Visualizing your Data

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Here's the plan…

— Examples of visualizations

— Visualization resources

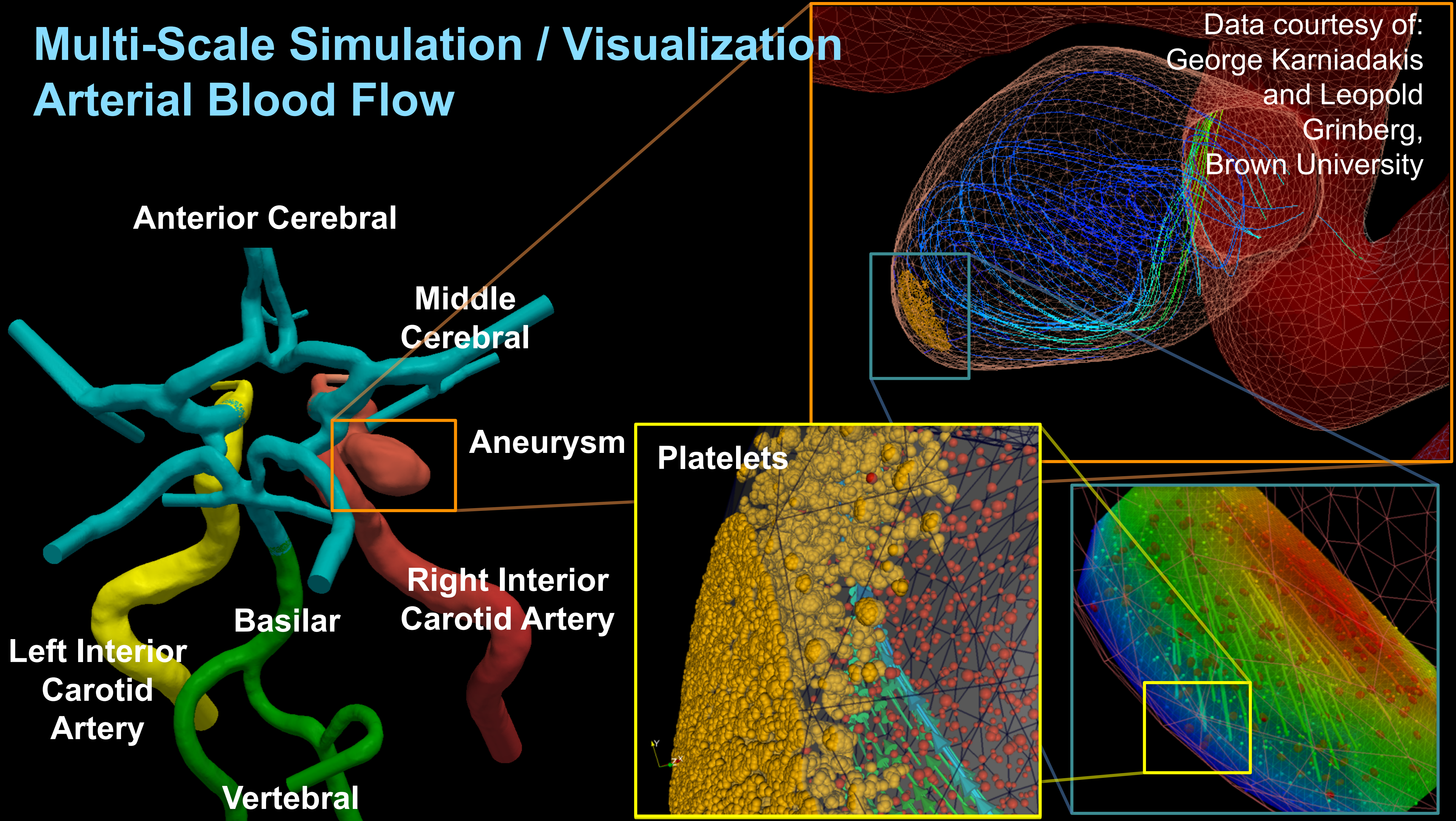
— Visualization tools and formats

— Data representations

— Visualization for debugging

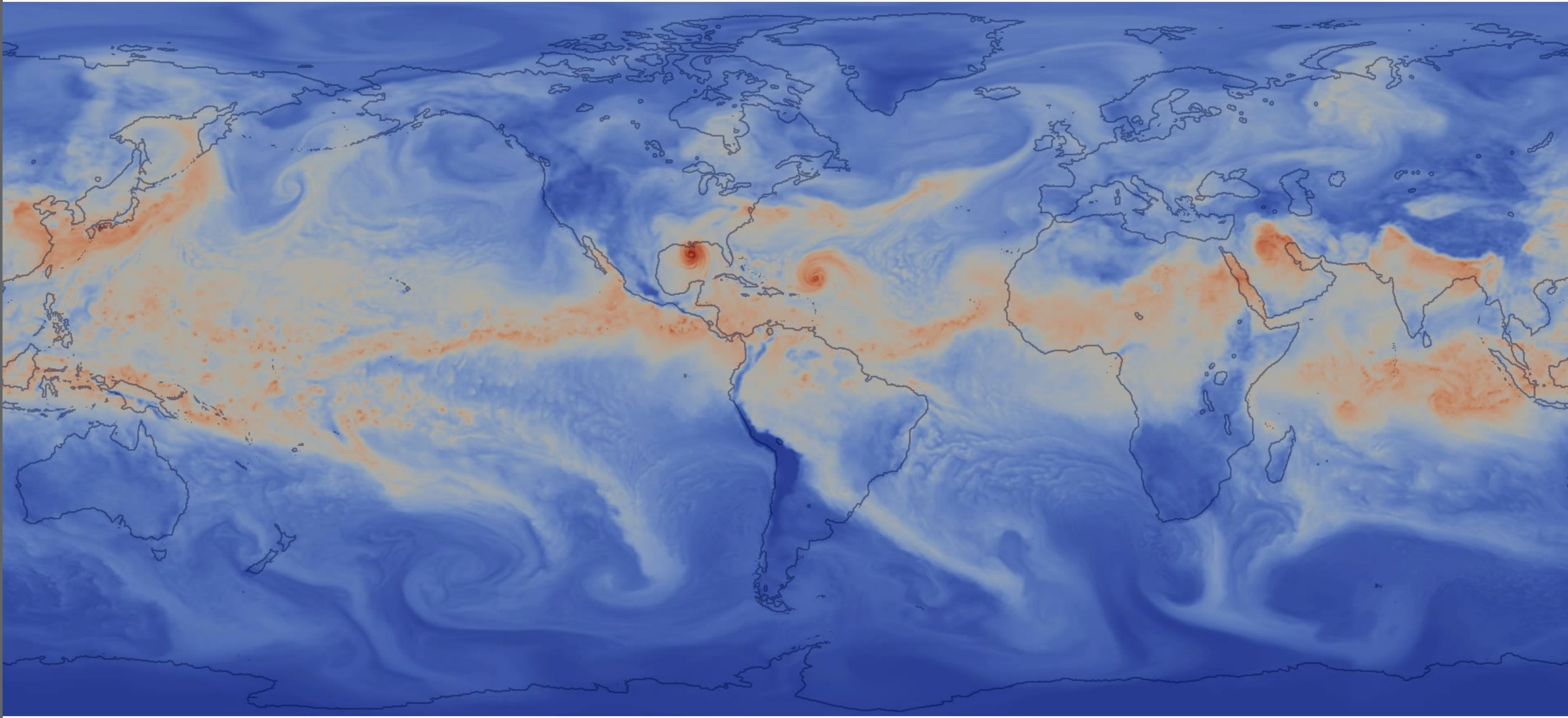
— In-Situ Visualization and Analysis

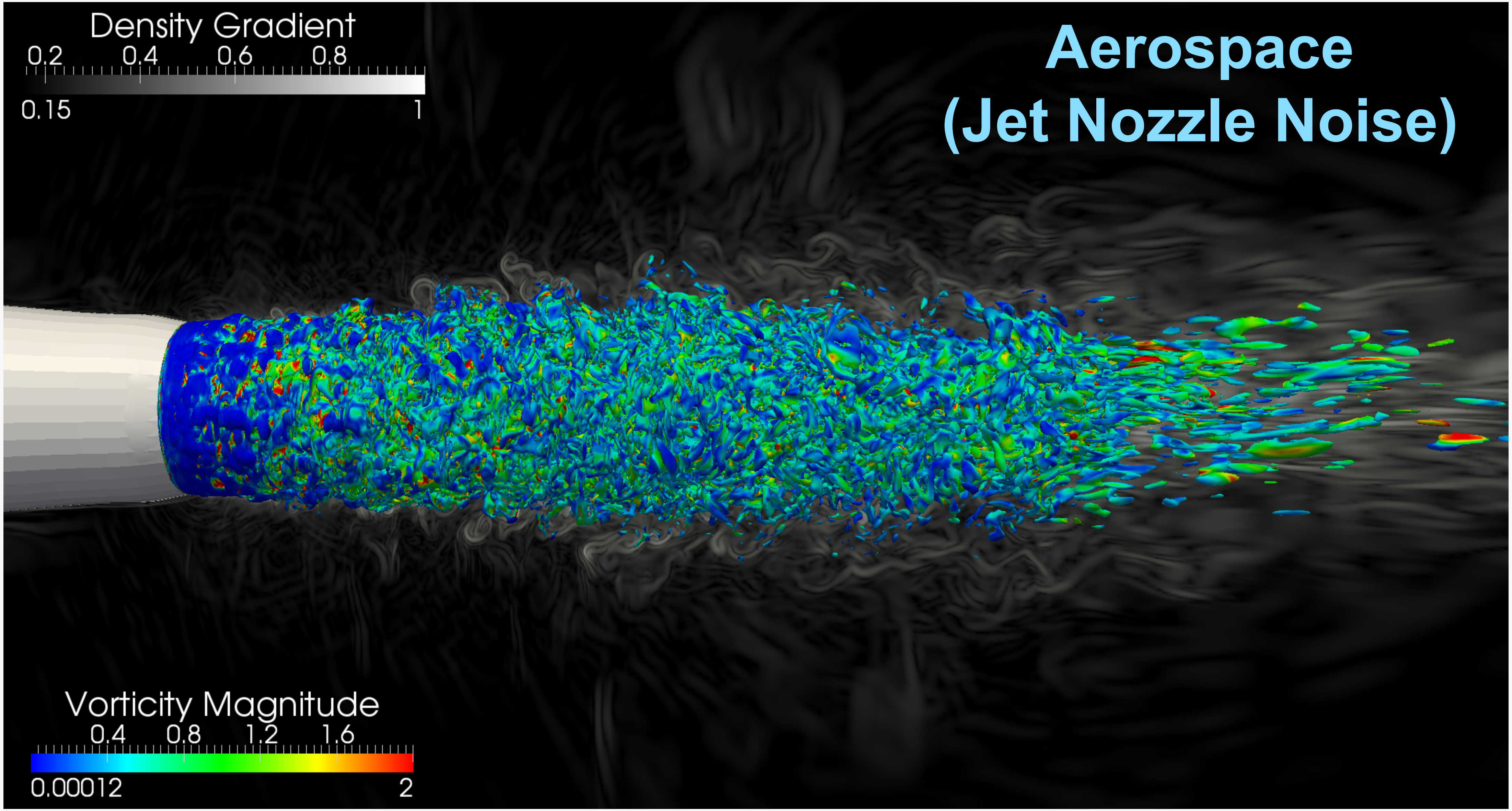
Multi-Scale Simulation / Visualization
Arterial Blood Flow



Climate

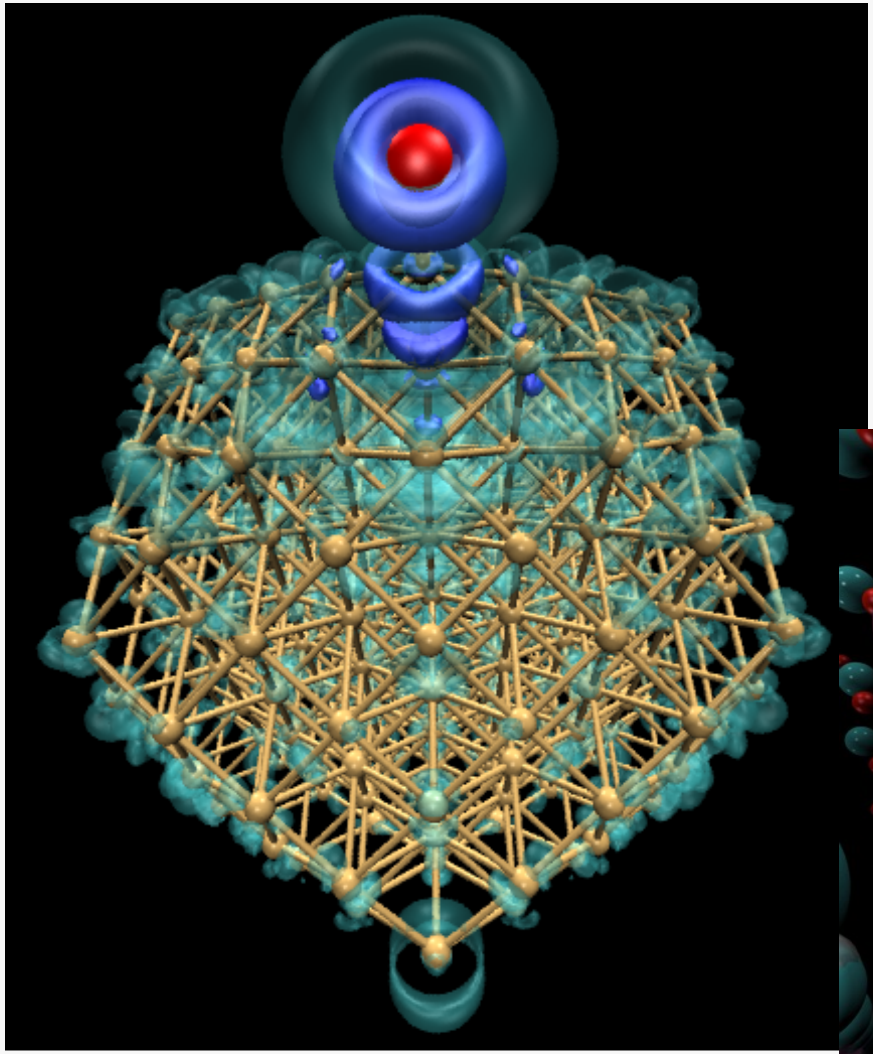
Data courtesy of: Mark Taylor, Sandia National Laboratory; Rob Jacob, Argonne National Laboratory; Warren Washington, National Center for Atmospheric Research



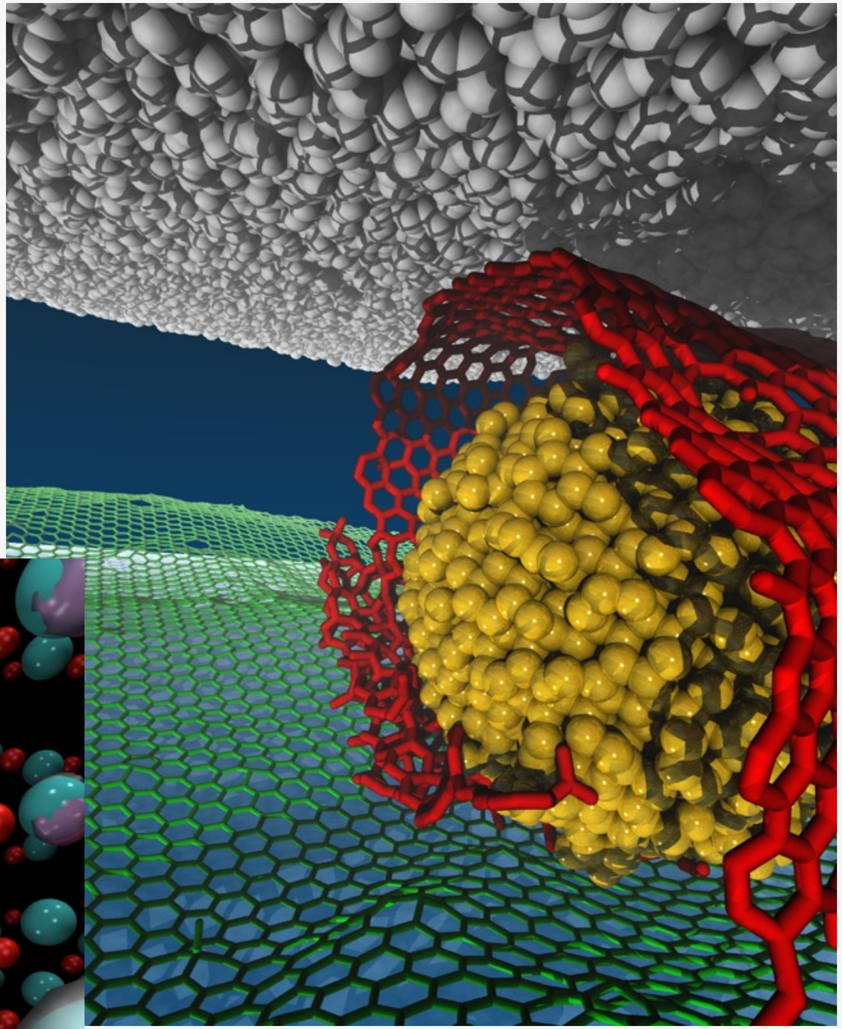


Data courtesy of: Anurag Gupta and Umesh Paliath, General Electric Global Research

