

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 reflects the buildings.

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 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)

SUPERCOMPUTERS



Argonne's Aurora Supercomputer, 2022/23

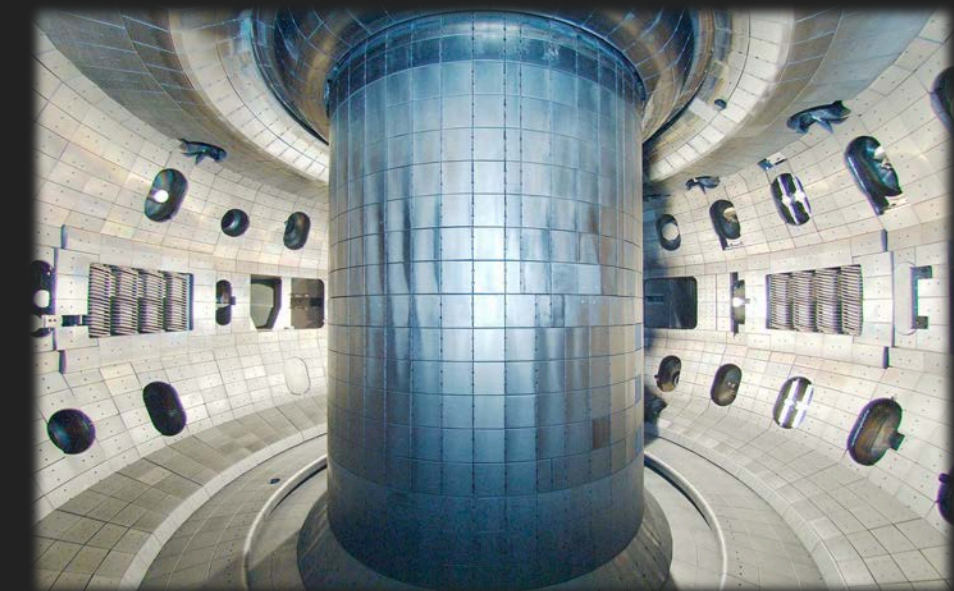
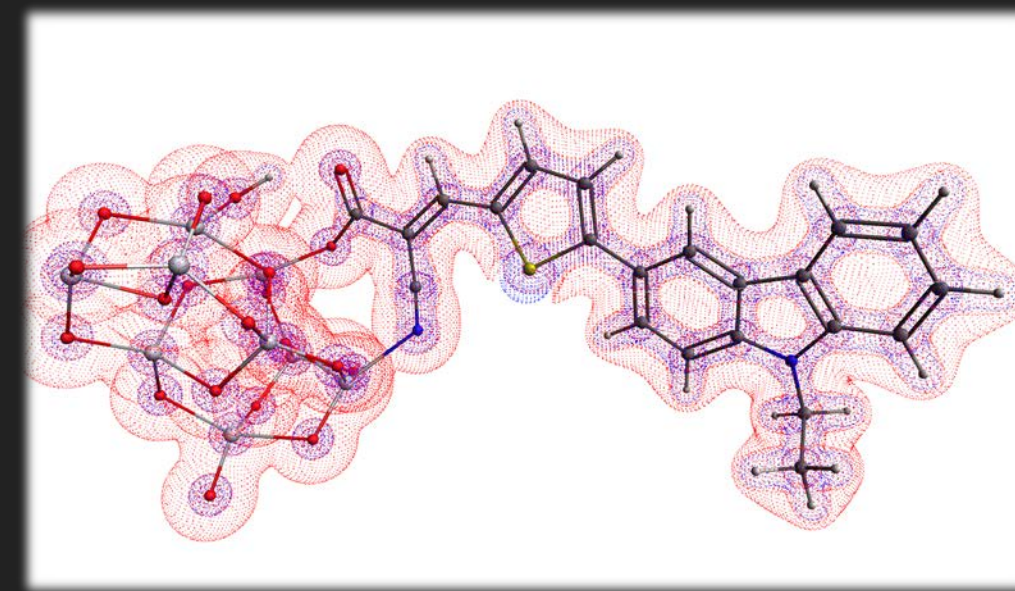
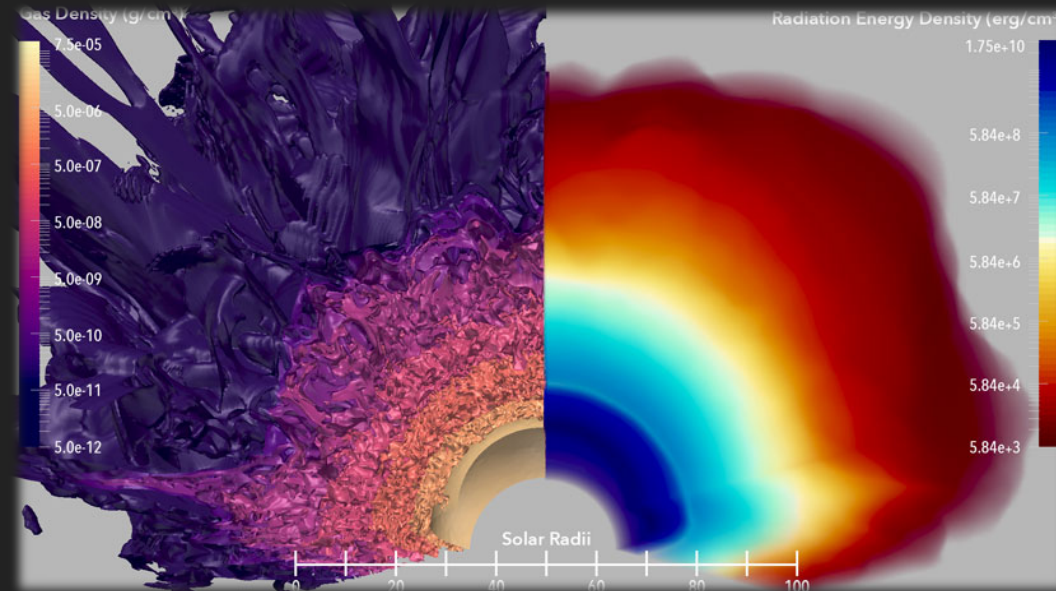
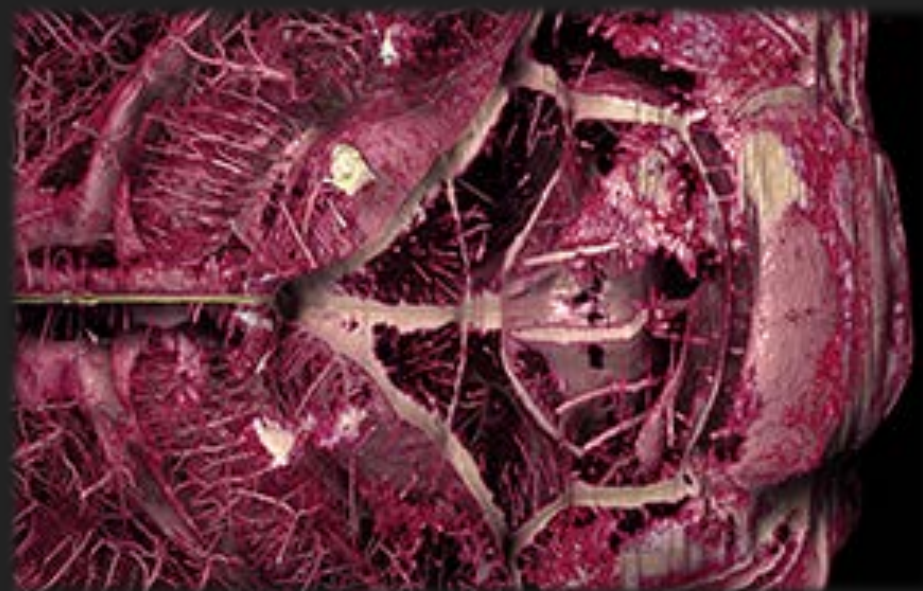
800megaFLOPS to ~2exaFLOPS

