ASCAC Early Career Virtual Panel

Panelists

Andrey Lokhov
Staff Scientist
Los Alamos National Laboratory

Joseph M. Lukens
Associate Professor
Purdue University

Ana Gainaru
Computer Scientist
Oak Ridge National Laboratory

Victor Mateevitsi
Computer Scientist
Argonne National Laboratory

Panel Moderator

Cindy Rubio González
Associate Professor
University of California, Davis

ASCAC Early Career Virtual Panel

Andrey Lokhov

Theoretical Division, Applied Mathematics Group

January 2024

Education and background

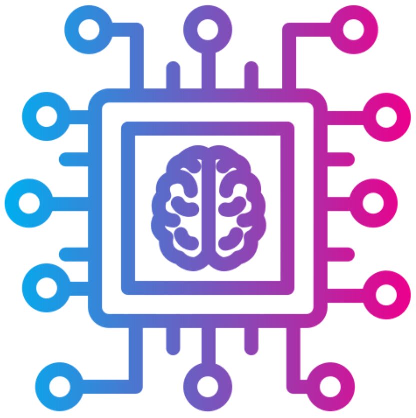
B.Sc. in **Physics** at Ecole Polytechnique, France

M.Sc. in **Theoretical Physics** at Ecole Polytechnique, France

Ph.D. in **Statistical Physics** at Universite Paris-Sud, France

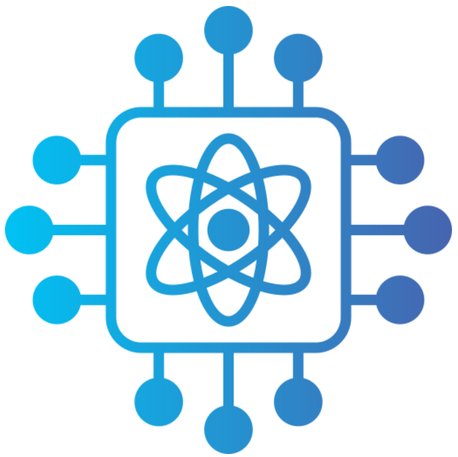
Postdoc → Scientist in **Applied Mathematics** at Los Alamos National Laboratory, USA

Main areas of my work and funding



Statistical Learning

Funding: DOE Office of Science ASCR Early Career

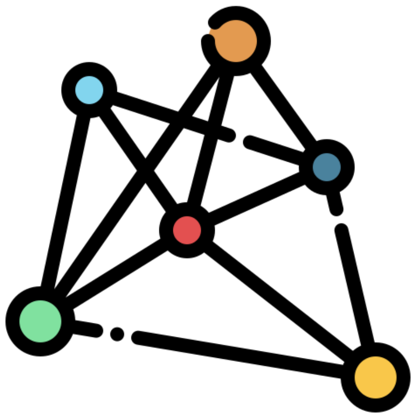


Quantum Computing

Funding: Defense Advanced Research Projects Agency (DARPA)

Power Grid

Funding: DOE Office of Electricity



Graph Algorithms

Funding: Laboratory Directed Research and Development (LDRD)

A Few Words on… Quantum Computing

Quantum Benchmarking Initiative

DARPA’s **Quantum Benchmarking Initiative (QBI)** aims to determine if it’s possible to build an industrially useful quantum computer much faster than conventional predictions.

Specifically, QBI is designed to rigorously **verify and validate** if any quantum computing approach can achieve utility-scale operation — meaning its computational value exceeds its cost — by the year 2033.

Funding: Defense Advanced Research Projects Agency (DARPA)

A Few Words on… Power Grid

U.S. Department of ENERGY

Grid Controls and Communications

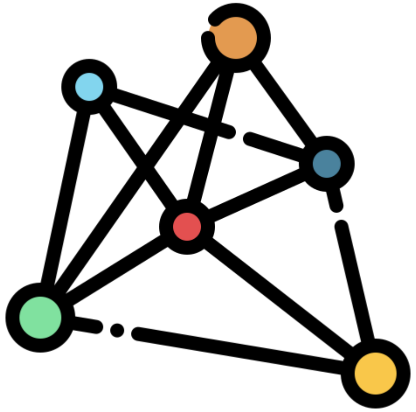
Real-time Valuation of Sensor Reliability:

Establish and benchmark a high-performance online sensor valuation method based on a novel idea for reliability assessment of measurements;

Use the developed metric to inform optimal sensor placement tools for enhanced grid reliability.

Funding: DOE Office of Electricity

A Few Words on… Graph Algorithms



LABORATORY DIRECTED RESEARCH & DEVELOPMENT
WHERE INNOVATION BEGINS

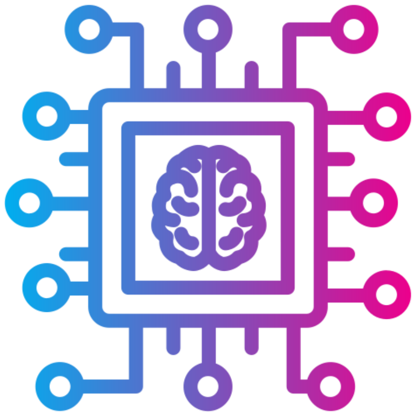
Novel Solutions for Out-of-Equilibrium Dynamics of Disordered Systems:

Is it possible to solve out-of-equilibrium reversible dynamics of disordered systems (epidemic spreading, dynamics of magnetic materials, *etc.*) and beat traditional Markov Chain Monte Carlo (MCMC) methods?

Making progress using a class of algorithms called dynamic message-passing (DMP)

Funding: Laboratory Directed Research and Development (LDRD)

A Few Words on… Statistical Learning



U.S. Department of ENERGY

Advanced Scientific Computing Research

Resurgence of Markov Random Fields for Scientific Machine Learning:
New Mathematics for an Old Framework

Advance mathematics behind machine learning methods for Markov Random Fields (MRFs);

Explore potential of MRFs to become a dominant paradigm for Scientific Machine Learning, and make impact in applications: many-body quantum physics, power grids, statistical physics, and field theories

Funding: DOE Office of Science ASCR Early Career Program

A Few Words on… Statistical Learning

Boltzmann distribution (Physics)

Gibbs measure (Mathematics)

Exponential family (Statistics)

Undirected graphical models, Markov random fields (Computer Science)

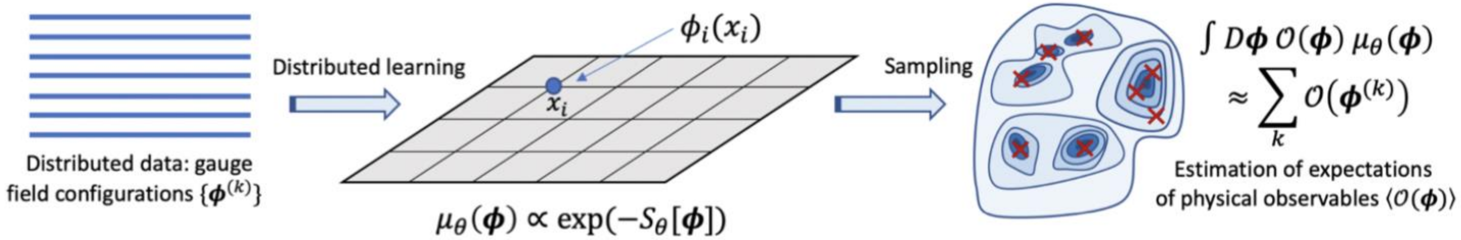
Log-linear model, Energy-based model, Boltzmann machine (Machine Learning)

$$\mu_\theta(\boldsymbol{x}) = \frac{1}{Z}\exp(-H_\theta[\boldsymbol{x}]) = \frac{1}{Z}\exp\left(-\sum_{k\in K}\theta_k\, q_k[\boldsymbol{x}]\right)$$

Gibbs distribution | "Hamiltonian" energy function | Parameters | Sufficient statistics

