

WITH MICHAEL E. PAPKA

November 16, 2021

DATA, DEVICES AND INTERACTION LABORATORY



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 Student)
- Argonne National Laboratory (Deputy Associate Laboratory Director, Division Director, Senior Scientist)
 - University of Chicago (Senior Fellow)
 - Illinois Institute of Technology (Research Professor)
- Northern Illinois University (Presidential Research, Scholarship, and Artistry Professor)





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

- Insley (Time Arts)
- Students
 - 1 PhD (Information Visualization)
 - 8 Undergraduates (IoT, VR, and HPC)

Joint with School of Art and Design and co-directed with Professor Joseph

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





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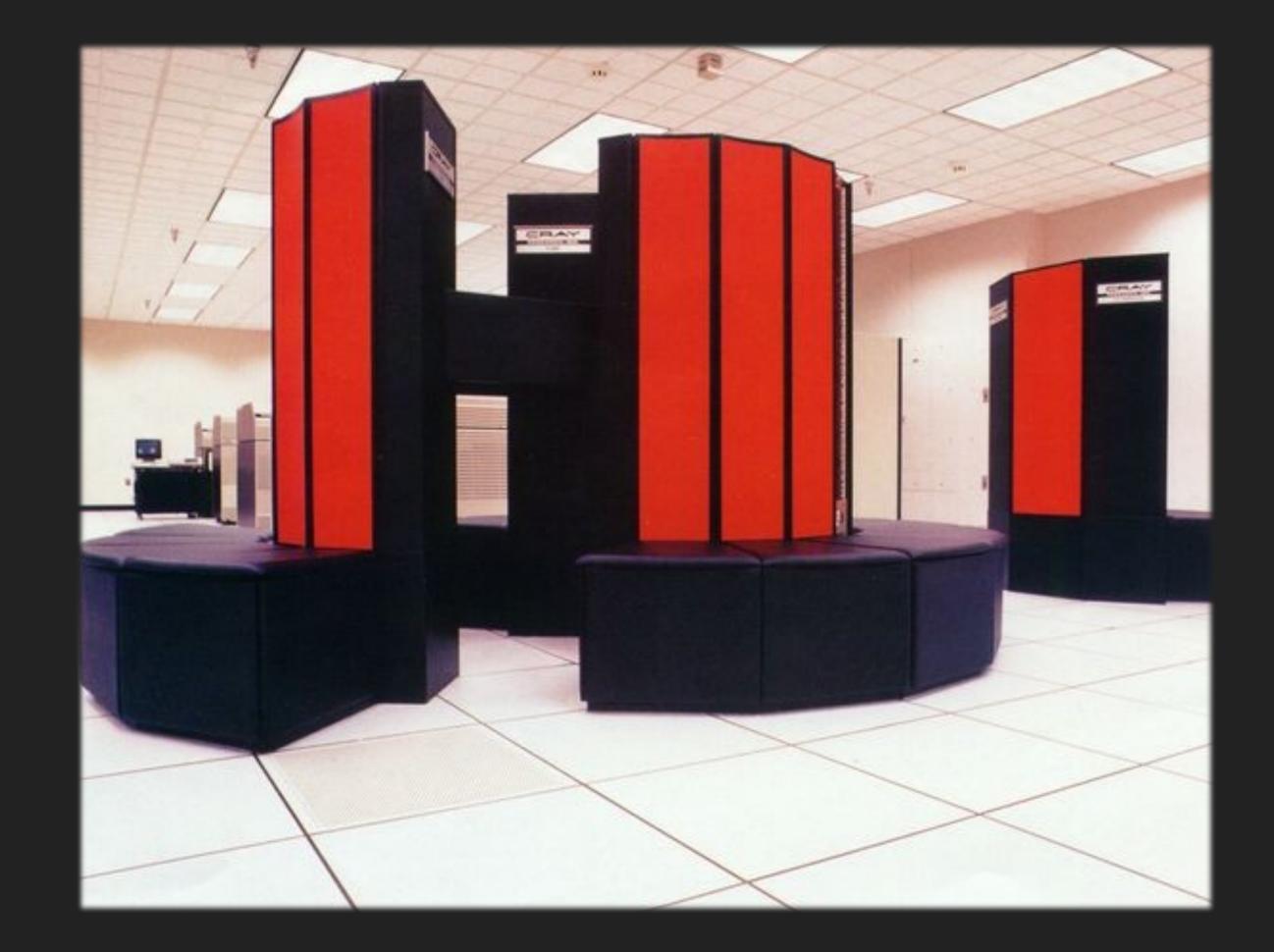


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SUPERCOMPUTERS







SUPERCOMPUTERS



Argonne's Aurora Supercomputer, 2022/23



800megaFL0PS to ~2exaFL0PS







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



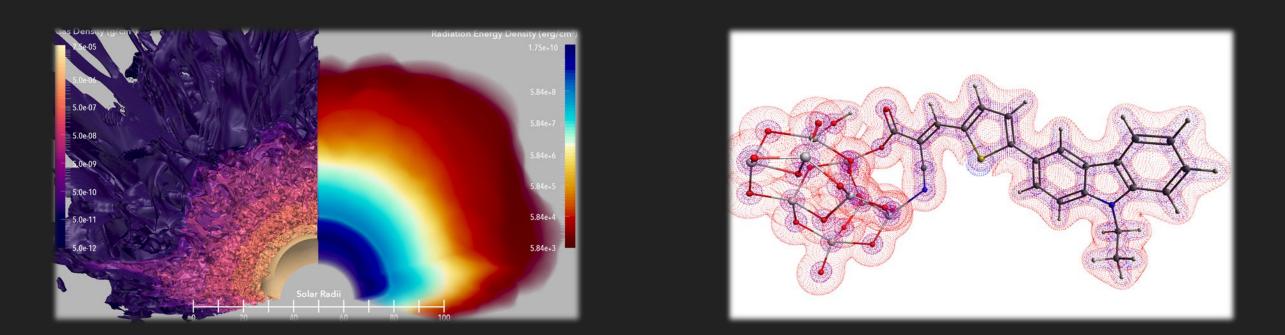




SO WHAT DOES ALL THAT COMPUTE POWER ENABLE?

