WORKSHOP

ALCF Hands-on HPC Workshop

September 23-25 & October 7-9, 2025
Argonne National Laboratory

Overview of Visualization

Joseph Insley, ALCF Visualization and Data Analytics Team Lead
Thursday, September 25

U.S. DEPARTMENT of ENERGY

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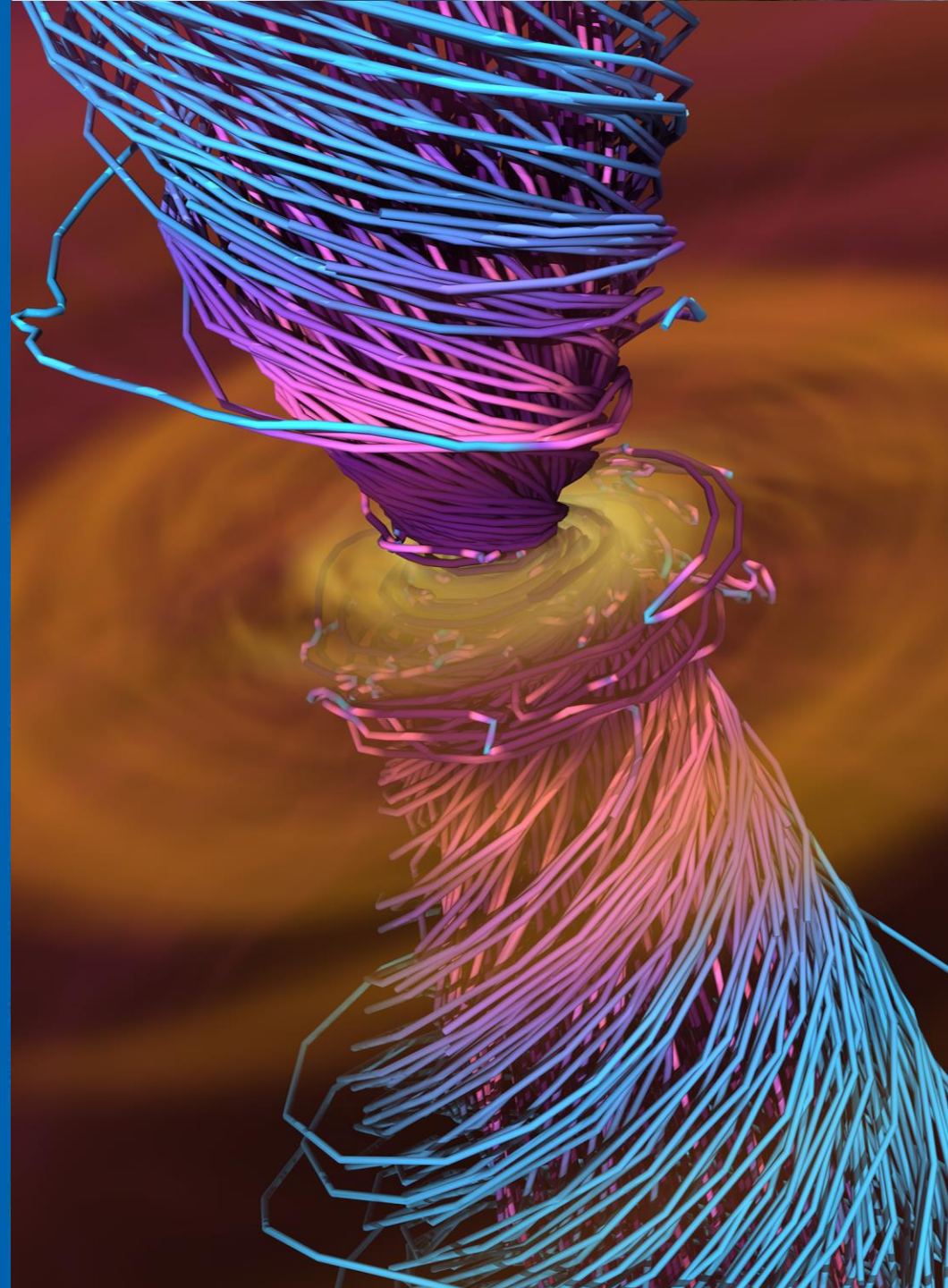
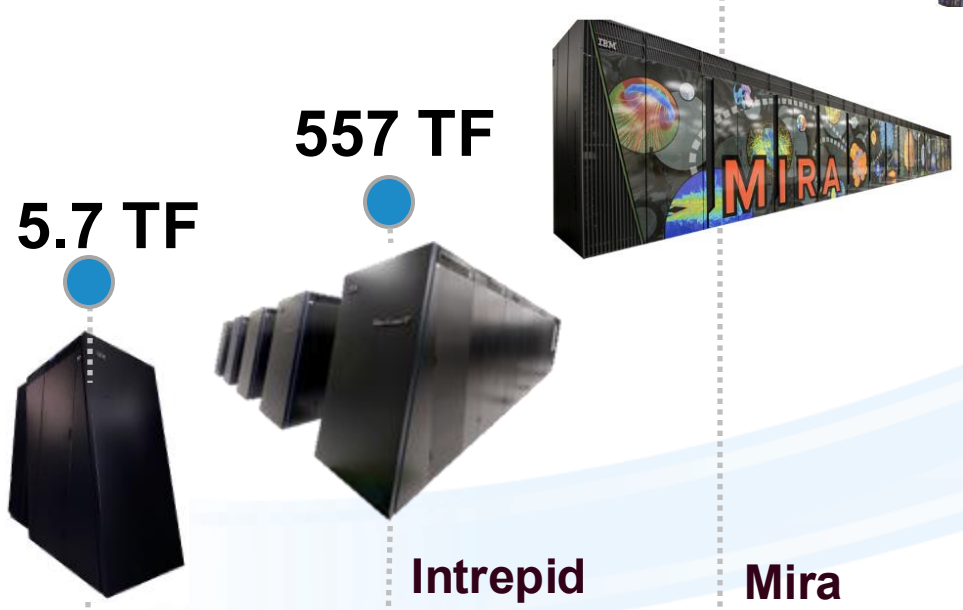