Applications:

- many-body quantum states
- power grids
- statistical physics
- field theories



Funding: DOE Office of Science ASCR Early Career Program

Team

Dr. Abhijith Jayakumar

Theory of MRF learning,
Quantum Computing

Dr. Minh Vu

Power grid dynamics

Dr. Shreya Shukla

Applications in field theories

Dr. Karthik Elamvazhuthi

Algorithms for MRF learning

Dr. Shiba Biswal

Algorithms for MRF sampling

Elmore Family School of Electrical and Computer Engineering

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Joseph M. Lukens

Purdue University

16 Jan. 2025

About myself: education

University of Alabama (2007–2011)

B.S. Electrical Engineering & Physics

Undergraduate research with Profs. Margaret Kim & Patrick Kung

Purdue University (2011–2015)

Ph.D. Electrical Engineering

Graduate research with Andy Weiner

In memoriam (1958–2024)

Dissertation

Novel applications of photonic signal processing: temporal cloaking and biphoton pulse shaping

About myself: career

Oak Ridge National Lab

- 2015–present
  - Eugene P. Wigner Fellow (2015–2018)
  - Research Scientist (2018–2022)
  - Joint Faculty Appointment (2022–present)
- Won Early Career Award from DOE ASCR in 2019
  - *Scalable Architectures for Hybrid Quantum/Classical Networking*

Arizona State University

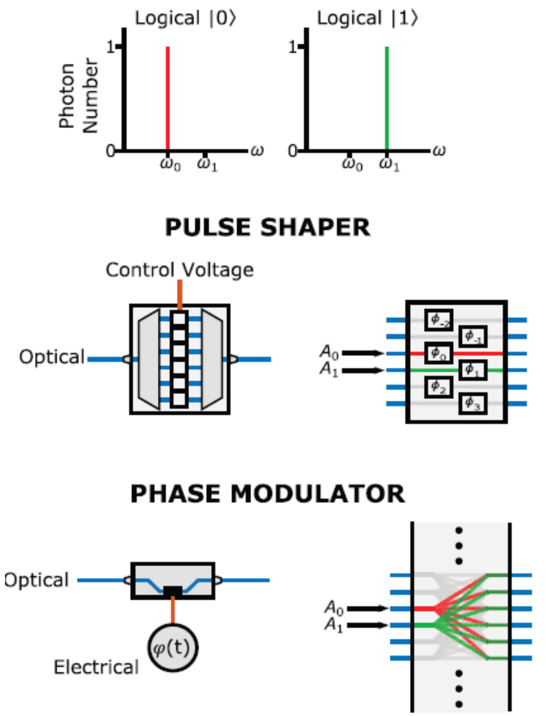
- 2022–present
  - Sr. Director of Quantum Networking & Research Professor (2022–2024)
  - Adjunct Professor (2025–present)

Purdue University

- 2025–present
  - Associate Professor of Electrical & Computer Engineering

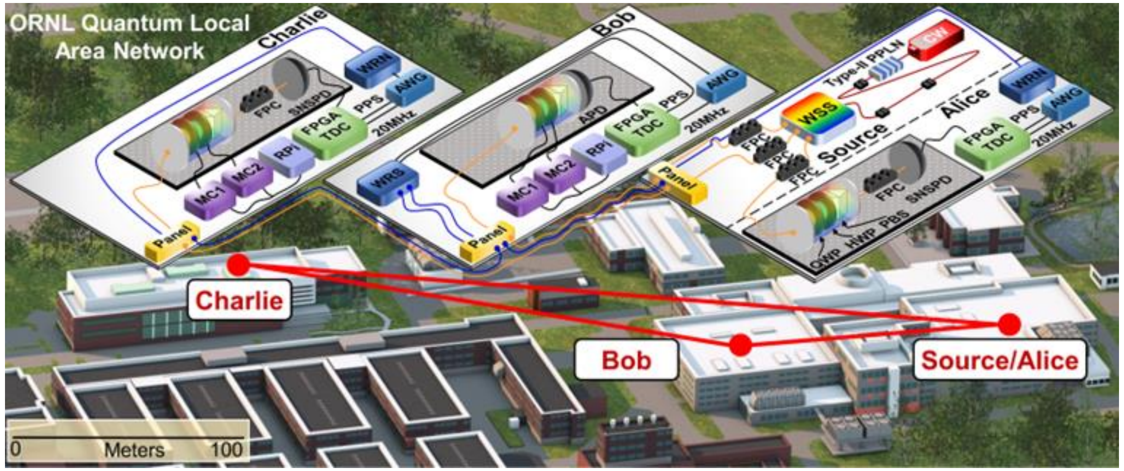
Research interests

Frequency-bin quantum information



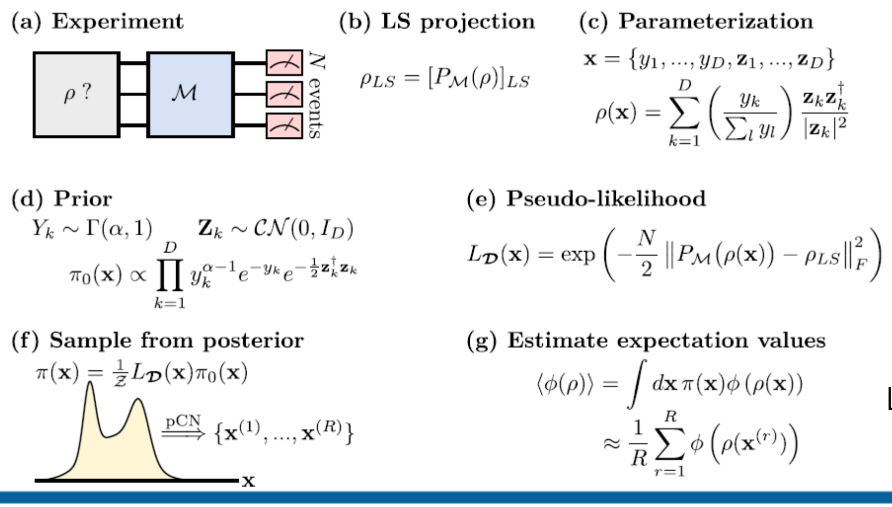
J. M. Lukens & P. Lougovski, *Optica* **4**, 8 (2017).

Quantum networking



M. Alshowkan, B. P. Williams, P. G. Evans, N. S. V. Rao, E. M. Simmerman, H.-H. Lu, N. B. Lingaraju, A. M. Weiner, C. E. Marvinney, Y.-Y. Pai, B. J. Lawrie, N. A. Peters, & J. M. Lukens, *PRX Quantum* **2**, 040304 (2021).

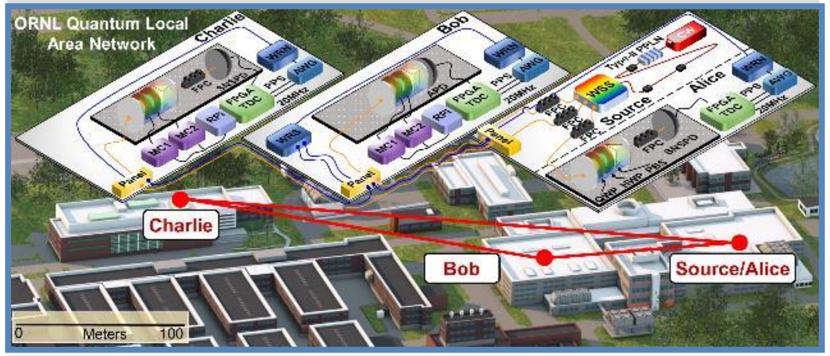
Bayesian quantum state tomography



J. M. Lukens, K. J. H. Law, A. Jasra, & P. Lougovski, *New J. Phys.* **22**, 063038 (2020).

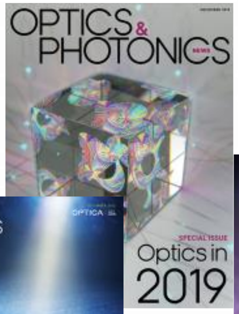
Early Career Award highlights

QLAN testbed



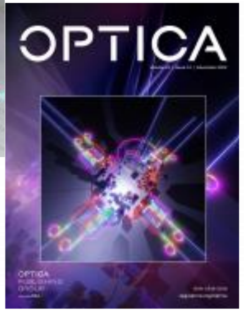
- First deployed **flex-grid** quantum network.
- Picosecond timing with **White Rabbit**.
- Secure classical comms with **QKD**.

