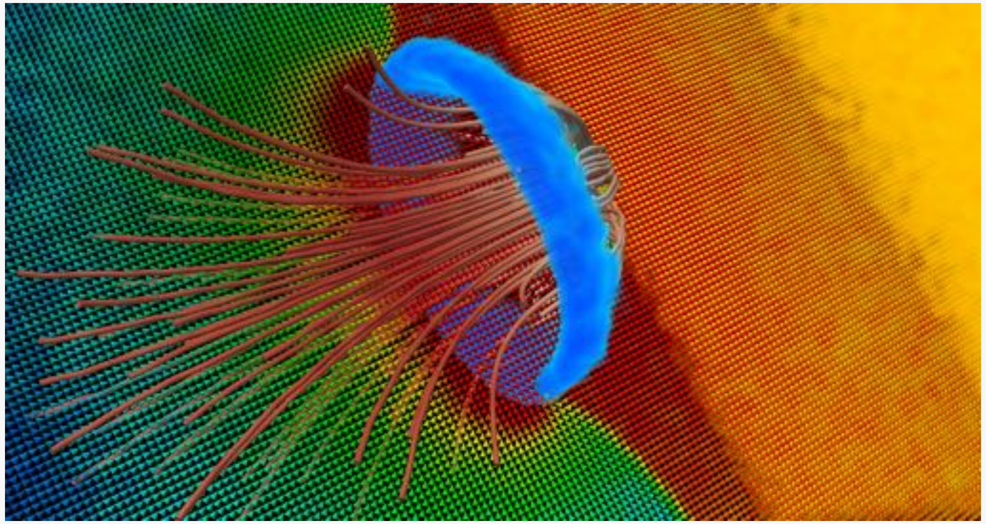
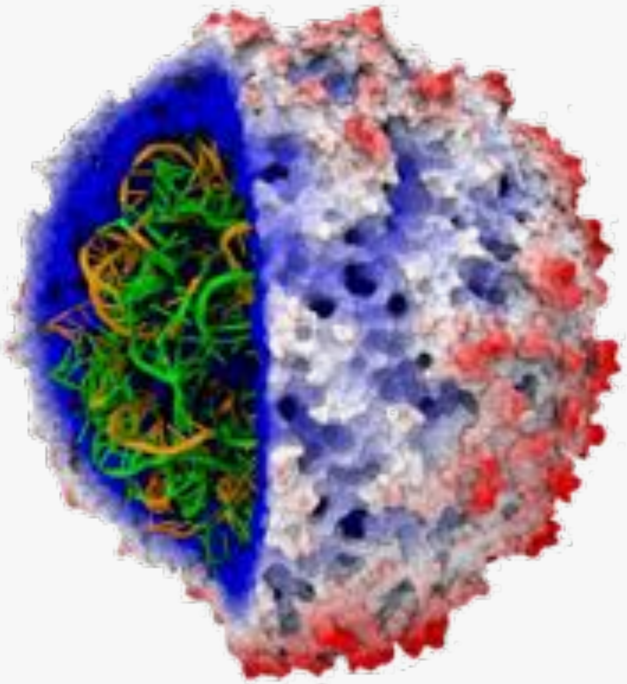
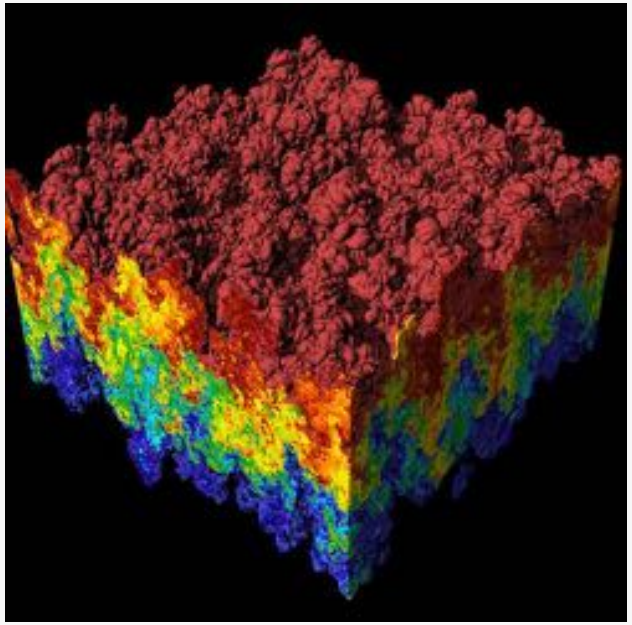
Argonne Training Program on Extreme-Scale Computing (ATPESC)

Data Analysis and Visualization







ECP
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U.S. DEPARTMENT OF ENERGY | Office of Science
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Visualization & Data Analysis

Time	Title of presentation	Lecturer
8:30 am	**Visualization Introduction**	Mike Papka, Joe Insley, Silvio Rizzi, ANL
9:30 am	**Large Scale Visualization with ParaView (Presentation)**	Dan Lipsa, Kitware
10:30 am	*Break*	
11:00 am	**Large Scale Visualization with ParaView (Hands-on Exercises)**	Dan Lipsa, Kitware
12:00 pm	**Visualization and Analysis of Massive Data with VisIt (Presentation)**	Cyrus Harrison, LLNL
12:30 pm	*Lunch*	
1:30 pm	**Visualization and Analysis of Massive Data with VisIt (Hands-on Exercises)**	Cyrus Harrison, LLNL
3:00 pm	*Break*	
3:30 pm	**Scalable Molecular Visualization and Analysis Tools in VMD**	John Stone, UIUC
4:30 pm	**Exploring Visualization with Jupyter Notebooks**	Mike Papka, Joe Insley, Silvio Rizzi, ANL
5:30 pm	***Dinner Talk: Visual Computing at the Electronic Visualization Laboratory***	Liz Marai, UIC
6:30 pm	*Hands-on Exercises*	

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Argonne Training Program on Extreme-Scale Computing (ATPESC)

Visualization Introduction

Mike Papka
Joe Insley
Silvio Rizzi
Argonne Leadership Computing Facility
Argonne National Laboratory

Q Center, St. Charles, IL (USA)
August 9, 2018

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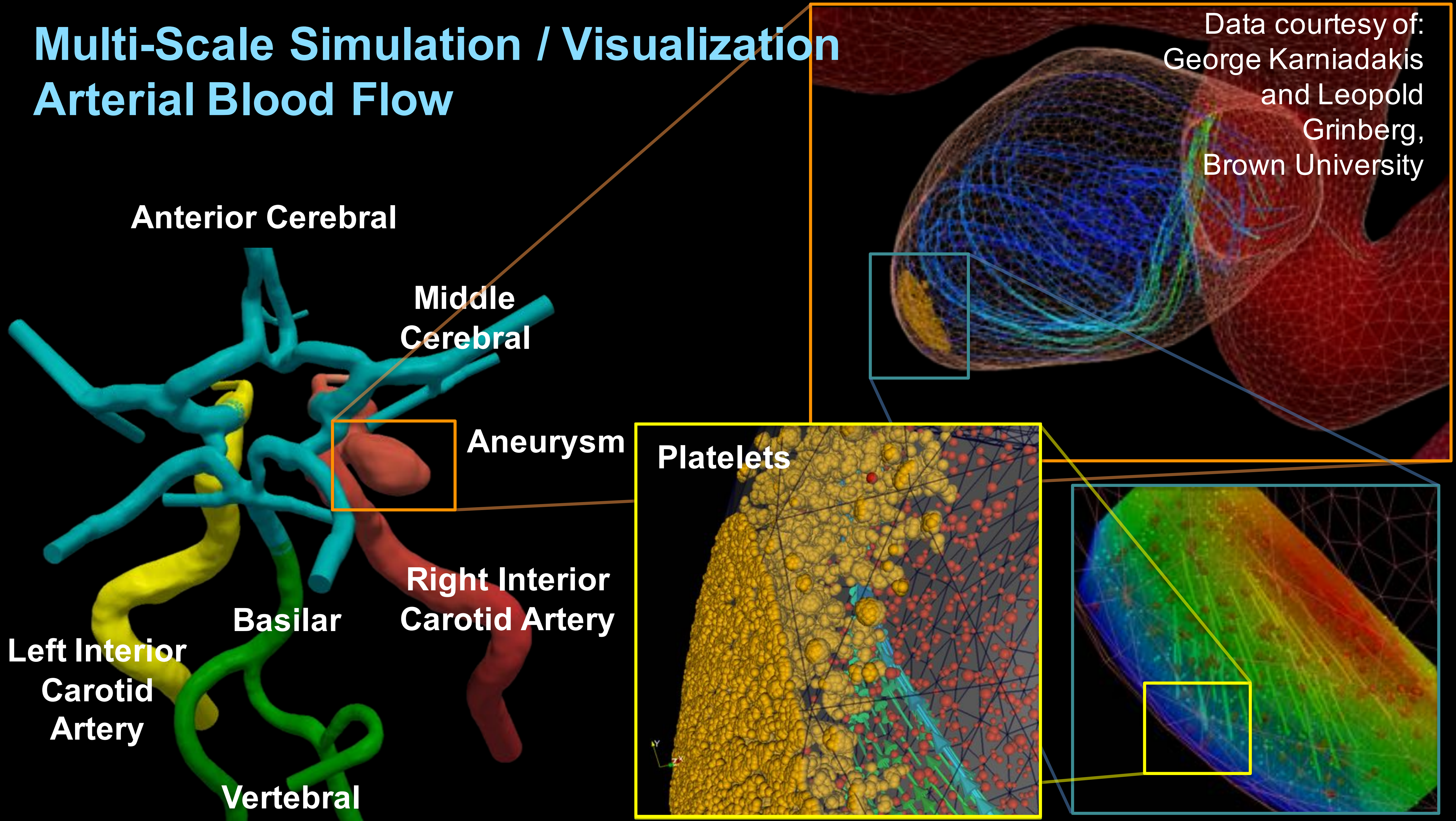
Here’s the plan…

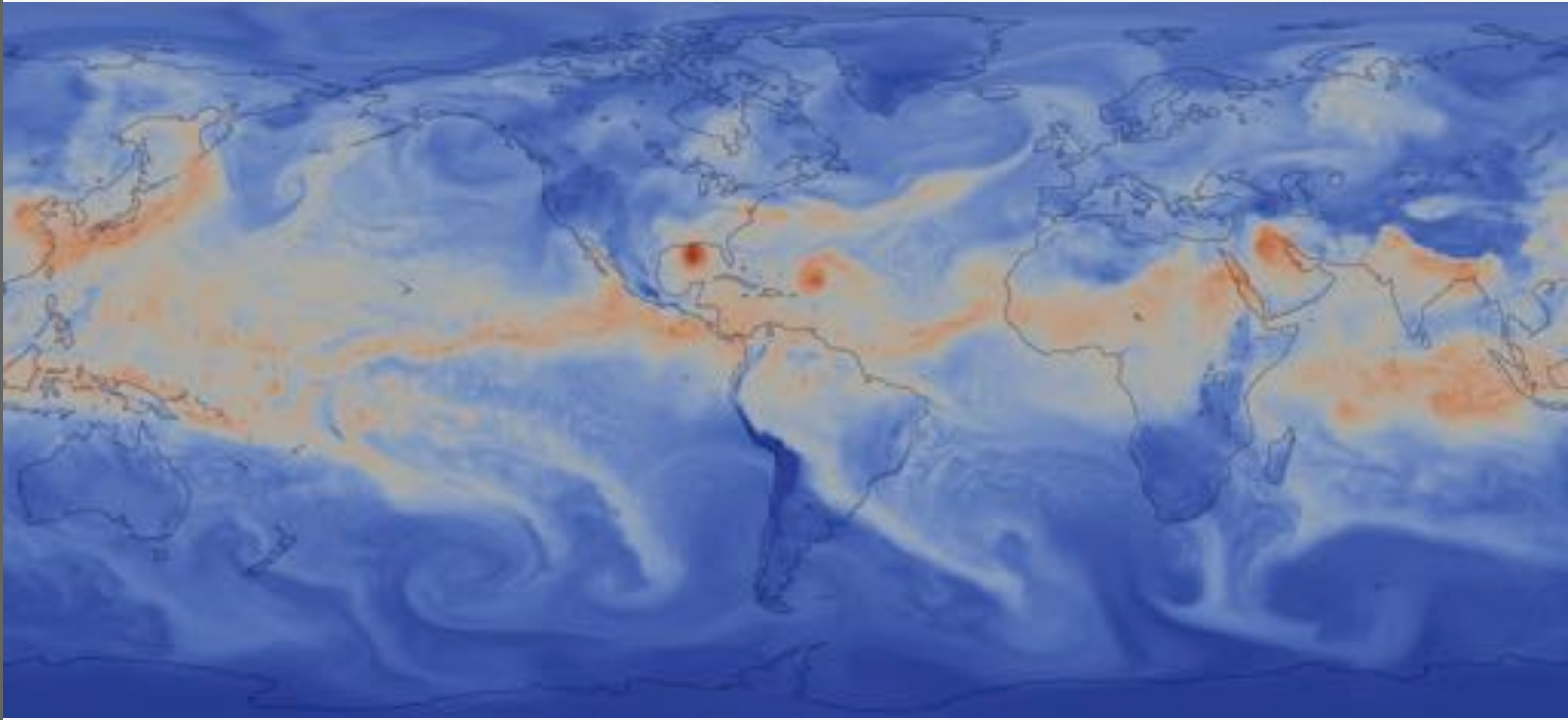
- Examples of visualizations
- Visualization resources
- Visualization tools and formats
- Data representations
- Visualization for debugging
- In-Situ Visualization and Analysis

