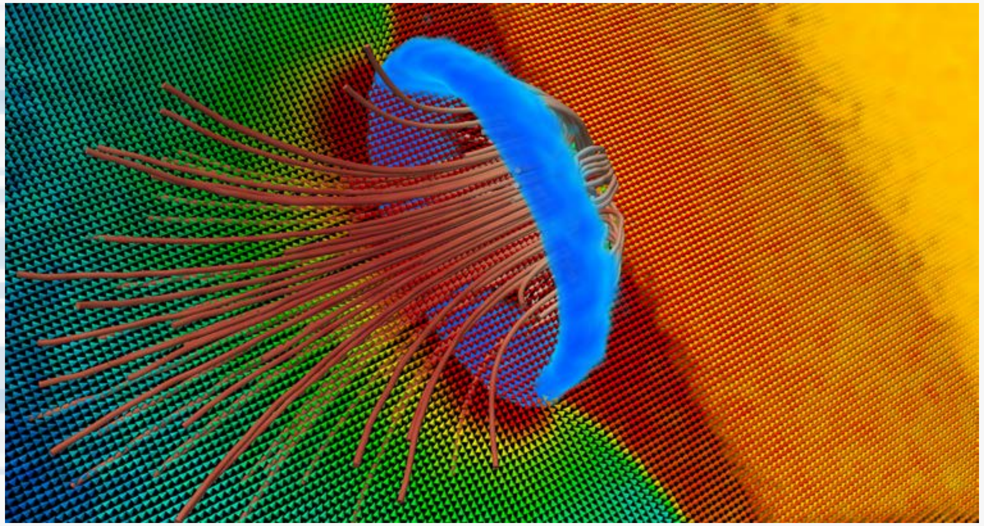
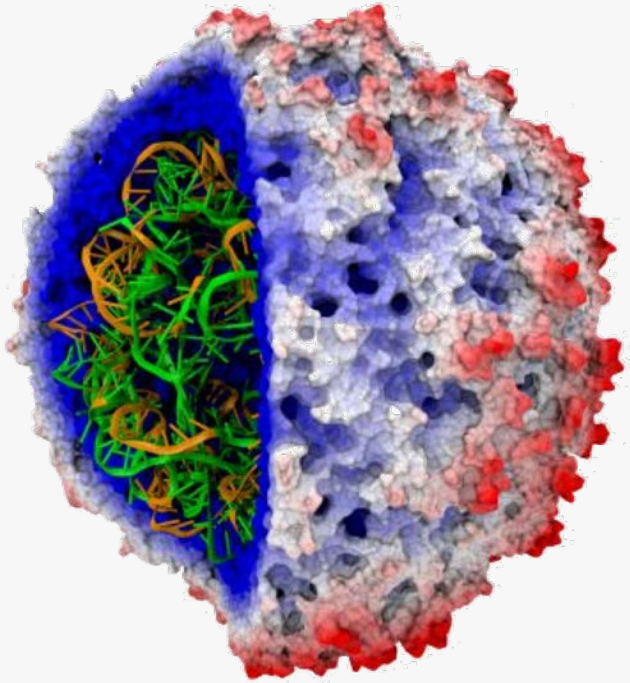
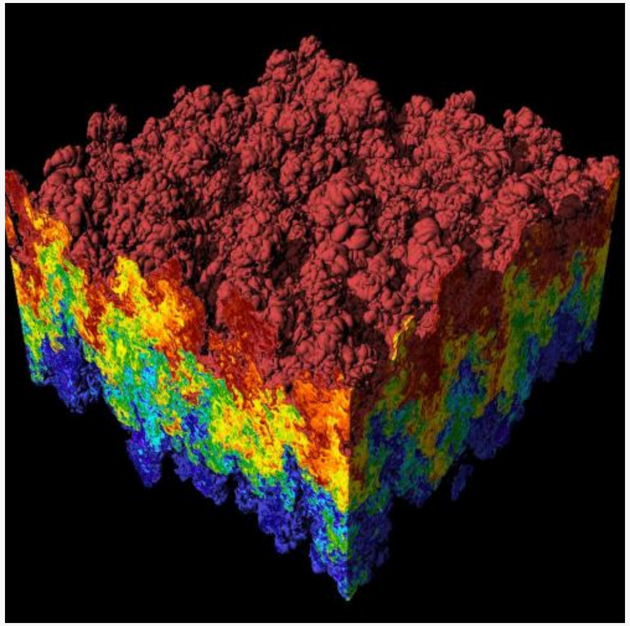
Argonne Training Program on Extreme-Scale Computing (ATPESC)

Data Analysis and Visualization







ECP
EXASCALE COMPUTING PROJECT

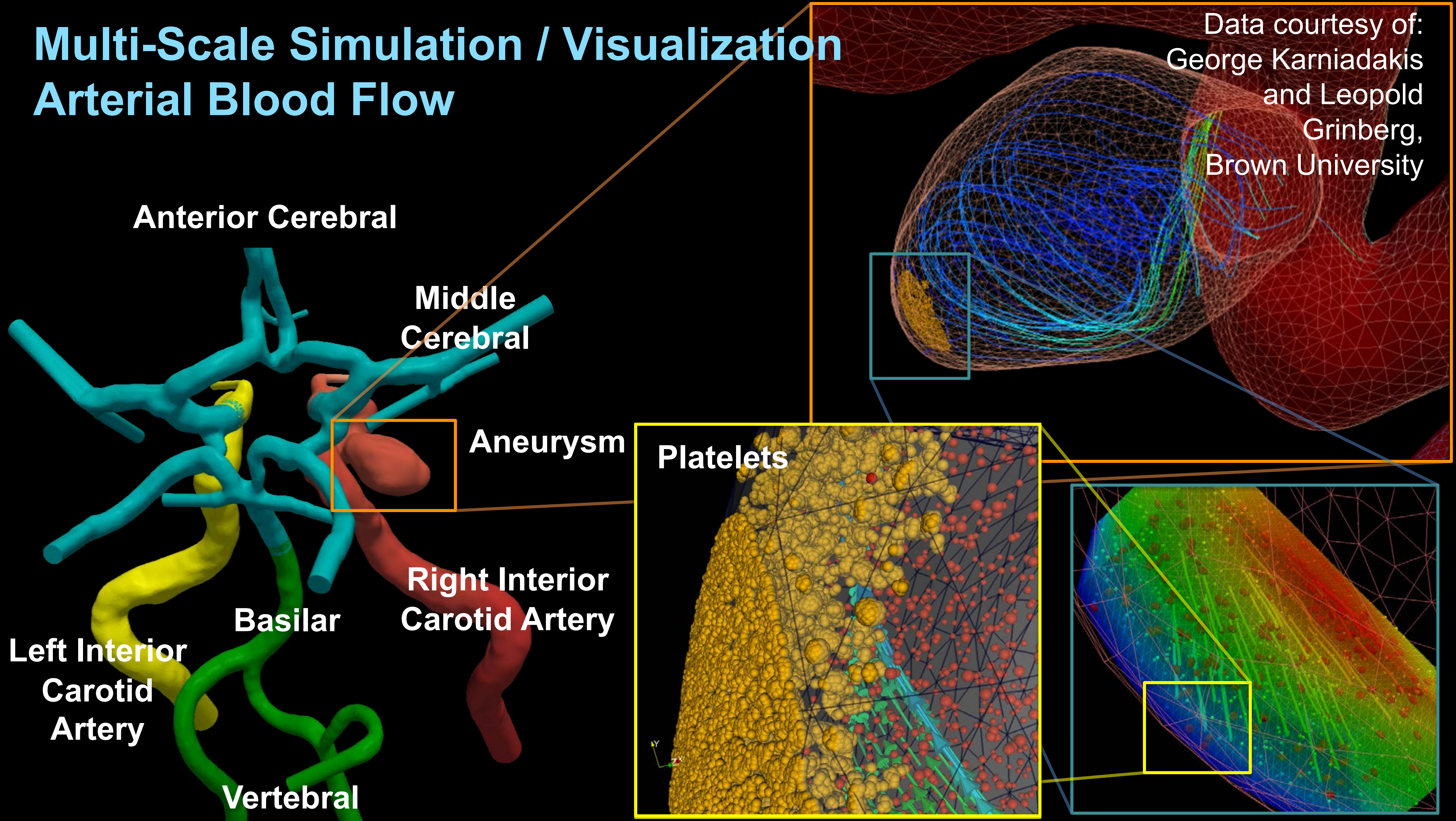
Visualization & Data Analysis

Time	Title of presentation	Lecturer
9:30 am	**Visualization Introduction**	Mike Papka, Joe Insley, Silvio Rizzi, ANL
10:15 am	*Break*	
10:45 am	**Large Scale Visualization with ParaView**	Dave DeMarle, Kitware
12:30 pm	*Lunch and Hands-on Exercises*	
1:30 pm	**Visualization and Analysis of Massive Data with VisIt**	Cyrus Harrison, LLNL
3:15 pm	*Break*	
3:45 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: DreamWorks Animation***	Mark Jackels
6:30 pm	*Hands-on Exercises*	

Here's the plan…

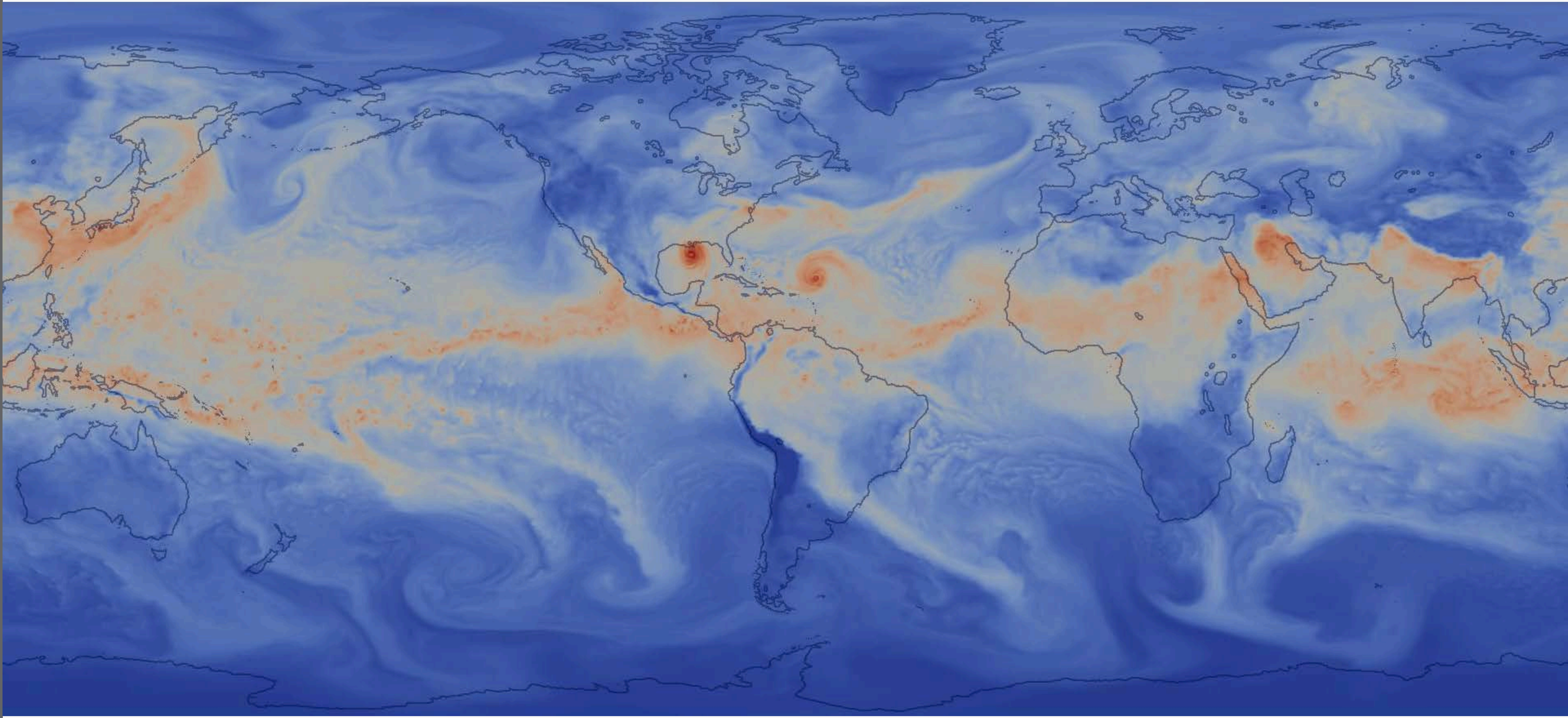
- Examples of visualizations
- Visualization resources
- Visualization tools and formats
- Data representations
- Visualization for debugging
- In Situ Visualization and Analysis

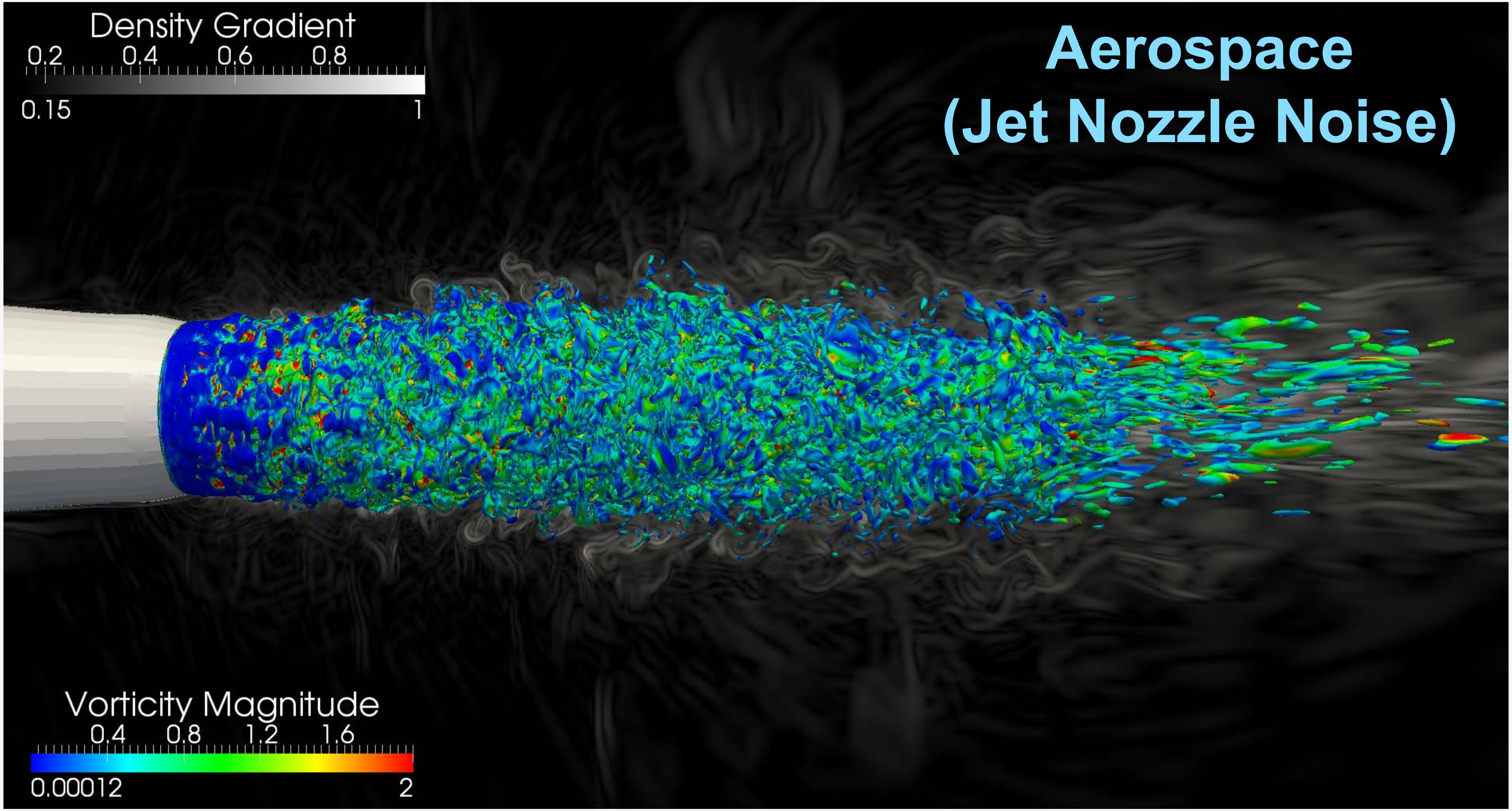
Multi-Scale Simulation / Visualization Arterial Blood Flow