M. Alshowkan *et al.*, *PRX Quantum* **2**, 040304 (2021).
M. Alshowkan *et al.*, *J. Opt. Commun. Netw.* **14**, 493 (2022).

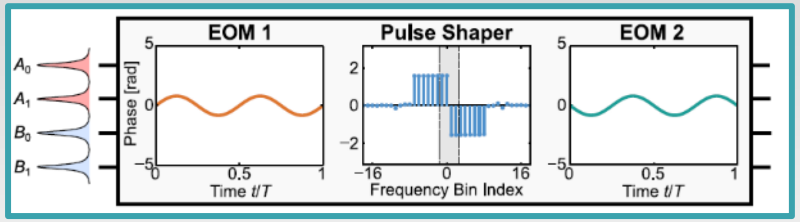


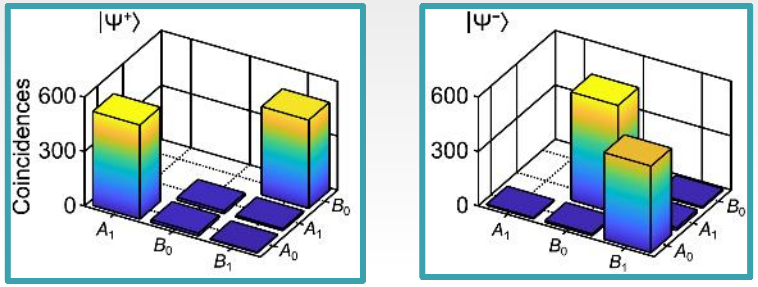
Artifacts

35 journal articles
47 conference papers
1 book chapter
1 patent



Frequency-bin networking

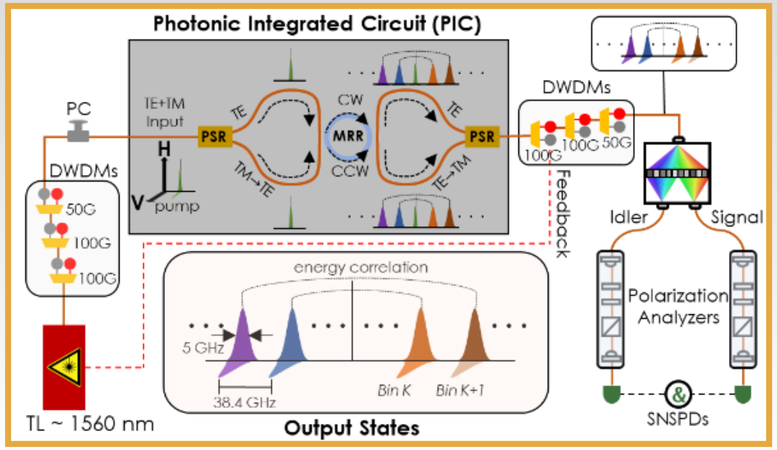




- First **Bell state analyzer** for frequency-bin qubits.
- Building block for **frequency-based quantum repeaters**.

N. B. Lingaraju *et al.*, *Optica* **9**, 280 (2022).

Silicon photonics



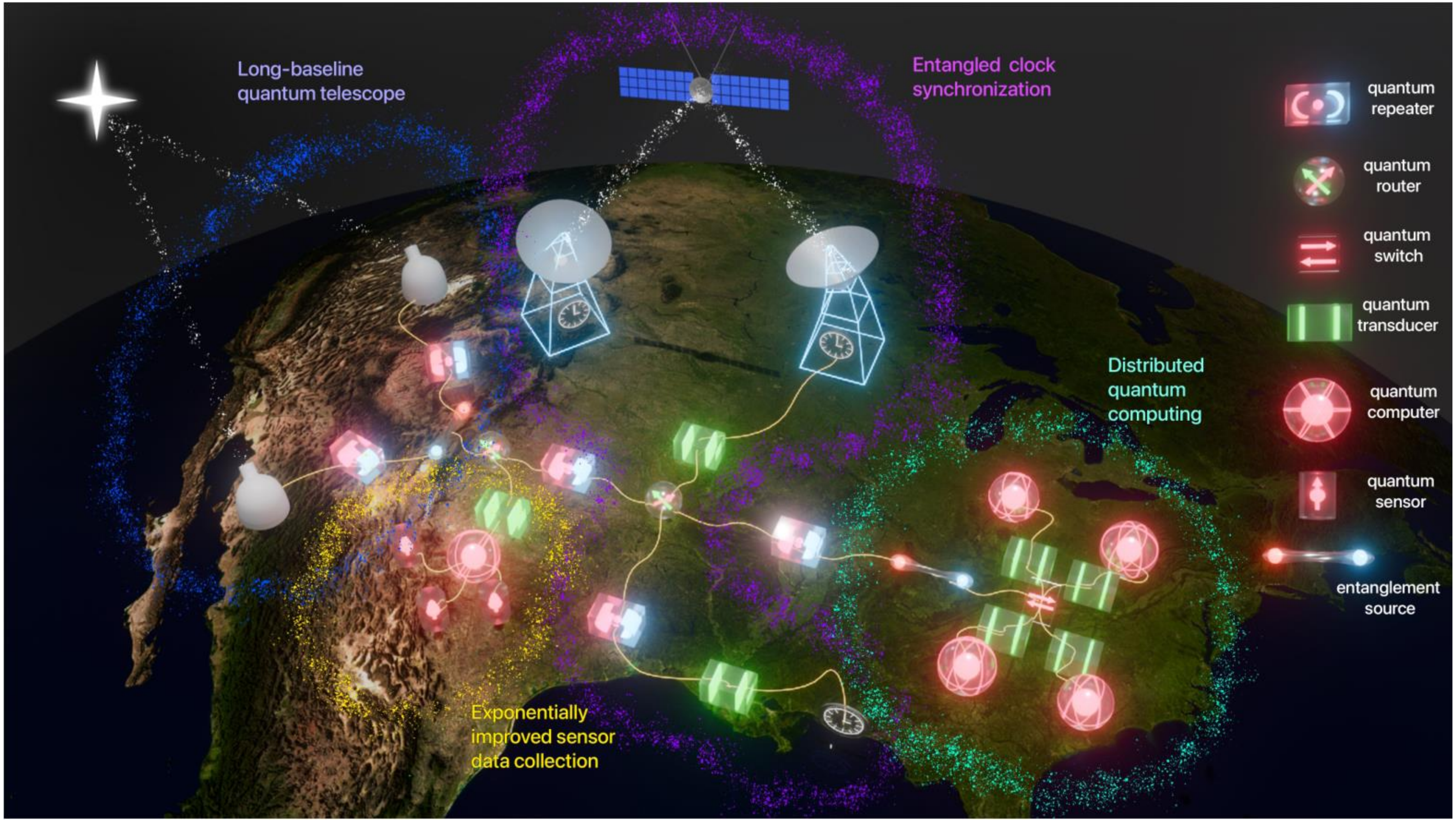
- **All-CMOS** design for frequency-polarization entanglement.
- Over **100 channels** of high-fidelity polarization states.