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

2,500,000,000x

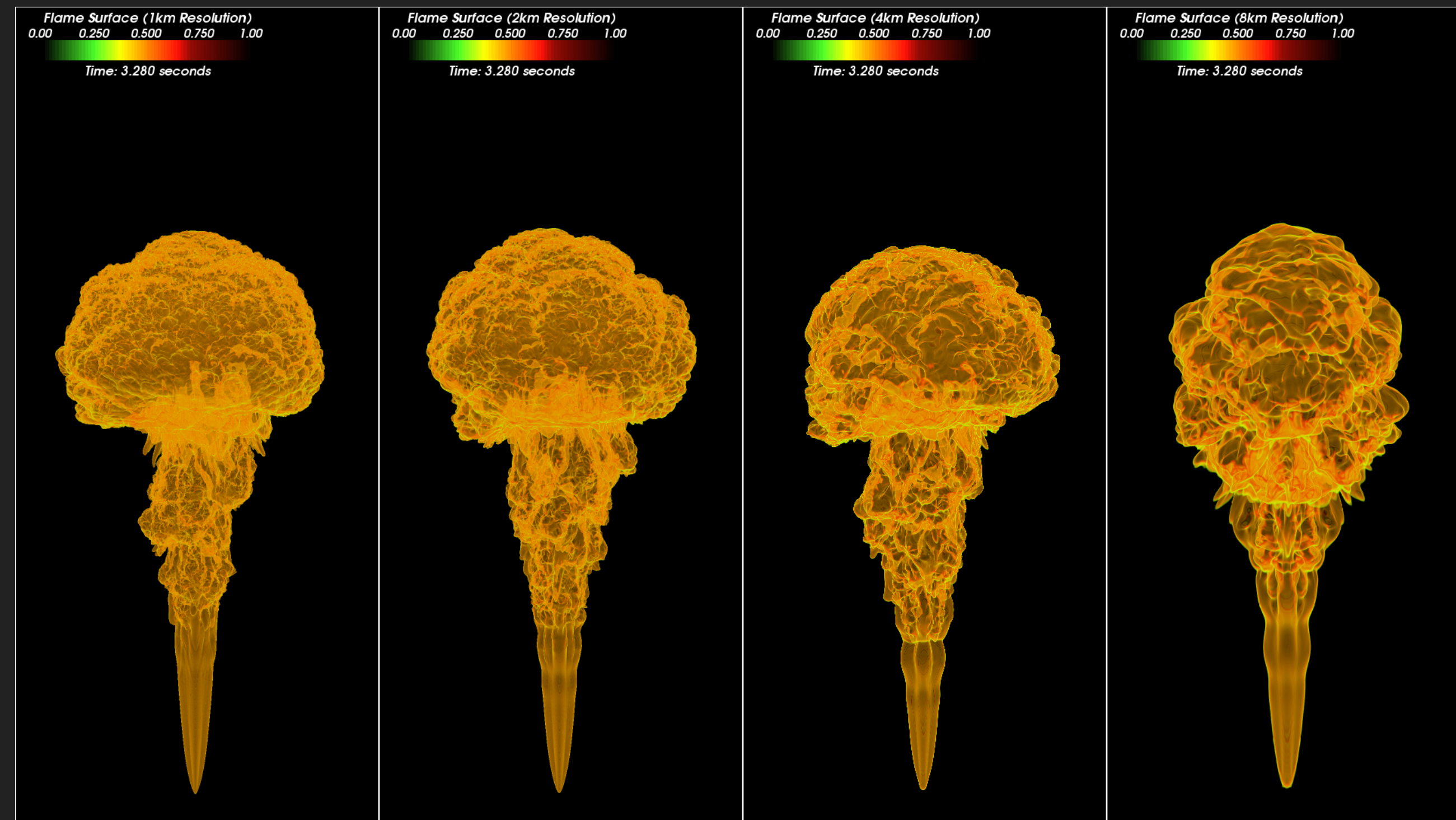
SO WHAT DOES ALL THAT COMPUTE POWER ENABLE?

- ▶ 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



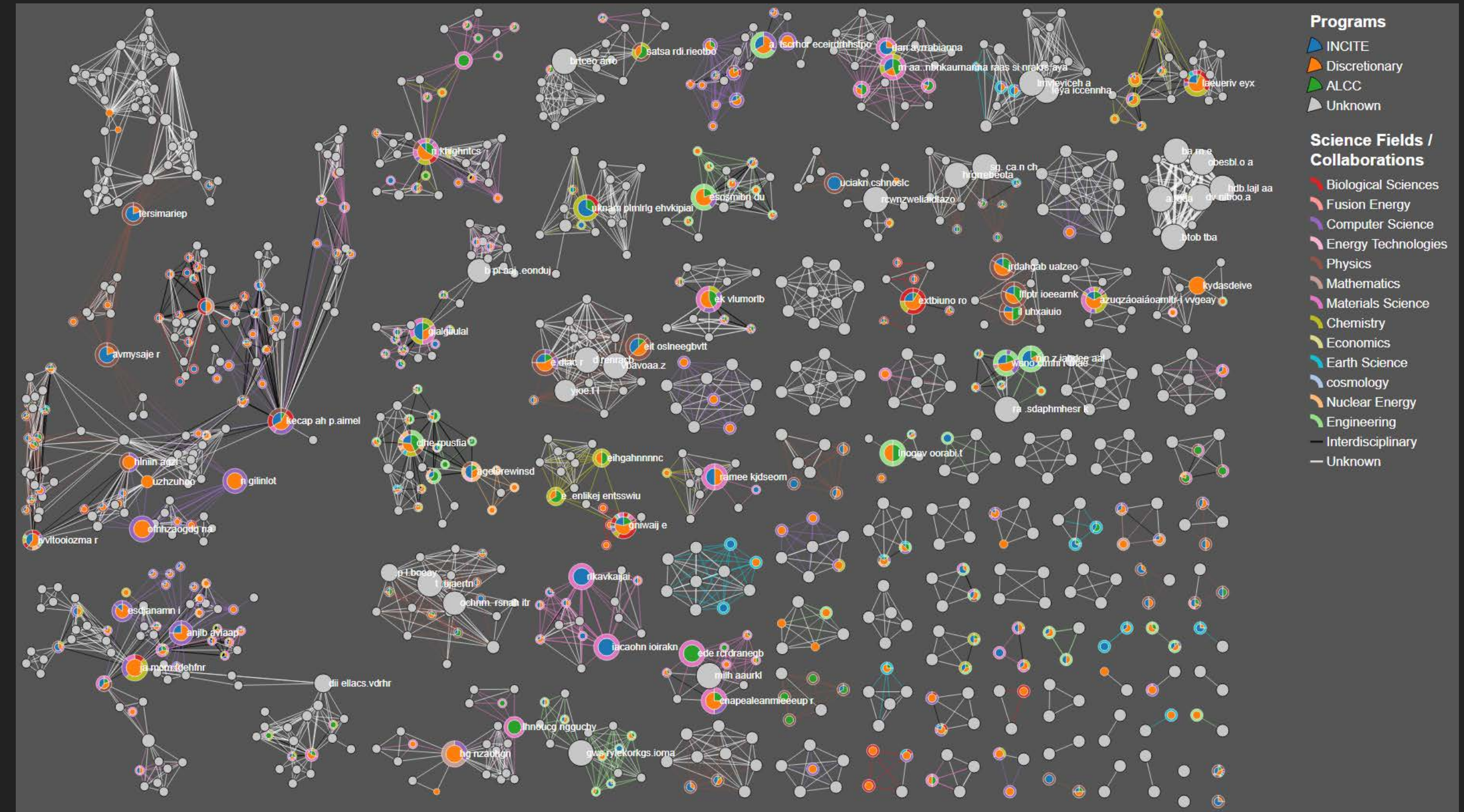
HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

- ▶ How do you translate theory into simulation?



HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

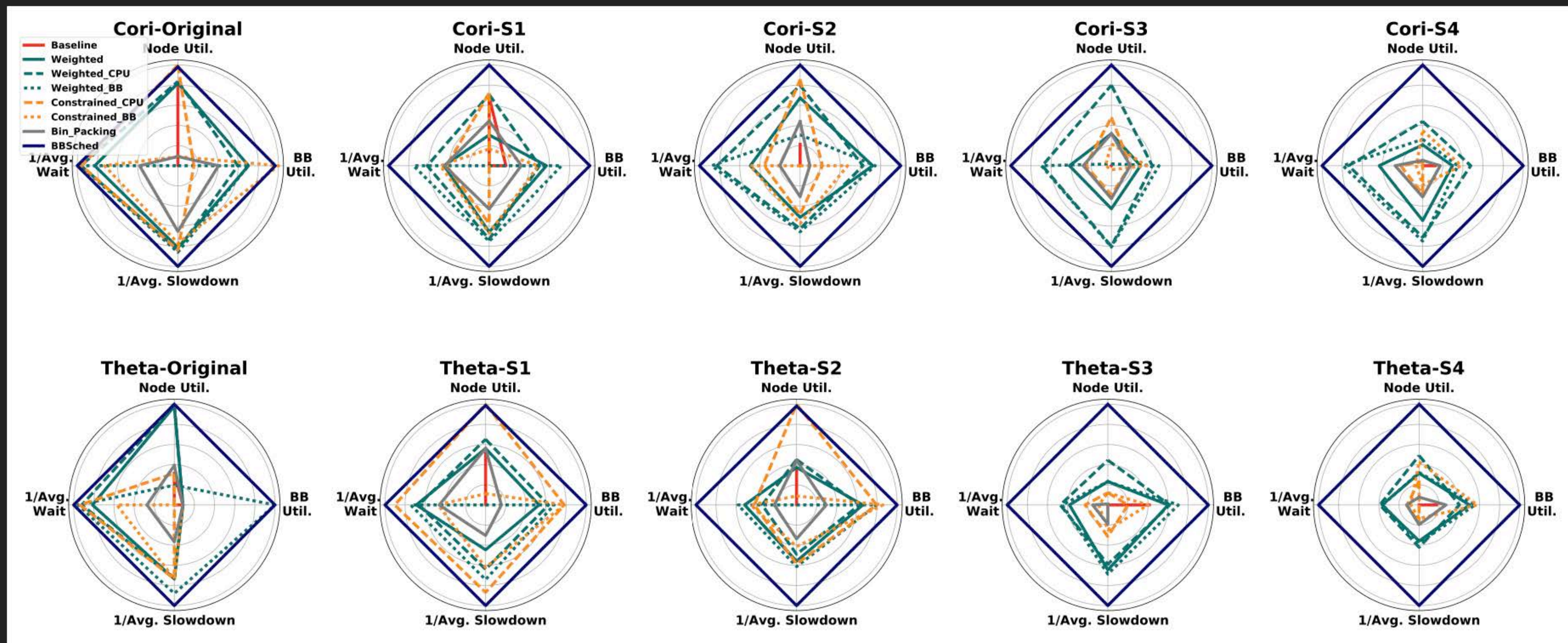
► How do you more efficiently operate a facility?



