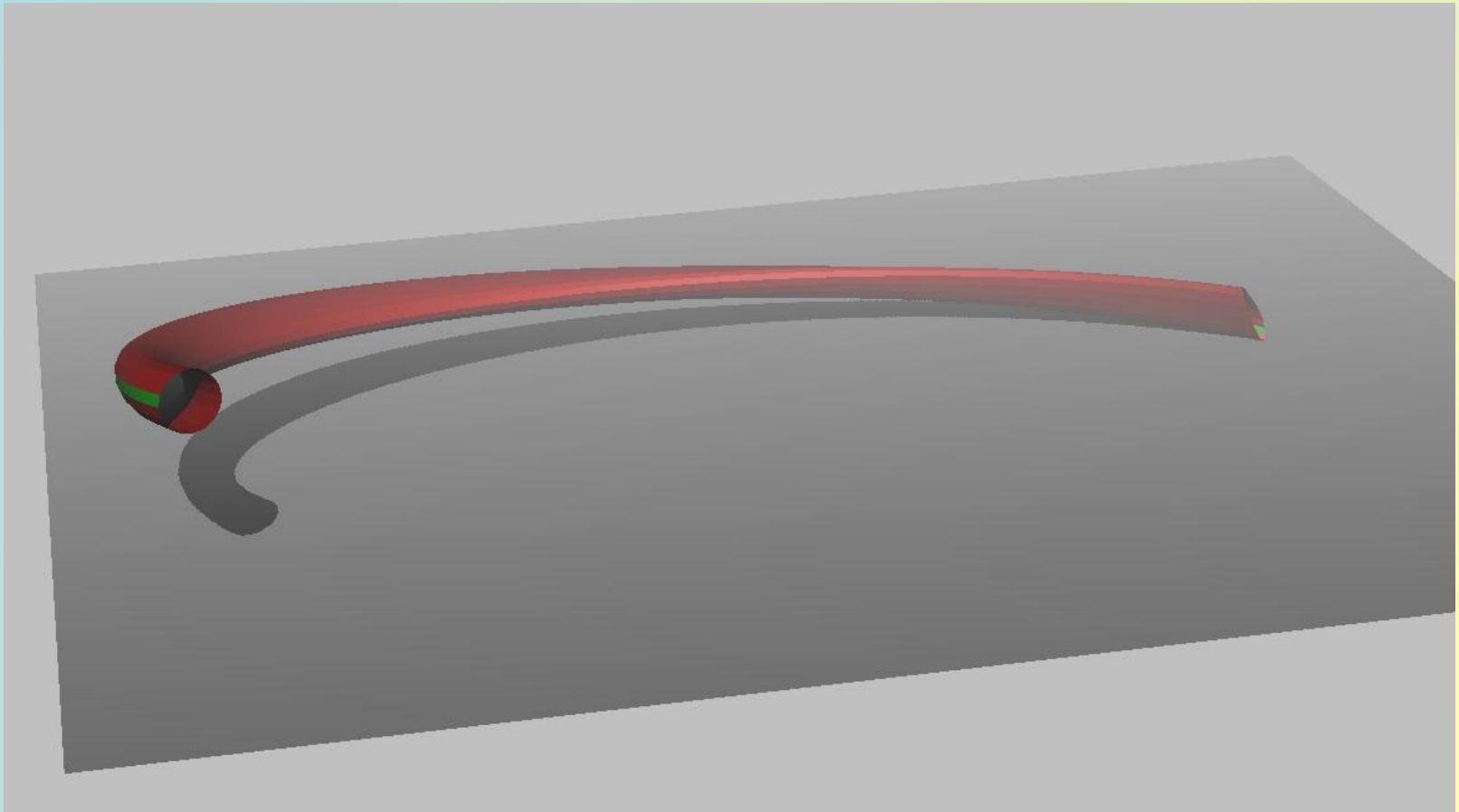
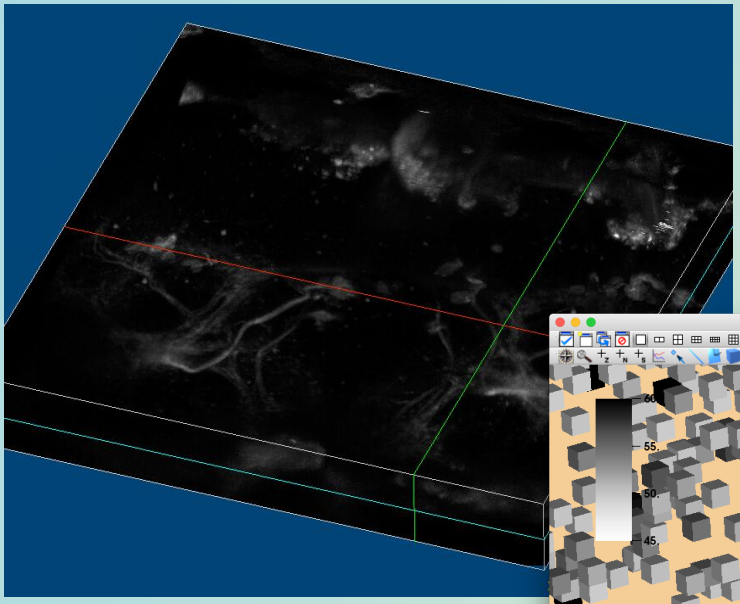
Scientific Visualization