A. Miloshevsky *et al.*, *Optica Quantum* **2**, 254 (2024).

Collaborators

A. M. Weiner — Purdue University
B. T. Kirby — DEVCOM Army Research Laboratory
T. J. Kippenberg — EPFL
S. M. Kim — The University of Alabama
K. J. H. Law — The University of Manchester
T. A. Searles — UIC
S. Estrella — Freedom Photonics, a Luminar company

A possible future…



from the *Quantum Information Science Applications Roadmap for the U.S. Department of Energy* (December 2024)

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Ana Gainaru

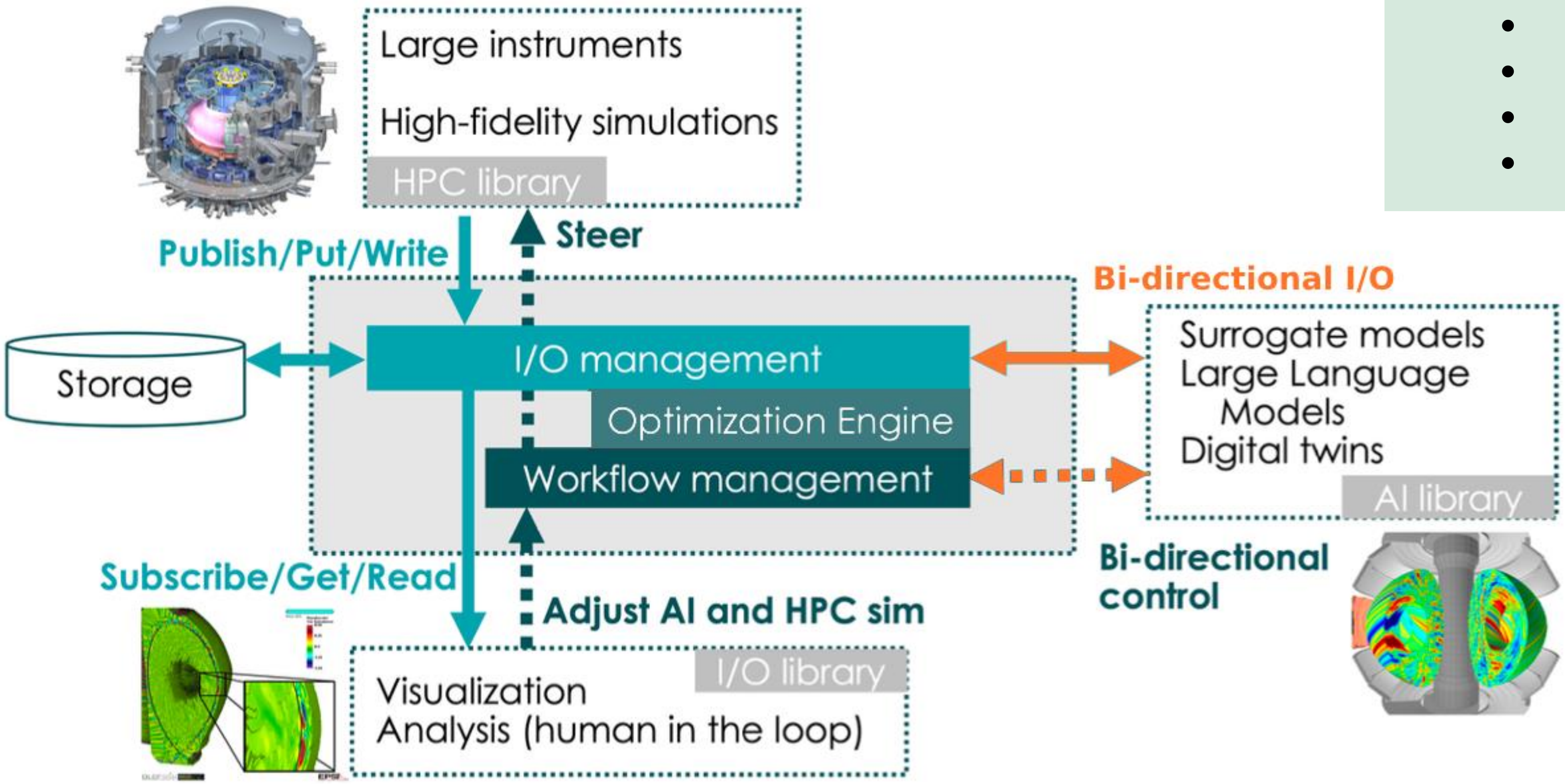
Workflow System Group, Data and AI systems Section

CSMD, Oak Ridge National Laboratory

Data and workflow management for complex scientific application

gainarua@ornl.gov

HPC application landscape



Applications are becoming proxy for experiments

Workflows combine
- High fidelity simulations
- Instruments
- Visualization services
- Analysis
- AI surrogate models
- Digital twins

SKA (Square Kilometer Array)
- Generating 1 TB/s data

Cancer research
- Ensemble runs for 10k+ images

Fusion
- Simulations training digital twins
  - Bi-directional feedback
  - Human in the loop

Background

- Interests
  - **Data fusion** with extreme and small data
  - **Coupling** between traditional HPC and AI
  - Extract **knowledge** from data
  - Smart **querying** capabilities
    - For data or for performance monitoring

- ASCR projects
  - SciDAC FES
  - Data management
  - RAPIDS

- PhD at **UIUC**
  - The Blue Waters project, **performance optimization and resilience**
  - Advisor: Marc Snir

ILLINOIS
UNIVERISTY OF ILLINOIS AT URBANA-CHAMPAIGN

- **Mellanox**
  - **Data transfer** optimization for MPI collective communication using **networking** features

- **Vanderbilt** University
  - **Scheduling** stochastic applications of HPC systems
  - Medical **AI applications**

- **ORNL** (since 2020)
  - **I/O** optimizations and **query** engine
  - **Workflow** modeling and scheduling

Research focusing on optimizing the performance of applications using HPC

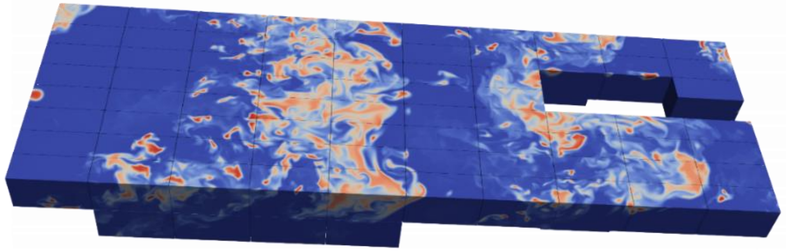
Oak Ridge National Laboratory

Highlights

Data management

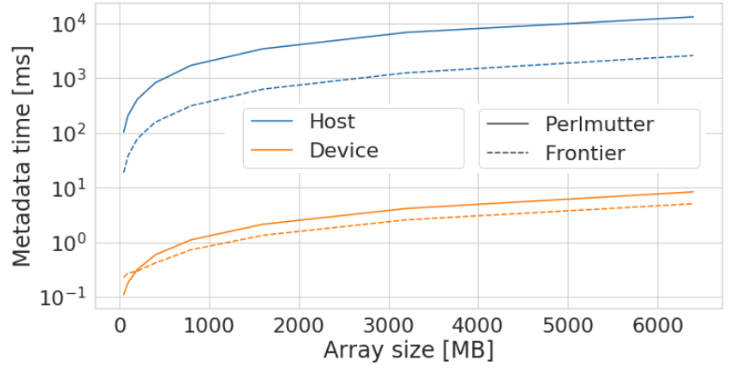
In-situ and remote analysis of S3D data

- Complex querying
  - Using quantities of interest
  - User-defined accuracy
  - On remote data



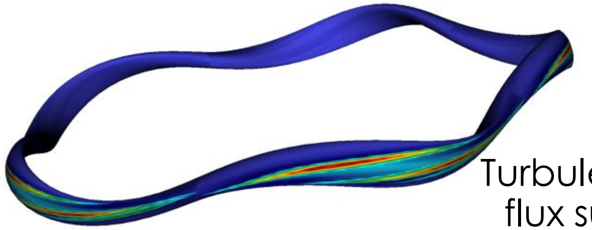
Local visualization in a region of interest with 0.1 accuracy

