

November 16, 2021

# Big Ideas

WITH MICHAEL E. PAPKA

DATA, DEVICES AND INTERACTION LABORATORY



Northern Illinois University



## 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
  - ▶ 1 PhD (Information Visualization)
  - ▶ 8 Undergraduates (IoT, VR, and HPC)

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**We are looking  
to hire MS and  
PhD students!!!!**





# 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**

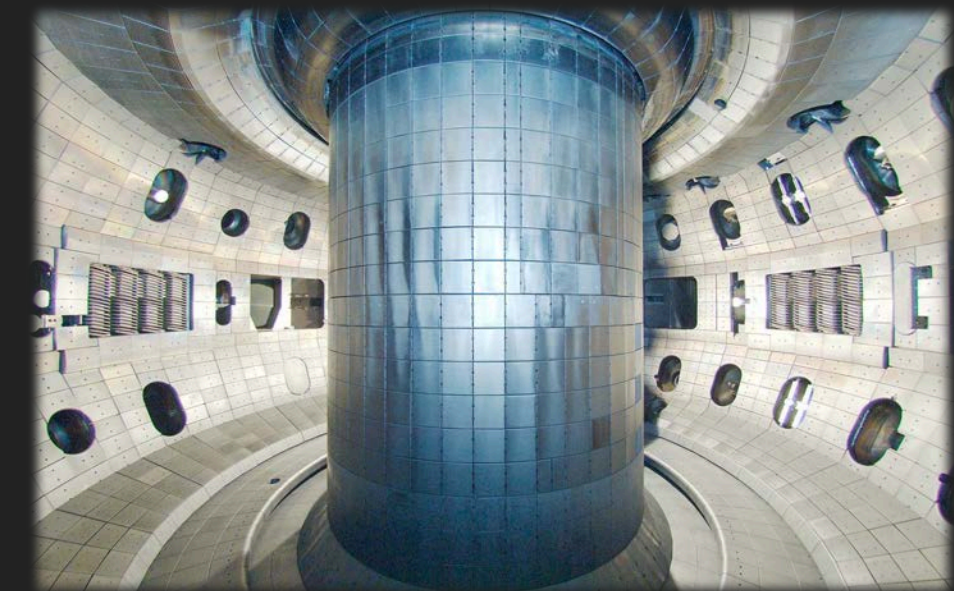
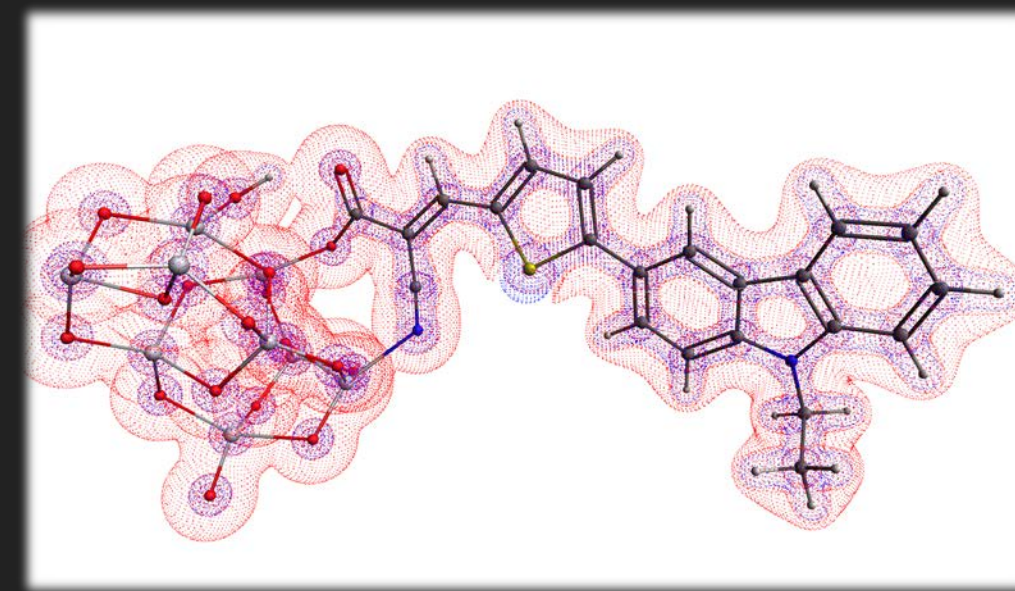
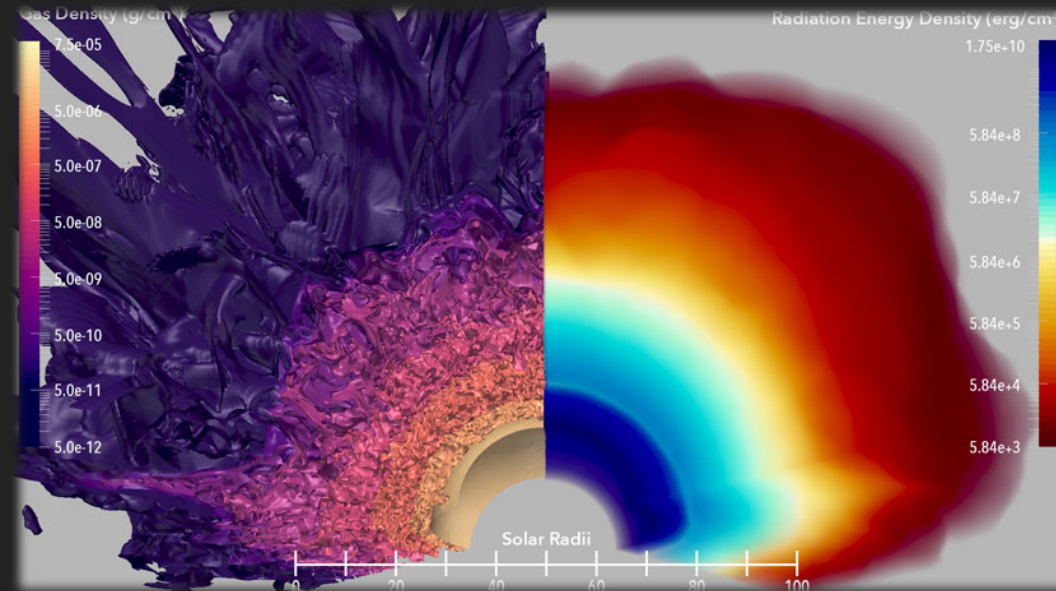
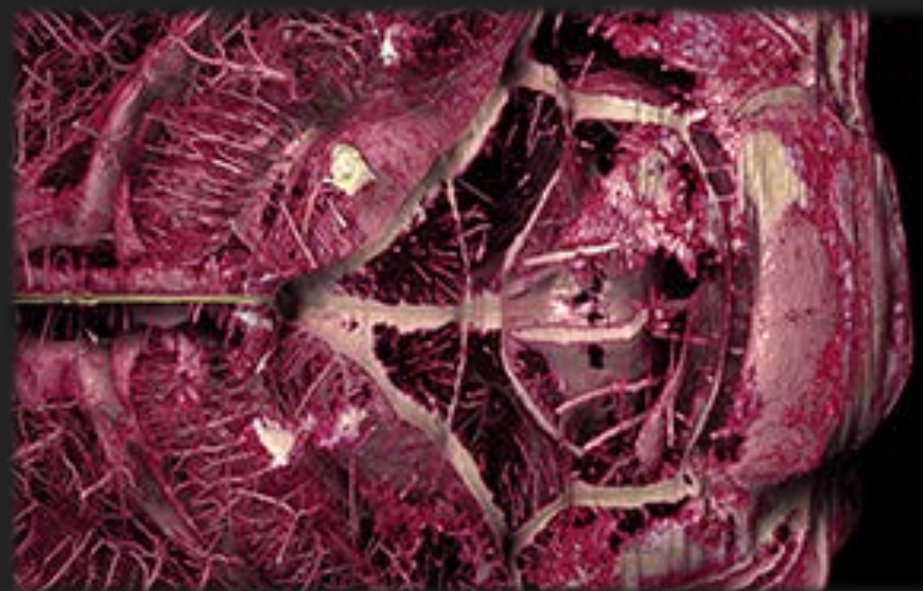


