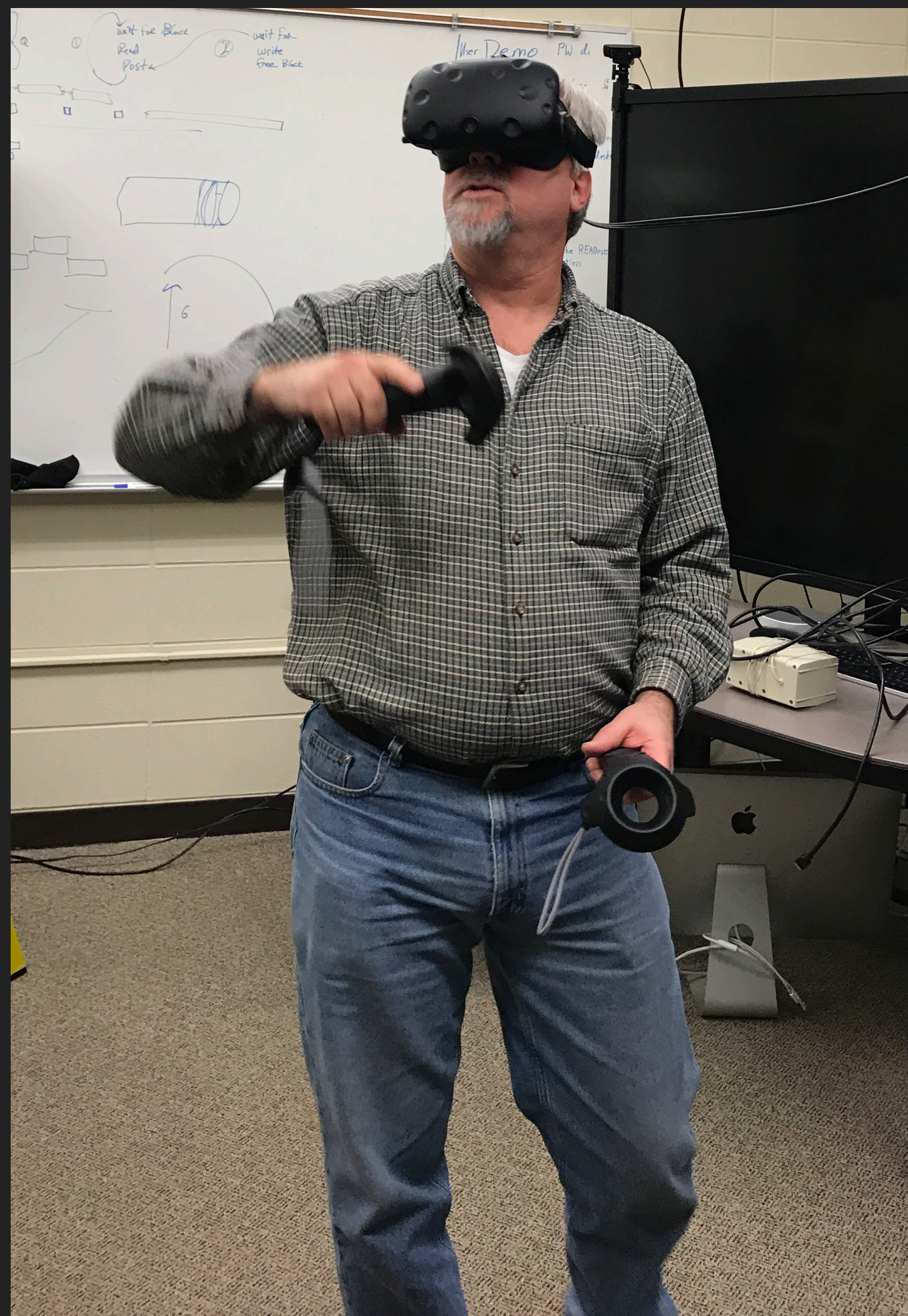


Use of **Virtual Reality** in Science

- ▶ 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.





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

35

**Sir Isaac Newton**