Workflow management



Metadata time between the CPU and GPU backend used by I/O libraries

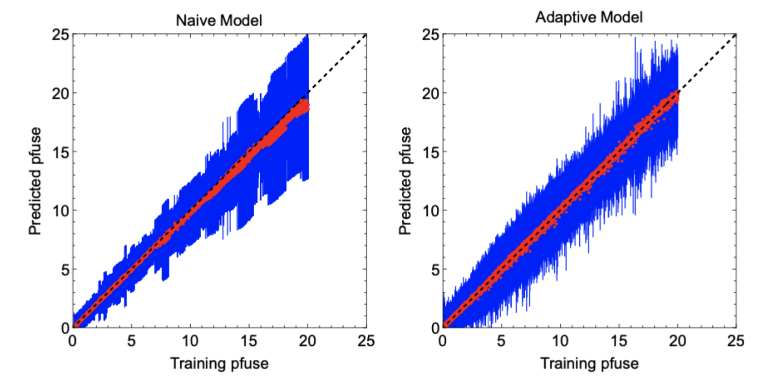
- Code coupling
  - The output time on Frontier is 17 times faster than the previous I/O interface
  - The cost of code coupling is less than 1%



Turbulence intensity on one of the islands flux surfaces obtained running GX with Trinity and Genray

Application impact

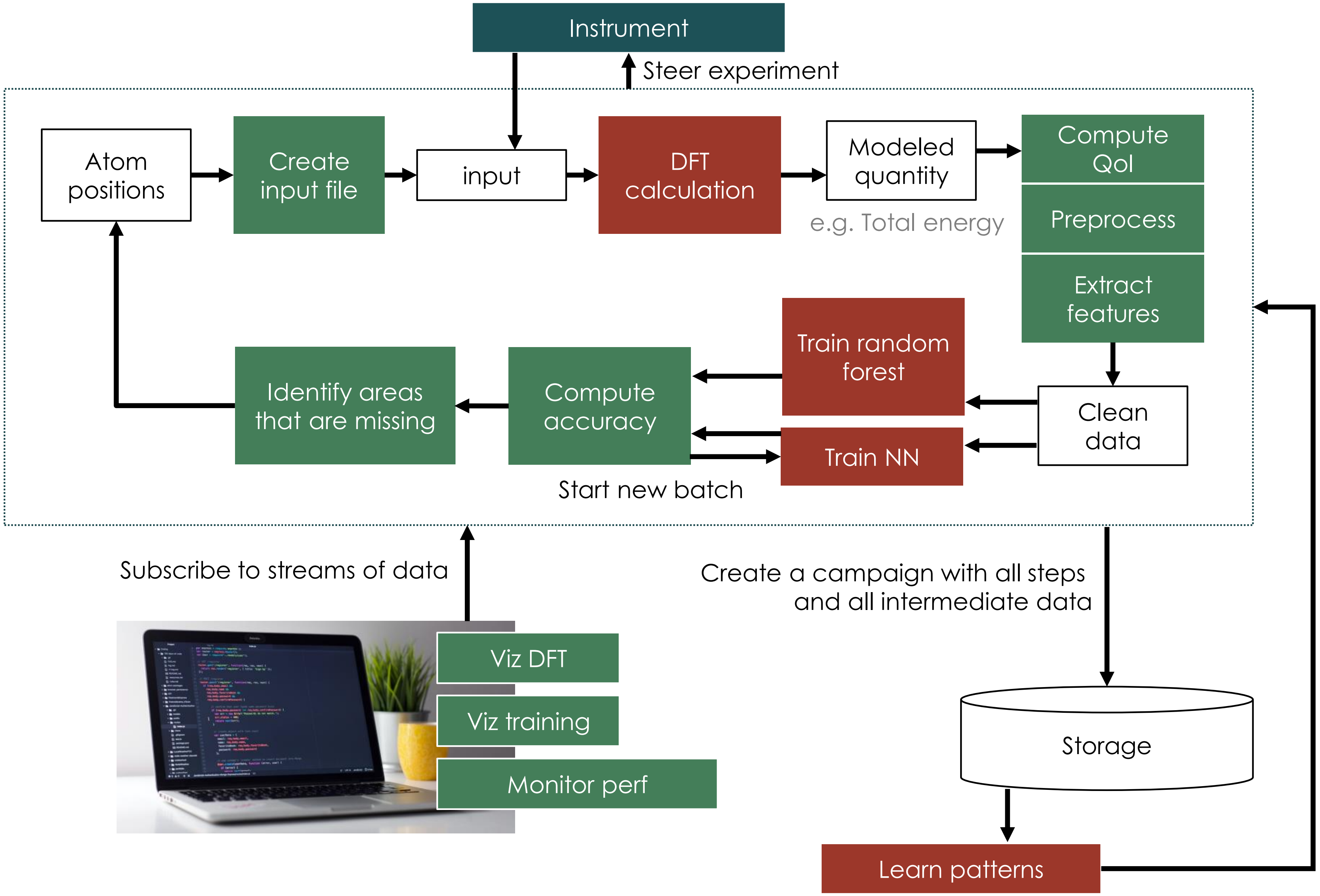
- Adaptive training workflow optimization
  - Streaming improved the I/O time by 75%
  - Having a GPU backend available in ADIOS improves I/O by 15%



An adaptively trained model provides more accurate prediction at high electron fusion power output.

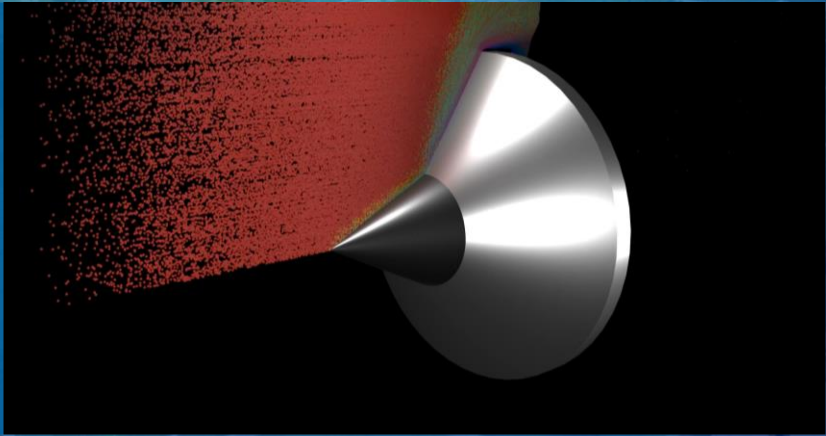
Future: AI driven workflows

- **Challenges**
  - Digital twin creation and updating
  - Query campaigns of runs
  - Schedule all intermediate analysis codes
    - Agent based
  - Keep track of intermediate representation of data
  - Learn from access patterns
    - Prefetch and pre-compute