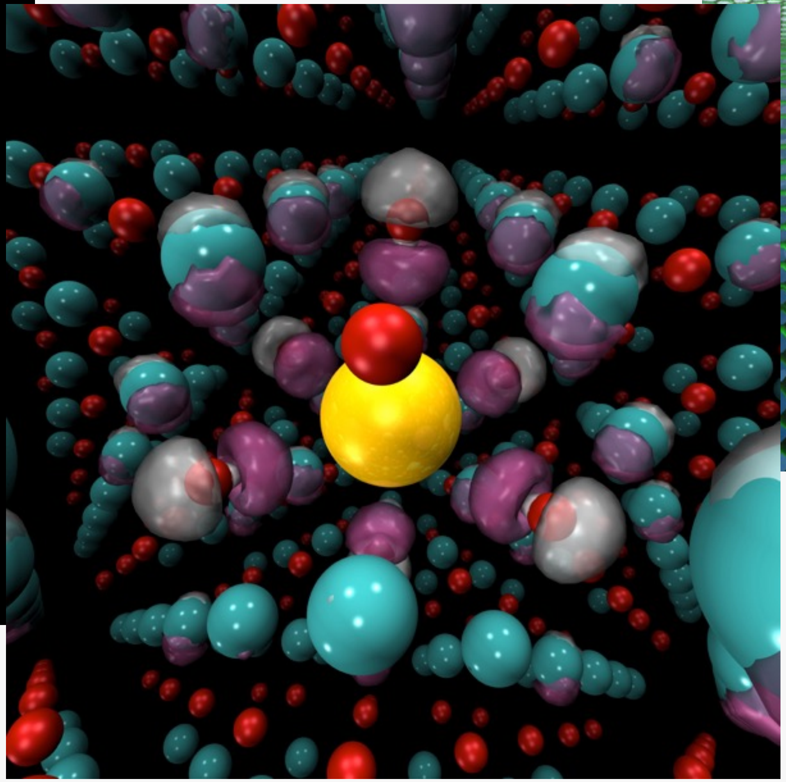
Materials Science / Molecular



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

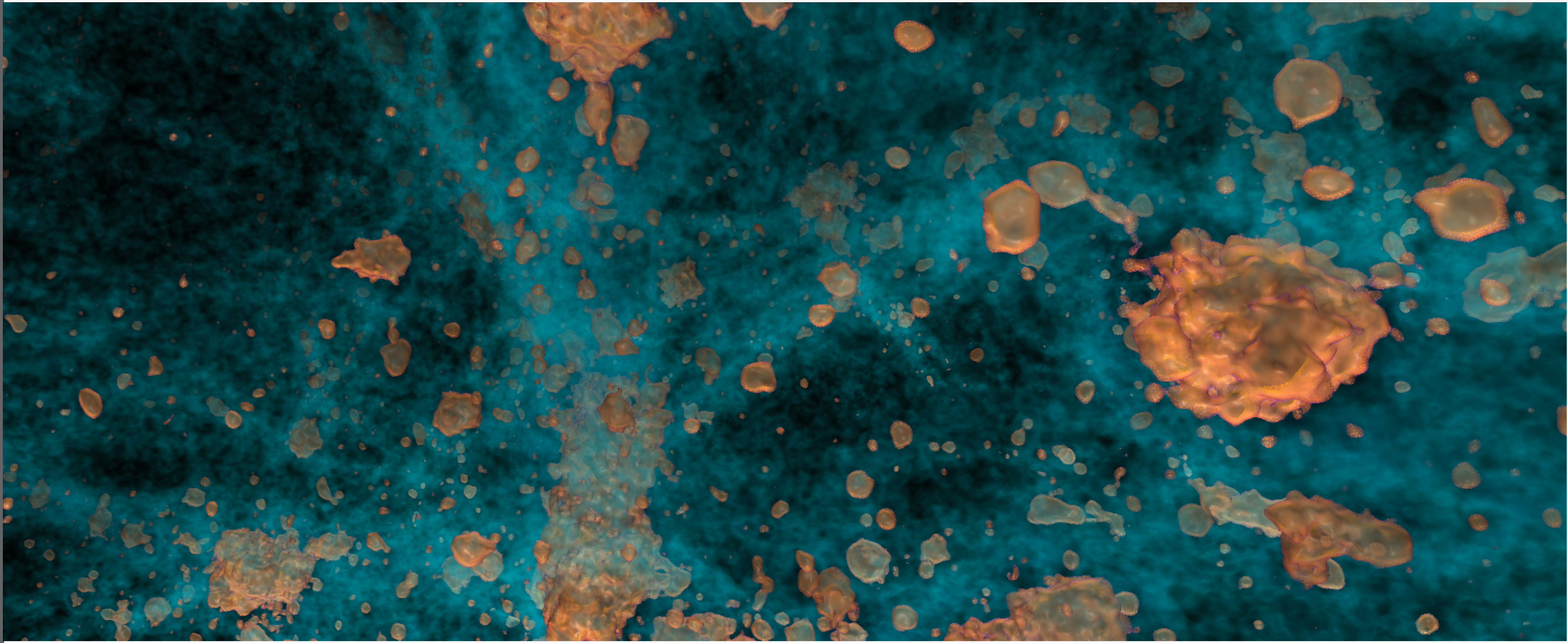


Data courtesy of: Subramanian Sankaranarayanan, Argonne National Laboratory



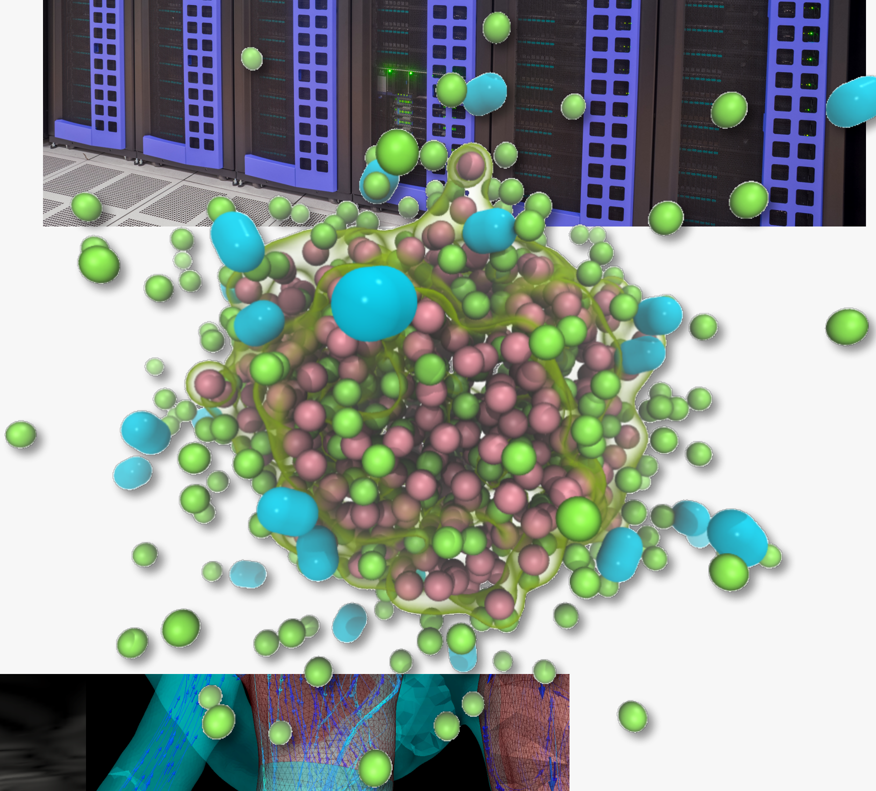
Data courtesy of: Paul Kent, Oak Ridge National Laboratory, Anouar Benali, Argonne National Laboratory

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

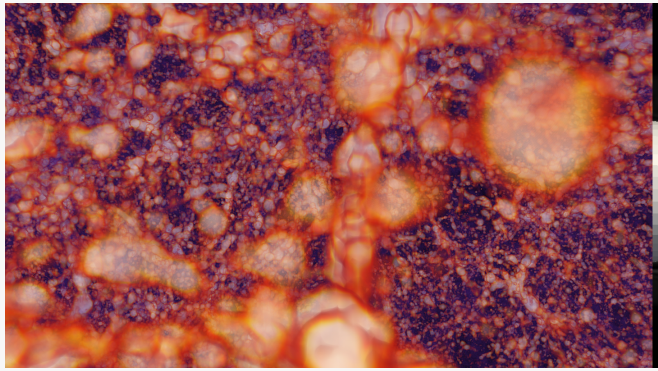
Aggregate RAM of 47 TB

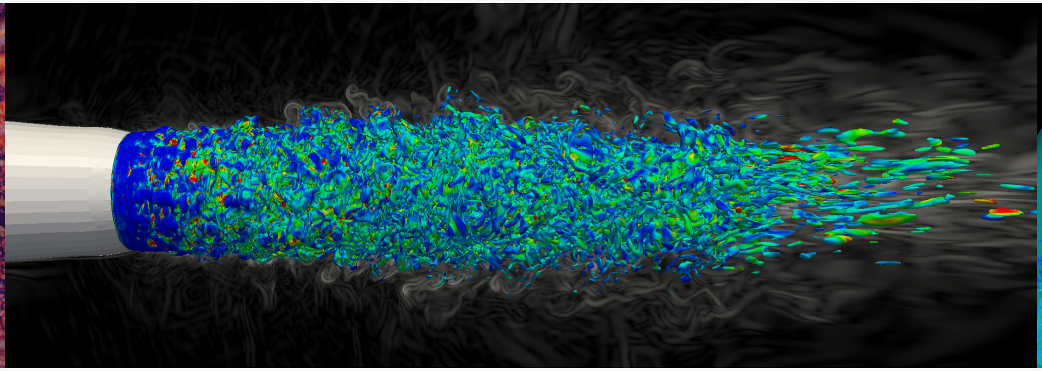
Aggregate GPU memory of ~3TB

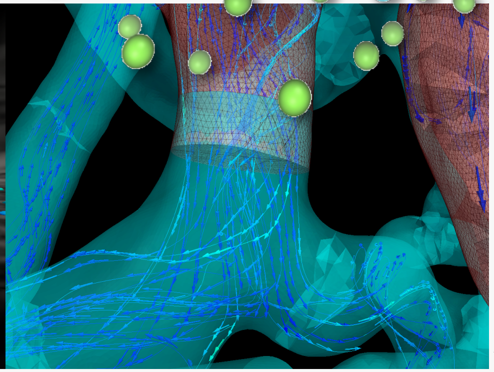
Cray CS System

216 port FDR IB switch with uplinks to our QDR infrastructure

Mounts the same 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

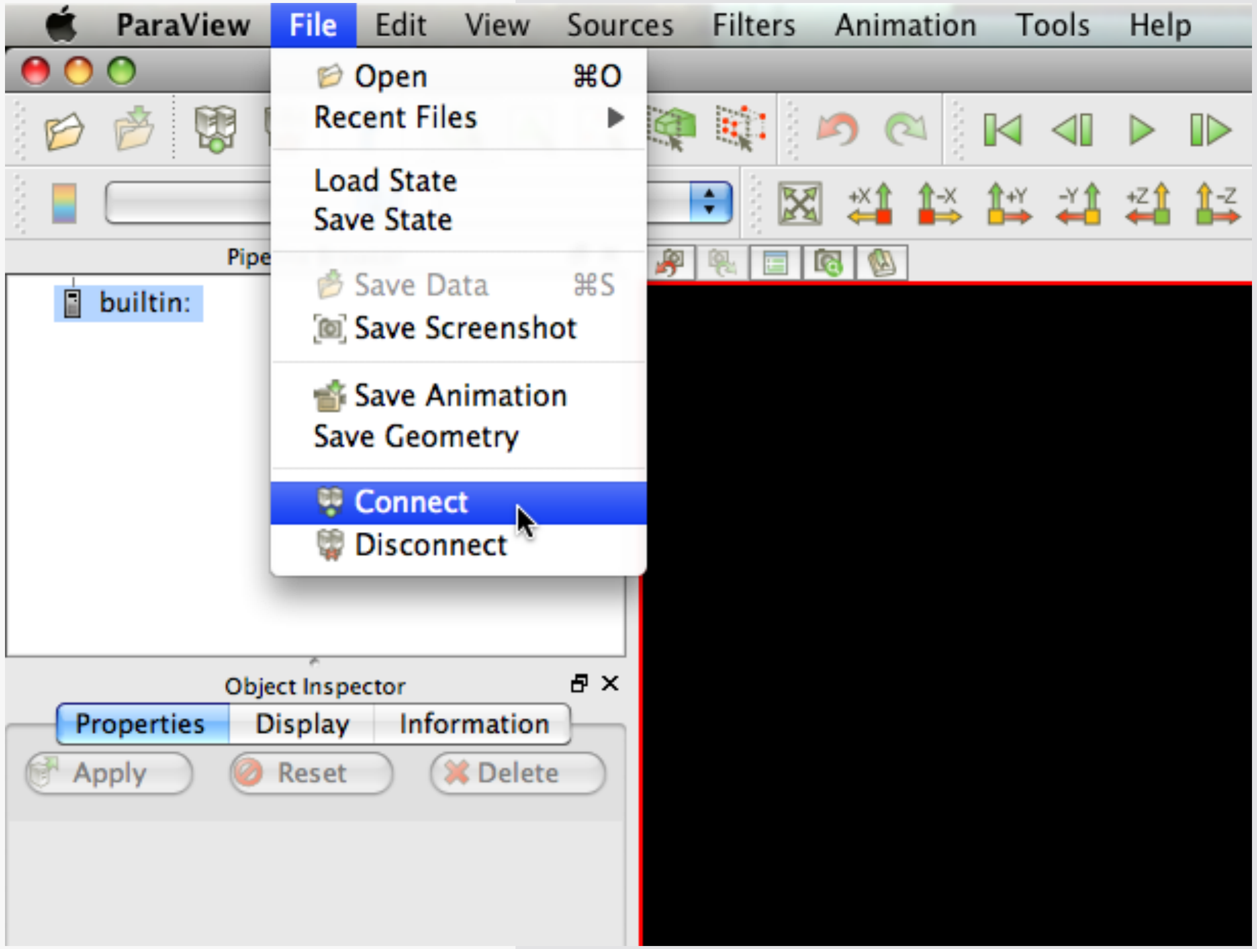
Tetrad
UNIC
VASP
ZeusMP
ANALYZE
BOV
GMV
Tecplot
Vis5D
Xmdv
XSF

ParaView on Theta

Version 5.5.2 (Client and Server versions must match)

After launching client locally

- Connect
- Fetch servers (first time only)
- Fetch Theta configuration
- Connect
- Configure server settings
- Connecting: Enter Password
- Open File