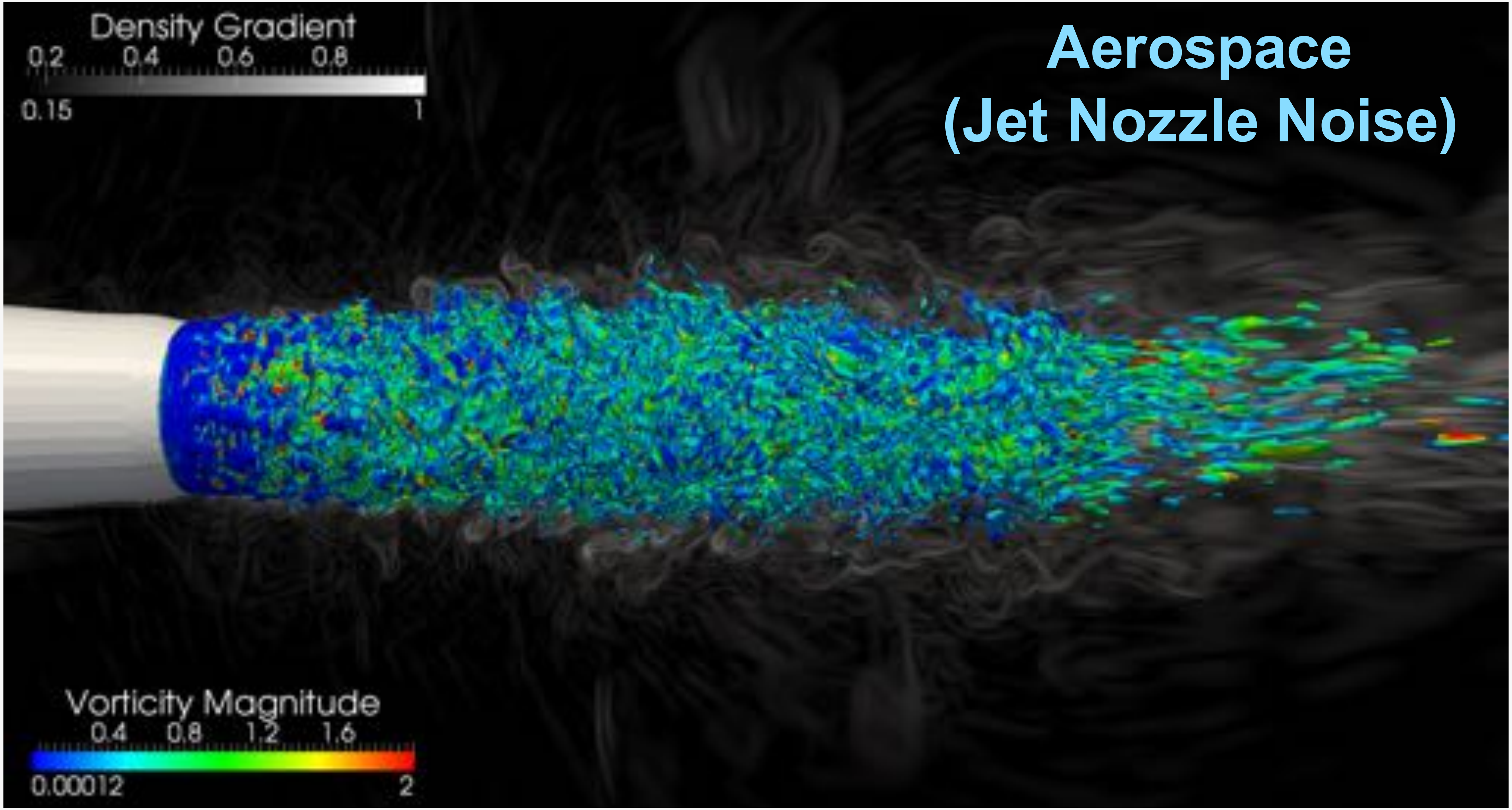
Multi-Scale Simulation / Visualization Arterial Blood Flow



Climate

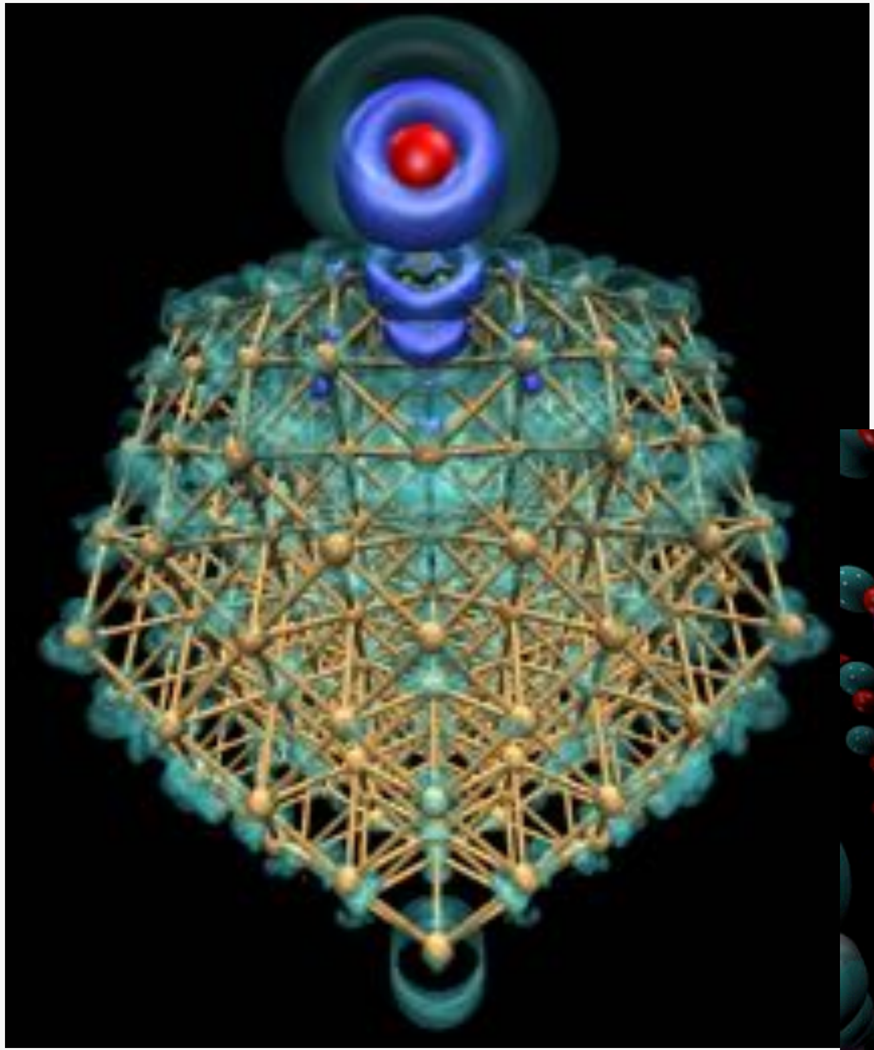
Data courtesy of: Mark Taylor, Sandia National Laboratory; Rob Jacob, Argonne National Laboratory; Warren Washington, National Center for Atmospheric Research





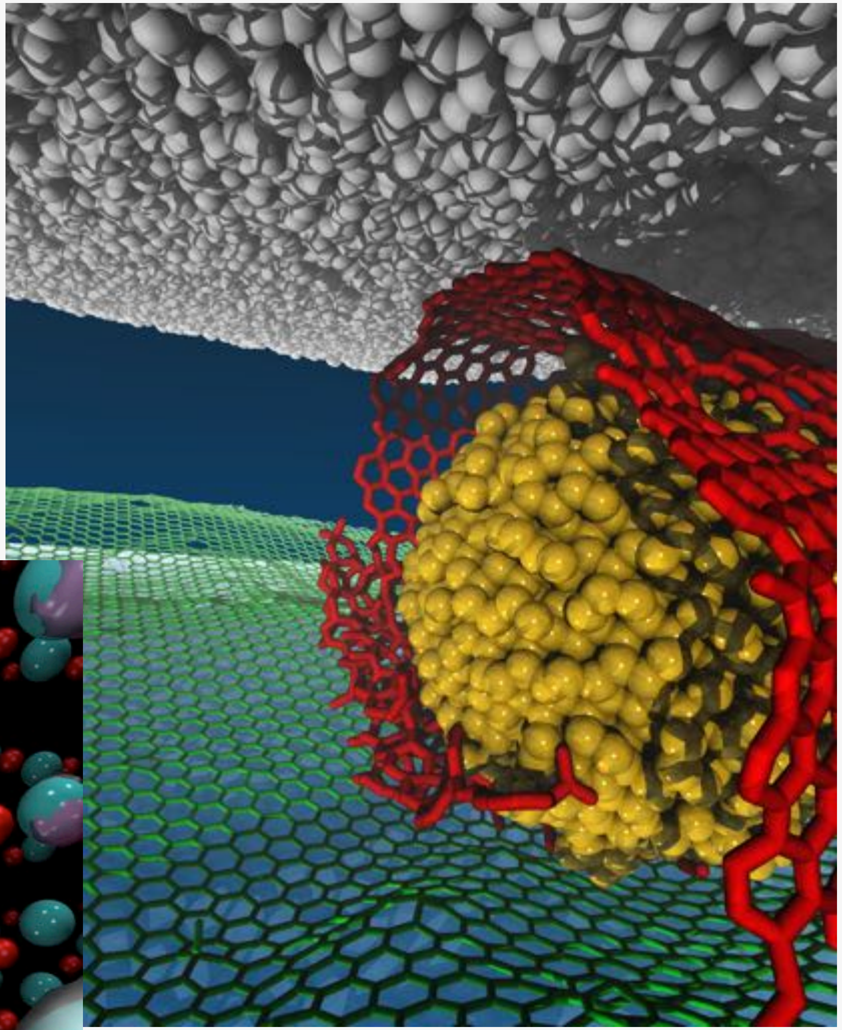
Data courtesy of: Anurag Gupta and Umesh Paliath, General Electric Global Research

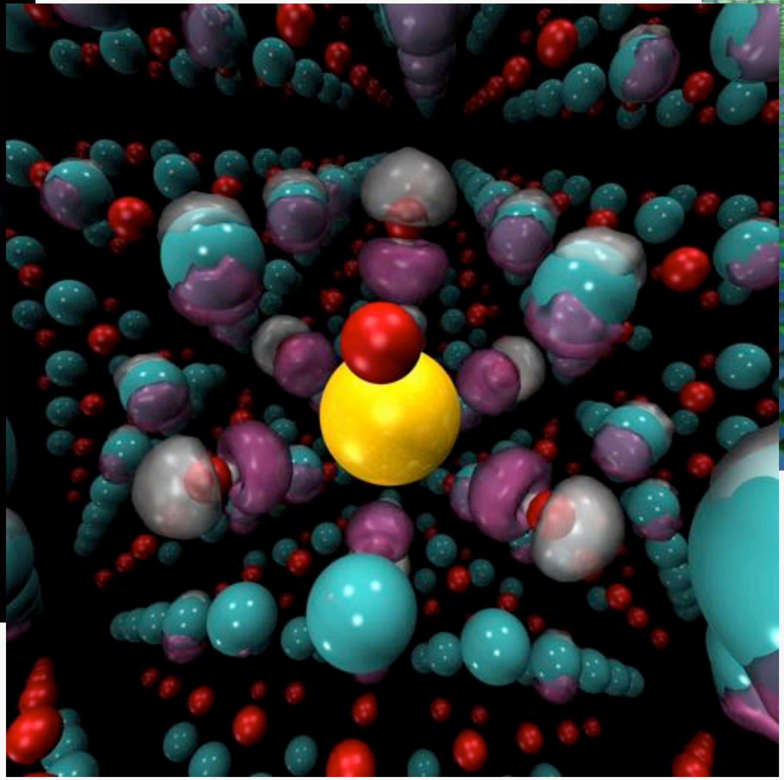
Materials Science / Molecular



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

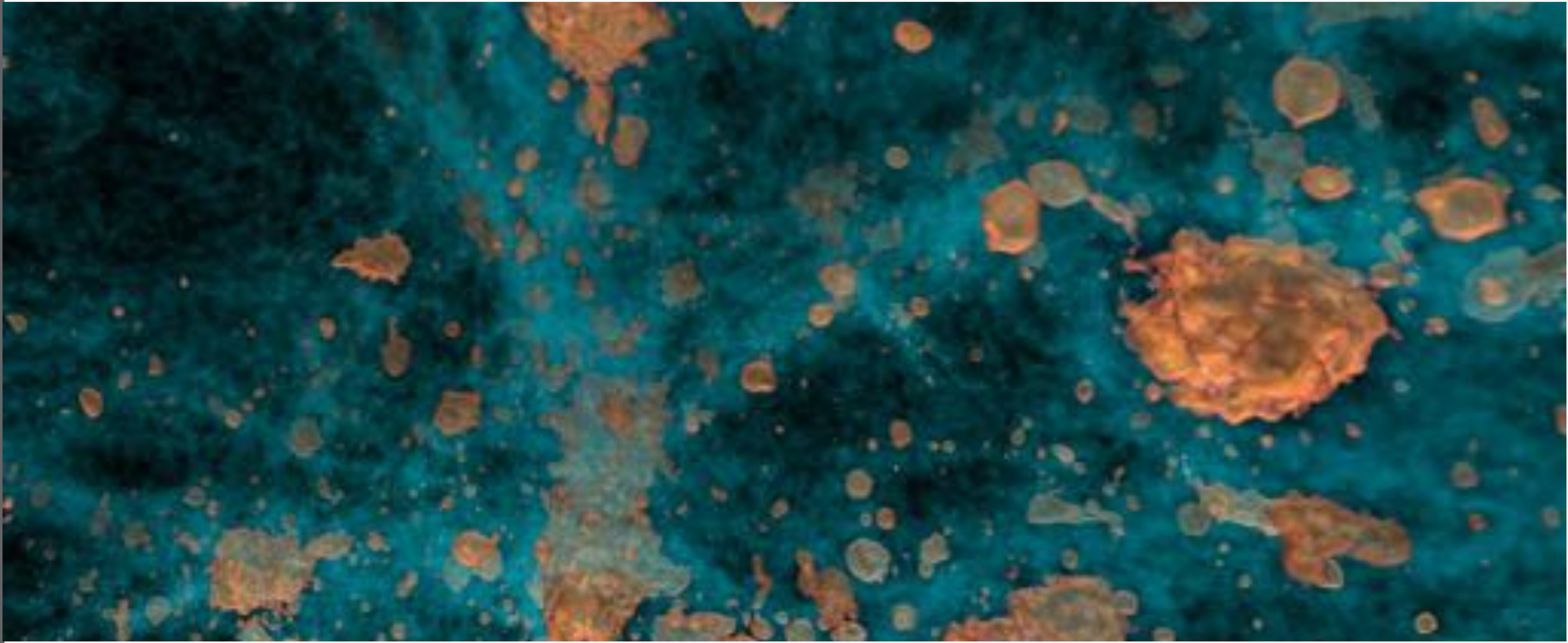
Data courtesy of: Subramanian Sankaranarayanan, Argonne National Laboratory