Climate

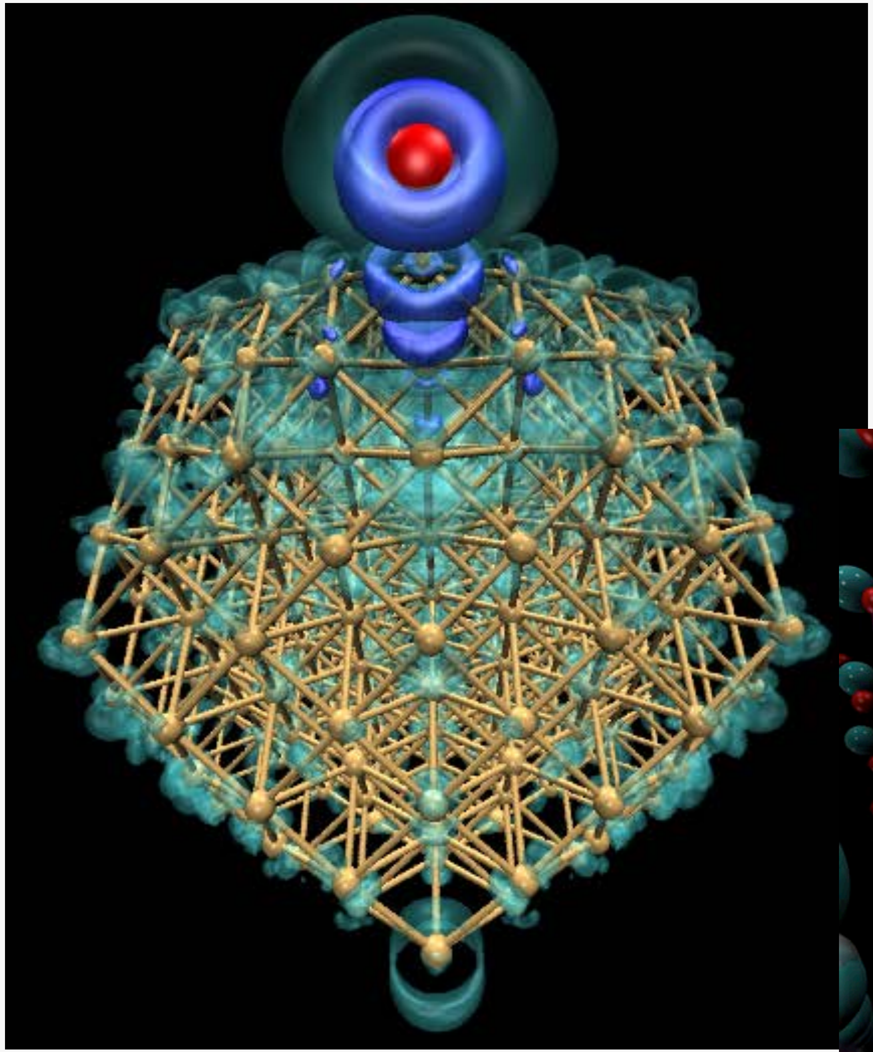
Data courtesy of: Mark Taylor, Sandia National Laboratory; Rob Jacob, Argonne National Laboratory; Warren Washington, National Center for Atmospheric Research





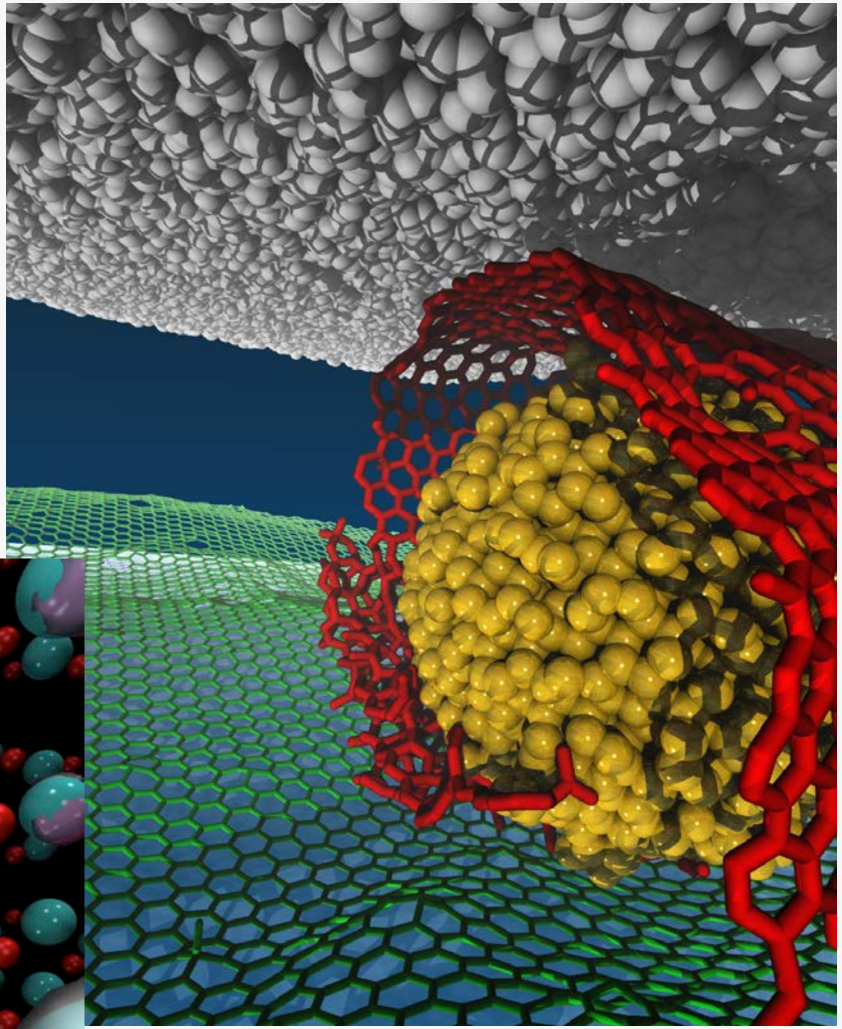
Data courtesy of: Anurag Gupta and Umesh Paliath, General Electric Global Research

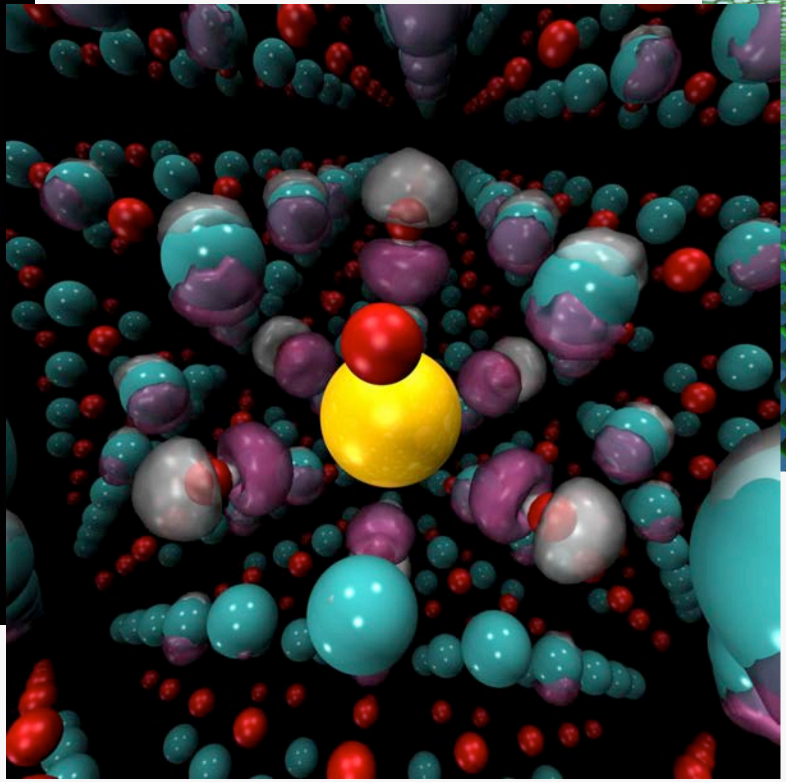
Materials Science / Molecular



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

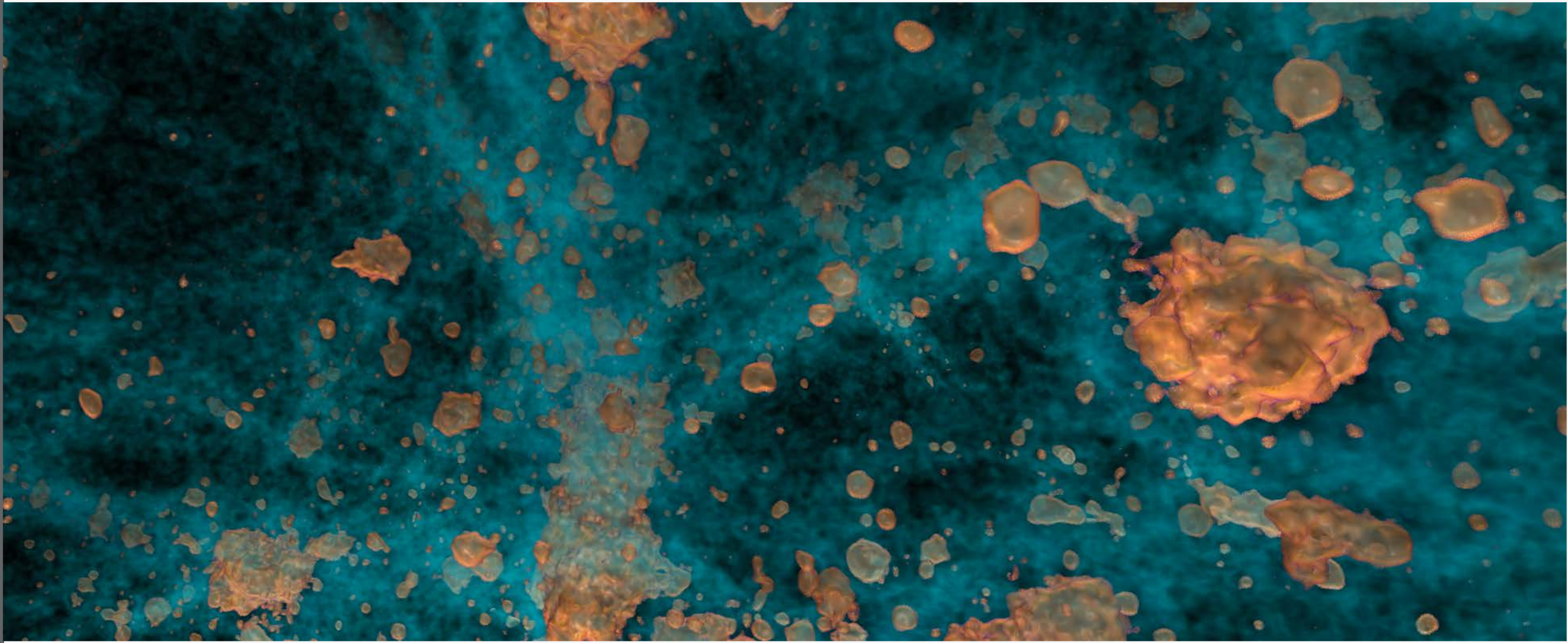
Data courtesy of: Subramanian Sankaranarayanan, Argonne National Laboratory





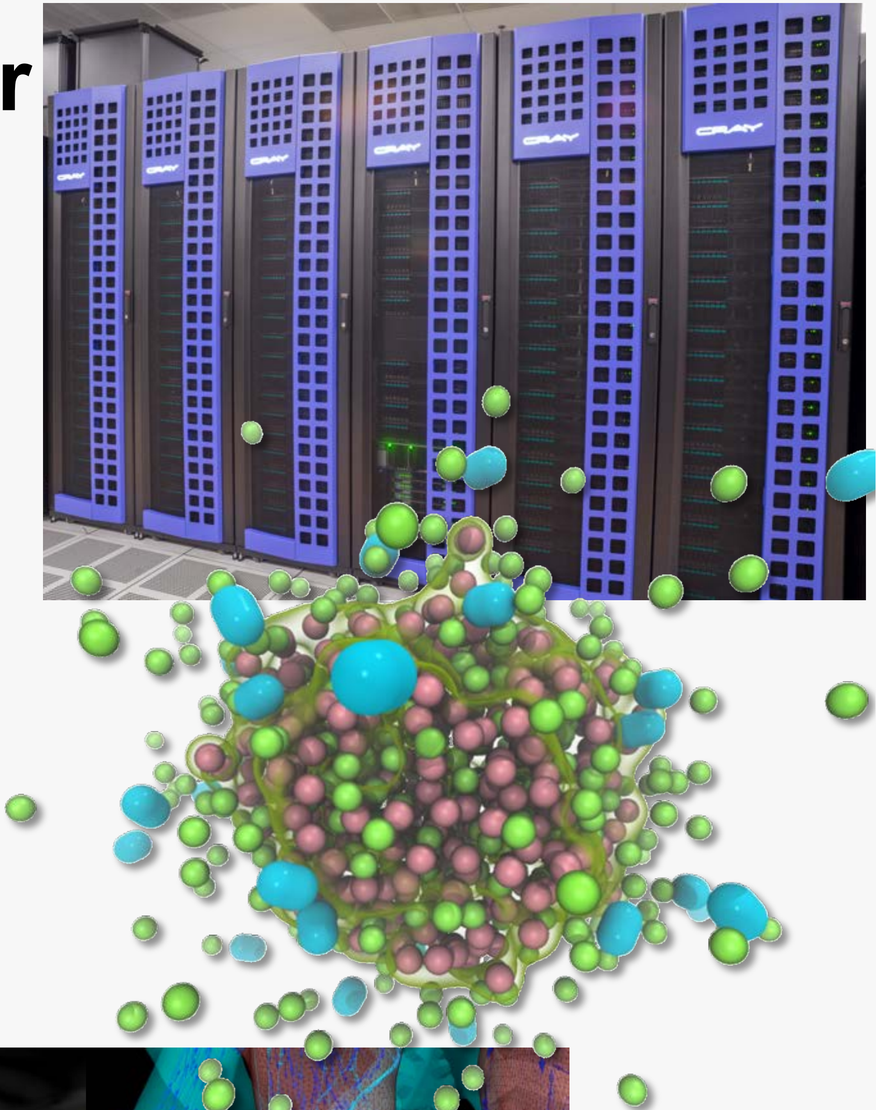
Data courtesy of: Paul Kent, Oak Ridge National Laboratory, Anouar Benali, Argonne National Laboratory