ALCF Systems Evolution



5.7 TF
IBM BG/L
2004

557 TF
Intrepid
IBM BG/P
2007

10 PF
Mira
IBM BG/Q
2012

11.7 PF
Theta
Intel-Cray XC40
2017

15.6 PF
ThetaGPU
NVIDIA
DGX A100
2020

34 PF
Crux
HPE-AMD
+
Polaris
HPE
2021

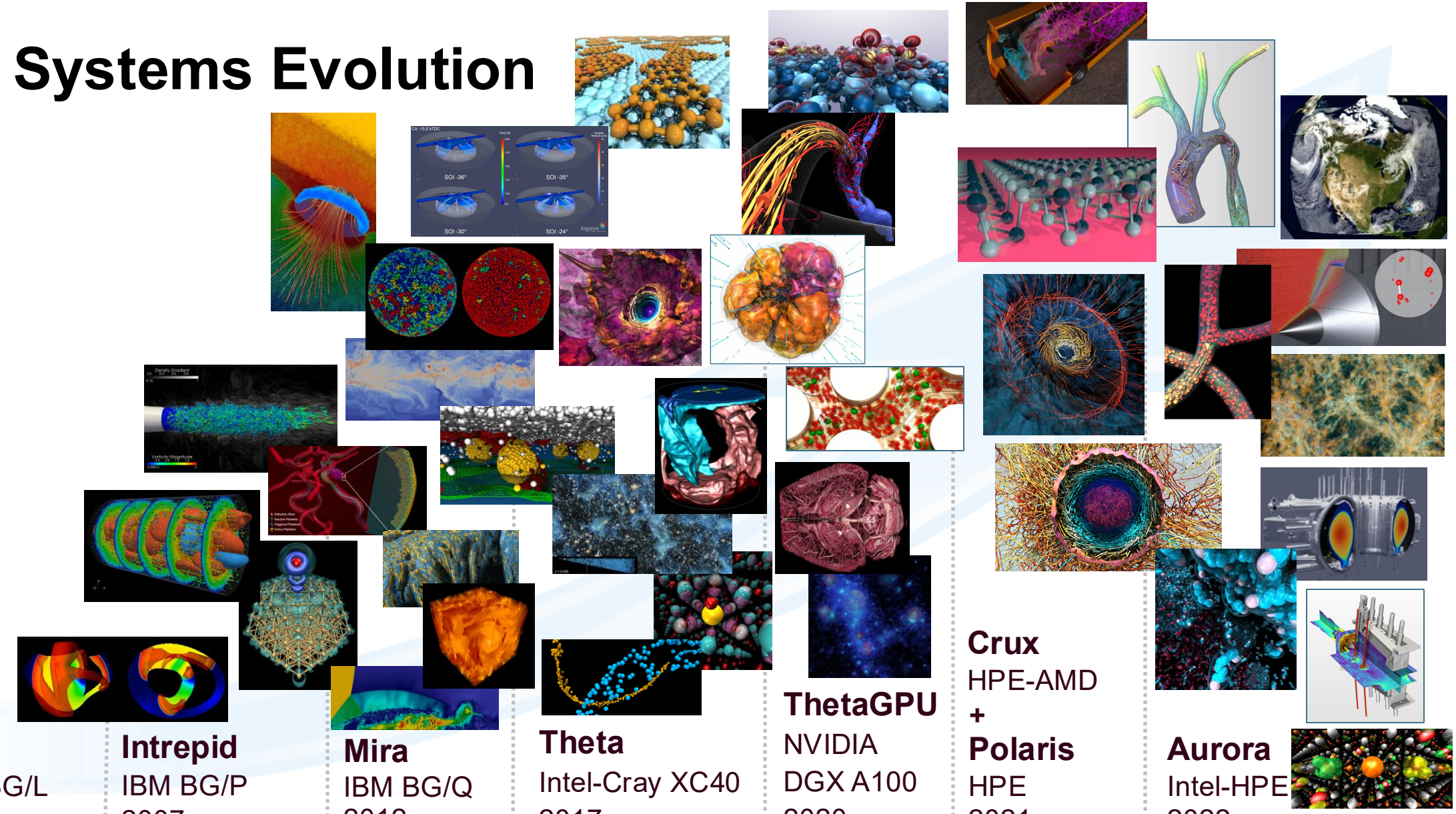
Exascale
Aurora
Intel-HPE
2022

JLSE (2013)

AI Testbed (2020)

Edge Testbed (2021)

ALCF Systems Evolution



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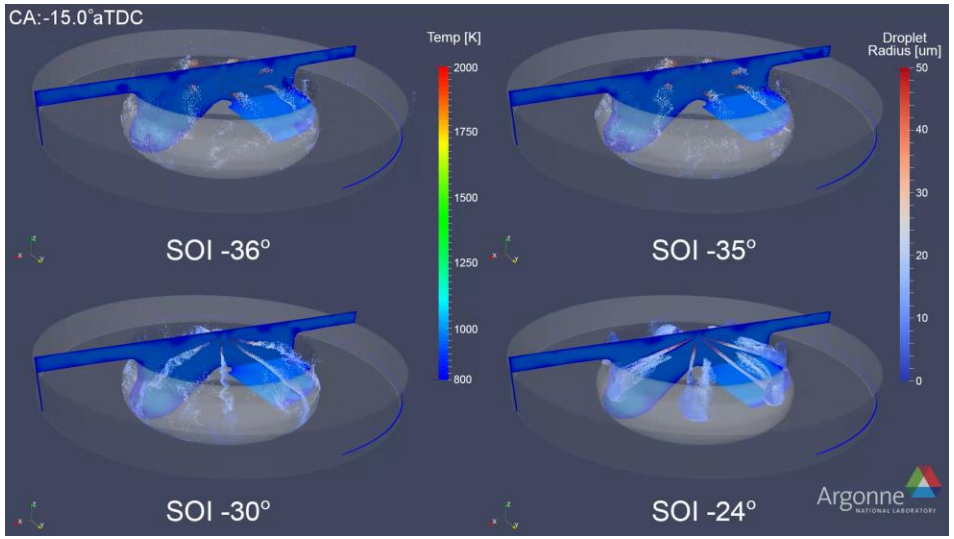
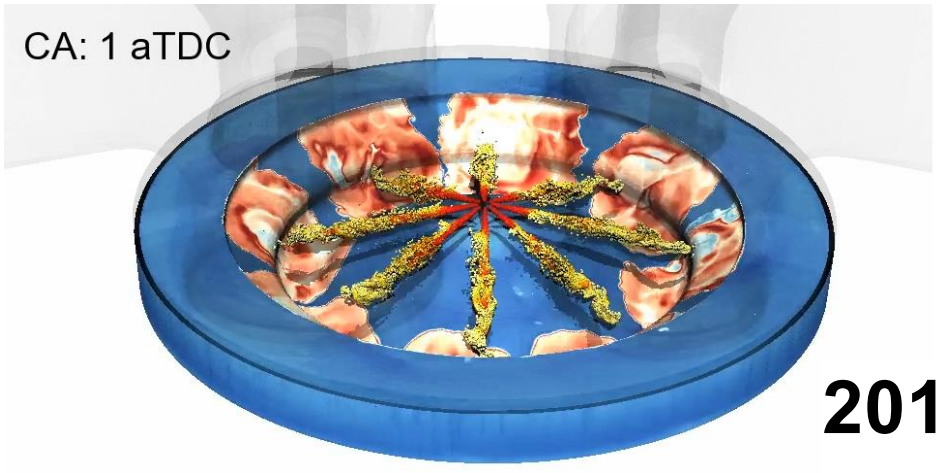
Engineering / Combustion / Biofuels