- 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



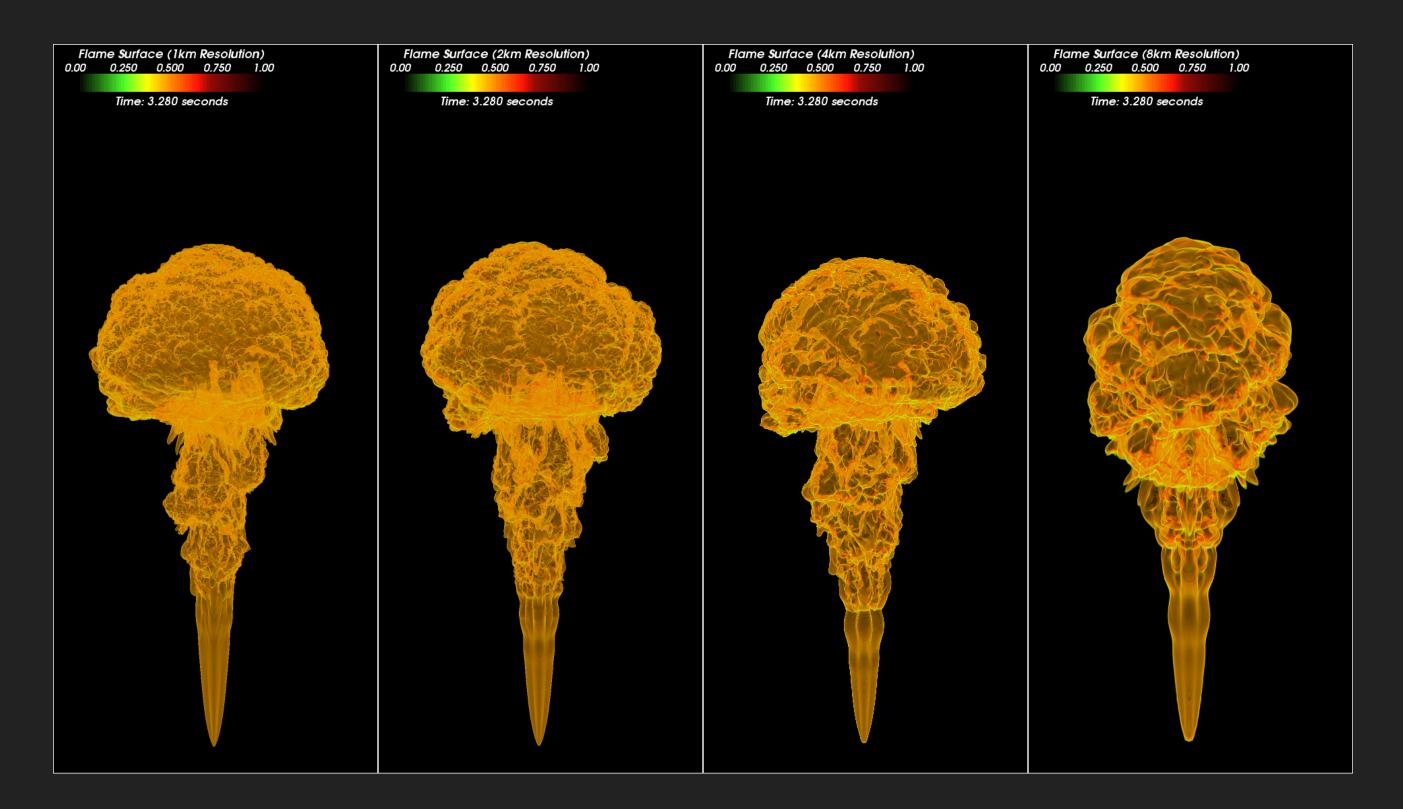


Doga Gursoy, Argonne National Laboratory | Lars Bildsten, University of California, Santa Barbara | Jaqueline M. Cole, University of Cambridge | David Schissel, General Atomics





How do you translate theory into simulation?



R. Fisher, L. Kadanoff, D. Lamb, A. Dubey, T. Plewa, A. Calder, F. Cattaneo, P. Constantin, I. Foster, M. E. Papka, S. I. Abarzhi, S. M. Asida, P. M. Rich, C. C. Glendenin, K. Antypas, D. J. Sheeler, L. B. Reid B. Gallagher, and S. G. Needham, Terascale Turbulence Computation Using the FLASH3 Application Framework on the IBM Blue Gene/L System, IBM Journal of Research and Development, 52(1.2):127-36, 2008.





How do you more efficiently operate a facility?



S. Read, M. E. Papka, Operational Metrics Reporting Processes at Scientific User Facilities: Comparing A High-Energy X-Ray Synchrotron Facility to a Supercomputing Facility, 2017 IEEE International Professional **Communication Conference (ProComm)**, pp. 1-6, Madison, WI, July 23, 2017.



Programs

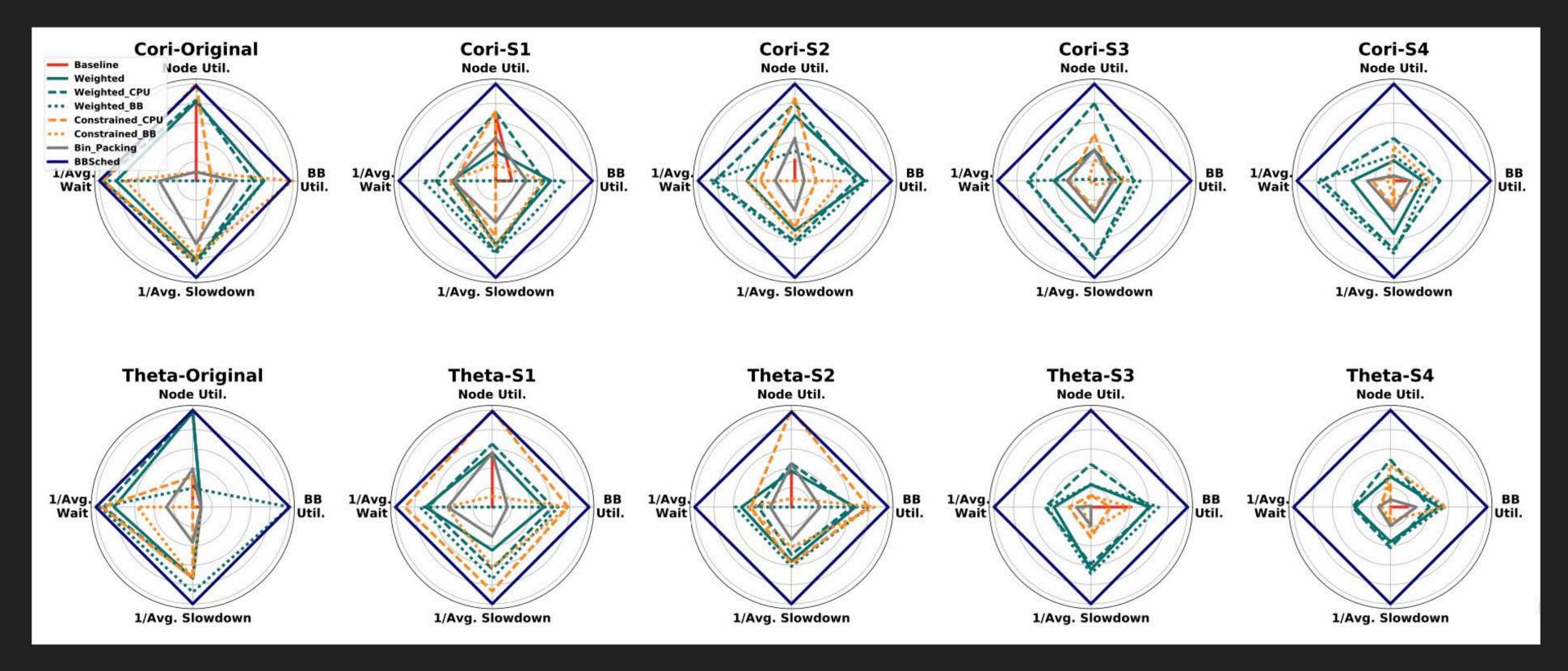
- INCITE
- Discretionary
- ALCC
- Unknown

Science Fields / porations

- **Biological Scienc**
- Fusion Energy
- Computer Scienc
- Energy Technologie
- Physics
- Mathematics
- Materials Scienc
- Chemistry
- Economics
- Searth Science
- cosmology
- Nuclear Energy
- Fngineering
- Interdisciplinar
- Unknowr



How do you effectively schedule and operate a resource?