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

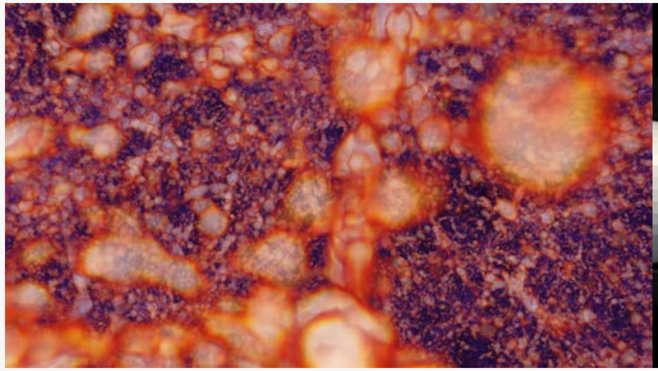
Aggregate RAM of 47 TB

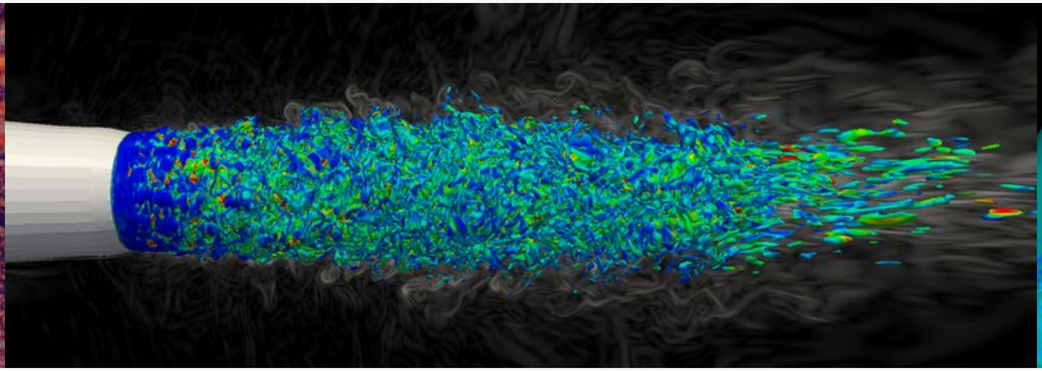
Aggregate GPU memory of ~3TB

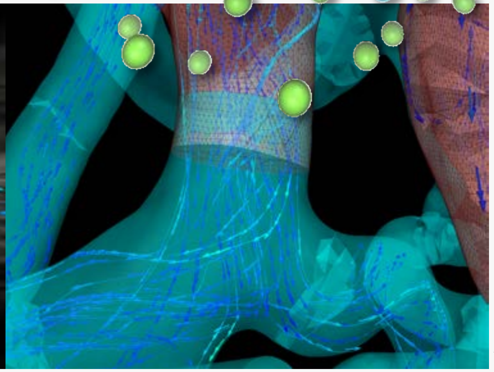
Cray CS System

216 port FDR IB switch with uplinks to our QDR infrastructure

Mounts the same file systems as Mira, Cetus, Theta







Visualization Tools and Data Formats

All Sorts of Tools

Visualization Applications
- VisIt *
- ParaView*
- EnSight

Domain Specific
- VMD, PyMol, Ovito

APIs
- VTK: visualization
- ITK: segmentation & registration

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

Analysis Environments
- Matlab
- Parallel R

Utilities
- GnuPlot
- ImageMagick

■ Available on Cooley

* Available on Theta

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

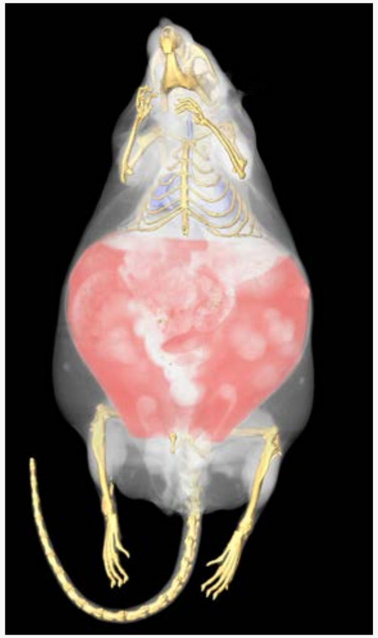
PLOT3D
SpyPlot CTH
HDF5 raw image data
DEM
VRML
PLY
Polygonal Protein Data Bank
XMol Molecule
Stereo Lithography
Gaussian Cube
Raw (binary)
AVS
Meta Image

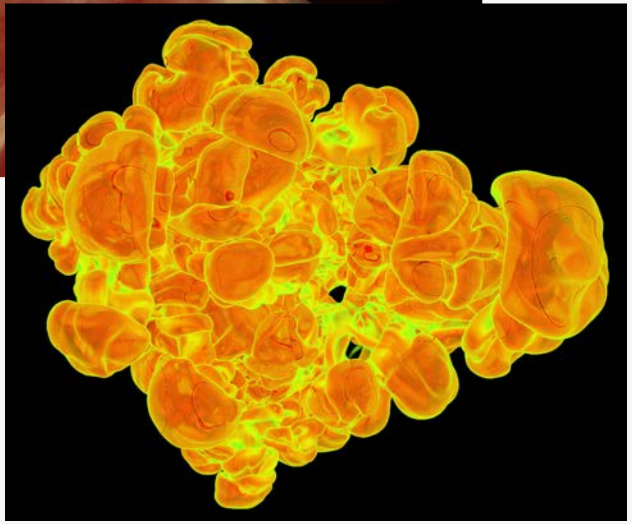
Facet
PNG
SAF
LS-Dyna
Nek5000
OVERFLOW
paraDIS
PATRAN
PFLOTRAN
Pixie
PuReMD
S3D
SAS

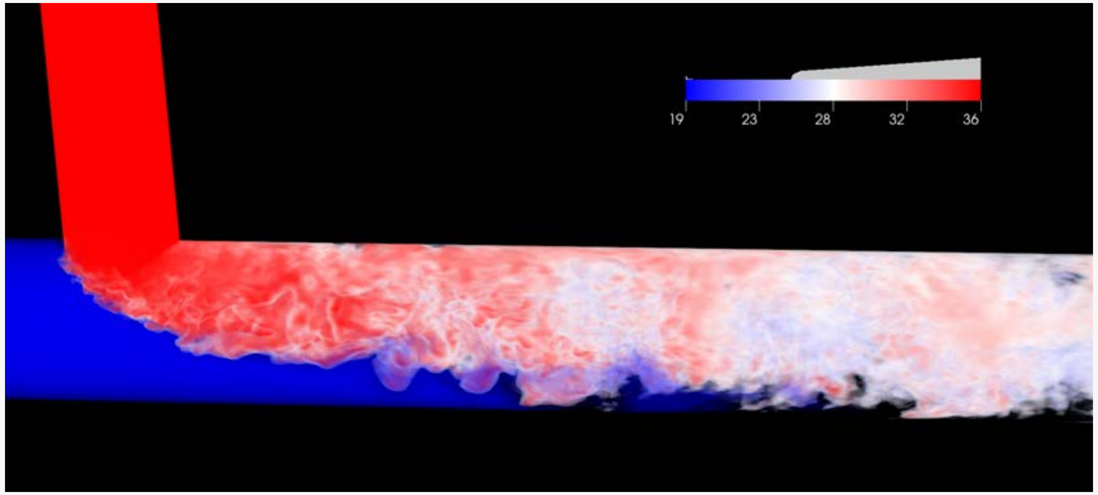
Tetrad
UNIC
VASP
ZeusMP
ANALYZE
BOV
GMV
Tecplot
Vis5D
Xmdv
XSF

Data Representations

Data Representations: Volume Rendering







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Data Representations: Glyphs