800,000,000 to  
~2,000,000,000,000,000,000  
FLOPS

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

## SO WHAT DOES ALL THAT COMPUTE POWER ENABLE?

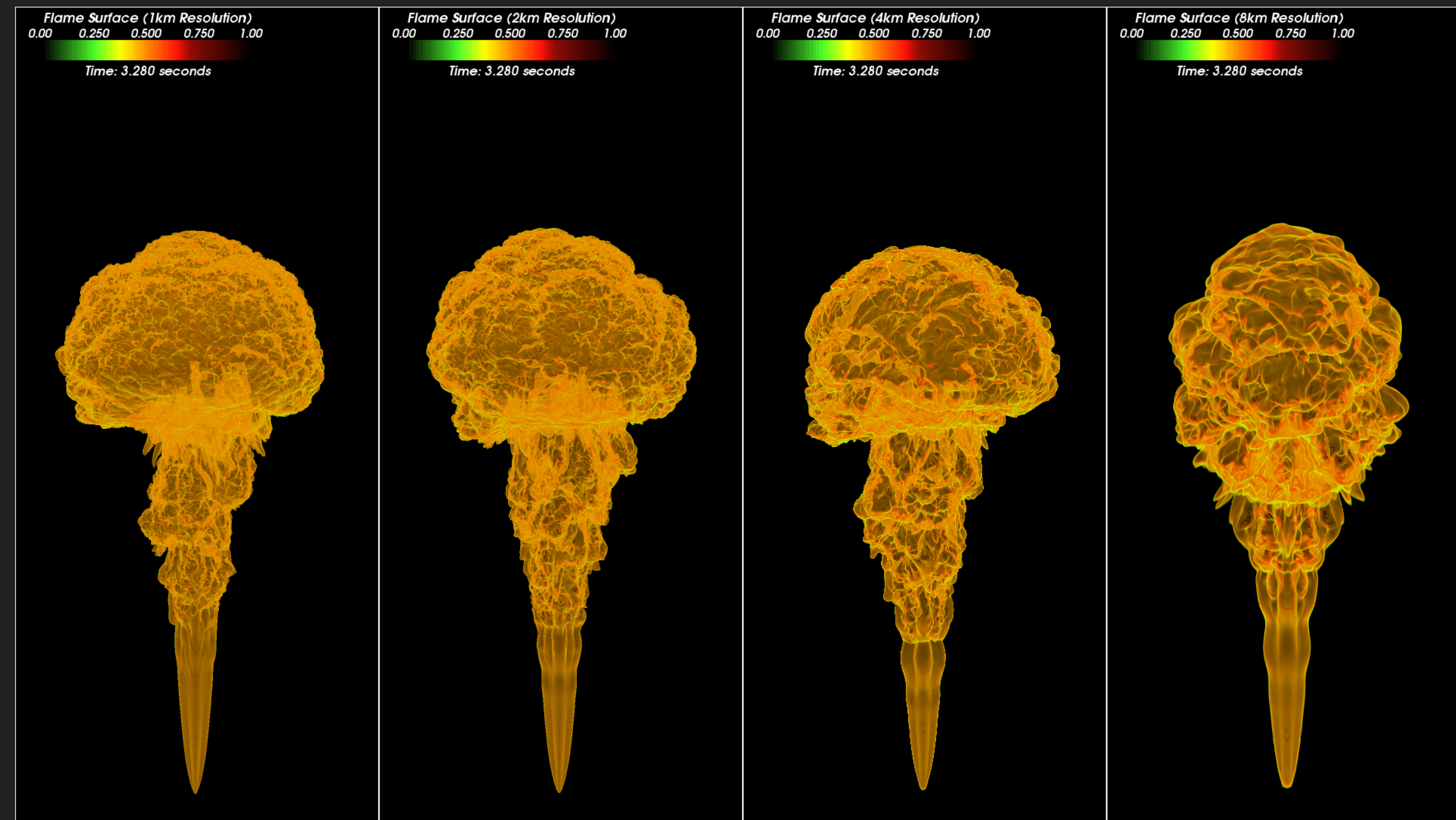
- ▶ Large-Scale Computing on the Connectomes of the Brain
- ▶ Global Radiation MHD Simulations of Massive Star Envelopes
- ▶ Molecular Design of Dye-Sensitized Solar Cells
- ▶ Real-time Computing in support of DIII-D National Fusion Facility





# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

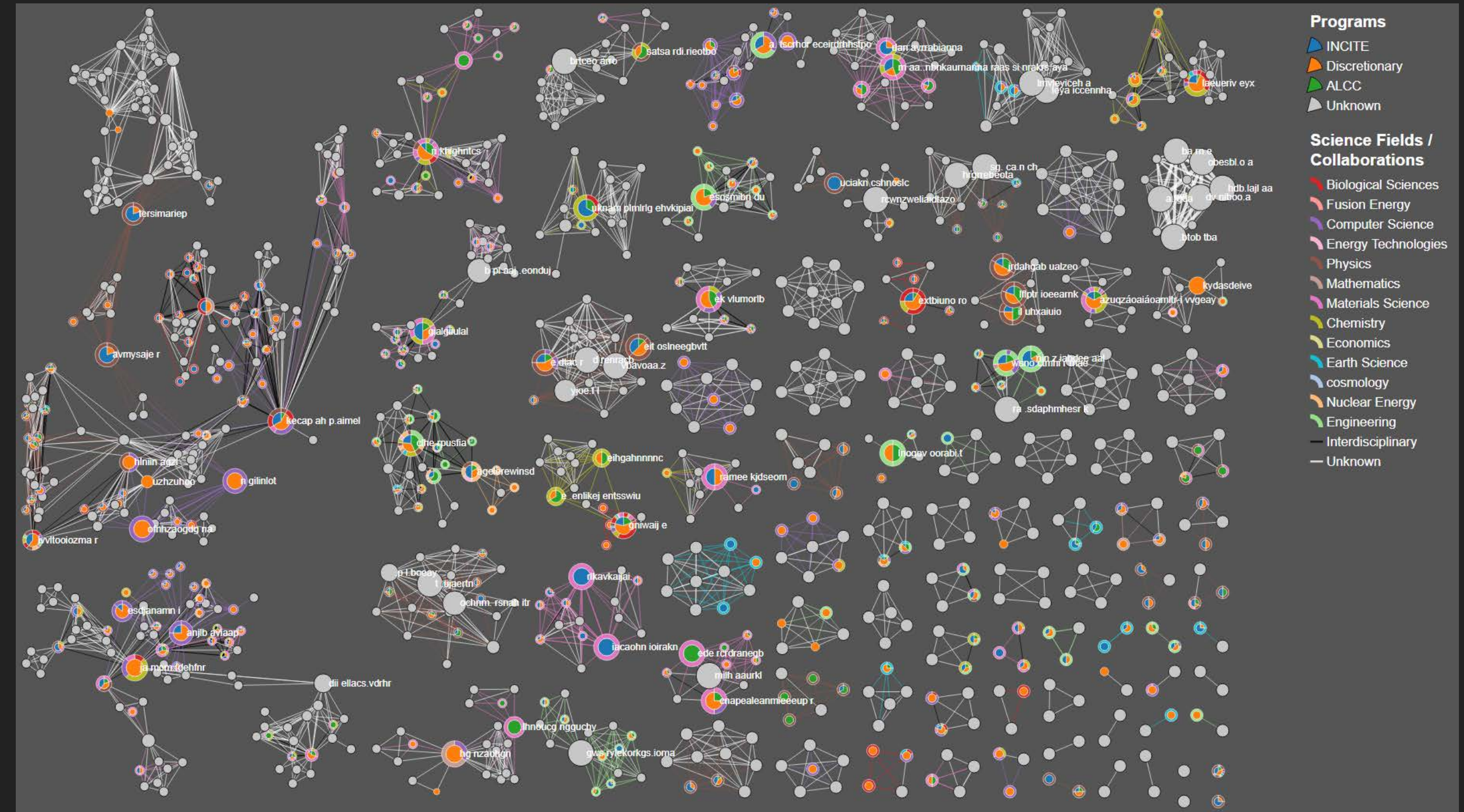
- ▶ How do you translate theory into simulation?





# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

► How do you more efficiently operate a facility?