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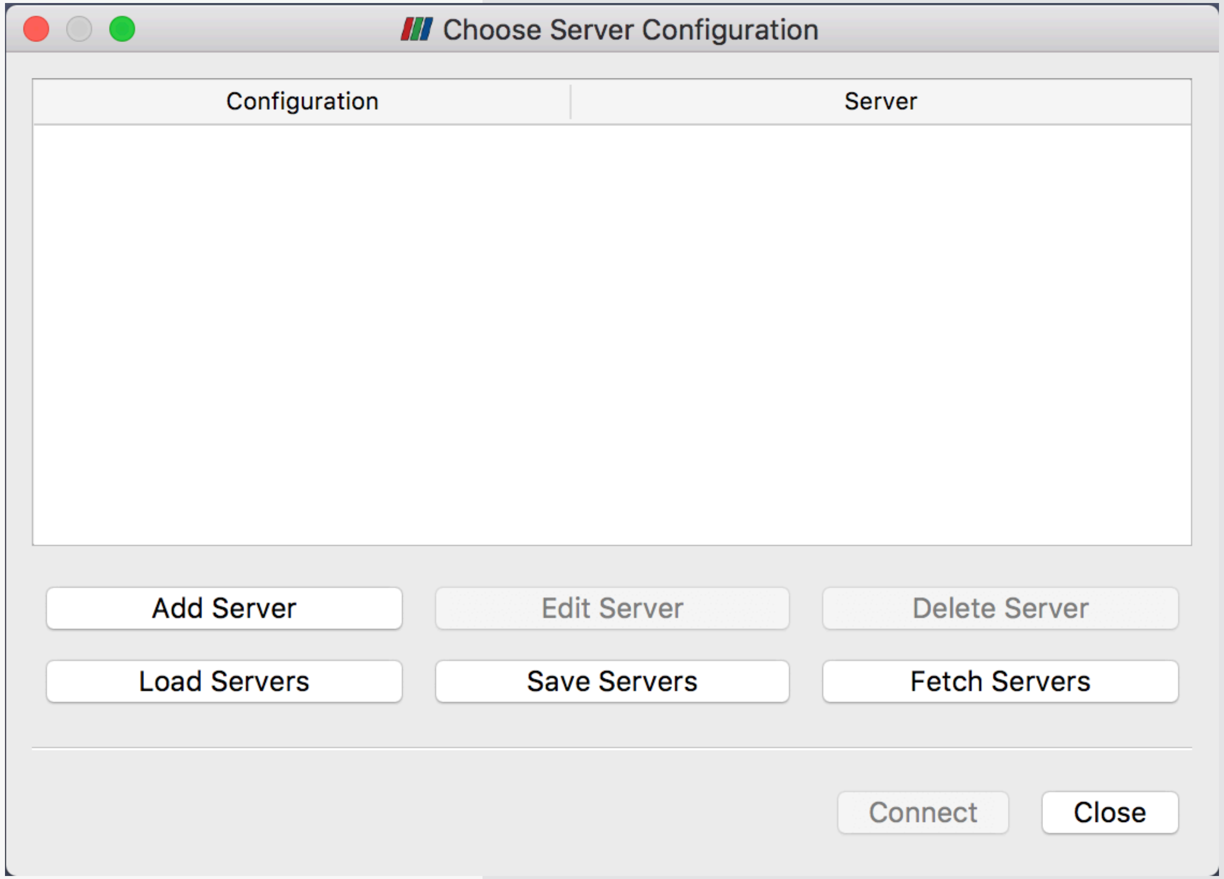

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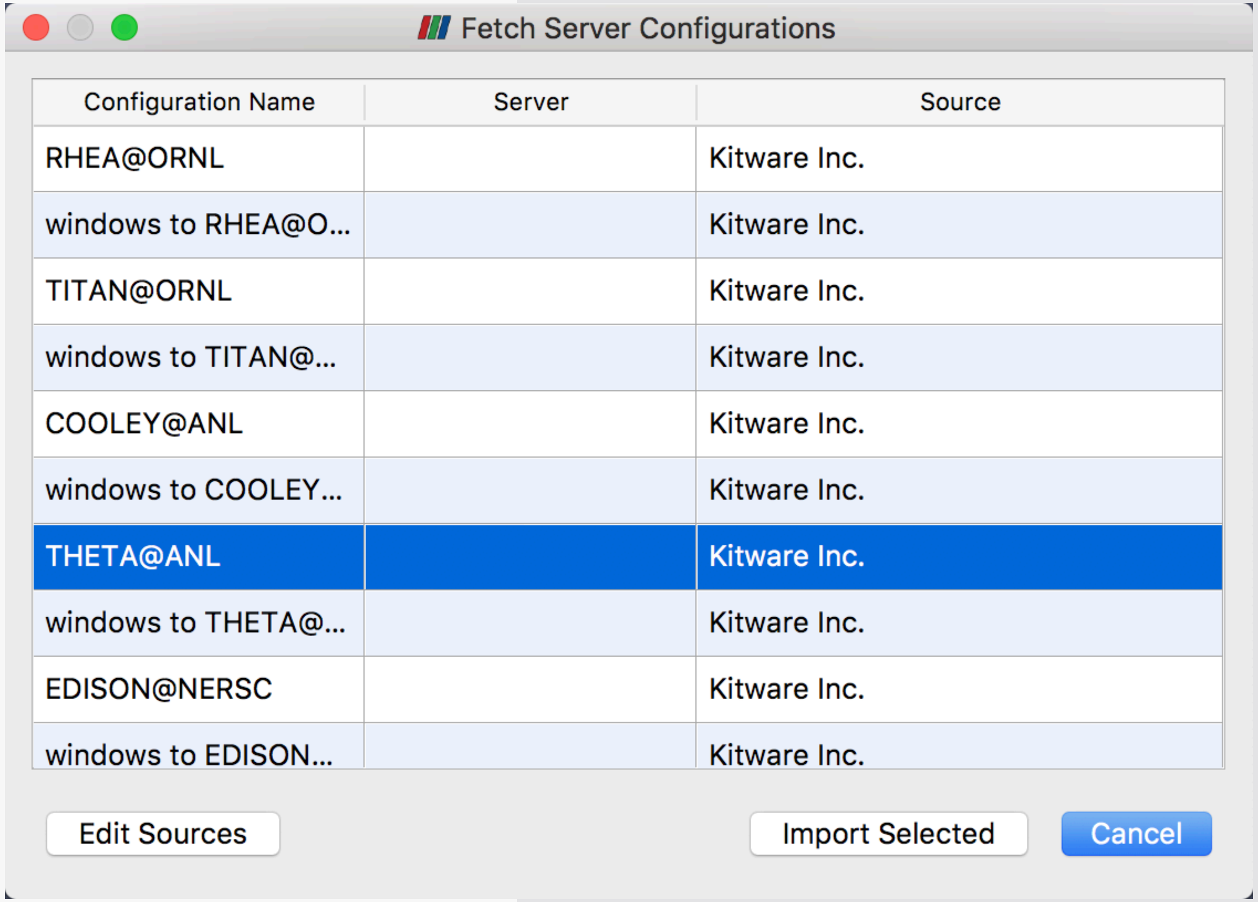

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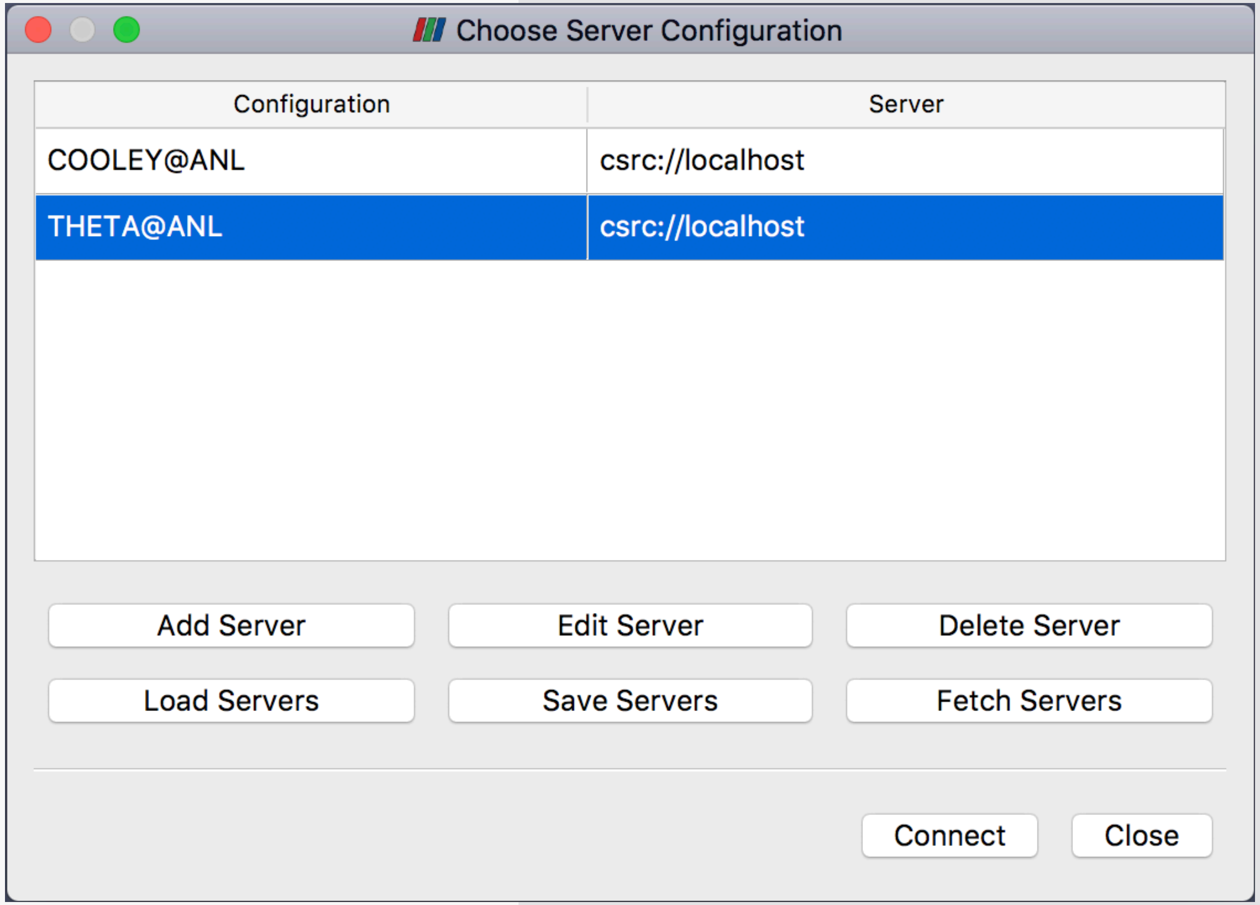

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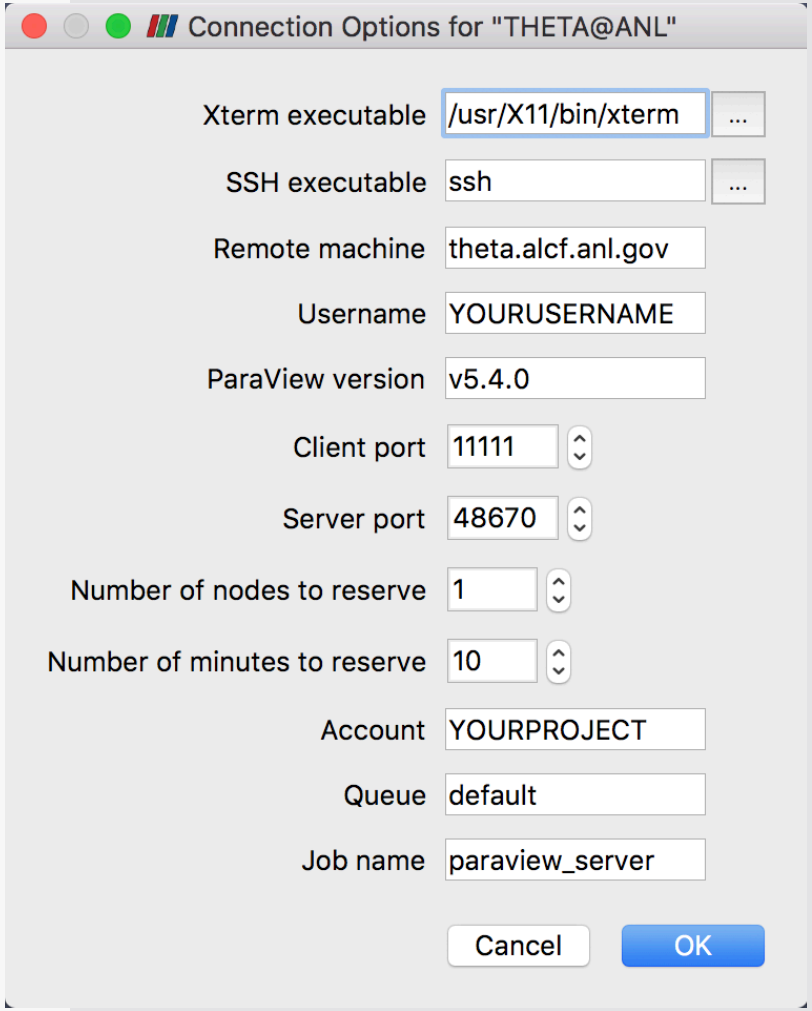

ParaView on Theta

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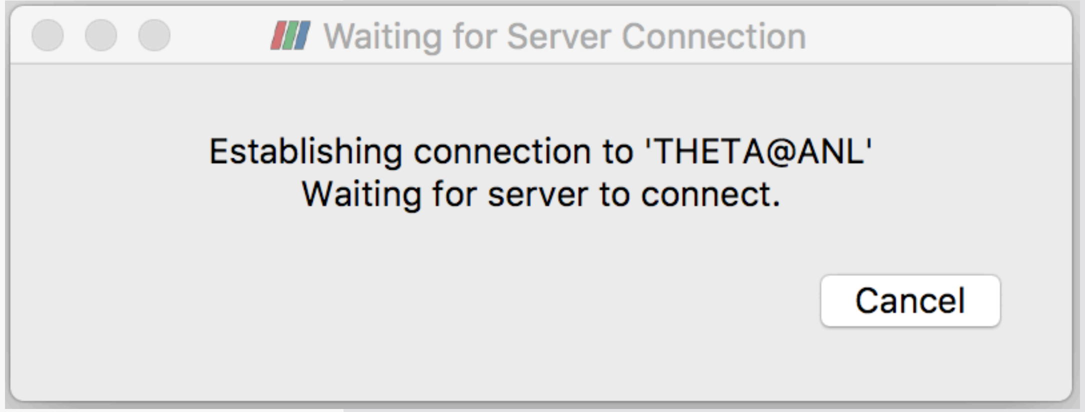
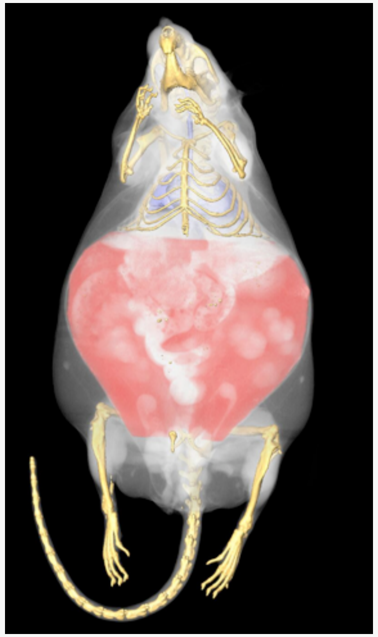
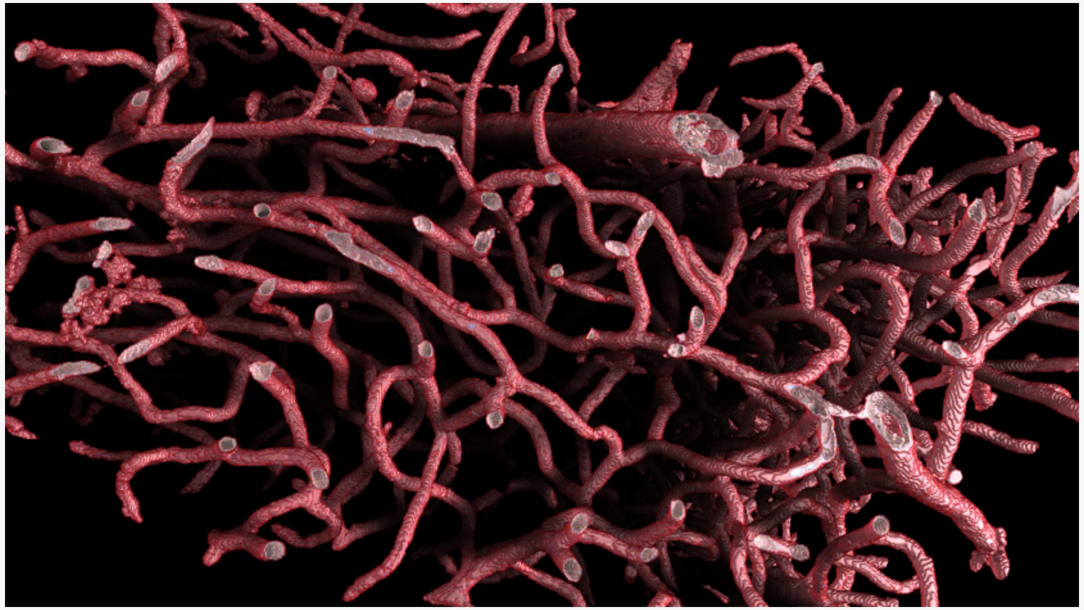
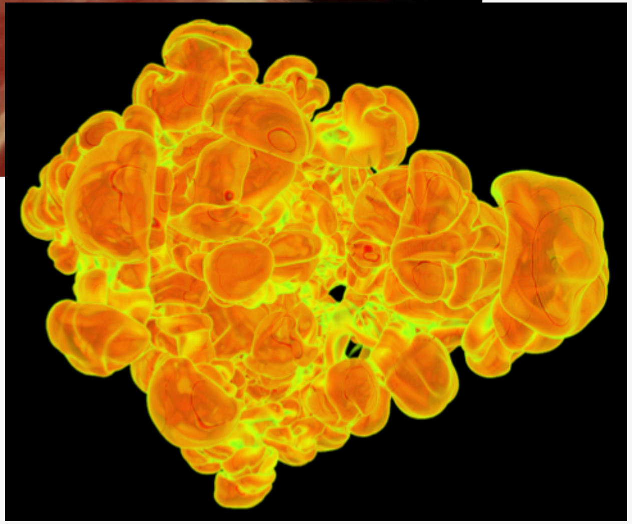


