

Visualization at ExaScale on Aurora

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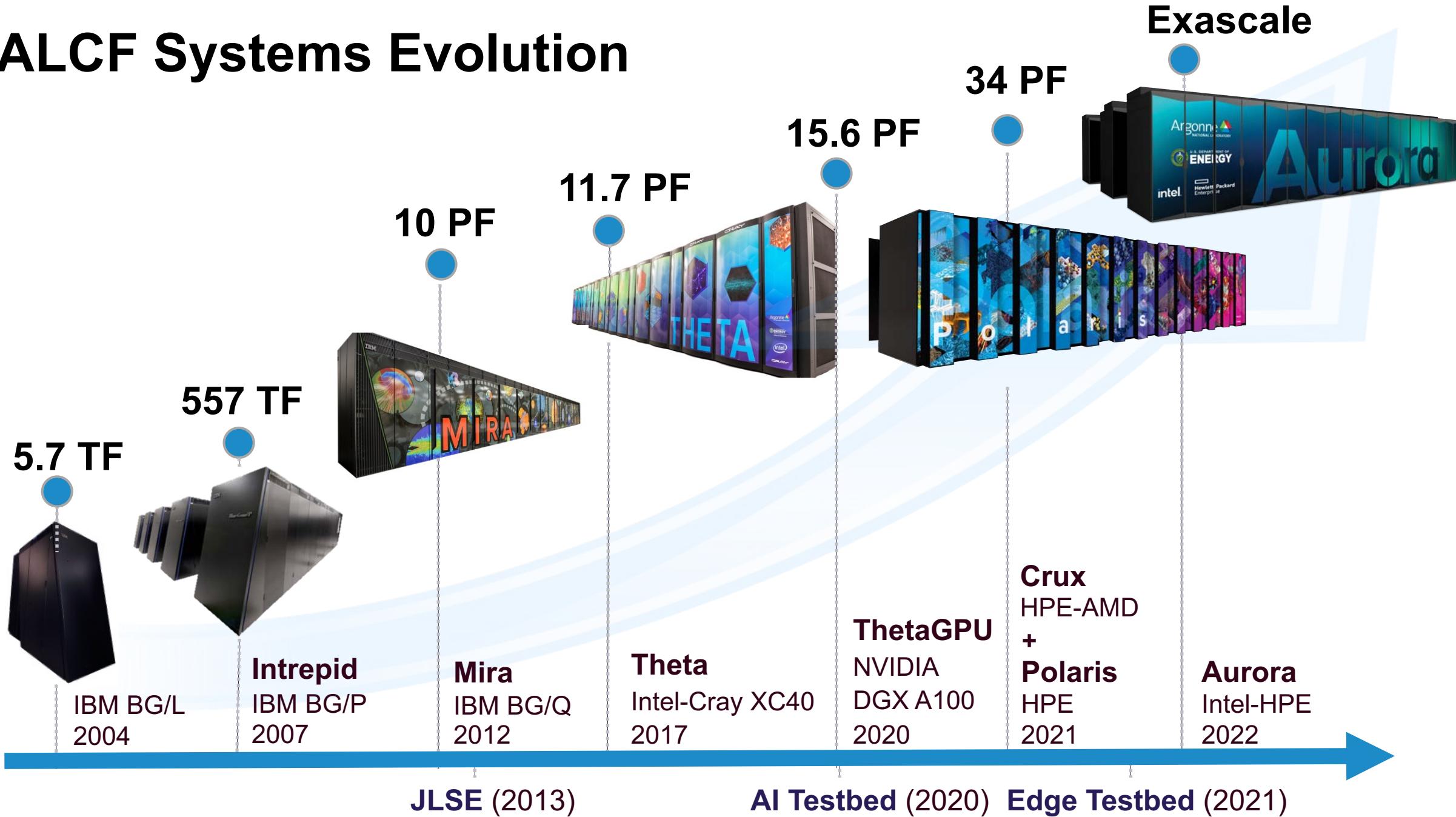
Silvio Rizzi

Argonne National Laboratory

Victor Mateevitsi

Argonne National Laboratory

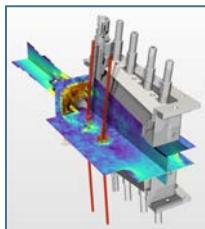
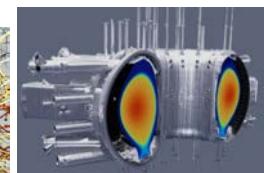
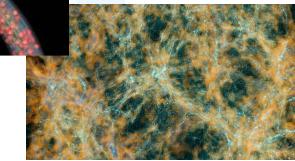
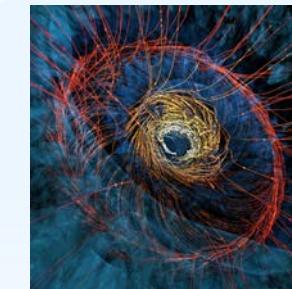
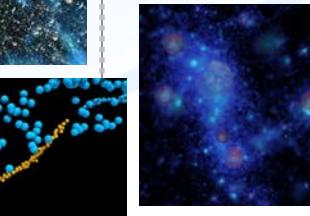
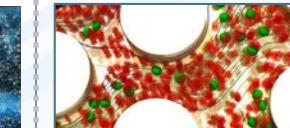
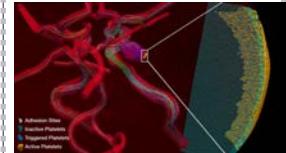
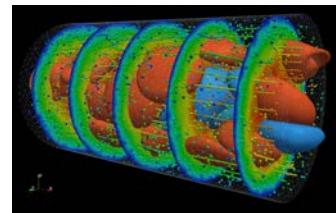
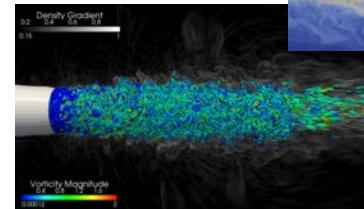
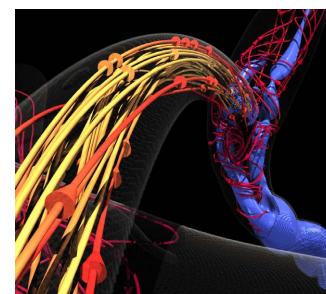
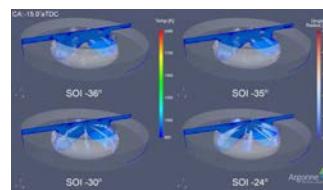
ALCF Systems Evolution



ALCF Systems Evolution

 **ParaView**

 **ParaView Catalyst**



IBM BG/L
2004

Intrepid
IBM BG/P
2007

Mira
IBM BG/Q
2012

Theta
Intel-Cray XC40
2017

ThetaGPU
NVIDIA
DGX A100
2020

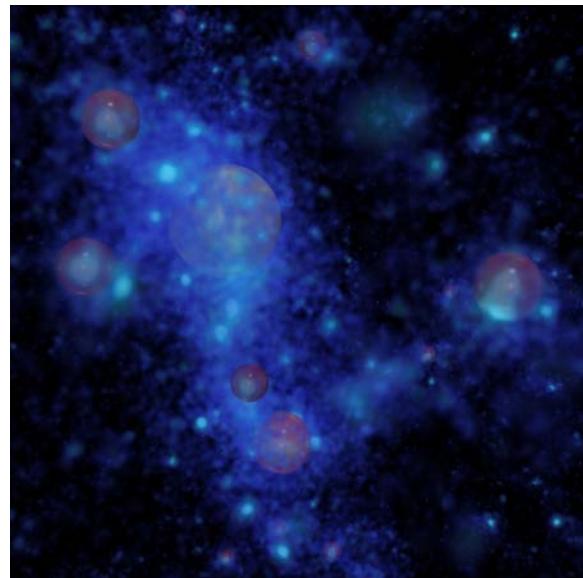
Crux
HPE-AMD
+
Polaris
HPE
2021

Aurora
Intel-HPE
2022

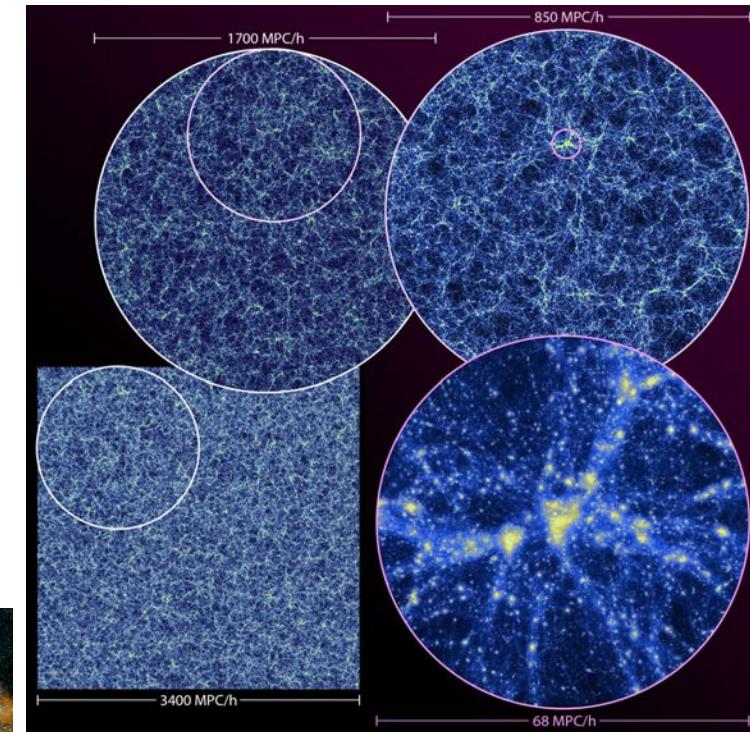
2018



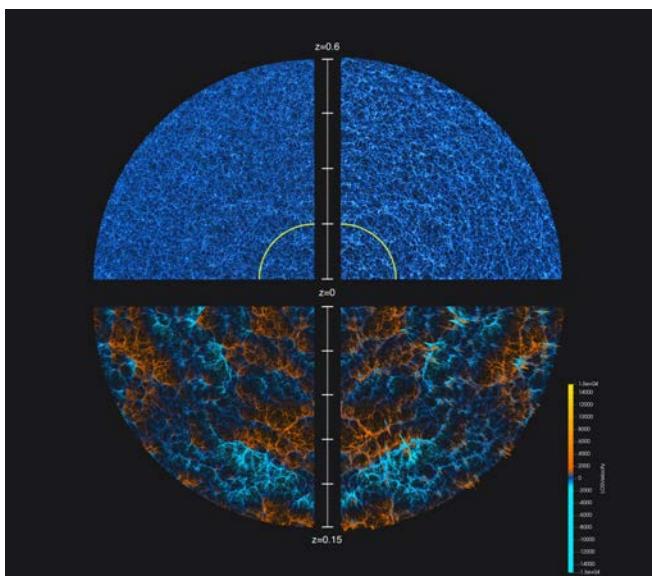
2020



2020



2021



Computed and Rendered on Aurora 2023

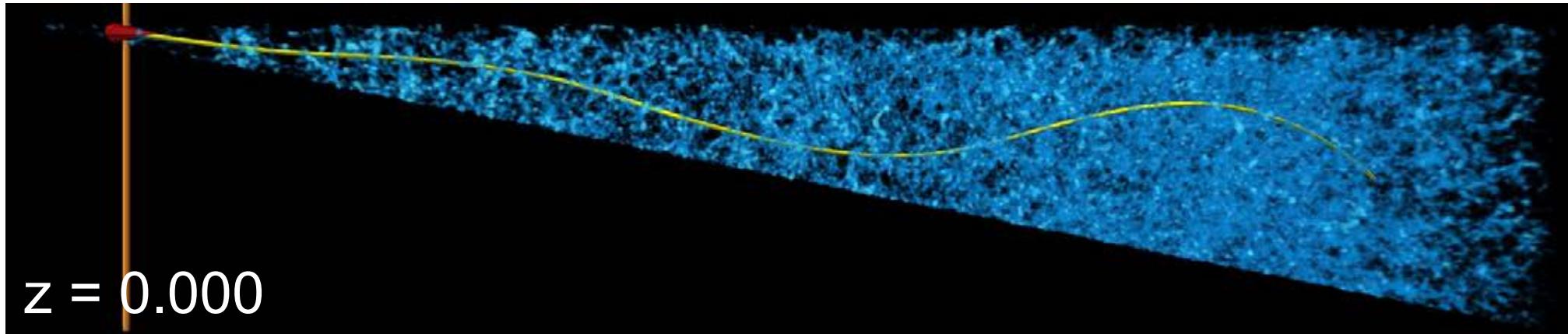
PI: Salman Habib and
HACC Team, Argonne
National Laboratory