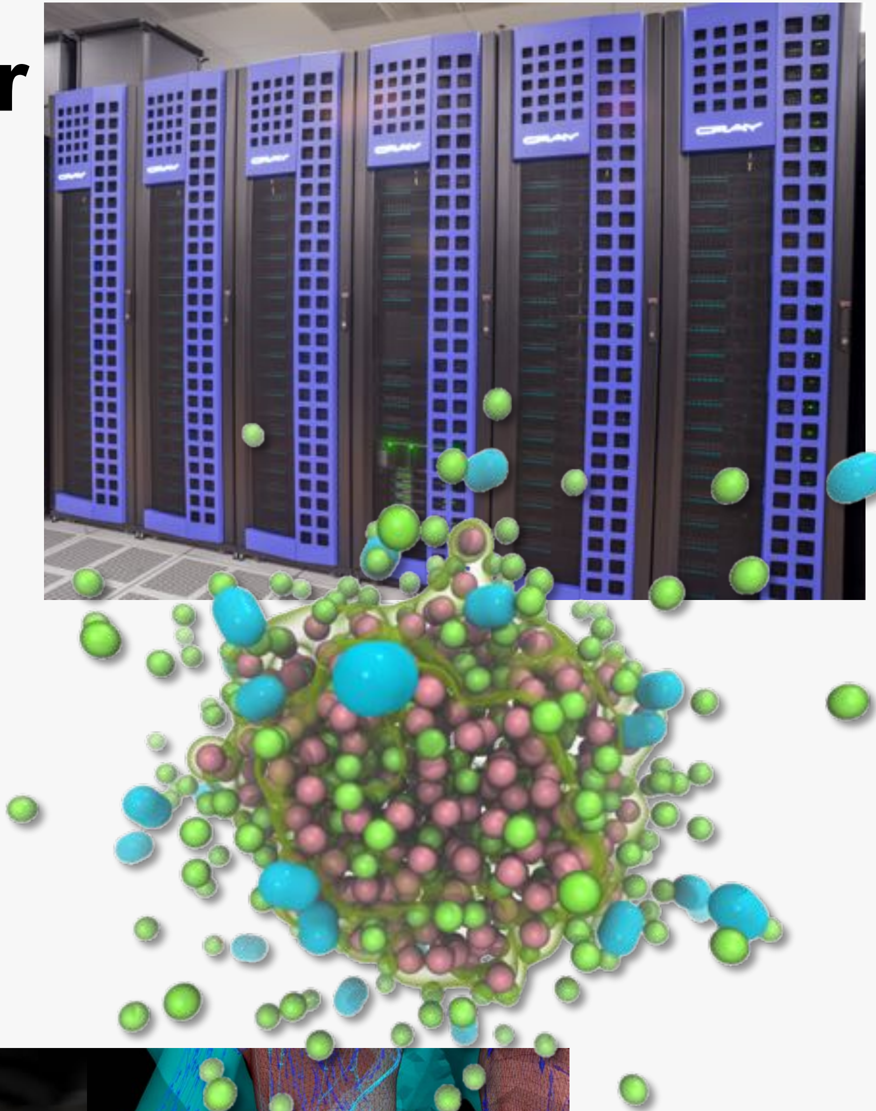
Data courtesy of: Paul Kent, Oak Ridge National Laboratory, Anouar Benali, Argonne National Laboratory

Cosmology



Data courtesy of: Salman Habib, Katrin Heitmann, and the HACC team, Argonne National Laboratory

Cooley: Analytics/Visualization cluster



Peak 223 TF

126 nodes; each node has

– Two Intel Xeon E5-2620 Haswell 2.4 GHz 6-core processors

– NVIDIA Telsa K80 graphics processing unit (24GB)

– 384 GB of RAM

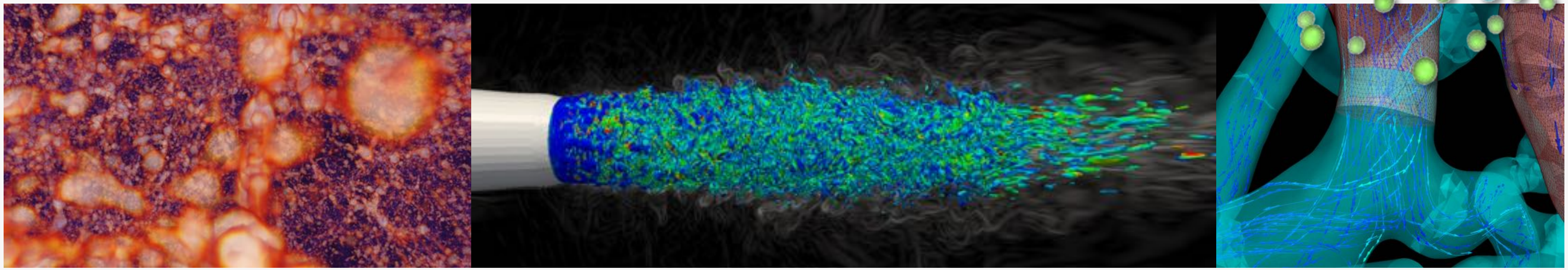
Aggregate RAM of 47 TB

Aggregate GPU memory of ~3TB

Cray CS System

216 port FDR IB switch with uplinks to our QDR infrastructure

Mounts the same GPFS file systems as Mira, Cetus



Visualization Tools and Data Formats

All Sorts of Tools

Visualization Applications
- VisIt
- ParaView
- EnSight

Domain Specific
- VMD, MegaMol, Ovito

APIs
- VTK: visualization
- ITK: segmentation & registration

GPU performance
- vl3: shader-based volume and particle rendering

Analysis Environments
- Matlab
- Parallel R

Utilities
- GnuPlot
- ImageMagick

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

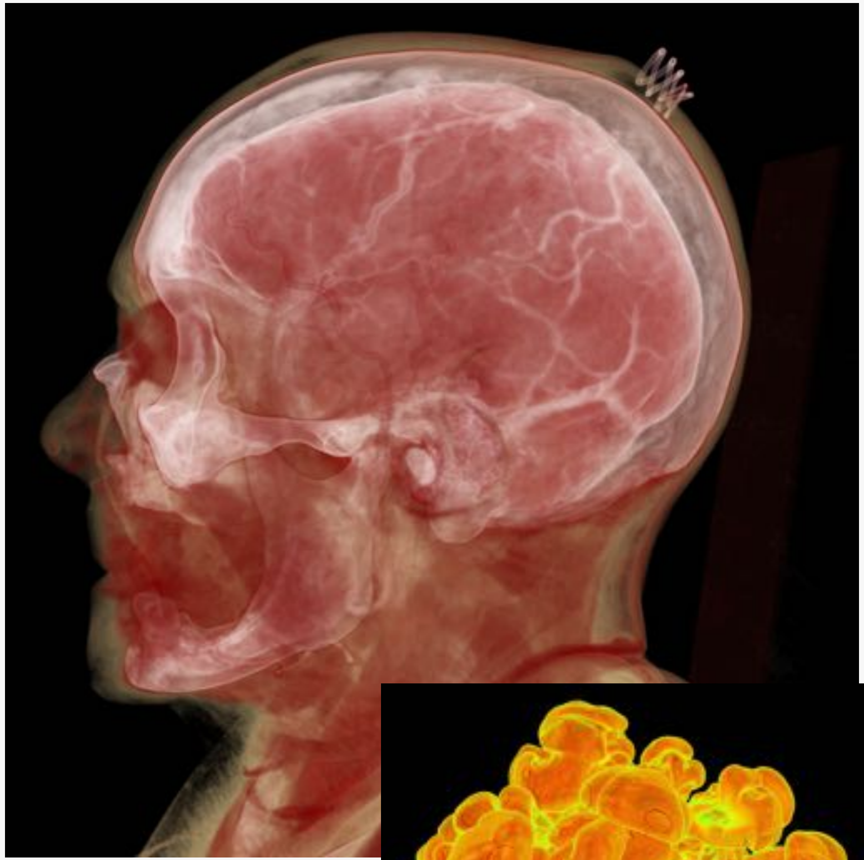
- Programming environment / API
- Additional capabilities, finer control
- Smaller memory footprint
- Requires more expertise (build custom applications)

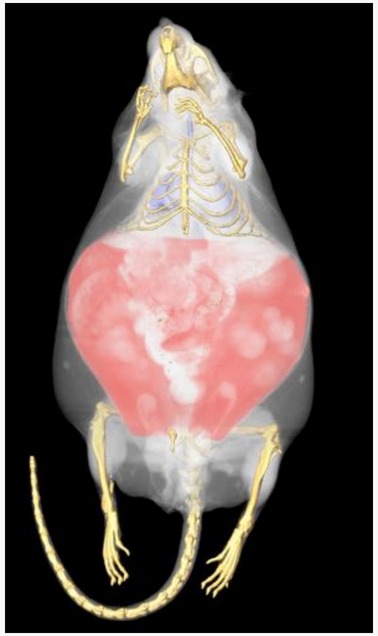
Data File Formats (ParaView & VisIt)

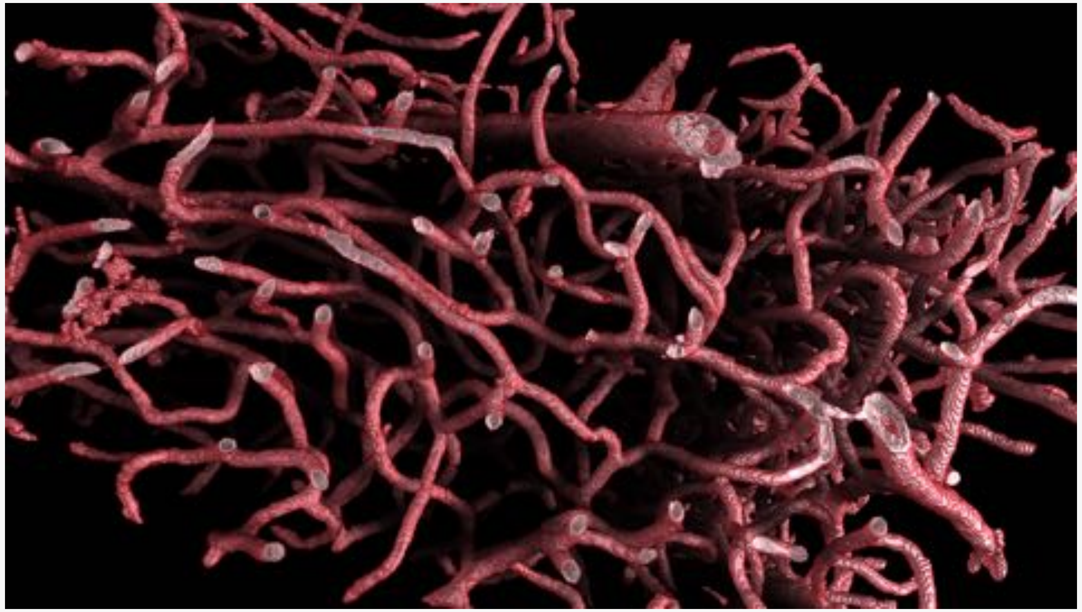
- VTK
- Parallel (partitioned) VTK
- VTK MultiBlock (MultiGroup, Hierarchical, Hierarchical Box)
- Legacy VTK
- Parallel (partitioned) legacy VTK
- EnSight files
- EnSight Master Server
- Exodus
- BYU
- XDMF
- PLOT2D
- PLOT3D
- SpyPlot CTH
- HDF5 raw image data
- DEM
- VRML
- PLY
- Polygonal Protein Data Bank
- XMol Molecule
- Stereo Lithography
- Gaussian Cube
- Raw (binary)
- AVS
- Meta Image
- Facet
- PNG
- SAF
- LS-Dyna
- Nek5000
- OVERFLOW
- paraDIS
- PATRAN
- PFLOTRAN
- Pixie
- PuReMD
- S3D
- SAS
- Tetrad
- UNIC
- VASP
- ZeusMP
- ANALYZE
- BOV
- GMV
- Tecplot
- Vis5D
- Xmdv
- XSF