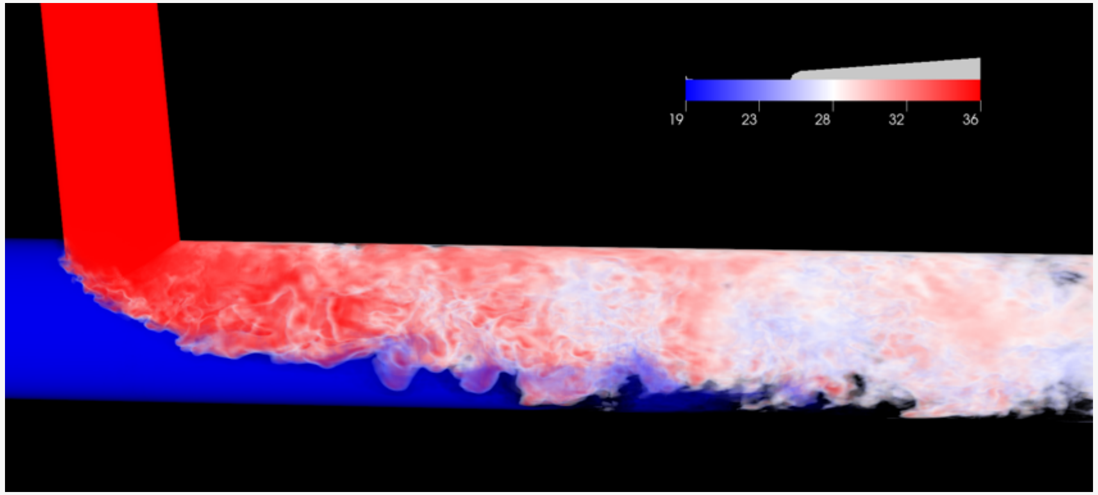
Data Representations

Data Representations: Volume Rendering









Data Representations: Glyphs

2D or 3D geometric object to represent point data

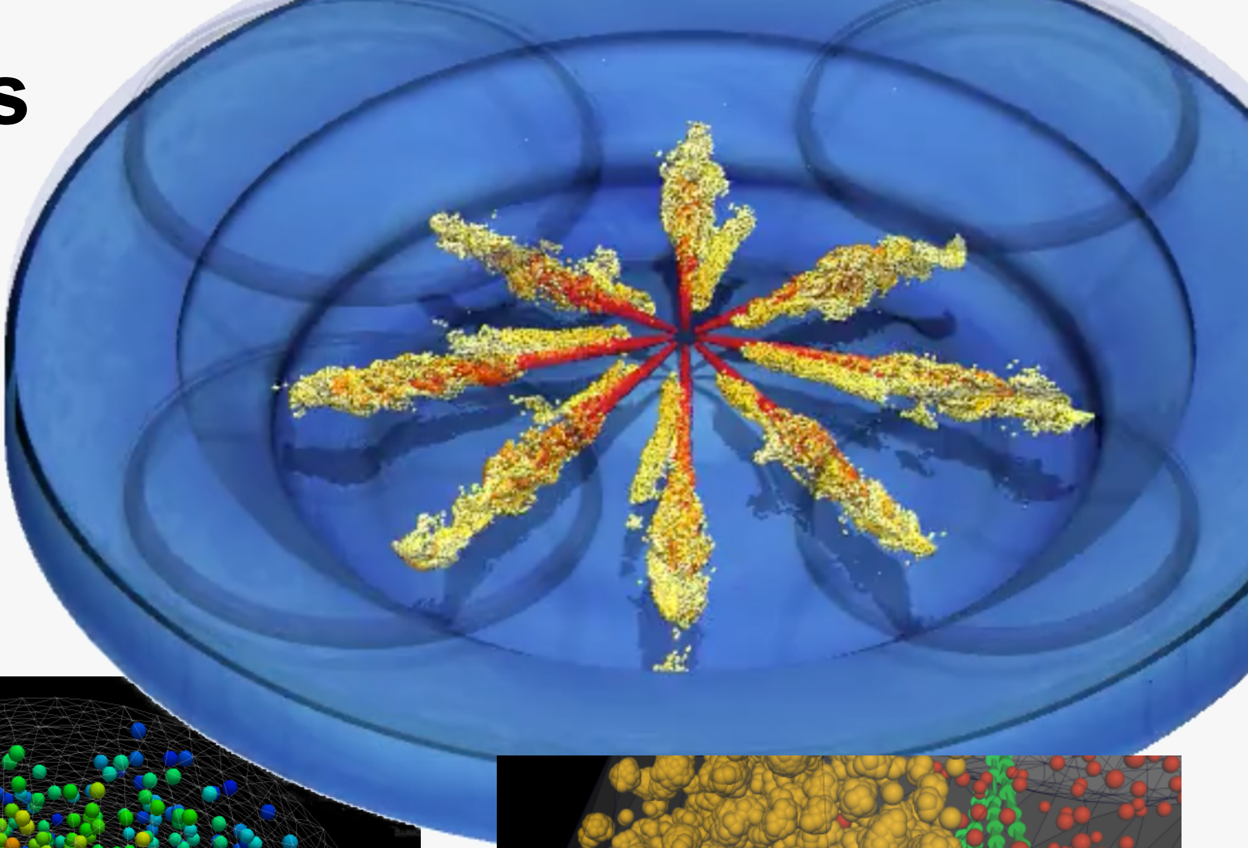
Location dictated by coordinate

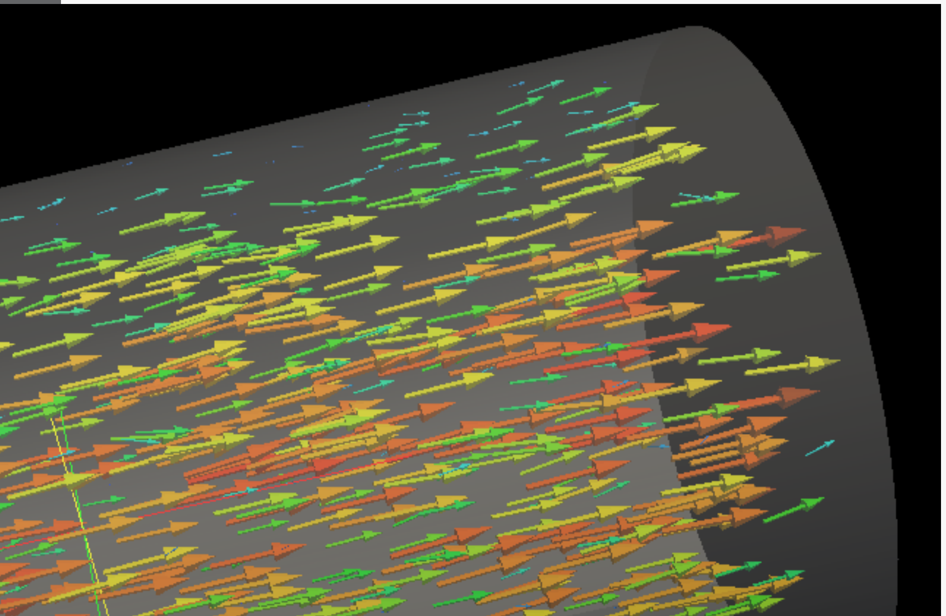
– 3D location on mesh

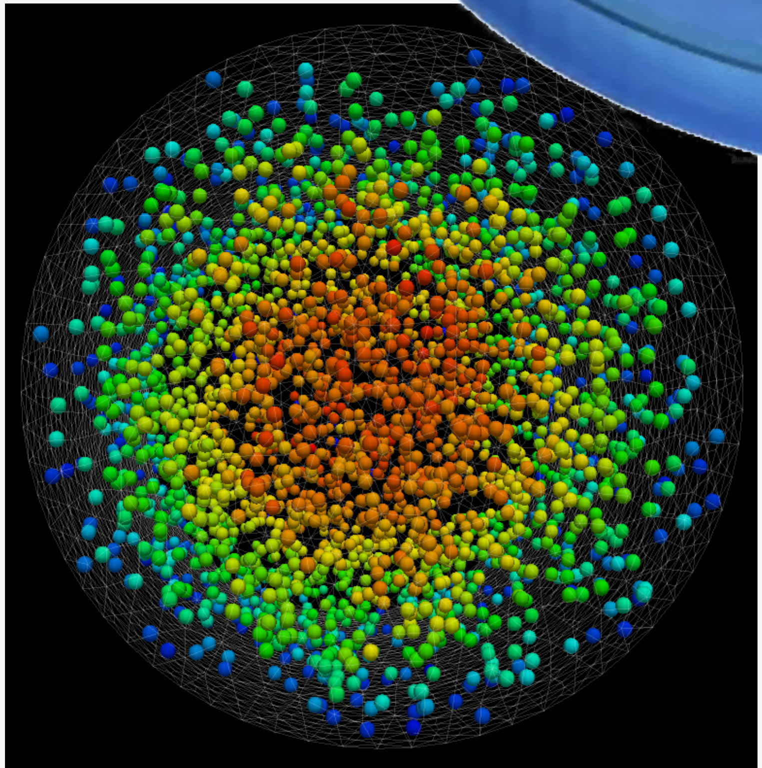
– 2D position in table/graph

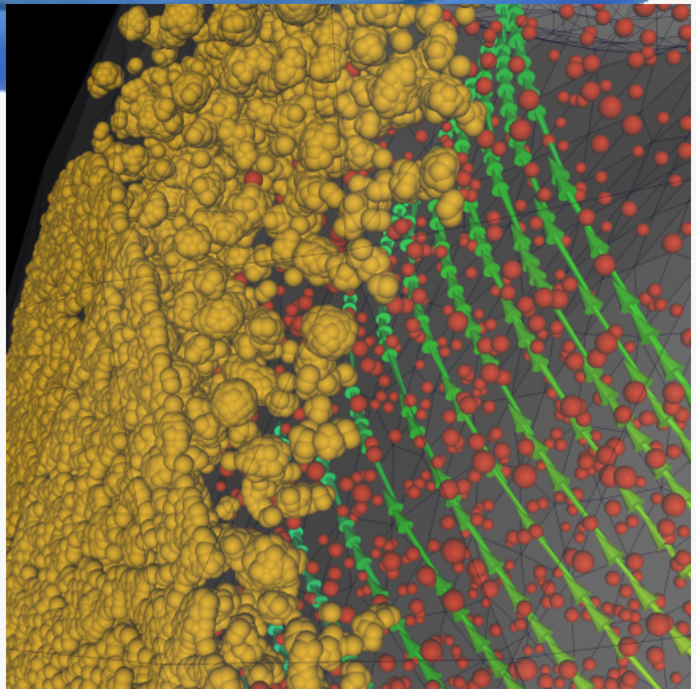
Attributes of graphical entity dictated by attributes of data

– color, size, orientation









Data Representations: Contours (Isosurfaces)

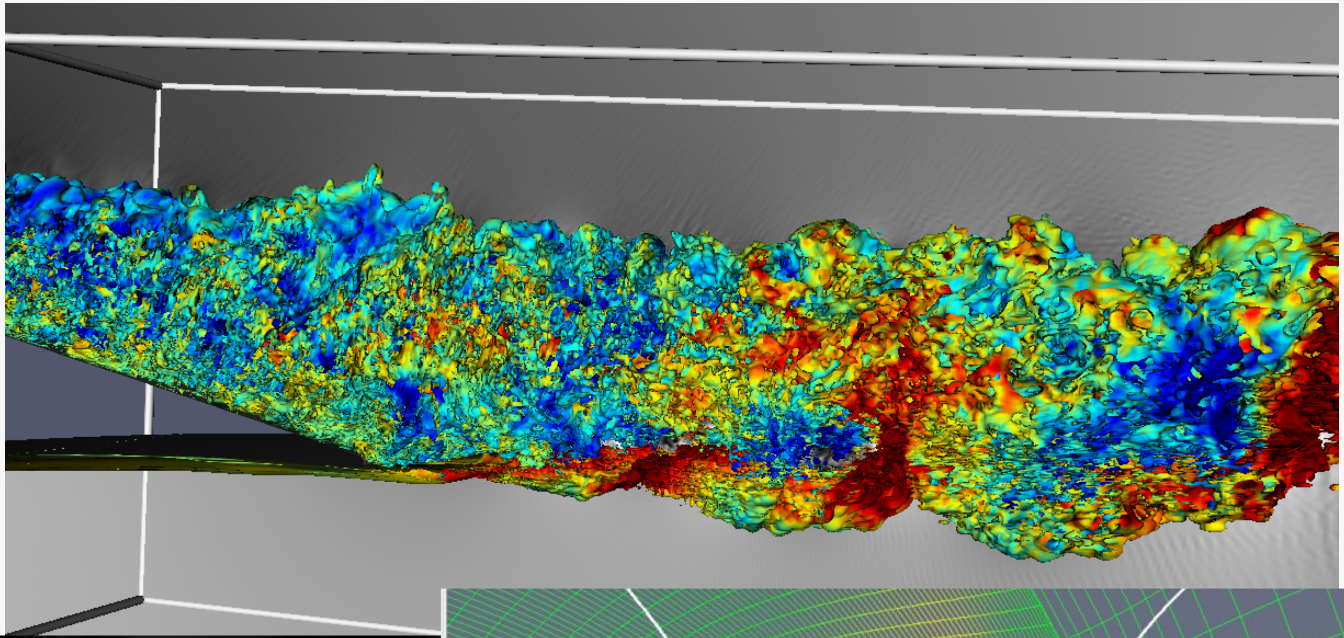
A Line (2D) or Surface (3D), representing a constant value

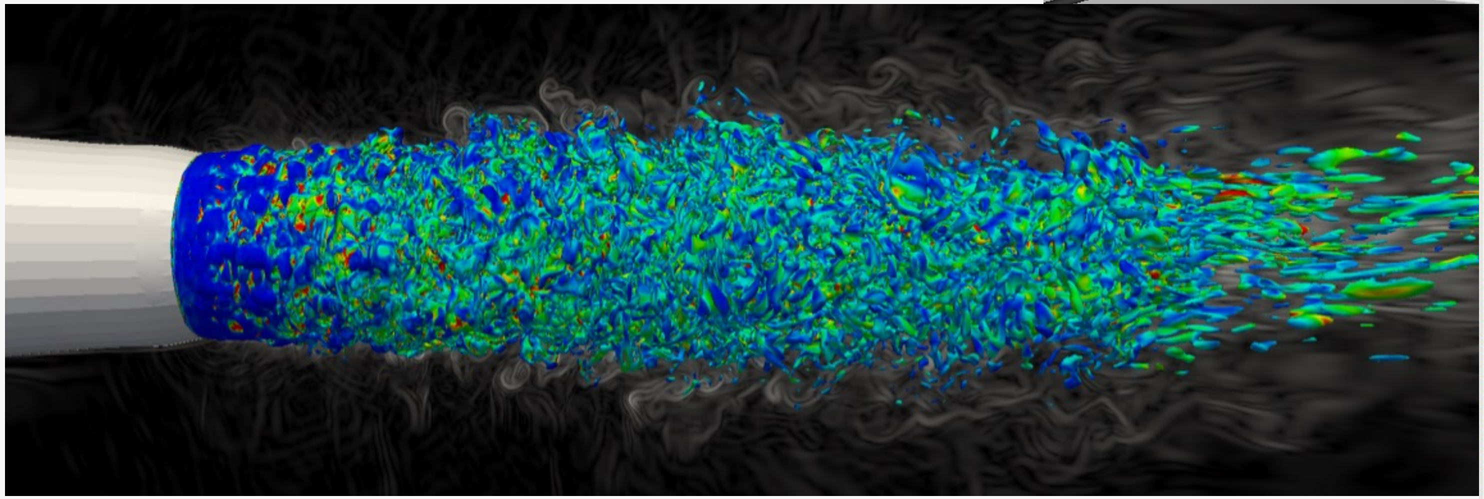
VisIt & ParaView:

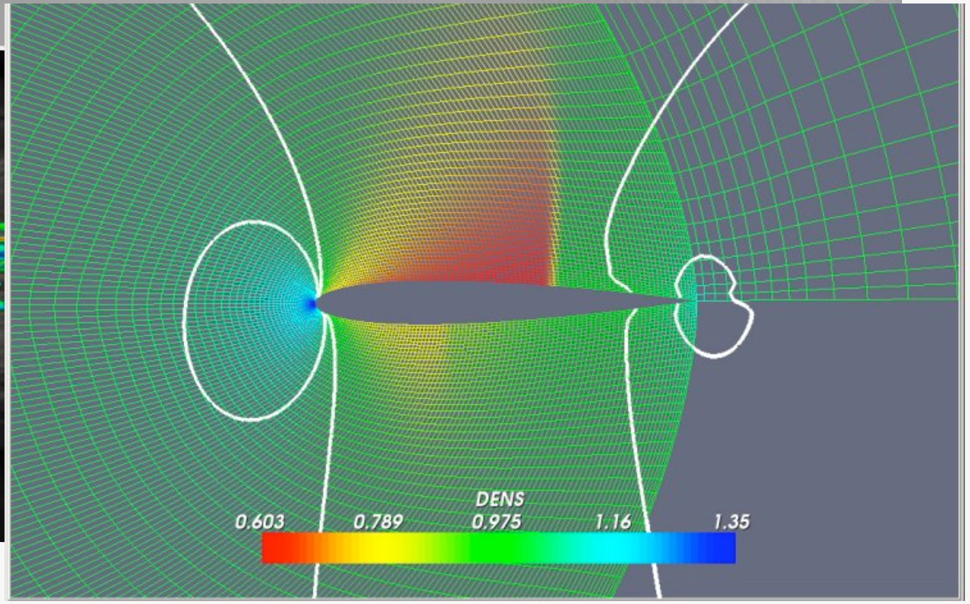
– good at this

vtk:

– same, but again requires more effort







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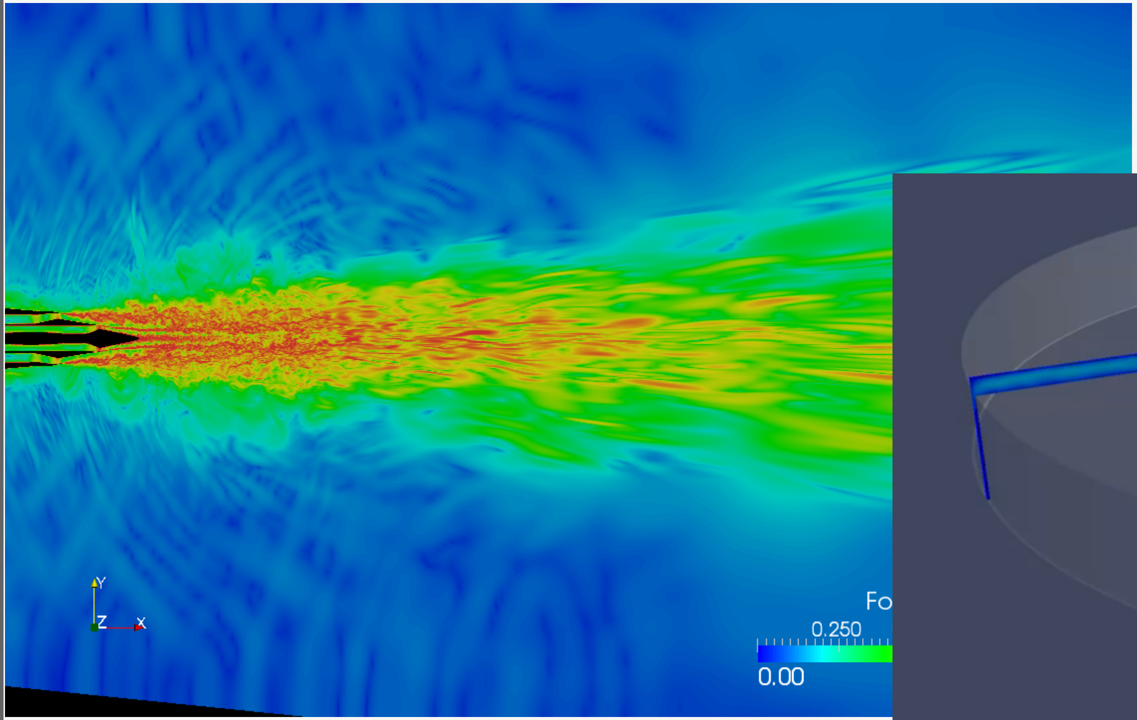
Data Representations: Cutting Planes

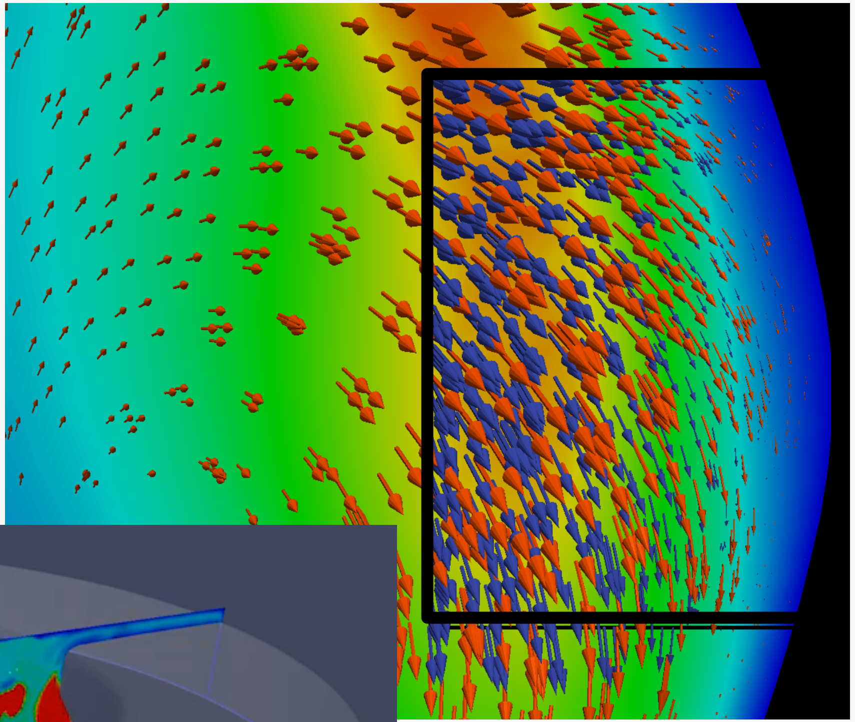
Slice a plane through the data

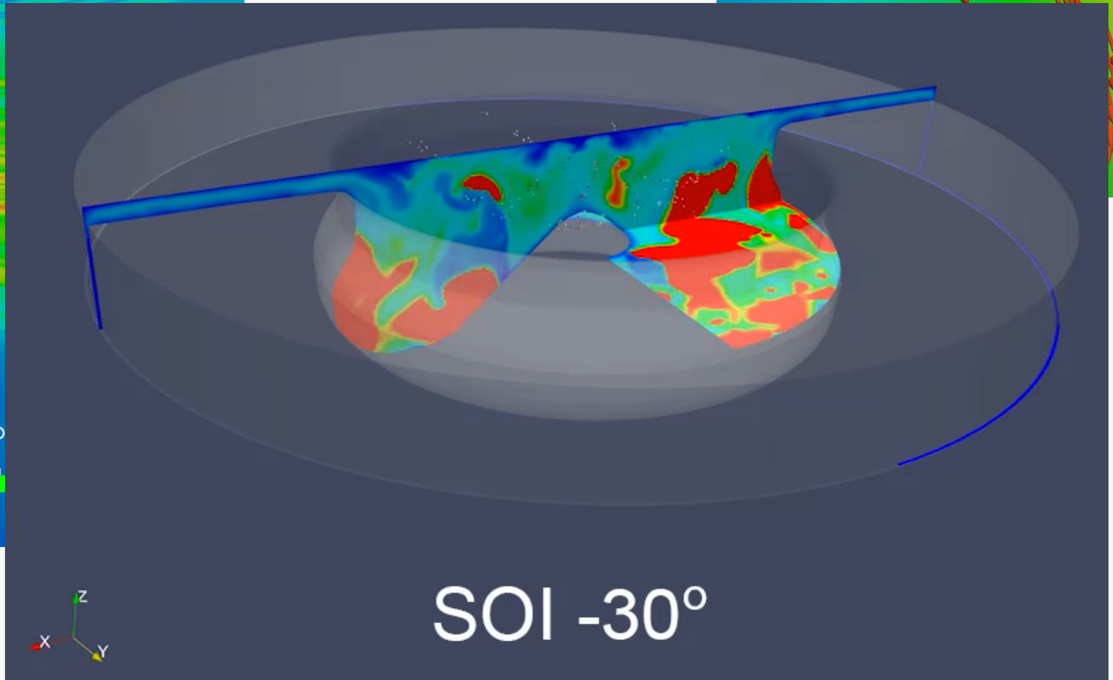
– Can apply additional visualization methods to resulting plane