2D or 3D geometric object to represent point data

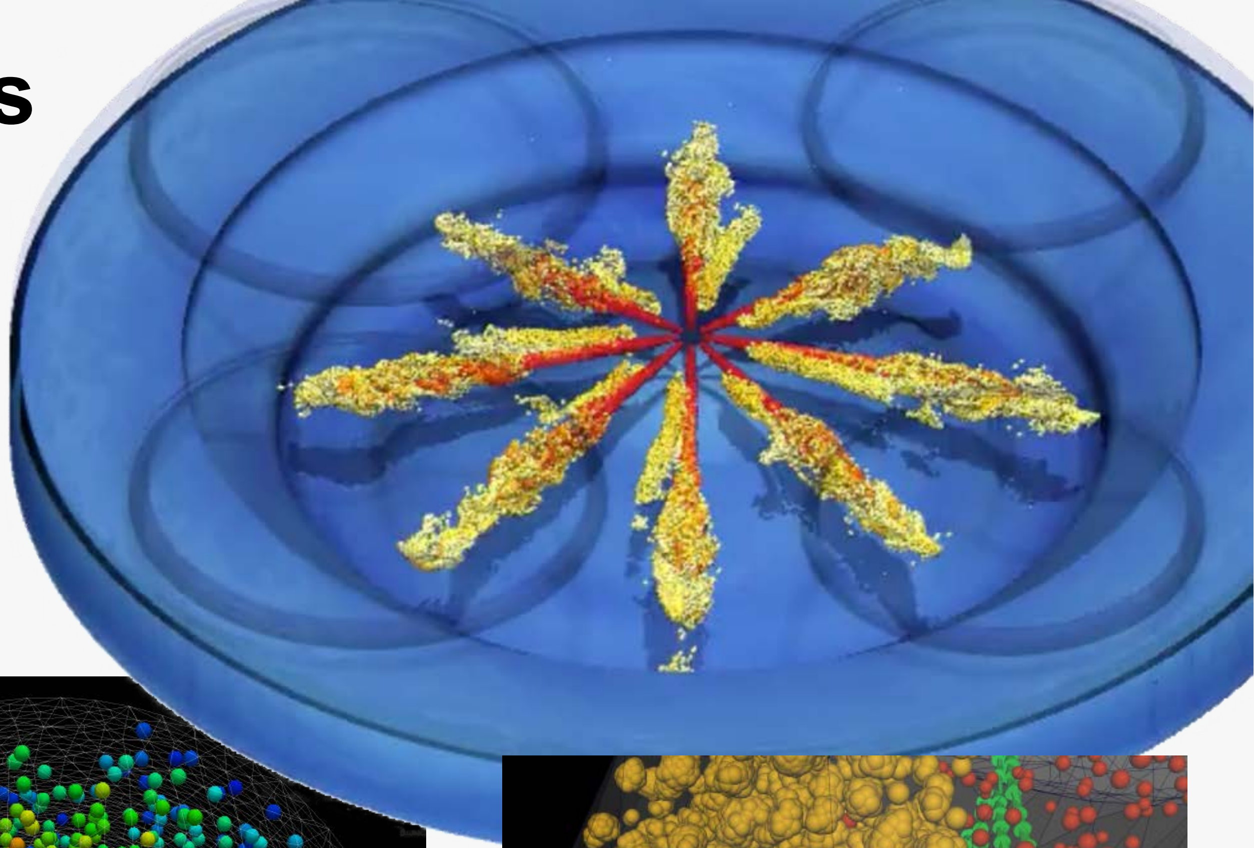
Location dictated by coordinate

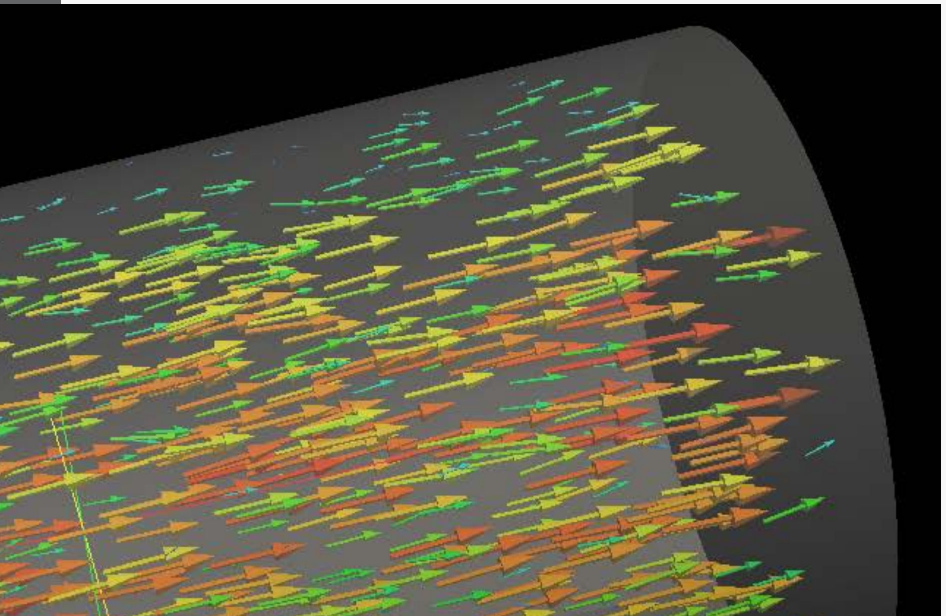
– 3D location on mesh

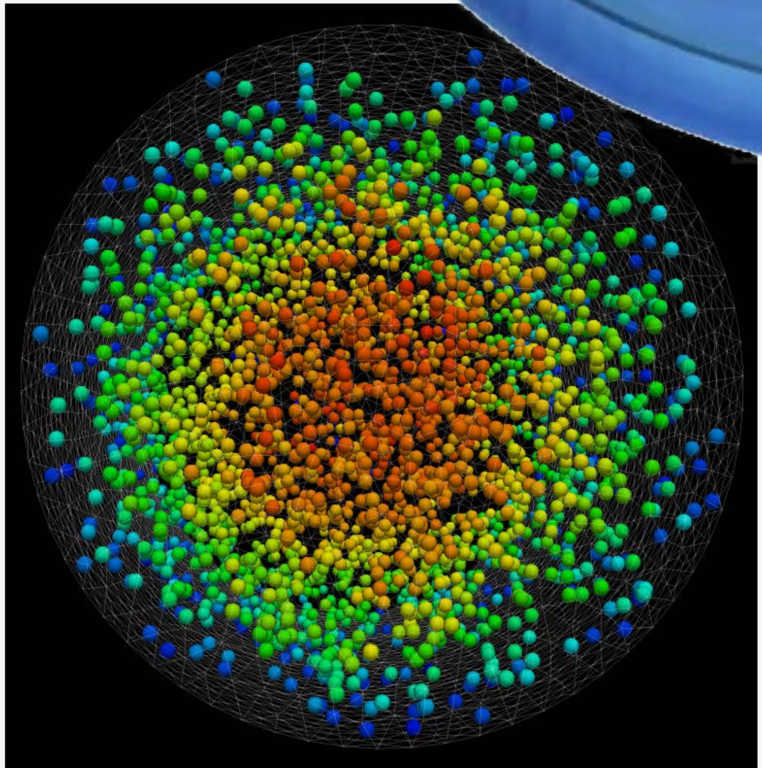
– 2D position in table/graph

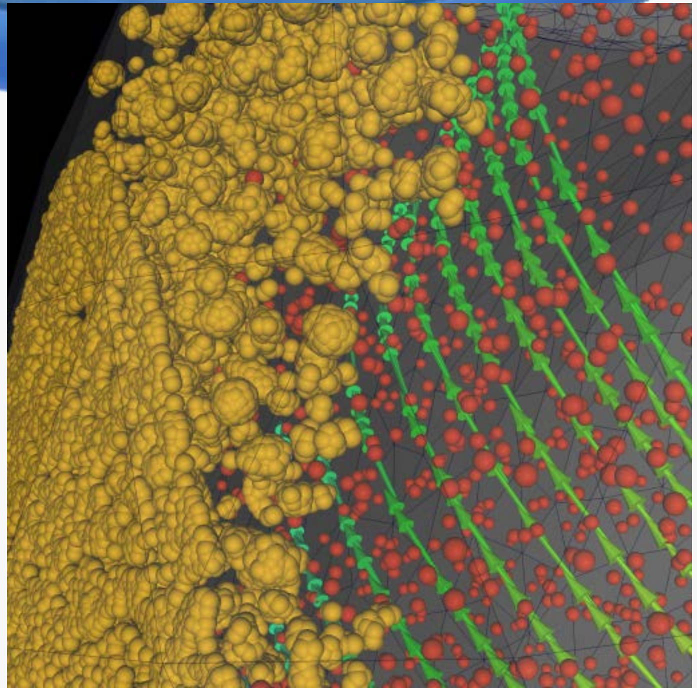
Attributes of graphical entity dictated by attributes of data

– color, size, orientation









Data Representations: Contours (Isosurfaces)

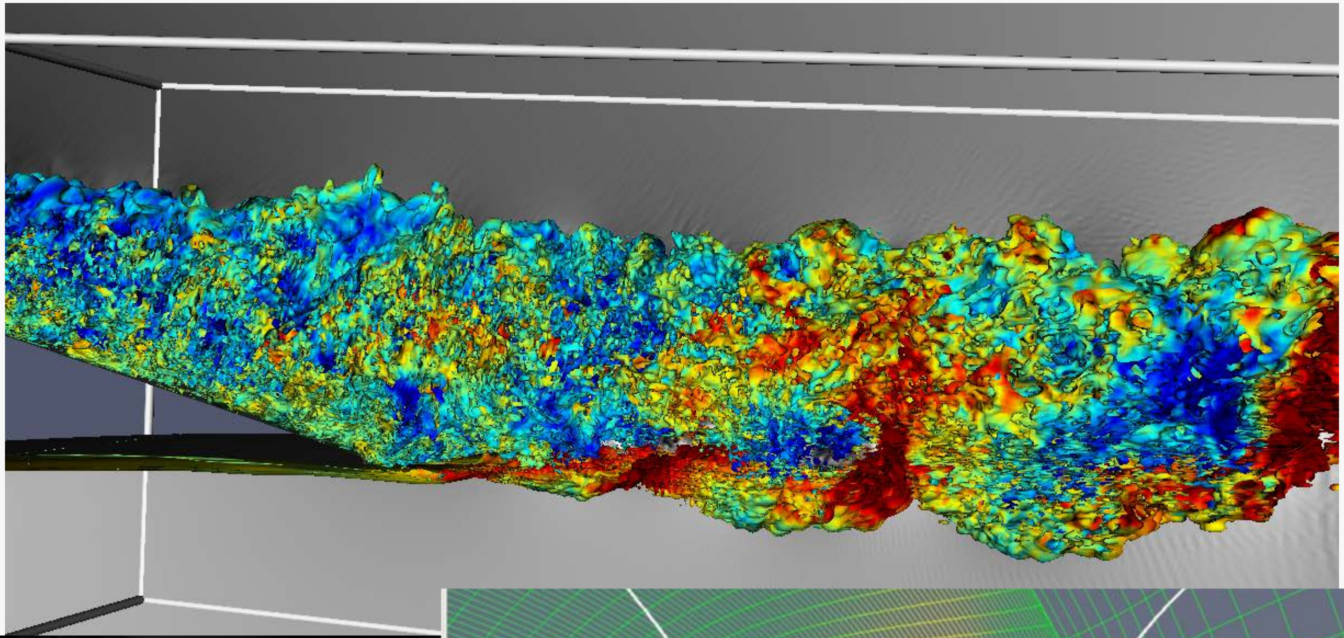
A Line (2D) or Surface (3D), representing a constant value

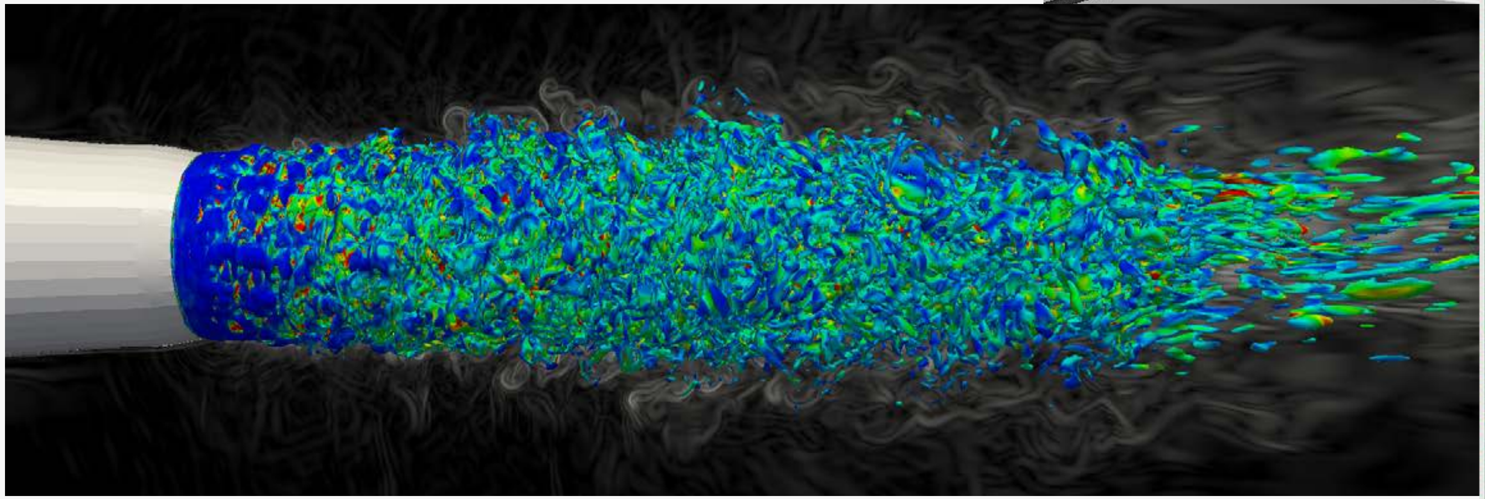
VisIt & ParaView:

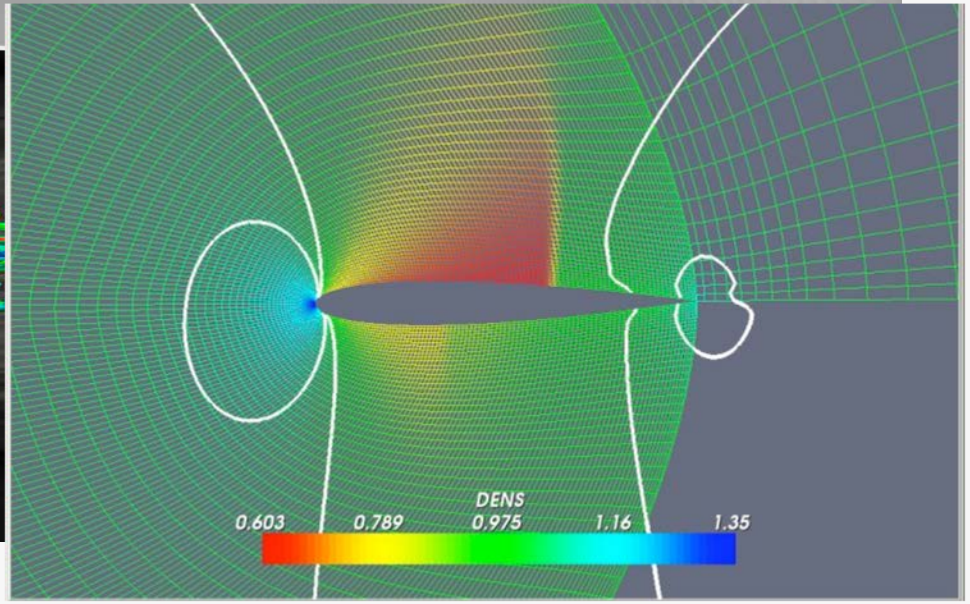
– good at this

vtk:

– same, but again requires more effort







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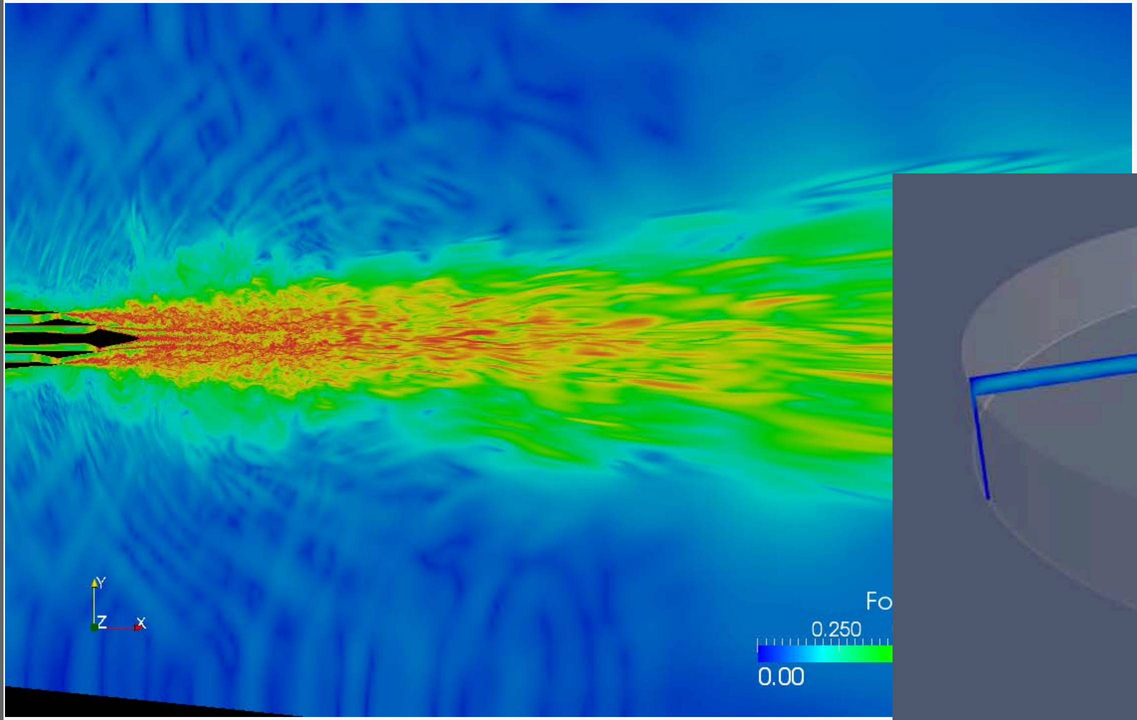
Data Representations: Cutting Planes