Eliot Feibush

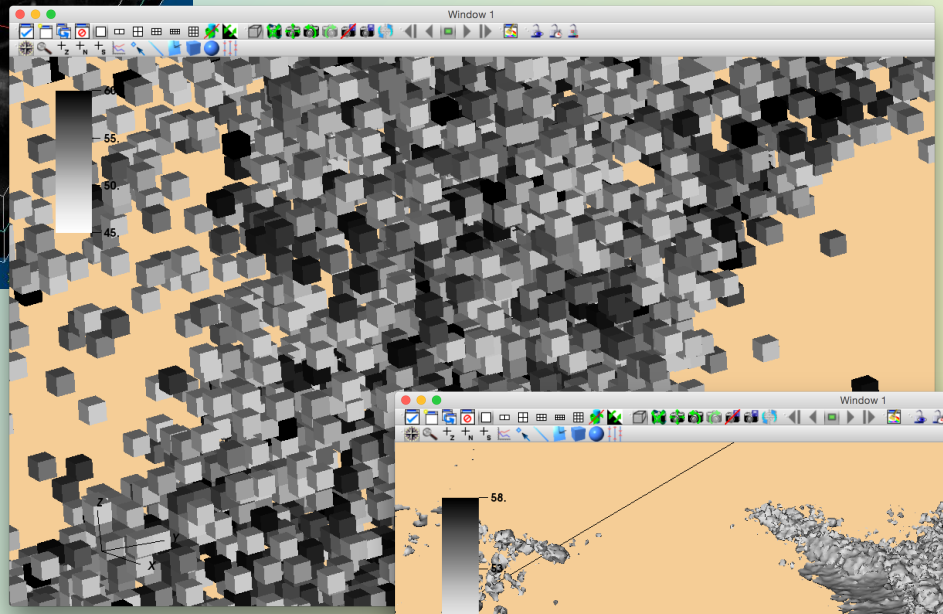
RESEARCH COMPUTING



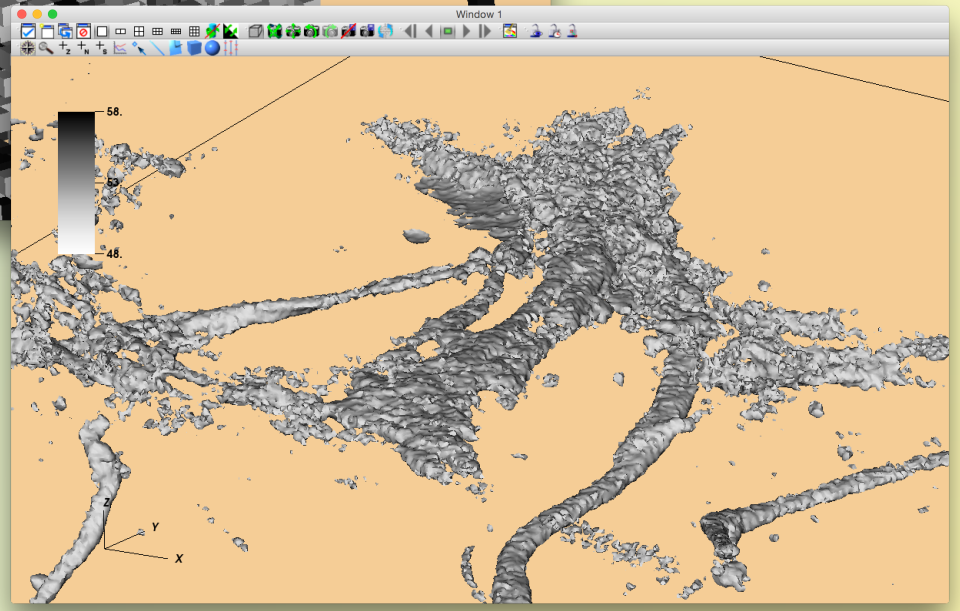
Acquire



Analyze



Visualize

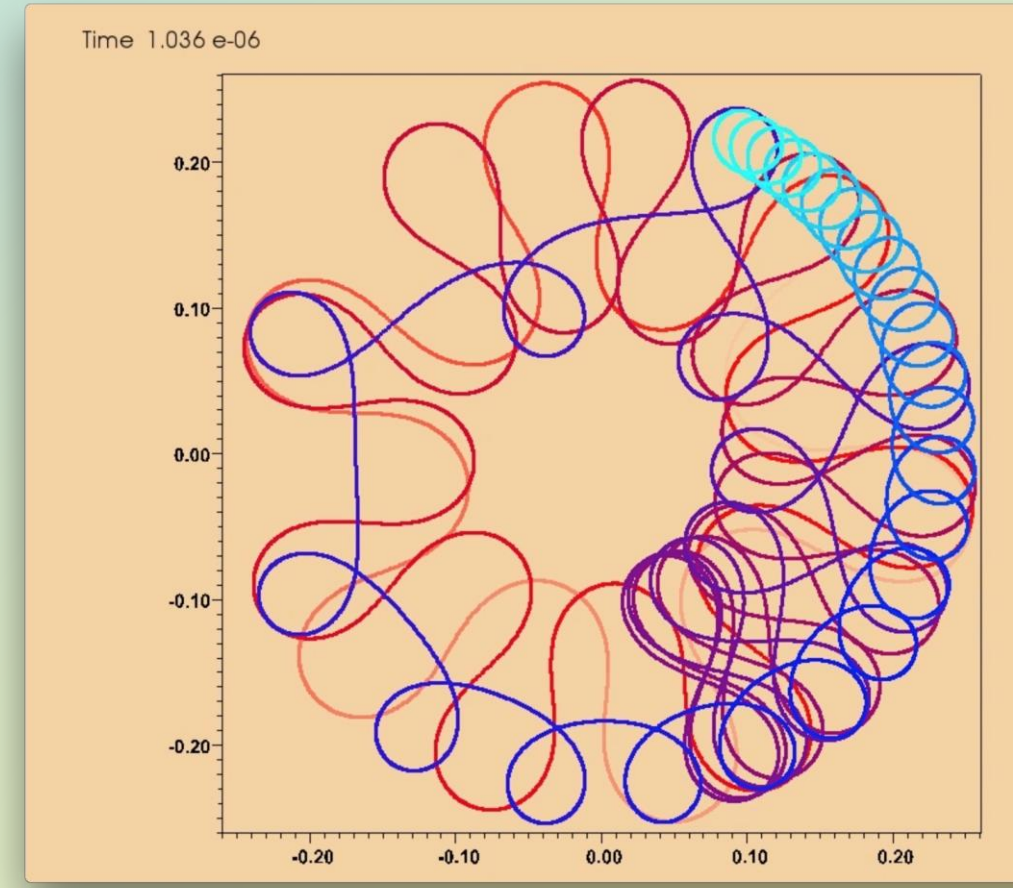


Work Flow

Visualization of 1 Particle Path Can Be Interesting:

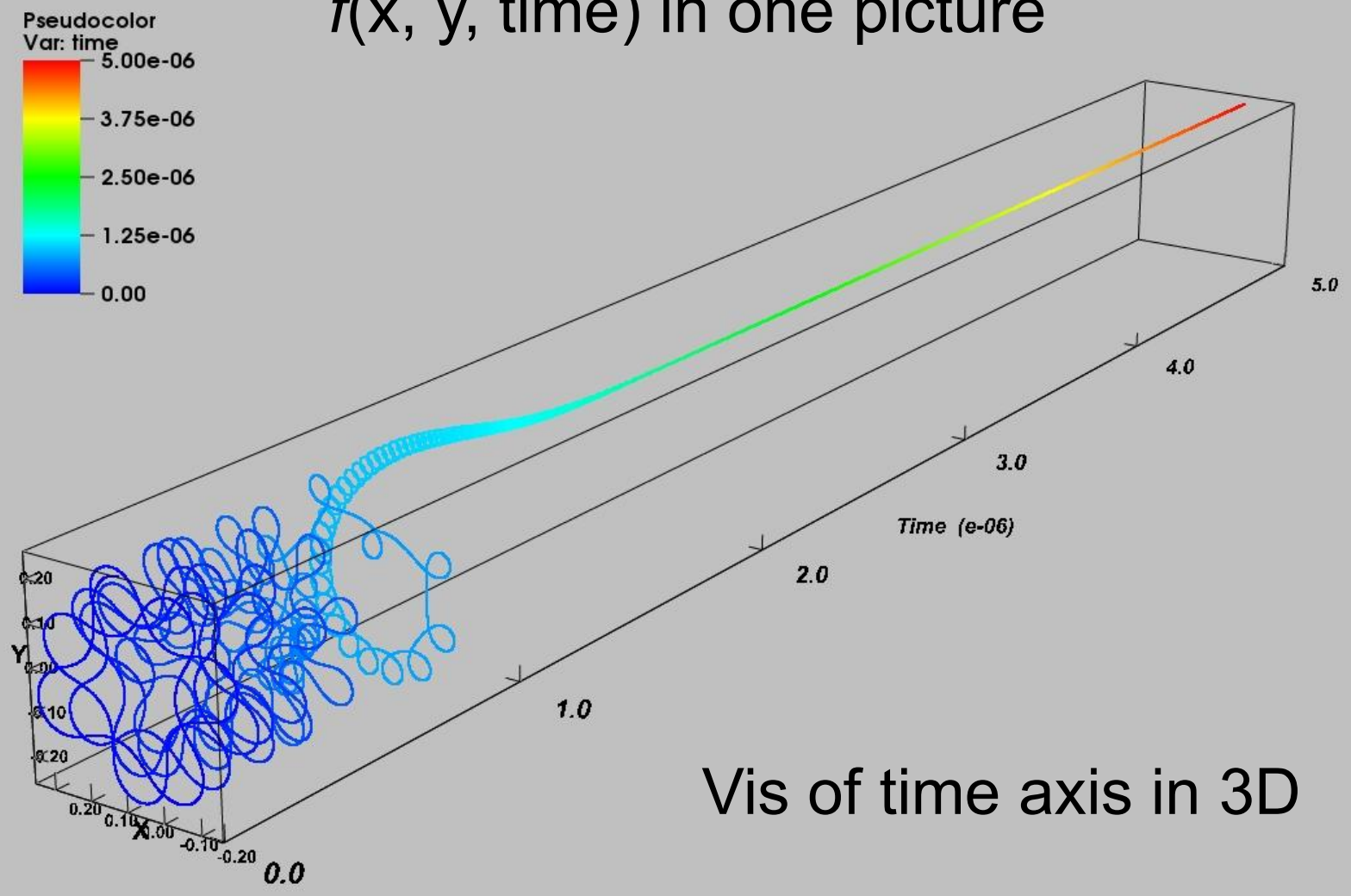
Simulation of Ion Path as Energy Decreases

Trajectory starts as betatron.
Transitions to Figure 8.
Finally becomes cyclotron.