VisIt & ParaView & vtk good at this

VMD has similar capabilities for some data formats





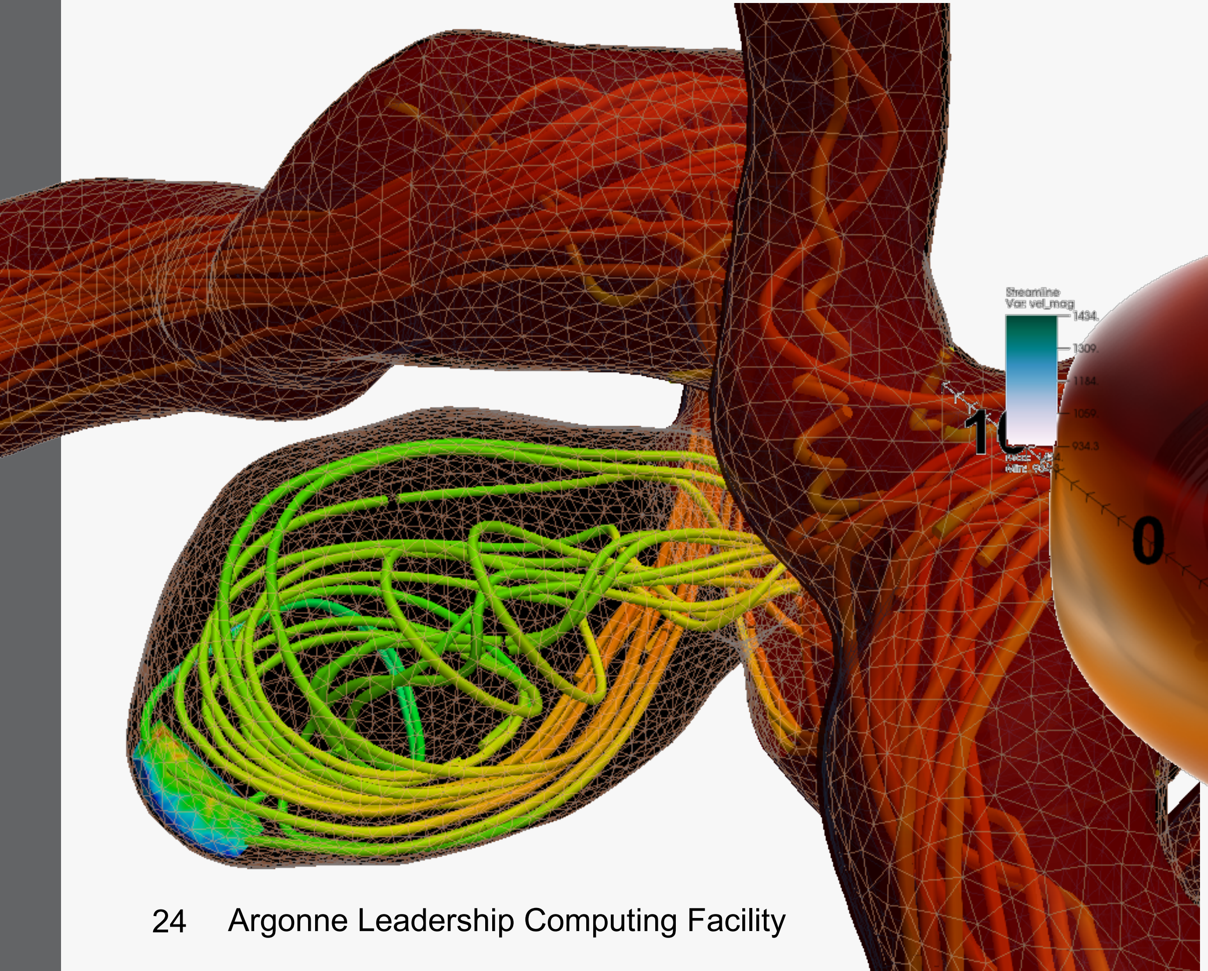


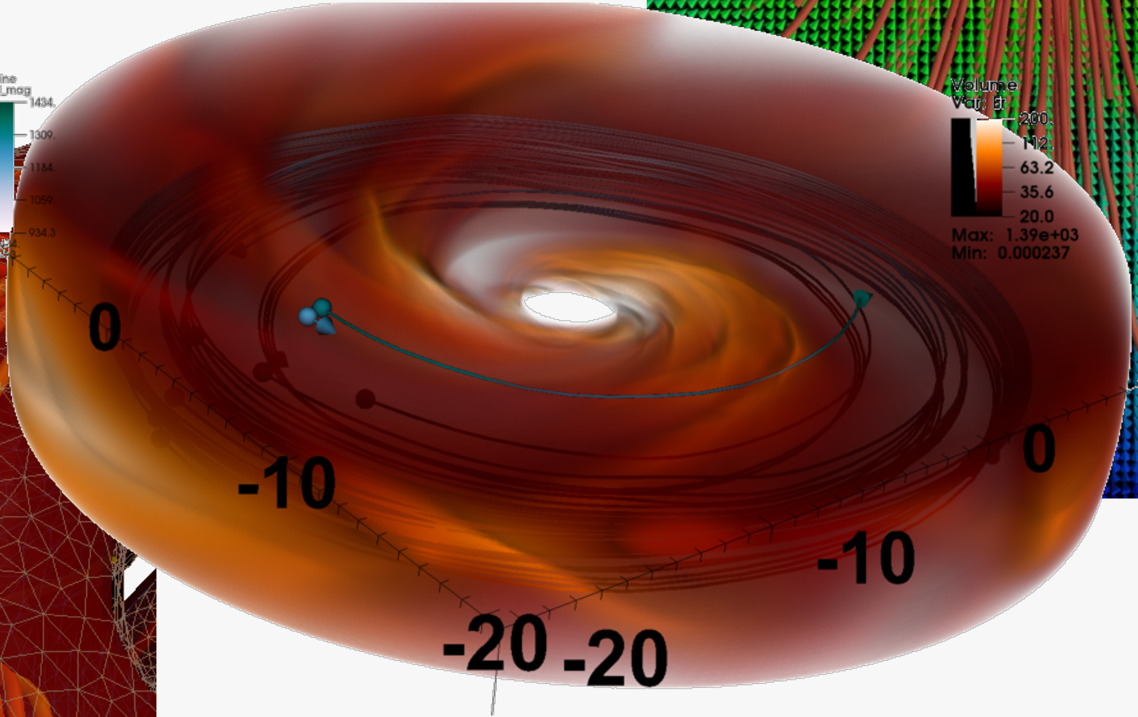
Data Representations: Streamlines

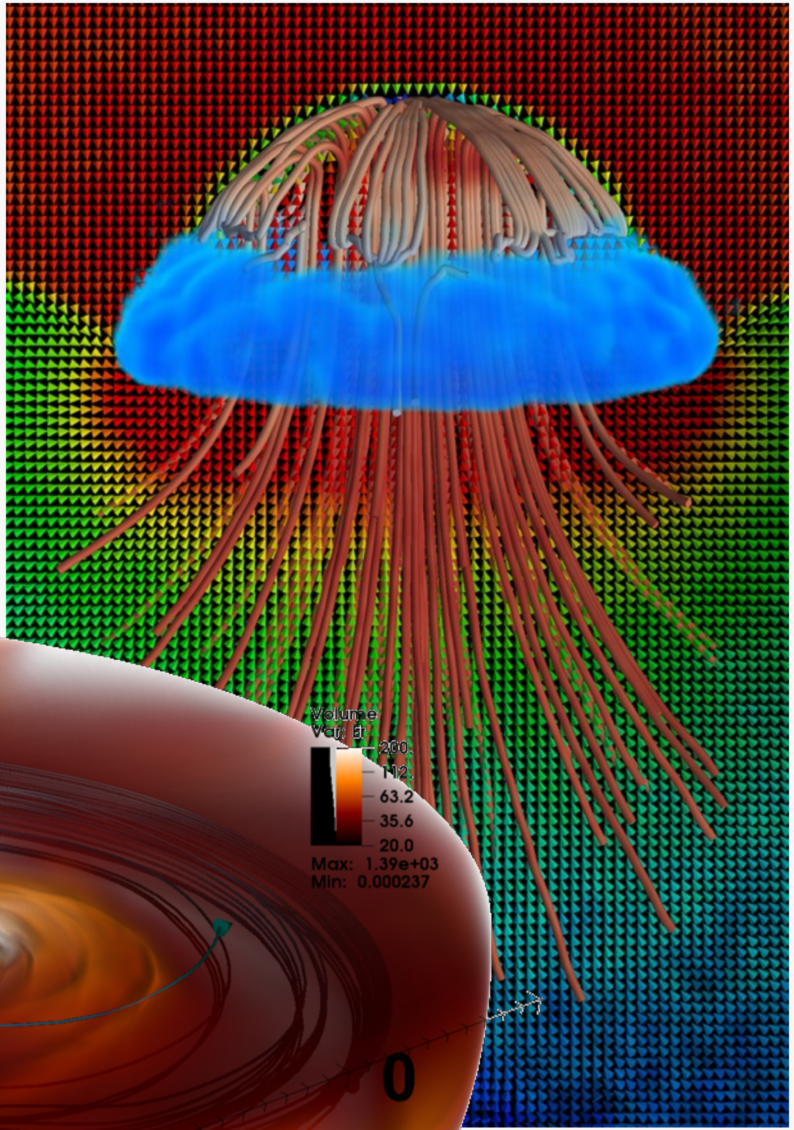
From vector field on a mesh (needs connectivity)

– 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:

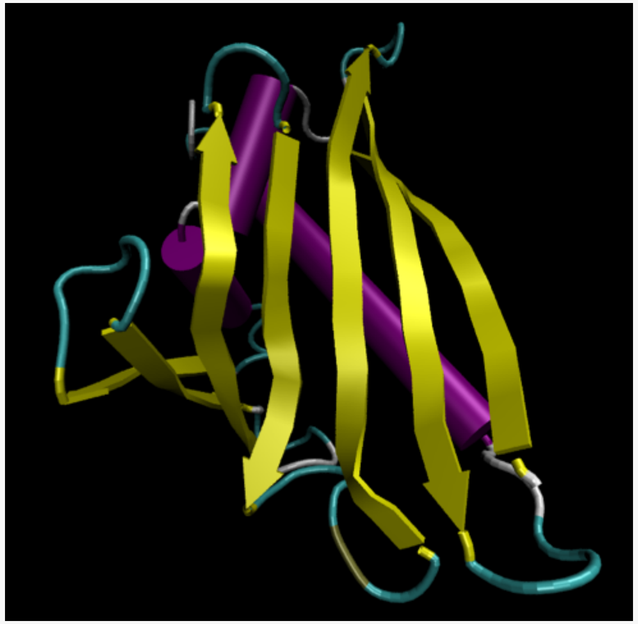
- Lots of domain-specific representations
- Many different file formats
- Animation
- Scriptable

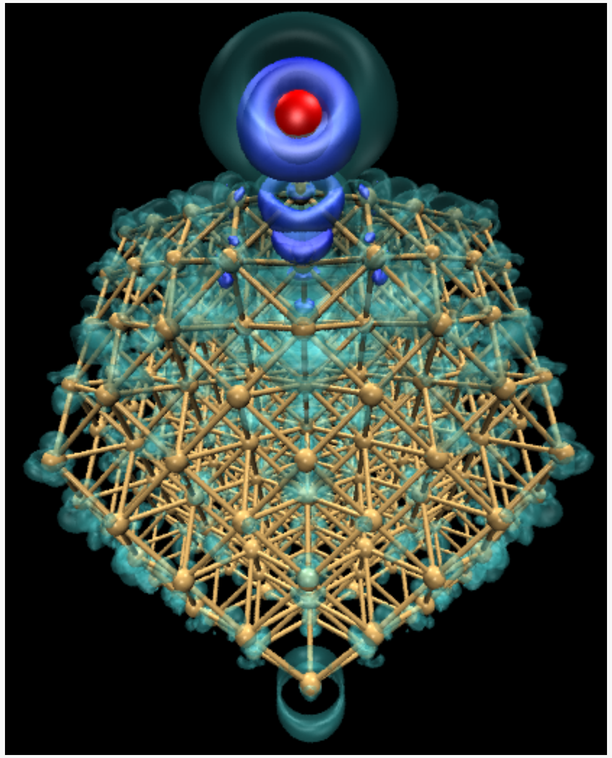
VisIt & ParaView:

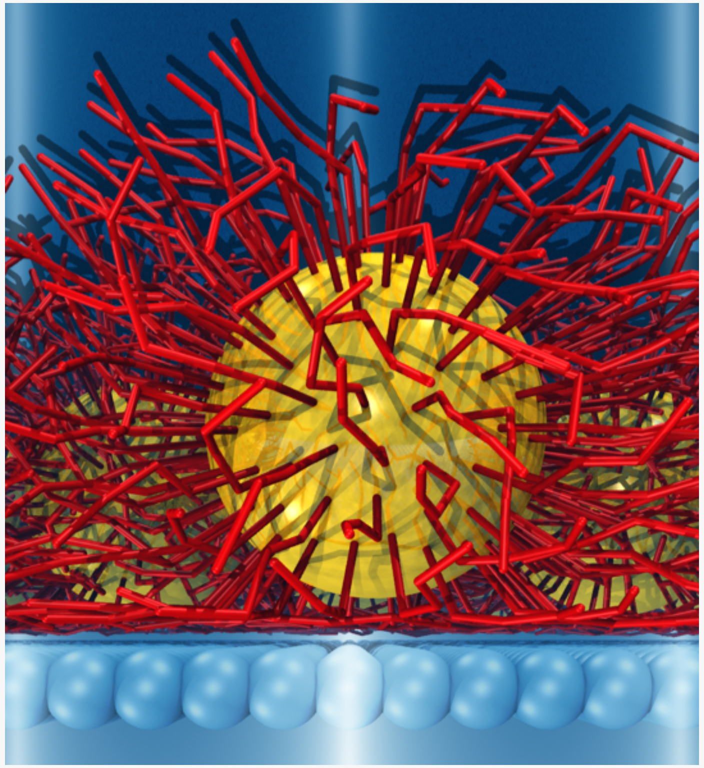
- Limited support for these types of representations, but improving

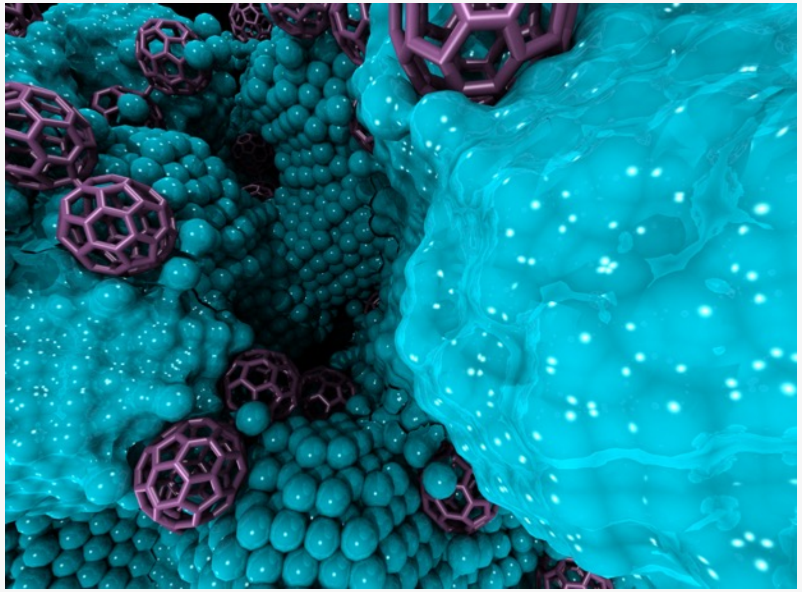
VTK:

- Anything's possible if you try hard enough



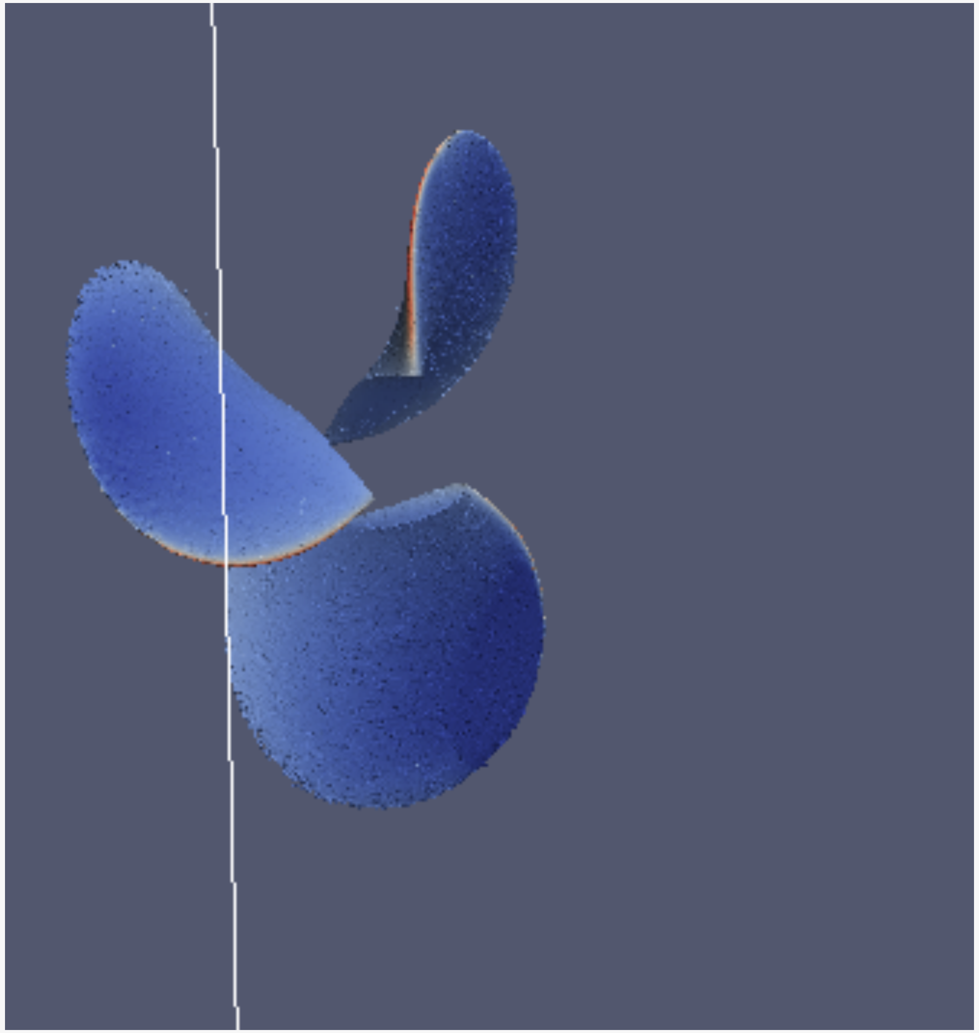






Visualization for Debugging

Visualization for Debugging



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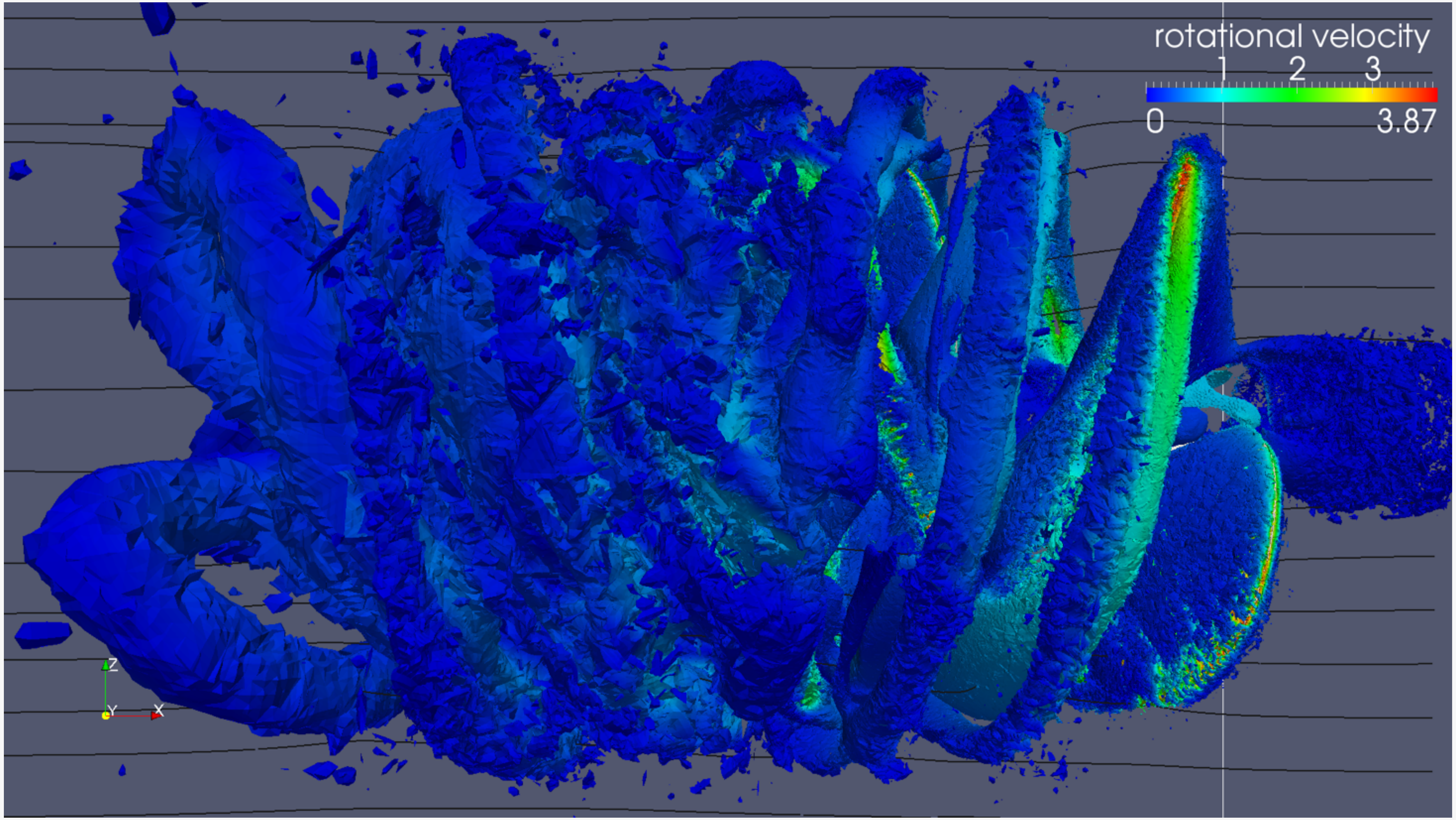
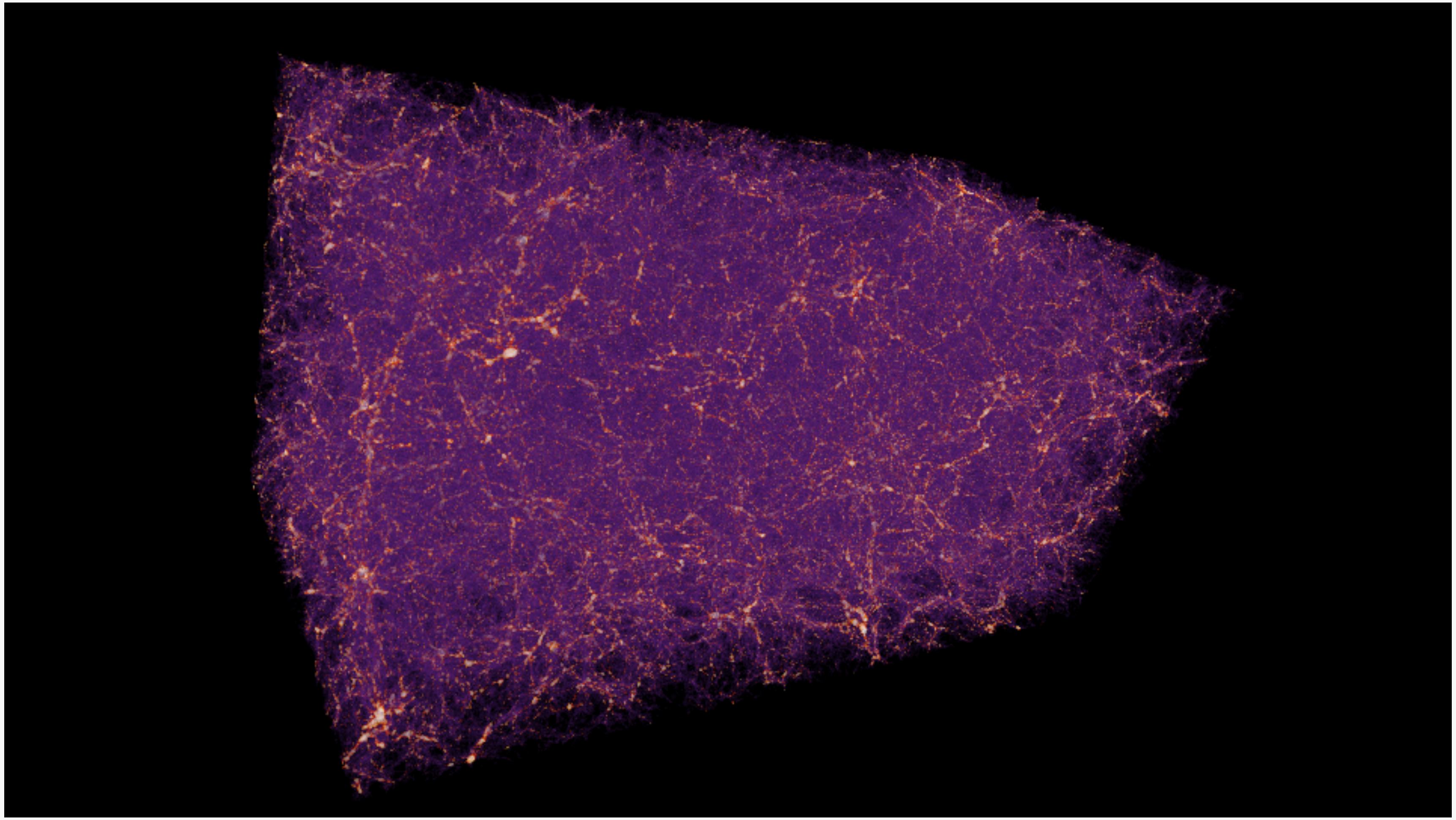