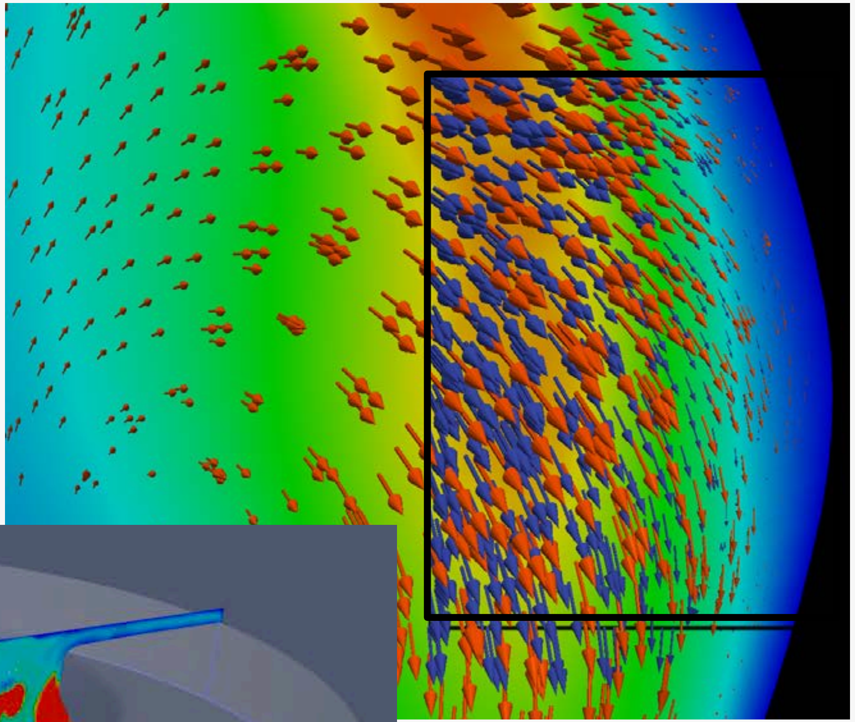
Slice a plane through the data

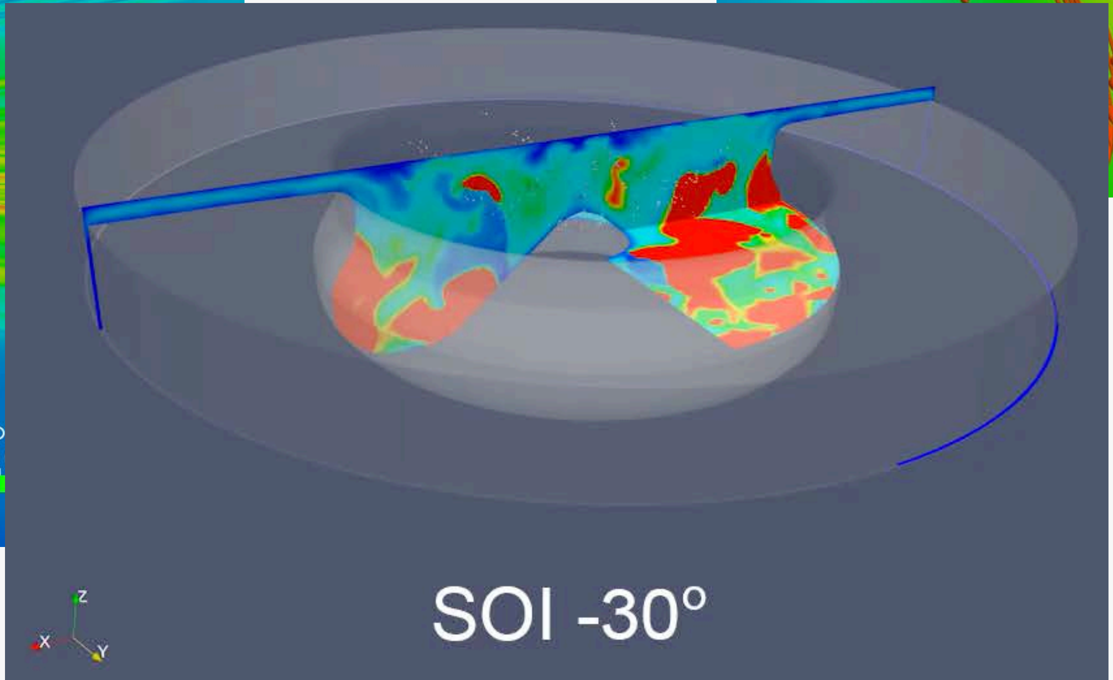
– Can apply additional visualization methods to resulting plane

VisIt & ParaView & vtk good at this

VMD has similar capabilities for some data formats





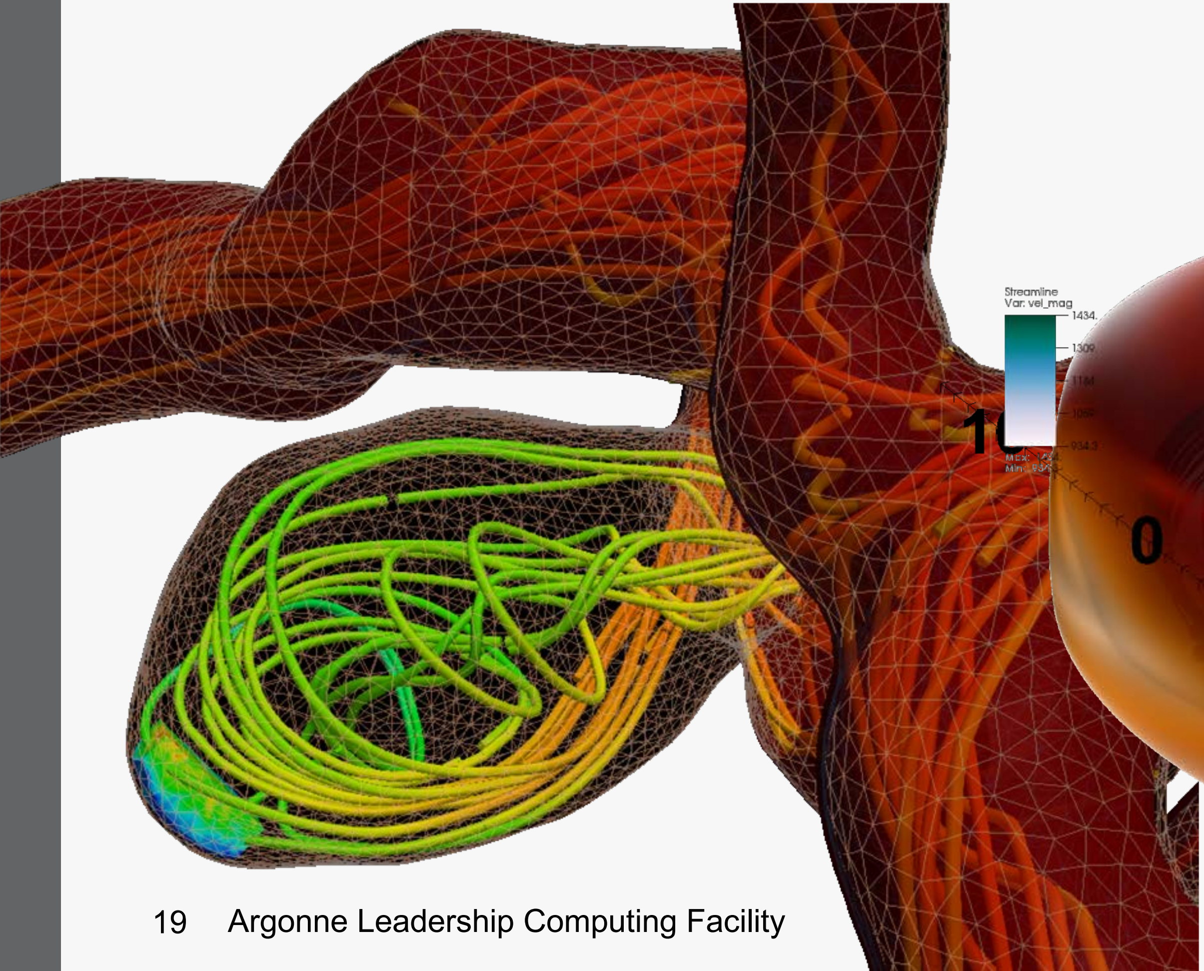


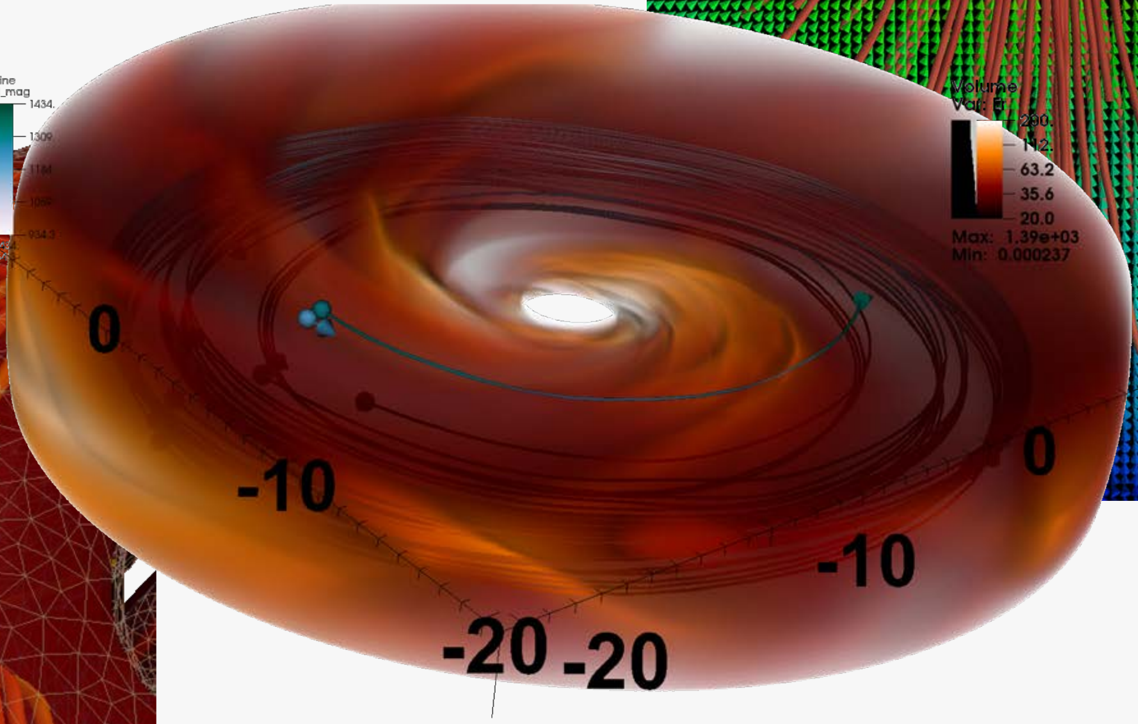
Data Representations: Streamlines

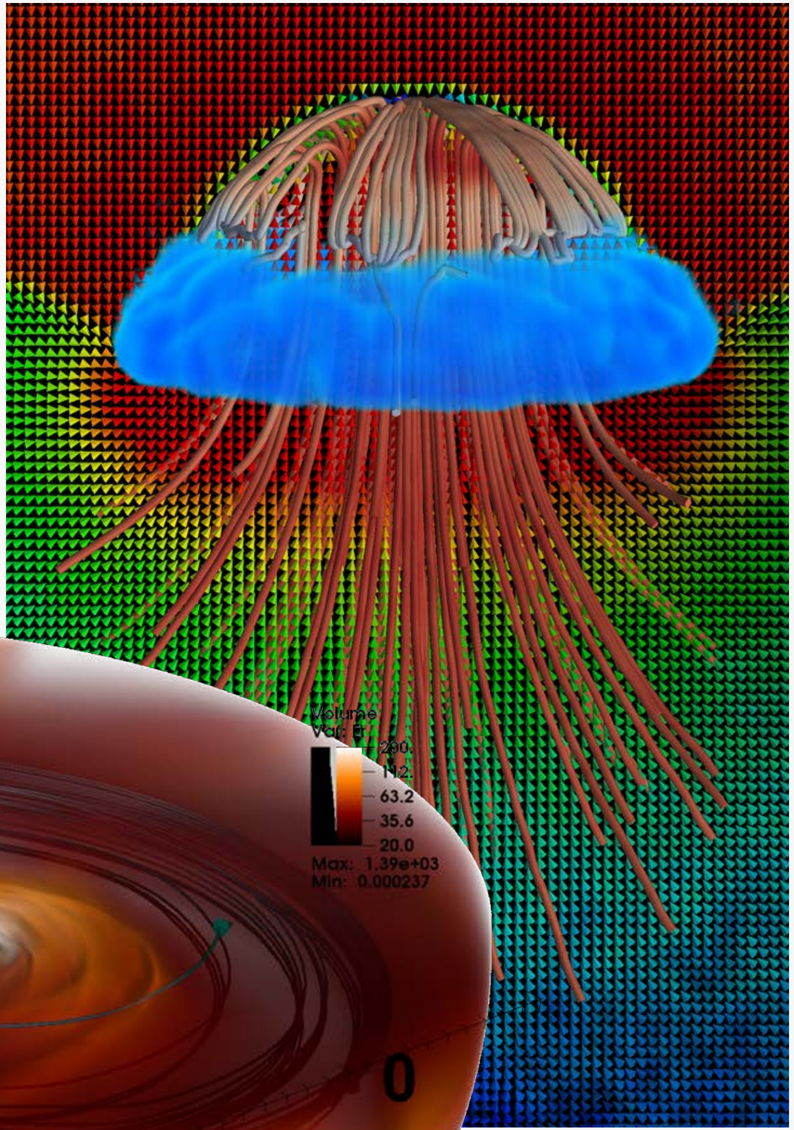
From vector field on a mesh (needs connectivity)

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

VisIt & ParaView & vtk good at this







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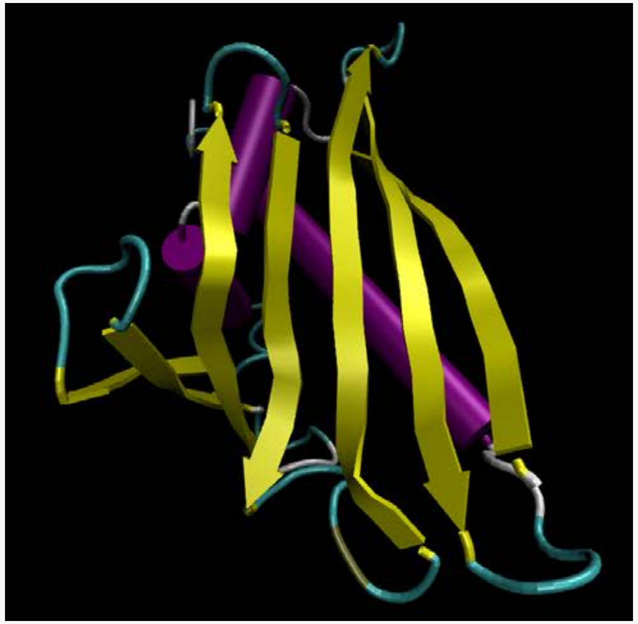
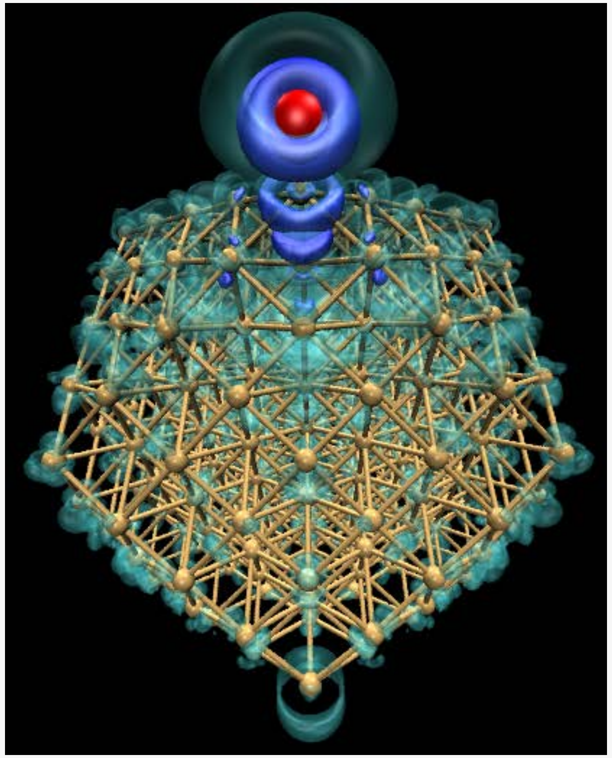
Molecular Dynamics Visualization