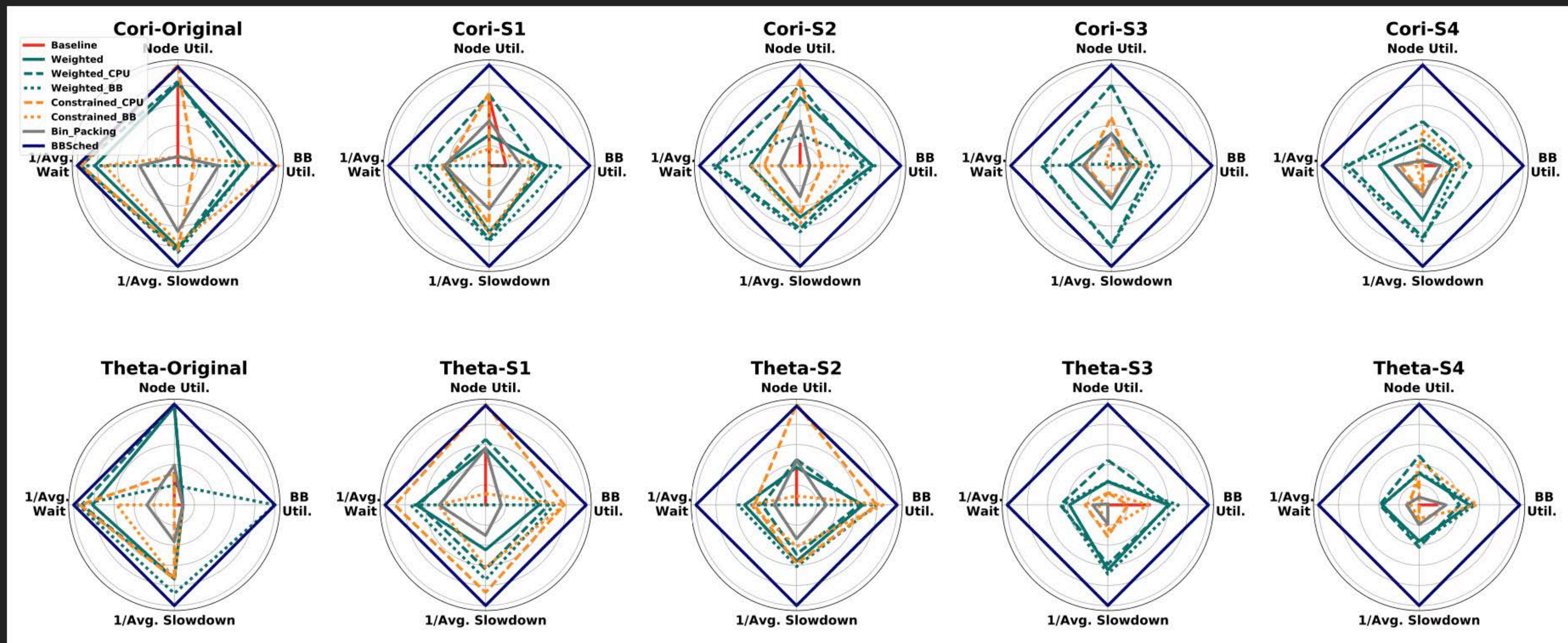


Bharat Kale, MS Thesis



# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

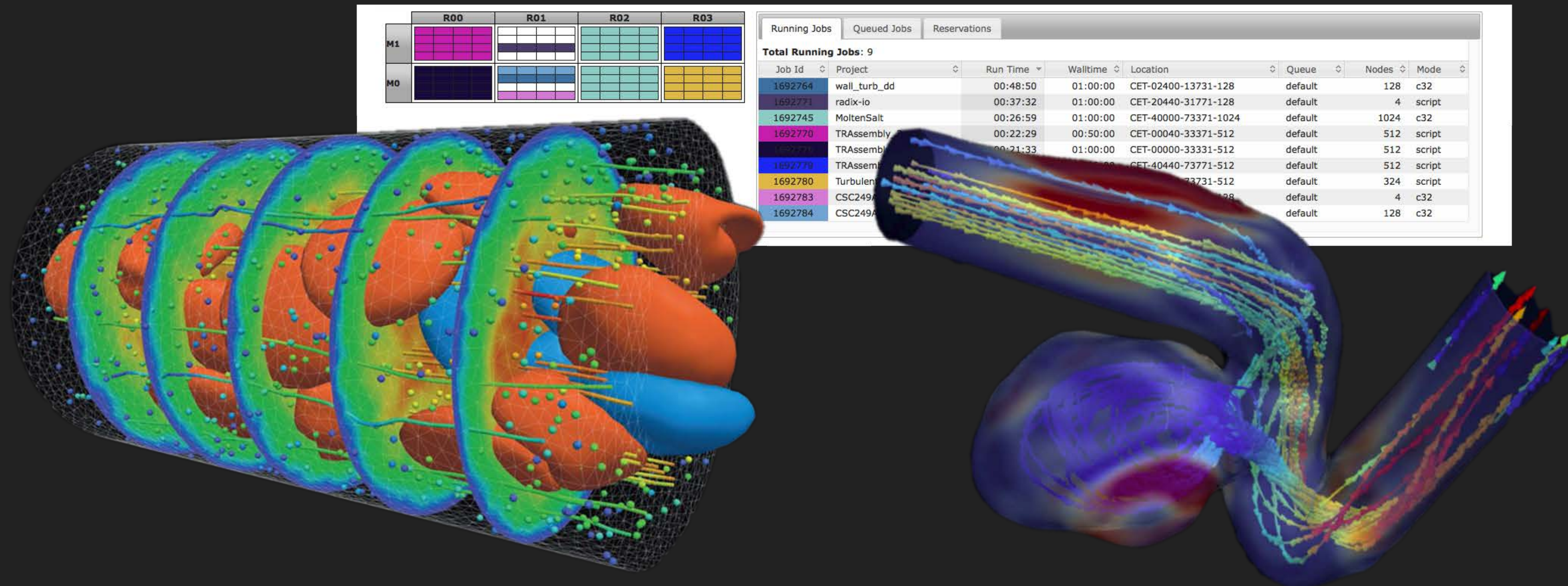
- ▶ How do you effectively schedule and operate a resource?





# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

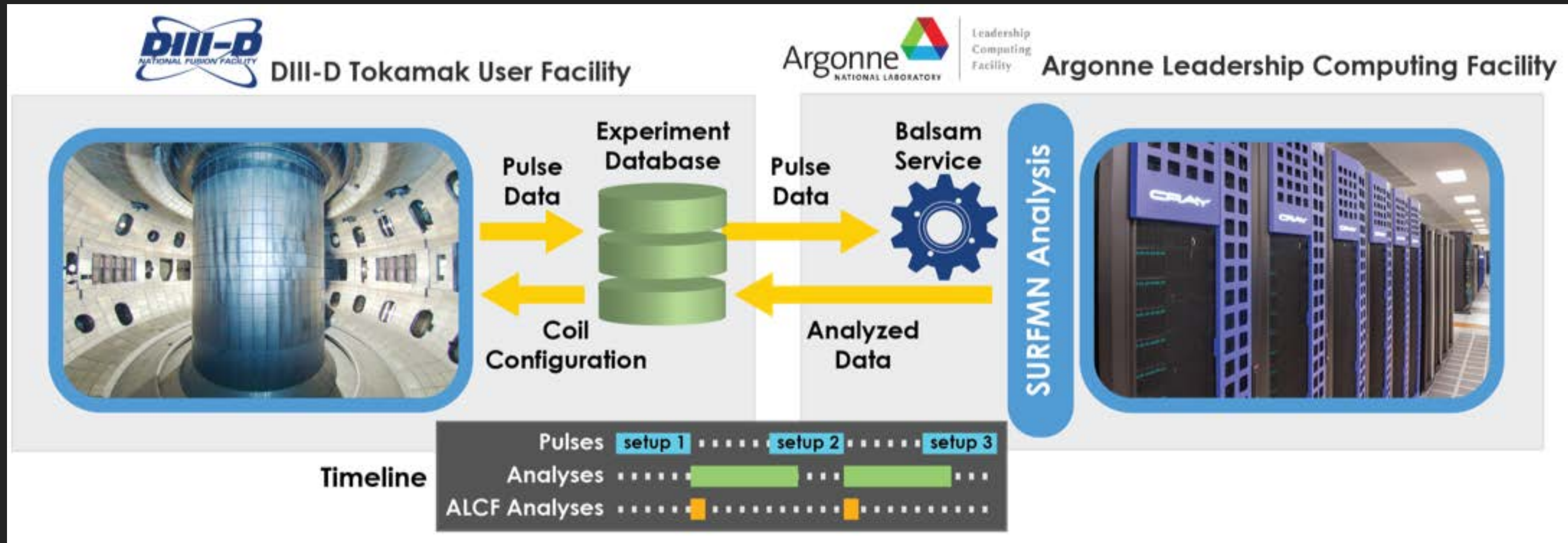
- ▶ How do you evolve traditional HPC environment?





# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

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

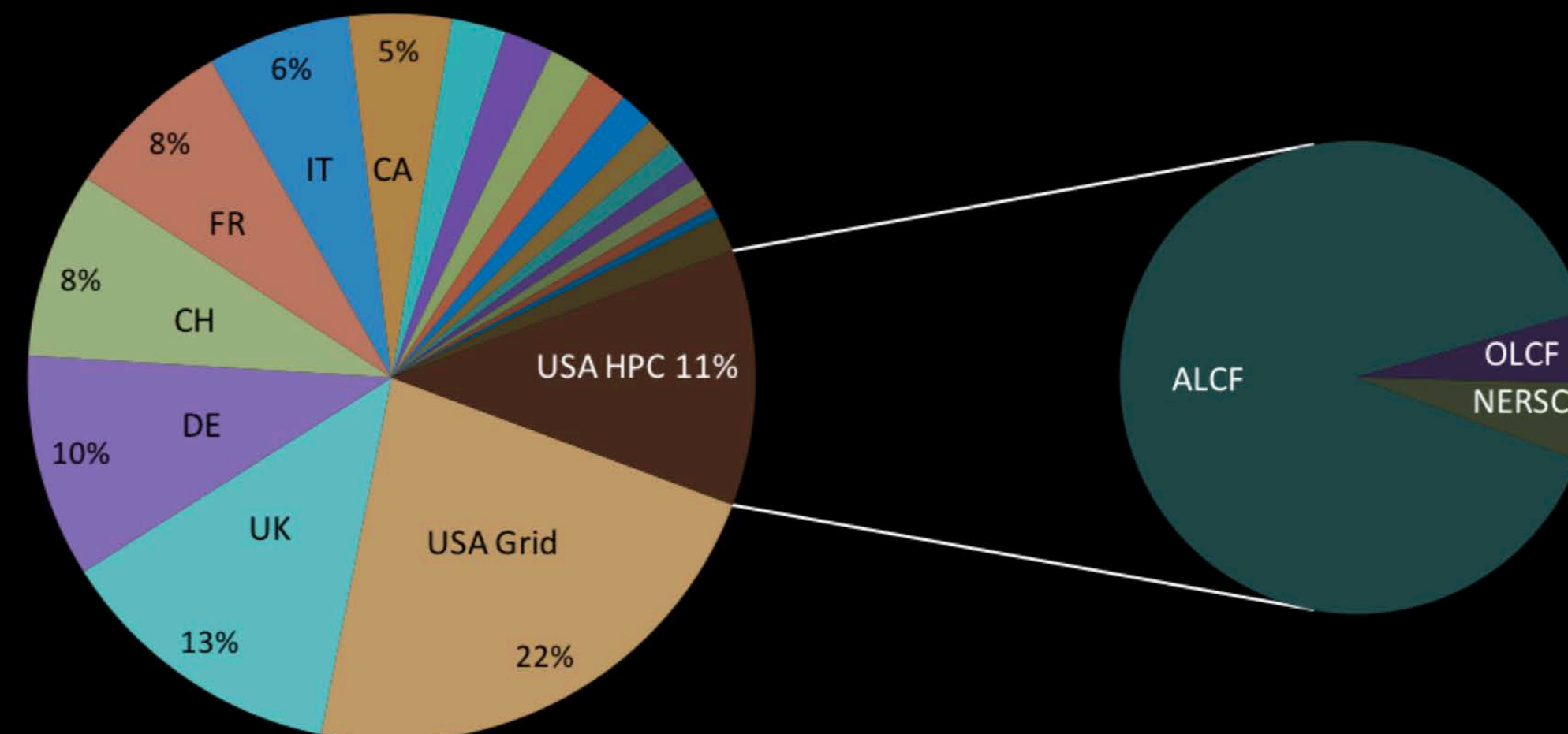


# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

- ▶ 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

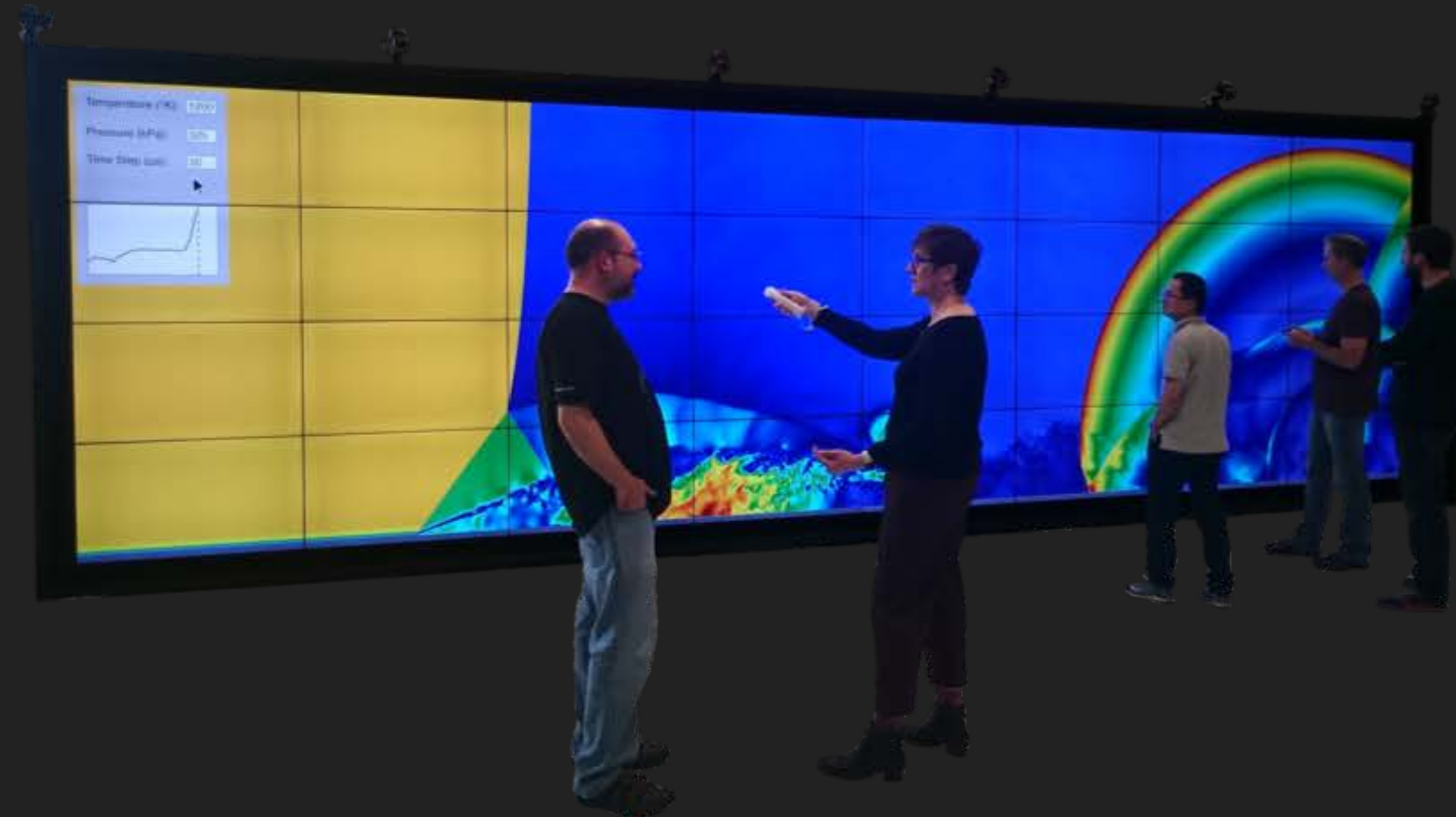
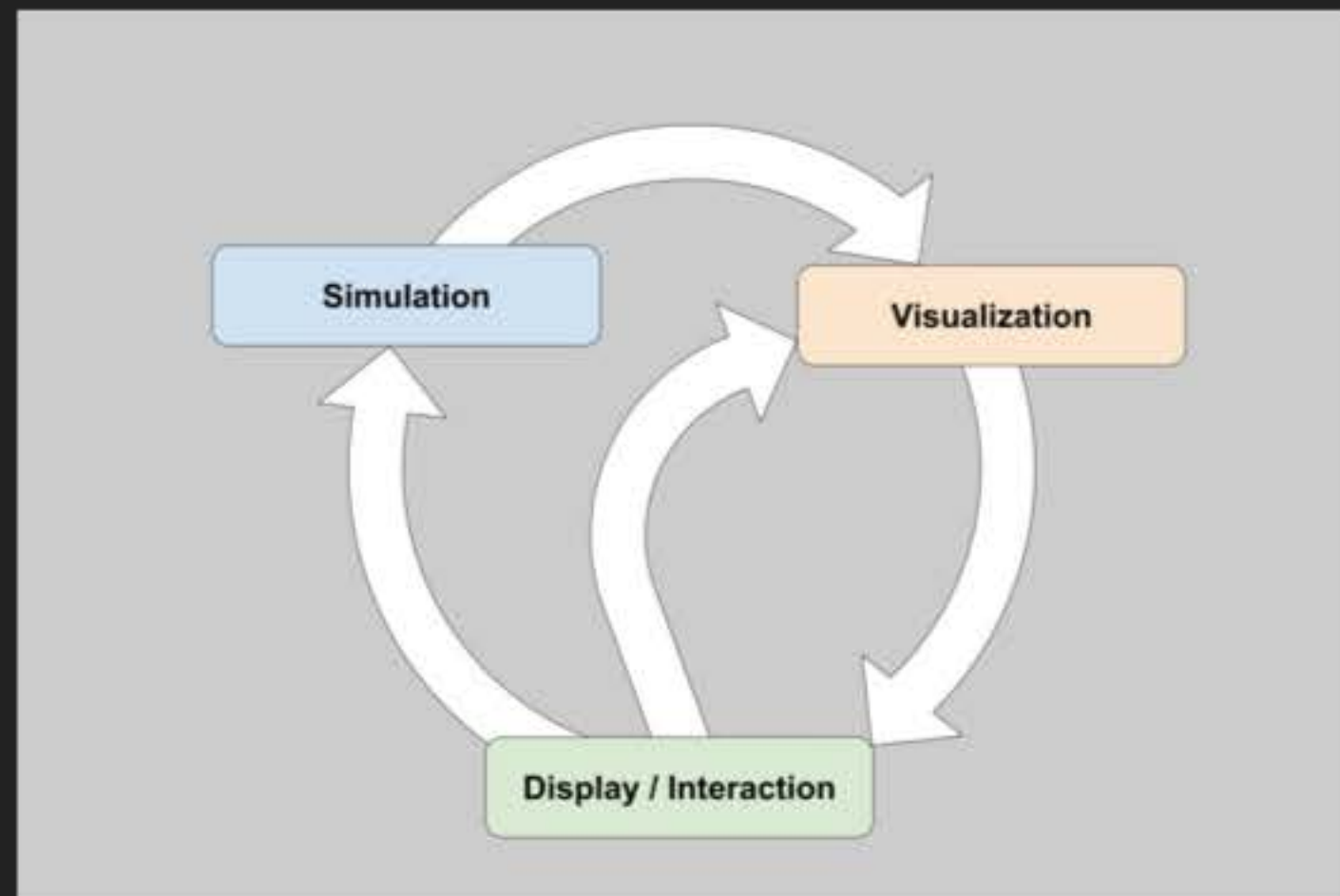
- These would still eventually be written without the US HPC effort, but they probably would not exist today: the **time-to-science has been dramatically shortened.**





# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

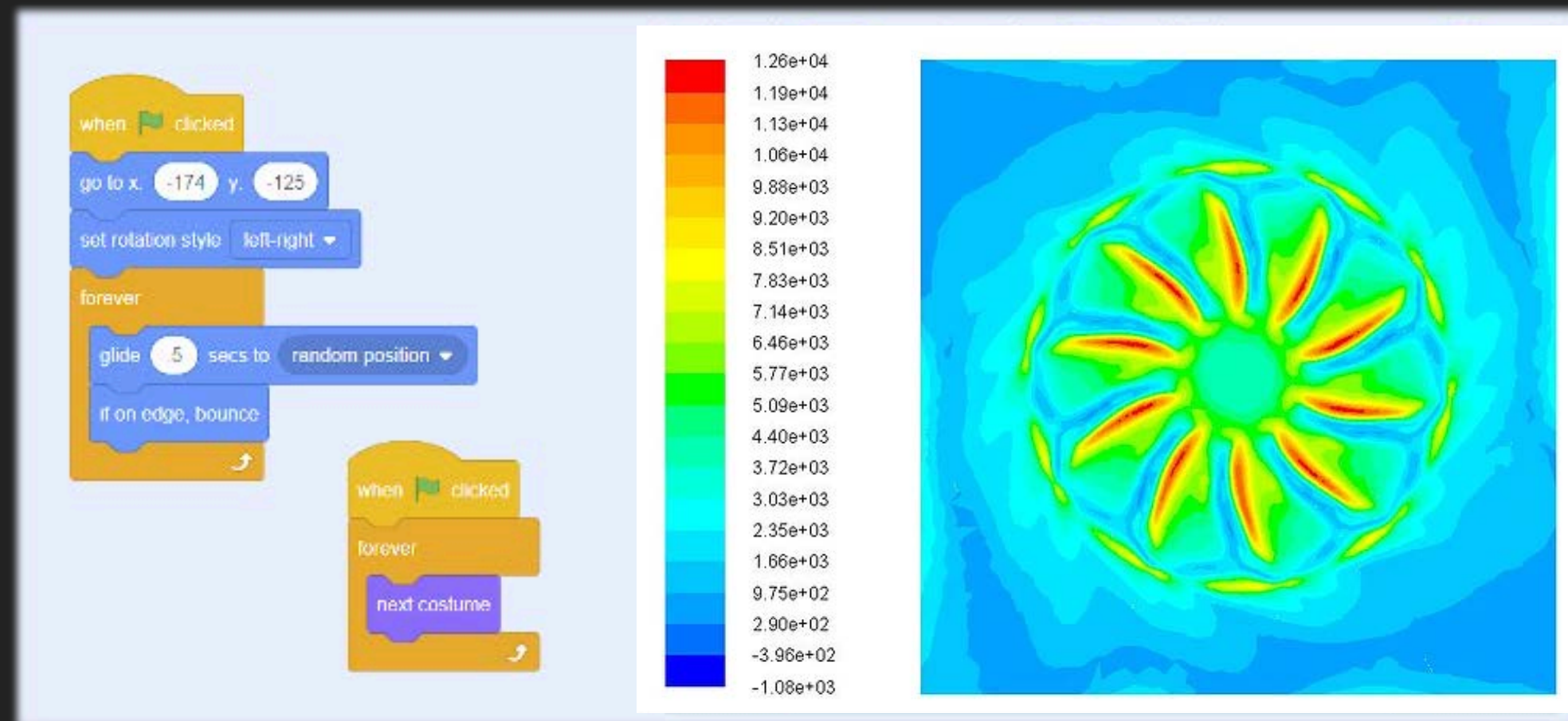
- ▶ How do you evolve traditional HPC environment to increase engagement?





# 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?

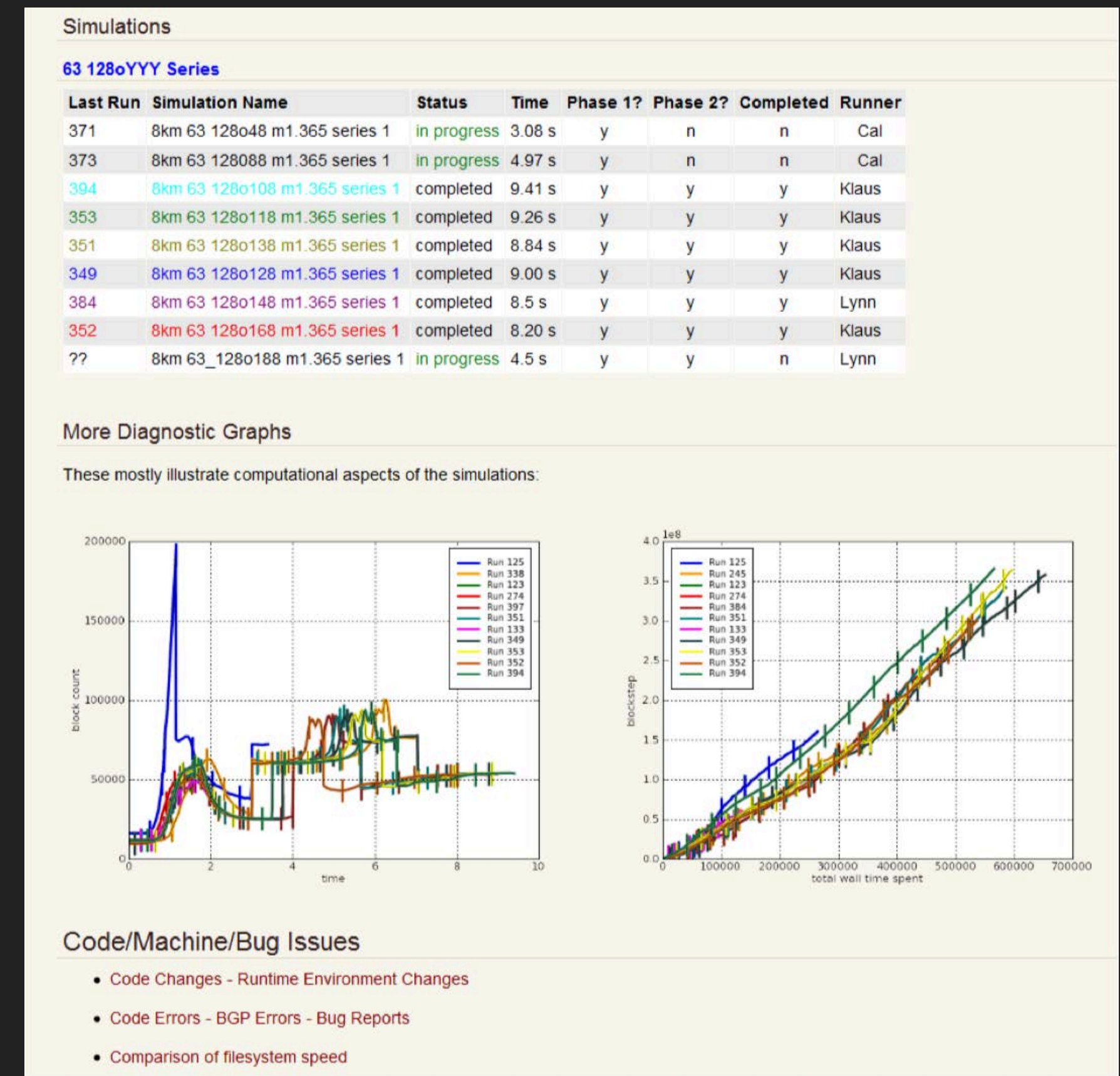






# HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

- ▶ 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 three screenshots of the Smaash/HACC web interface, illustrating the workflow for managing and viewing simulation data.

**Left Screenshot: Model: MiraU / M019 / L2100**

This view shows a plot of  $\rho(k)$  versus  $k$  on a log-log scale. The plot displays multiple curves representing different simulation runs. Below the plot is a table of runs:

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

Below the runs table is a 'Files' section showing a single file:

Path	Date	Size	Type
/homes/turam/dev/smaash/data/631/pk.png	09/27/2017 6:21 a.m.	149367	png

**Middle Screenshot: Run: MiraU / M019 / run001 / L2100**

This view shows a table of timesteps for a specific run:

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

Below the timesteps table is a 'Files' section showing three files:

Path	Date	Size	Type
/homes/turam/dev/smaash/data/606/hacc_gpu_m019.log	09/27/2017 6:21 a.m.	1.0 MB	txt
/homes/turam/dev/smaash/data/607/hacc_gpu_m019.err	09/27/2017 6:21 a.m.	119.6 KB	txt
/homes/turam/dev/smaash/data/608/indat.params	09/27/2017 6:21 a.m.	7.4 KB	txt