HACC: SPHEREx

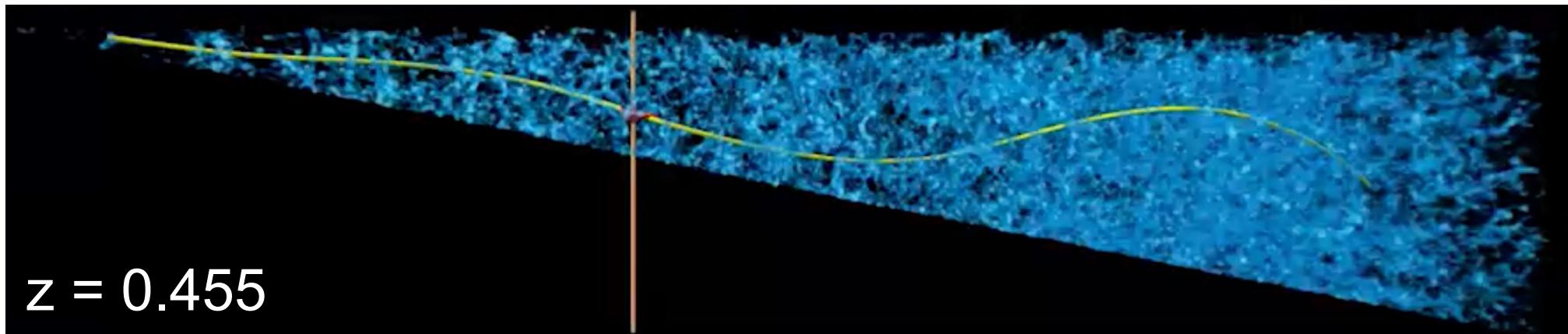
2018



HACC: SPHEREx



$z = 0.000$

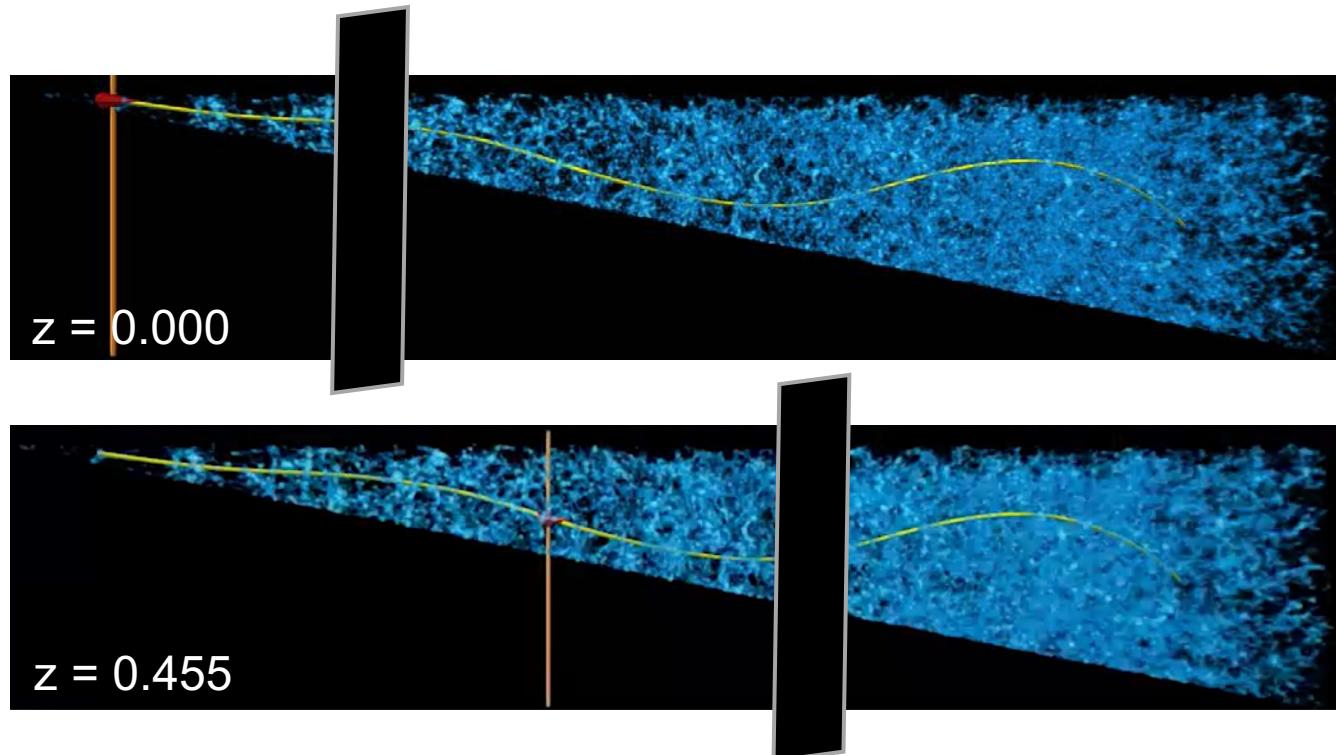


$z = 0.455$

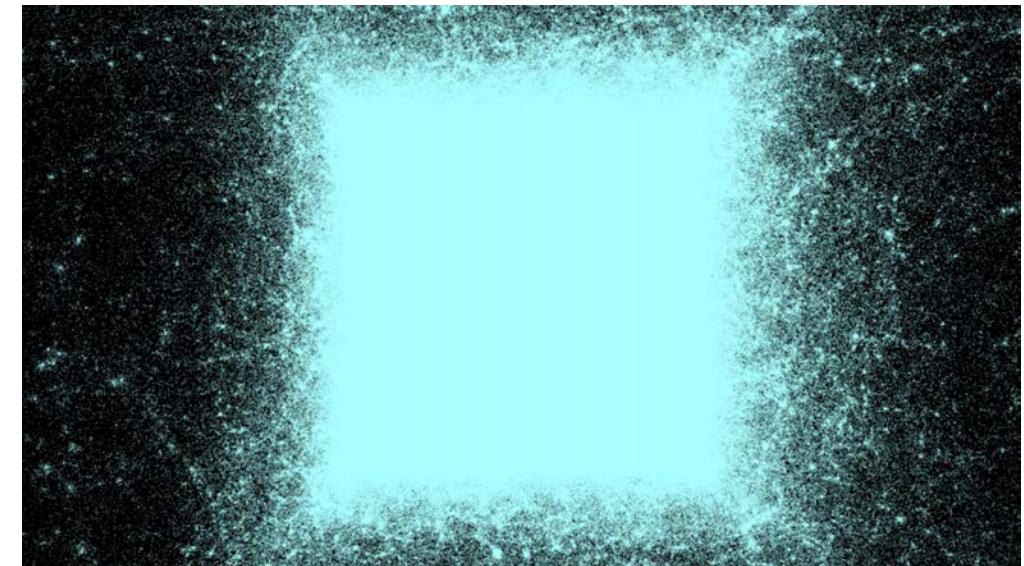
- **Light cone**
 - Particles projected onto a regular grid and volume rendered
 - Shows path of the camera

HACC: SPHEREx

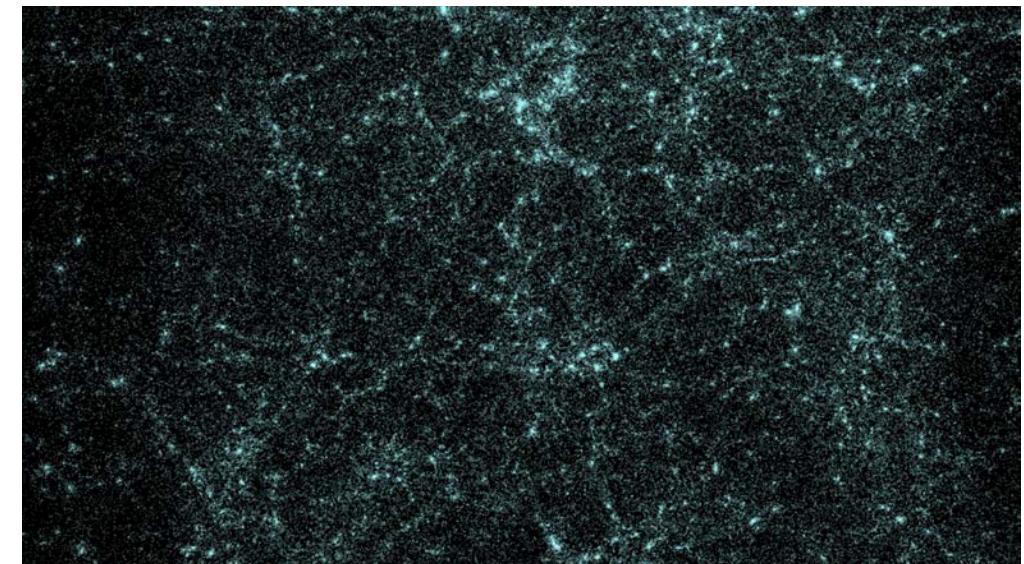
- Particles as particles
- Moving plane to avoid the brick



No plane

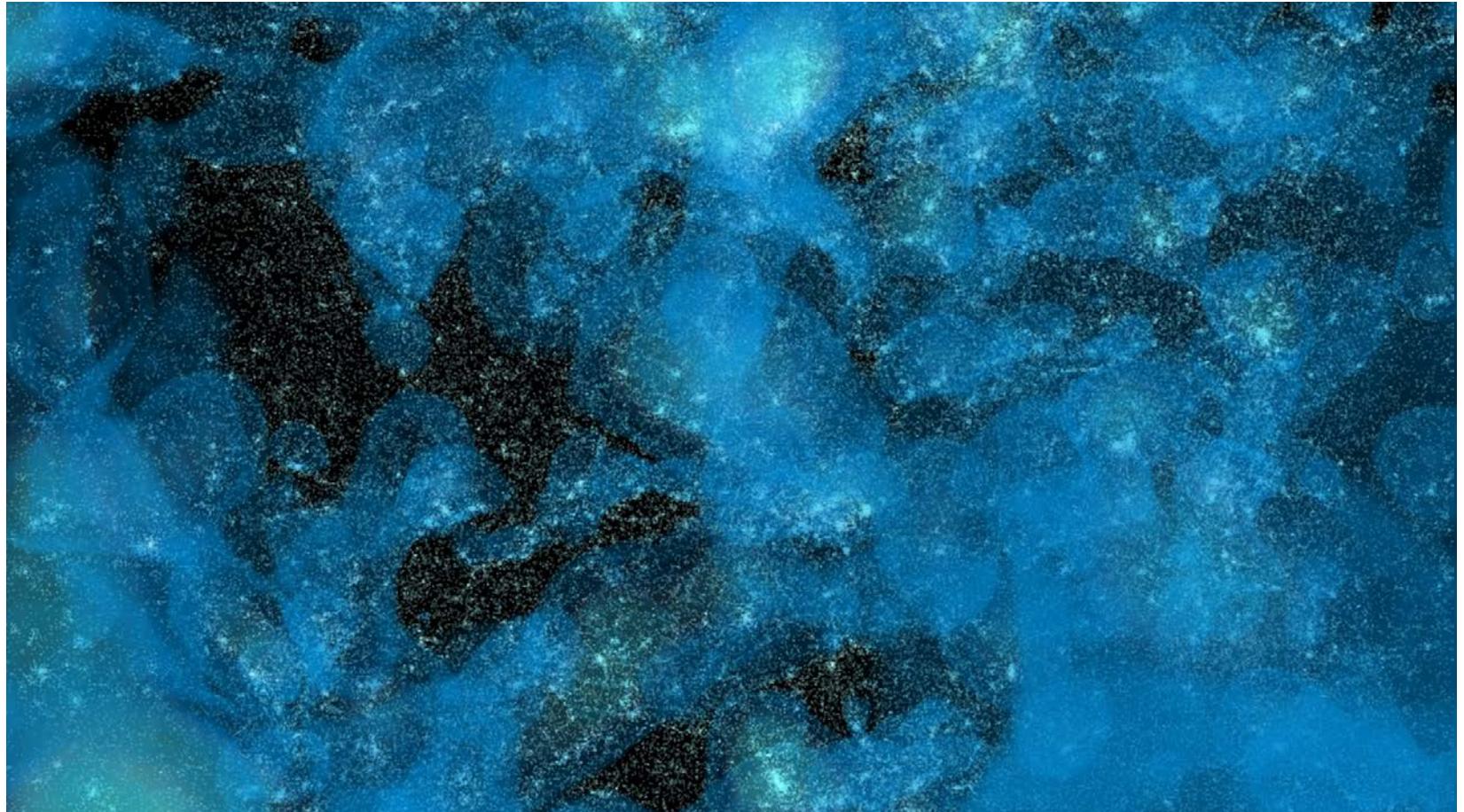


With plane



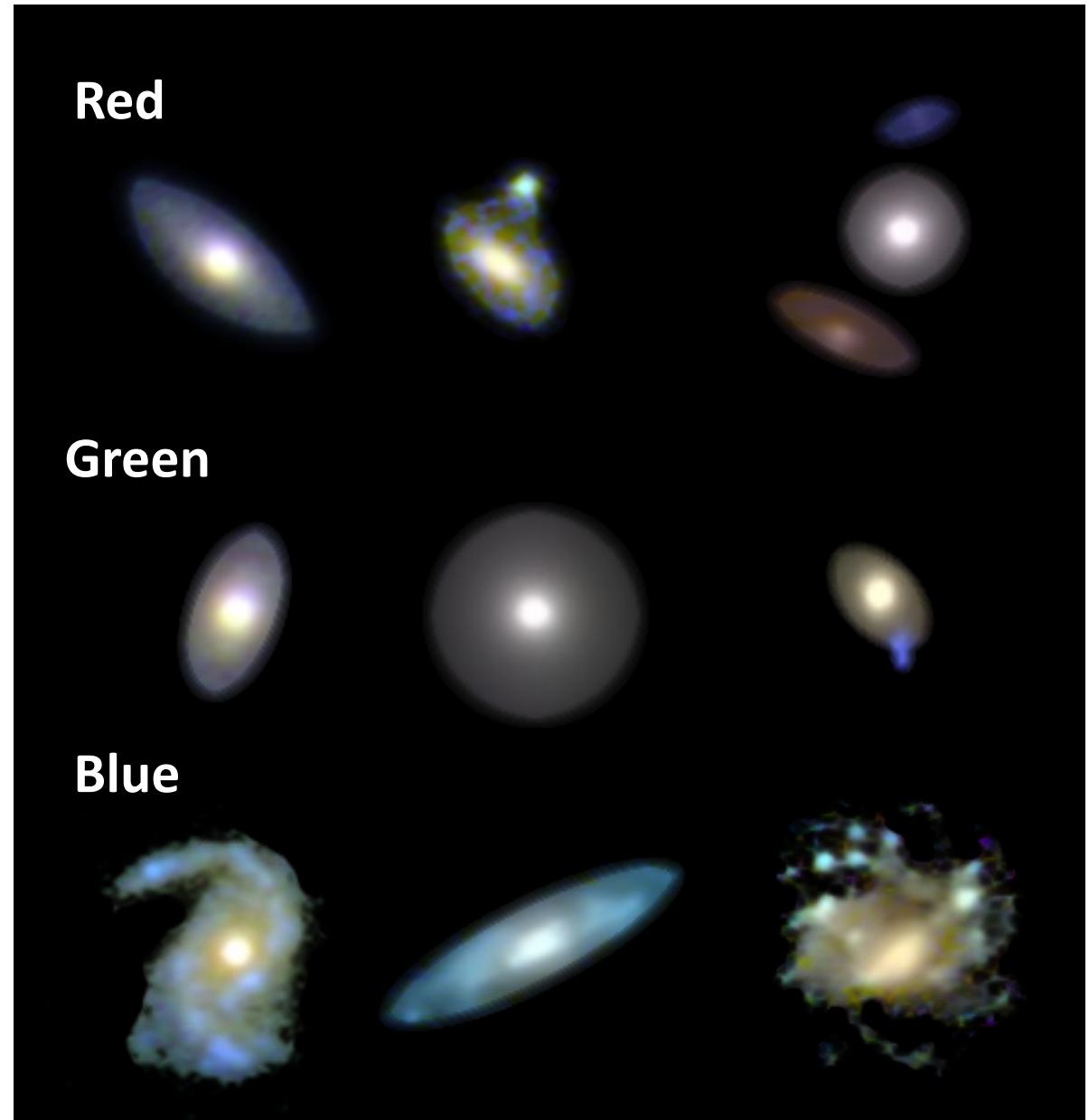
HACC: SPHEREx

- Density as volume



HACC: SPHEREx

- Galaxies as textures
 - Categorized as Red, Green, or Blue
 - Rotated at random angle
 - Perpendicular to camera



HACC: SPHEREx

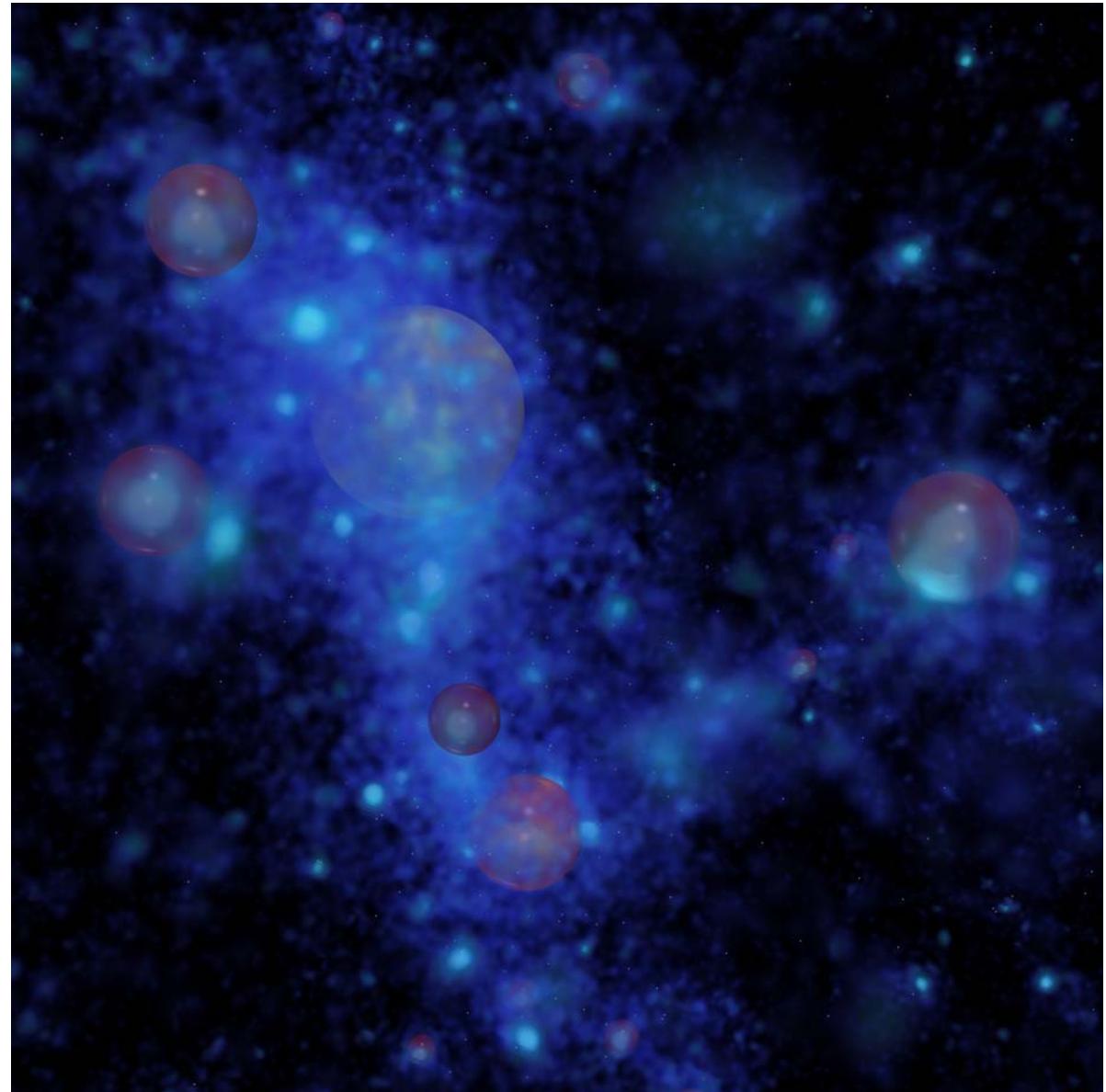
Animation: https://www.youtube.com/watch?v=l0D7_0Kus8g