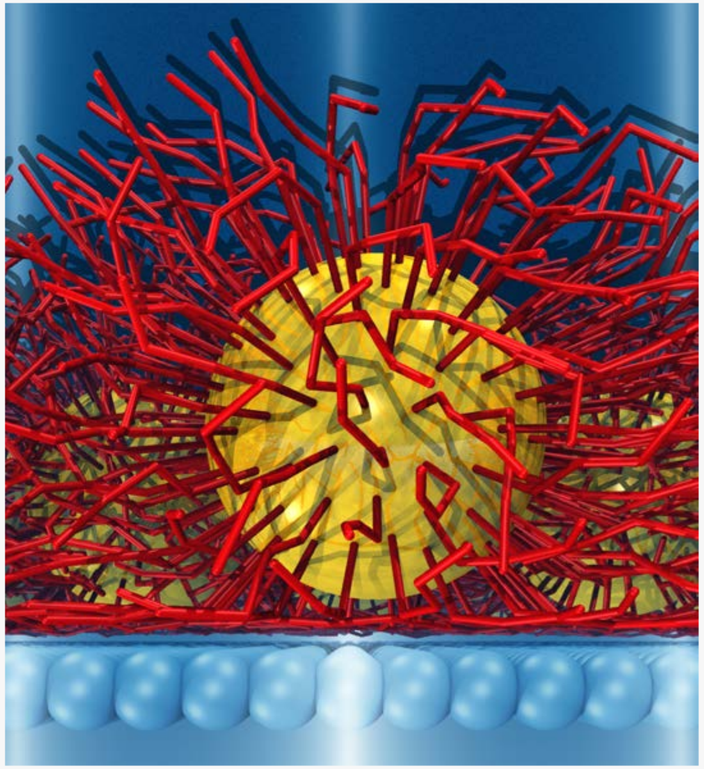




VMD:

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

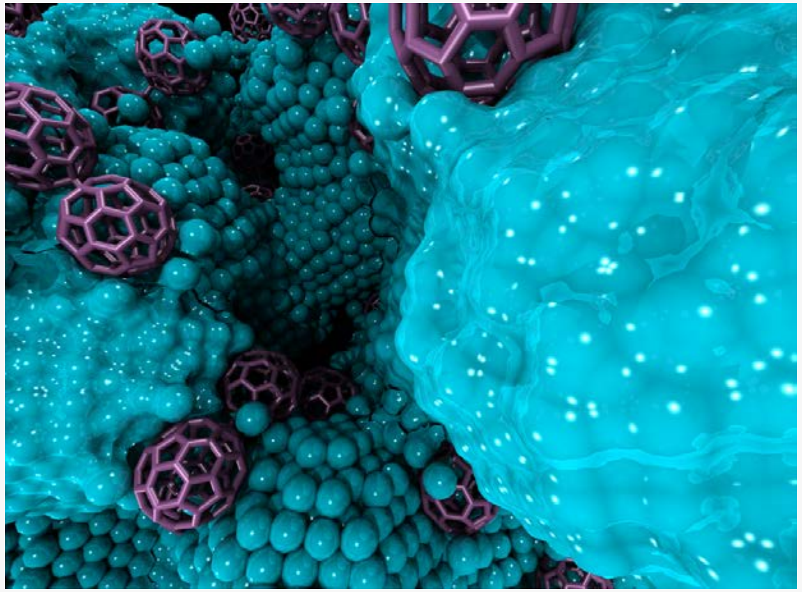
VisIt & ParaView:



- Limited support for these types of representations, but improving

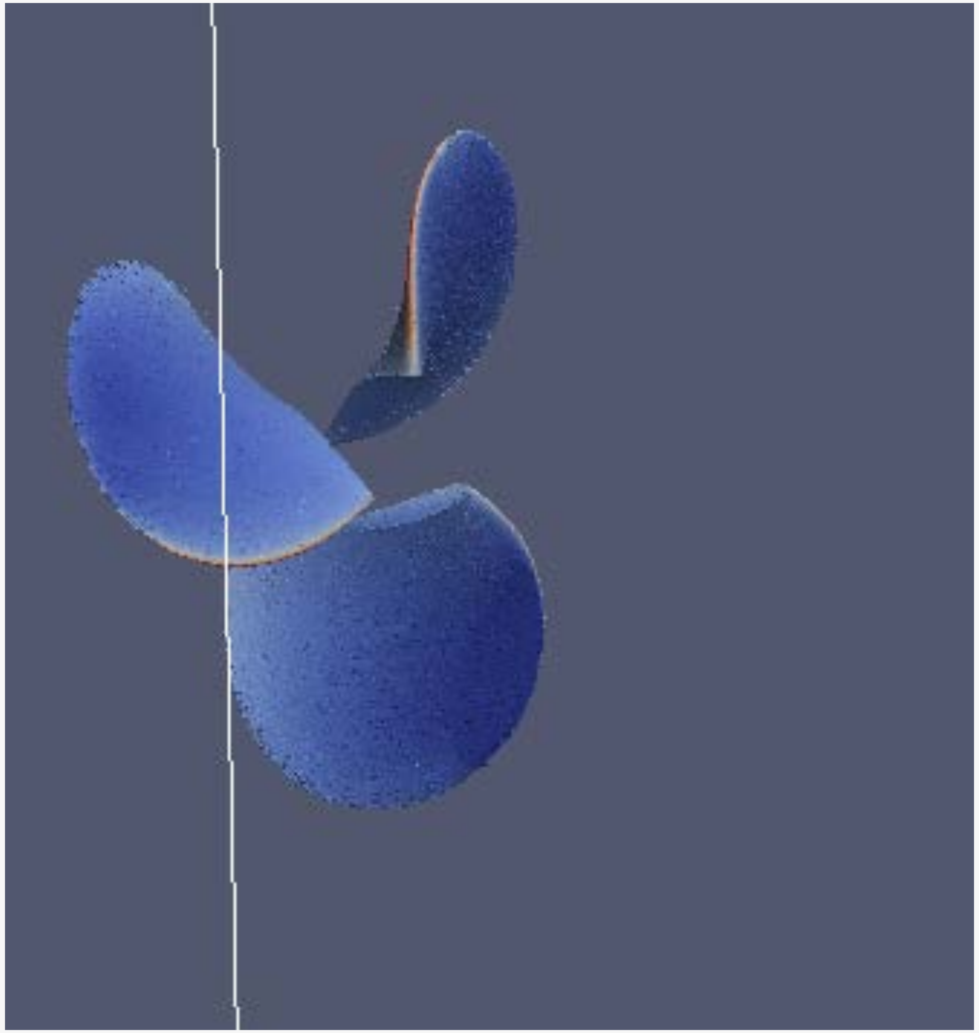
VTK:

- Anything's possible if you try hard enough

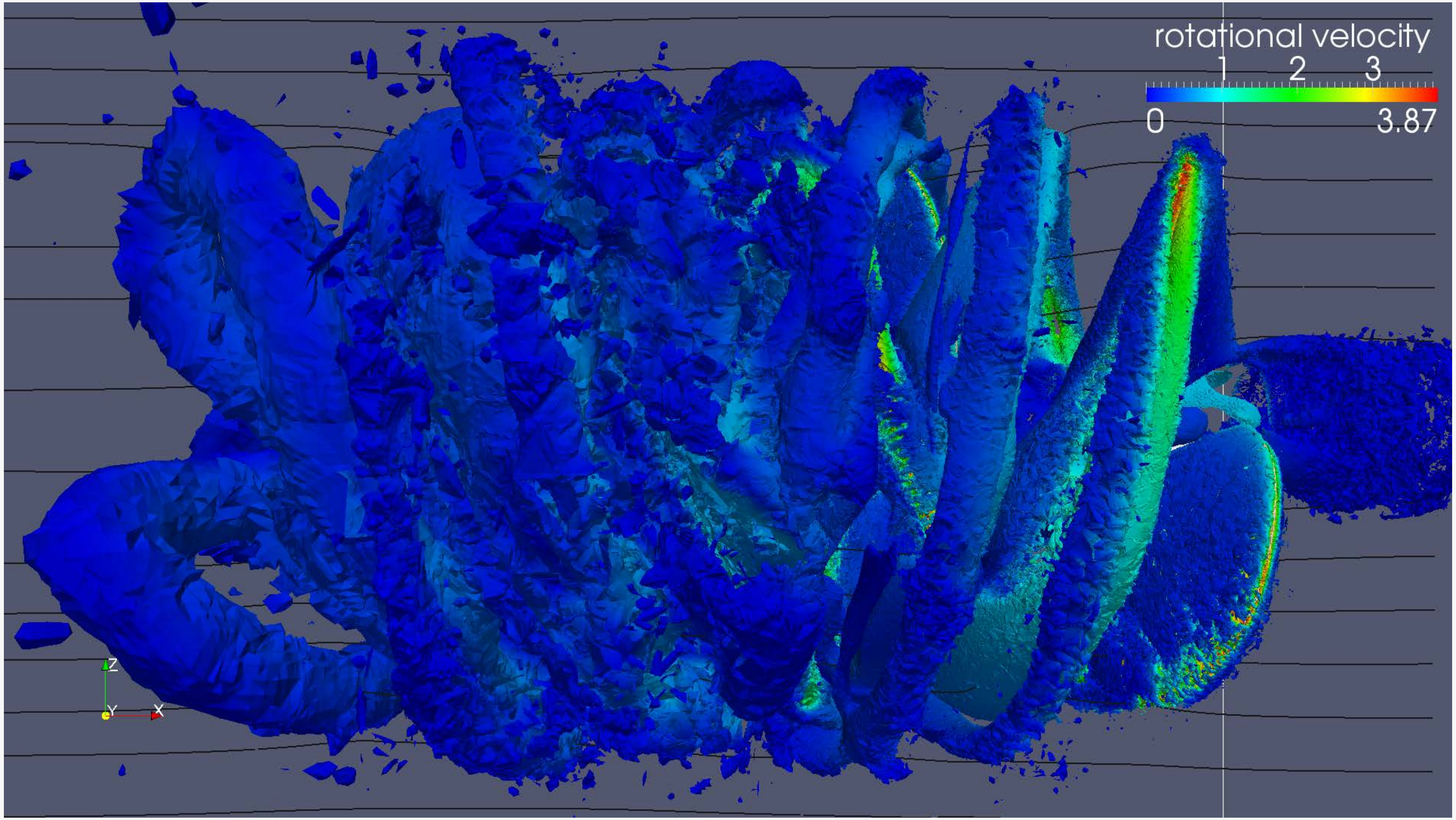


Visualization for Debugging

Visualization for Debugging



Visualization for Debugging



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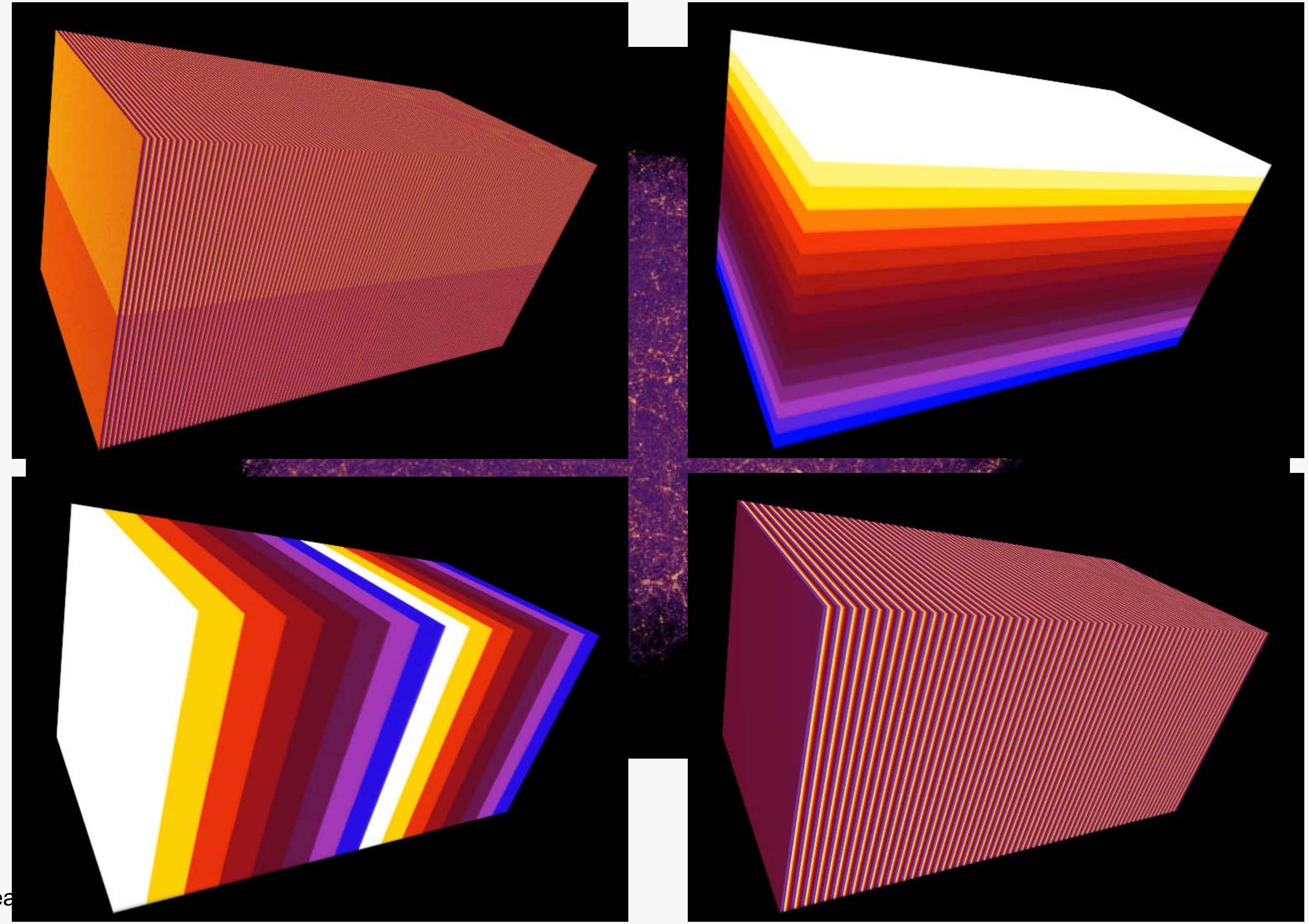
Visualization as Diagnostics: Color by Thread ID



In Situ Visualization and Analysis

In situ visualization and analysis with SENSEI

Slides courtesy SENSEI in situ project:

www.sensei-insitu.org

SENSEI
in situ

BERKELEY LAB

Argonne NATIONAL LABORATORY

OAK RIDGE National Laboratory

Intelligent Light

Kitware

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.