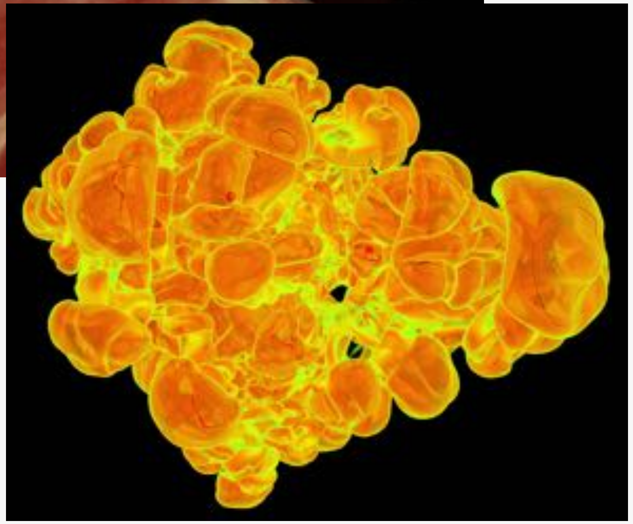
Data Representations

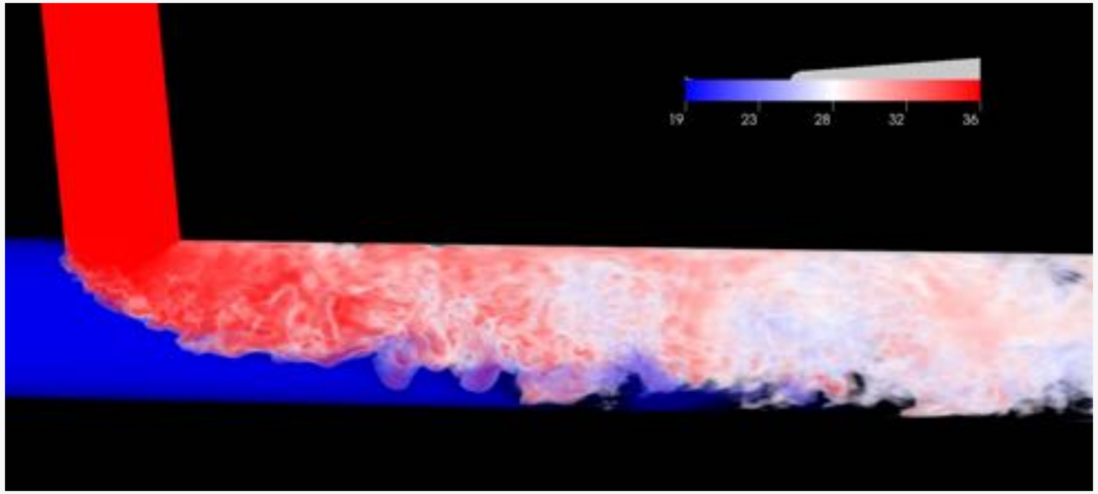
Data Representations: Volume Rendering





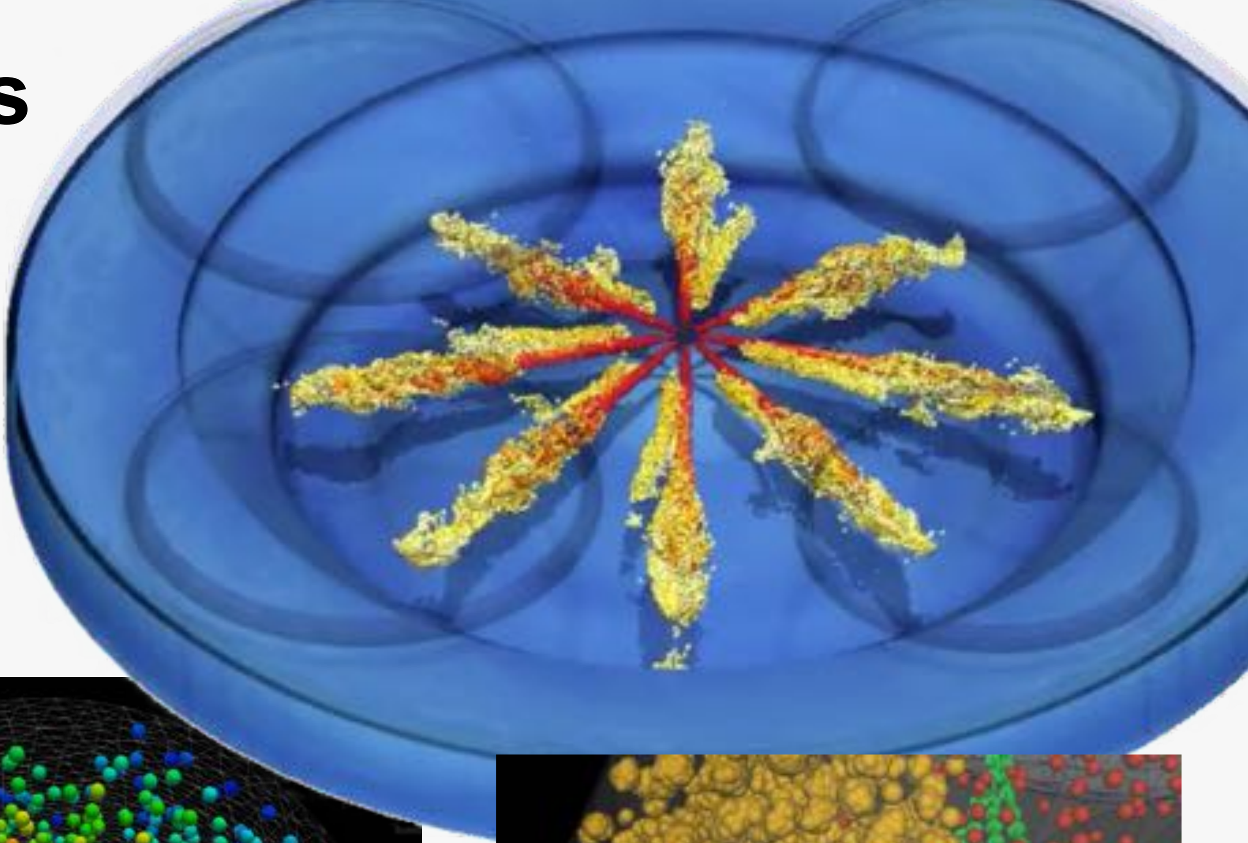


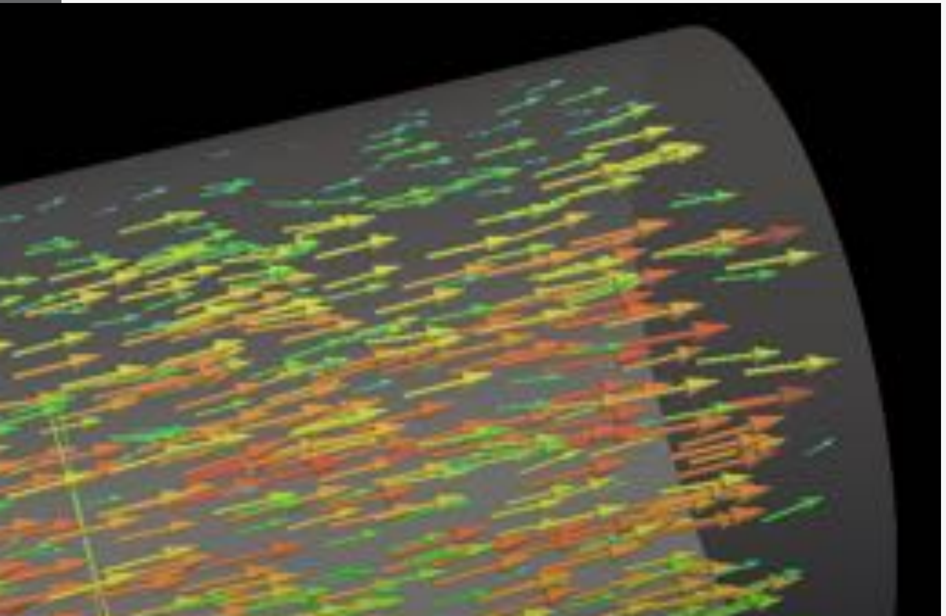


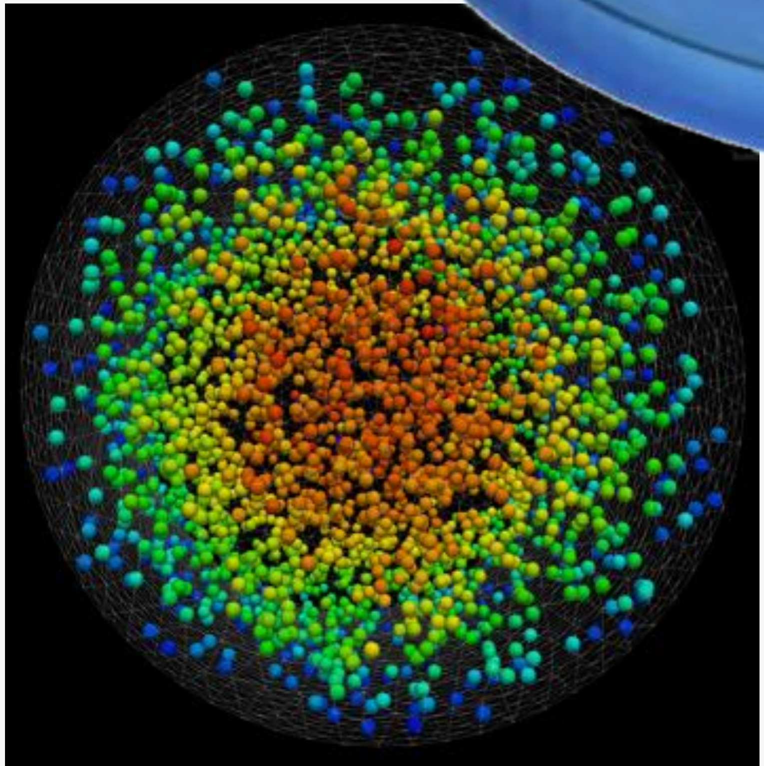


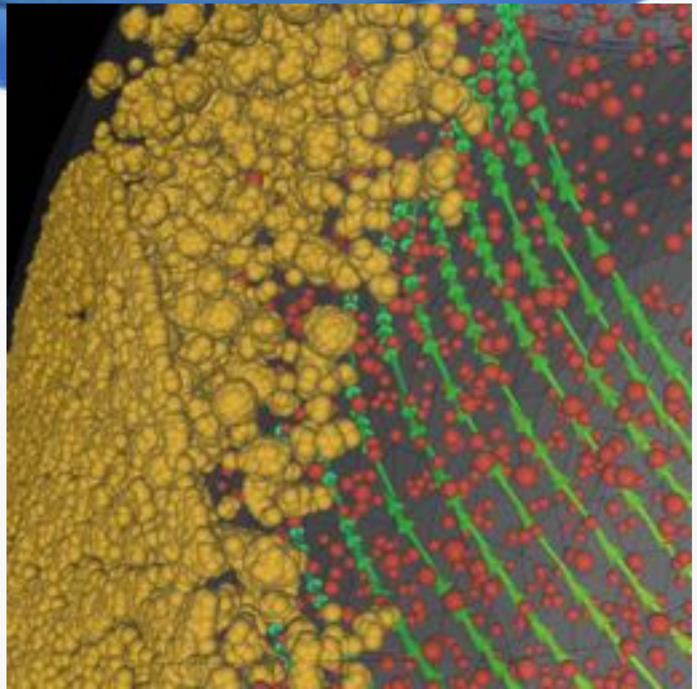
Data Representations: Glyphs

- 2D or 3D geometric object to represent point data
- Location dictated by coordinate
  - – 3D location on mesh
  - – 2D position in table/graph
- Attributes of graphical entity dictated by attributes of data
  - – color, size, orientation









Data Representations: Contours (Isosurfaces)

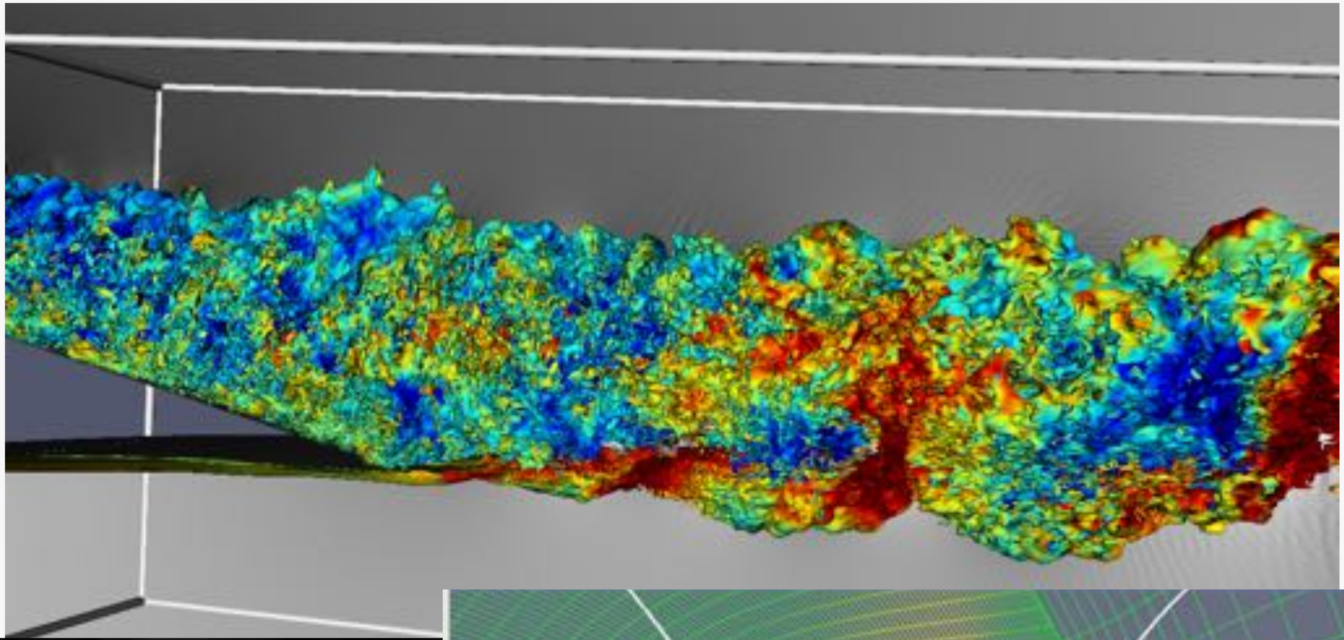
A Line (2D) or Surface (3D), representing a constant value