HACC: Last Journey

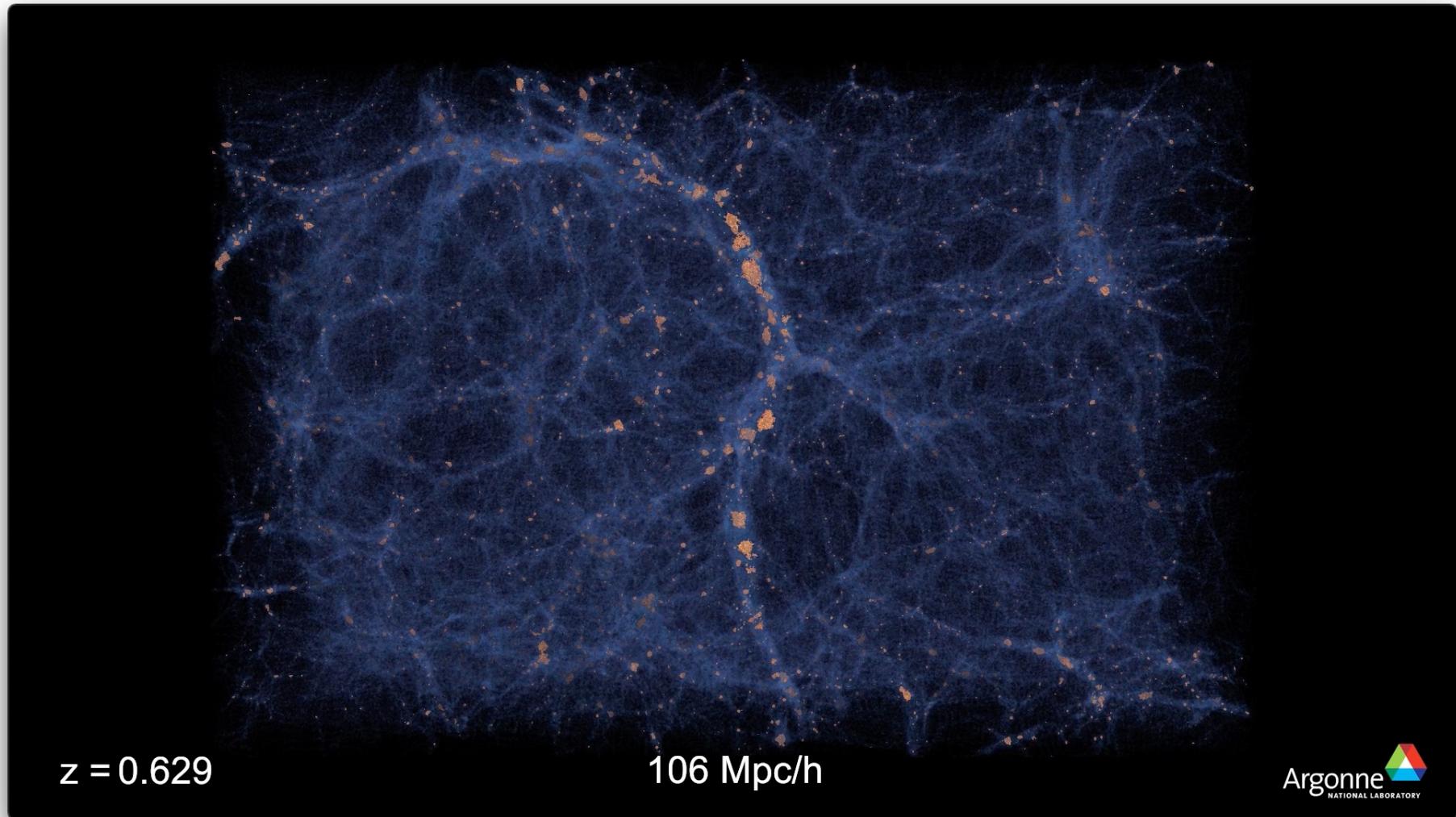
2020

- Final simulation to run on Mira
- 1.24 trillion particles



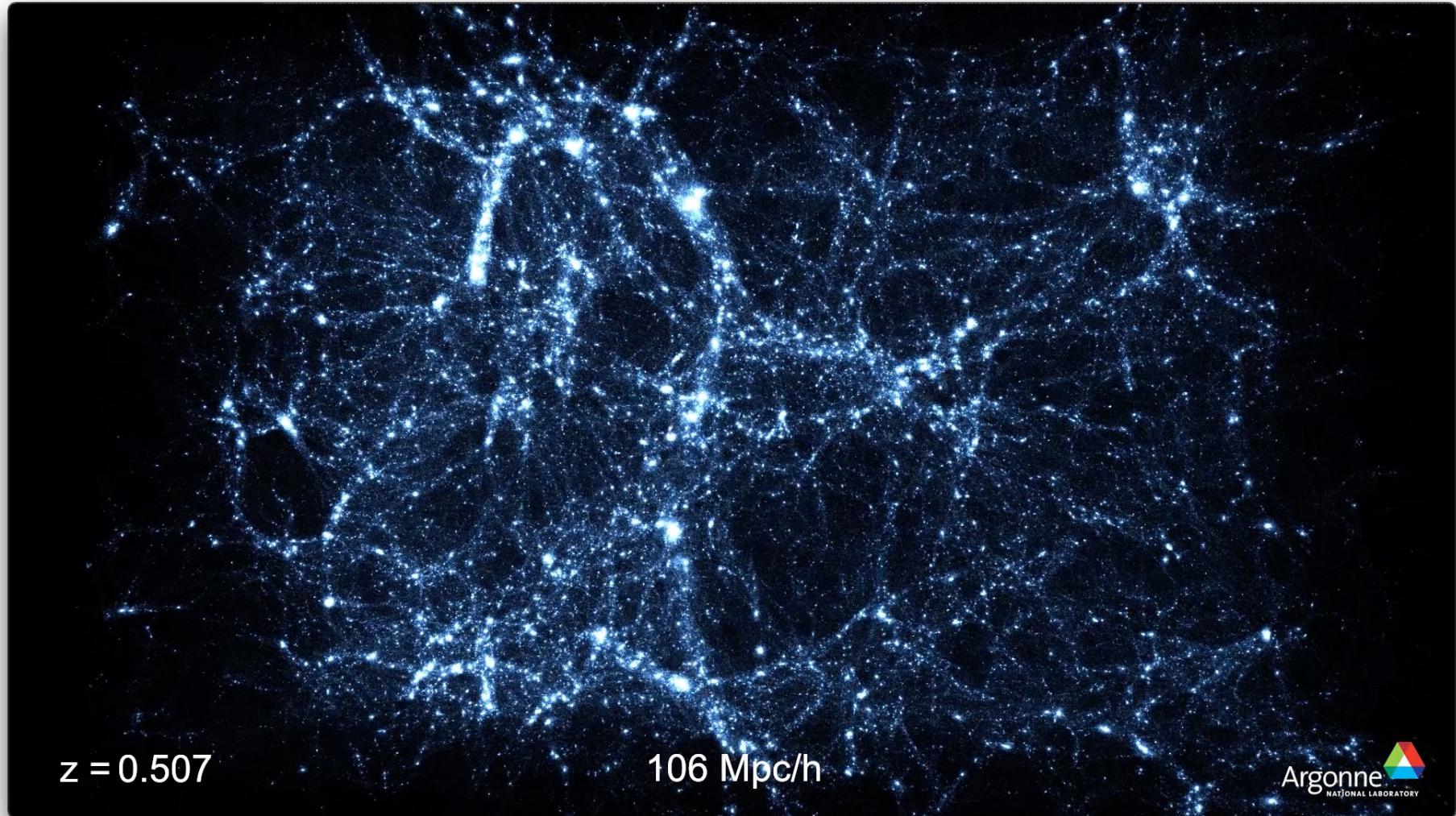
HACC: Last Journey

- **Volume rendering
of particle density**



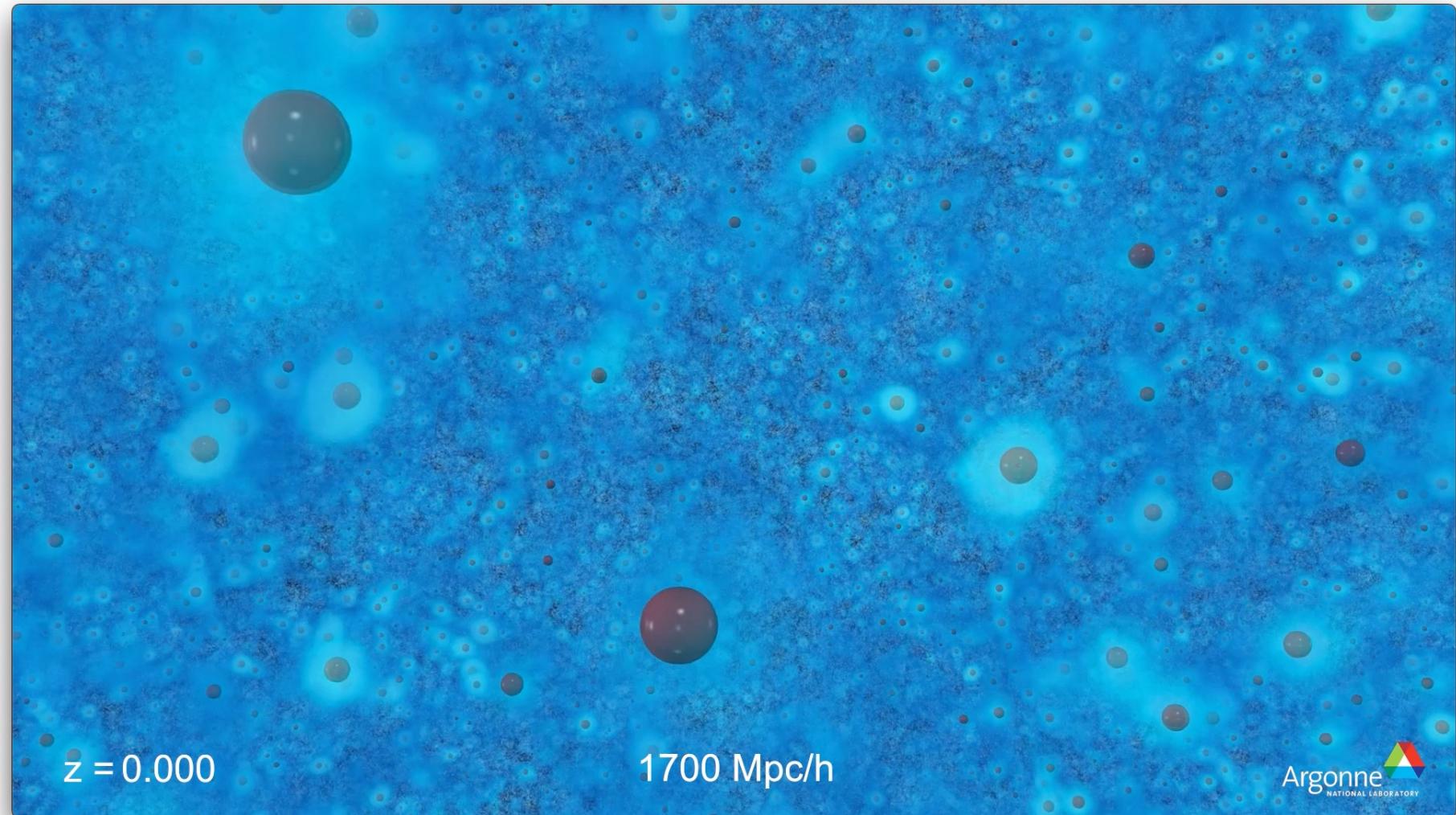
HACC: Last Journey

- Particle rendering
to reveal
individual particle
behavior



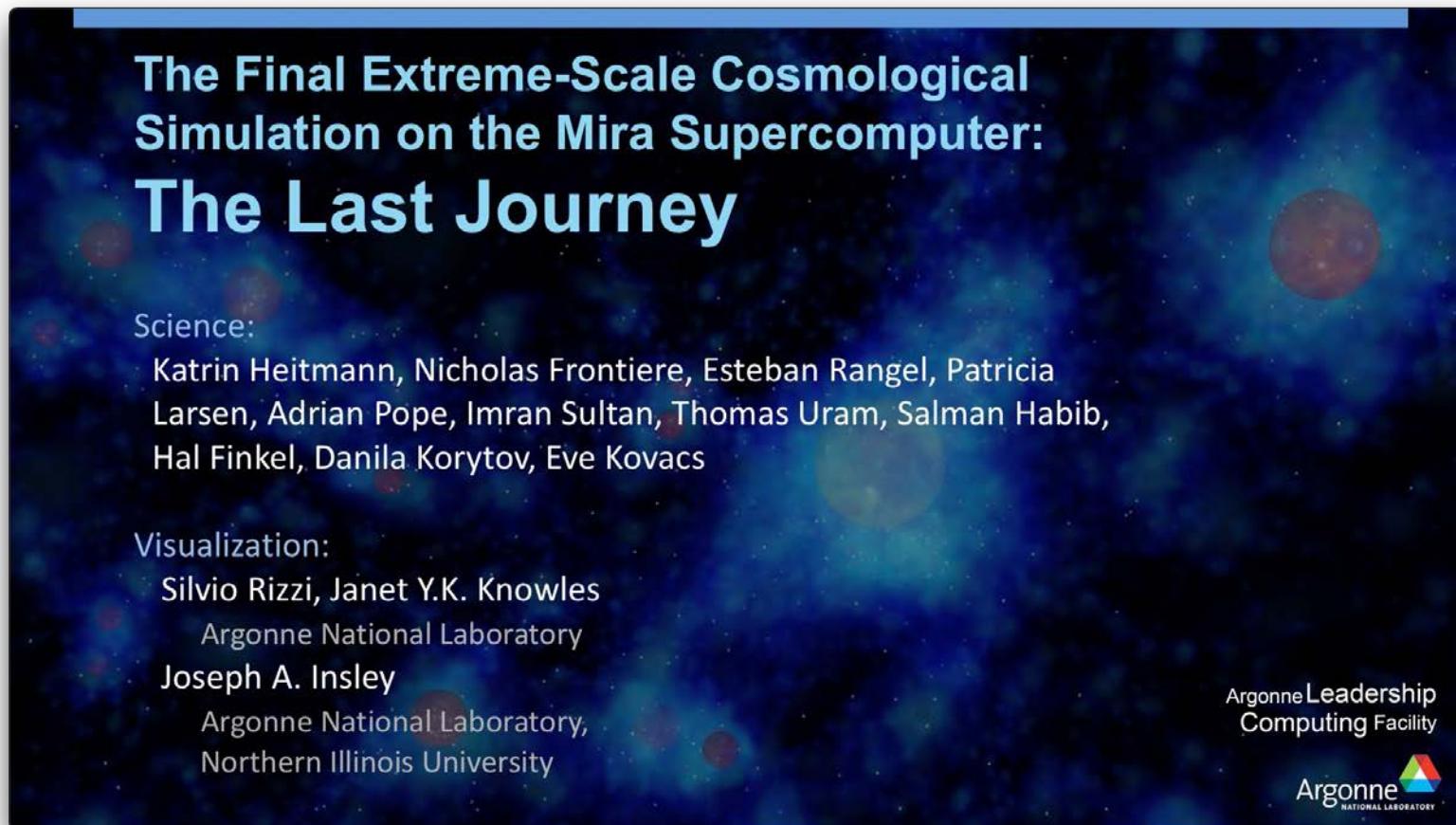
HACC: Last Journey

- Halos represented as spheres
 - Colored and scaled by mass



HACC: Last Journey

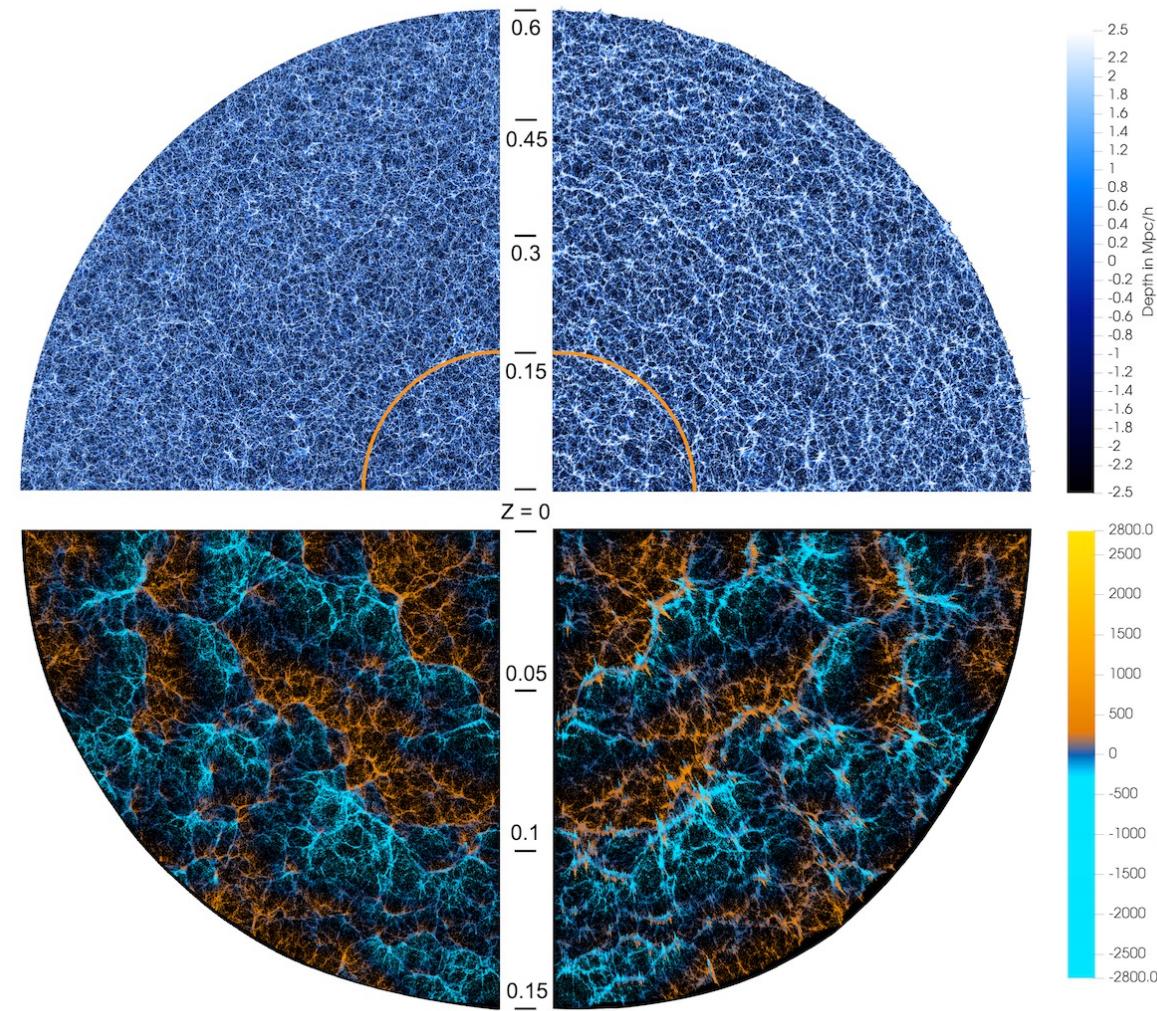
Animation: https://www.youtube.com/watch?v=JAyrpJCC_dw