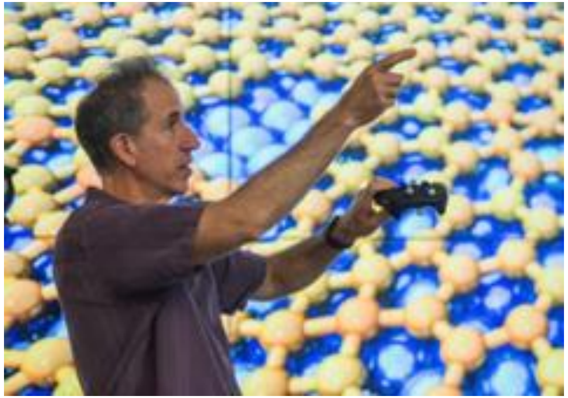
JANUARY 16, 2025

DOE ASCAC EARLY CAREER VIRTUAL PANEL

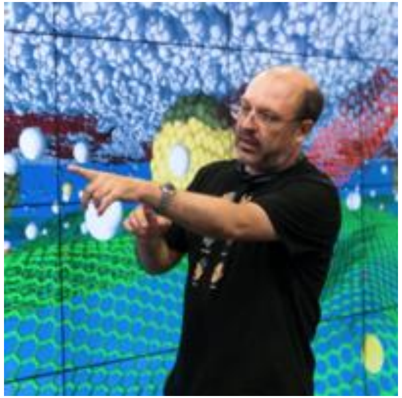


VICTOR MATEEVITSI
Assistant Computer Scientist

ALCF VISUALIZATION AND DATA ANALYTICS GROUP



Joe Insley
Team Lead



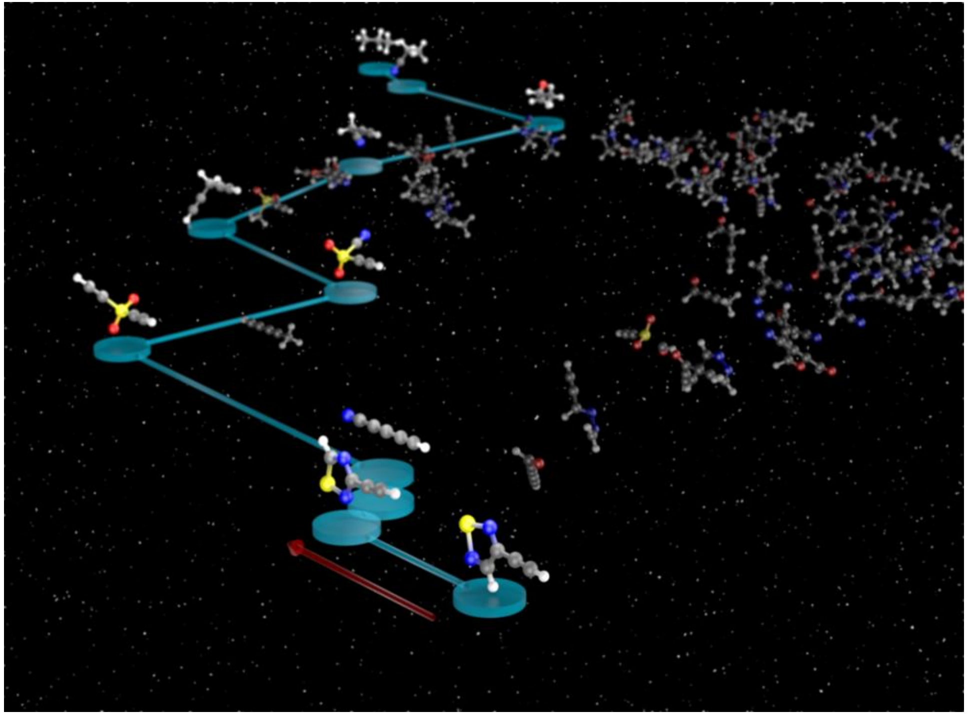
Silvio Rizzi
Computer Scientist

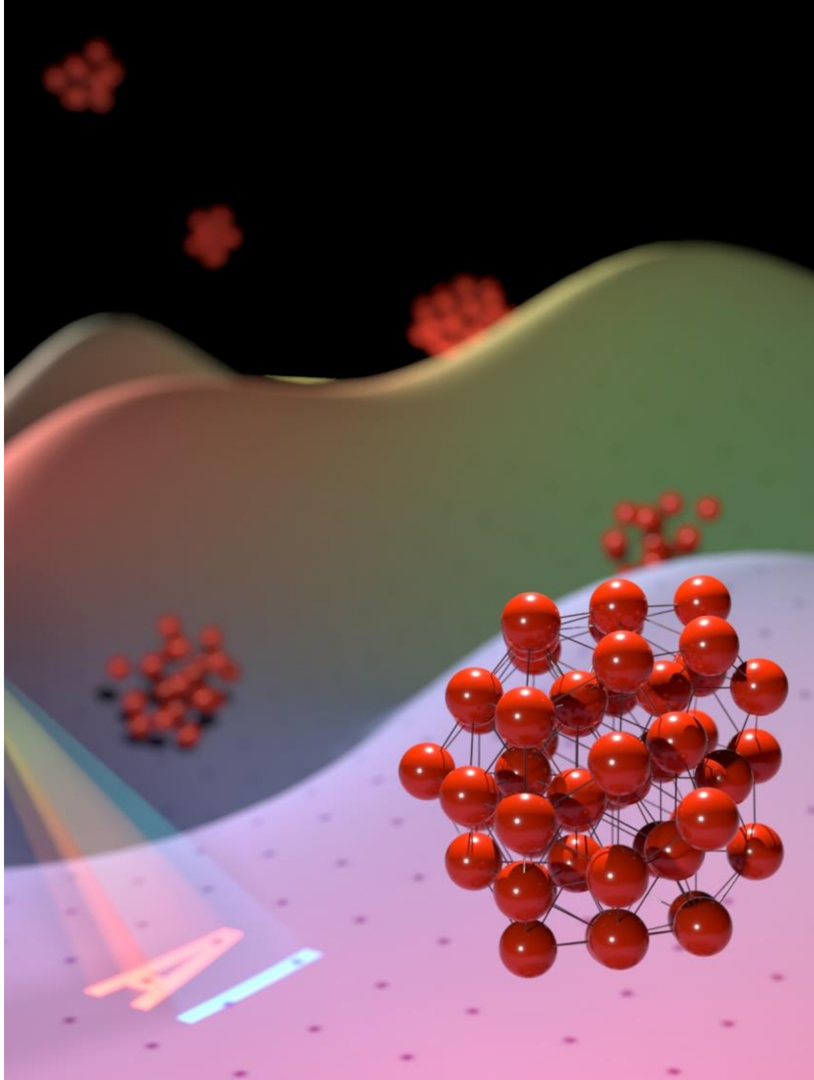
Victor Mateevitsi
Assistant Computer Scientist

Janet Knowles
Principal Software Engineering Specialist

Geng Liu
Postdoctoral Appointee

PRODUCTION VIS





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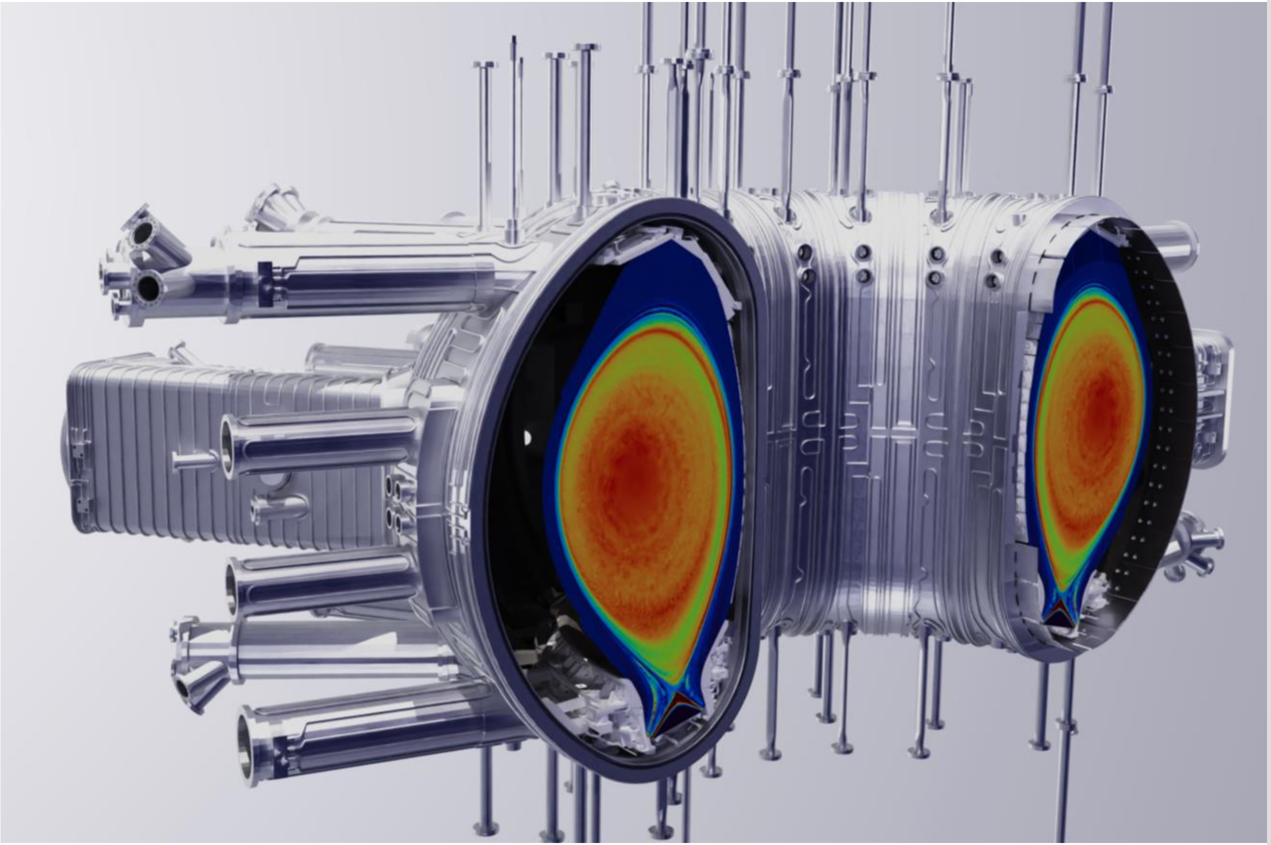