http://www.princeton.edu/~efeibush/movies/m3_720.mp4

Visualization of 1 Particle Path



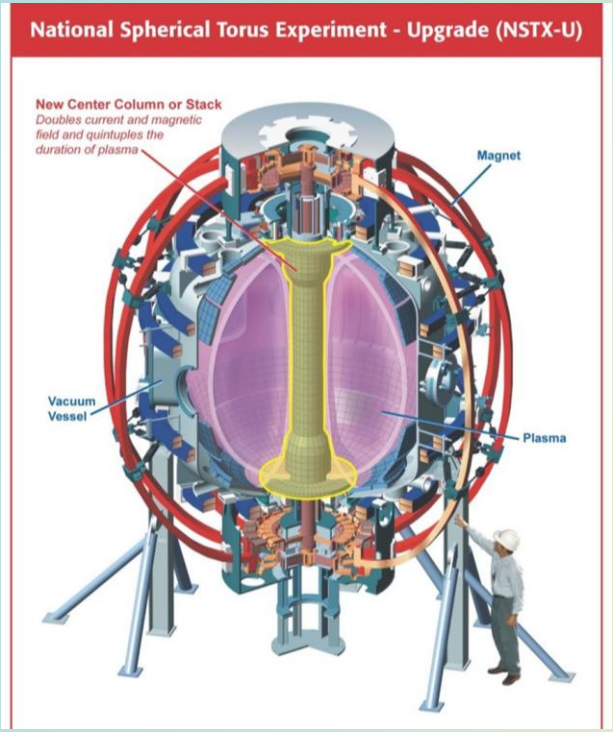
f(x, y, time) in one picture

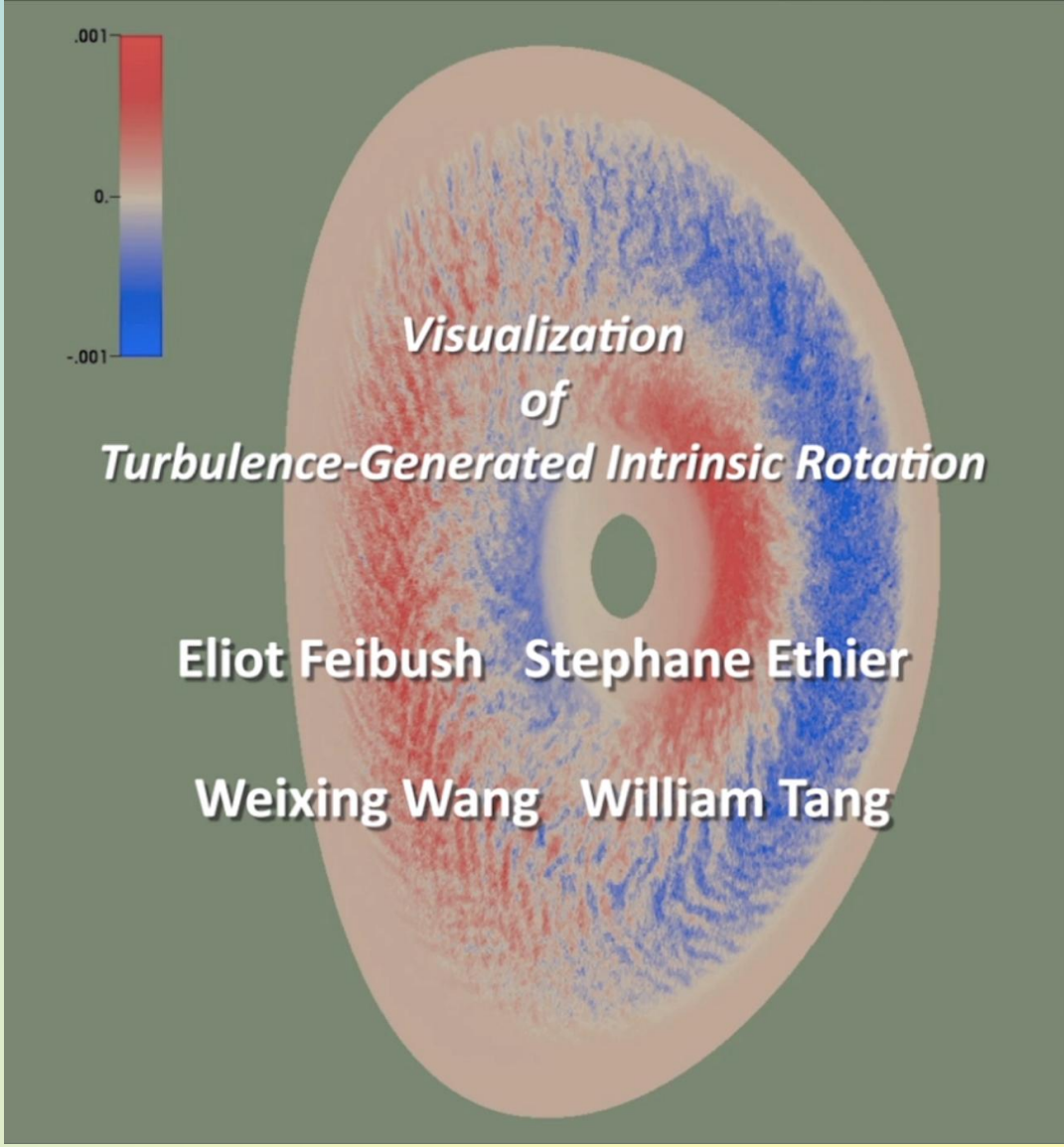
Vis of time axis in 3D

Time Step Simulation

Render each time step to a PNG image file.

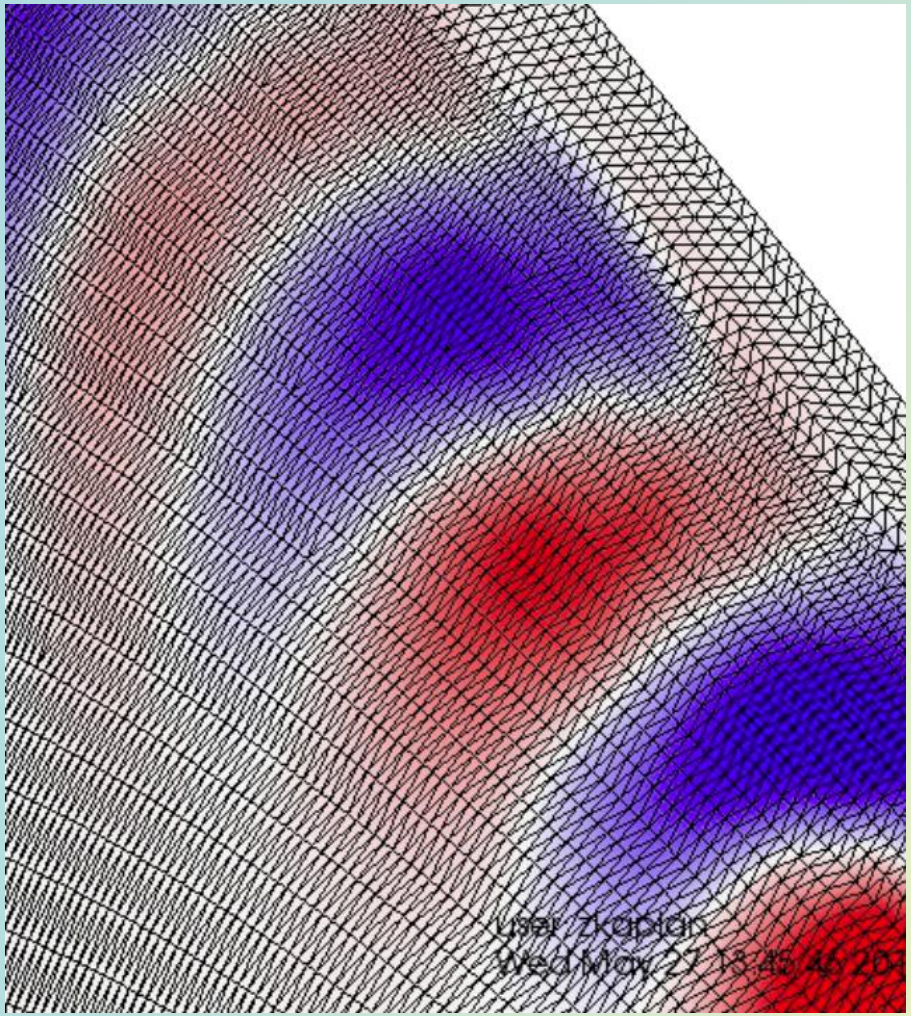
Combine images to create animation.