PI: Sibendu Som, Argonne National Laboratory

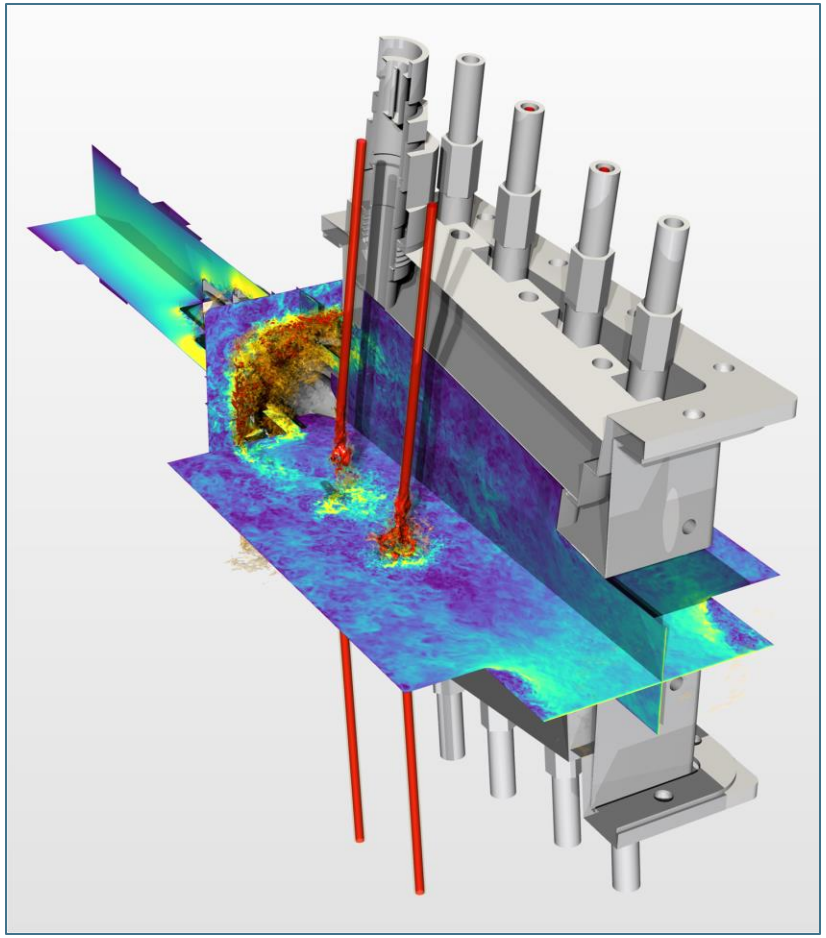


2015



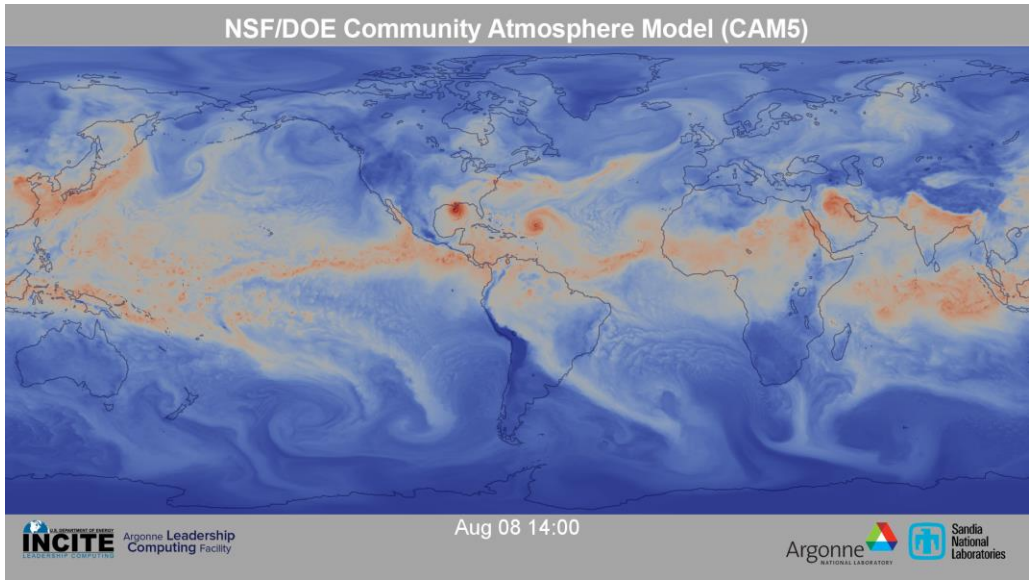
2017

2021



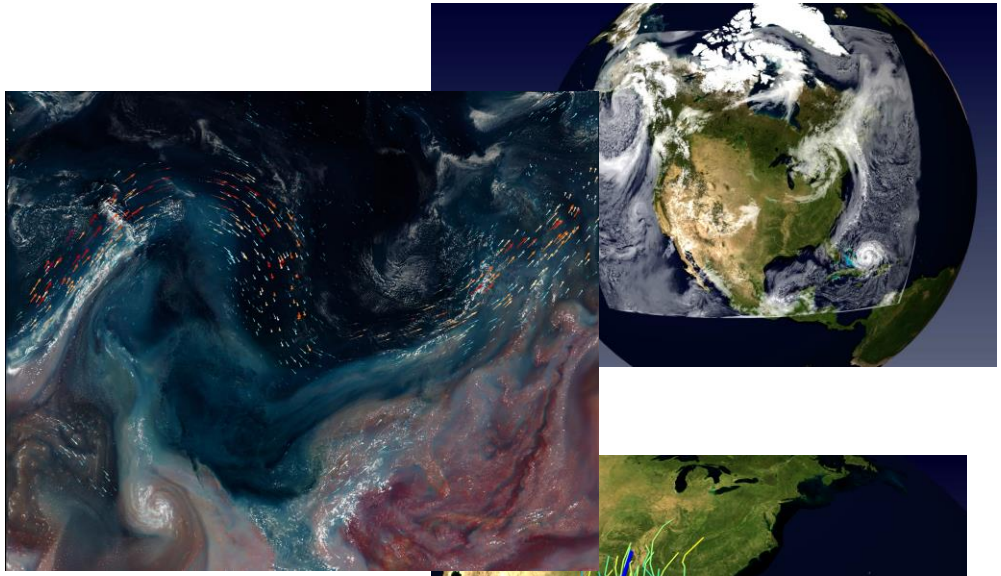
2023

Earth Systems Science

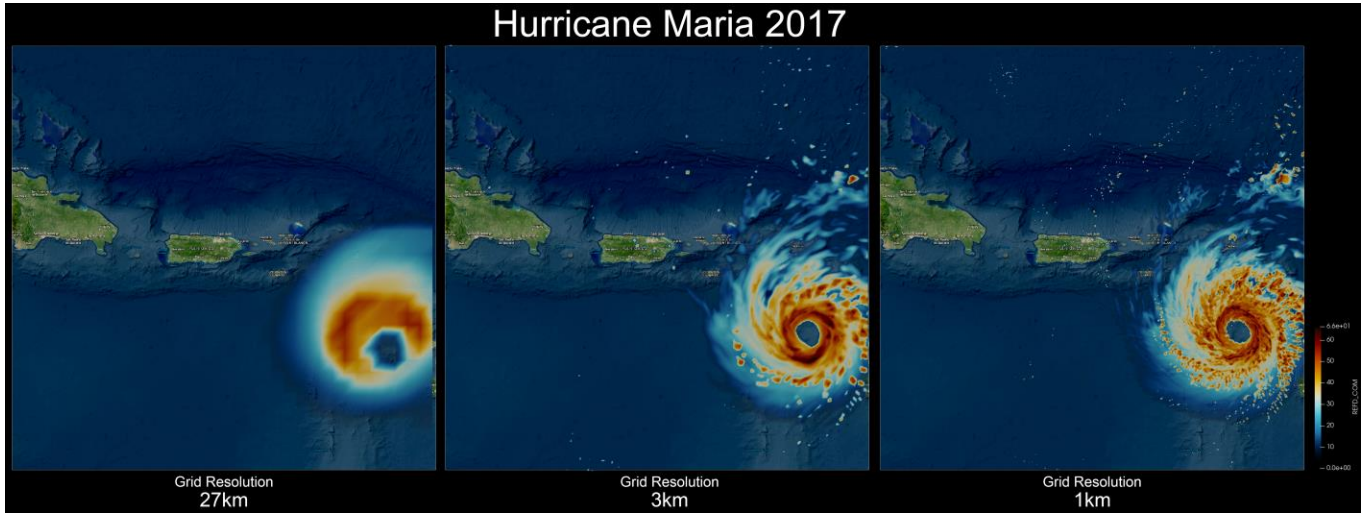


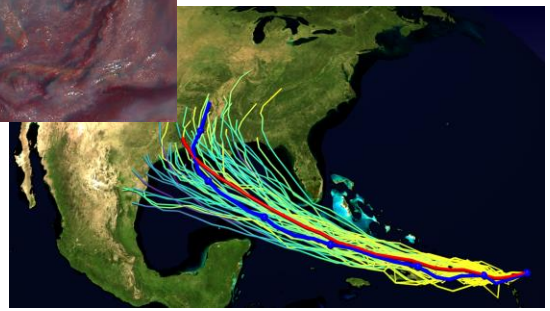
PI: Warren Washington, National Center for Atmospheric Research