OUR APPROACH

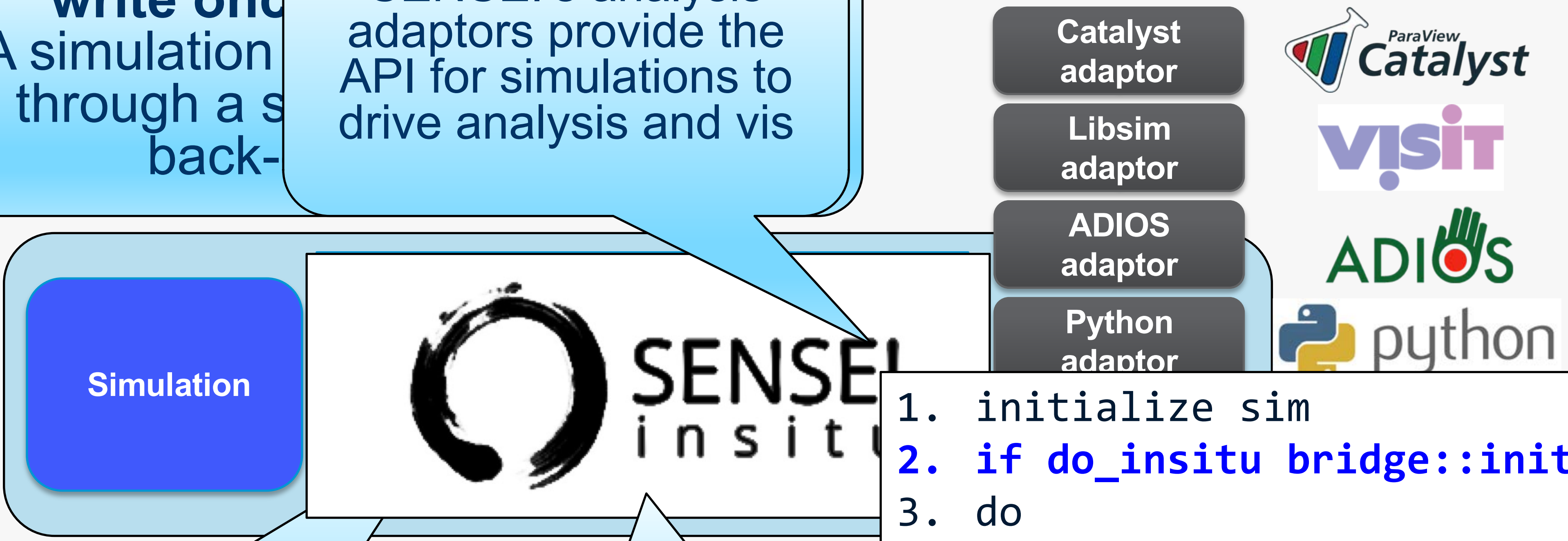
Data model – to pass data between Simulation & Analysis

API – for instrumenting simulation and analysis codes

SENSEI In Situ Architecture

“write onc
A simulation
through a s
back-

SENSEI’s analysis adaptors provide the API for simulations to drive analysis and vis




```
initialize sim
if do_insitu bridge::initialize
do
  compute new state
  if do_io write plot file
  if do_insitu bridge::execute
while !done
if do_insitu bridge::finalize
finalize sim
```

SENSEI’s data adaptor
API and data r
expose simulati
structures to the
back-end

Bridge/instrumentation code is added to call SENSEI Analysis. Typically: Initialize, Execute, Finalize

Using the configurable analysis adaptor

- Enable analysis in .xml file
- Run instrumented simulation

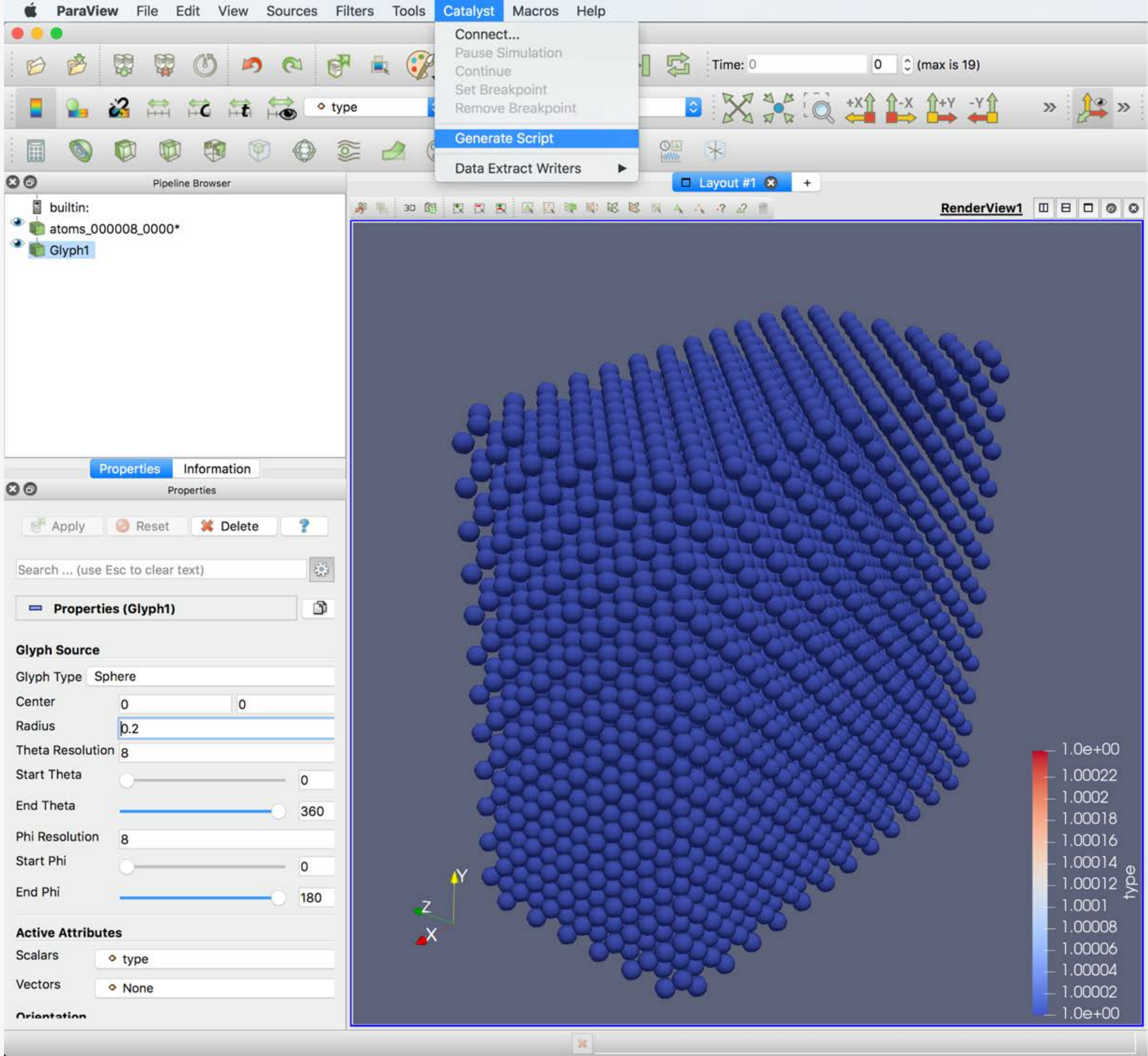
```xml
<sensei>
  <!-- Custom Analyses -->
  <analysis type="histogram" mesh="atoms" array="type" association="point"
    bins="10" enabled="0" />

  <analysis type="histogram" mesh="atoms" array="id" association="point"
    bins="10" enabled="1" />

  <!-- Available with ENABLE_VTK_IO -->
  <analysis type="PosthocIO" mode="paraview" output_dir="./vtkio" enabled="0">
    <mesh name="atoms">
        <point_arrays> type, id</point_arrays>
    </mesh>
  </analysis>
</sensei>
```

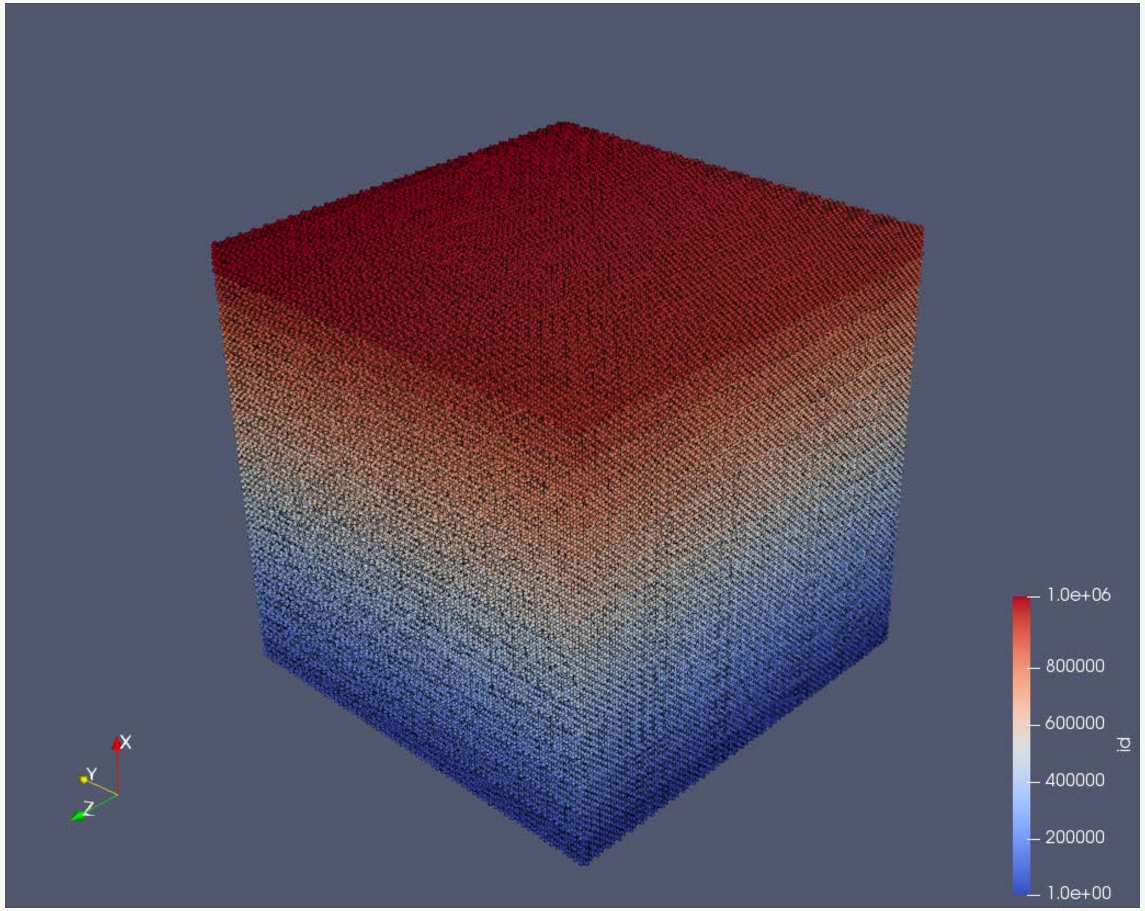
Catalyst example

- Load a representative dataset in ParaView
- Define your visualization pipeline
- Export Catalyst Python script

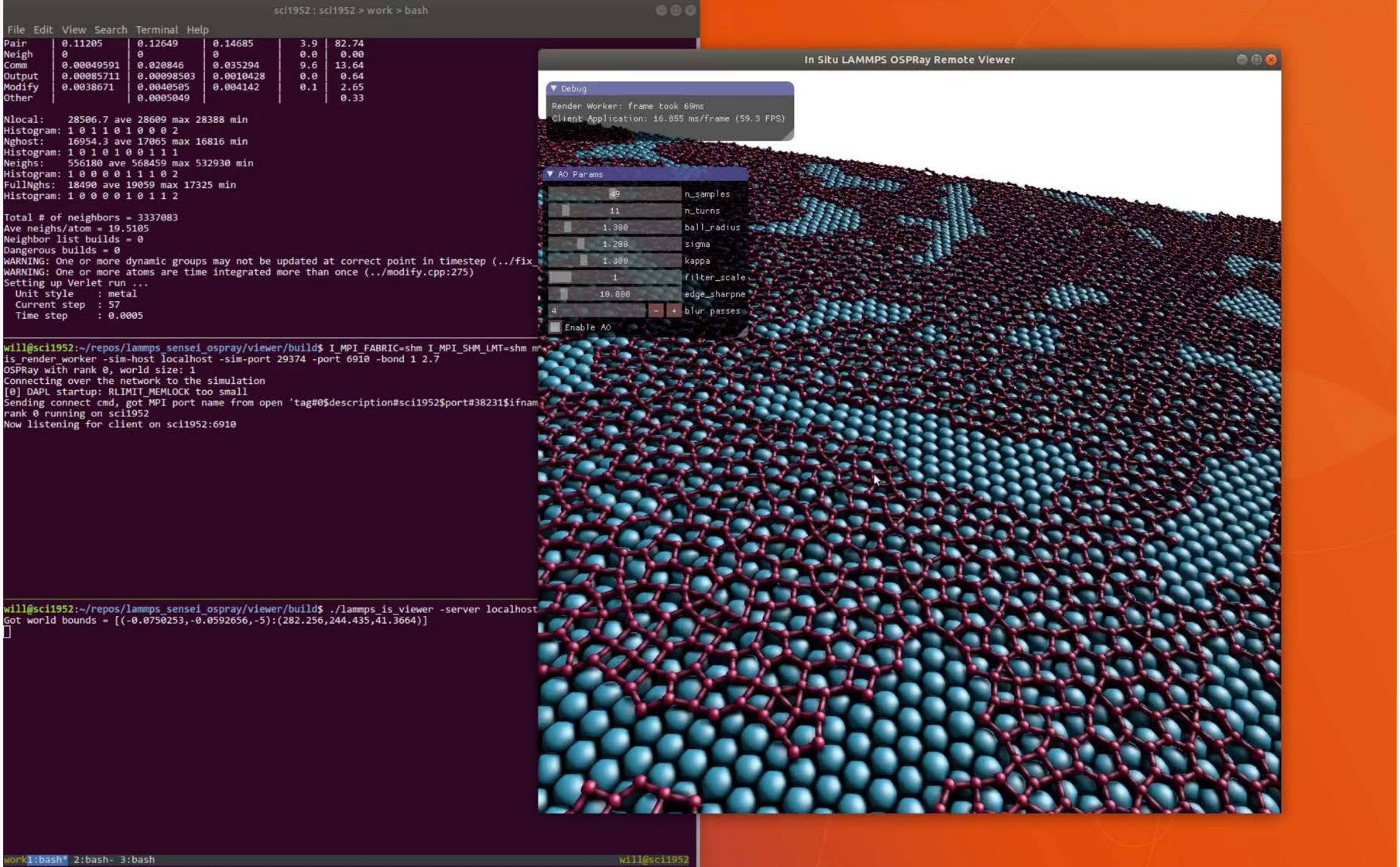


Catalyst example

- Configure XML file
- Run instrumented simulation
- Result: one .png image per simulation timestep




```xml
<sensei>
  <!-- Available with ENABLE_CATALYST -->
  <analysis type="catalyst" pipeline="pythonscript"
    filename="gaussianptsbyid.py" enabled="1" />
</sensei>
```