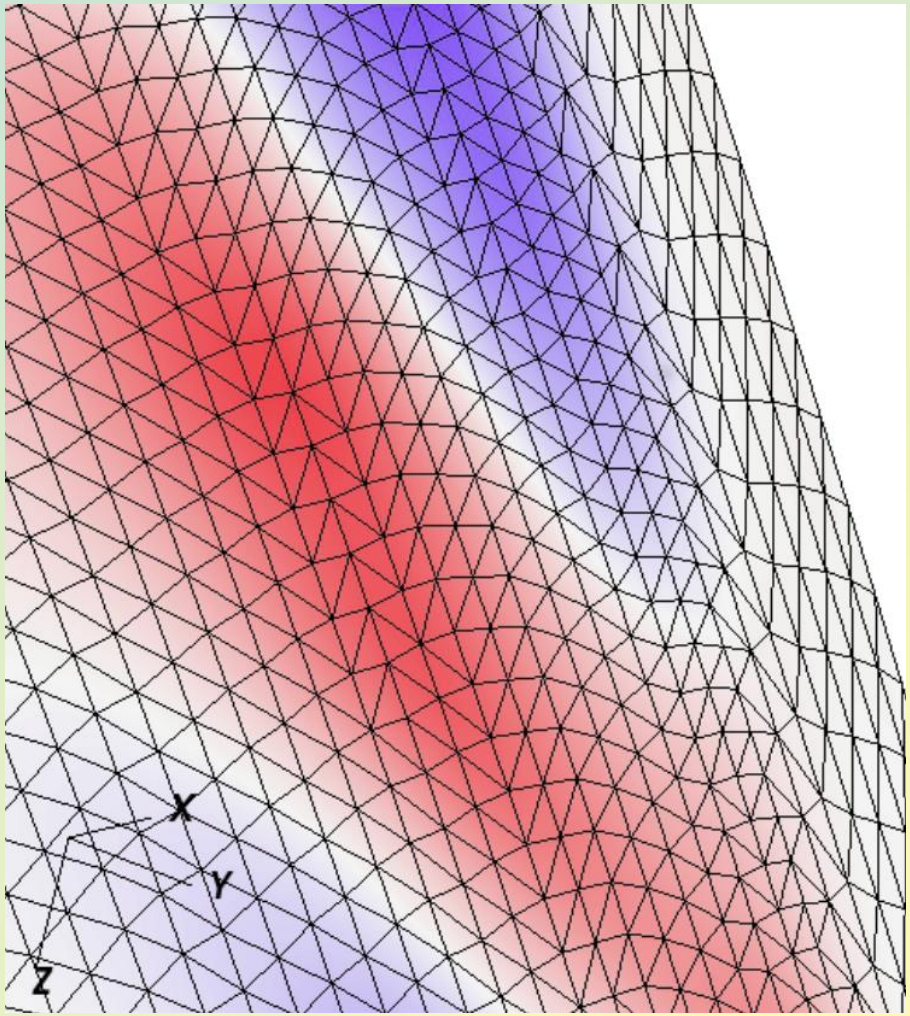




http://www.princeton.edu/~efeibush/movies

Complex Compute Grid – Concentric Rings





Gaining insight …

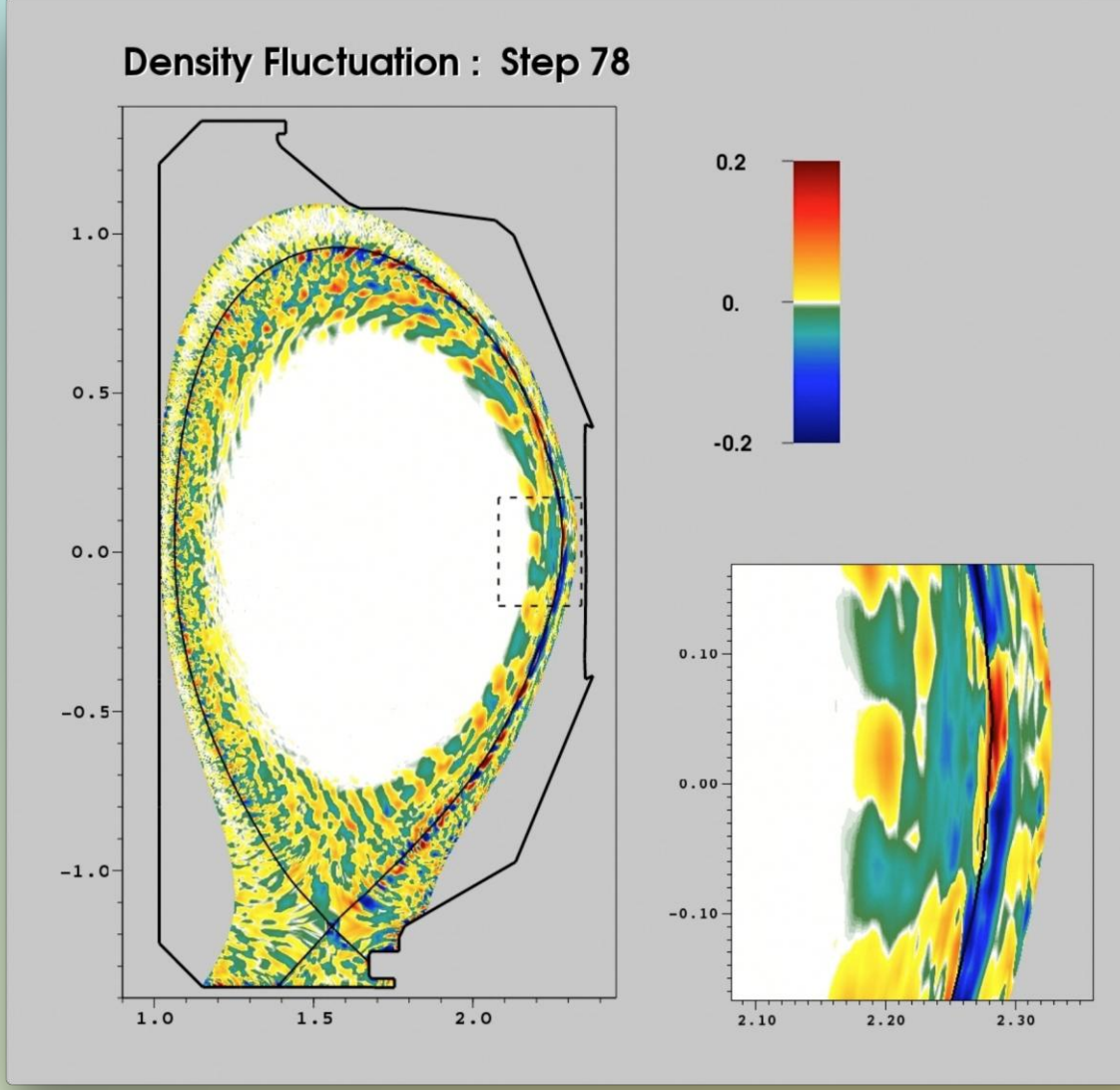
Time Step Simulation

Render overview

+

Region of Interest

Combine images into movie.



http://www.princeton.edu/~efeibush/movies

deninsetb1080.mp4

Scientific Visualization

Simulations generate data

Acquire data from experiments

- Biology
- Chemistry
- Physics
- Engineering
  - ...

Explore

Communicate

Based on computer graphics

- points
- lines
- polygons, surface mesh
  - 3D transformations
  - hidden surface removal
  - shading
  - lighting

Vis Plot Types
(Based on graphics primitives)

Points

Lines

Vectors

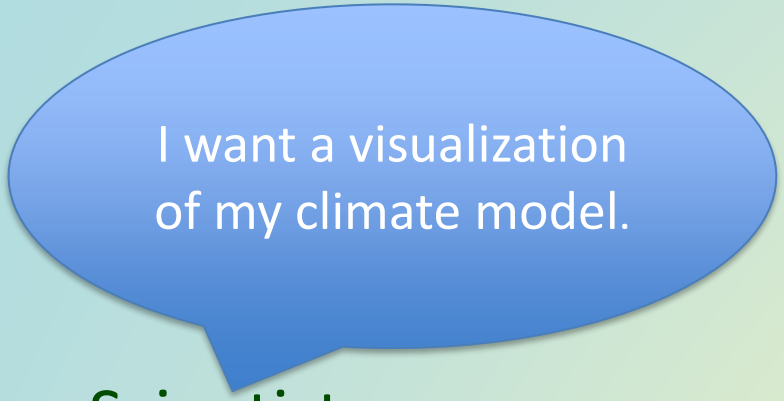
Contour lines & isosurfaces

Polygons, mesh

Volume

Molecule

Designing a Visualization



Scientist

Vis Guy

2-D/3-D Compute grid:

scalar or vector

per point, per cell

Selection + Operators

Getting to Know Your Data

Geometric range

Numerical domain (min, max)

- Histogram
- Outliers
- Features
- Local / Global (steps)

Data Science / Science of Data

n-Dimensions of Data

f(x)

f(x, time) f(x, i)

f(x, y)

f(x, y, time)

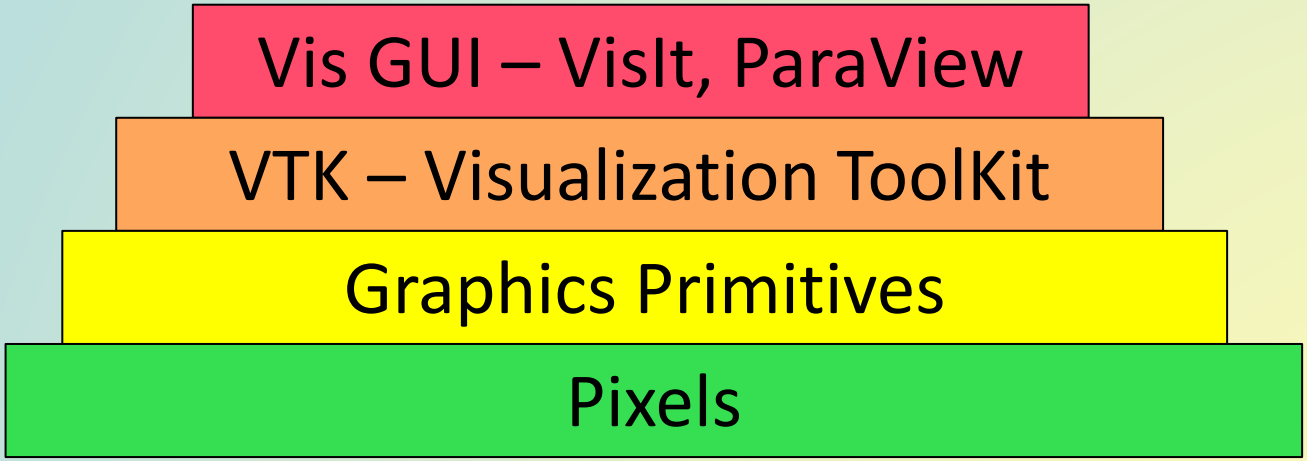
f(x, y, z)

f(x, y, z, time)

Understanding Complexity !

Time dependent data is a good candidate for animation.