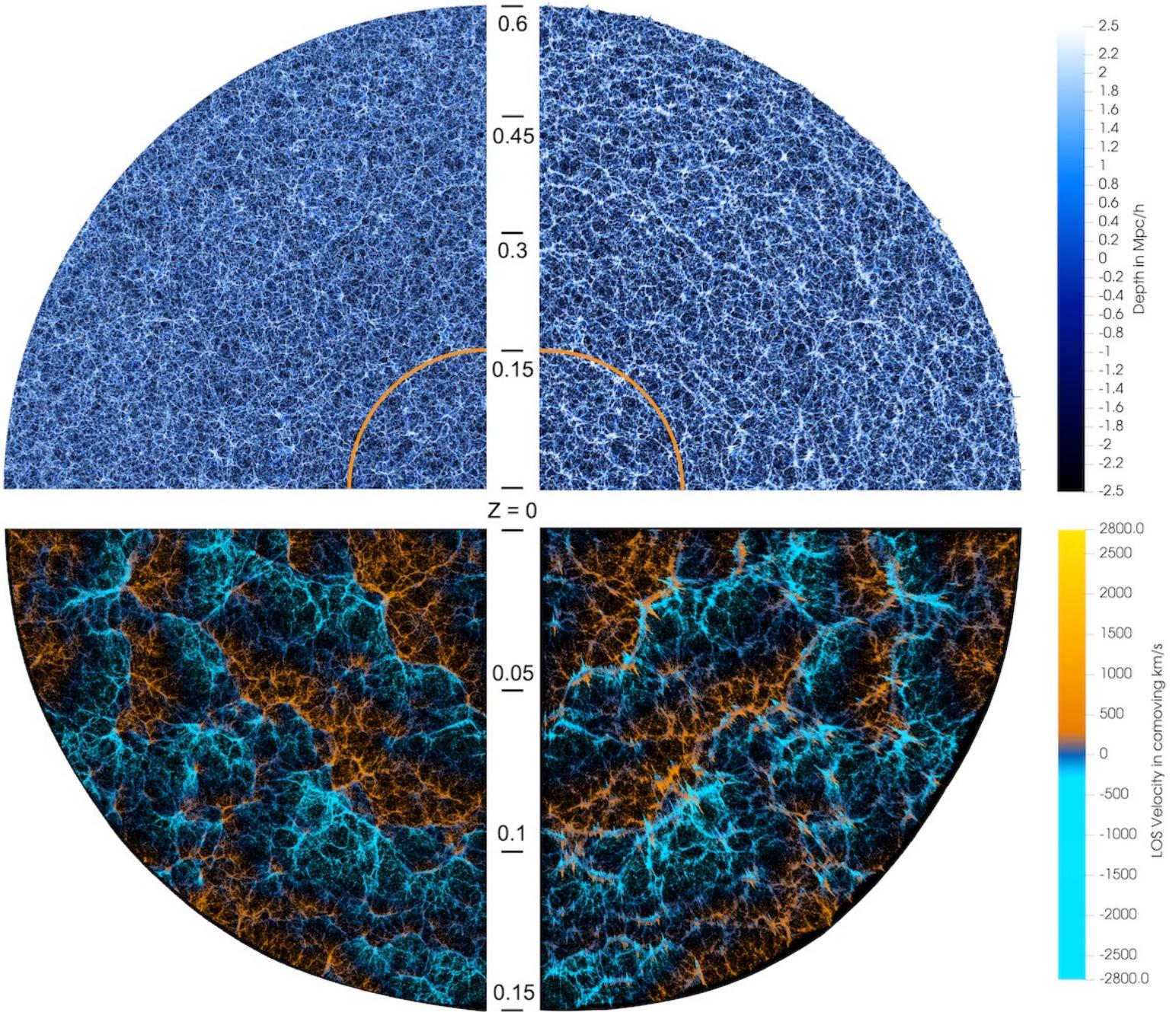
HACC - Farpoint: A High-resolution Cosmology Simulation at the Gigaparsec Scale

2022

- Visualization of the particle light cone data out to $z = 0.6$ (upper panels) and a zoom-in to $z = 0.15$ (lower panels)
- The orange curve in the upper panels shows the $z = 0.15$ boundary
- The color in the upper panels represents depth in the disk of particles (in Mpc h^{-1})
- In the lower panels, color represents LOS velocities (in comoving km s^{-1})
- The left panels render the comoving particle positions while the right panels demonstrate the so-called *Fingers of God* effect from redshift space distortion.



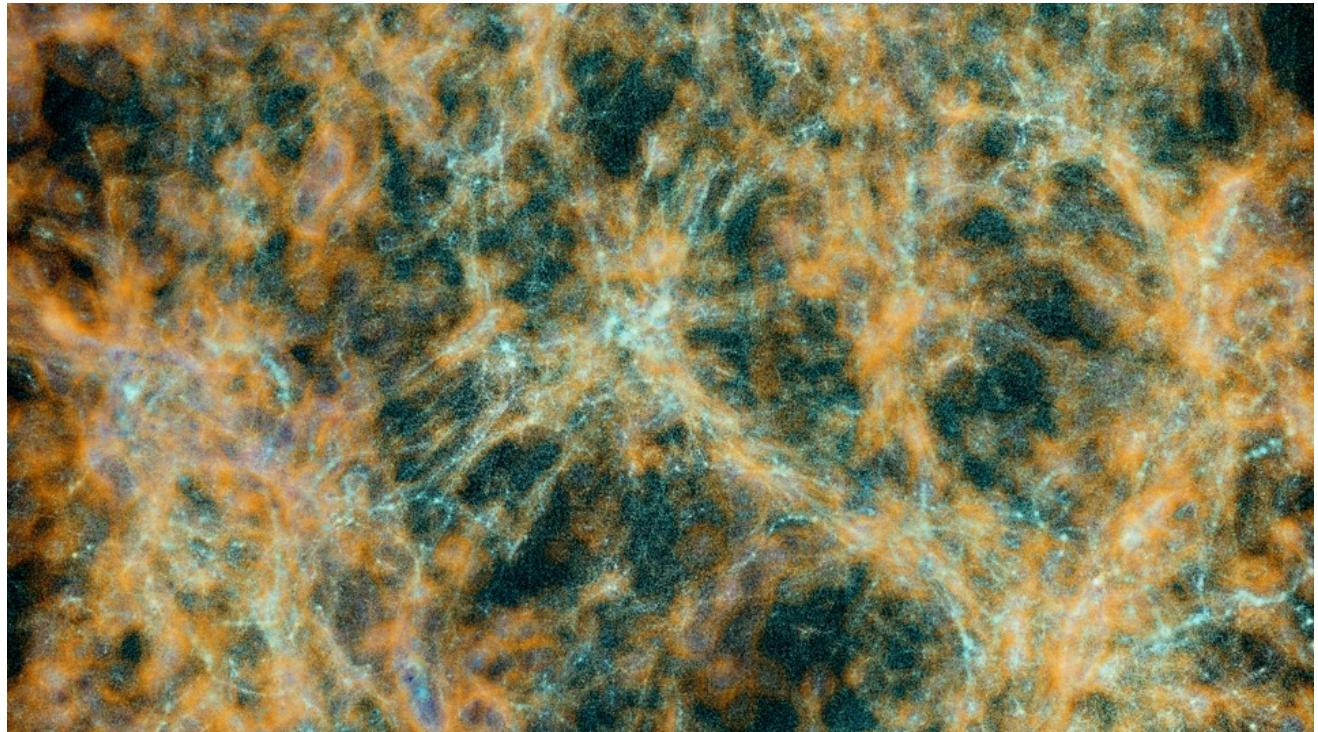
Frontiere, N., Heitmann, K., Rangel, E., Larsen, P., Pope, A., Sultan, I., Uram, T., Habib, S., Rizzi, S., Insley, J. and HACC Collaboration, 2022. Farpoint: A High-resolution Cosmology Simulation at the Gigaparsec Scale. *The Astrophysical Journal Supplement Series*, 259(1), p.15.



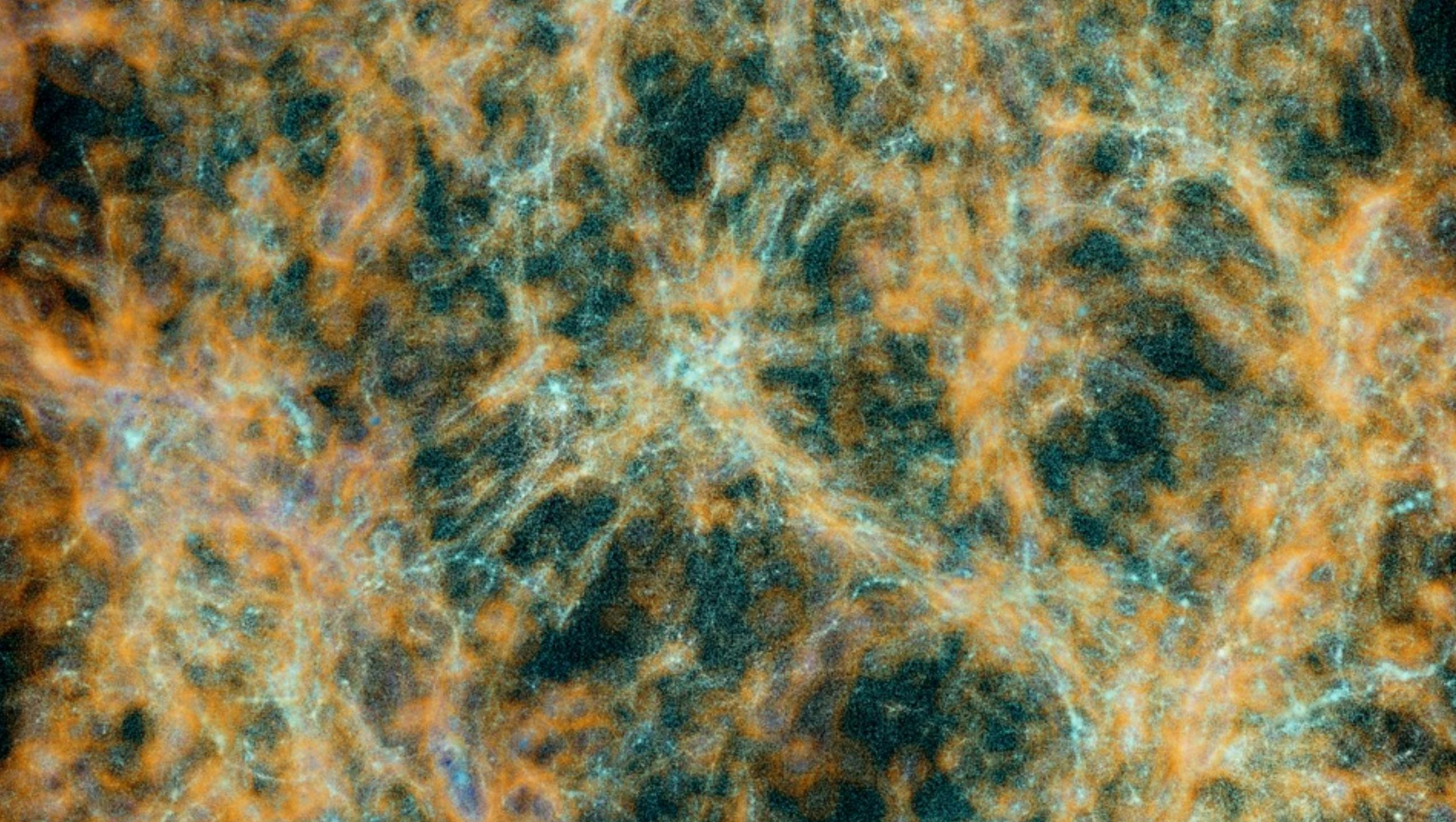
HACC: Leveraging Aurora Exascale to show where our Universe has been and predicting where it may go

2023

- Simulations and predictions enabled by HACC deployed at Exascale will help deepen our understanding of the structure of the universe and its underlying physics.
- New generations of cosmological instruments, such as the Vera Rubin Observatory, alongside with the Aurora exascale simulations, will help deliver a host of new scientific insights.
- To date, HACC has already demonstrated runs on over 1.5K Aurora nodes



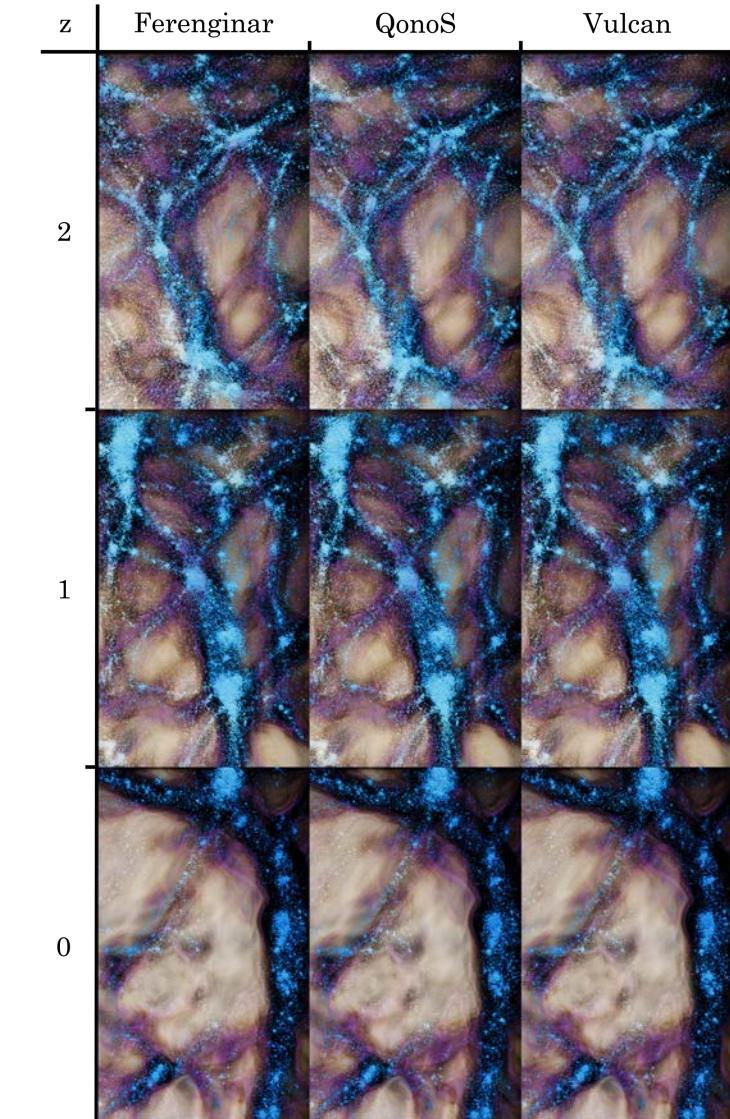
Baryons overlaid on the internal energy (proportional to the gas temperature) from a HACC simulation carried out on Aurora.