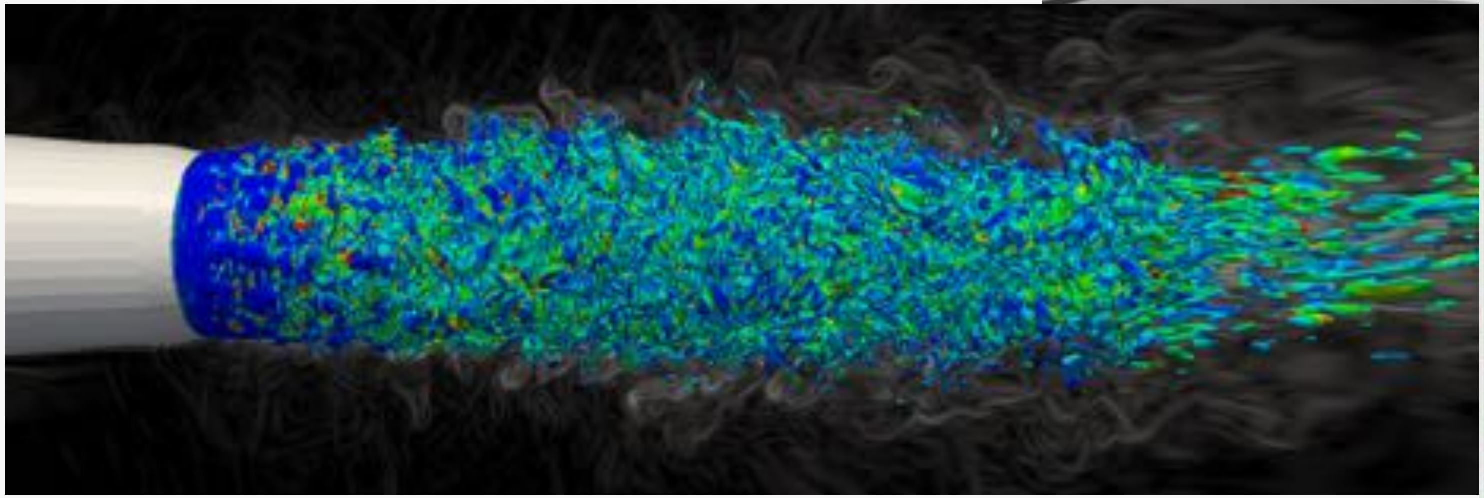
VisIt & ParaView:

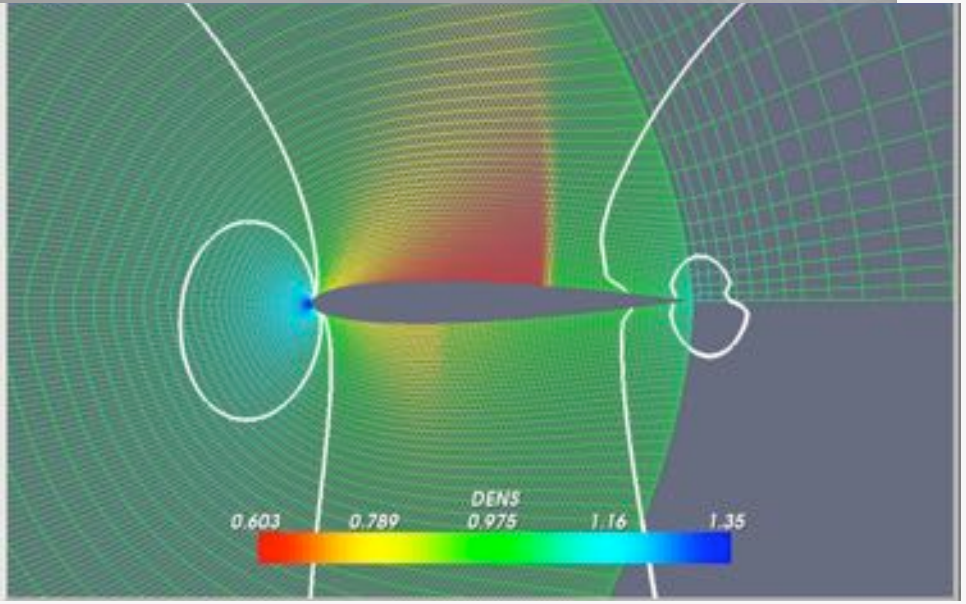
– good at this

vtk:

– same, but again requires more effort







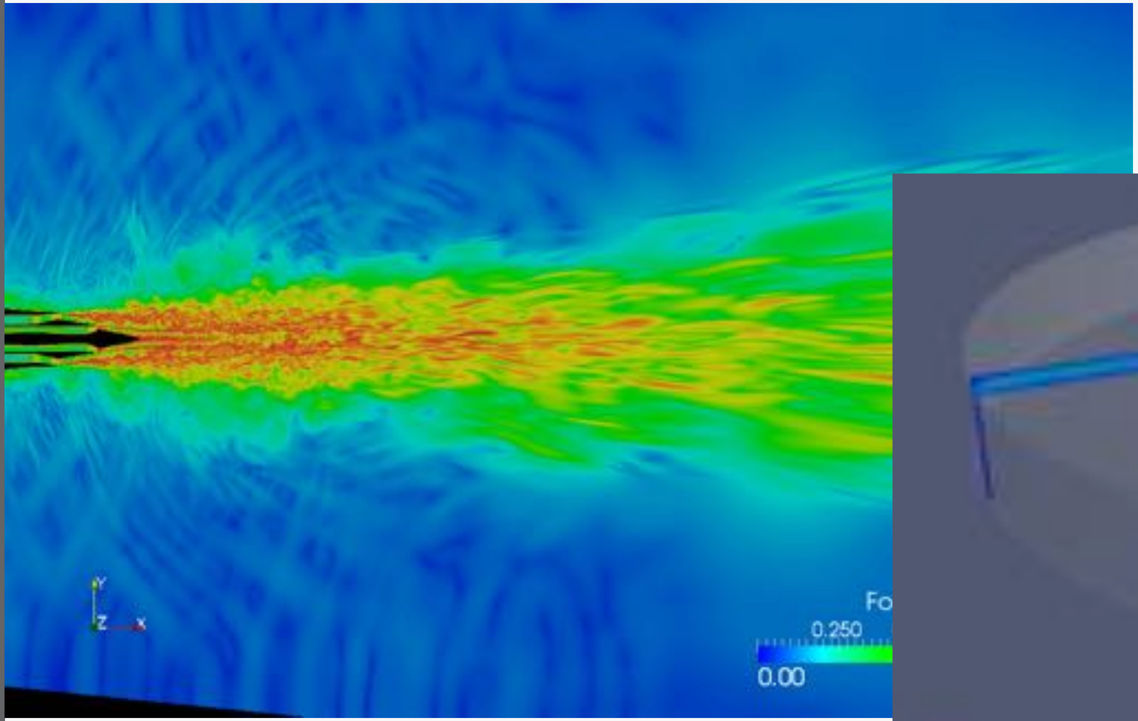
Data Representations: Cutting Planes

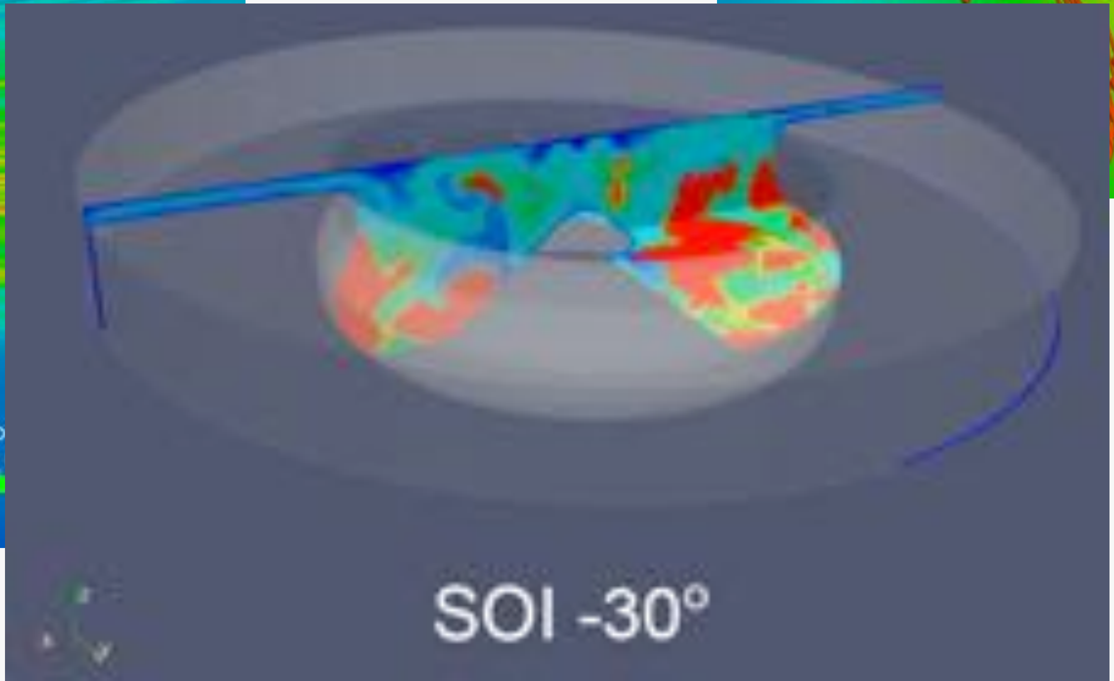
Slice a plane through the data

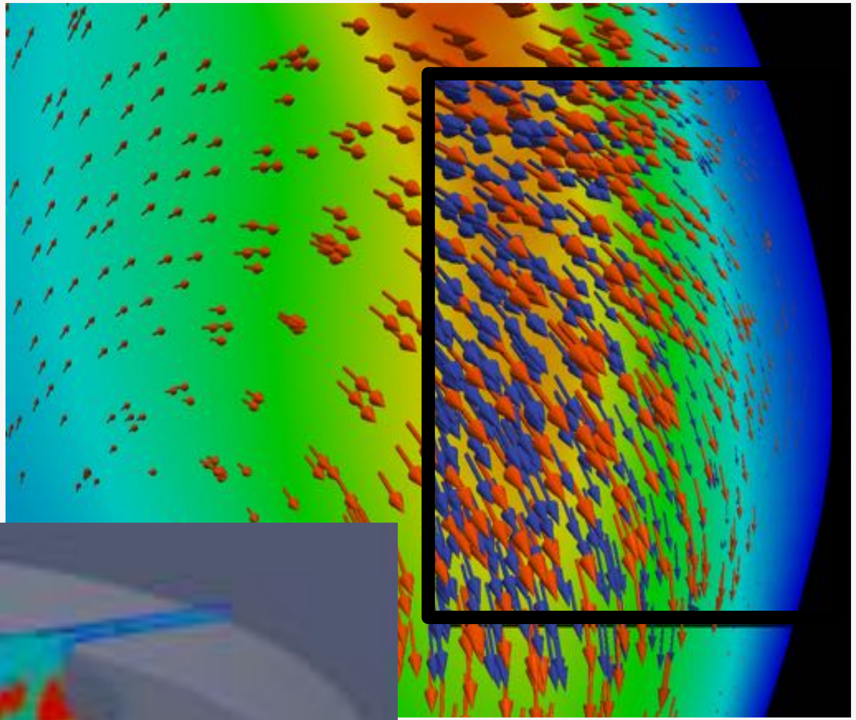
– Can apply additional visualization methods to resulting plane