Bharat Kale, MS Thesis

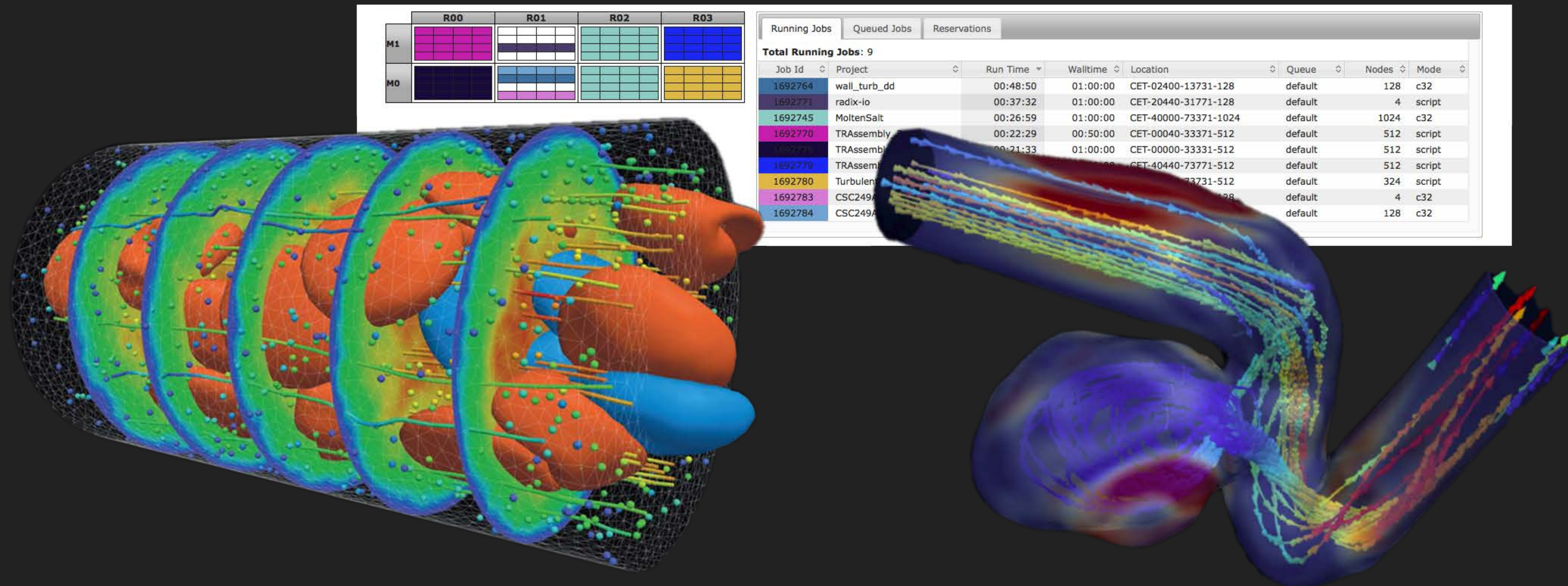
HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

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



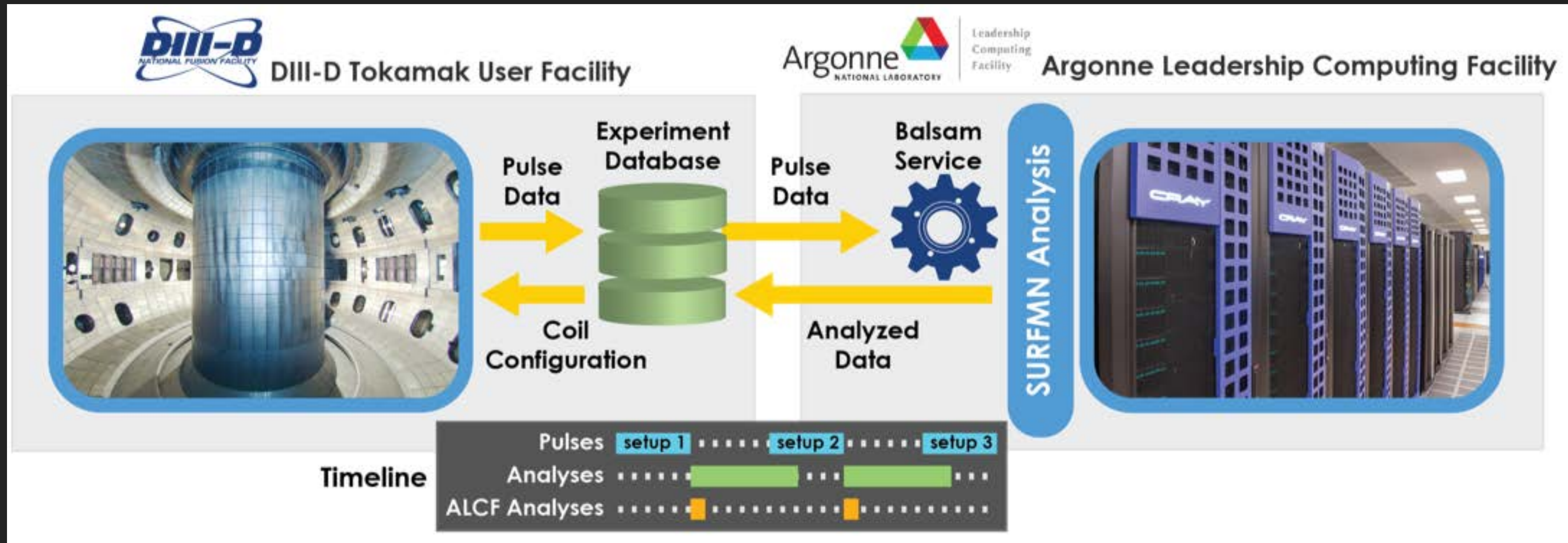
HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

- ▶ How do you evolve traditional HPC environment?



HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

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

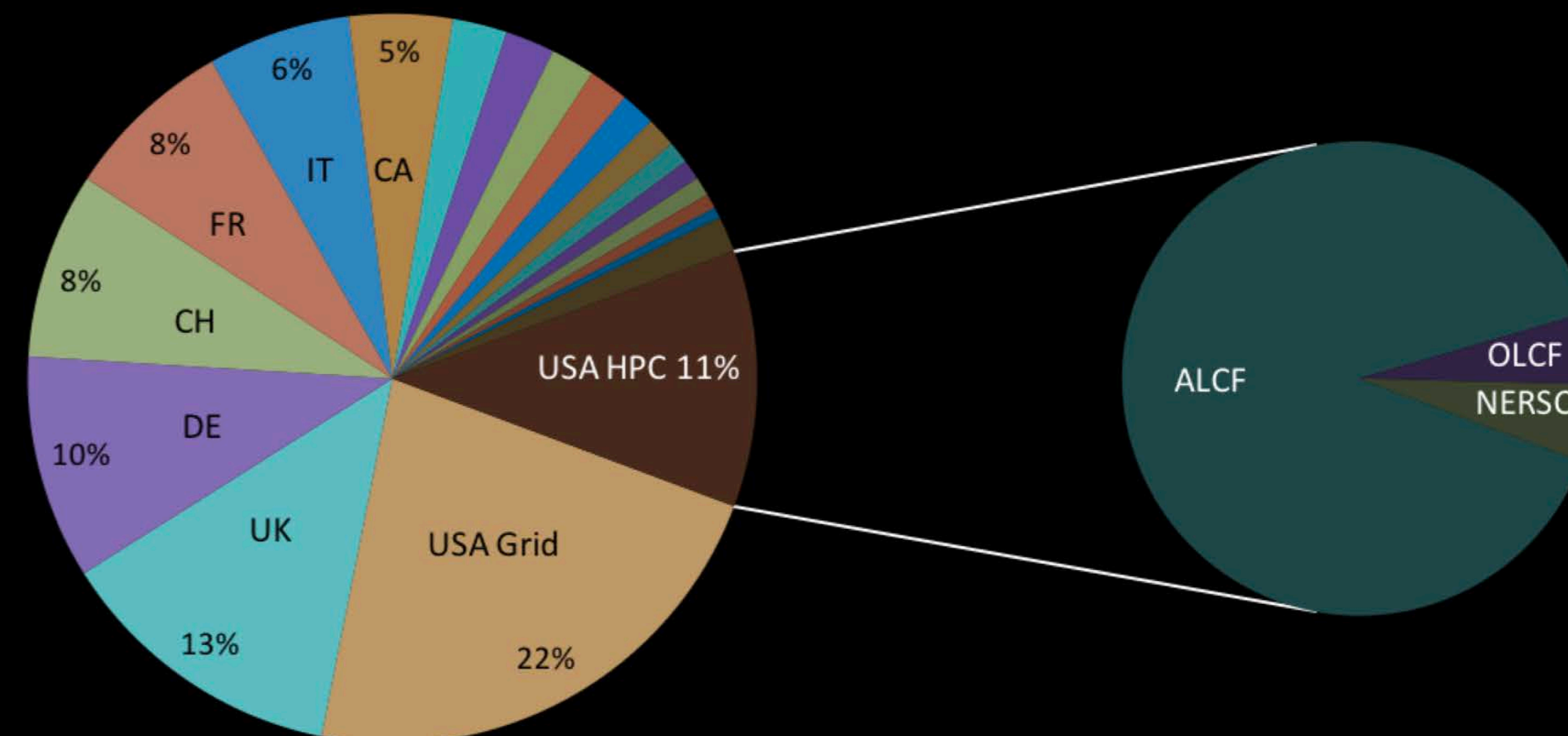


HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

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

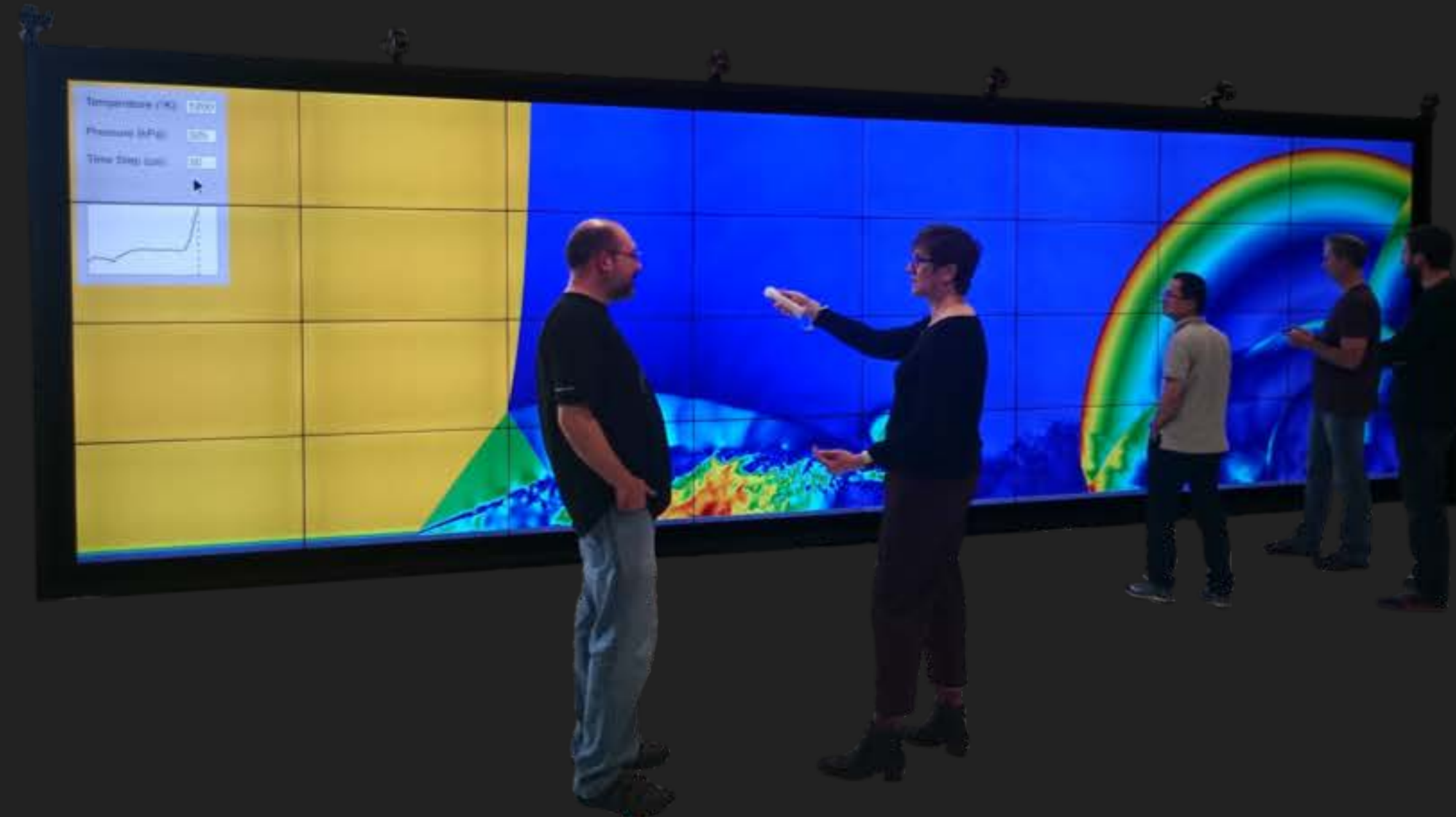
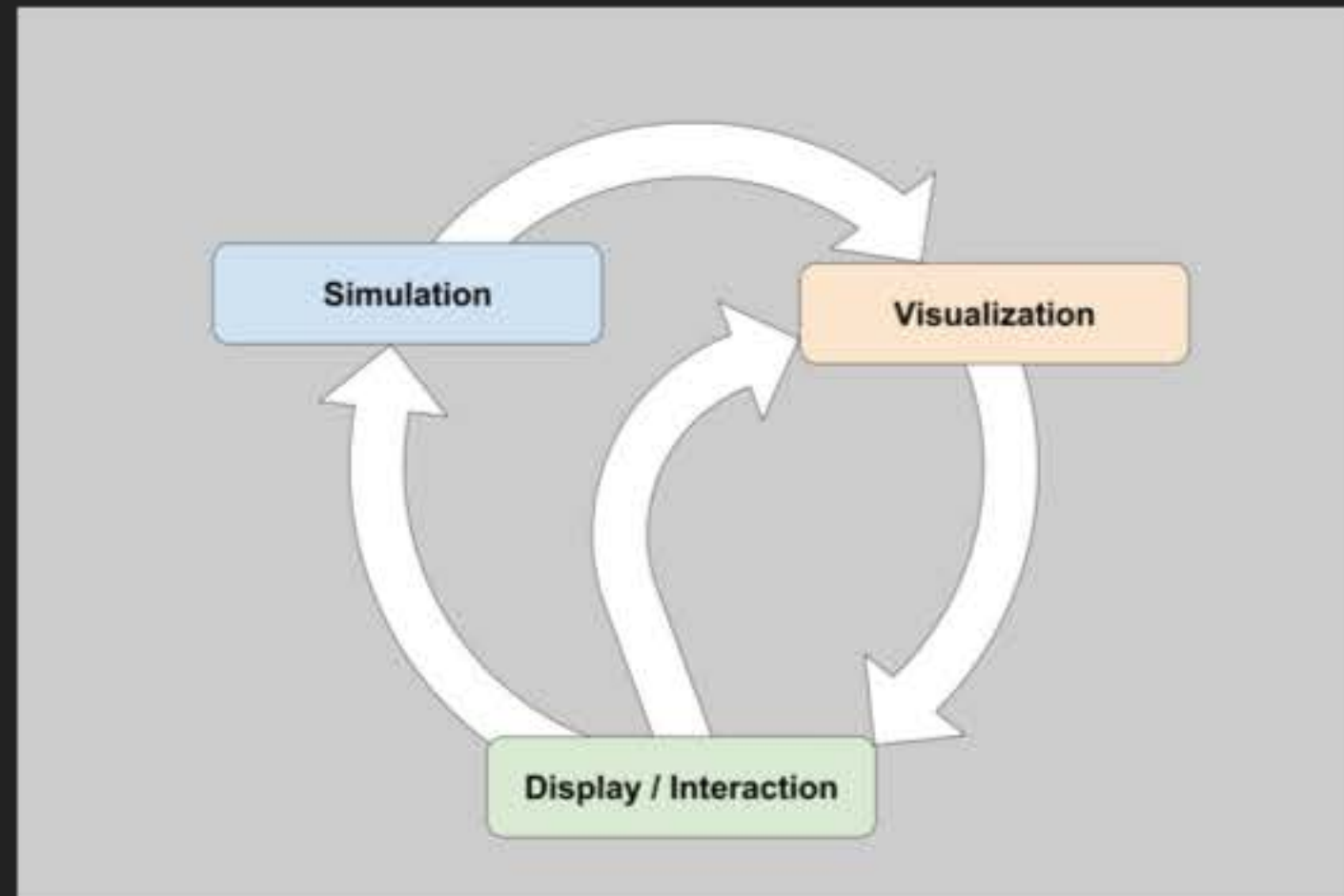
50% of the ATLAS papers based on 2015 data use the HPC-produced computing in a demonstrable manner

- 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.**



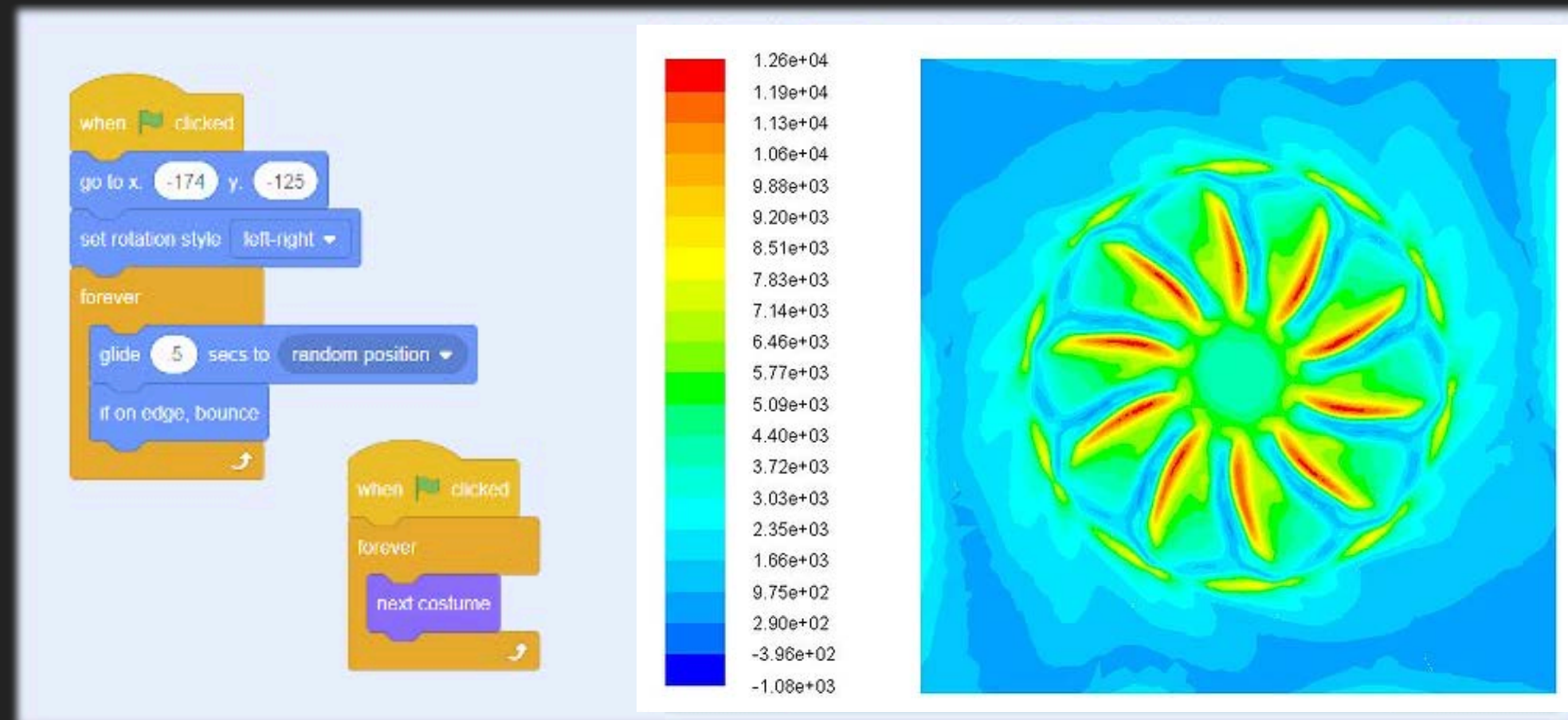
HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