HACC: The New Worlds Simulations: Large-scale Simulations across Three Cosmologies

2024

- Three very large cosmology simulations that were carried out on the Summit supercomputer with HACC.
- The simulations cover three different cosmologies, one Λ CDM model, consistent with measurements from Planck, one simulation with massive neutrinos, and one simulation with a varying dark energy equation of state.
- Zoom-in visualization at three redshifts $z = 2, 1, 0$ (top to bottom) for the three different simulations.
- Particles are overlayed on the density representation.
- Differences are clearly visible at early times, the Ferenginar simulation shows tighter and larger structures in the high-density regions.
- Over time, the structures appear more and more similar.



Heitmann, K., Uram, T., Frontiere, N., Habib, S., Pope, A., Rizzi, S. and Insley, J., 2024. The New Worlds Simulations: Large-scale Simulations across Three Cosmologies. arXiv preprint arXiv:2406.07276.

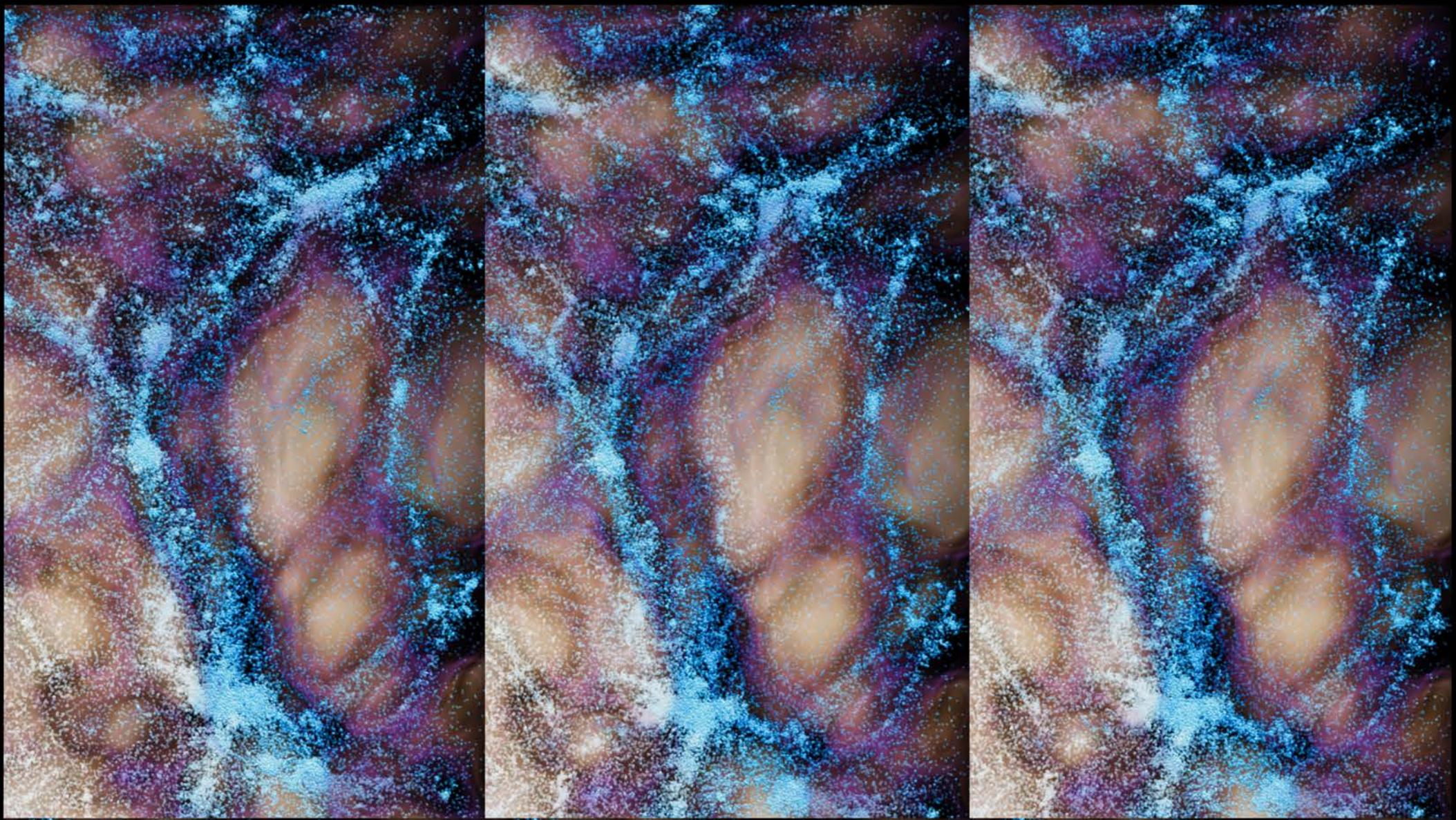
z

Ferenginar

QonoS

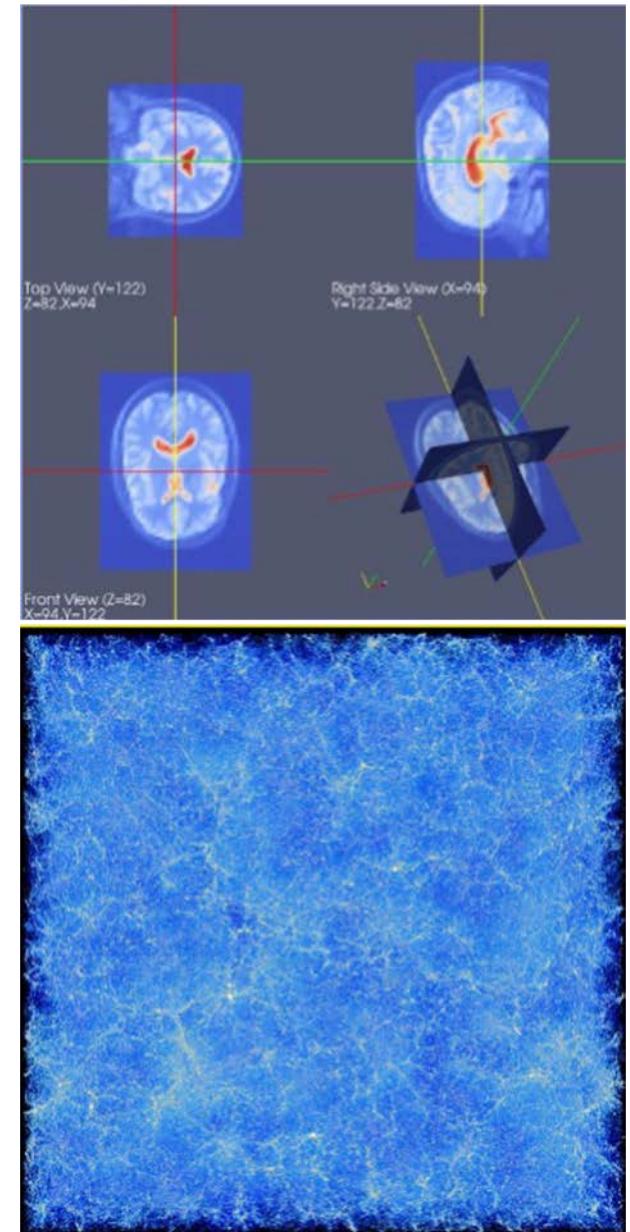
Vulcan

2



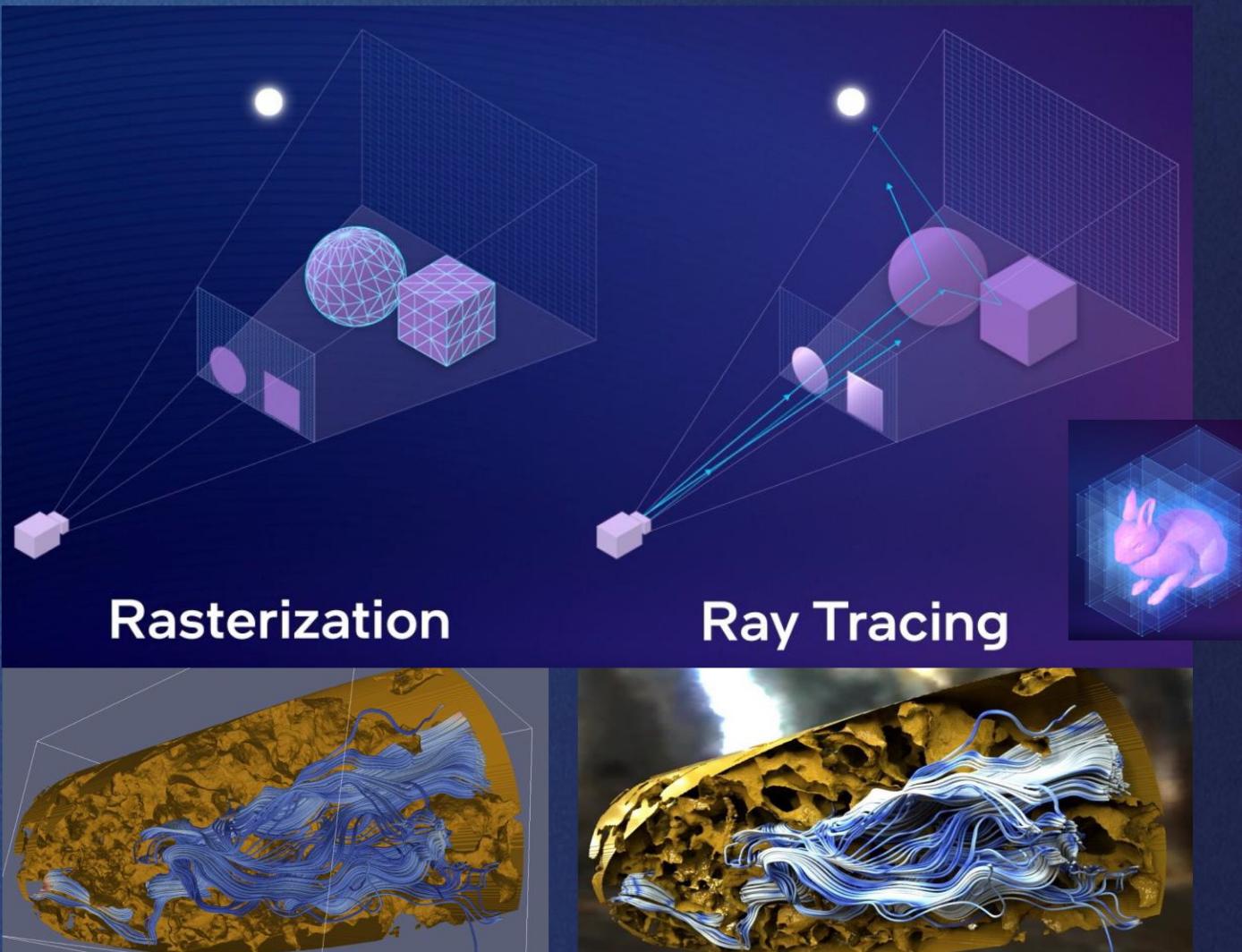
OSPRay on Intel X^e GPUs (PVC)

- Objectives
 - Advance state of the art in GPU accelerated Ray Tracing
 - Aurora first supercomputer where GPU accelerated ray tracing is the primary renderer
- Port OSPRay, and supporting libraries to GPU
- Scalability and compatibility
 - Across multiple GPUs in a node
 - Across multiple nodes



The following slides courtesy of Roba Binyahib
and Dave Demarle of Intel

Rendering

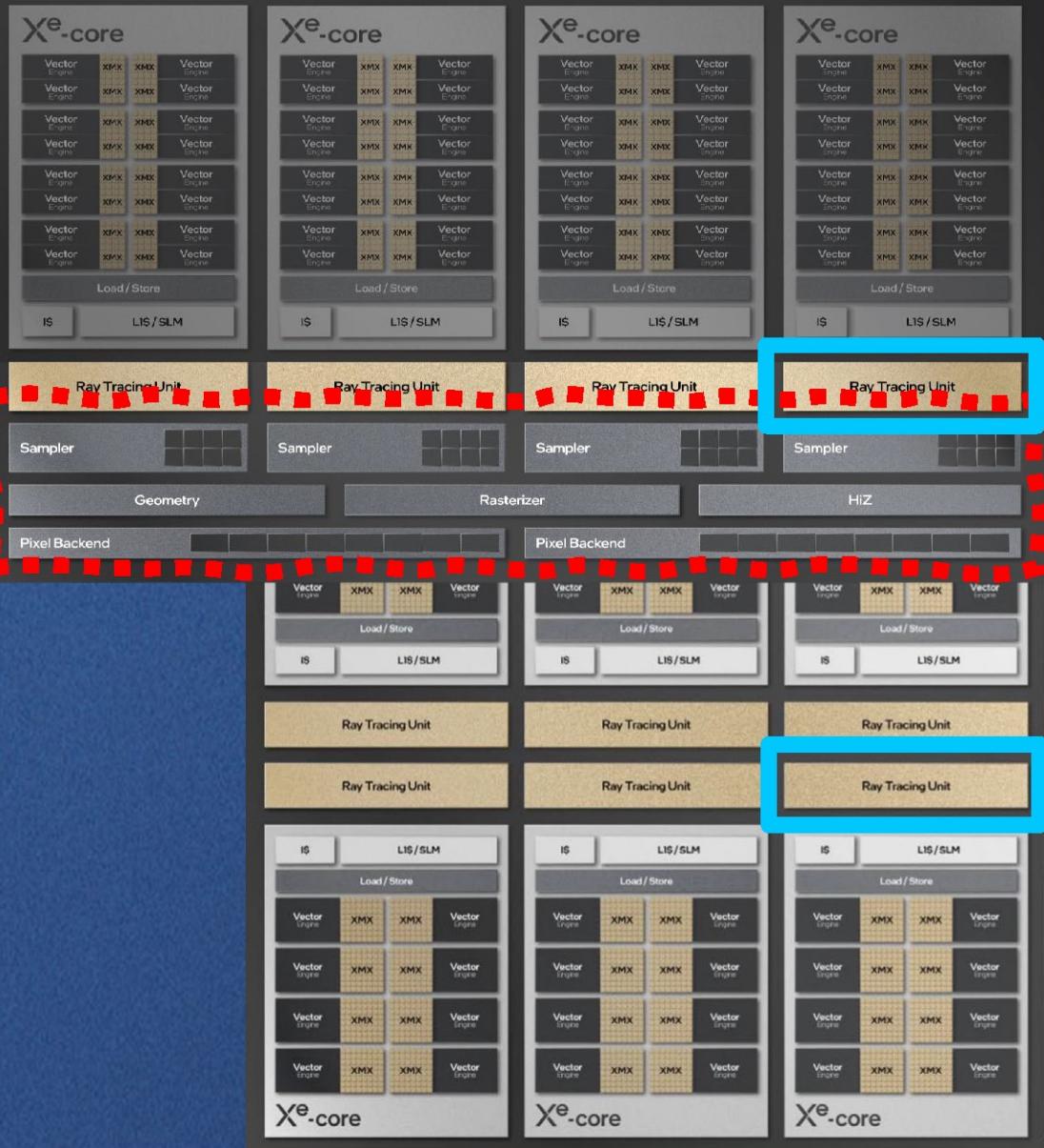


Visualizing water flowing through a limestone karst from a South Florida ground core sample. Credit: Data courtesy of Michael Sukop, Sade Garcia, Florida International University and Kevin Cunningham, United States Geological Survey. Visualization: Carson Brownlee, Aaron Knoll, Paul Navratil, Texas Advanced Computing