**Right Screenshot: Run: MiraU / M019 / run000 / L2100**

This view shows the content of the 'indat.params' file:

```
#####
# 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
# SSB: 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
SSB 0.854654384
NS 1.026482126
W_DE -0.981272382
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 page includes a header with the Argonne logo and a 'Create a Job' button. Below the header, there are four main 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 page includes a header with the Argonne logo and a 'Create a Job' button. Below the header, there are eight job status cards arranged in a 2x4 grid:

- Top row: APS Basic Job (Jan. 15, 2016, 11:47 a.m., No Comments) - Complete; APS Basic Job (Jan. 15, 2016, 11:41 a.m., No Comments) - Processing...; APS Basic Job (Jan. 15, 2016, 11:11 a.m., No Comments) - Processing...; HA\_tube5\_test2 Basic Job (Dec. 8, 2015, 6:14 p.m., No Comments) - Complete.
- Bottom row: HA\_tube5\_test2 Basic Job (Dec. 8, 2015, 6:04 p.m., No Comments) - In Progress; HA\_tube5\_test2 Basic Job (Dec. 8, 2015, 5:23 p.m., No Comments) - In Progress; hacc\_160x160x160\_float\_little\_endian.bin Basic Job (Dec. 4, 2015, 3:39 p.m., No Comments) - In Progress; hacc\_160x160x160\_float\_little\_endian.bin Basic Job (Dec. 4, 2015, 10:06 a.m., No Comments) - In Progress.

Argonne HPC portal interface showing video and image galleries. The page includes a header with the Argonne logo and a 'Create a Job' button. Below the header, there are two main sections:

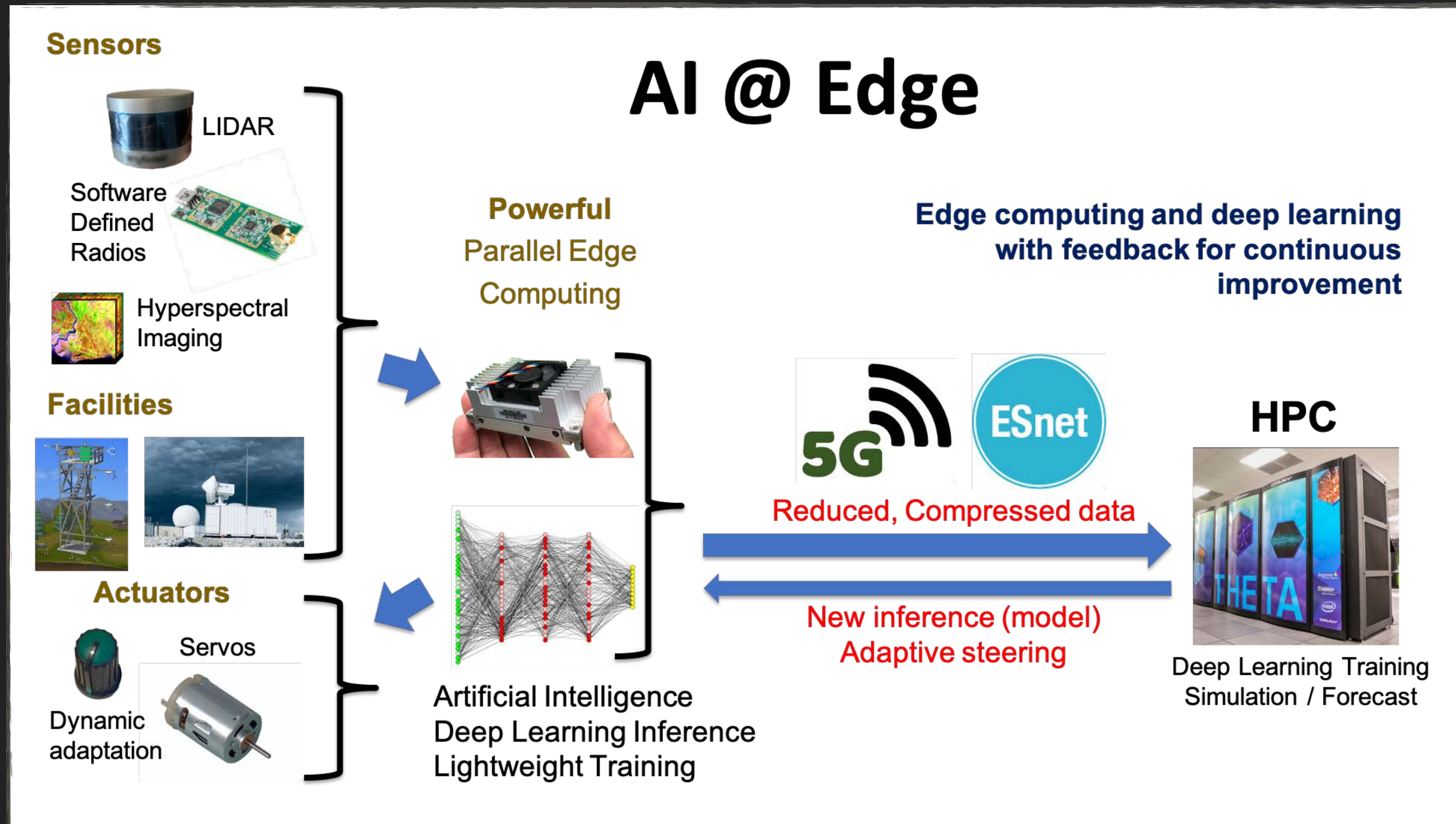
- Videos**: A single video thumbnail.
- Images**: A grid of 24 image thumbnails.