Implementation



VisIt Can Read Data Files

- Silo
- Chombo
- GTC
- M3D
- H5Nimrod
- SAMRAI
- S3D
- Enzo
- ITAPS
- XDMF
- Exodus
- FLASH
- EnSight
- VTK **VTK is Internal Format**
- NetCDF
- CGNS
- NASTRAN
- TecPlot
- Protein Databank (PDB)
- Plot3D
- GIS (ESRI Shapefile, DEM, many more)
- Image formats

Variable types

- Scalar
- Vector
- Tensor
- Arrays
- Label
- Material
- Species
- X,Y pairs

Database reader plug-ins can be developed for new formats

Install VisIt on Your Computer

https://visit-dav.github.io/visit-website

Downloads

Releases

Web search for: “visit visualization”

visitusers.org search …

Start Running VisIt

Mac

Magnifying Glass:

Top Hit: VisIt

Finder

Applications

Visit

Windows

Taskbar

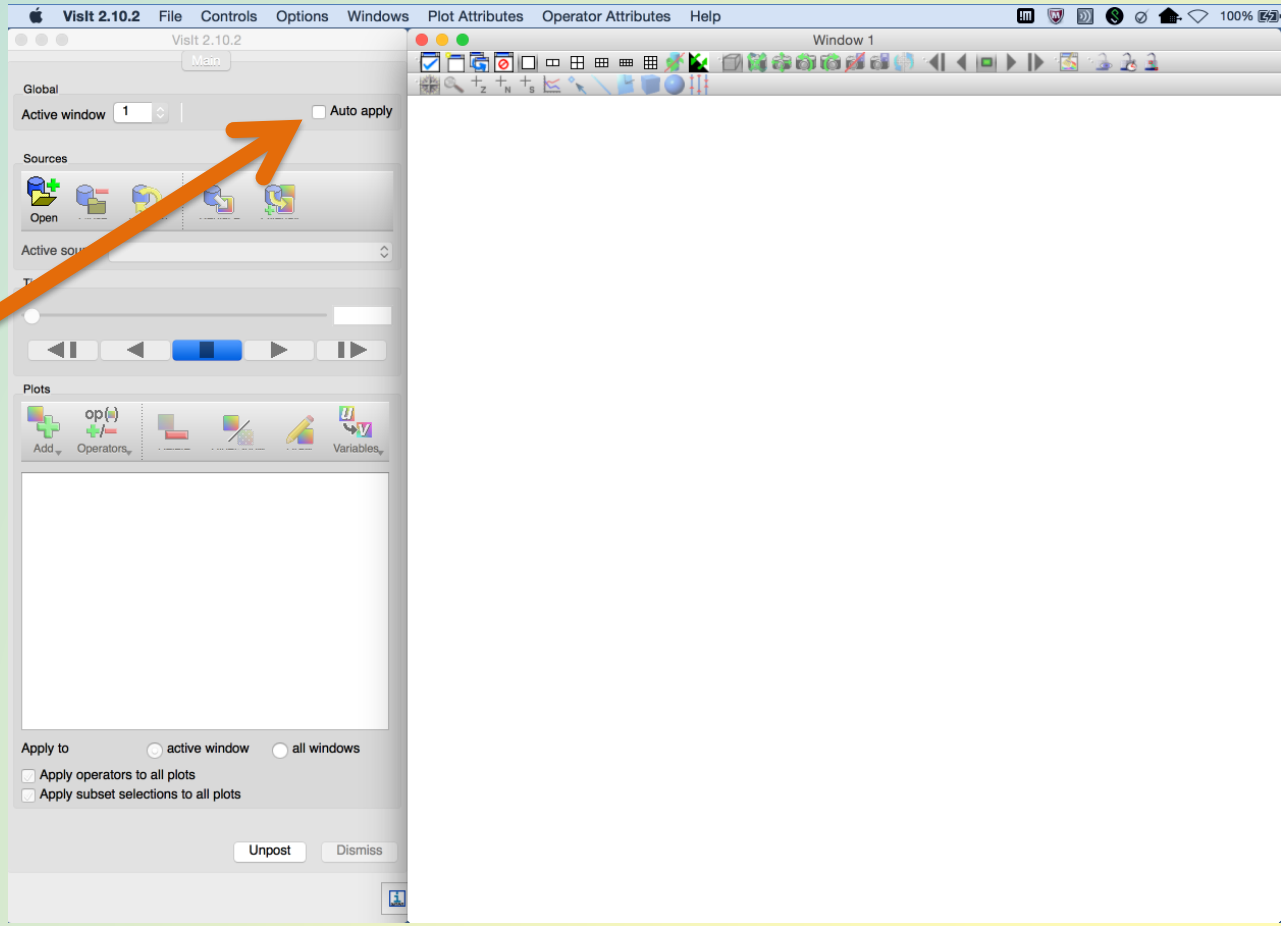
Search:

Visit

VisIt icon on the desktop

Get Started

Check “Auto apply”



Continuous 3D Grids

3D volume of data defined at compute points

f(x,y,z)

VisIt interpolates among grid points in all 3 directions.

Specify data at grid locations.

Apply Operators to explore & examine data.

Try It - part 1

Download Data File:

https://www.princeton.edu/~efeibush/viscourse/visit_data/

Open File strpts3d.vtk

Add Mesh

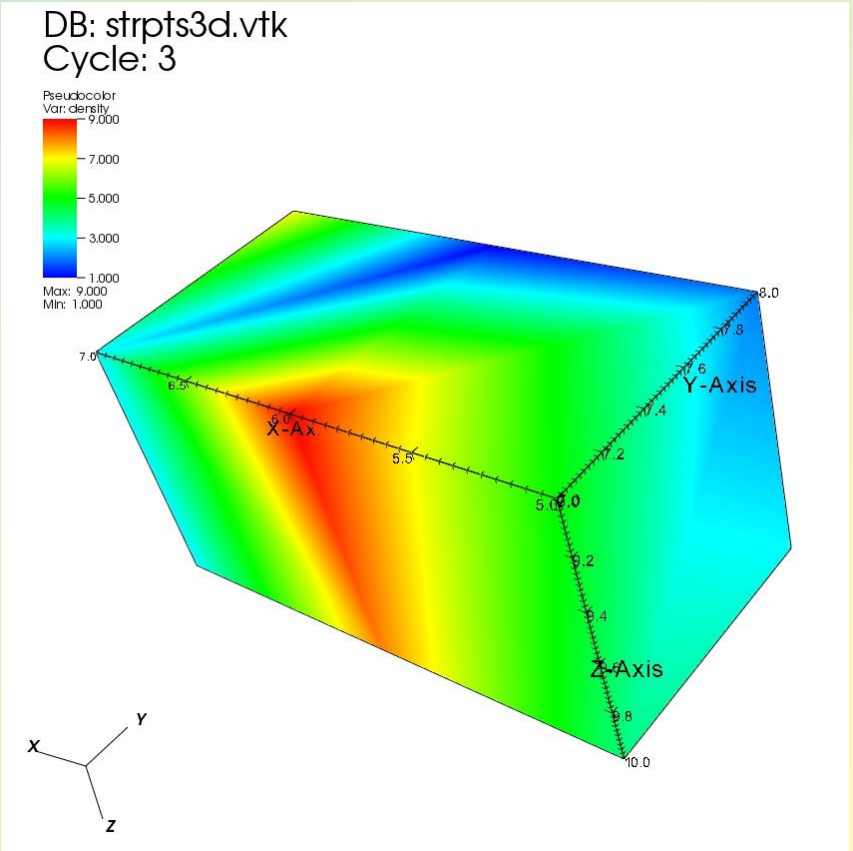
Add Pseudocolor→density

VTK:

STRUCTURED_POINTS

3 x 2 x 2 = 12 points

SCALARS density double



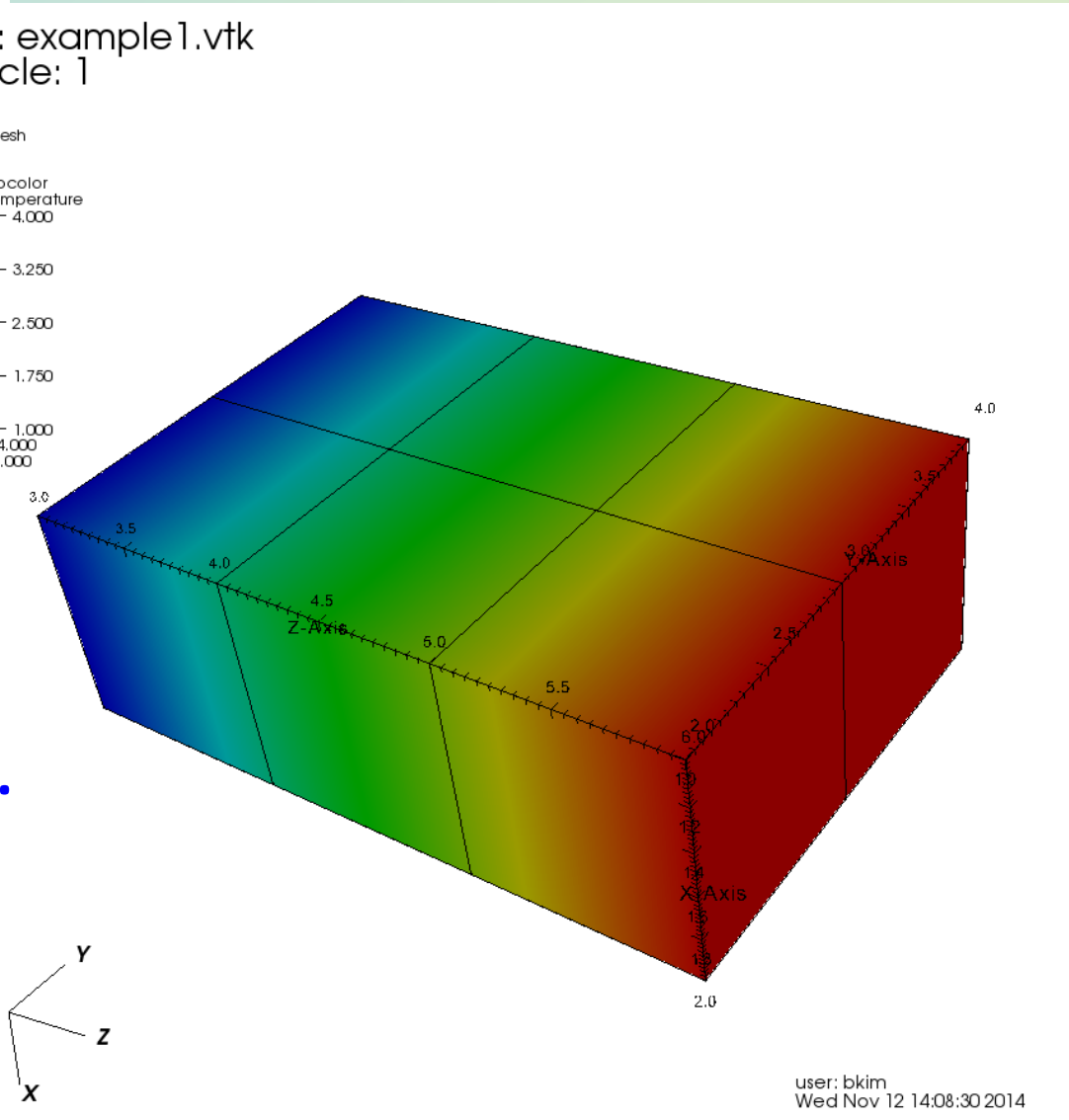
Structured Points

```
# vtk DataFile Version 3.0
VTK format
ASCII
DATASET STRUCTURED_POINTS
DIMENSIONS 2 3 4
ORIGIN 1. 2. 3.
SPACING 1. 1. 1.
POINT_DATA 24
SCALARS temperature int
LOOKUP_TABLE default
1
1
1
1
1
1
1
2
2
2
2
2
2
2
3
3
3
3
3
3
4
4
4
4
4
4
4
```

Continuous volume of data.

Uniform spacing per axis.

Value at each point.



Structured Points Ordering

```
# Example python loop to write values
to vtk file


for z in range(4):
    for y in range(3):
        for x in range(2):
            # write f(x,y,z) value to file
```