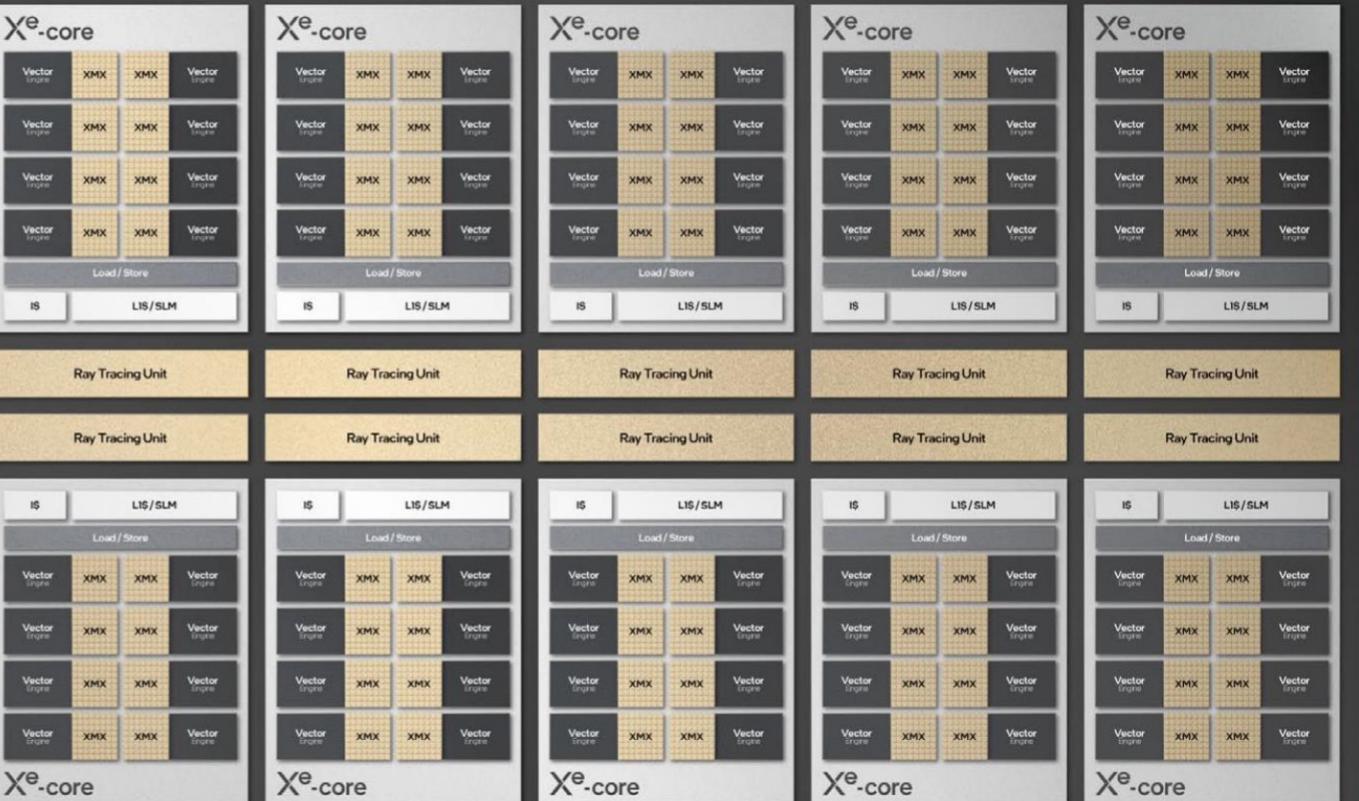
Render slice

Alchemist "DG2"



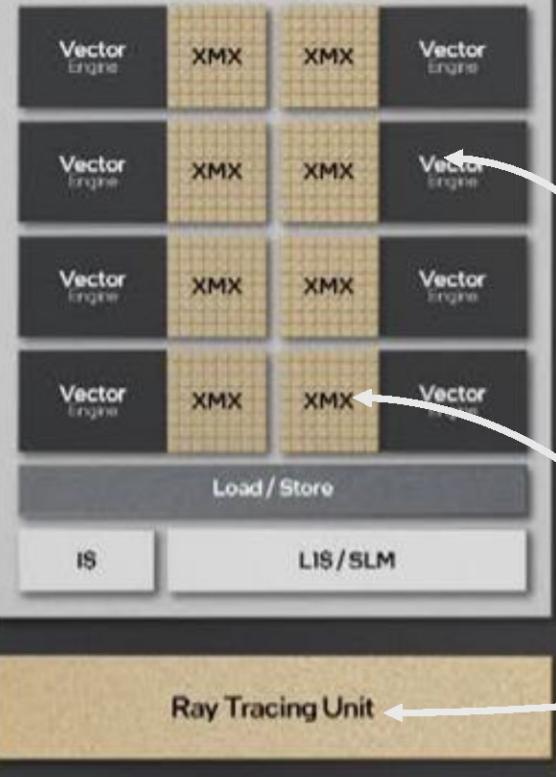
x10000 -> Aurora has 7.6M Ray Tracing Units
x6 + 2 SPR = node aka "blade"
x2 = GPU aka "device"
x4 = Tile aka "subdevice"

Max GPU ("PVC")



Xe HPC slice

Xe-core



Application/InSitu library
ParaView/Catalyst, VisIt/libSim, /SENSEI, OSPRay Studio/

Intel® OSPRay

Scalable rendering engine, API and SDK
Distributed MPI Rendering via OSPRay MPI



Intel® implementation of the Khronos ANARI specification (<https://www.khronos.org/anari>)

<http://www.ospray.org>

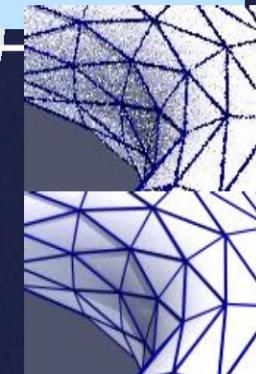
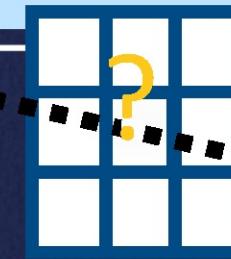
Intel® Embree

Optimized geometry ray tracing kernels
- BVH builders, traversal and intersection
<http://www.embree.org>

Intel® Open VKL

API for volume sampling, traversal,
interpolation and classification
<http://www.openvkl.org>

Intel® Open Image Denoise
AI / DL – based denoising of sampling
artifacts from path tracing
<http://www.openimagedenoise.org>



intel.

Intra Node (MultiDevice)

Delegate work to one or more subdevices in an image parallel fashion
Since OSPRay v2.7.0.

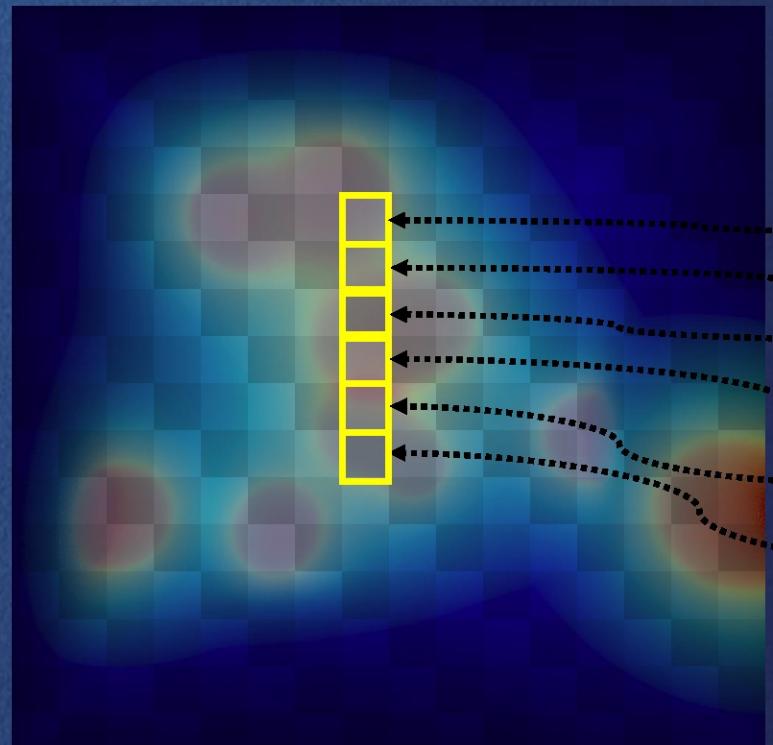
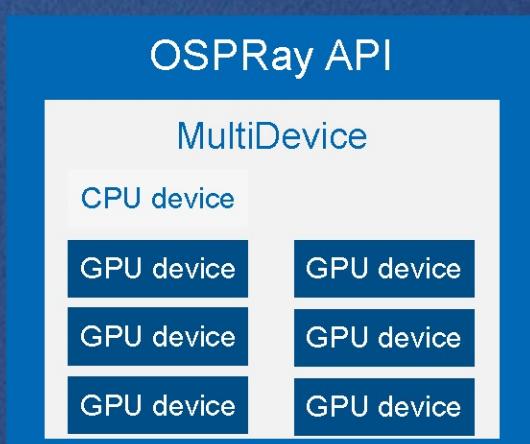
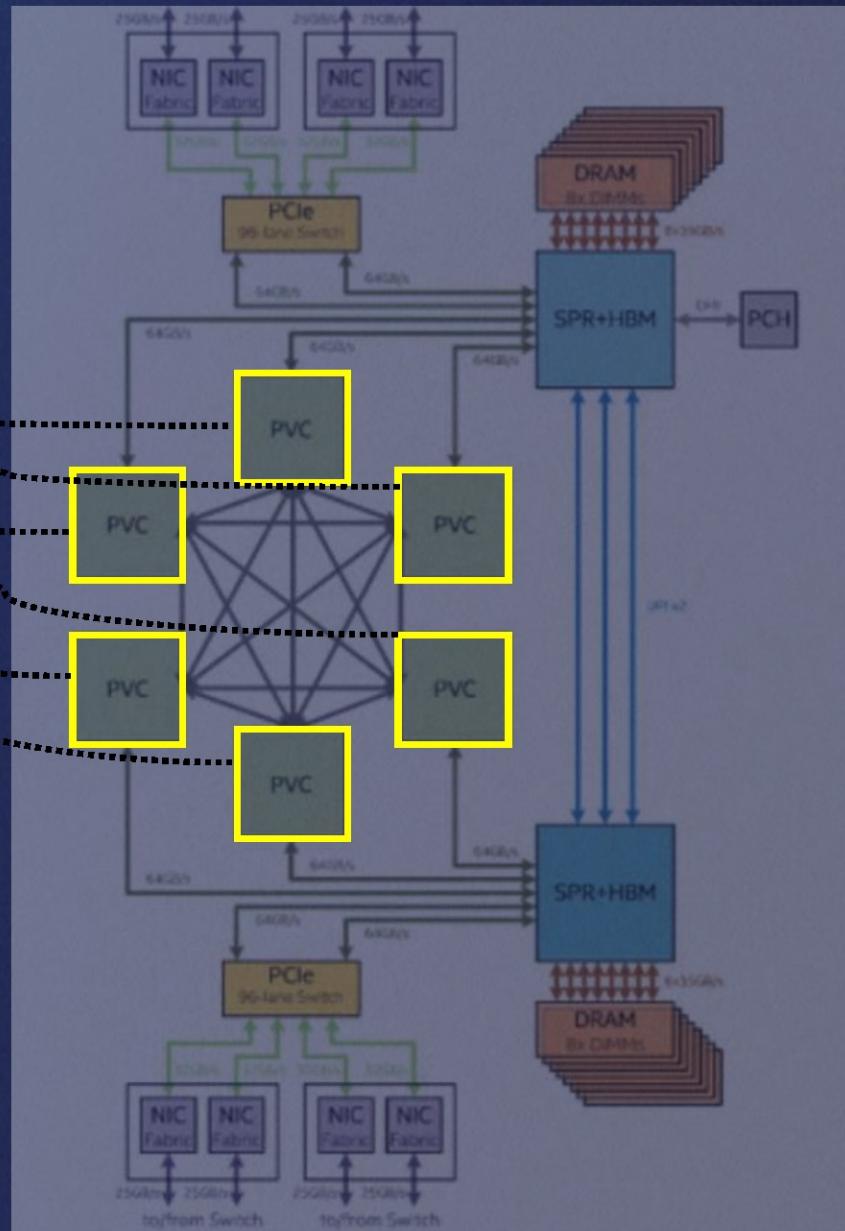


image parallel, data replicated



Inter Node (Data Scalability)

MPIDistributed Device

Strategy

Run copies of the same in situ sim or vis application

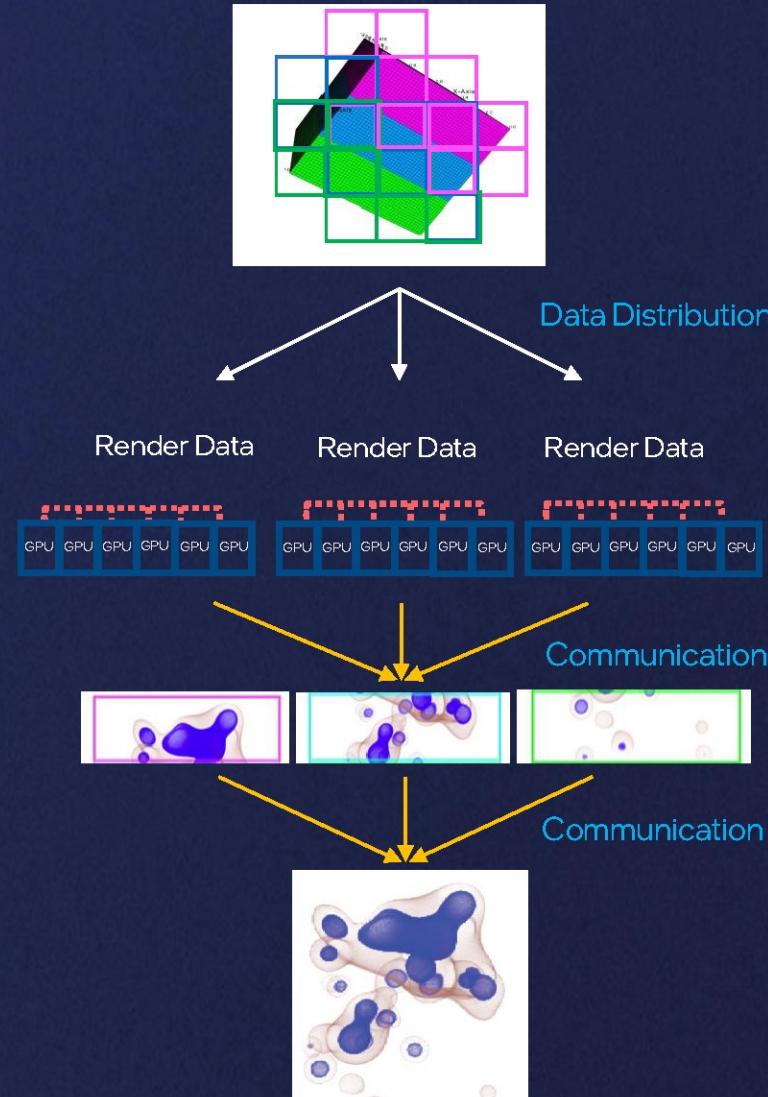
Each runs the same operations

Each operates on different subsets of the data

Each renders only the subsets of pixels (tiles) their data intersects

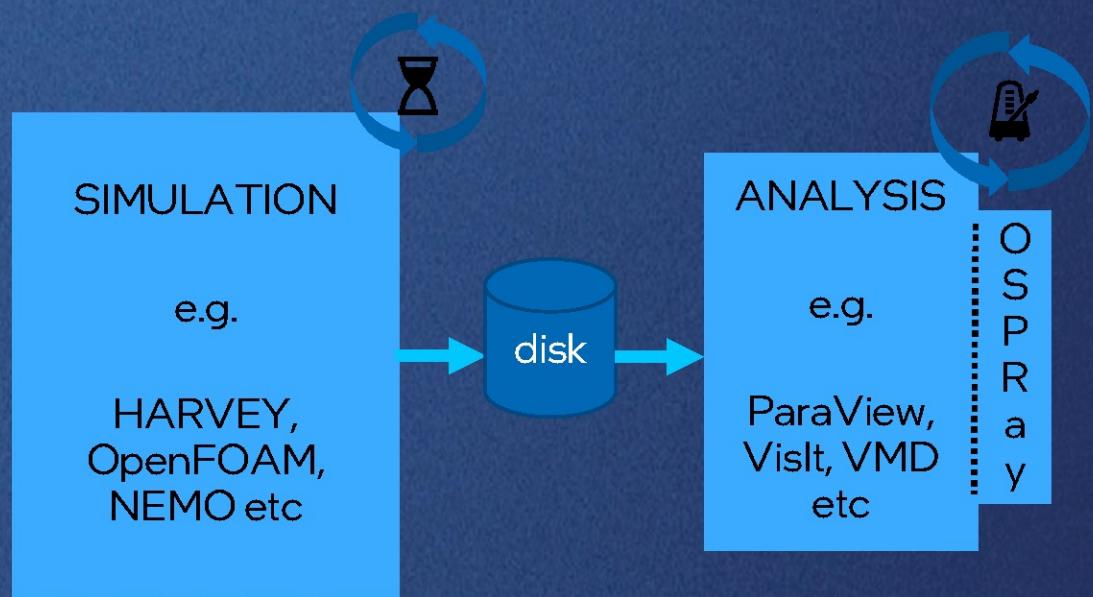
Composite tiles in flight using OSPRay's distributed frame buffer or more typically Sandia's IceT library

1MPI rank per GPU x N ranks -> up to N x GPU RAM



Post Hoc

- Traditional human in the loop analysis
- Run simulation, save timesteps to disk
- At some later point, load data into analysis package