2012



2022





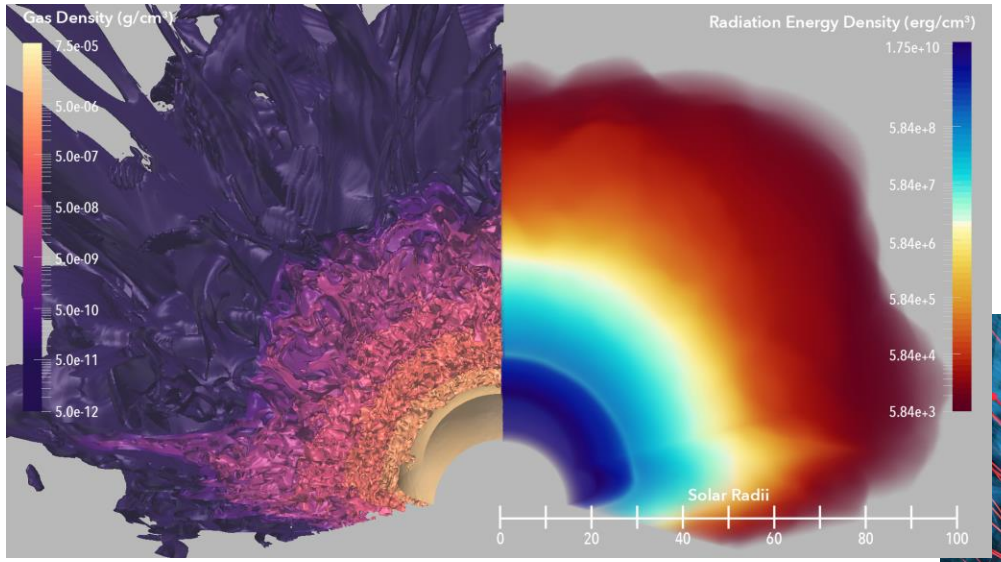
2024 / 2025

PI: Rao Kotamarthi, Argonne National Laboratory

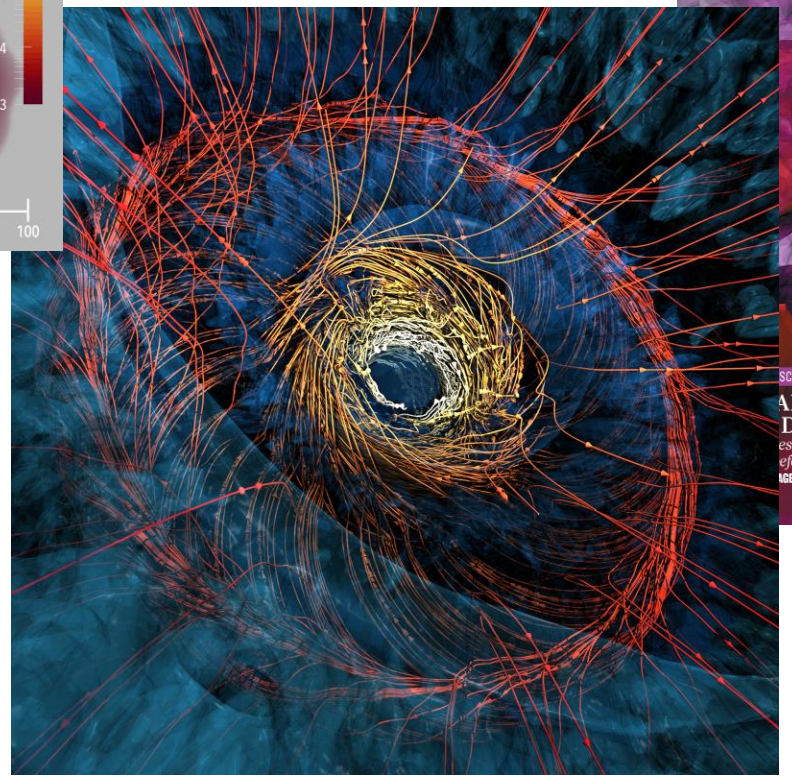
Physics: Stellar Radiation

PI: Lars Bildsten, University of California, Santa Barbara

2018



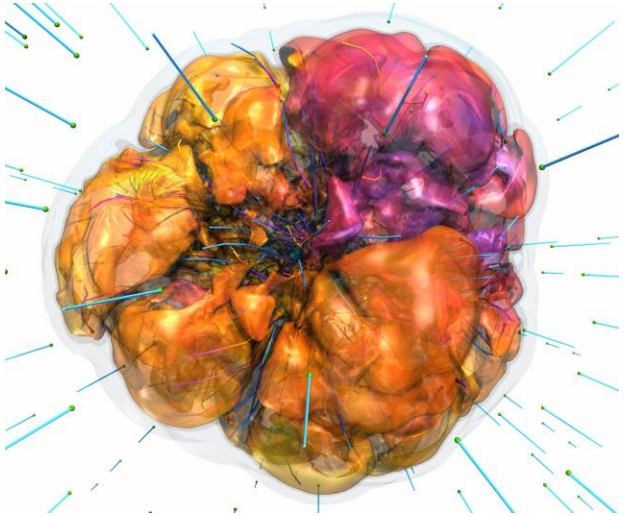
2017



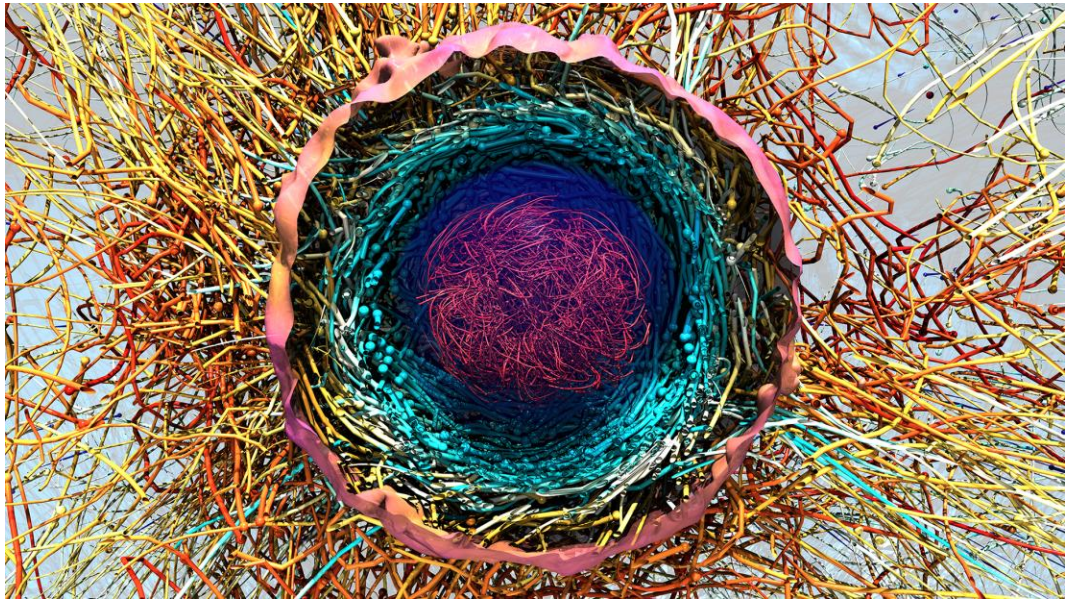
2021

Astrophysics