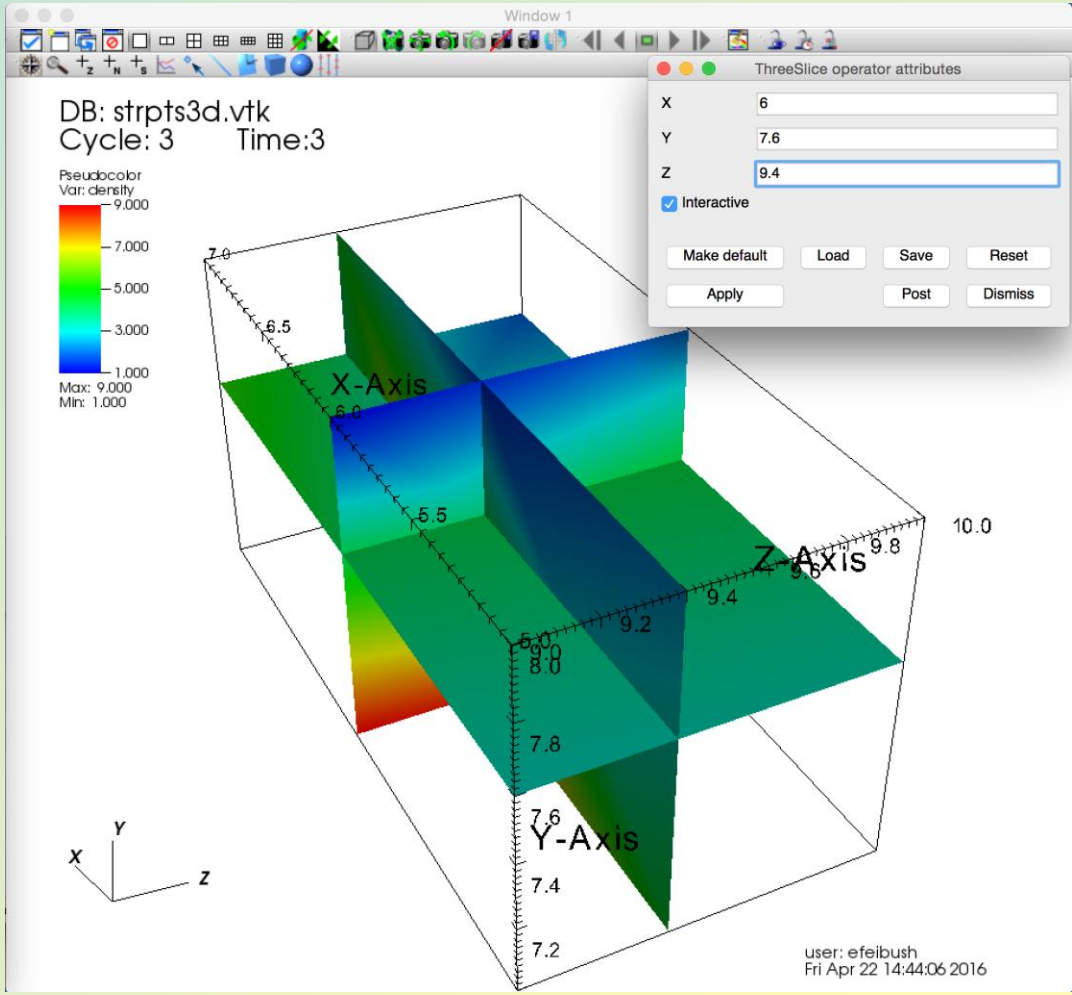
Try It - part 2

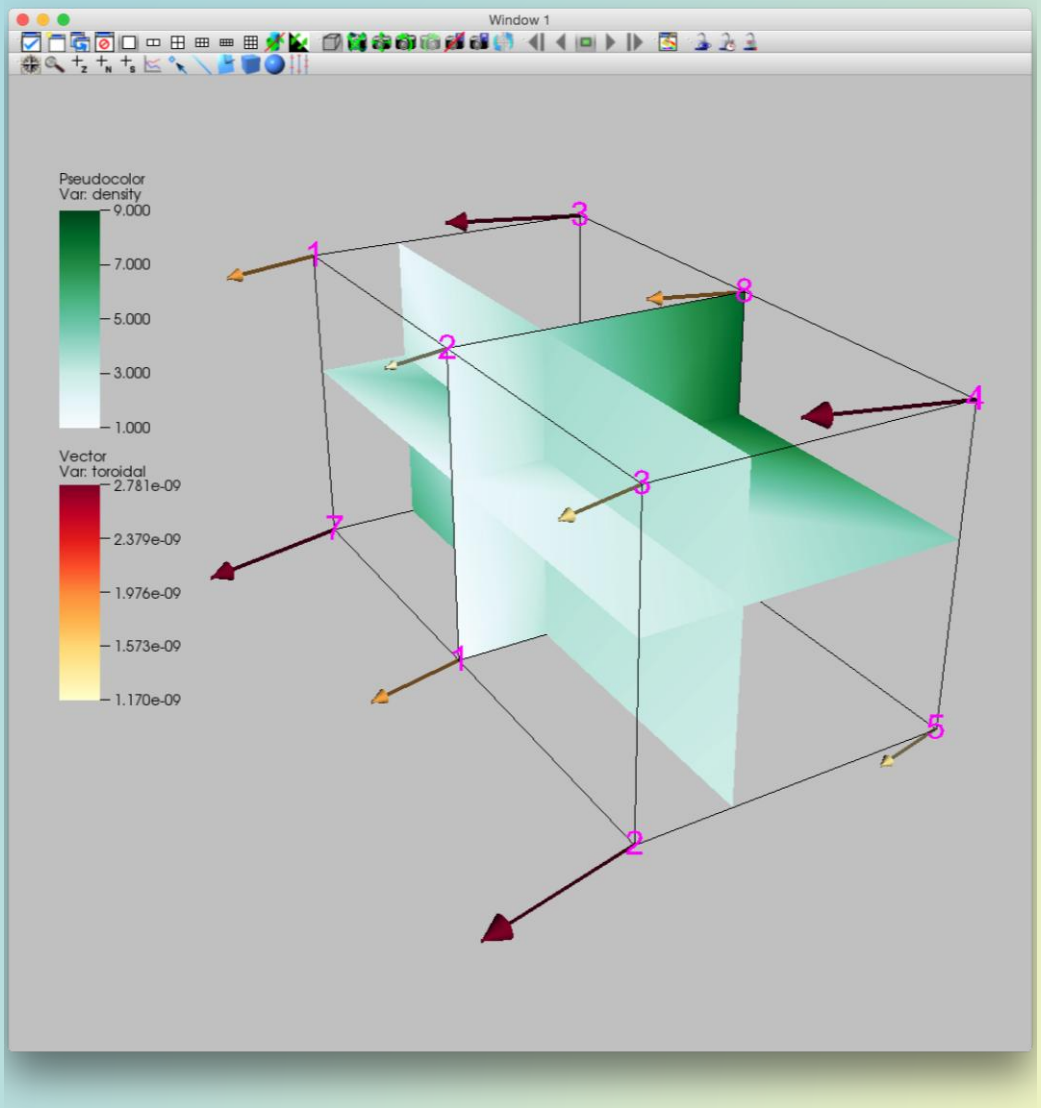
Open File strpts3d.vtk

Add Pseudocolor→density

Operators

- Slicing
  - ThreeSlice
    - X = 6
    - Y = 7.5
    - Z = 9.5





Add→Vector toroidal

Add→Label density

Different color maps for different variables.

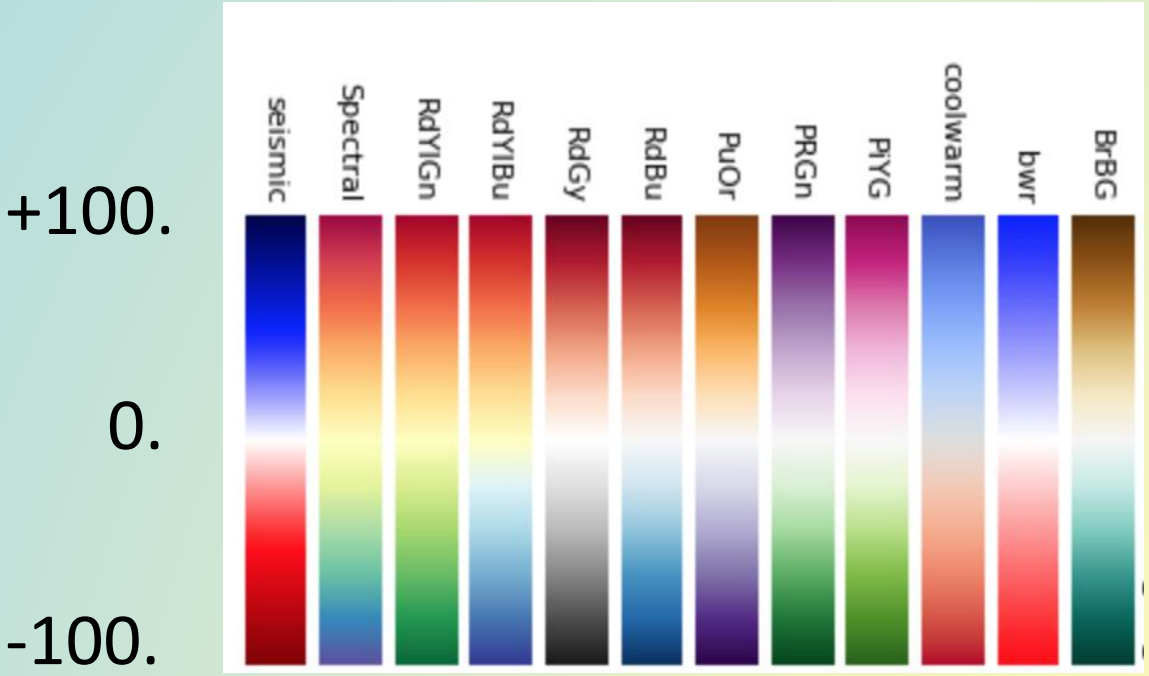
Lighting – off.

Gray background.

Density labels at mesh points.

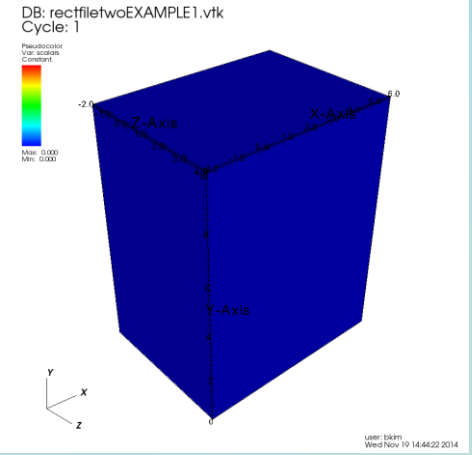
Color Maps

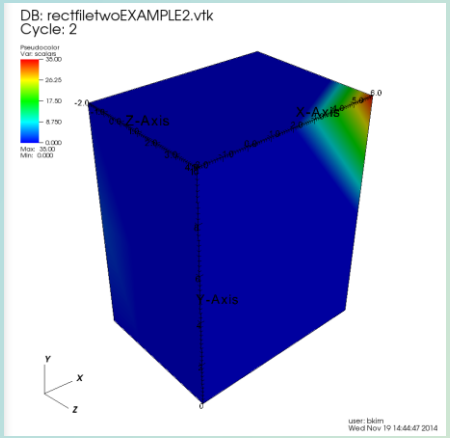
Divergent color maps

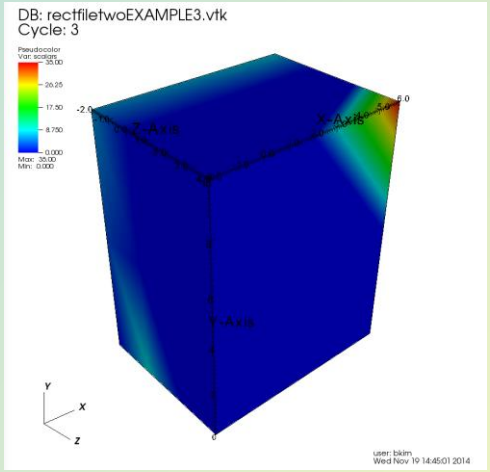


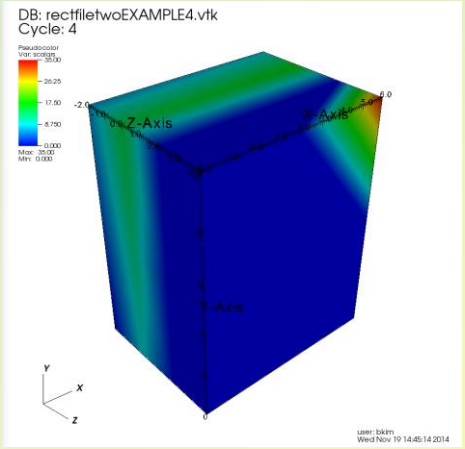
Time Steps *f(x,y,z,t)*

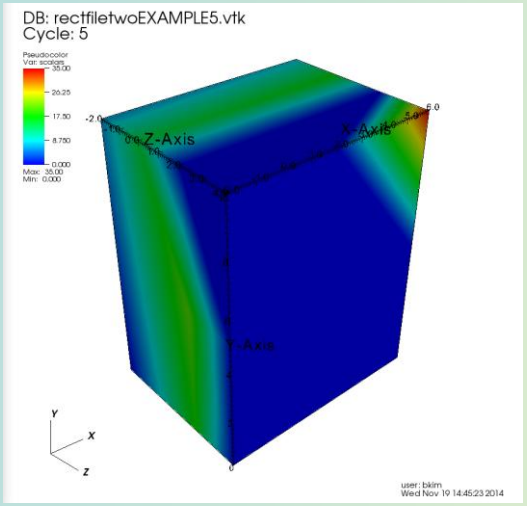
VisIt automatically reads files named in numerical order for time step visualization.