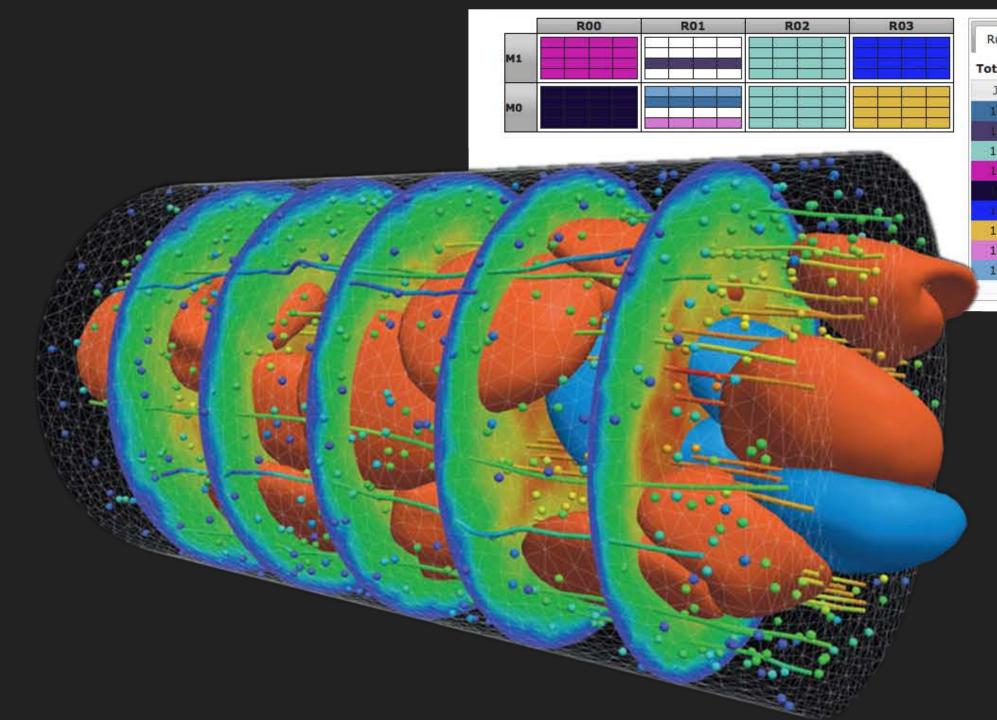


97-108, June 2019.

Y. Fan, Z. Lan, P. Rich, W. E. Allcock, M. E. Papka, B. Austin, D. Paul, Scheduling Beyond CPUs for HPC, Proceedings of the 28th International Symposium on High-Performance Parallel and Distributed Computing, pp.

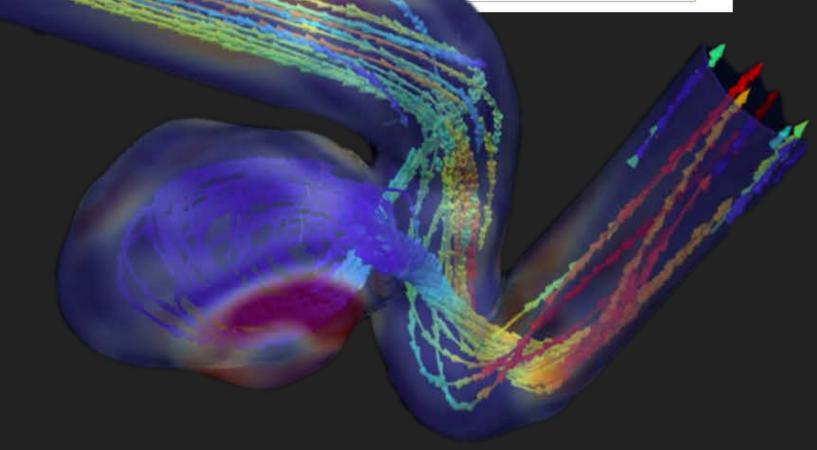


How do you evolve traditional HPC environment?



L. Grinberg, J. A. Insley, D. Fedosov, V. A. Morozov, M. E. Papka, G. E. Karniadakis, Tightly Coupled Atomistic-Continuum Simulations of Brain Blood Flow on Petaflop Supercomputers, Computing in Science and Engineering, 14(6):58-67, 2012.

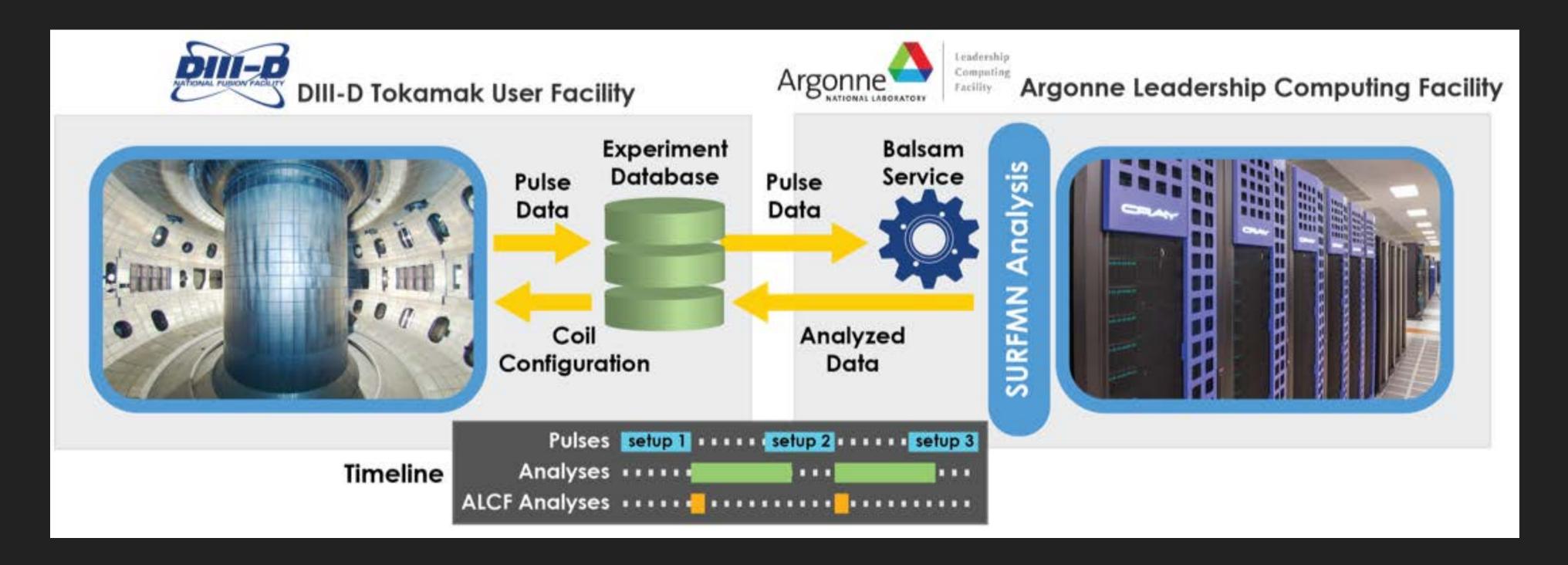
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How do you evolve traditional HPC environment to address real-time needs?