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



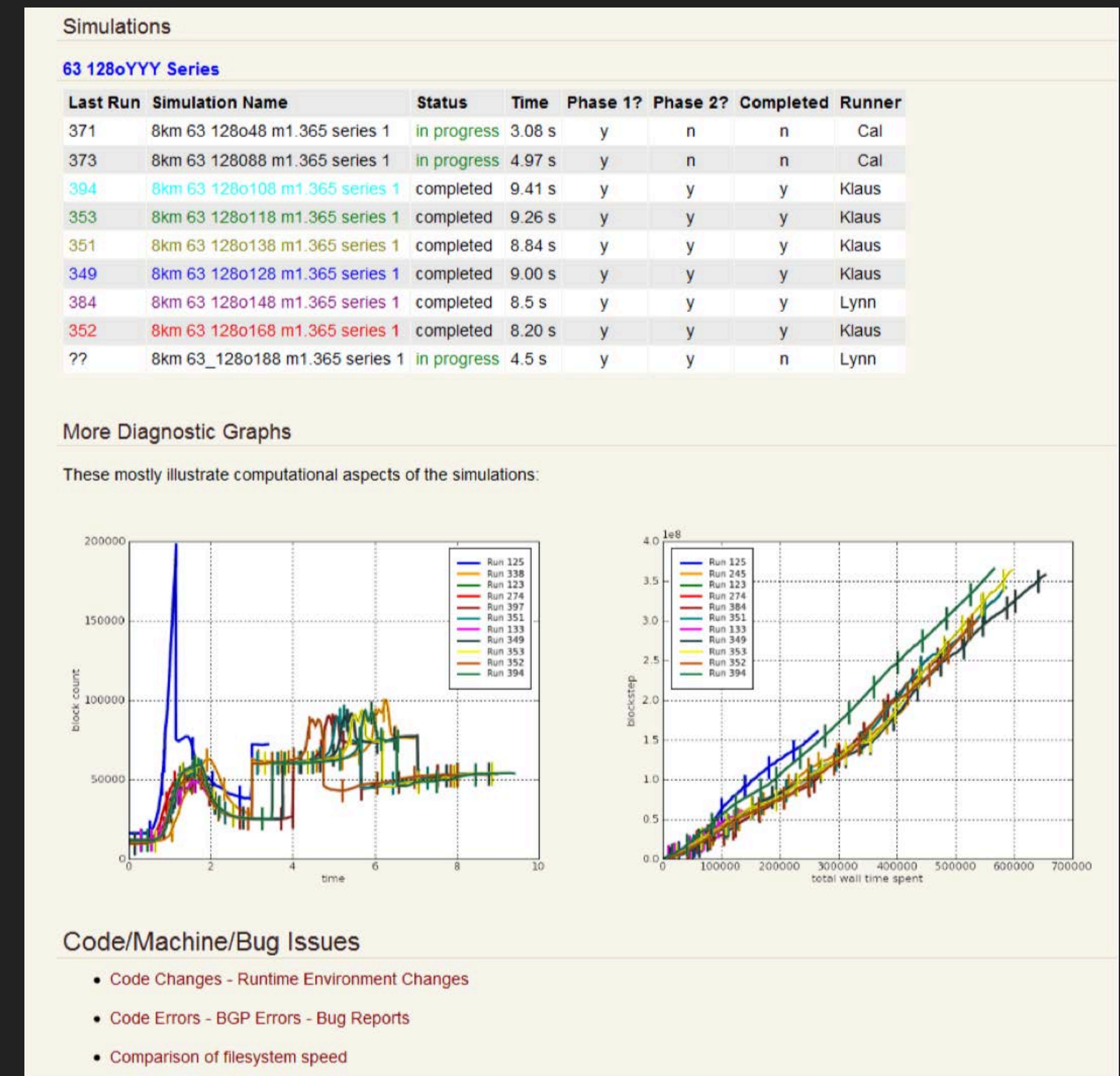
HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

- ▶ 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 three sequential screenshots of the Smaash/HACC web interface, illustrating the workflow from model selection to data analysis.

Left Screenshot: Model: MiraU / M019 / L2100
 This view shows a log-log plot of $\rho(k)$ versus k . The plot contains multiple colored lines representing different simulation parameters. A legend on the right lists parameters such as m019.pk.50, m019.pk.96, m019.pk.121, etc., up to m019.pk.499. Below the plot, there are sections for 'Runs' and 'Files'. The 'Runs' section shows a table with columns for Run, Model, Simulation, Date, and Size. The 'Files' section shows a single file: /homes/turam/dev/smaash/data/631/pk.png.

Run	Model	Simulation	Date	Size
run000	M019	MiraU	1 day, 16 hours ago	1
run001	M019	MiraU	1 day, 16 hours ago	1
run002	M019	MiraU	1 day, 16 hours ago	1

Middle Screenshot: Run: MiraU / M019 / run001 / L2100
 This view provides a detailed look at a specific run. It features a 'Timesteps' table and a 'Files' section. The 'Timesteps' table lists individual simulation steps with their respective dates and sizes. The 'Files' section shows three files: /homes/turam/dev/smaash/data/606/hacc_gpu_m019.log, /homes/turam/dev/smaash/data/607/hacc_gpu_m019.err, and /homes/turam/dev/smaash/data/608/indat.params.

Timestep	Run	Model	Simulation	Date	Size
496	run001	M019	MiraU	1 day, 16 hours ago	1
495	run001	M019	MiraU	1 day, 16 hours ago	1
494	run001	M019	MiraU	1 day, 16 hours ago	1
493	run001	M019	MiraU	1 day, 16 hours ago	1
492	run001	M019	MiraU	1 day, 16 hours ago	1
491	run001	M019	MiraU	1 day, 16 hours ago	1
490	run001	M019	MiraU	1 day, 16 hours ago	1
489	run001	M019	MiraU	1 day, 16 hours ago	1
488	run001	M019	MiraU	1 day, 16 hours ago	1
487	run001	M019	MiraU	1 day, 16 hours ago	1

Right Screenshot: Run: MiraU / M019 / run000 / L2100
 This view shows the parameter file for a run. A window titled 'Viewing /homes/turam/dev/smaash/data/589/indat.params' is open, displaying the raw parameter text. The parameters include cosmological constants like HUBBLE, OMEGA_CDM, and OMEGA_NU, as well as simulation-specific settings like N_DE, WA_DE, and N_EFF_MASSLESS.

```

#####
# Header version information
#####
HACC_HEADER_VERSION 1.0.0

#####
# Cosmological Parameters
# Length scales are measured in Mpc/h
# OMEGA_CDM and OMEGA_NU given for Omega_cdm and Omega_nu (no $h^2$)
# DEUT=Omegab+h^2
# HUBBLE: Hubble constant/100 km/s/Mpc
# SS8: target value for sigma_8
# NS: index of the primordial power spectrum
# W_DE: constant dark energy equation of state
# Currently flat universe only
#####
OMEGA_CDM 0.145884
DEUT 0.02217382692
OMEGA_NU 0.00686393
HUBBLE 0.825136069
SS8 0.854654384
NS 1.026482126
W_DE -0.981272302
WA_DE -0.339335368548398
T_CMB 2.726
N_EFF_MASSLESS 0.0
N_EFF_MASSIVE 3.04

#####
# Initializer Set-up and read-ins
# ZIN: Starting redshift
# USE_WHITE_NOISE_INIT: YES: real space, NO: k space
# Input type: INIT|RECORD|BLOCK|COSMO|RESTART
# INIT: generates internal initial conditions, rest if for read-ins
# distrib. type: ROUND_ROBIN|ALL_TO_ALL|ONE_TO_ONE|restart_step
# (ignored if INPUT_TYPE is INIT)
# ROUND_ROBIN indicates particles must be looked at by all processors
# ONE_TO_ONE indicates that particles physically reside on matching processor
# ALL_TO_ALL improved ROUND_ROBIN
# For restart: specify time step and modify INPUT_BASE_NAME
# TRANS: Transfer function: Read in CAMB file (specify name in INPUT_BASE_NAME)
# or internal TF (KH, HS, PD, BBKS)
#####
Z_IN 200.0
USE_WHITE_NOISE_INIT YES
TRANS CMB
INPUT_BASE_NAME cmbM019.tf
INPUT_TYPE INIT
DISTRIBUTE_TYPE LAST
MAX_MINUTES 700
    
```


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 top bar includes the Argonne logo, a 'Create a Job' button, and the user name 'Tom'. The main content area displays four visualization options:

- 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.