PI: Adam Burrows, Princeton University

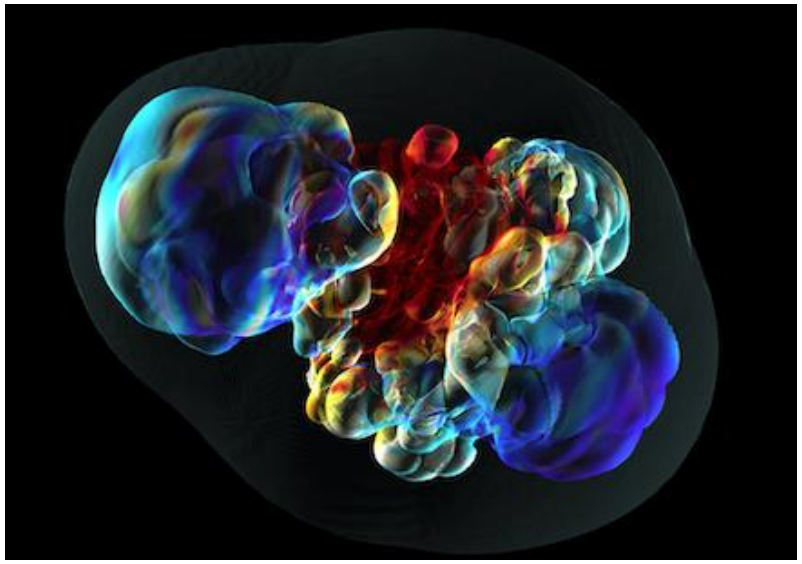


2019

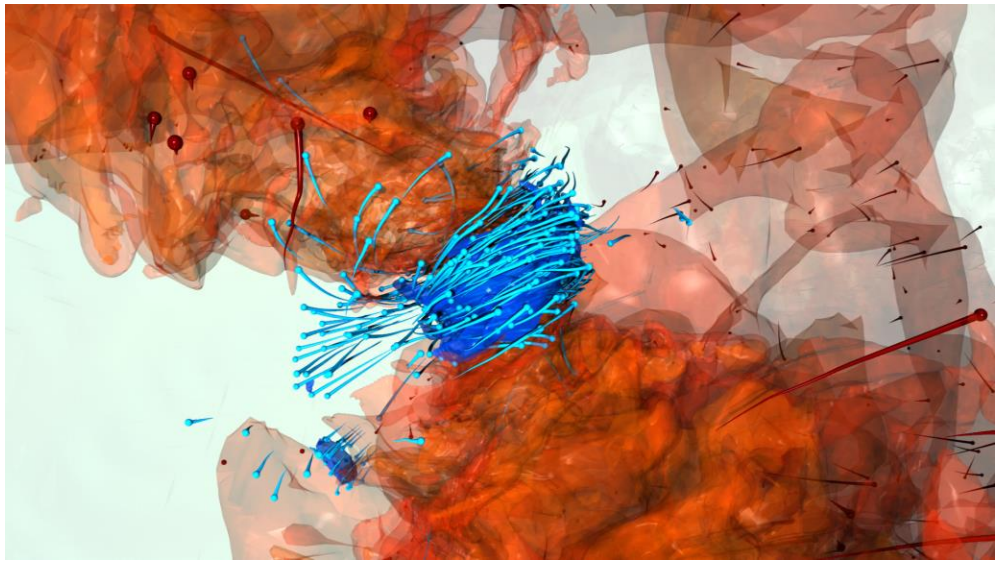


2021

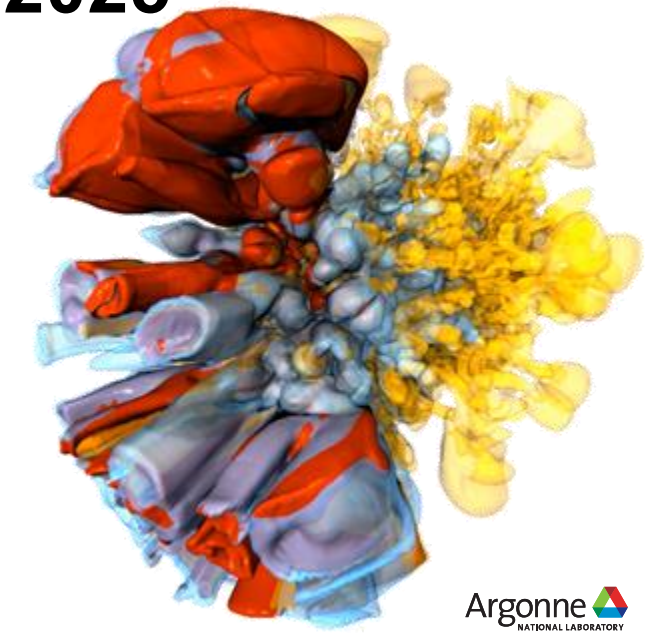
2022



2023



2025



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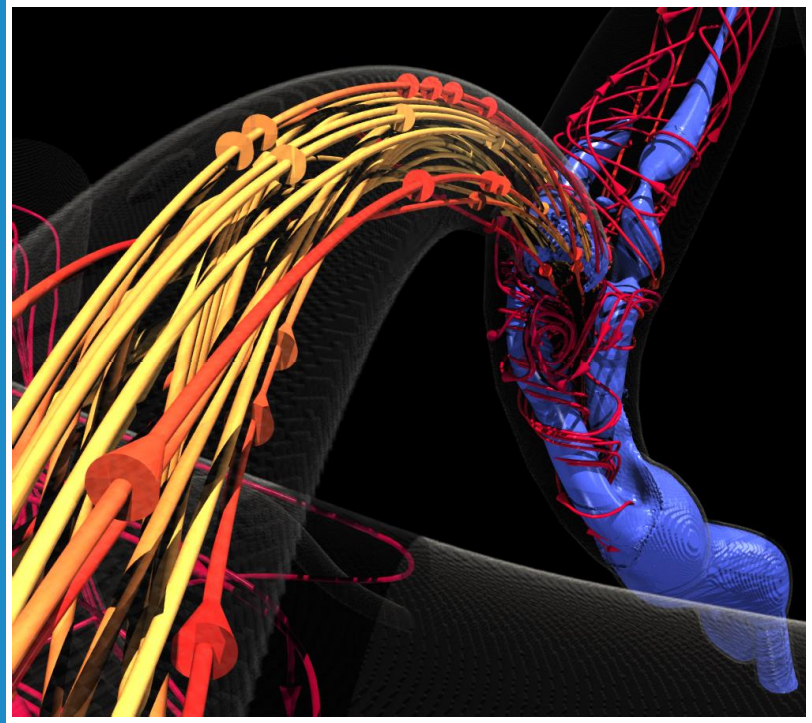
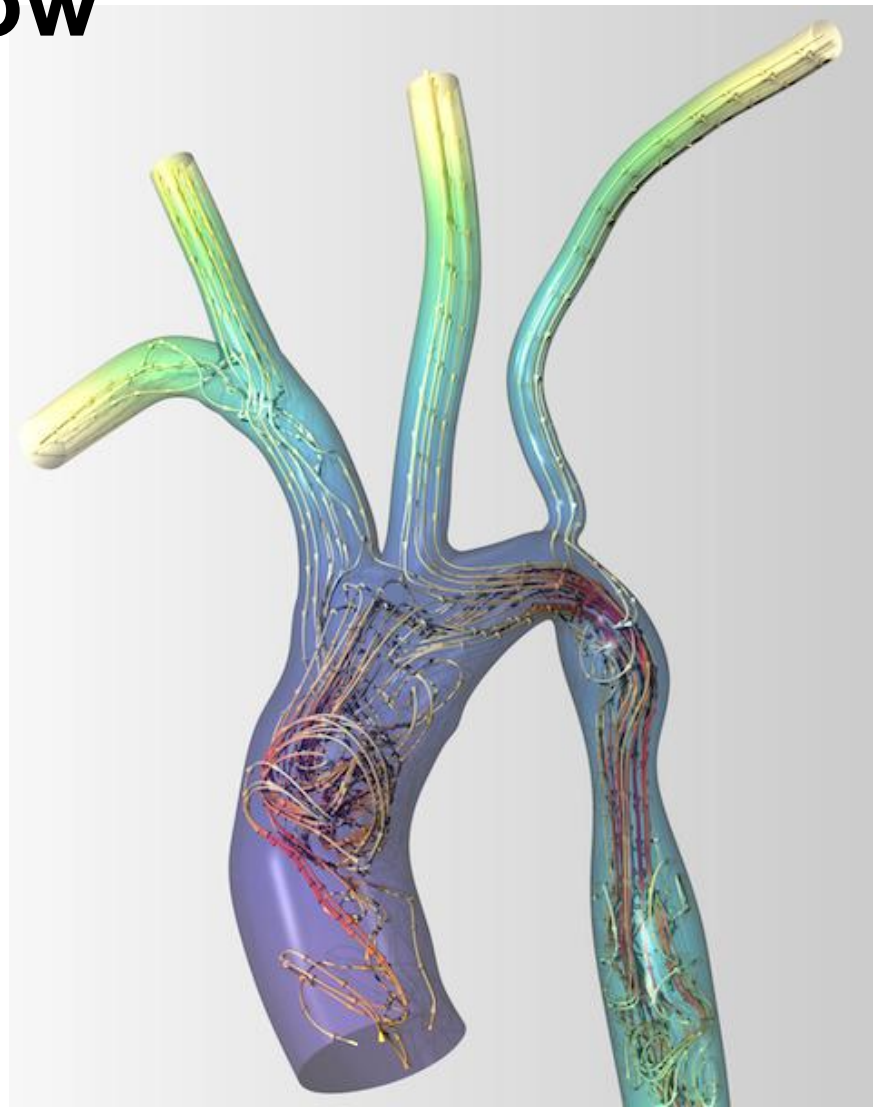
Arterial Blood Flow