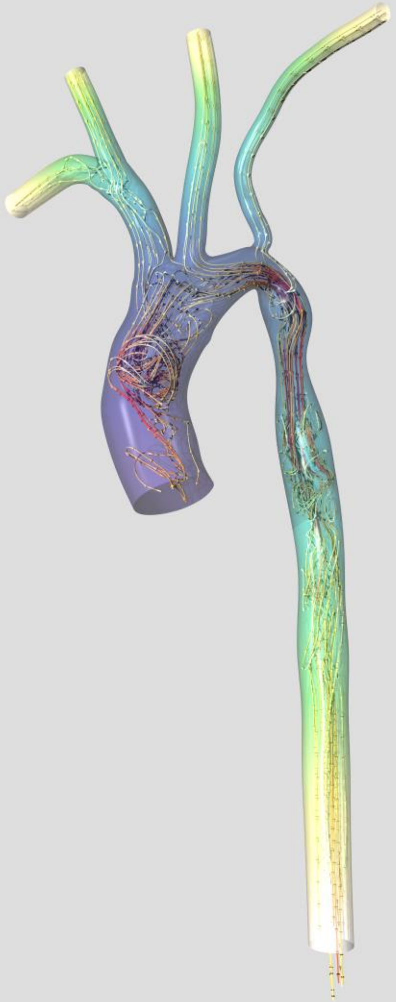

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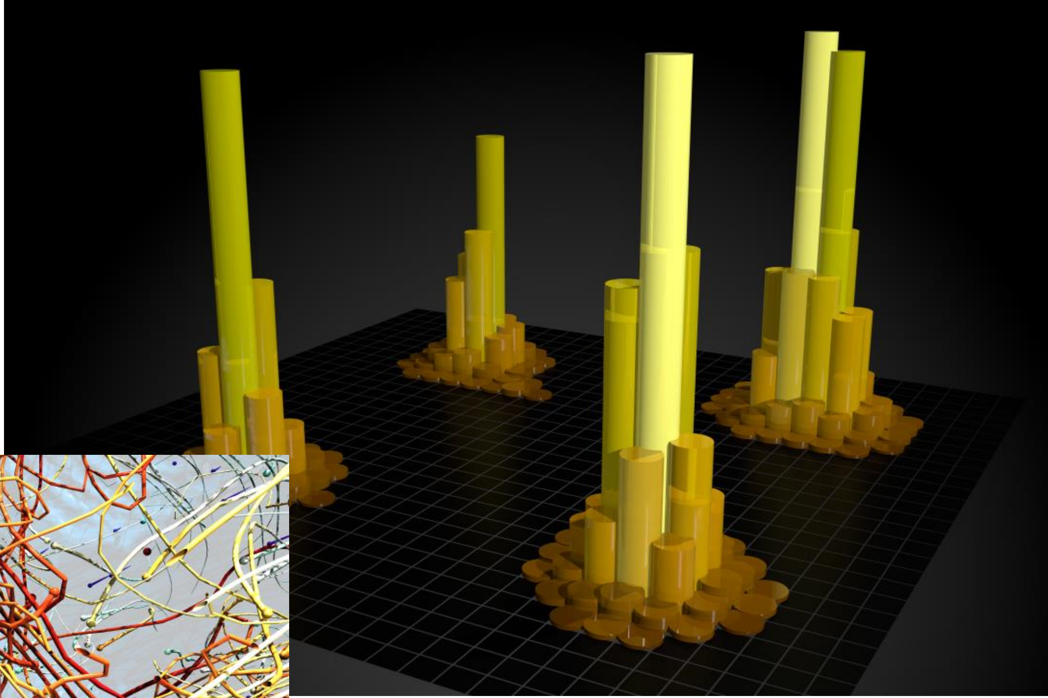
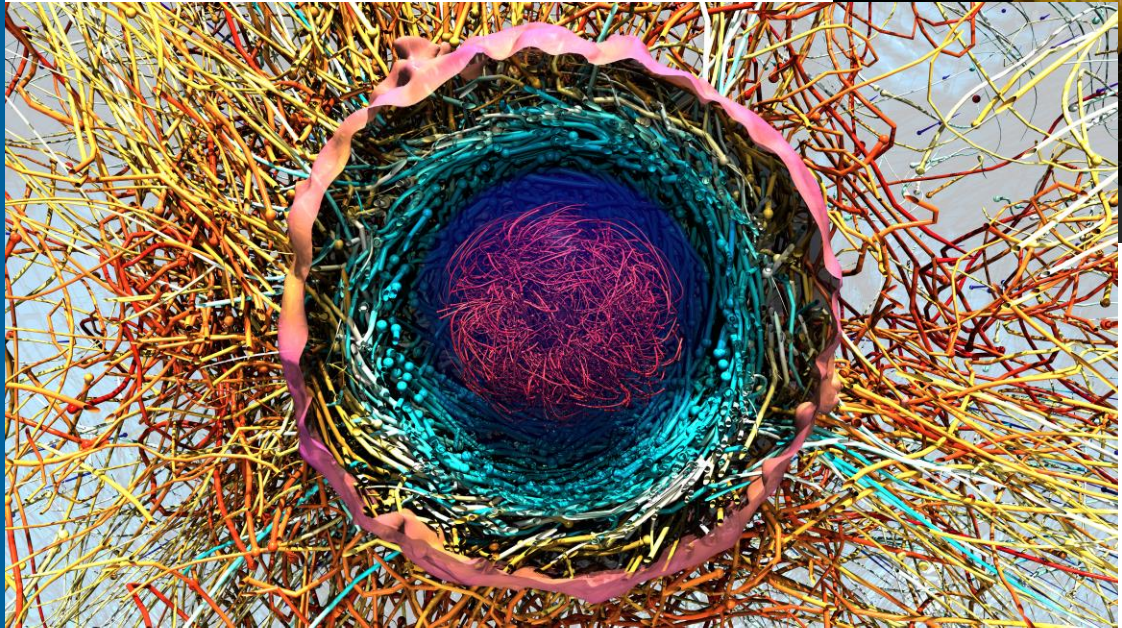
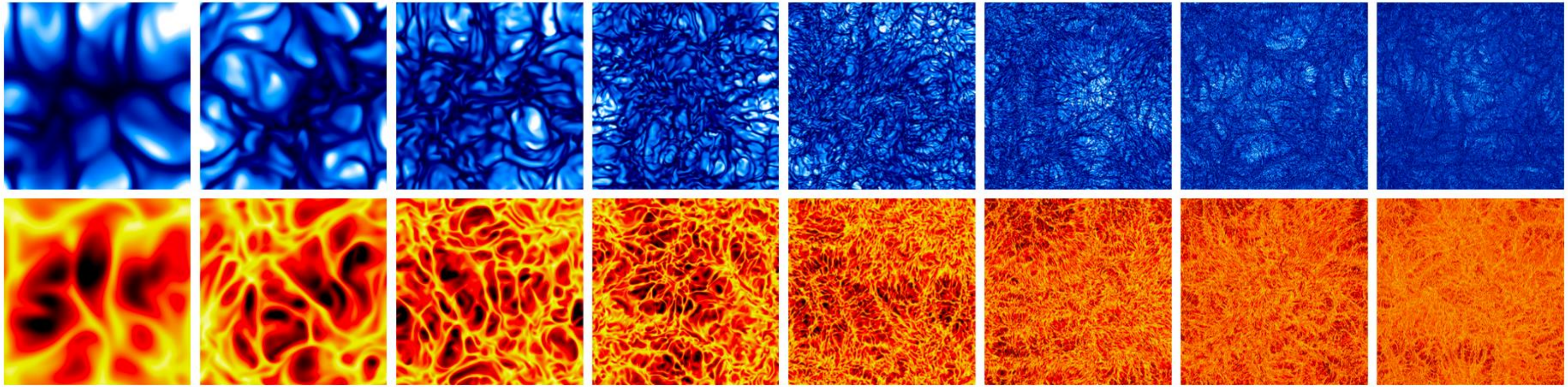