On the right side, there is a metadata panel for 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]

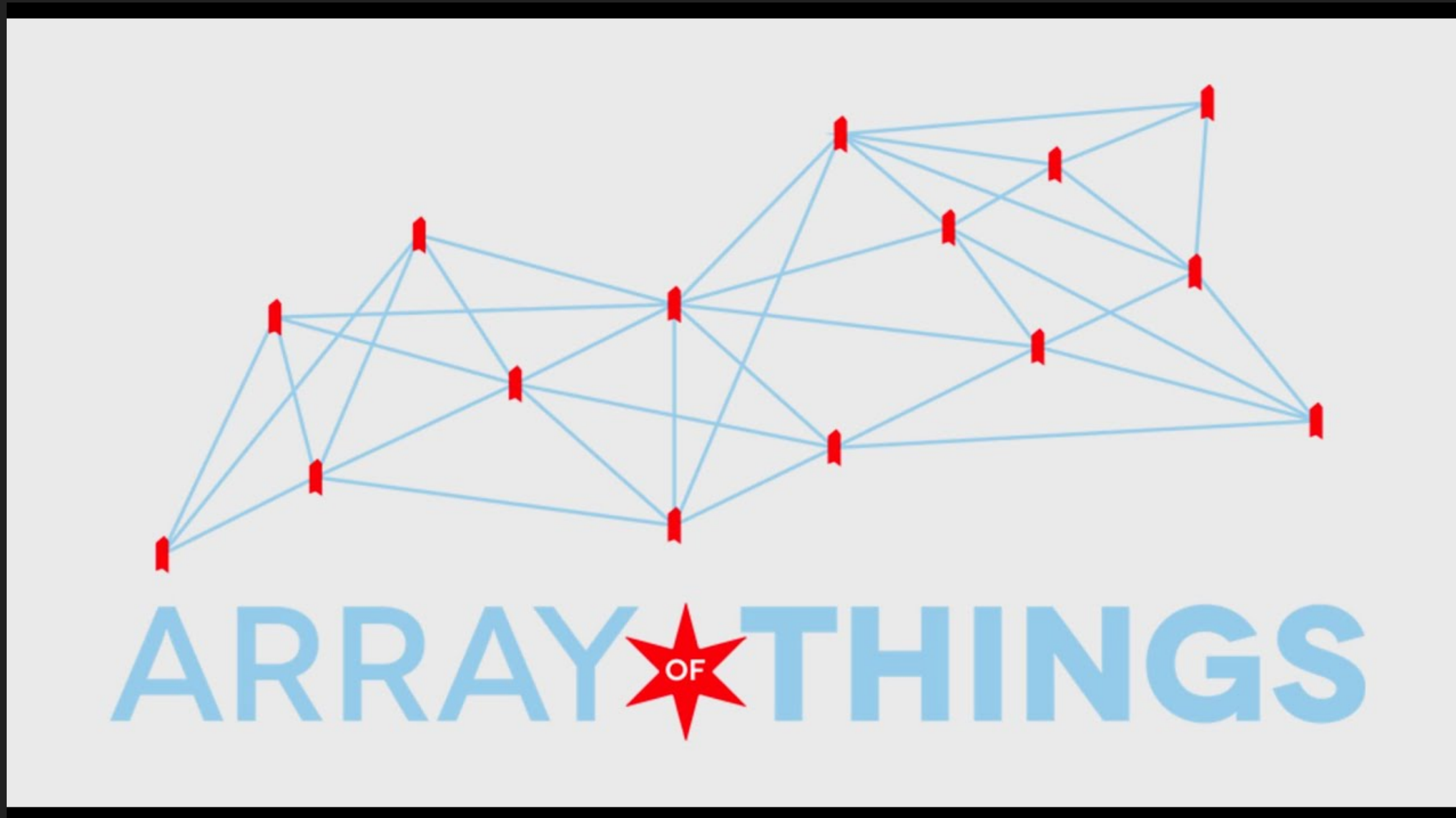


# INTERNET OF THINGS (COMPUTING CONTINUUM) [EDGE COMPUTING]



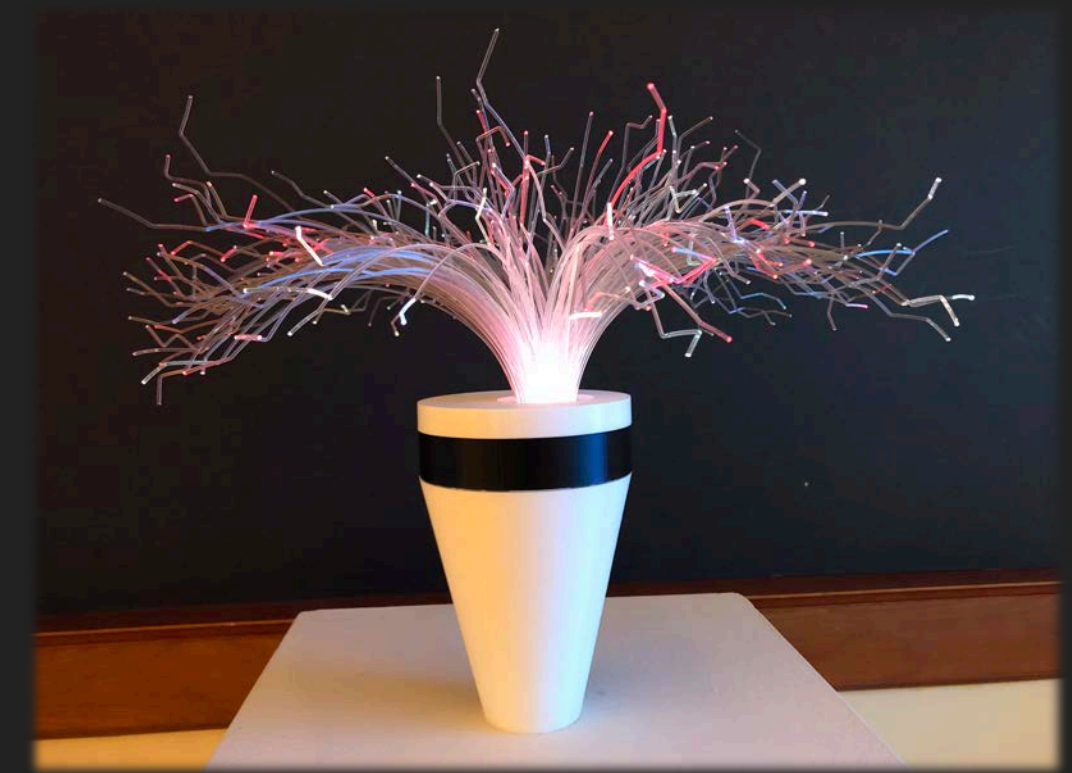
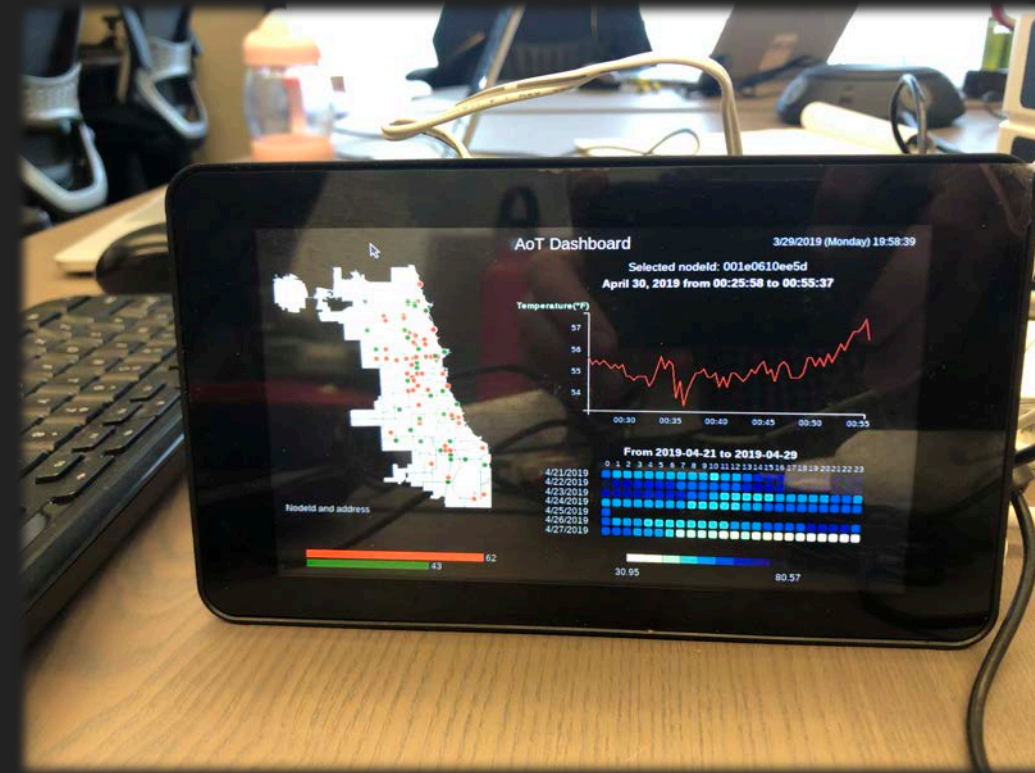


# INTERNET OF THINGS (COMPUTING CONTINUUM) [EDGE COMPUTING]



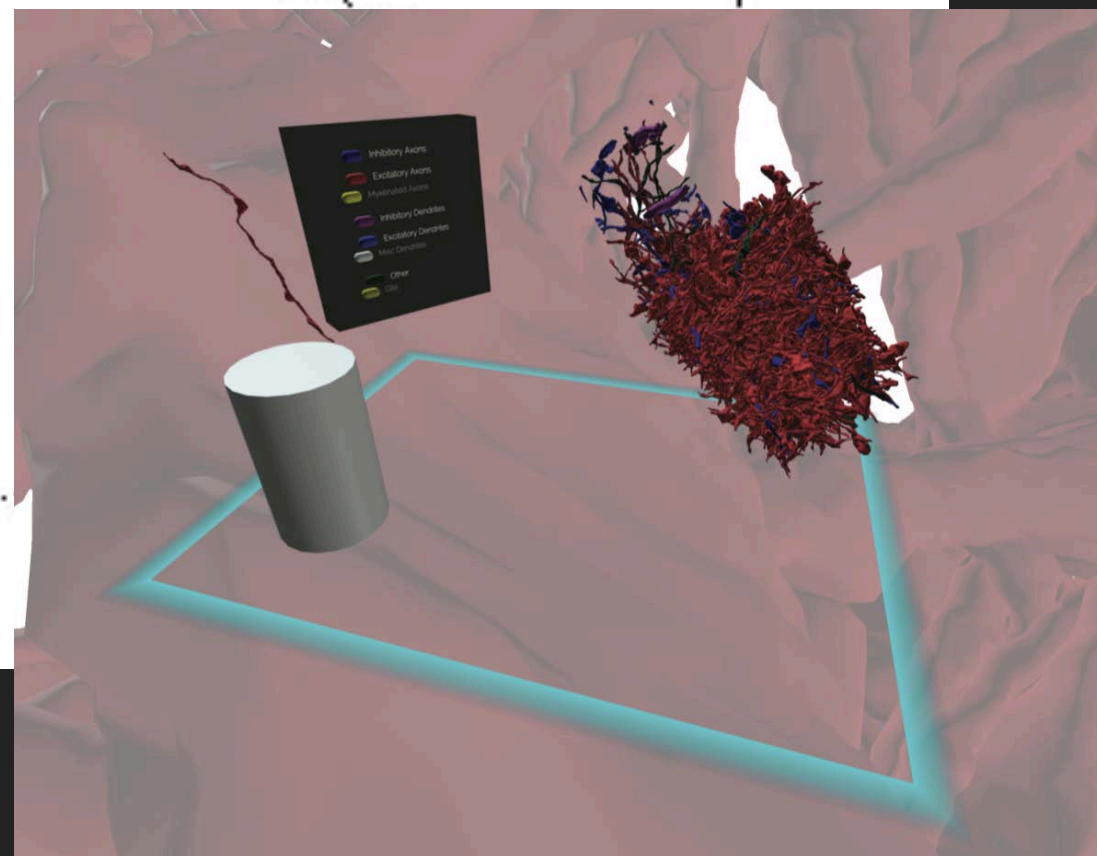
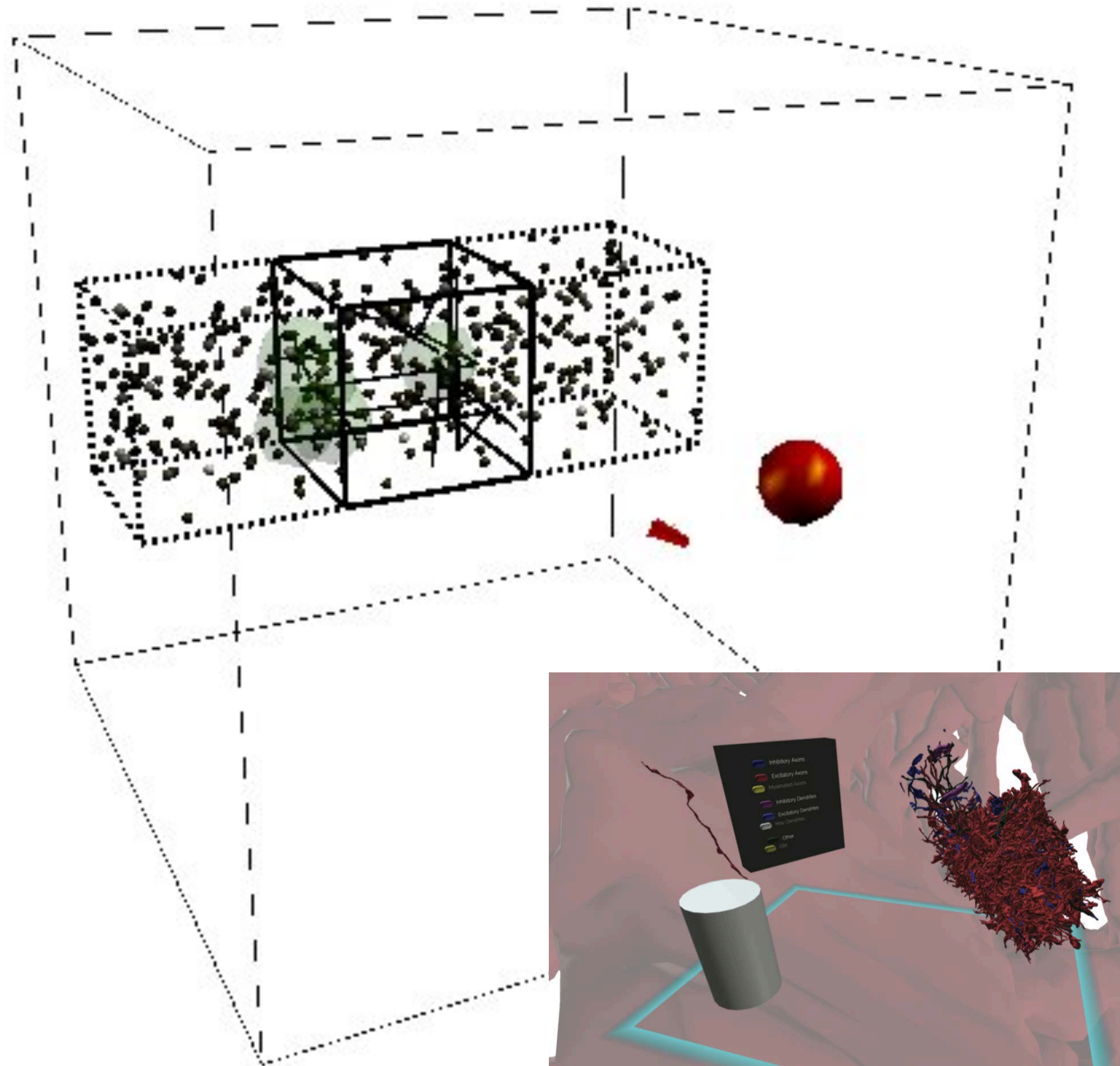


# INTERNET OF THINGS (COMPUTING CONTINUUM) [EDGE COMPUTING]





# VIRTUAL REALITY

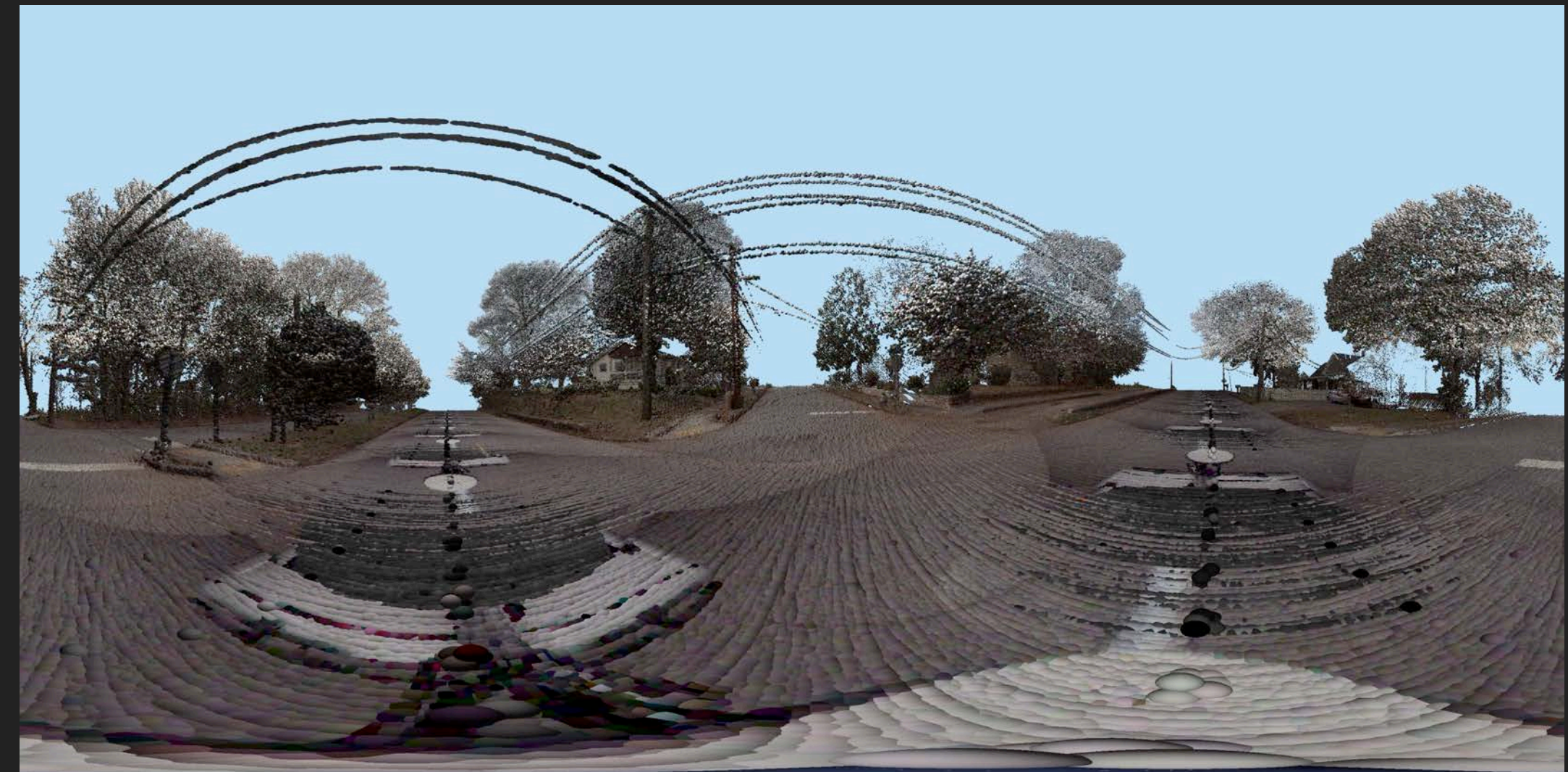
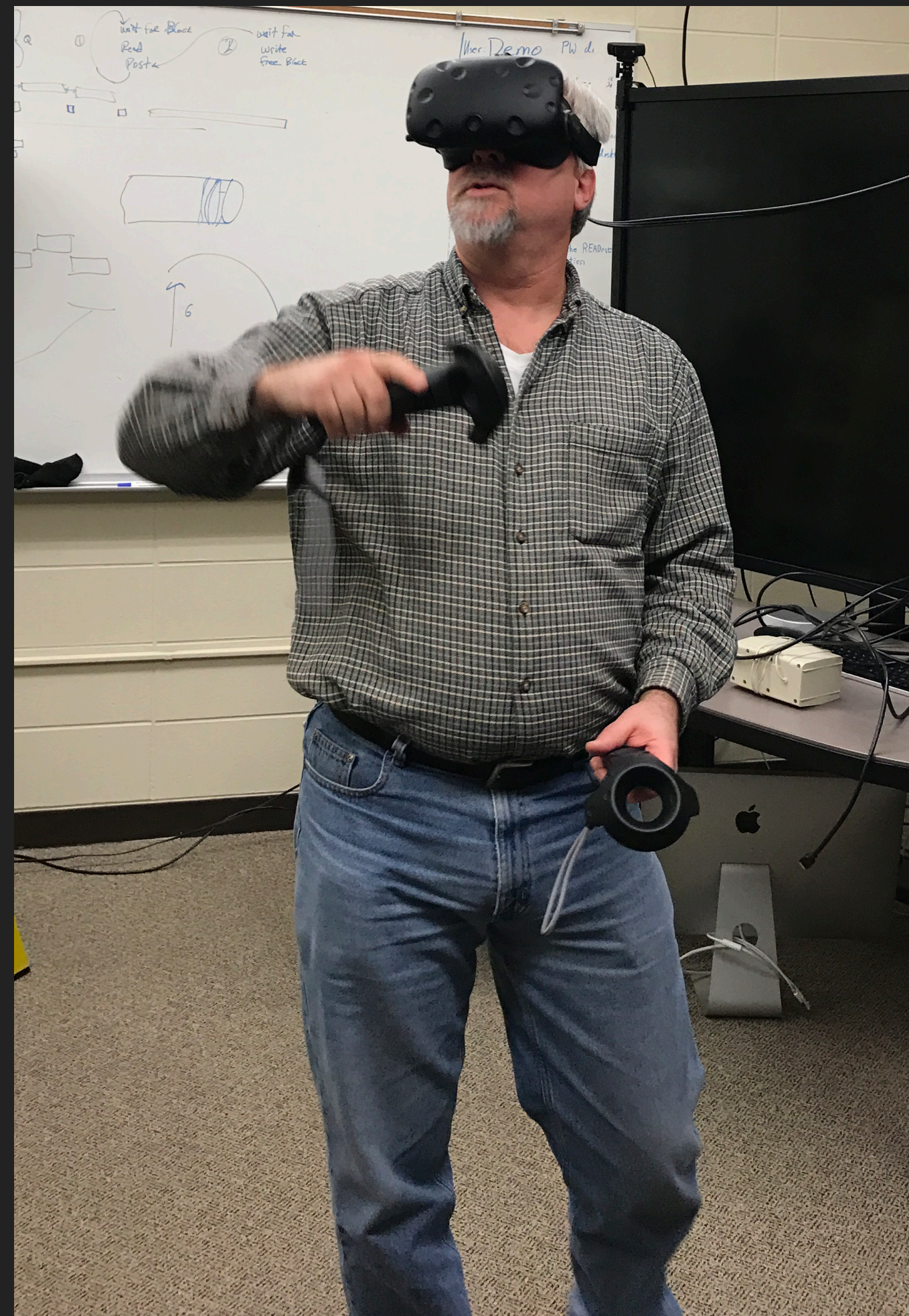


Use of **Virtual Reality** in Science

- ▶ 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 and CCF-2119056.
- ▶ 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.**

36

**Sir Isaac Newton**