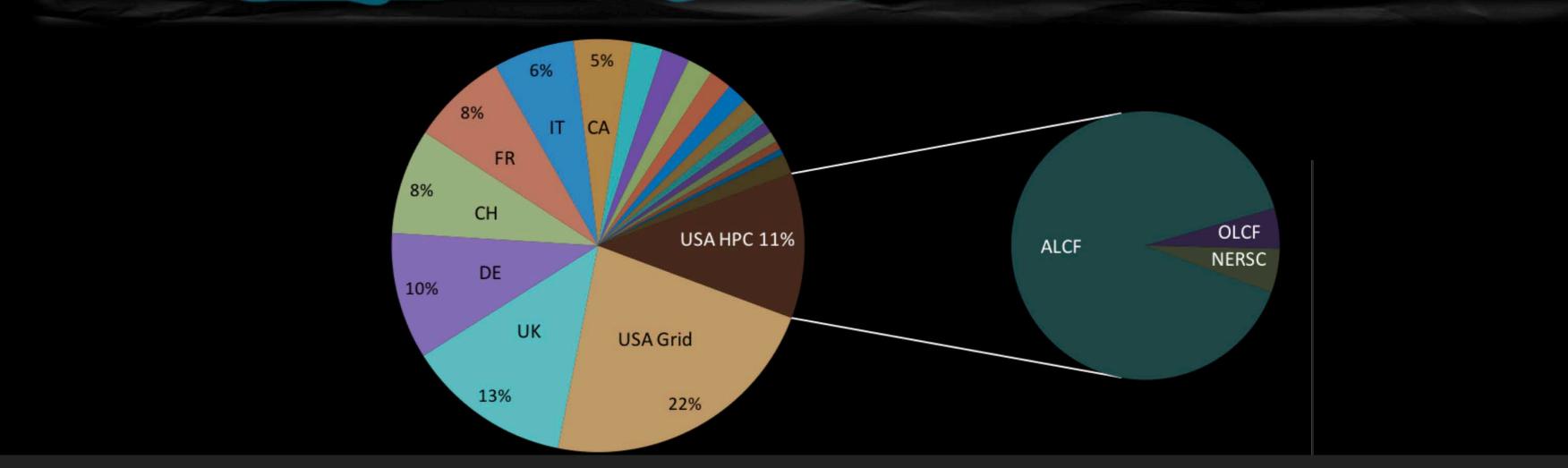
M. Kostuk, T. D. Uram, T. Evans, D. M. Orlov, M. E. Papka, D. Schissel, Automatic Between-Pulse Analysis of DIII-D Experimental Data Performed Remotely on a Supercomputer at Argonne Leadership Computing Facility, Fusion **Science and Technology**, September 2017.



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.

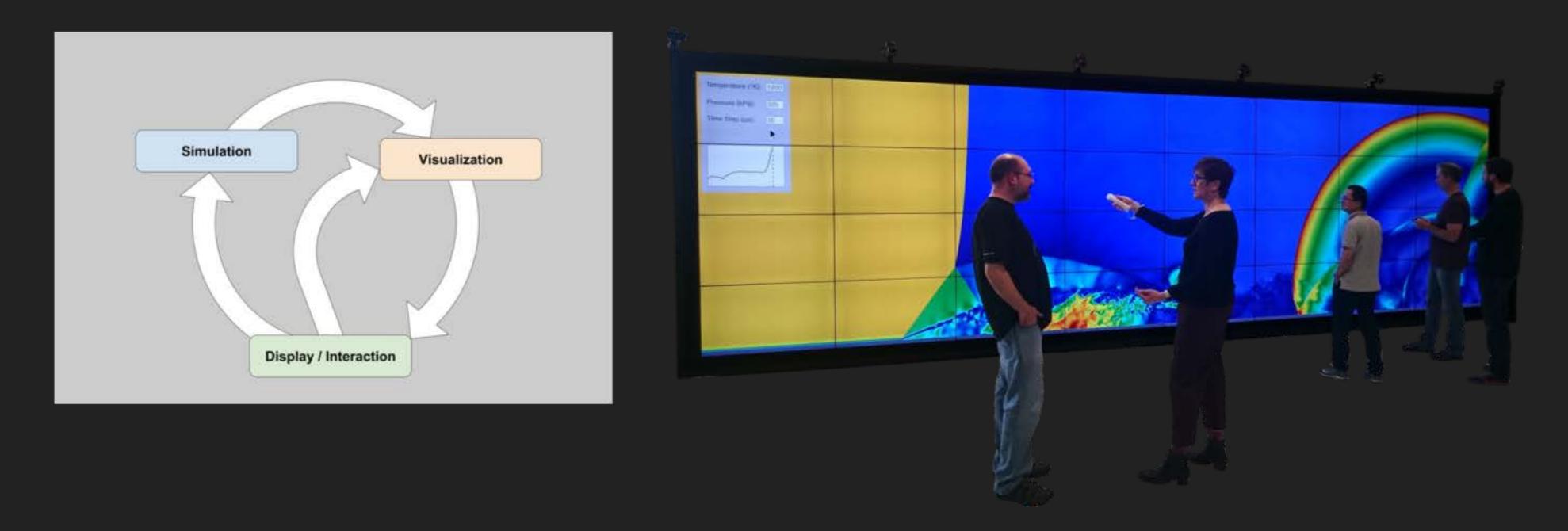


T. LeCompte(HEP){06/02/2016} and J. T. Childers, T. D. Uram, D. Benjamin, T. J. LeCompte, M. E. Papka, An Edge Service for Managing HPC Workflows, Proceedings of the Fourth International Workshop on HPC User Support Tools (HUST'17), Denver, CO, November 12, 2017





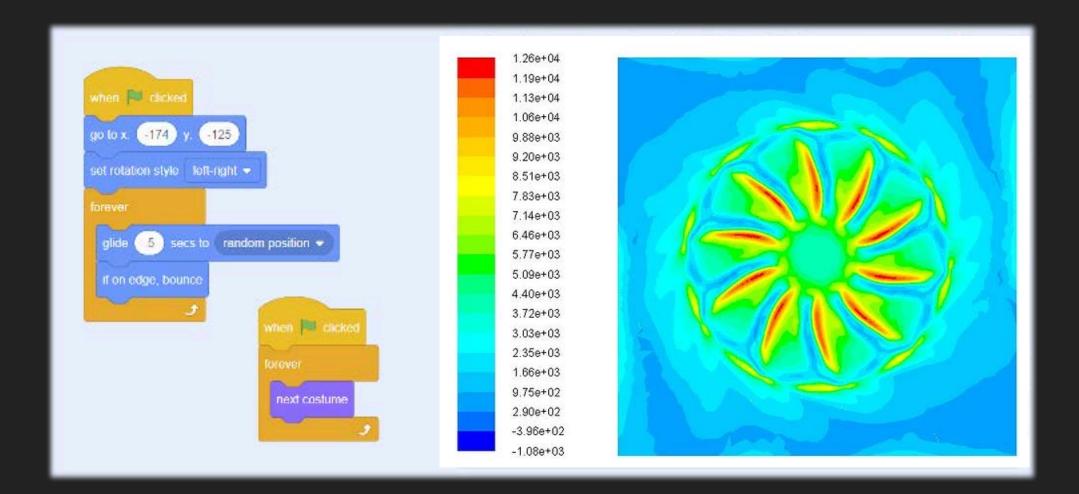
How do you evolve traditional HPC environment to increase engagement?