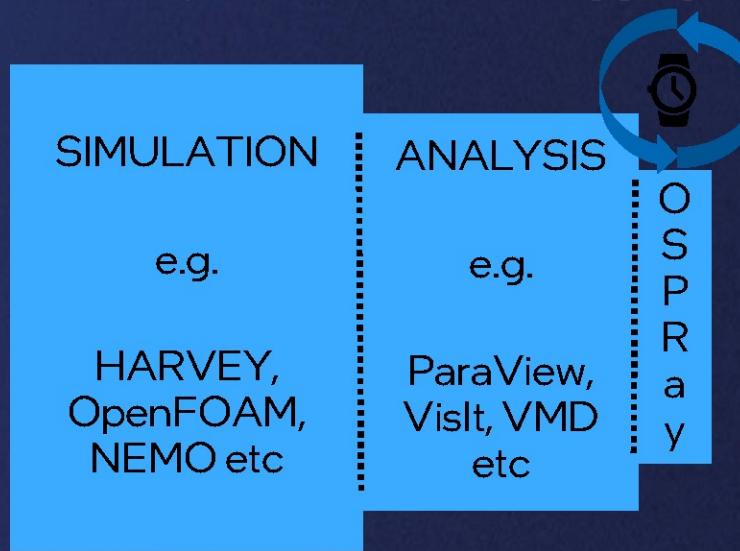


traditional aka "*post hoc*" visualization

vs

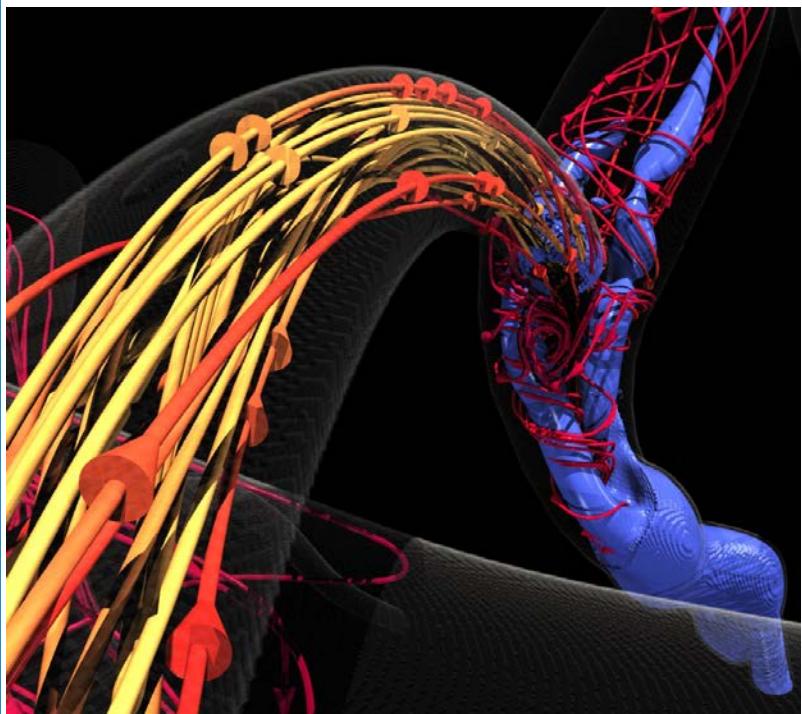
In Situ

- Analyze and render data concurrently with computation
- i.e. bypass IO, call analysis directly ("in line") or send raw data to ("in transit")
- Orders of magnitude less IO
- Increased scalability
- Increase visibility/resolution in temporal dimension - between restarts
- Pathway to enhanced debugging and steering

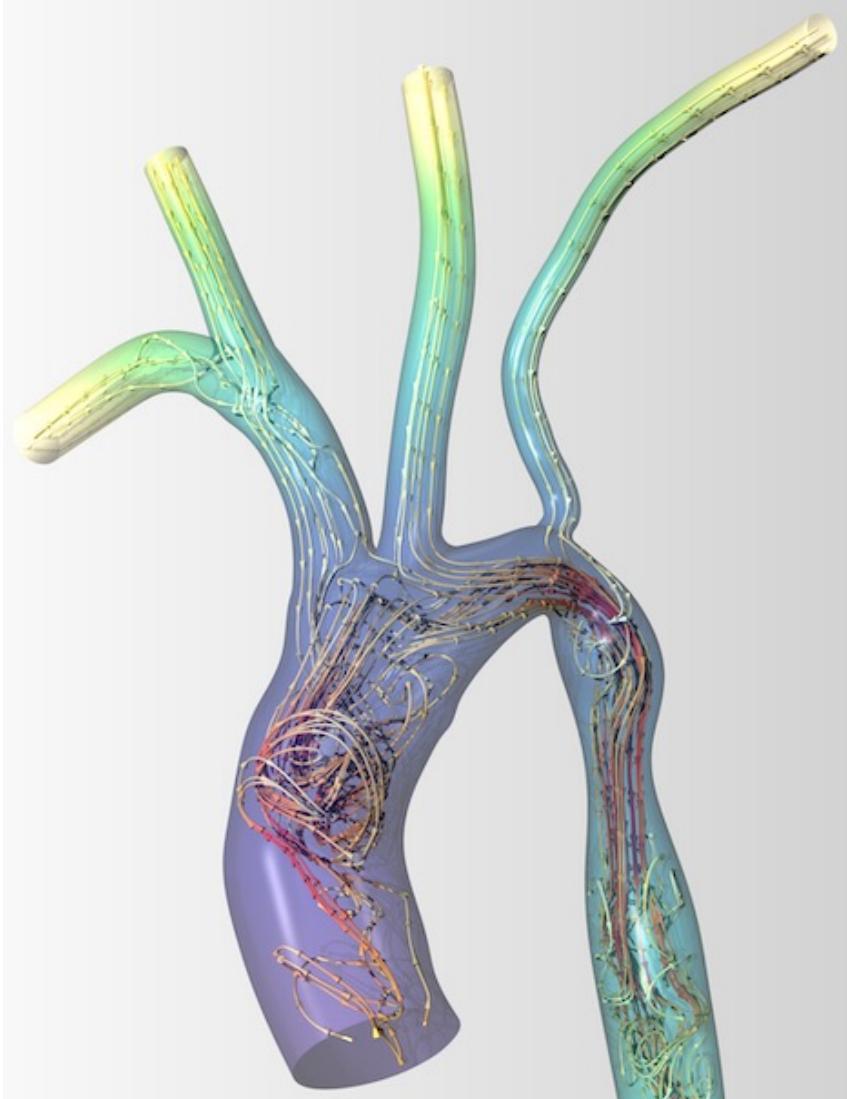


in situ visualization (specifically "in line")

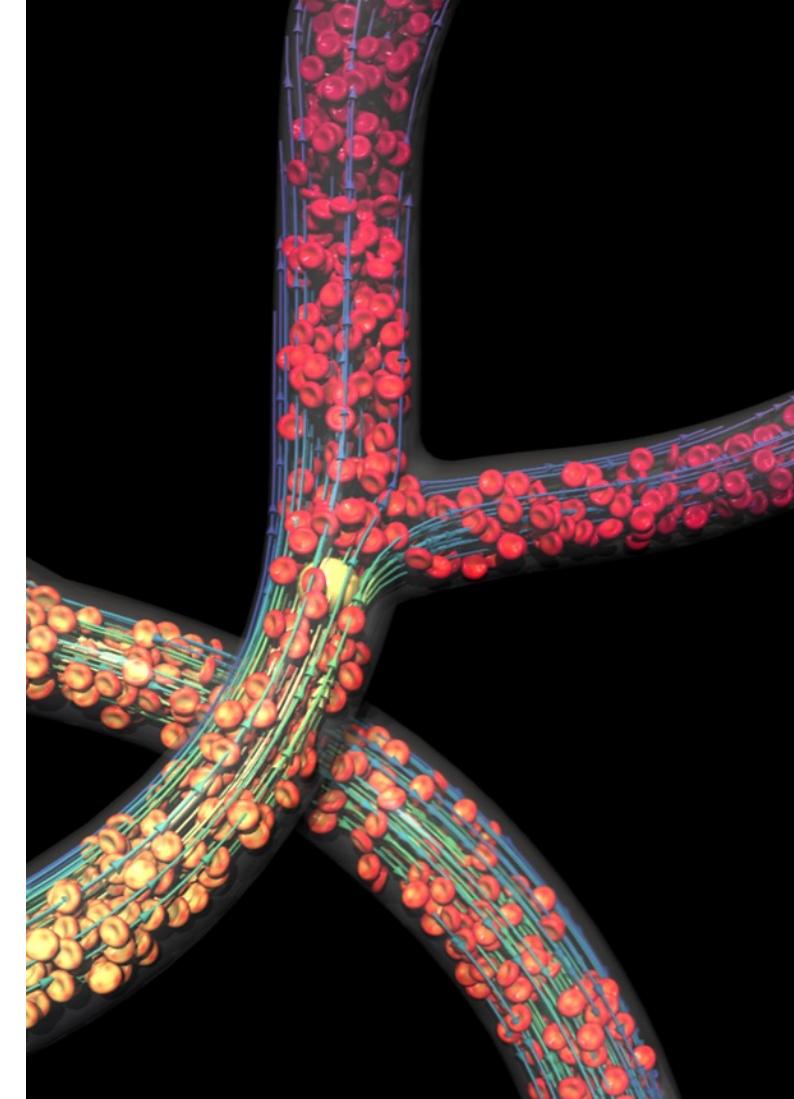
PI: Amanda Randles, Duke University



2020



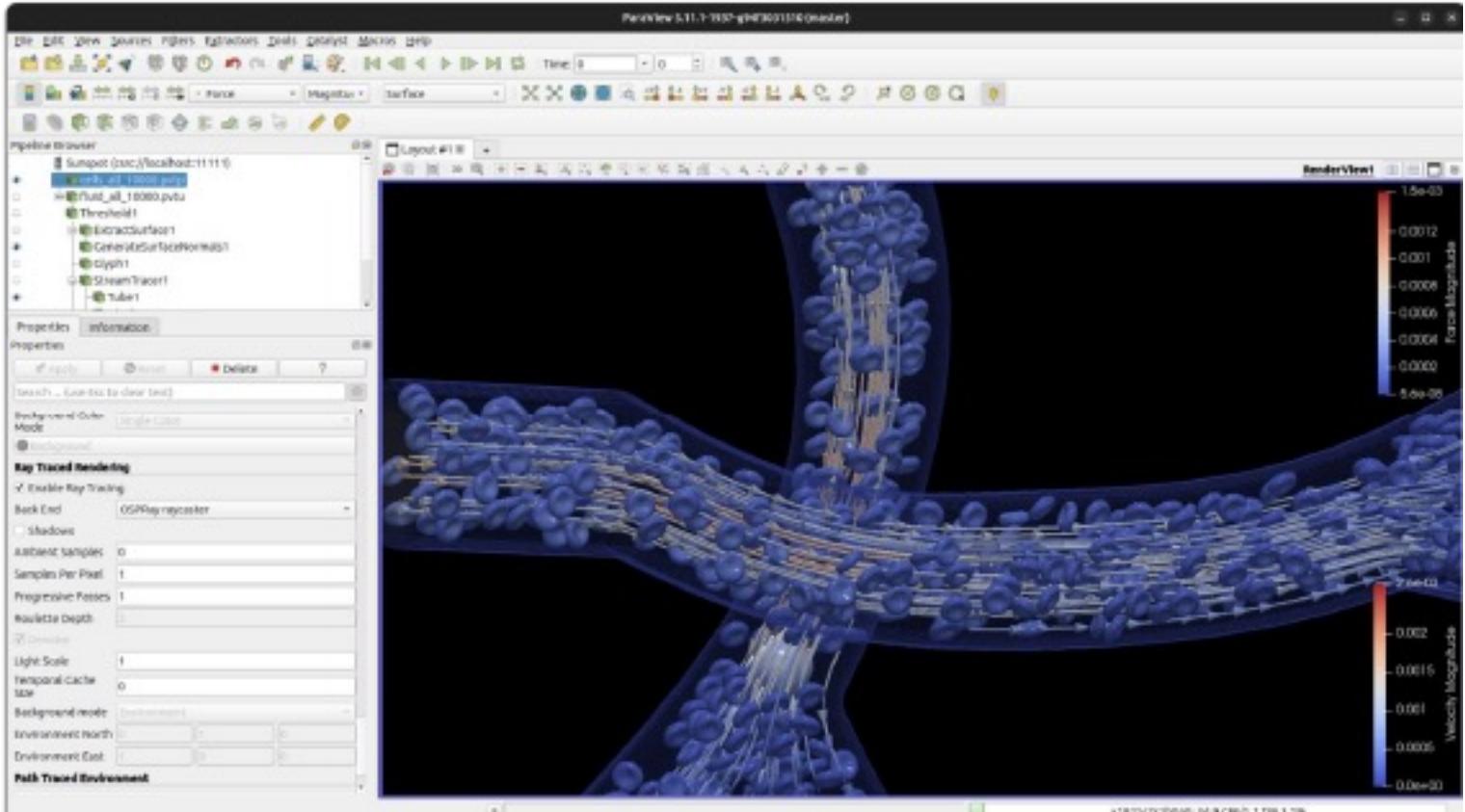
2023 Rendered on Aurora



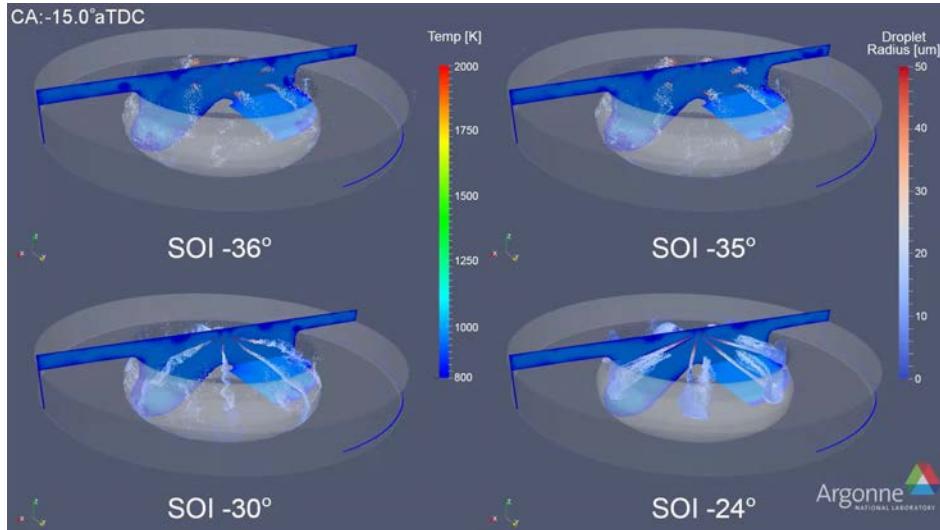
2023 Rendered on Aurora

SC23 Live Demo

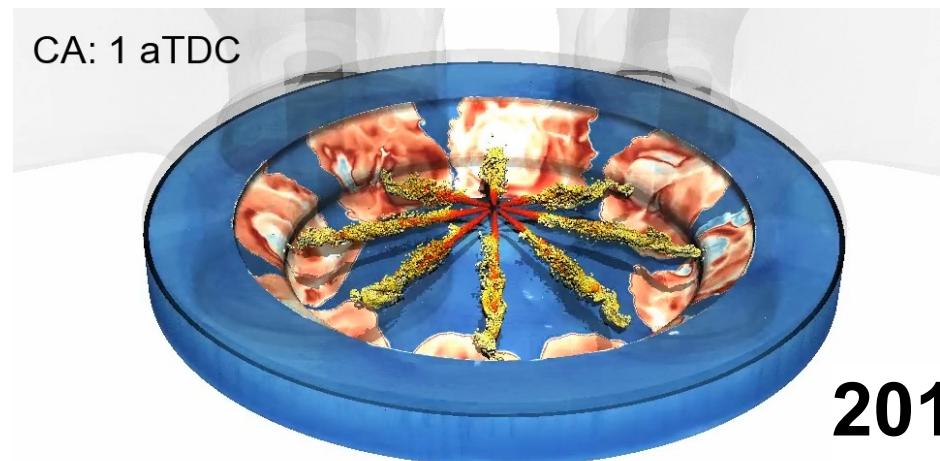
- ParaView server running on 16 nodes (96 GPUs) on Sunspot
- ParaView client running on SC23 show floor