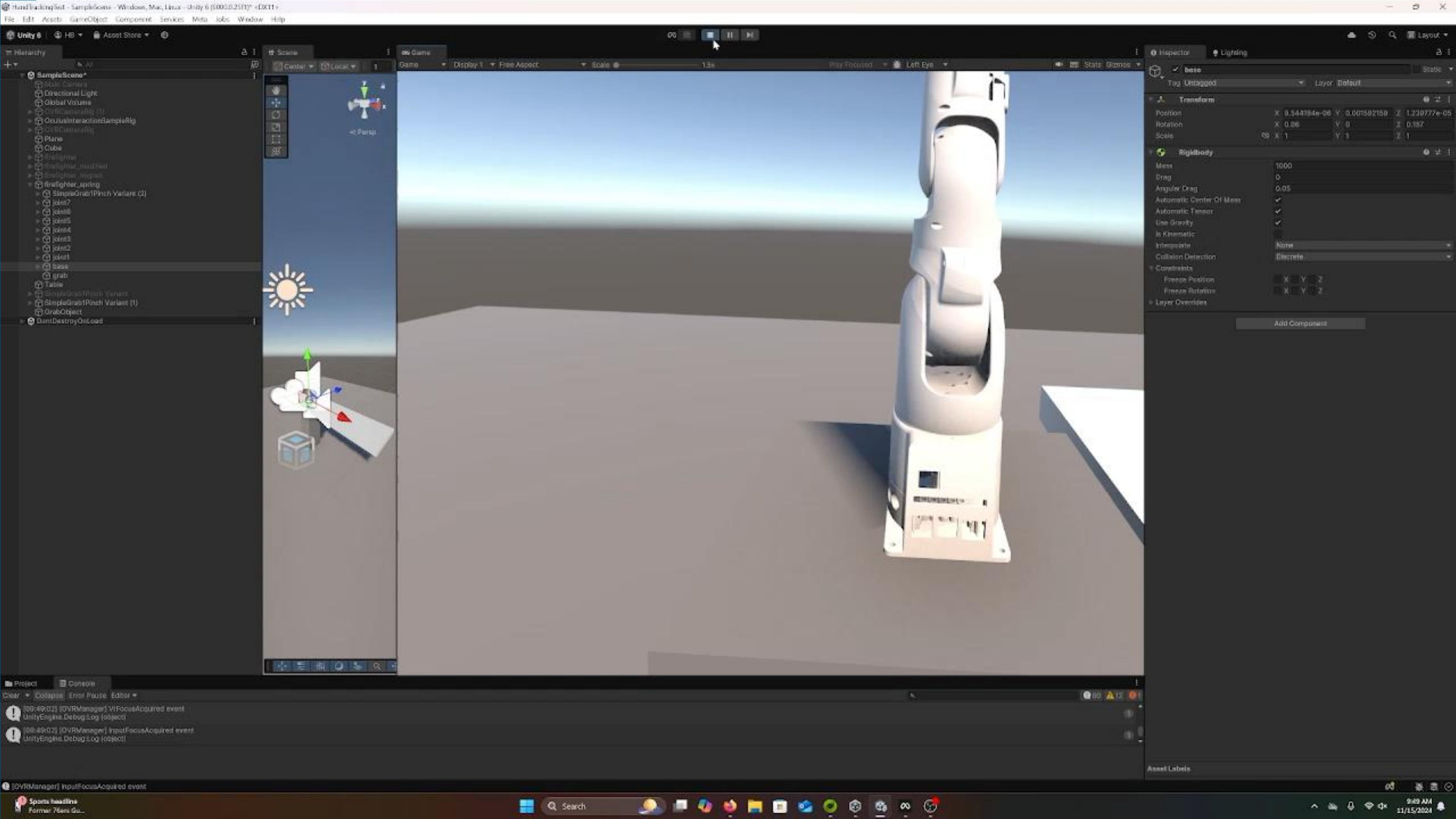


INSITU VIS

- In-situ visualization of NekRS (CFD code) 🥇
- Bi-directional steering 🥇
- Concurrent CPU (LDAV poster)



TELE-ROBOTICS TO TELE-AUTONOMOUS ROBOTICS FOR ISOTOPE PRODUCTION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Unity 6
Asset Store
Hierarchy
SampleScene*
Directional Light
Global Volume
OculusInteractionSampleRig
Plane
Cube
firefighter_spring
SimpleGrab1Pinch Variant (2)
joint7
joint6
joint5
joint4
joint3
joint2
joint1
base
grab
Table
SimpleGrab1Pinch Variant (1)
GrabObject
DontDestroyOnLoad
Scene
Game
Display 1
Free Aspect
Scale
1.5x
Left Eye
Stats
Gizmos
< Persp
Inspector
Lighting
base
Tag Untagged
Layer Default
Transform
Position
Rotation
Scale
Rigidbody
Mass 1000
Drag 0
Angular Drag 0.05
Automatic Center Of Mass
Automatic Tensor
Use Gravity
Is Kinematic
Interpolate None
Collision Detection Discrete
Constraints
Freeze Position
Freeze Rotation
Layer Overrides
Add Component
Asset Labels
Project
Console
Clear
Collapse
Error Pause
Editor
[09:49:02] [OVRManager] VrFocusAcquired event
UnityEngine.Debug:Log (object)
[09:49:02] [OVRManager] InputFocusAcquired event
UnityEngine.Debug:Log (object)
[OVRManager] InputFocusAcquired event
Search

DIGITAL TWINS AND AI-ENABLED & IMMERSIVE ENVIRONMENTS FOR AUTOMATED SCIENTIFIC LABORATORIES (DAIMSL)

Goal: create **automated**, **self-driving laboratories** by integrating robotics, augmented/virtual reality (AR/VR), and digital twin (DT) technologies.

- AI driven-process automation: Record human-operated robotic tasks to **train AI models** that automate these tasks over time

- Digital Twins: model and simulate lab processes in real-time to predict and prevent risks, ensure protocols are followed, and optimize experimental outcomes.

THANK YOU!

- Questions?