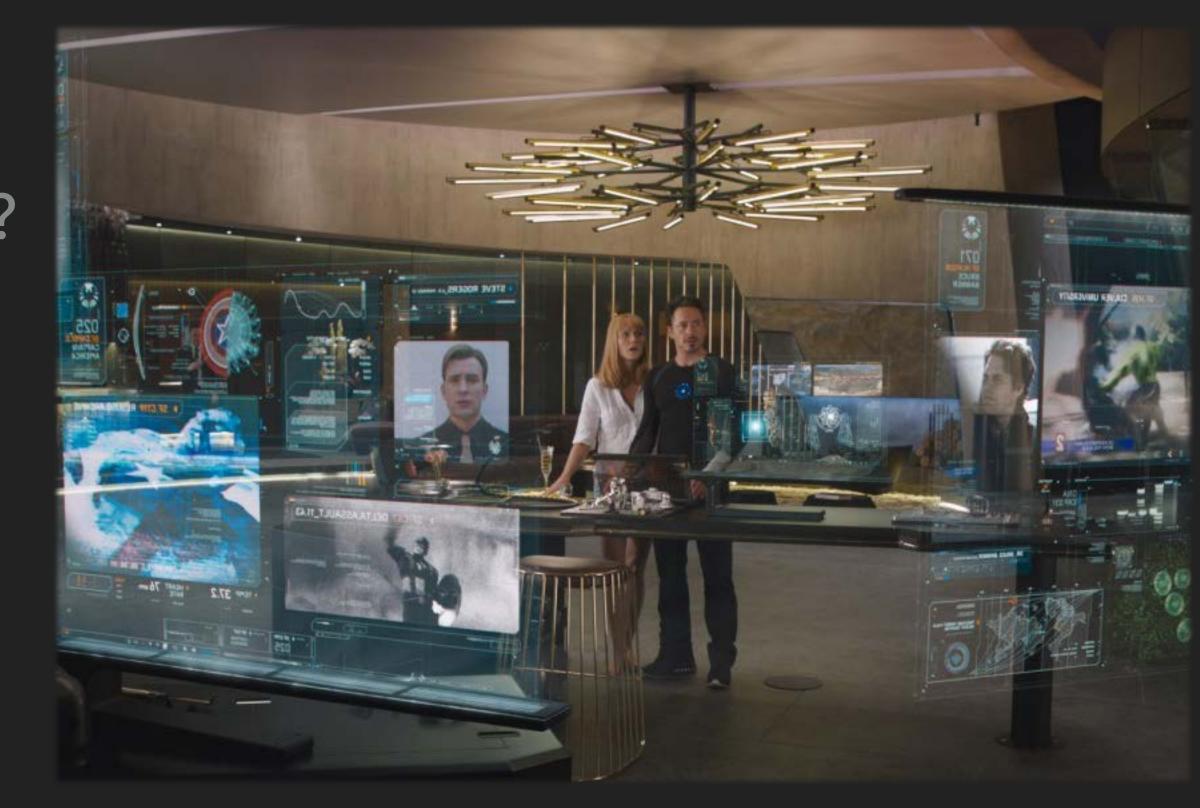
T. Marrinan, A. Nishimoto, J. A. Insley, S. Rizzi, A. Johnson, M. E. Papka, Interactive Multi-Modal Display Spaces for Visual Analysis, Proceedings of the 2016 ACM on Interactive Surfaces and Spaces, pp. 421-426, Niagara Falls, Canada, November 6, 2016.



- - How do we improve usability?
 - How do simplify supercomputing?



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





- 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



- 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

R. Hudson, J. Norris, L. B. Reid, K. Weide, G. C. Jordan, and M. E. Papka, Experiences Using Smaash to Manage Data-Intensive Simulations, Proceedings of the 20th International Symposium on High-Performance Parallel and Distributed Computing, pp. 205-15, San Jose, CA, June 2011.

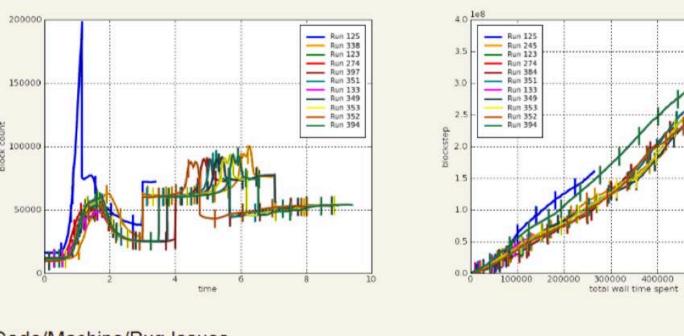
Simulations

63 128oYYY Series

Last Run	Simulation Name	Status	Time	Phase 1?	Phase 2?	Completed	Runner
371	8km 63 128048 m1.365 series 1	in progress	3.08 s	у	n	n	Cal
373	8km 63 128088 m1.365 series 1	in progress	4.97 s	У	n	n	Cal
394	8km 63 1280108 m1.365 series 1	completed	9.41 s	У	У	У	Klaus
353	8km 63 1280118 m1.365 series 1	completed	9.26 s	У	У	у	Klaus
351	8km 63 1280138 m1.365 series 1	completed	8.84 s	У	У	у	Klaus
349	8km 63 1280128 m1.365 series 1	completed	9.00 s	у	У	У	Klaus
384	8km 63 1280148 m1.365 series 1	completed	8.5 s	У	У	У	Lynn
352	8km 63 1280168 m1.365 series 1	completed	8.20 s	У	У	у	Klaus
??	8km 63_1280188 m1.365 series 1	in progress	4.5 s	у	у	n	Lynn

More Diagnostic Graphs

These mostly illustrate computational aspects of the simulations



Code/Machine/Bug Issues

- Code Changes Runtime Environment Changes
- Code Errors BGP Errors Bug Reports
- · Comparison of filesystem speed