PI: Sibendu Som, Argonne National Laboratory

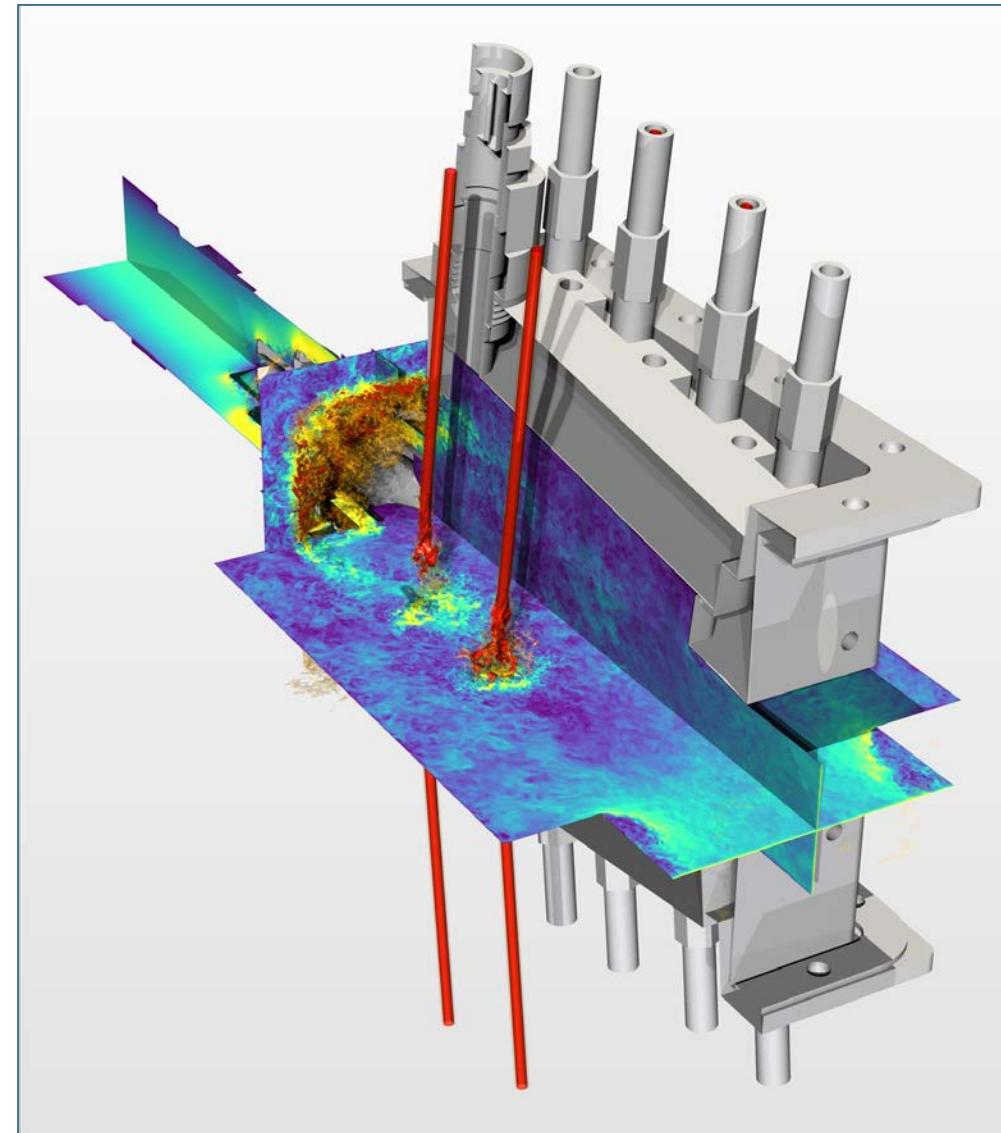


2015

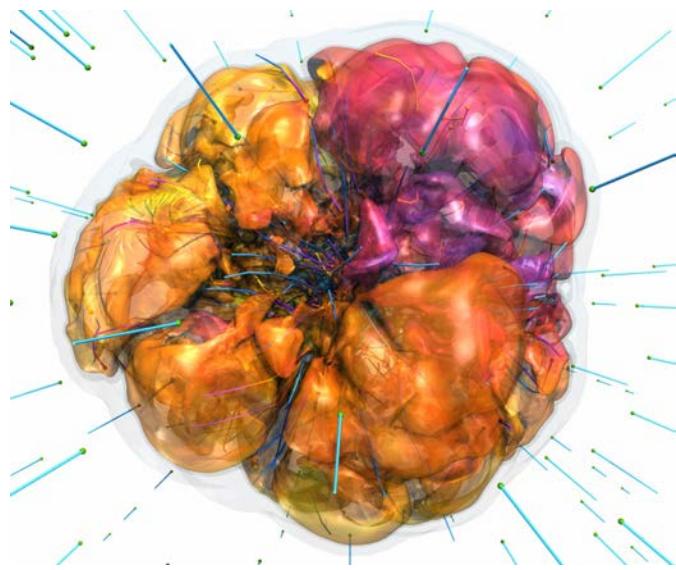


2017

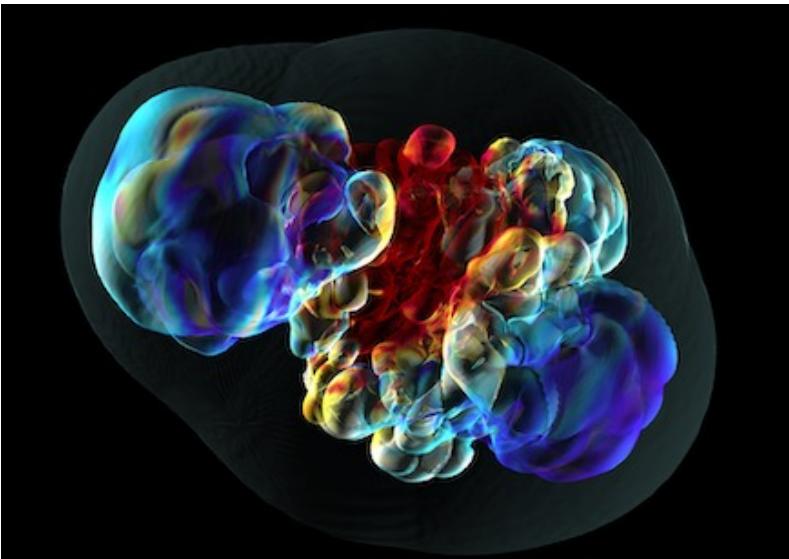
2023



PI: Adam Burrows, Princeton University

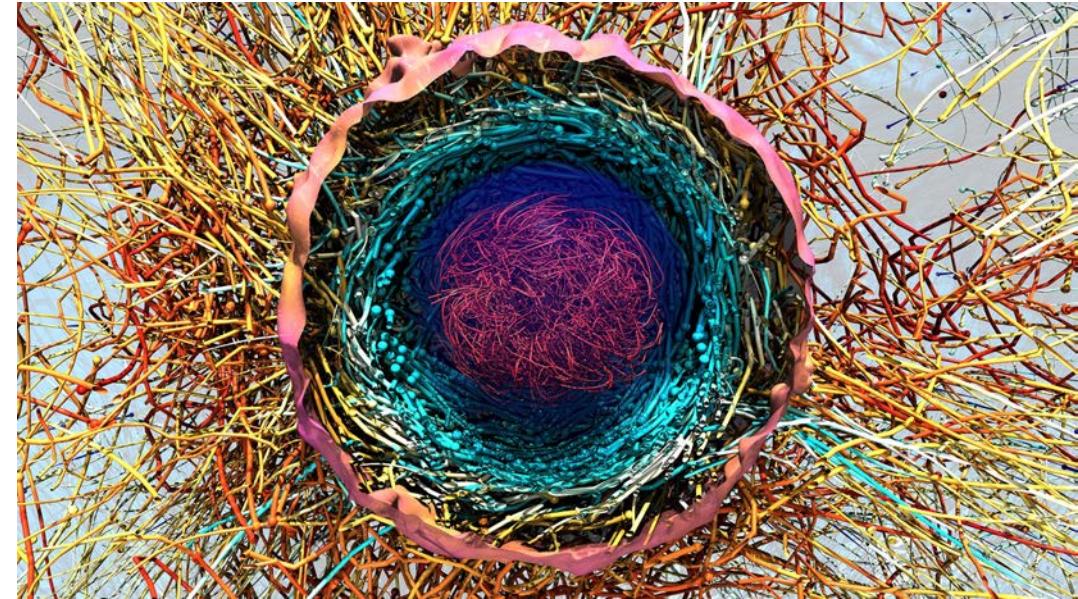


2019



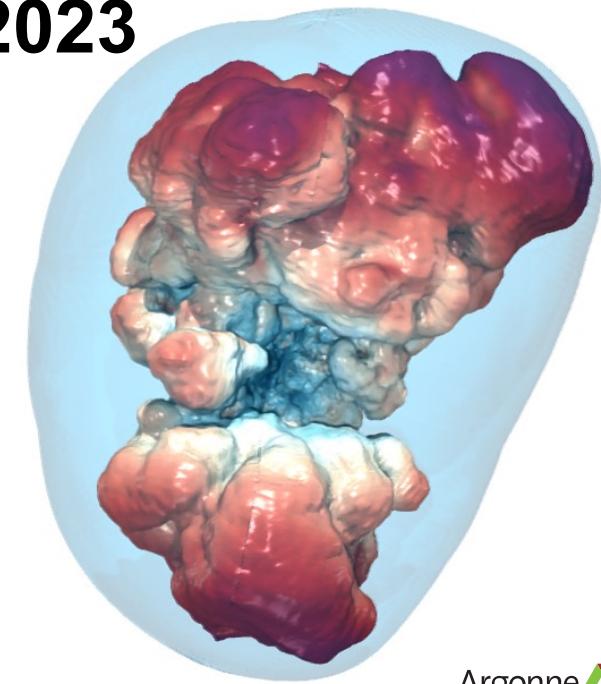
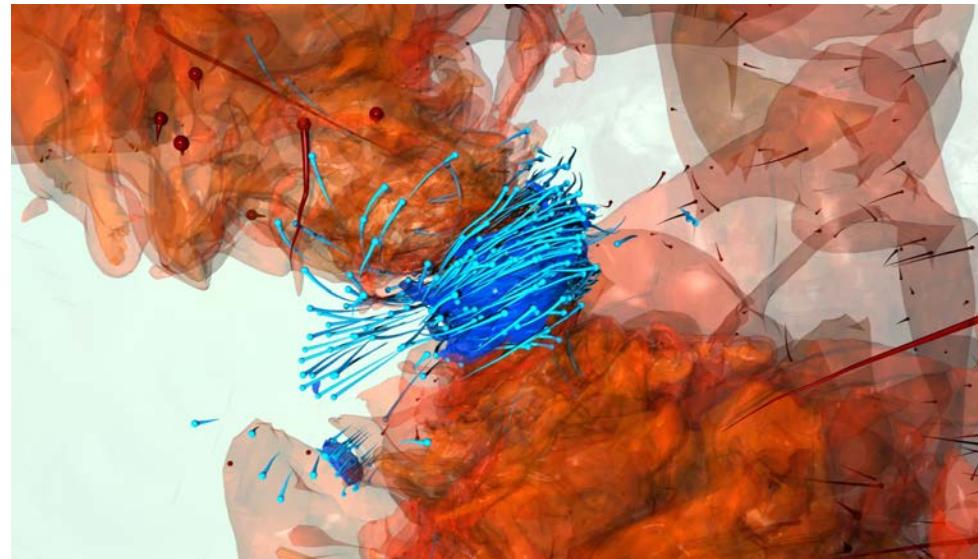
2022

2023

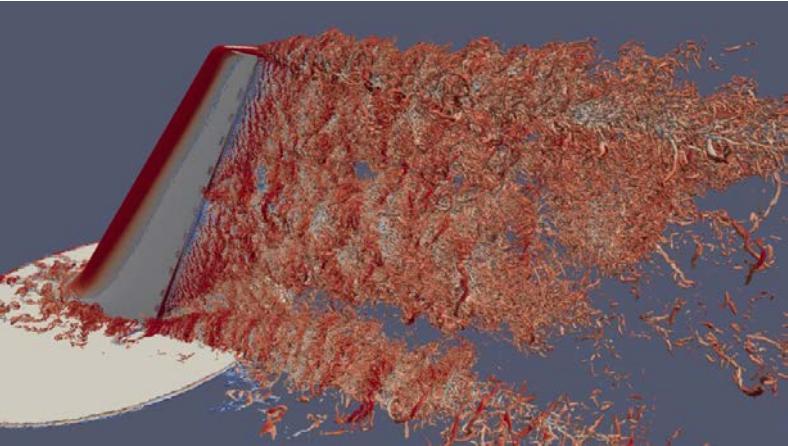


2021

2023

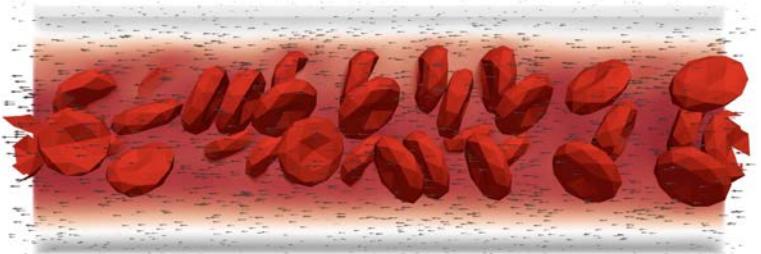
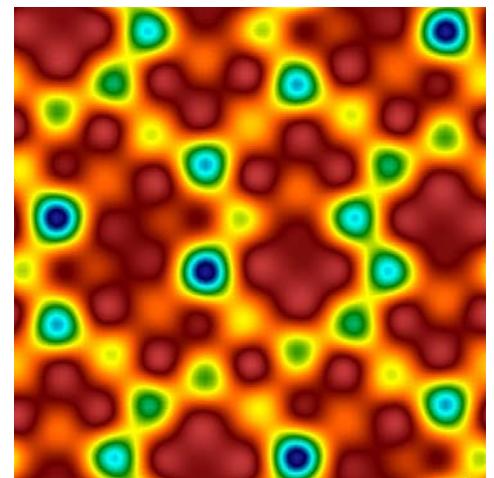


In Situ



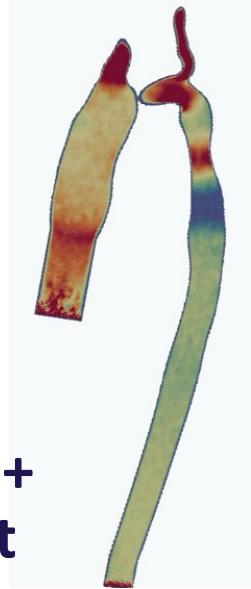
~2014
**PHASTA, Catalyst,
Ken Jansen**

2018
**Nek5000,
SENSEI**



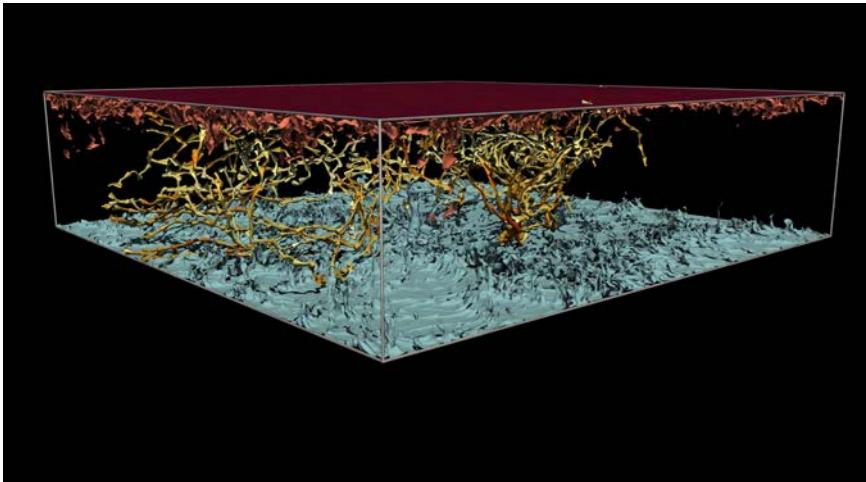
2021 - 2024

**Palabos+LAMMPS,
SENSEI + Catalyst,
bi-directional**

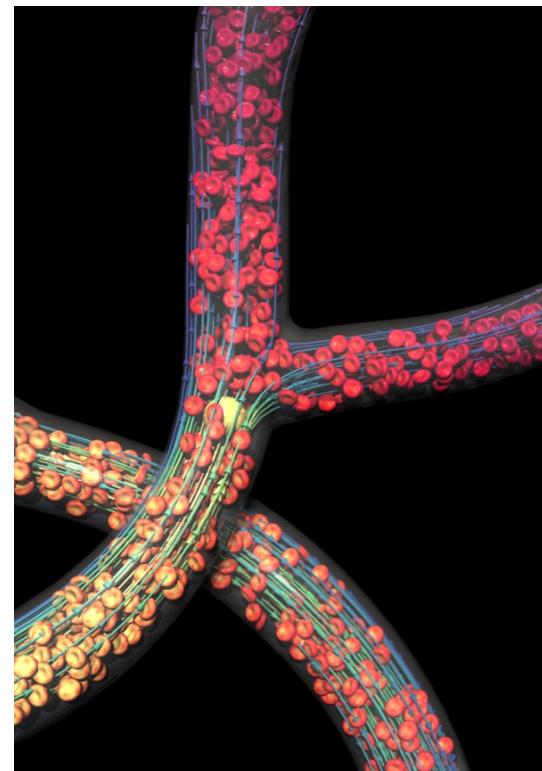


2019
**SENSEI +
Catalyst**

2024
**nekRS,
Ascent +
Catalyst**



HARVEY
**Ascent +
Catalyst** **2024**



THANKS

- Argonne Leadership Computing Facility at Argonne National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under contract DE-AC02-06CH11357.

QUESTIONS?

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