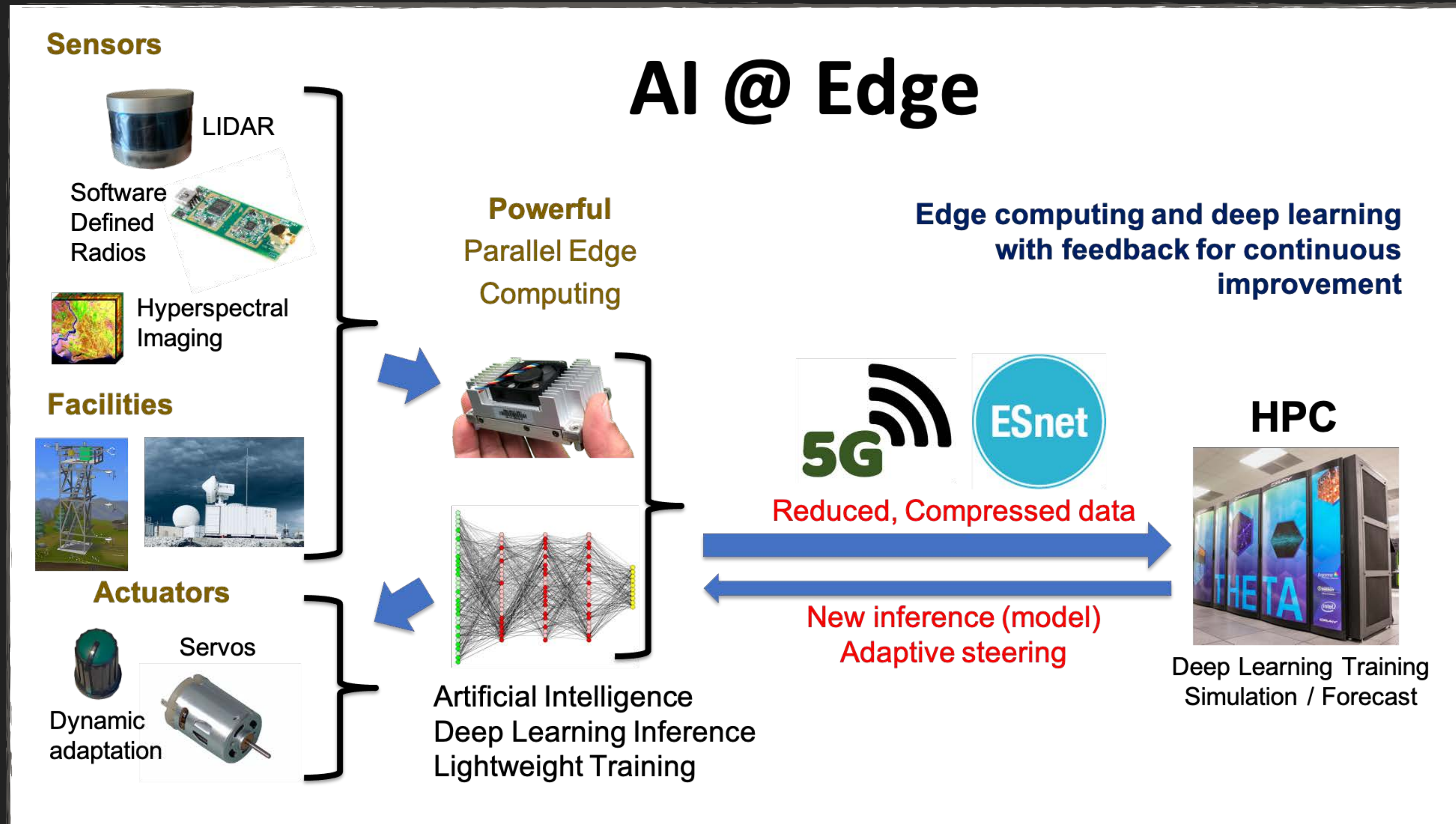
Argonne HPC portal interface showing job status. The top bar includes the Argonne logo, a 'Create a Job' button, and the user name 'Tom'. The main content area displays a grid of job status cards:

- Two 'Complete' jobs (APS Basic Job) with completion dates: Jan. 15, 2016, 11:47 a.m. and Jan. 15, 2016, 11:41 a.m.
- Two 'In Progress' jobs (APS Basic Job) with completion dates: Jan. 15, 2016, 11:11 a.m. and Jan. 15, 2016, 11:41 a.m.
- Two 'Complete' jobs (HA_tube5_test2 Basic Job) with completion dates: Dec. 8, 2015, 6:14 p.m. and Dec. 8, 2015, 6:14 p.m.
- Two 'In Progress' jobs (HA_tube5_test2 Basic Job) with completion dates: Dec. 8, 2015, 6:04 p.m. and Dec. 8, 2015, 5:23 p.m.
- Two 'In Progress' jobs (hacc_160x160x160_float_little_endian.bin Basic Job) with completion dates: Dec. 4, 2015, 3:39 p.m. and Dec. 4, 2015, 10:06 a.m.

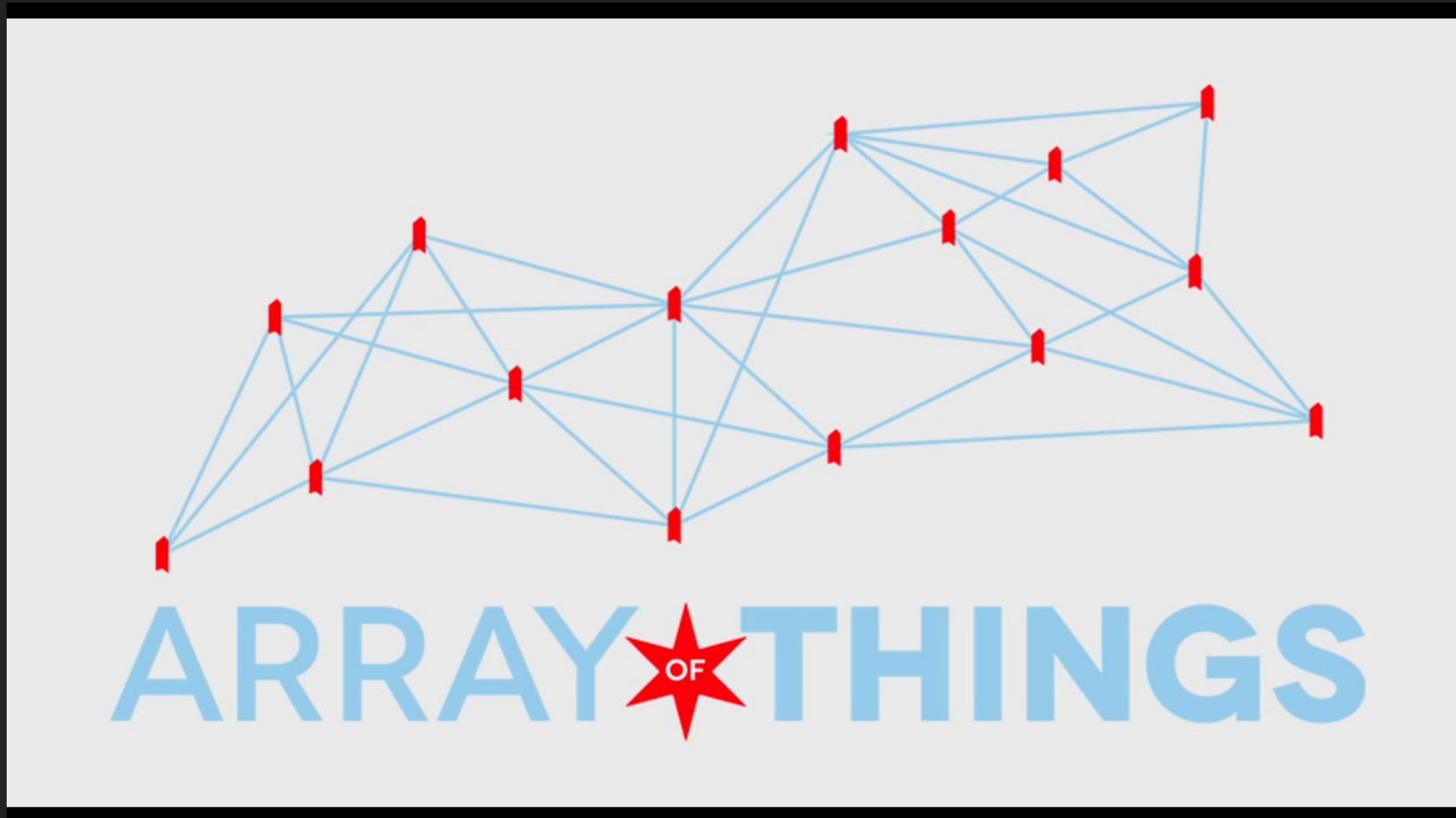
Argonne HPC portal interface showing job details and snapshots. The top bar includes the Argonne logo, a 'Create a Job' button, and the user name 'Tom'. The main content area displays:

- Videos**: A single video thumbnail.
- Images**: A grid of 60 snapshots.
- 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: [Download icon]