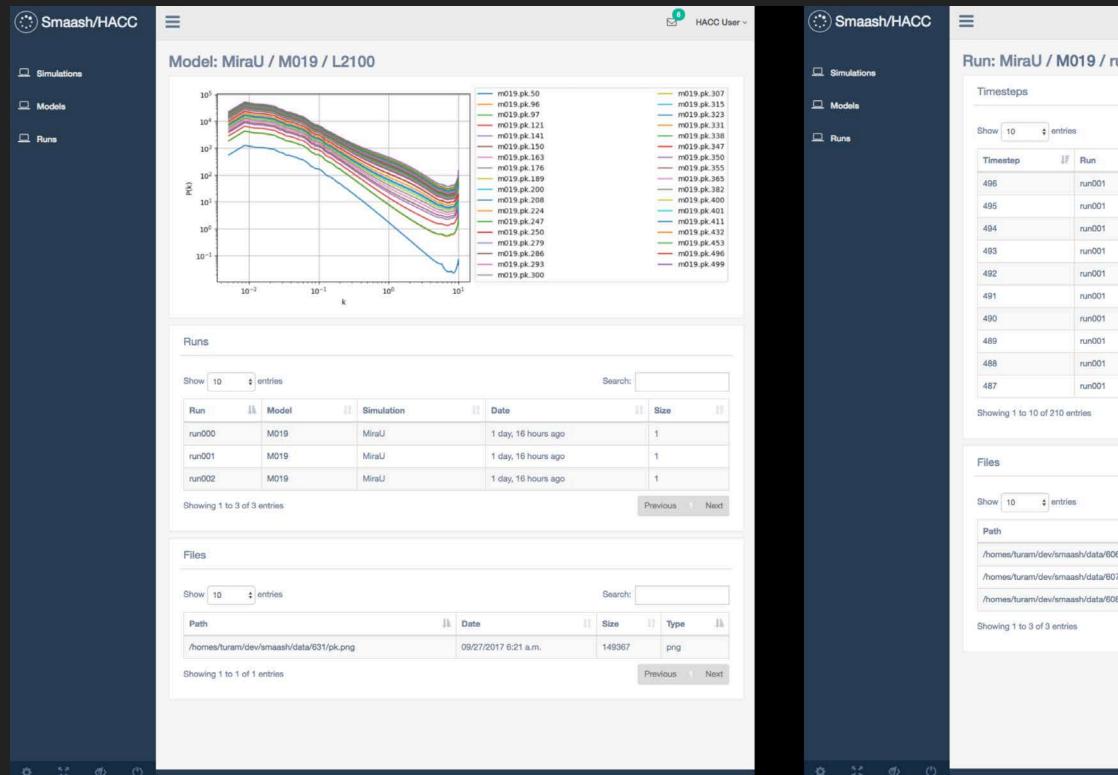




BIG IDEAS

HIGH PERFORMANCE COMPUTING RESEARCH OPPORTUNITIES

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



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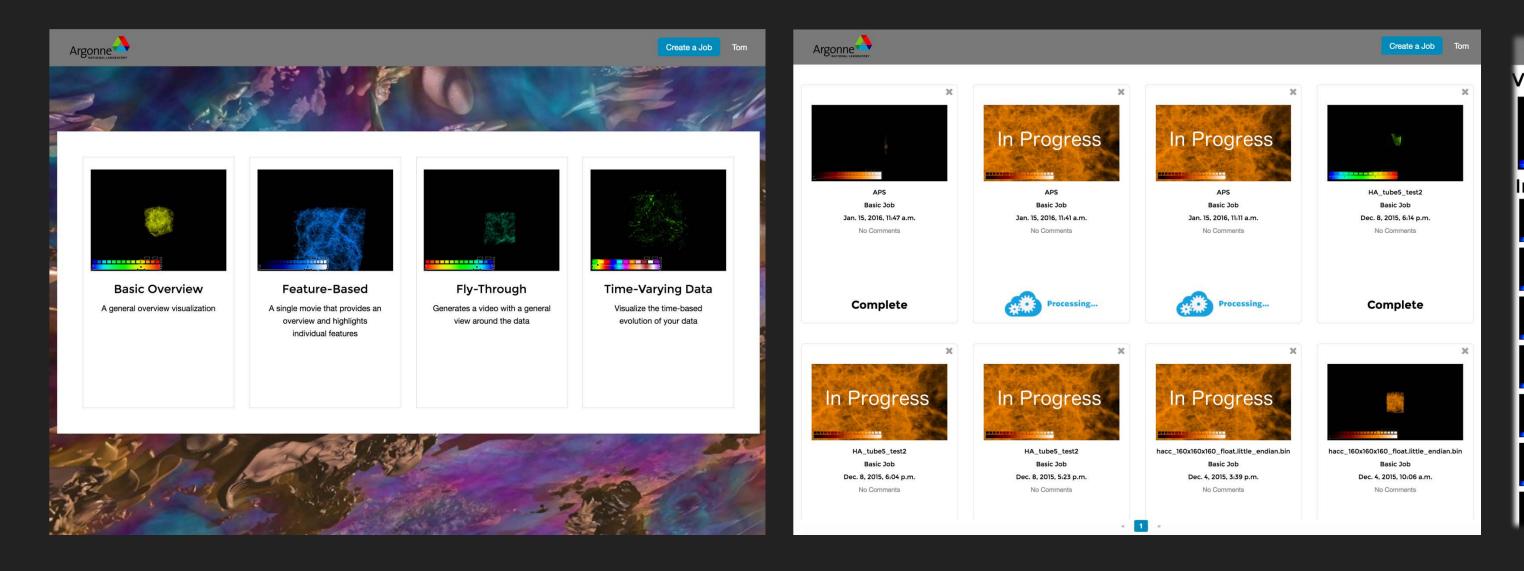
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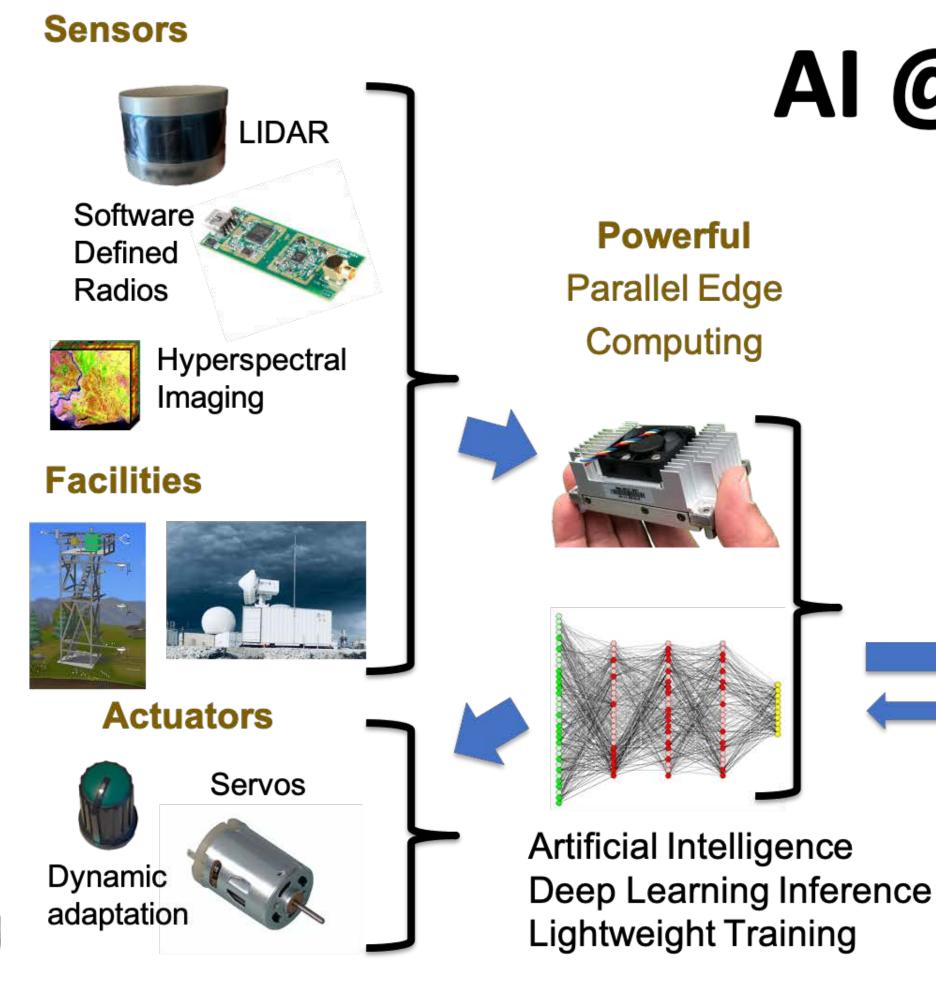
How do we enable scientists to be the most productive from start to finish?