Visualization as Diagnostics: Color by Thread ID



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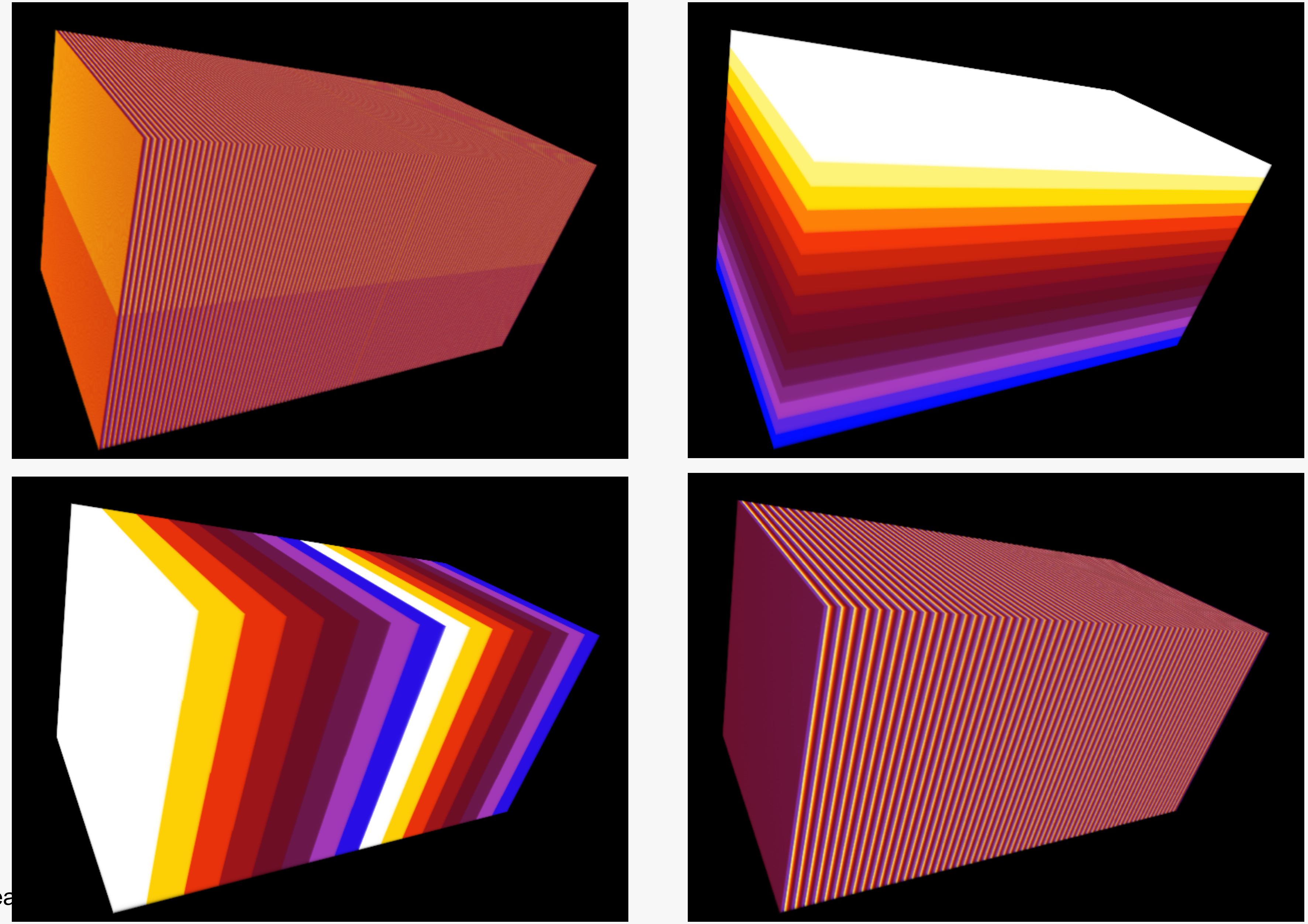


In Situ Visualization and Analysis

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

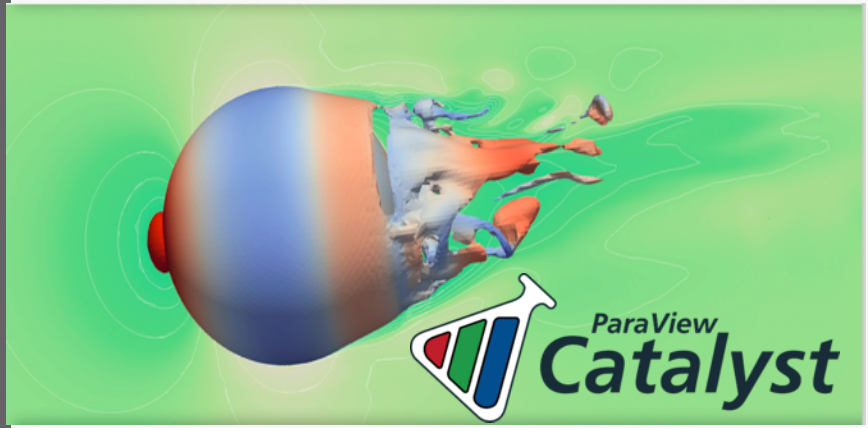
– will make full-resolution, I/O-intensive post hoc analysis prohibitively expensive, if not impossible.

Slides courtesy SENSEI in situ project:

www.sensei-insitu.org

SENSEI
in situ

Multiple in-situ infrastructures



LibSim

ADIOS

Can We….

Enable use of any in situ framework?

Develop analysis routines that are portable between codes?

Make it easy to use?

OUR APPROACH

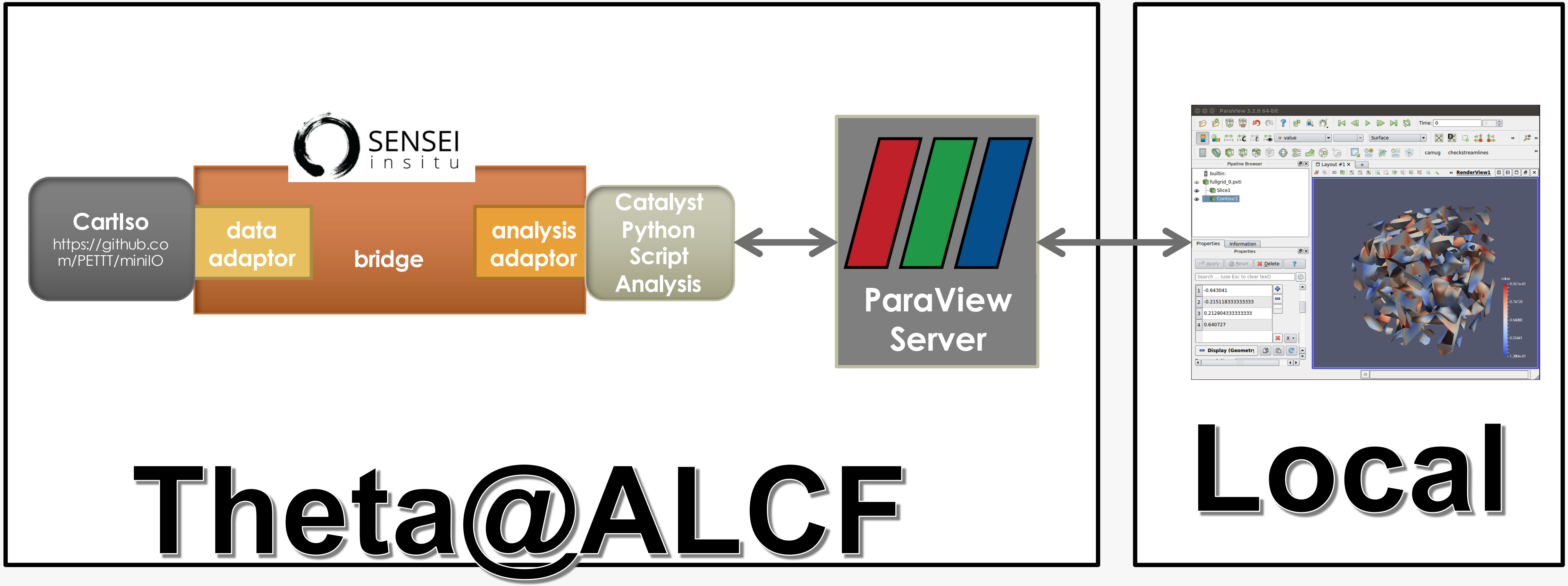
Data model – to pass data between Simulation & Analysis

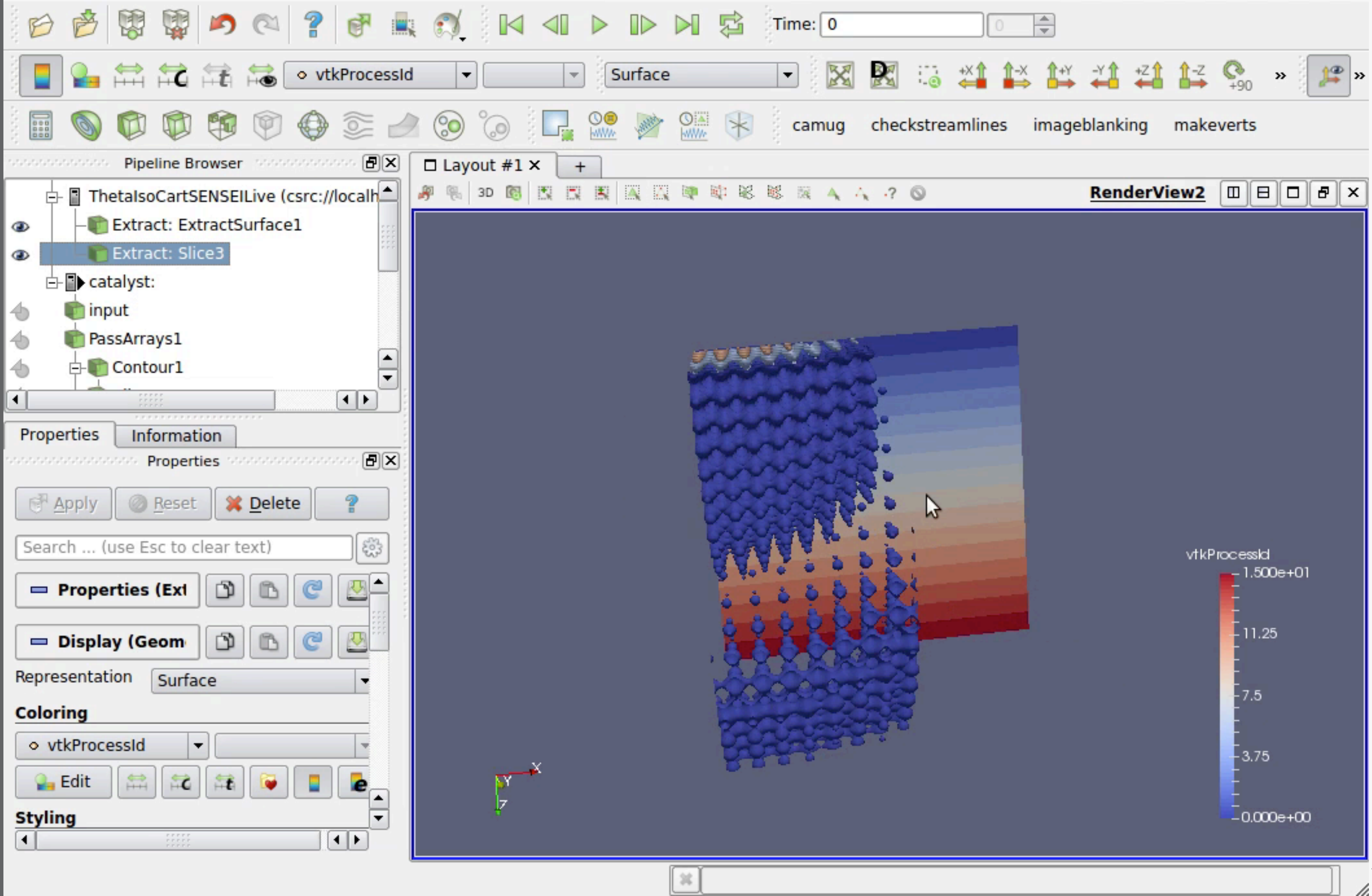
API – for instrumenting simulation and analysis codes

SENSEI

in situ

Miniapp instrumentation with SENSEI





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Instrumenting Applications

- Write Bridge and Data Adaptor code
  - Recommended to use SENSEI miniapp examples as starting point

- Three minor modifications in application code:
  1. Call Bridge Init() method after initializing MPI and pass MPI communicator
  2. Call Bridge Execute() method after computing every timestep
  3. Call Bridge Finalize() method before MPI finalize

- Write an XML file for SENSEI generic analysis adaptor …
  - All the currently supported analysis backends can be enabled using this method