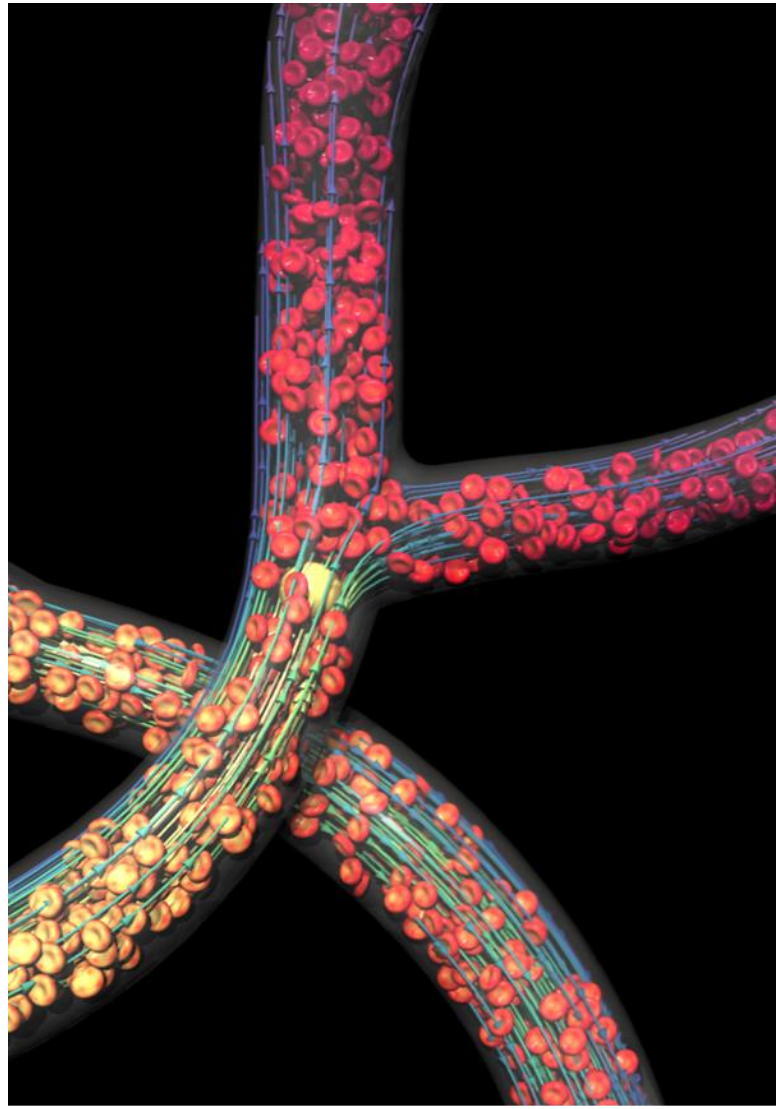
PI: Amanda Randles, Duke University



2020

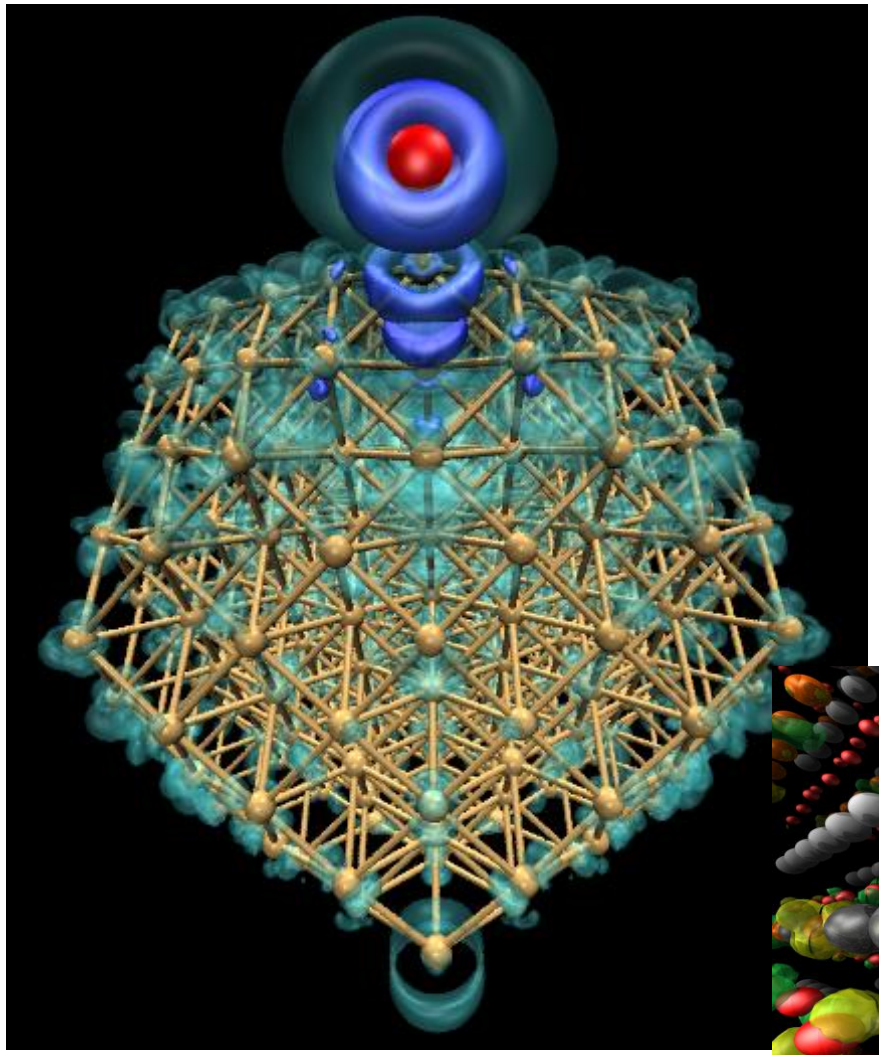


2023 Rendered on Aurora



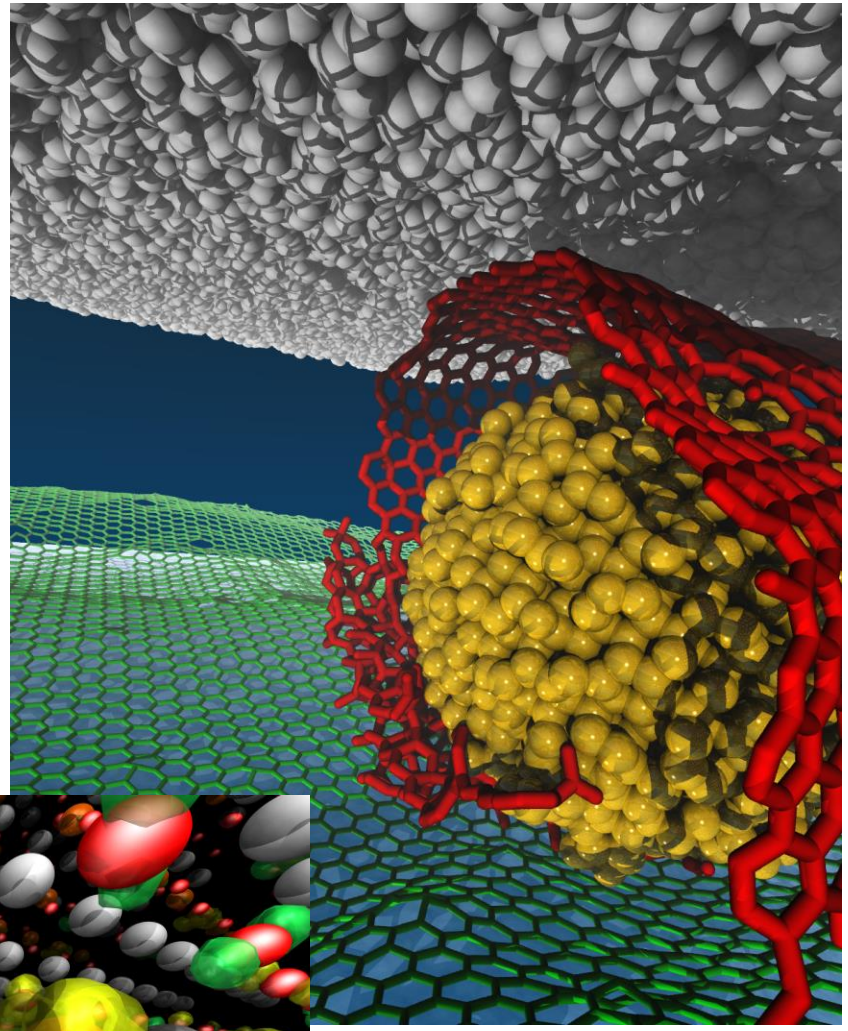
2023 Rendered on Aurora

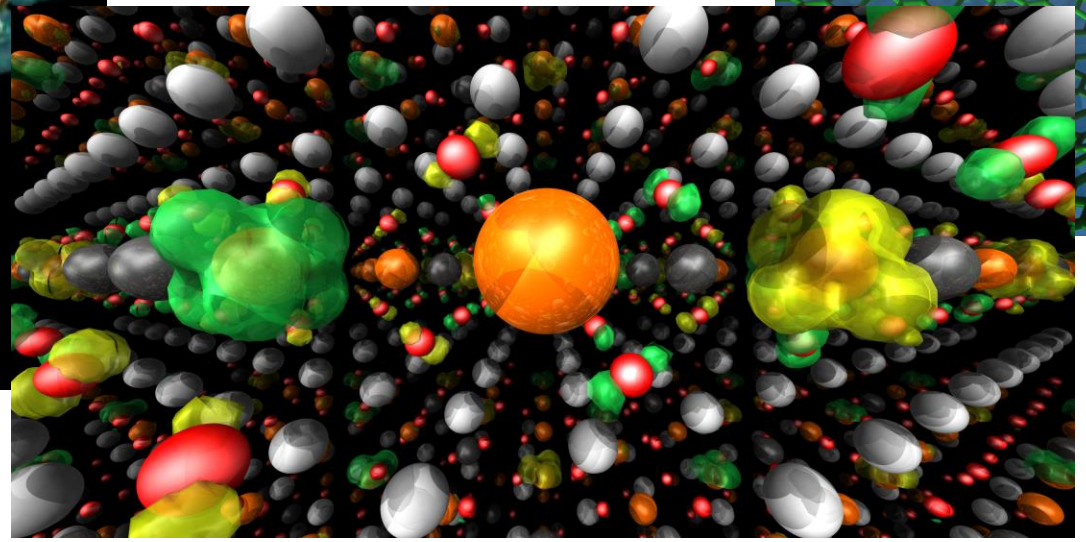
Materials Science / Molecular



Data courtesy of: Jeff Greeley, Nichols Romero, Argonne National Laboratory

Data courtesy of: Subramanian Sankaranarayanan, Argonne National Laboratory





Data courtesy of: Paul Kent, Oak Ridge National Laboratory, Anouar Benali, Argonne National Laboratory