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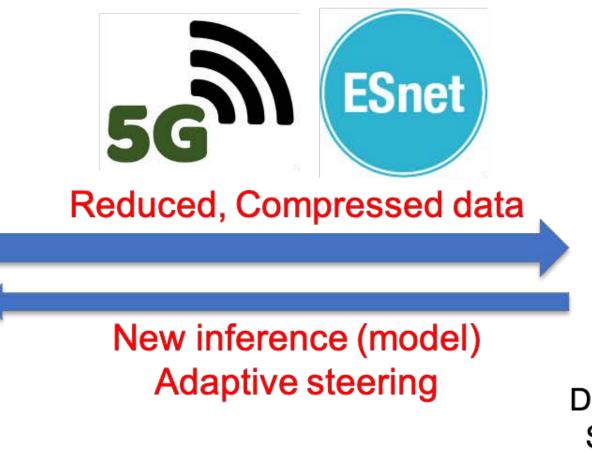


INTERNET OF THINGS (COMPUTING CONTINUUM) [EDGE COMPUTING]



Al @ Edge

Edge computing and deep learning with feedback for continuous improvement



HPC



Deep Learning Training Simulation / Forecast

Slide: Pete Beckman (ANL/NWU)





INTERNET OF THINGS (COMPUTING CONTINUUM) [EDGE COMPUTING]

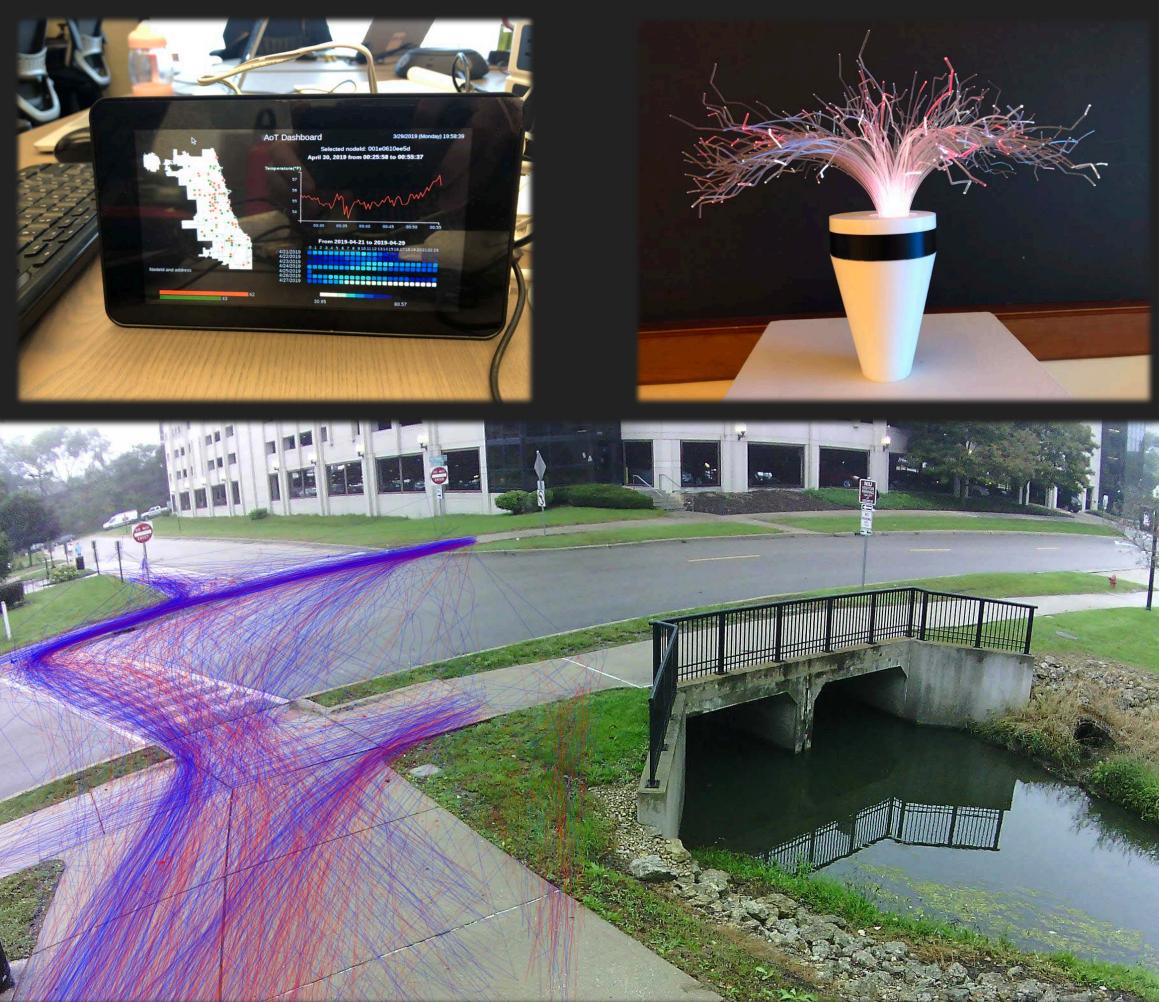




INTERNET OF THINGS (COMPUTING CONTINUUM) [EDGE COMPUTING]



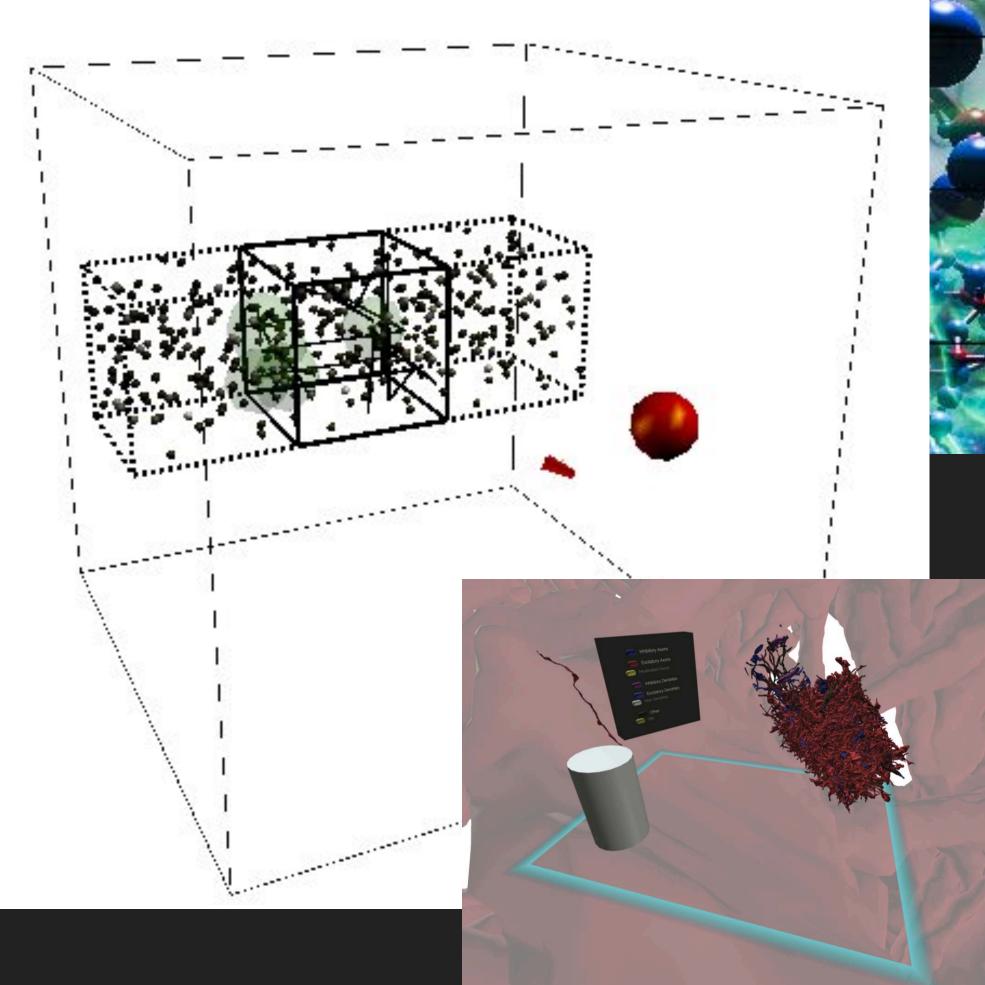
C. Catlett, P. Beckman N. Ferrier, H. Nusbaum, M. E. Papka, M. G. Berman, R. Sankaran, Measuring Cities with Software-Defined Sensors, Journal of Social Computing, 1(1), pp. 14 - 27, September 2020.