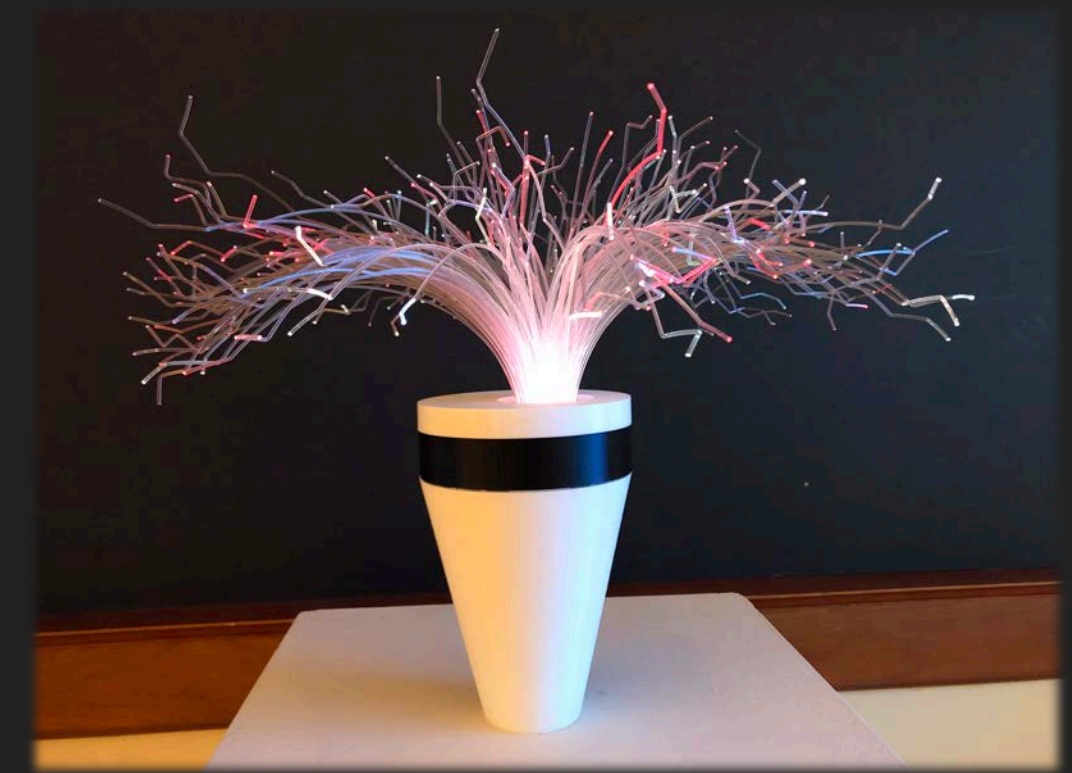
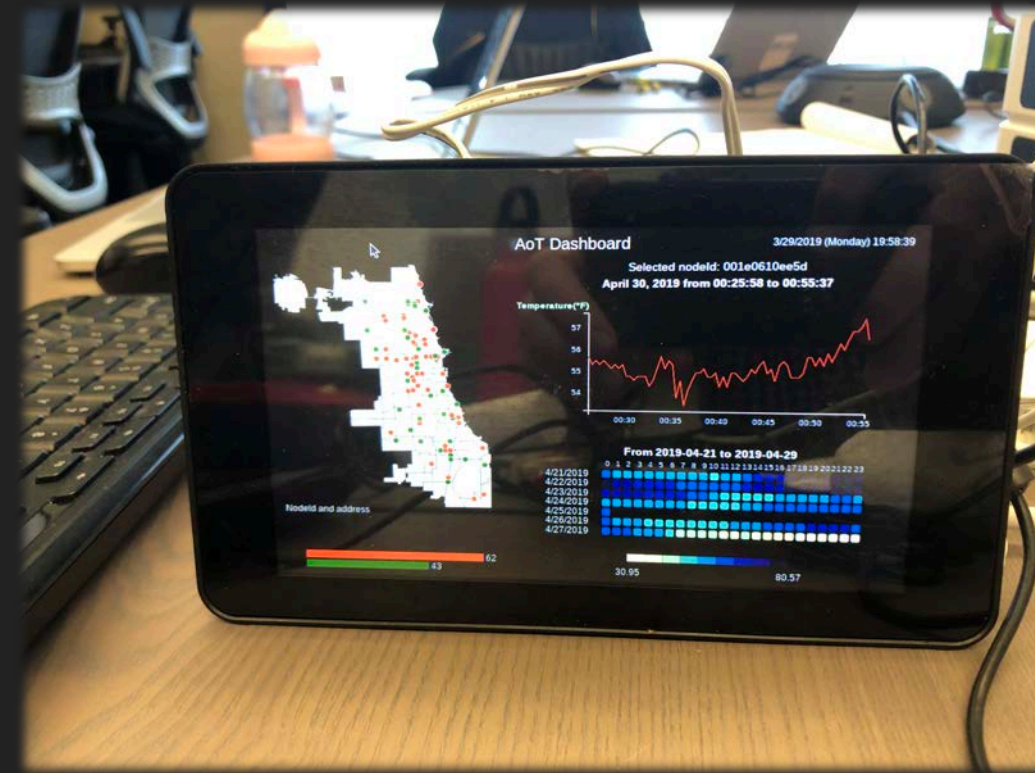
INTERNET OF THINGS (COMPUTING CONTINUUM) [EDGE COMPUTING]



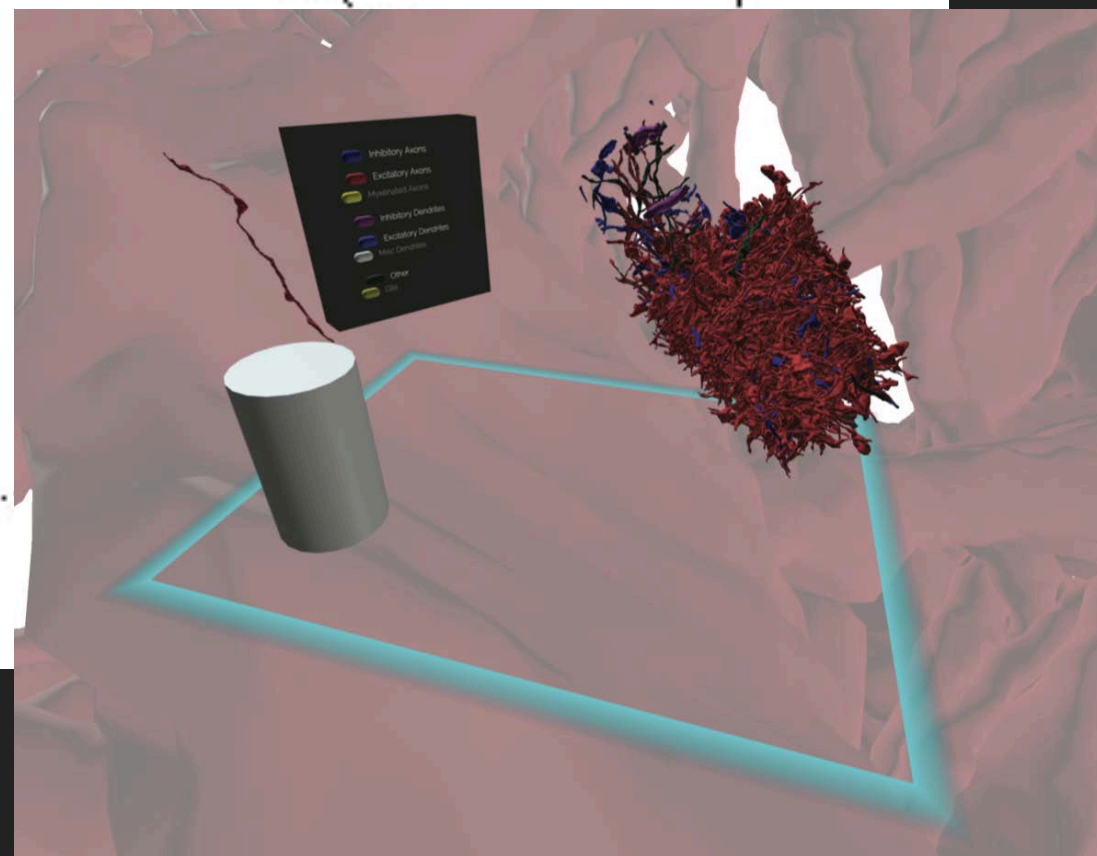
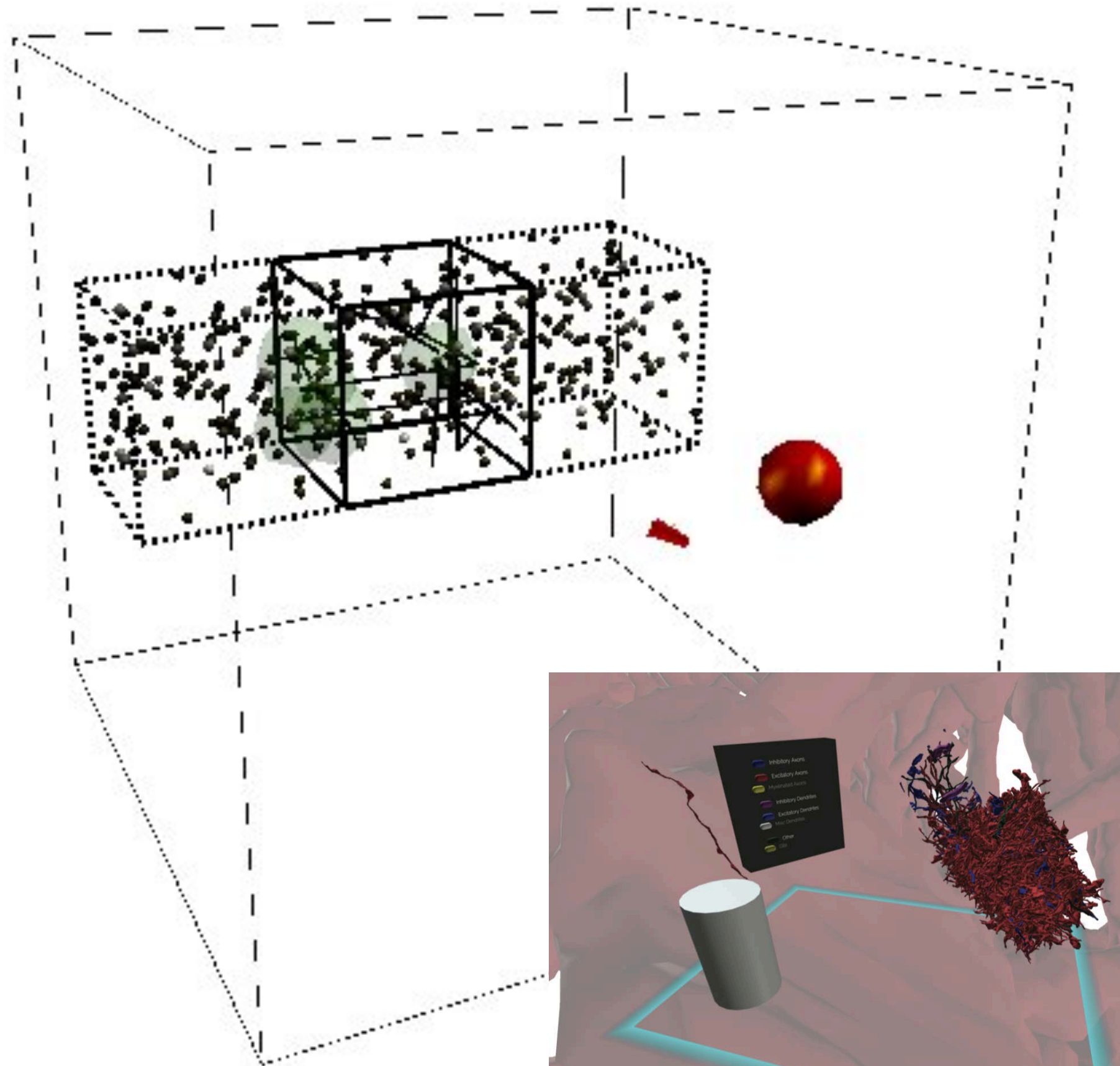
INTERNET OF THINGS (COMPUTING CONTINUUM) [EDGE COMPUTING]