- … or write your own analysis adaptor

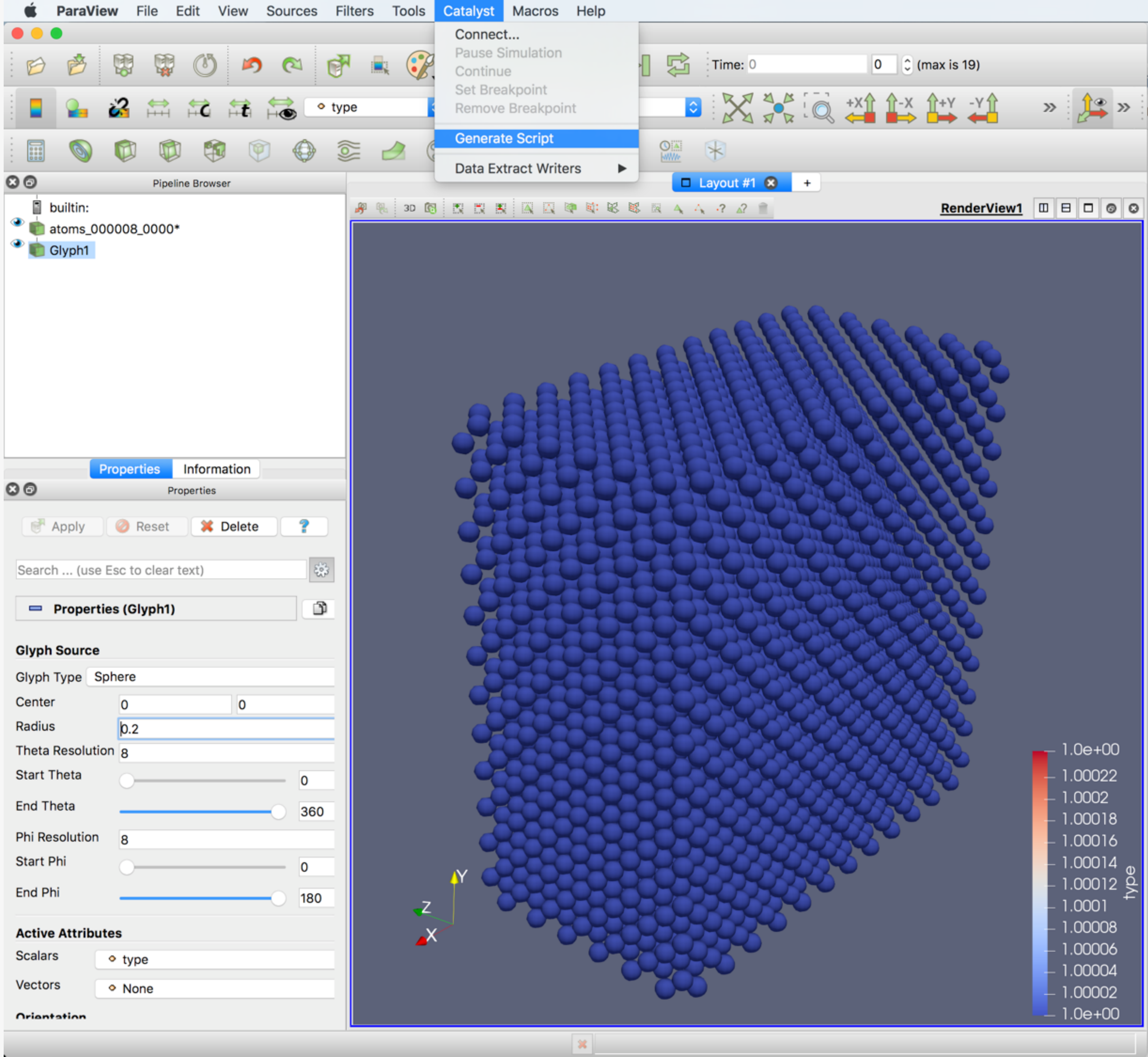
Using the configurable analysis adaptor

- Enable analysis in .xml file
- Run instrumented simulation

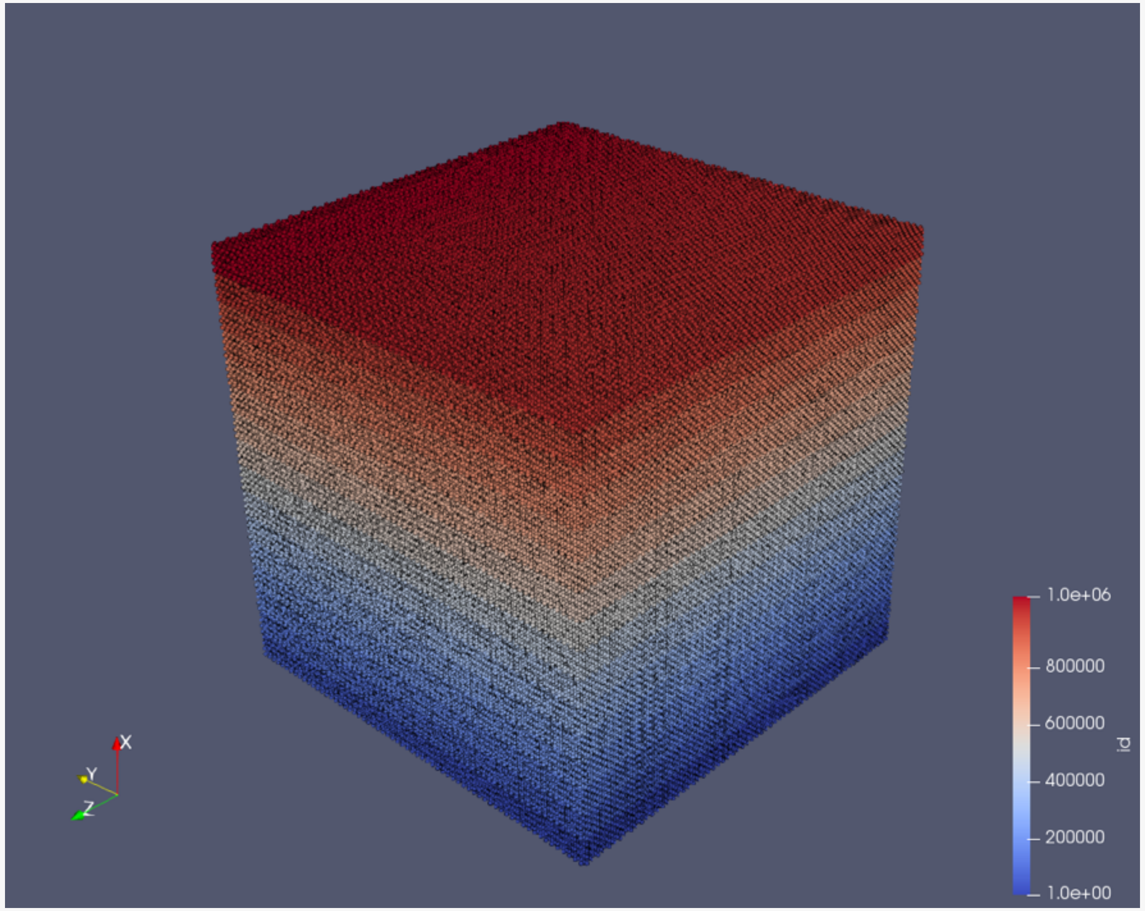
```xml
<sensei>
  <!-- Custom Analyses -->
  <analysis type="histogram" mesh="atoms" array="type" association="point"
    bins="10" enabled="0" />

  <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



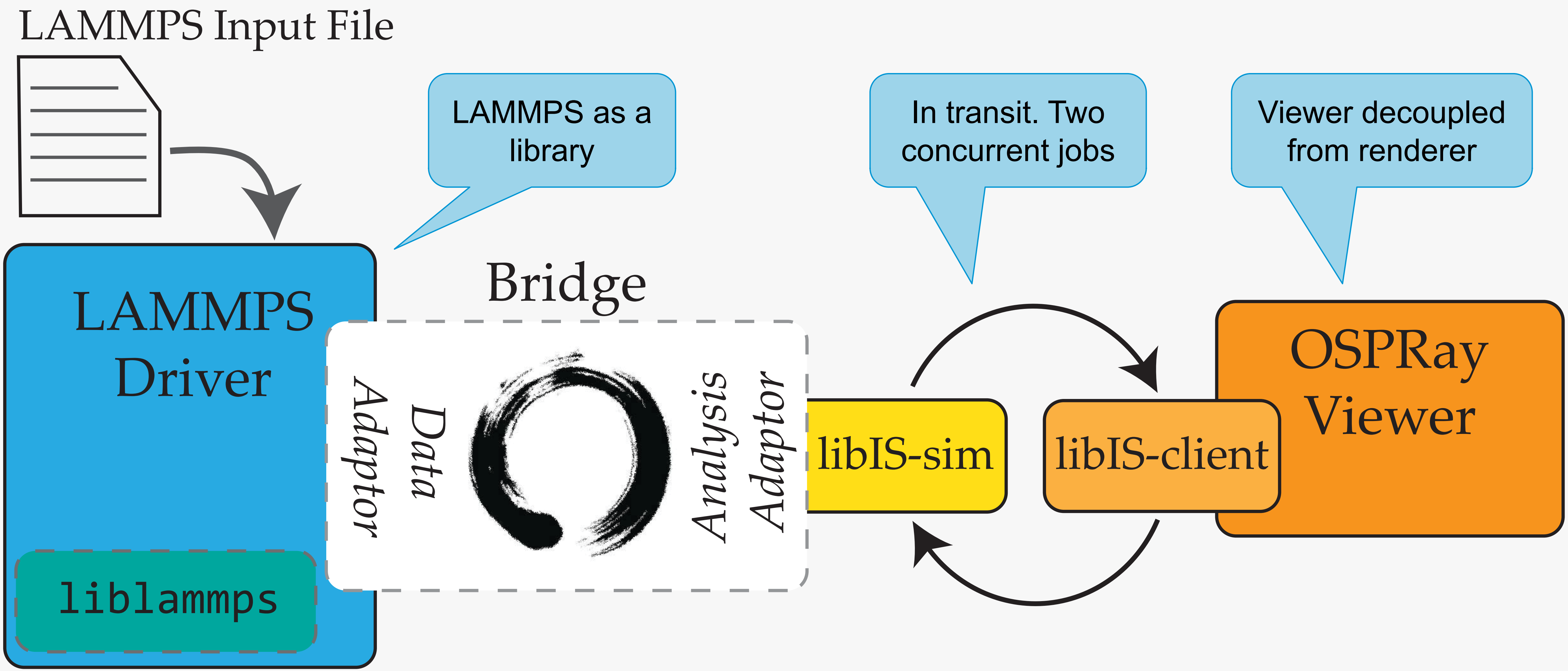
Catalyst example



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

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

LAMMPS instrumentation with SENSEI and OSPRay



Callback function from LAMMPS (every timestep)

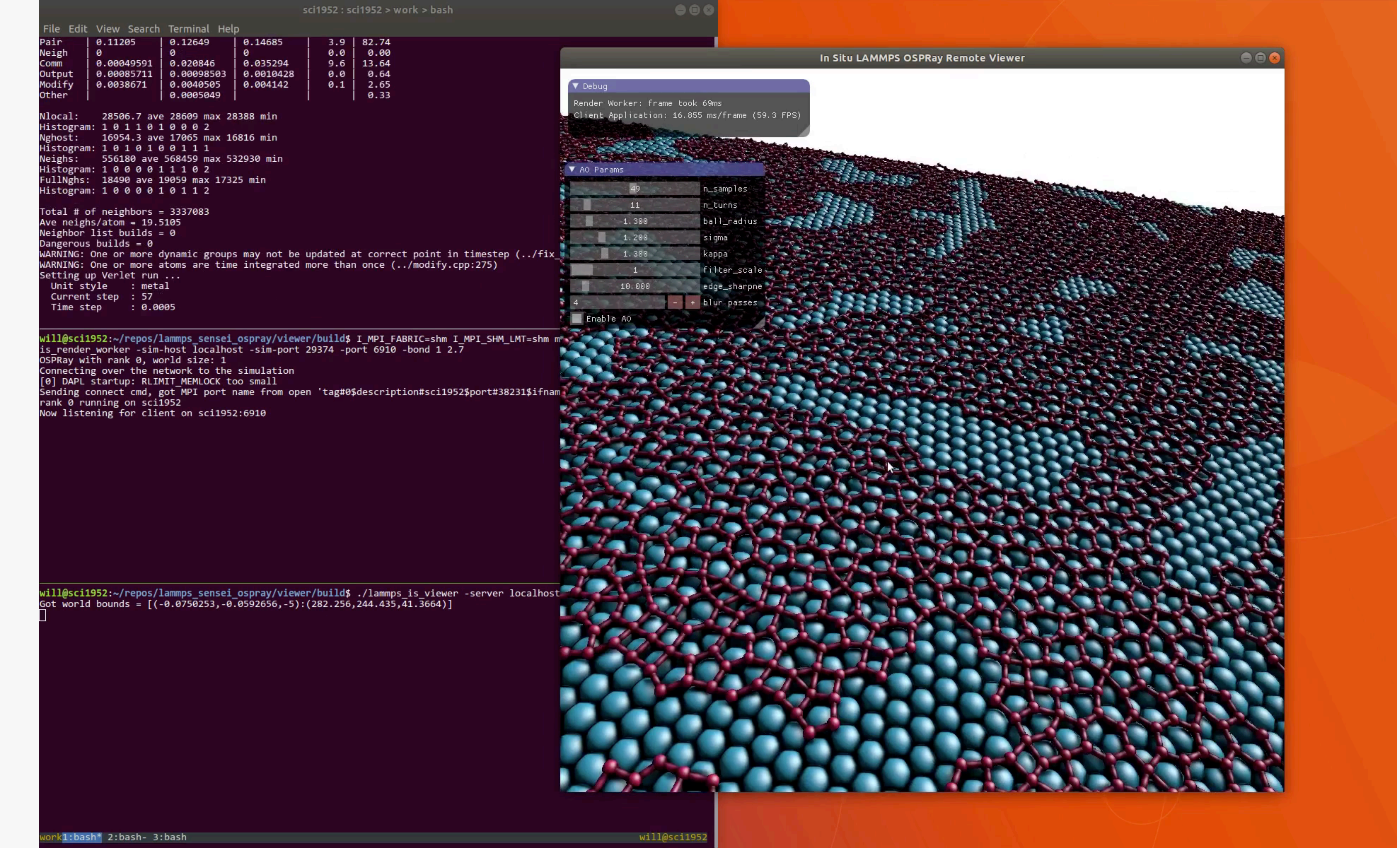
```
void LAMMPSCallback(void *ptr, bigint ntimestep,
                    int nlocal, int *id, double **x, double **f)
{
    Info *info = (Info *) ptr;

    // extents
    double boxxlo = *((double *) lammps_extract_global(info->lmp,"boxxlo"));
    double boxxhi = *((double *) lammps_extract_global(info->lmp,"boxxhi"));
    double boxylo = *((double *) lammps_extract_global(info->lmp,"boxylo"));
    double boxyhi = *((double *) lammps_extract_global(info->lmp,"boxyhi"));
    double boxzlo = *((double *) lammps_extract_global(info->lmp,"boxzlo"));
    double boxzhi = *((double *) lammps_extract_global(info->lmp,"boxzhi"));

    // get pointer to atom types
    int    *type = (int *) lammps_extract_atom(info->lmp,"type");

    // update SENSEI bridge
    bridge::Set_data(nlocal, id, type, x, boxxlo, boxylo, boxzlo, boxxhi, boxyhi, boxzhi);

    // visualize
    bridge::Execute();
}
```

XYZ atom coords from LAMMPS

get atom types from LAMMPS

Update SENSEI bridge

Visualize


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)]
work1: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

Additional Resources

- SENSEI source code and build instructions
  https://gitlab.kitware.com/sensei/sensei

- SENSEI SC17 Tutorial
  Slides and Virtual Machine
  https://data.kitware.com/#collection/5a007cb58d777f31ac64ddfd/folder/5a049b808d777f31ac64e77d

- SENSEI SC18 Tutorial
  SENSEI Cross-Platform View of In Situ Analytics
  Sunday, November 11^{th},1:30pm - 5pm
  https://sc18.supercomputing.org/presentation/?id=tut142&sess=sess255

Resources for optional hands-on session

- ParaView installers
  Download version 5.5.2
  https://www.paraview.org/download/

- ALCF ParaView Red Blood Cell Tutorial
  https://www.alcf.anl.gov/user-guides/vis-paraview-red-blood-cell-tutorial

- ParaView on Cooley
  https://www.alcf.anl.gov/user-guides/paraview-cooley

- Data on Cooley
  `/projects/SDL_Workshop/visualization/BLOODFLOW_TUTORIAL_DATA`

QUESTIONS?

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