BIG IDEAS

VIRTUAL REALITY





32

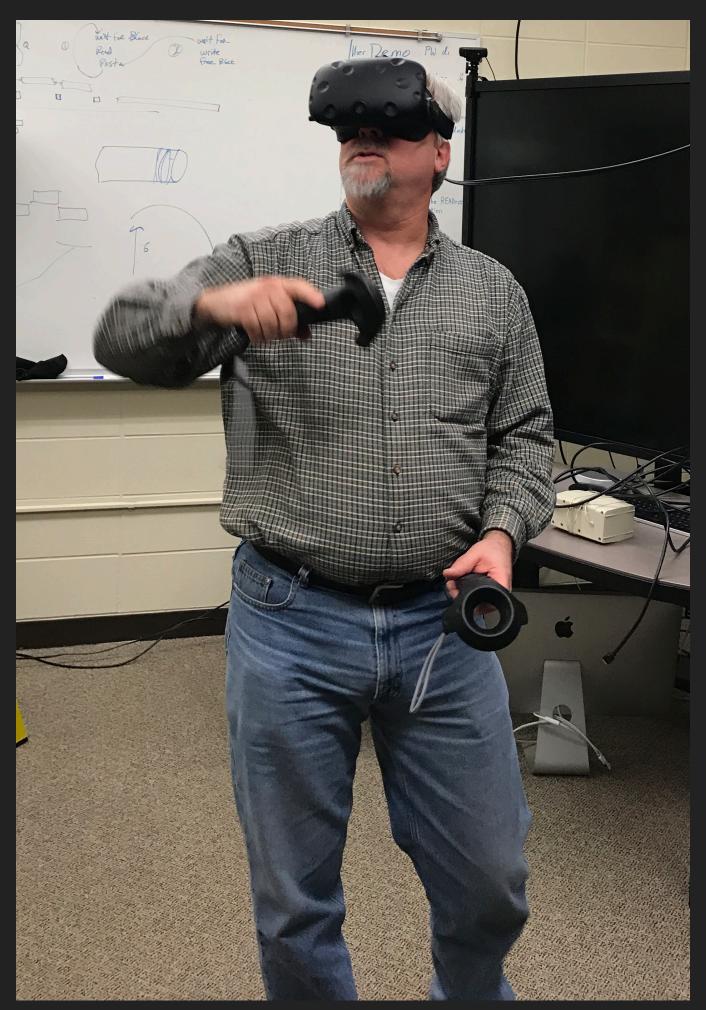
Use of Virtual Reality in Science

Usability, virtual interactions

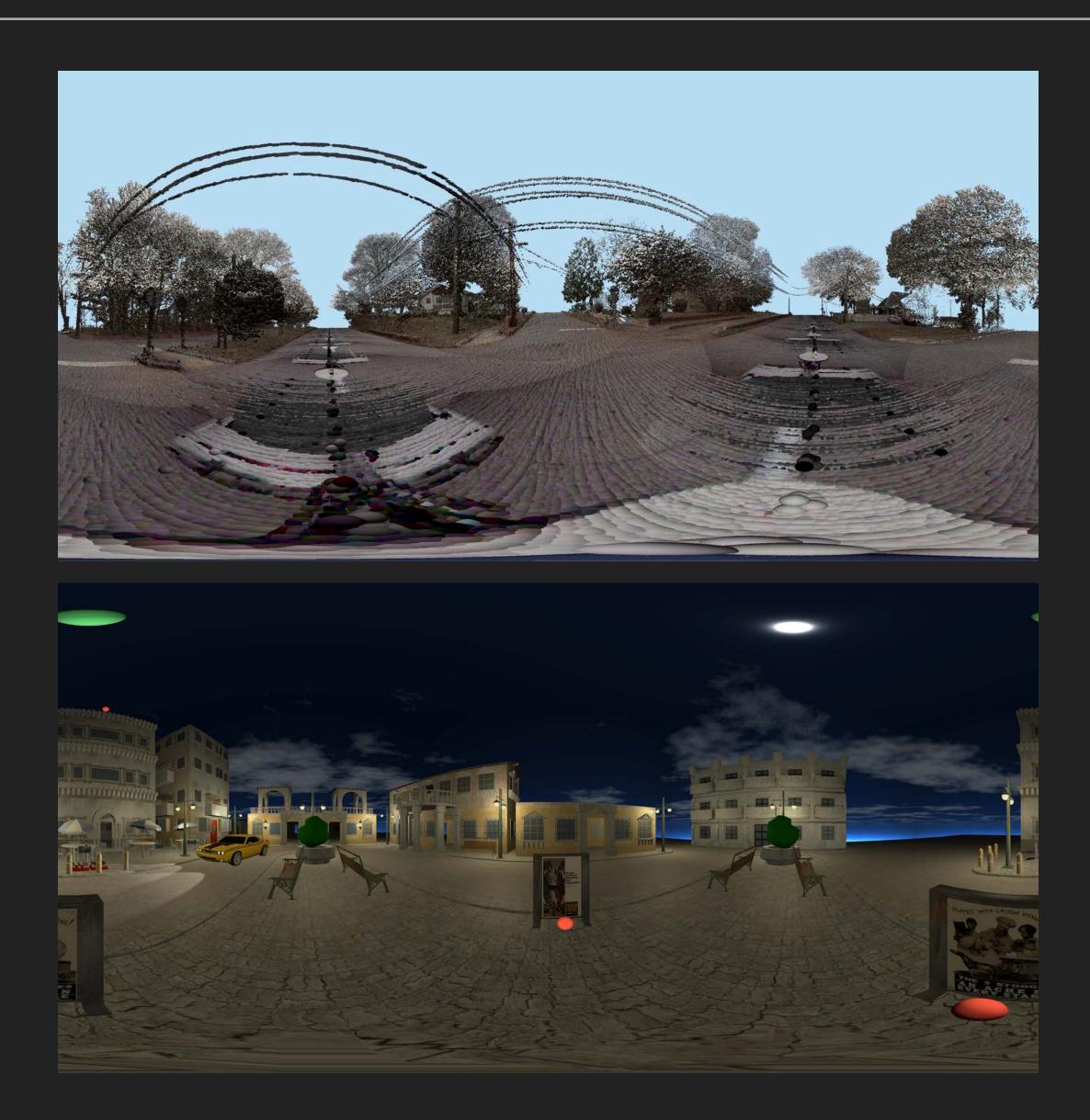
Rendering, realistic data in VR time

BIG IDEAS

VIRTUAL REALITY



T. Marrinan, M. E. Papka, Real-Time Omnidirectional Stereo Rendering: Generating 360° Surround-View Panoramic Images for Comfortable Immersive Viewing, Proceedings of IEEE VR 2021, Lisbon, Portugal, 03/27 - 04/01/2021.





SUMMER RESEARCH OPPORTUNITIES (IN PERSON NORMALLY, CURRENTLY VIRTUAL)



www.anl.gov/hr/argonne-career-and-internship-opportunities





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.





Spring 2019 ddiLab





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

Sir Isaac Newton