VisIt & ParaView & vtk good at this

VMD has similar capabilities for some data formats







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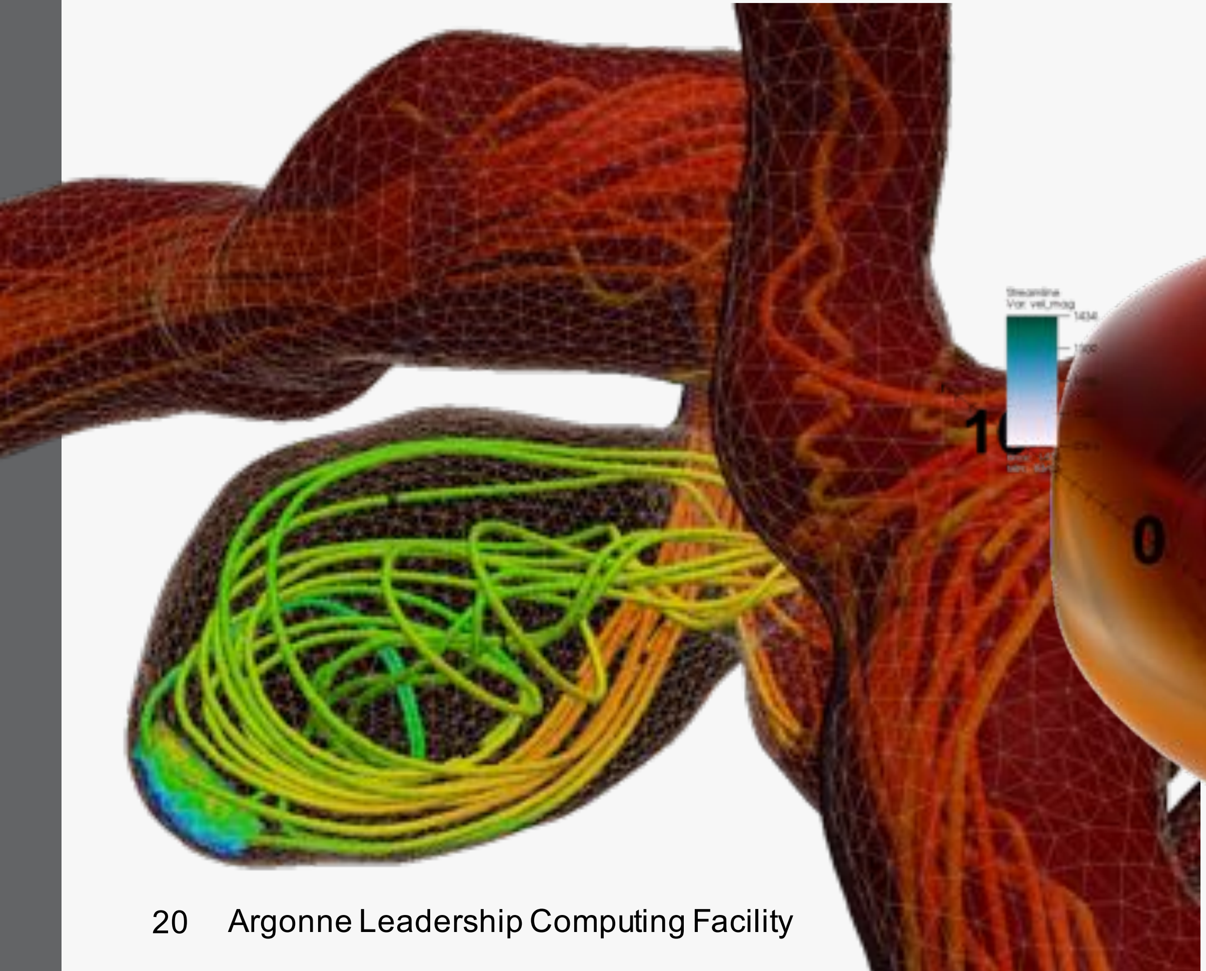
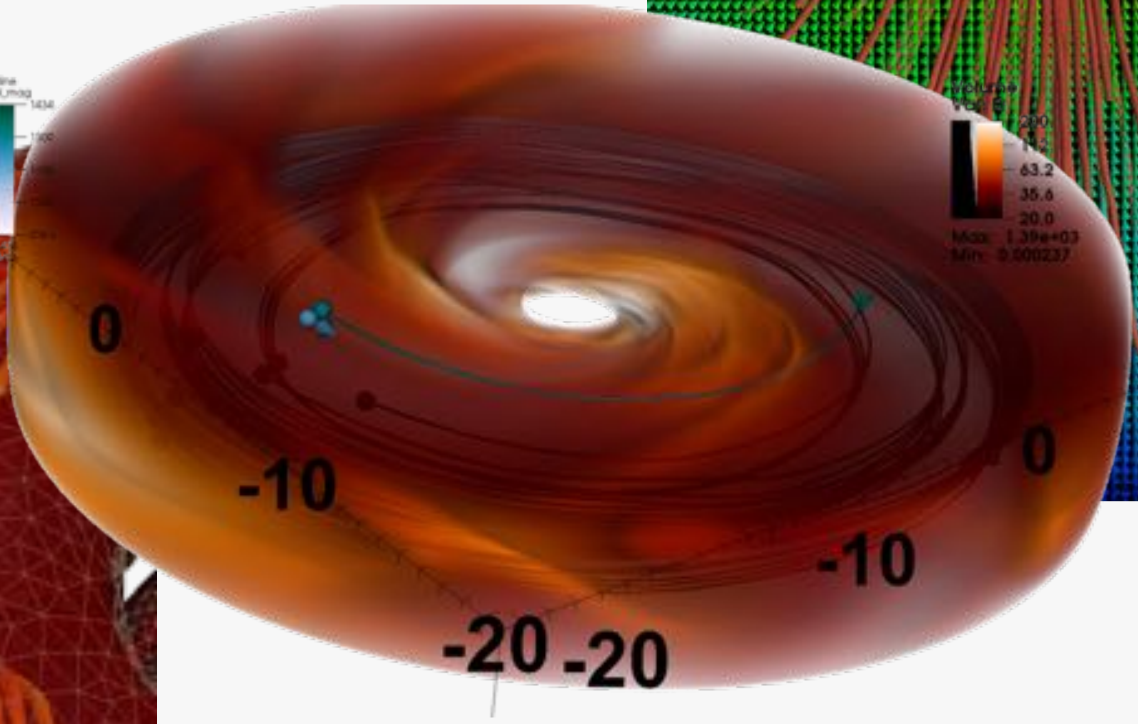
Data Representations: Streamlines

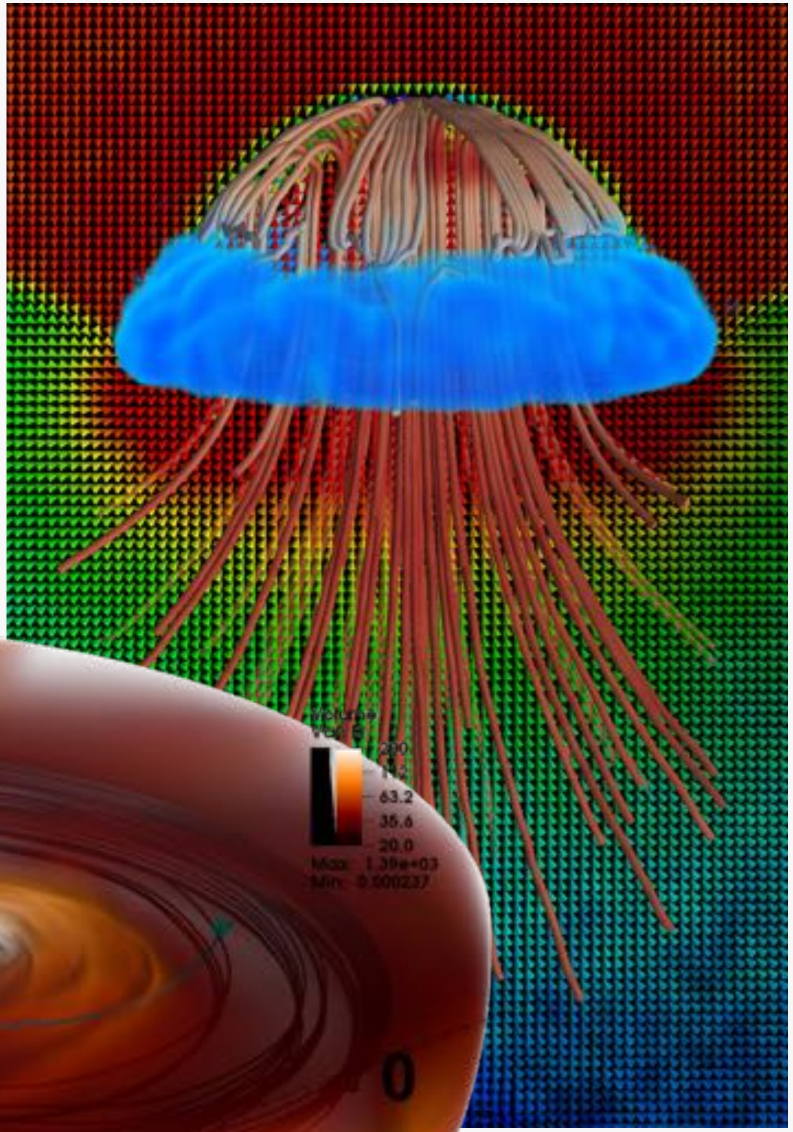
From vector field on a mesh (needs connectivity)

– Show the direction an element will travel in at any point in time.

VisIt & ParaView & vtk good at this





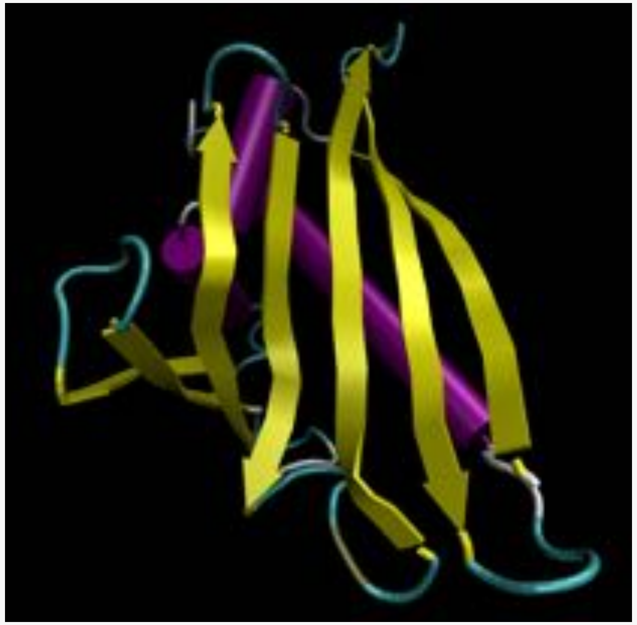


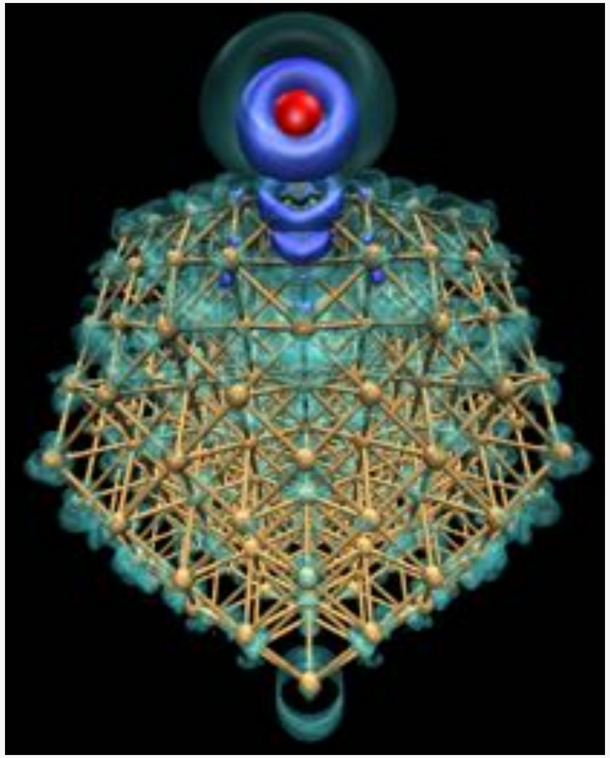
Molecular Dynamics Visualization

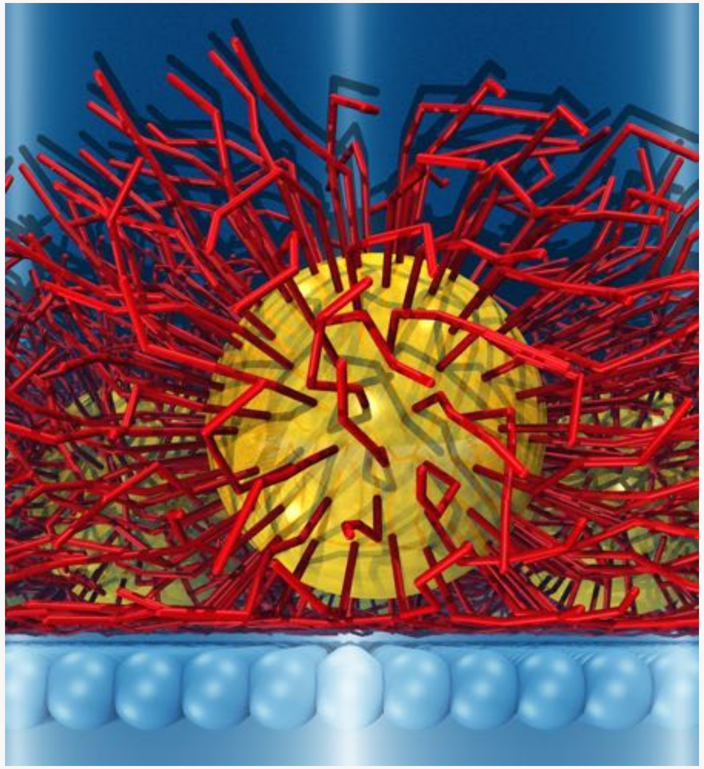
VMD:
- Lots of domain-specific representations
- Many different file formats
- Animation
- Scriptable

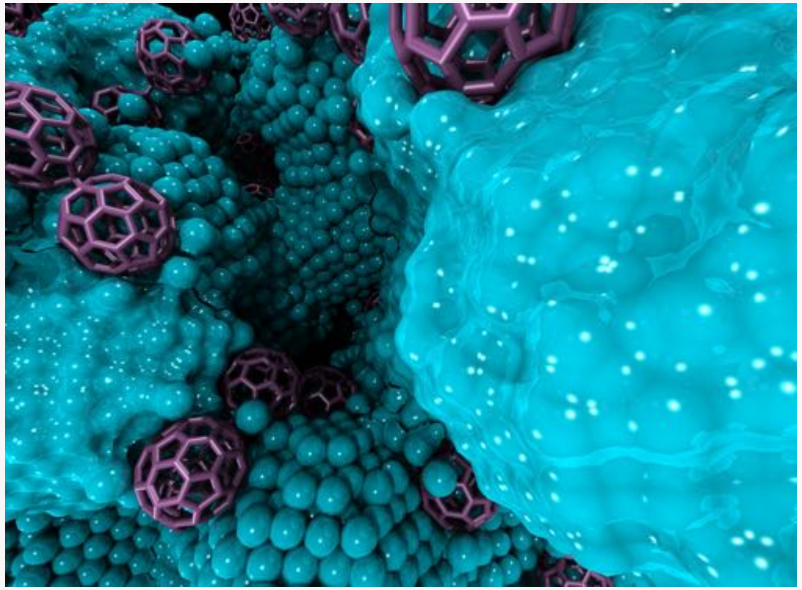
VisIt & ParaView:
- Limited support for these types of representations, but improving