Visualization Tools on Aurora and Polaris

Visualization Applications
- VisIt
- ParaView

Domain Specific
- VMD

APIs
- VTK: visualization

Utilities
- ImageMagick
- ffmpeg
- VNC

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ParaView & VisIt vs. vtk

ParaView & VisIt

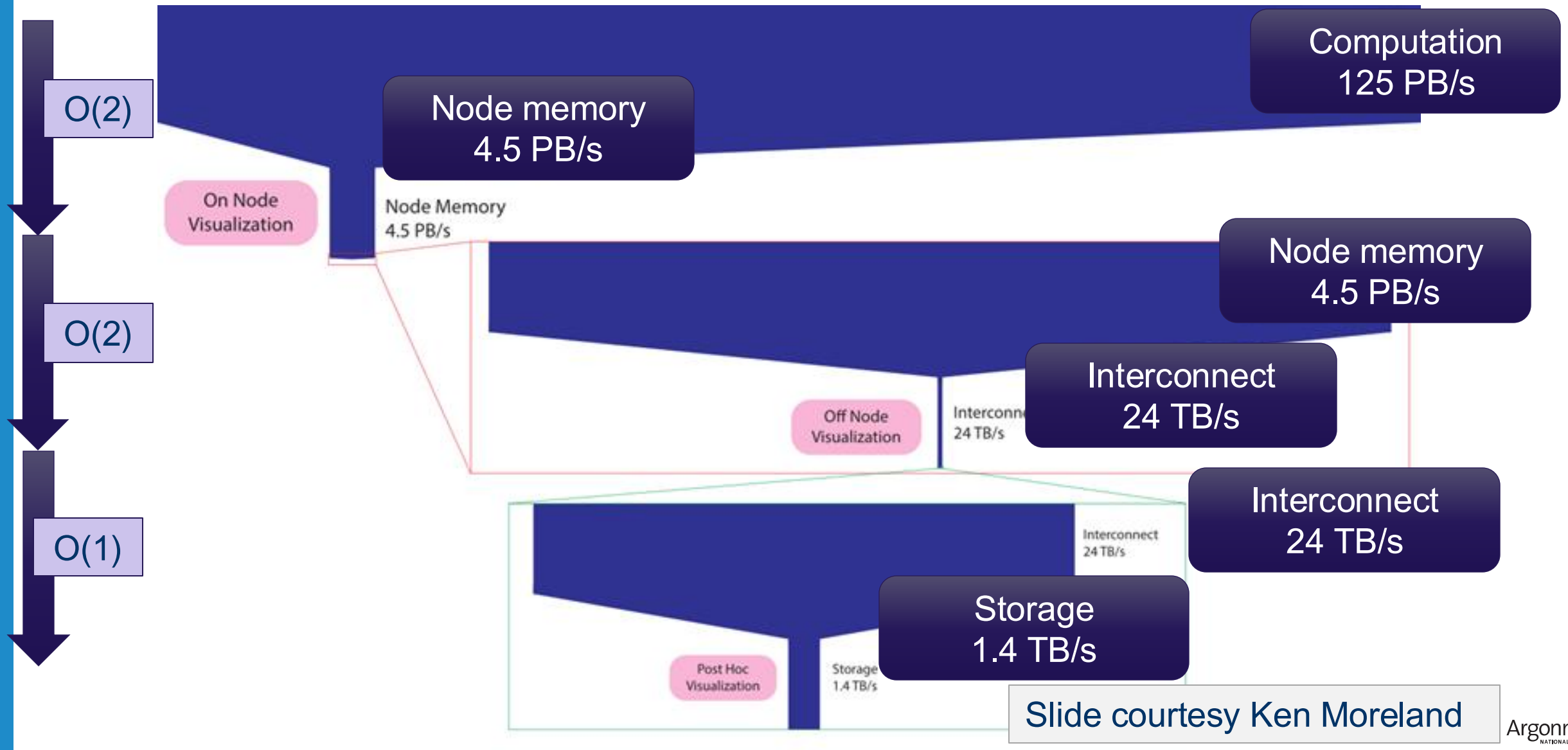
- General purpose visualization applications
- GUI-based
- Client / Server model to support remote visualization
- Scriptable / Extendable
- Built on top of vtk (largely)
- *In situ* capabilities

vtk

- Programming environment / API
- Additional capabilities, finer control
- Smaller memory footprint
- Requires more expertise (build custom applications)

In Situ Visualization and Analysis

Five orders of magnitude between compute and I/O capacity on Titan Cray system at ORNL



Slide courtesy Ken Moreland

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In Situ vis and Analysis Problem:

- FLOPS to I/O Bottleneck
  - —Frontier
    - Peak Performance: 1.6 EF
    - Storage: 2-4x Summit's I/O 2.5TB/s. At best 10TB/s
    - 5 orders of magnitude difference
  - —Aurora
    - Peak Performance: 1.012 EF
    - Storage: 31TB/s
    - 5 orders of magnitude difference

Problem

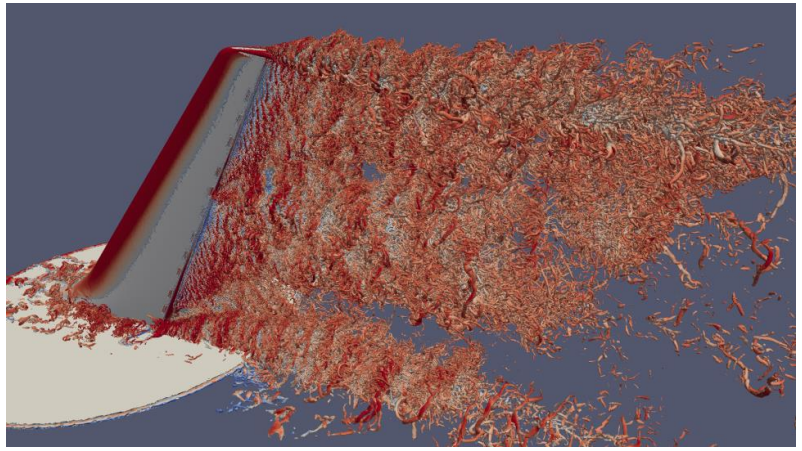
- I/O is too expensive
- Scientists cannot save every timestep, and/or resolution
- Lost cycles: simulation waits while I/O is happening
- Lost discoveries: scientists might miss discoveries

- Solution: *In situ* visualization and analysis

What is *In Situ* vis and analysis

- Traditionally visualization and analysis happens post hoc
  - —E.g.: Data gets saved to the disk, scientist opens it after the simulation has ended
- *In situ*
  - —Data gets visualized/analyzed **while** in memory.
  - —If zero-copy used, there is no data movement
  - —Ideally the data is on the GPU and stays on the GPU