sci1952 : sci1952 > work > bash
File Edit View Search Terminal Help
Pair | 0.11205 | 0.12649 | 0.14685 | 3.9 | 82.74
Neigh | 0 | 0 | 0 | 0.0 | 0.00
Comm | 0.00049591 | 0.020846 | 0.035294 | 9.6 | 13.64
Output | 0.00085711 | 0.00098503 | 0.0010428 | 0.0 | 0.64
Modify | 0.0038671 | 0.0040505 | 0.004142 | 0.1 | 2.65
Other | | 0.0005049 | | | 0.33
Nlocal: 28506.7 ave 28609 max 28388 min
Histogram: 1 0 1 1 0 1 0 0 0 2
Nghost: 16954.3 ave 17065 max 16816 min
Histogram: 1 0 1 0 1 0 0 1 1 1
Neighs: 556180 ave 568459 max 532930 min
Histogram: 1 0 0 0 0 1 1 1 0 2
FullNghs: 18490 ave 19059 max 17325 min
Histogram: 1 0 0 0 0 1 0 1 1 2
Total # of neighbors = 3337083
Ave neighs/atom = 19.5105
Neighbor list builds = 0
Dangerous builds = 0
WARNING: One or more dynamic groups may not be updated at correct point in timestep (../fix_
WARNING: One or more atoms are time integrated more than once (../modify.cpp:275)
Setting up Verlet run ...
Unit style : metal
Current step : 57
Time step : 0.0005
will@sci1952:~/repos/lammps_sensei_ospray/viewer/build$ I_MPI_FABRIC=shm I_MPI_SHM_LMT=shm m
is_render_worker -sim-host localhost -sim-port 29374 -port 6910 -bond 1 2.7
OSPRay with rank 0, world size: 1
Connecting over the network to the simulation
[0] DAPL startup: RLIMIT_MEMLOCK too small
Sending connect cmd, got MPI port name from open 'tag#0$description#sci1952$port#38231$ifnam
rank 0 running on sci1952
Now listening for client on sci1952:6910
will@sci1952:~/repos/lammps_sensei_ospray/viewer/build$ ./lammps_is_viewer -server localhost
Got world bounds = [(-0.0750253,-0.0592656,-5):(282.256,244.435,41.3664)]
work 1:bash* 2:bash- 3:bash
will@sci1952
In Situ LAMMPS OSPRay Remote Viewer
Debug
Render Worker: frame took 69ms
Client Application: 16.855 ms/frame (59.3 FPS)
AO Params
49 n_samples
11 n_turns
1.300 ball_radius
1.200 sigma
1.300 kappa
1 filter_scale
10.000 edge_sharpne
4 blur passes
Enable AO

In Situ Visualization and Analysis with Ascent

Slides courtesy:

Hank Childs, University of Oregon
Matthew Larsen, Lawrence Livermore National Laboratory
Cyrus Harrison, Lawrence Livermore National Laboratory
Kenneth Moreland, Sandia National Laboratories
David Rogers, Los Alamos National Laboratory

Ascent focuses on ease of use and efficient in-situ execution

Ascent Delivers

An easy to use API

- Designed to enable three use cases
  - Making Pictures
  - Transforming Data
  - Capturing Data
- Leverages Conduit (http://software.llnl.gov/conduit)
  - Underpins support for C, C++, Fortran, and Python
  - Simplifies handoff of mesh-based simulation data
  - Convention for specifying data called “Blueprint”

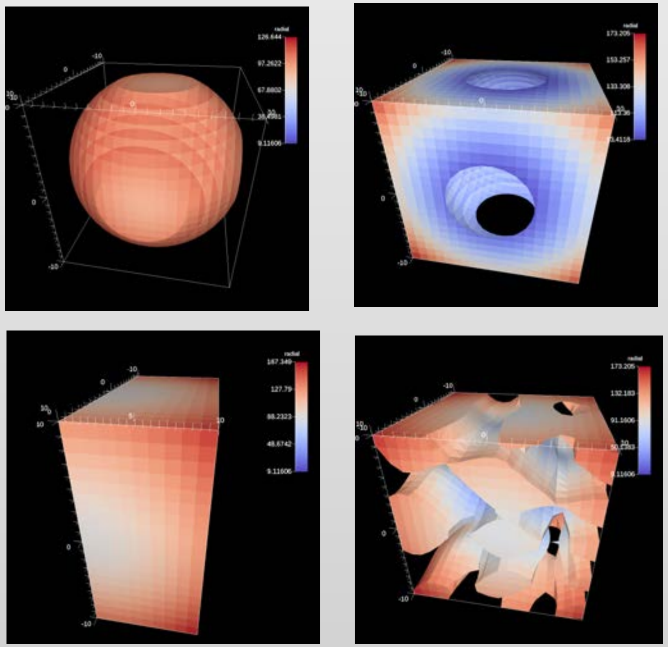
```
//
// Run Ascent
//

Ascent ascent;
ascent.open();
ascent.publish(data);
ascent.execute(actions);
ascent.close();
```

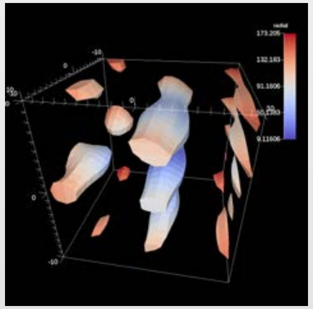
A flyweight design

- Efficient distributed-memory + many-core execution
  - Leverages MPI, VTK-m (http://m.vtk.org/)
- Lower memory requirements then current tools
- Less dependencies than current tools (ex: no OpenGL)

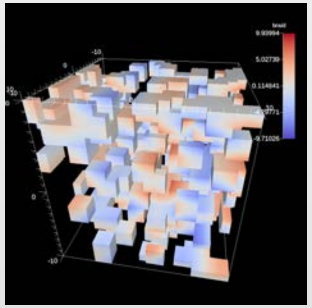
Ascent is ready for common visualization use cases



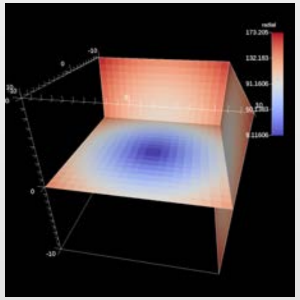
Clips



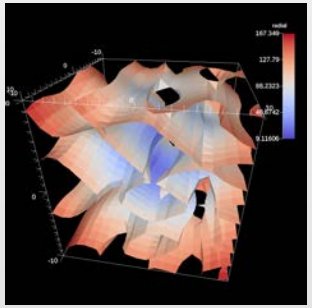
Iso-Volume



Threshold

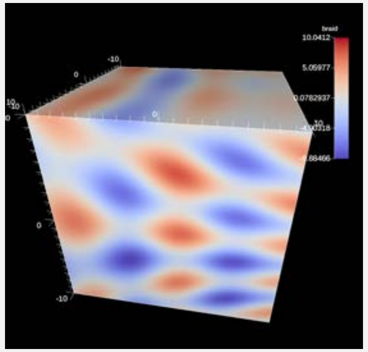


Slice

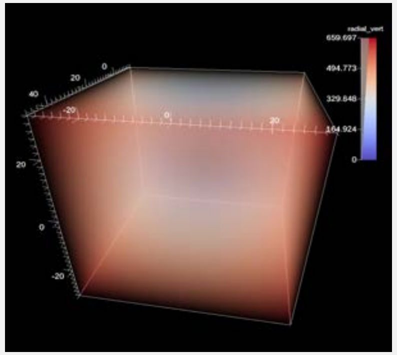


Contour

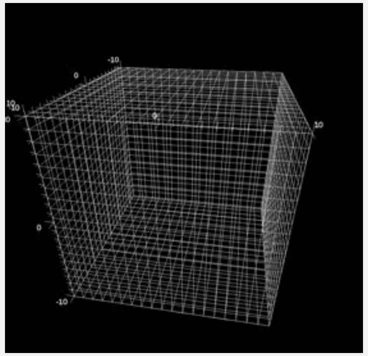
Rendering



Pseudocolor



Volume



Mesh

Design Goal: Support custom analysis as a first class citizen

Mainstream visualization only gets you so far

– Scientists often want something other than a contour

In-situ visualization frameworks need to be

– Flexible
– Easy to use
– Easy to connect with other “things”

Ascent supports multiple languages and output types

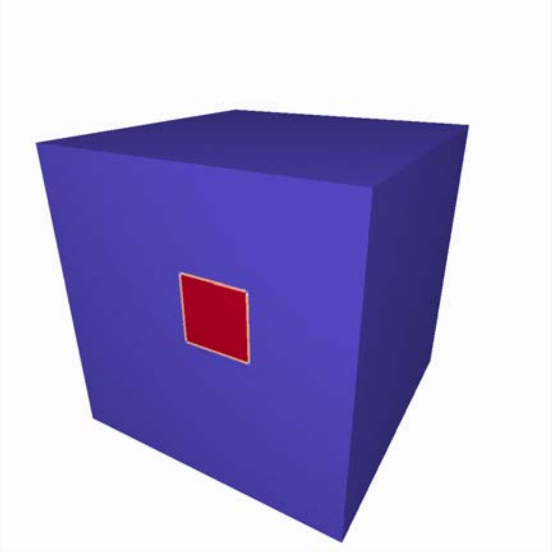
Language Bindings

- C/C++
- python™
- Fortran

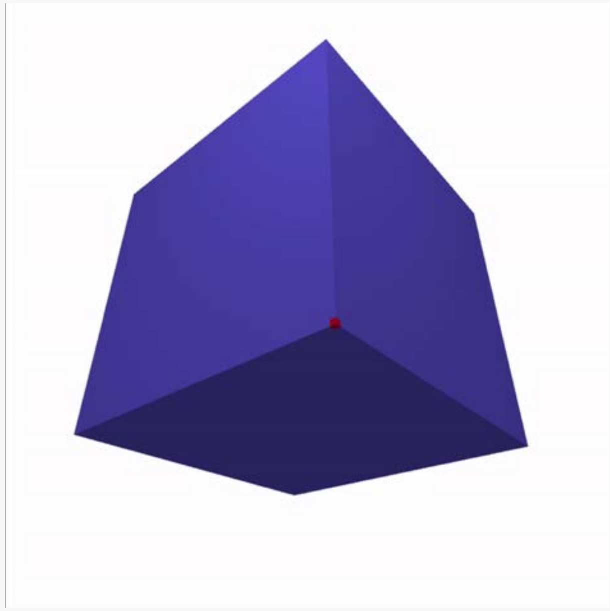
Output Types

- HDF
- ADIOS
- CINEMA

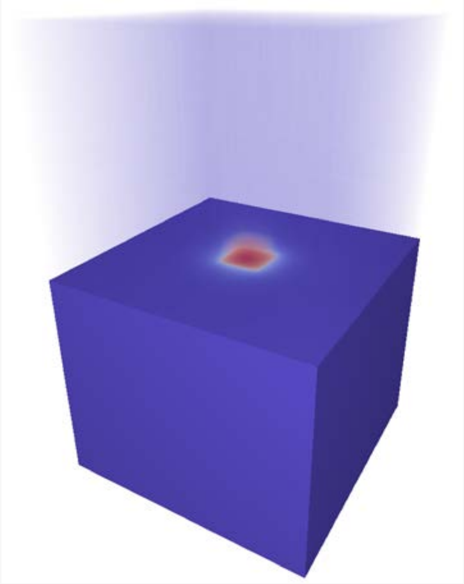
Ascent provides example integrations that also serve as built-in data sources



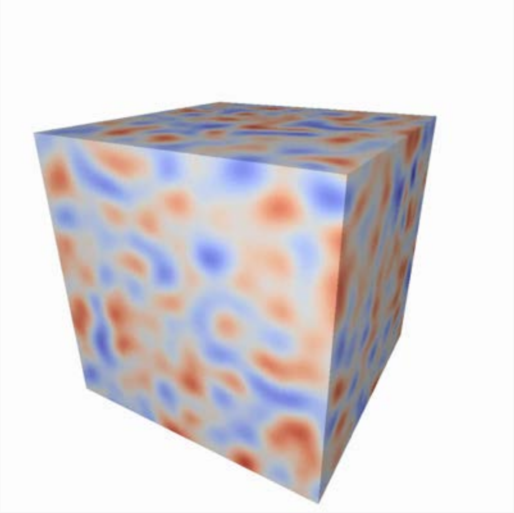
Cloverleaf3D



Lulesh



Kripke



Smooth Noise

Additional Resources

SENSEI additional resources

- SENSEI project page
  https://sensei-insitu.org/

- Gitlab repo
  https://gitlab.kitware.com/sensei/sensei

- SENSEI SC18 Tutorial - Slides and Virtual Machine
  https://sensei-insitu.org/tutorials/sc18.html

Ascent additional resources

Website + Docs:

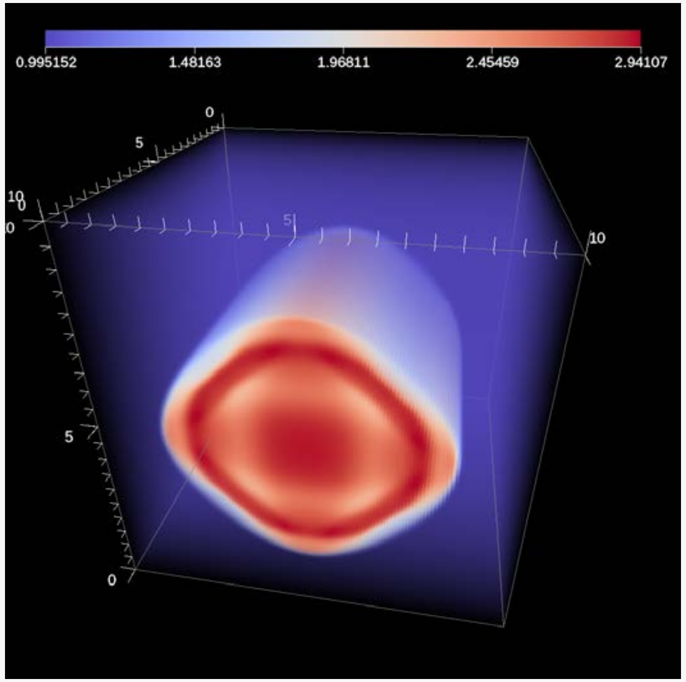
http://ascent-dav.org

GitHub Repo:

https://github.com/Alpine-DAV/ascent

Email Help:

help@ascent-dav.org



Example in-situ rendering created using Ascent

QUESTIONS?

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