INTERNET OF THINGS (COMPUTING CONTINUUM) [EDGE COMPUTING]



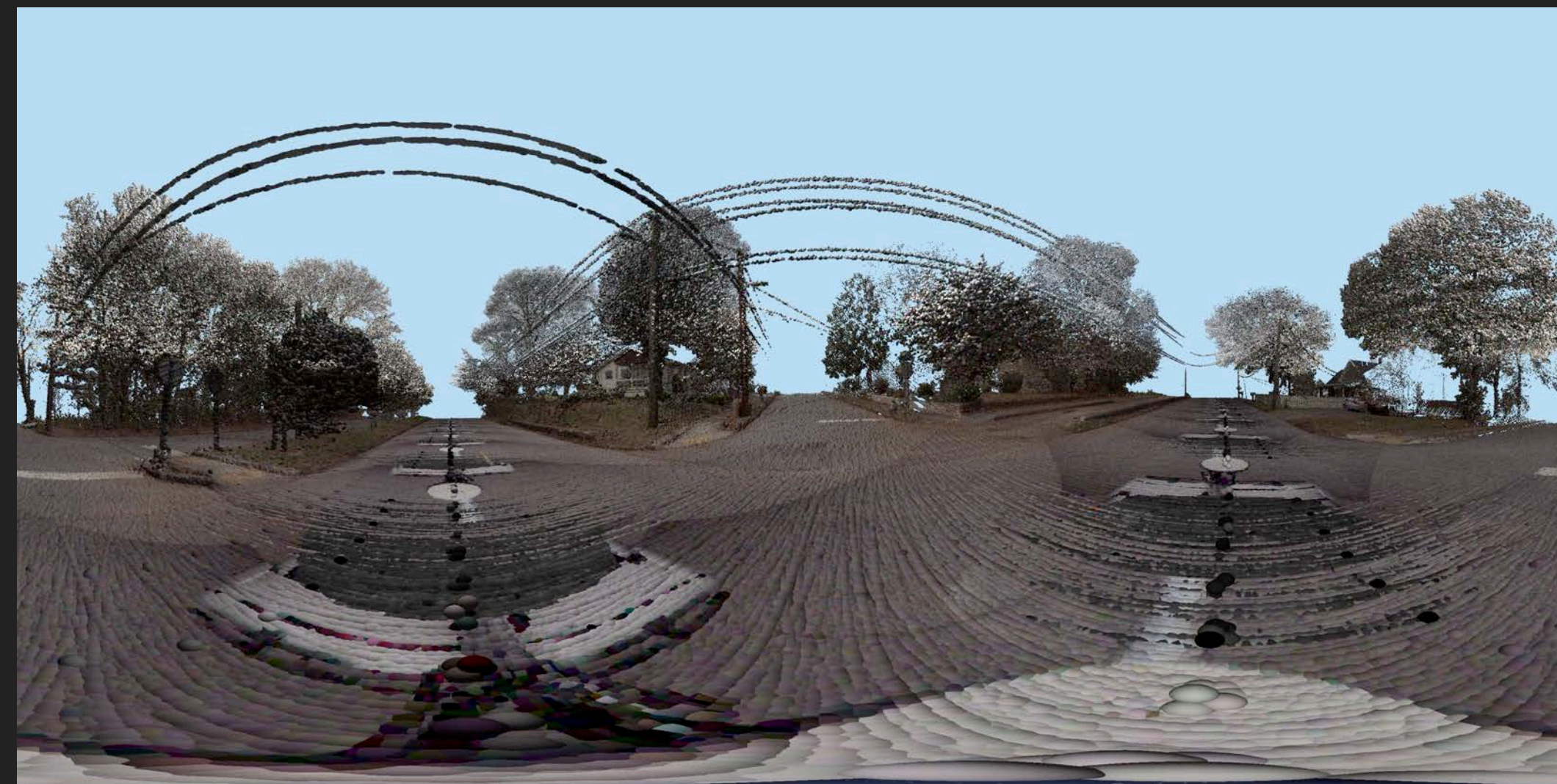
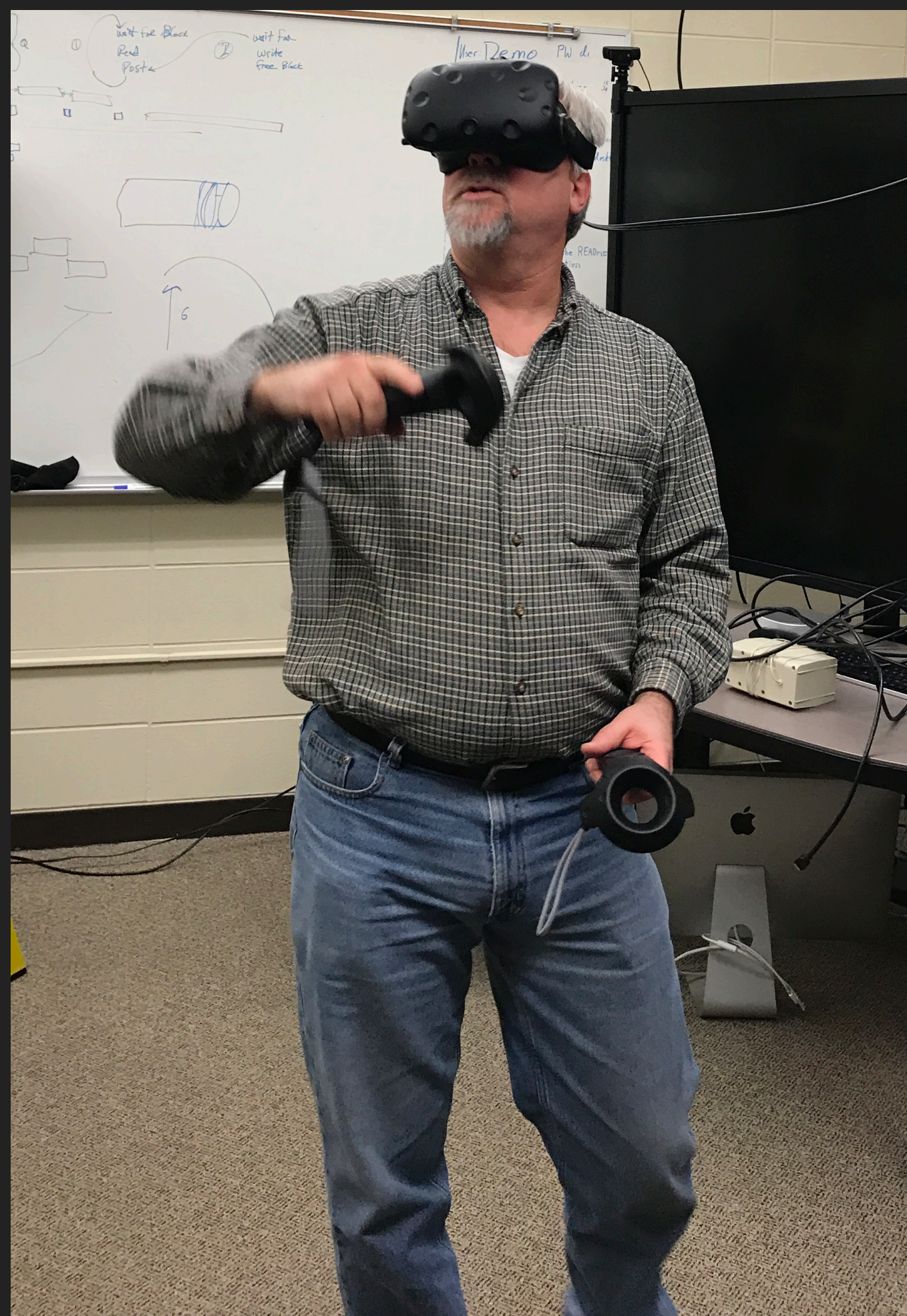
VIRTUAL REALITY



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