In Situ

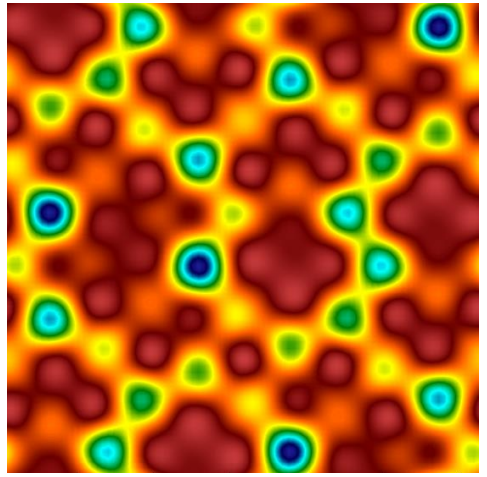


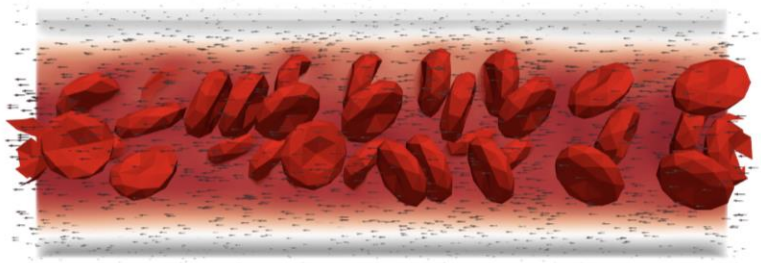
~2014

PHASTA, Catalyst, Ken Jansen

2018

Nek5000, SENSEI



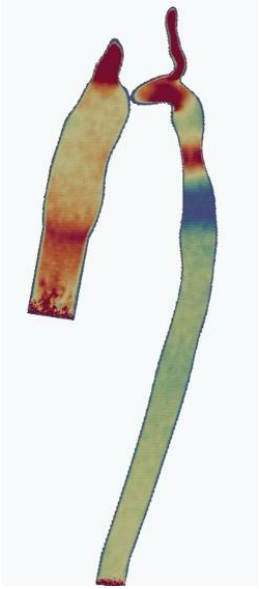


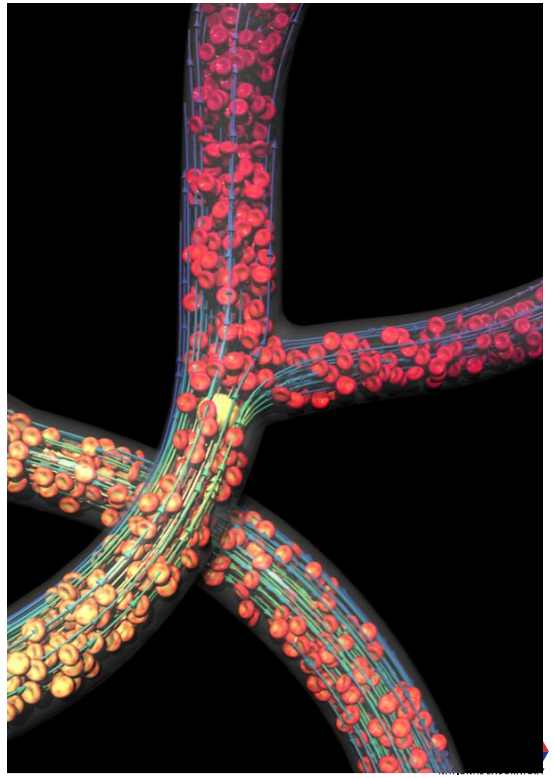
2021 - 2024

Palabos+LAMMPS, SENSEI + Catalyst, bi-directional

2019

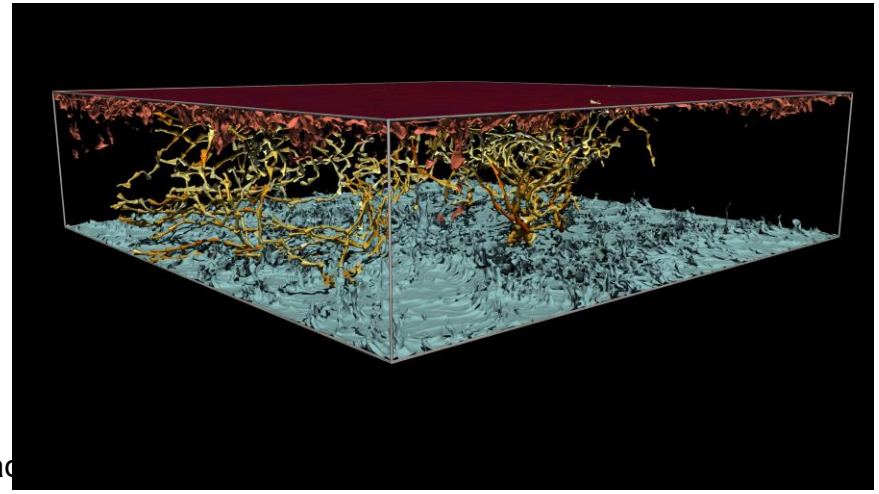
SENSEI + Catalyst





2024

nekRS, Ascent + Catalyst



HARVEY

Ascent + Catalyst

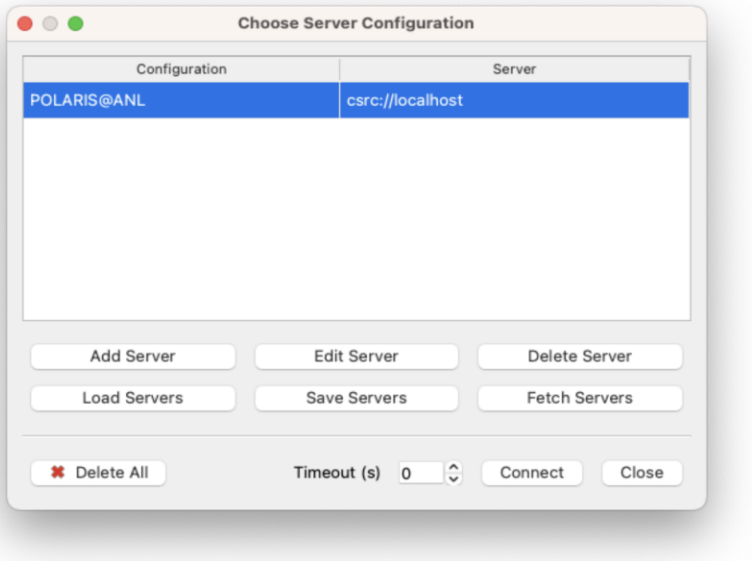
2024

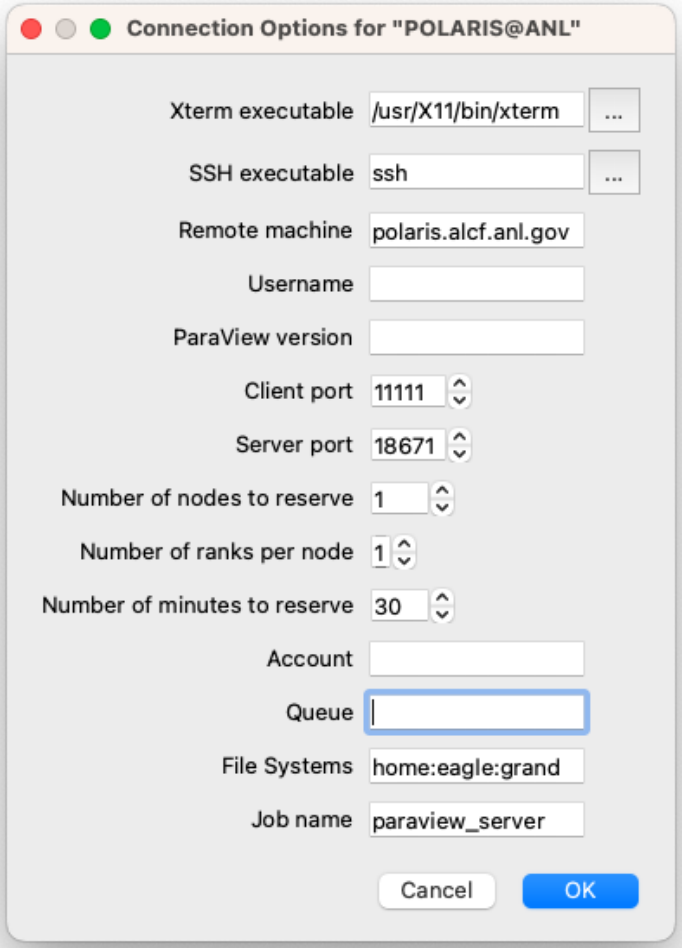
In Situ Frameworks and Infrastructures at ALCF

Name	Description
Ascent	The Ascent in situ infrastructure is designed for leading-edge supercomputers, and has support for both distributed-memory and shared-memory parallelism.
Catalyst	In situ use case library, with an adaptable application programming interface (API), that orchestrates the delicate alliance between simulation and analysis and/or visualization tasks
Cinema	Cinema is an innovative way of capturing, storing, and exploring both extreme scale scientific data and experimental data. It is a highly interactive image-based approach to data analysis and visualization that promotes investigation of large scientific datasets.
Viskores (vtk-M)	Viskores is a toolkit of scientific visualization algorithms for emerging processor architectures. Viskores supports the fine-grained concurrency for data analysis and visualization algorithms required to drive extreme scale computing.

Launching ParaView on Polaris

1. Connect
2. Fetch Server (first time only)
3. Select Server
4. Connect





4. Enter password in terminal

Additional Resources

ParaView

- www.paraview.org
- docs.alcf.anl.gov/aurora/visualization/paraview/

VisIt

- visit-dav.github.io/visit-website/
- docs.alcf.anl.gov/aurora/visualization/visit/

Questions?

Joe Insley
insley@anl.gov