VTK:
- Anything's possible if you try hard enough





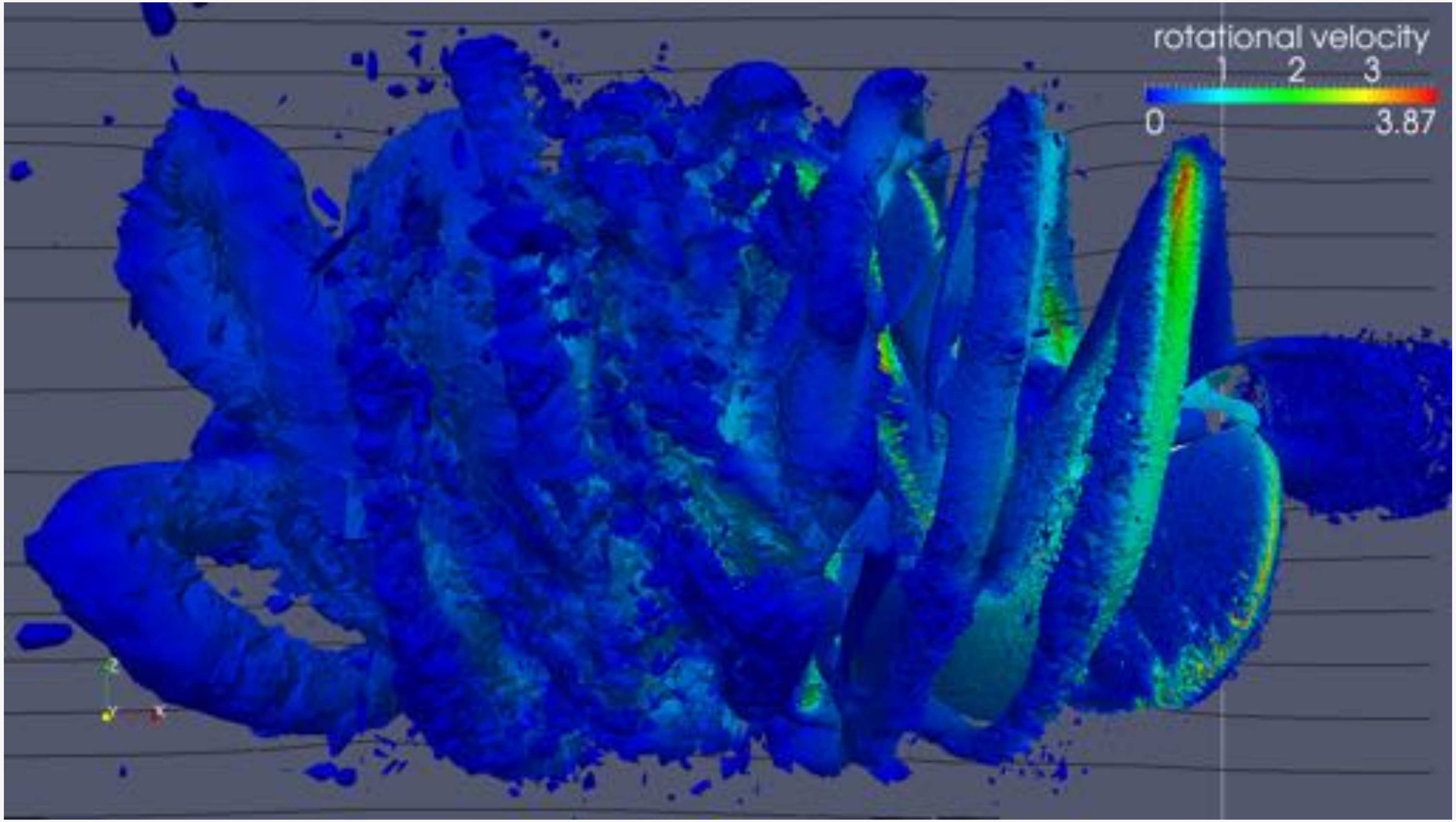




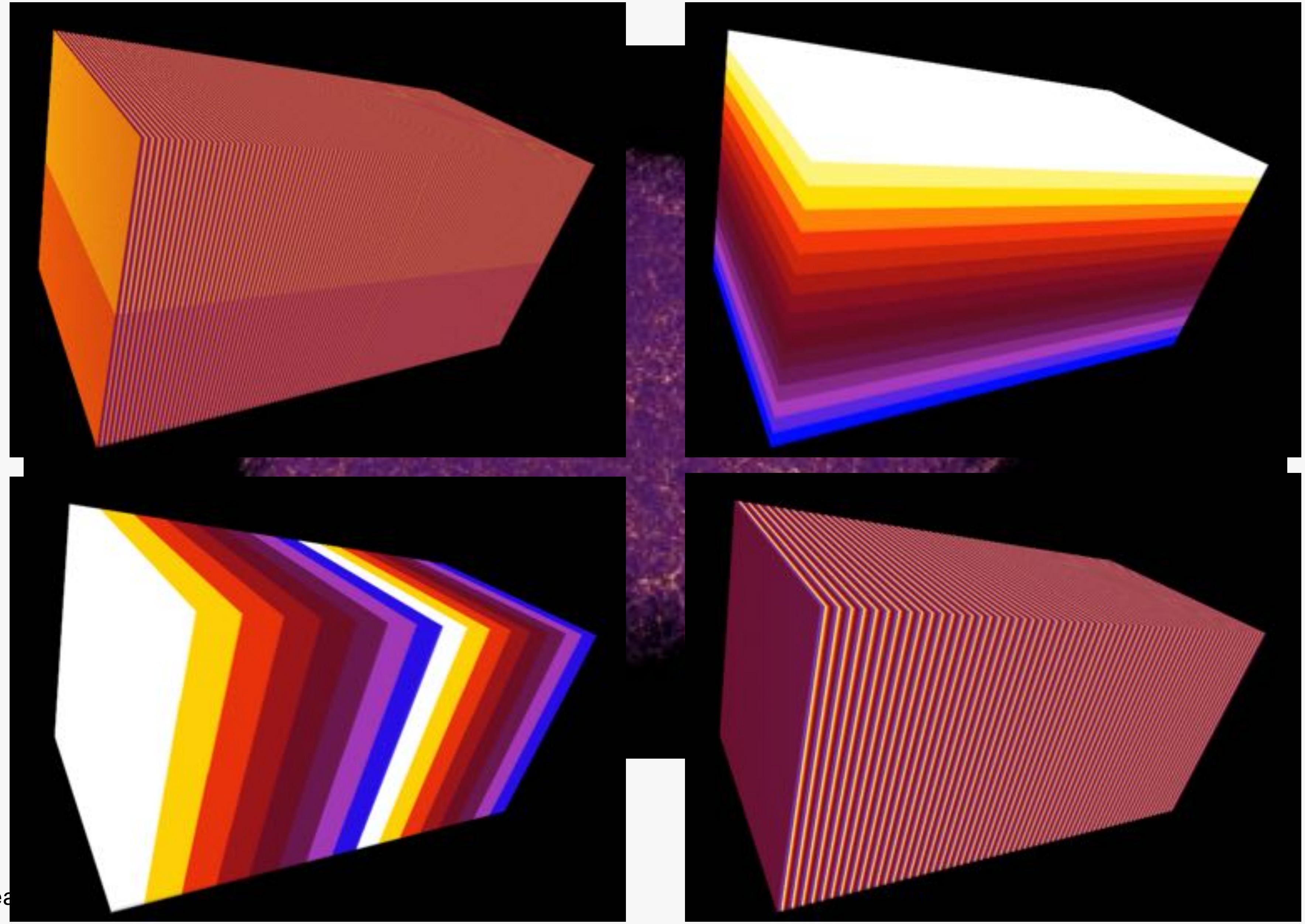
Visualization for Debugging

Visualization for Debugging

Visualization for Debugging



Visualization as Diagnostics: Color by Thread ID



In Situ Visualization and Analysis

The Need of *In Situ* Analysis and Visualization

Research challenges for enabling scientific knowledge discovery at extreme-scale concurrency

Widening gap between FLOPs and I/O capacity

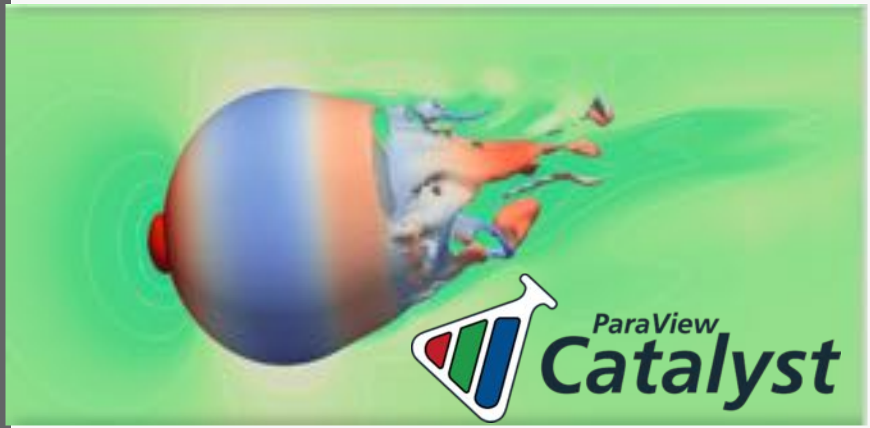
– will make full-resolution, I/O-intensive post hoc analysis prohibitively expensive, if not impossible.

Slides courtesy SENSEI in situ project:

www.sensei-insitu.org

SENSEI
in situ

Multiple in-situ infrastructures



ADIOS

LibSim

Can We….

Enable use of any in situ framework?

Develop analysis routines that are portable between codes?

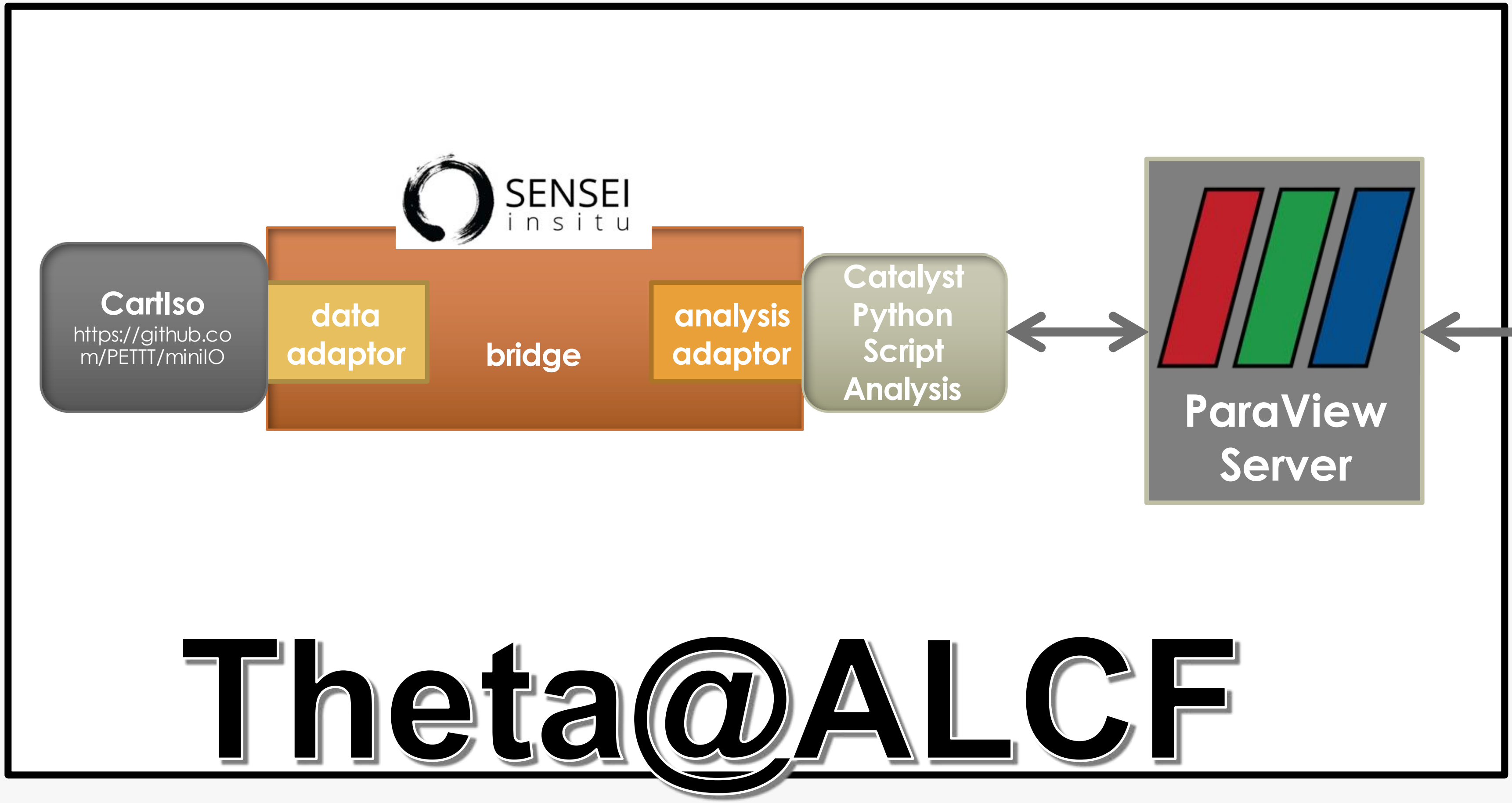
Make it easy to use?

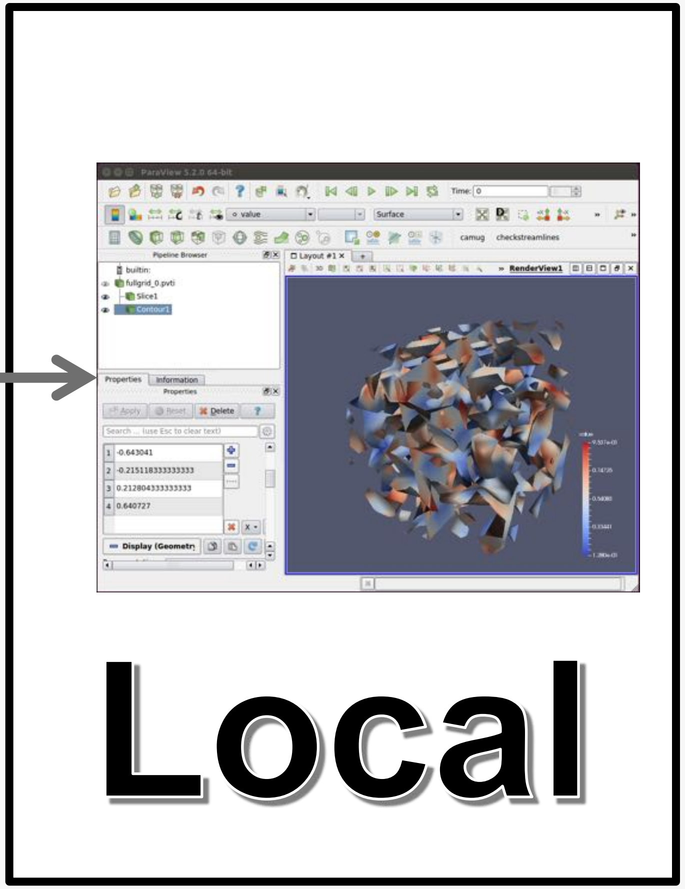
OUR APPROACH

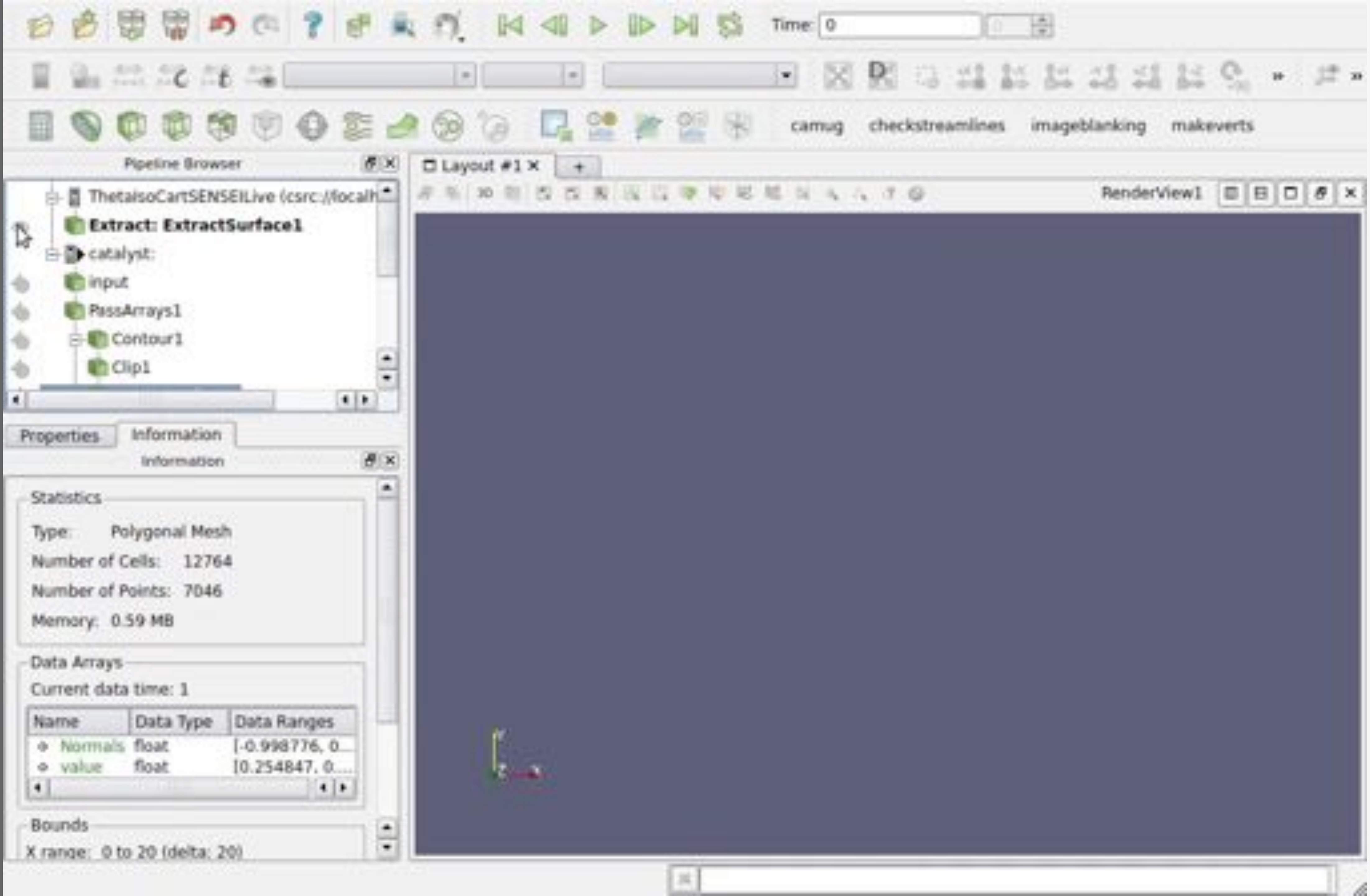
Data model – to pass data between Simulation & Analysis

API – for instrumenting simulation and analysis codes

Miniapp instrumentation with SENSEI



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Extract: ExtractSurface1
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input
PassArrays1
Contour1
Clip1
Layout #1
RenderView1
Properties
Information
Information
Statistics
Type: Polygonal Mesh
Number of Cells: 12764
Number of Points: 7046
Memory: 0.59 MB
Data Arrays
Current data time: 1
Name
Data Type
Data Ranges
Normals
float
[-0.998776, 0...
value
float
[0.254847, 0...
Bounds
X range: 0 to 20 (delta: 20)

Ospray for Interactive *In Situ* Visualization

OSPRay

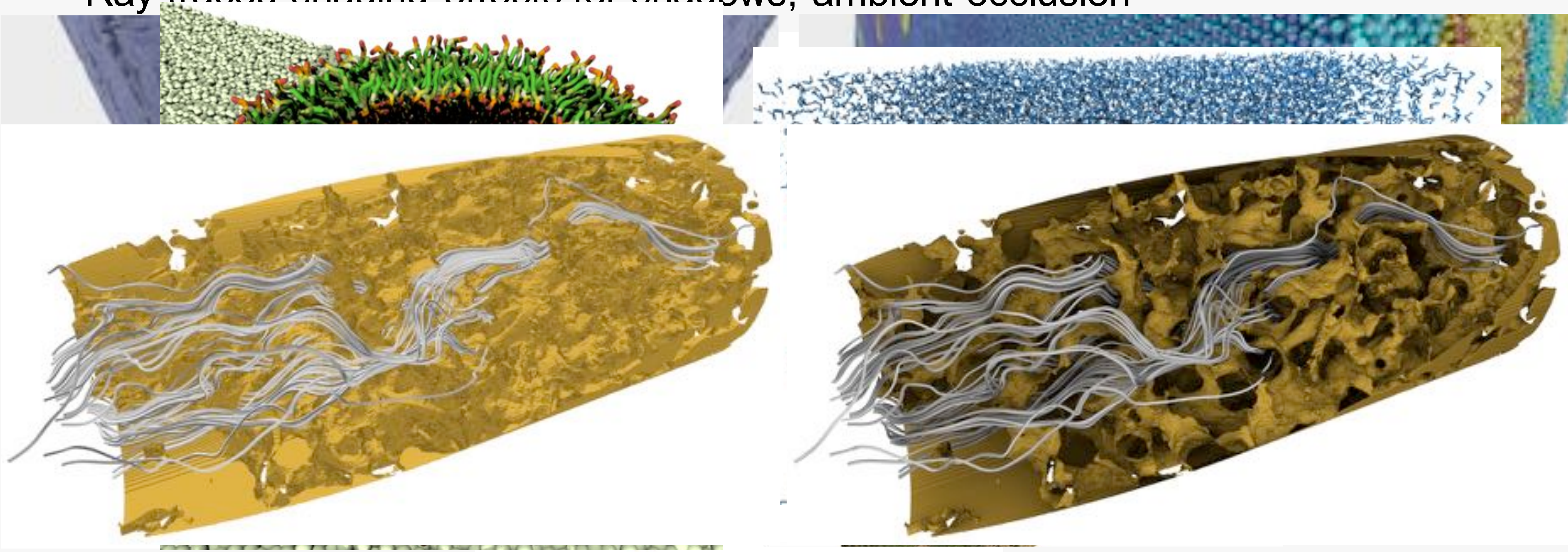
Slide courtesy OSPRay team @ Intel

Wald, Ingo, Gregory P. Johnson, J. Amstutz, Carson Brownlee, Aaron Knoll, J. Jeffers, J. Günther, and P. Navratil. "OSPRay-A CPU Ray Tracing Framework for Scientific Visualization." IEEE transactions on visualization and computer graphics 23, no. 1 (2017): 931-940.

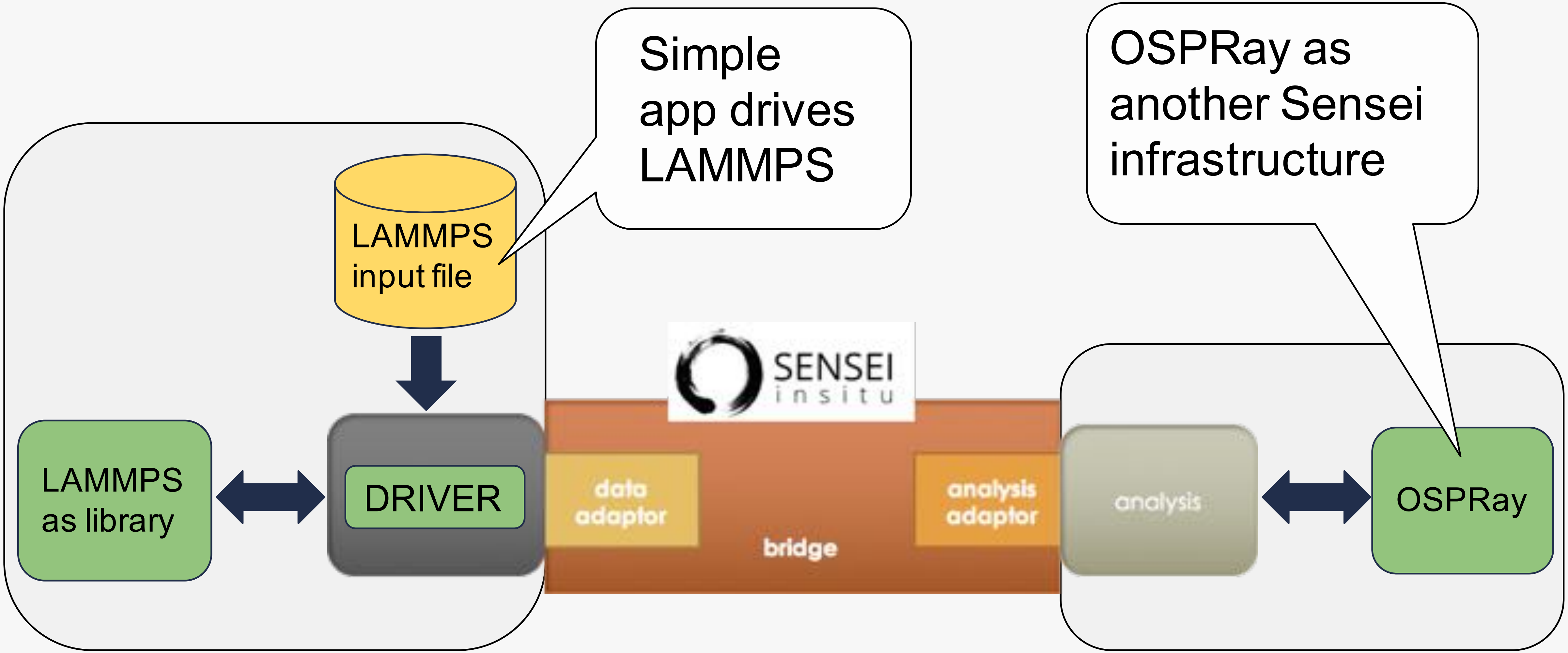
Ray tracer for interactive scientific visualization-style rendering

– Volumes, triangle meshes, non-polygonal geometry (spheres, cylinders,…)

– Ray traced shading effects for shadows, ambient occlusion



LAMMPS instrumentation with SENSEI and ospray



In Situ Visualization of LAMMPS with SENSEI and OSPRay

Will Usher, Silvio Rizzi, Jefferson Amstutz, Joe Insley,
Venkatram Vishwanath, Nicola Ferrier, Ingo Wald,
Michael E. Papka and Valerio Pascucci

QUESTIONS?

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