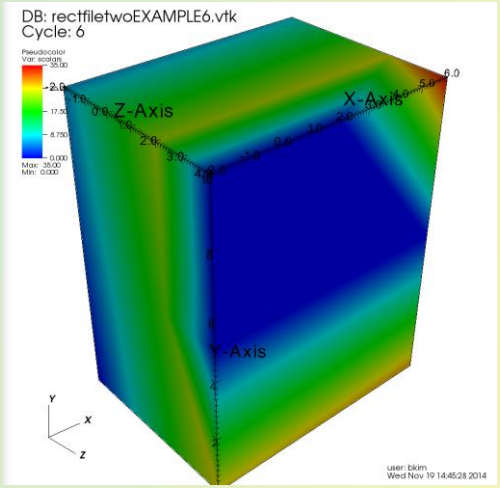


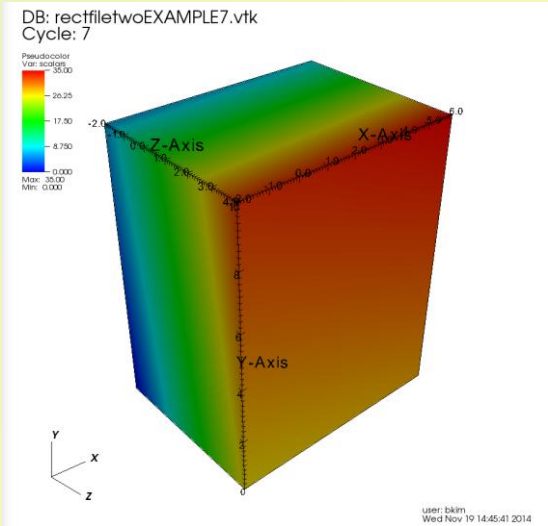












Demonstration

Open File:

poloidalplane.vtk

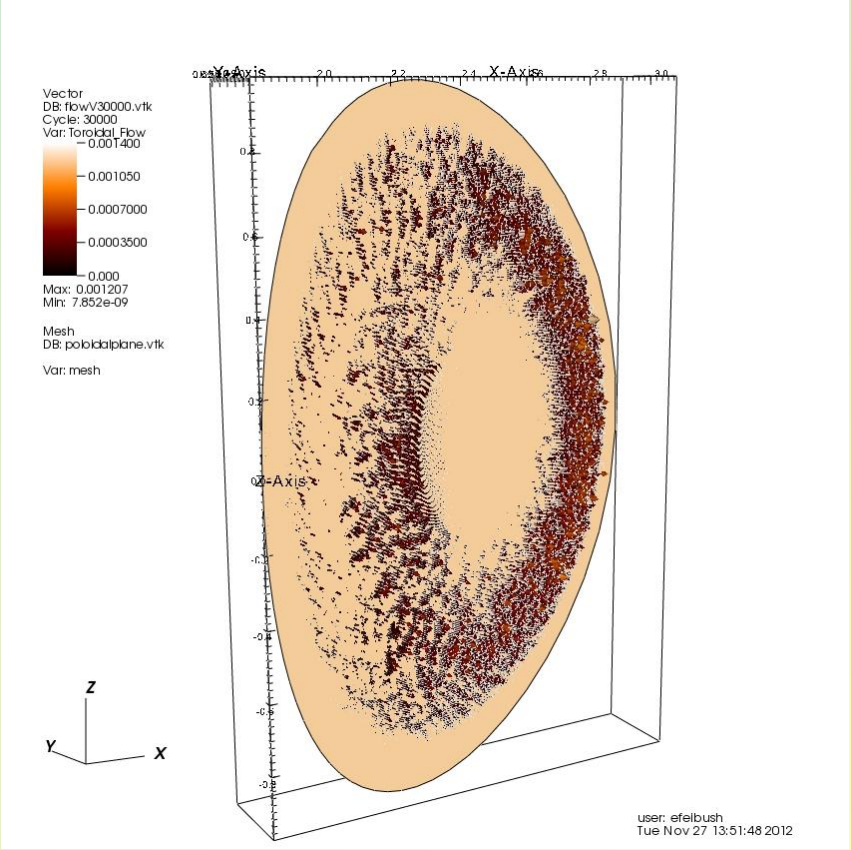
Add Mesh→mesh

Attributes

Open File

flowV*.vtk database *

Add Vector→Toroidal_Flow



* “Smart” File grouping

(Turn off Grouping to load 1 file)

Time Step Movie - Demonstration

File → Save Movie

New Simple Movie

QuickTime

→

4 Frames per second

Click the arrow to apply your config

mpeg2encode in VisIt software distribution

`mpeg1 format only - MPEG`

Combine Images into Movies

ffmpeg

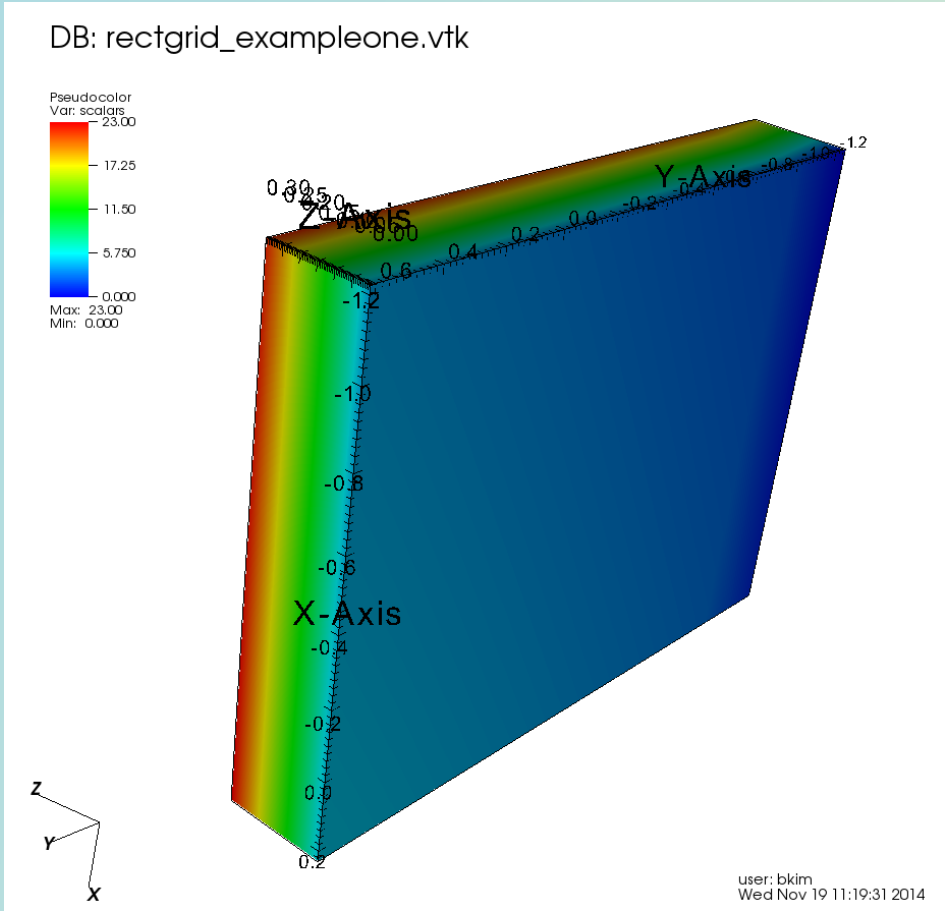
Most comprehensive: .mp4, compression

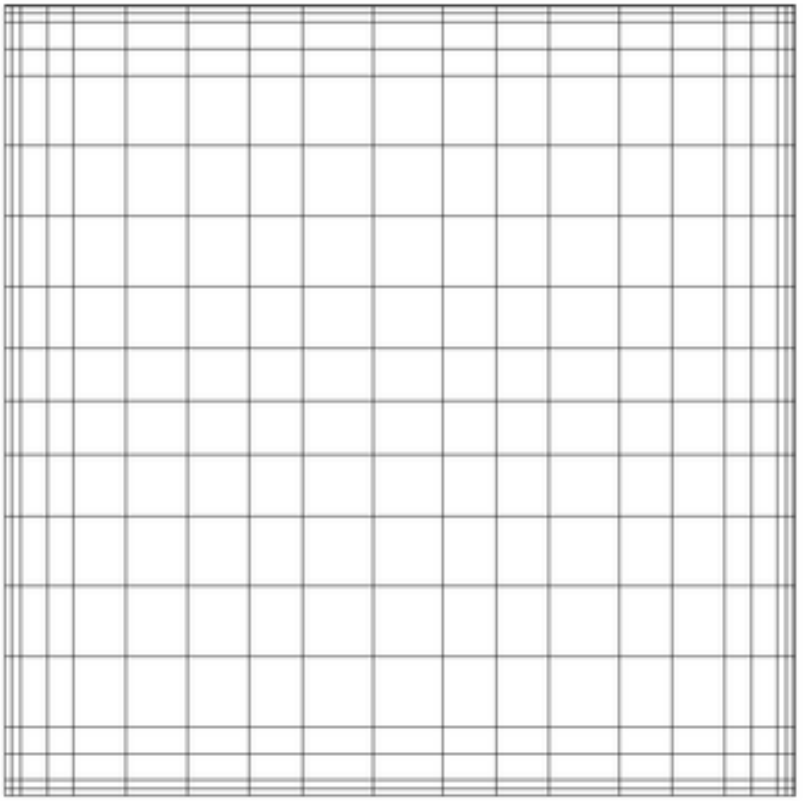
Command line Linux, Mac

Princeton Research Computing cluster

Free downloads for Mac, Windows, Linux

Rectilinear Grids

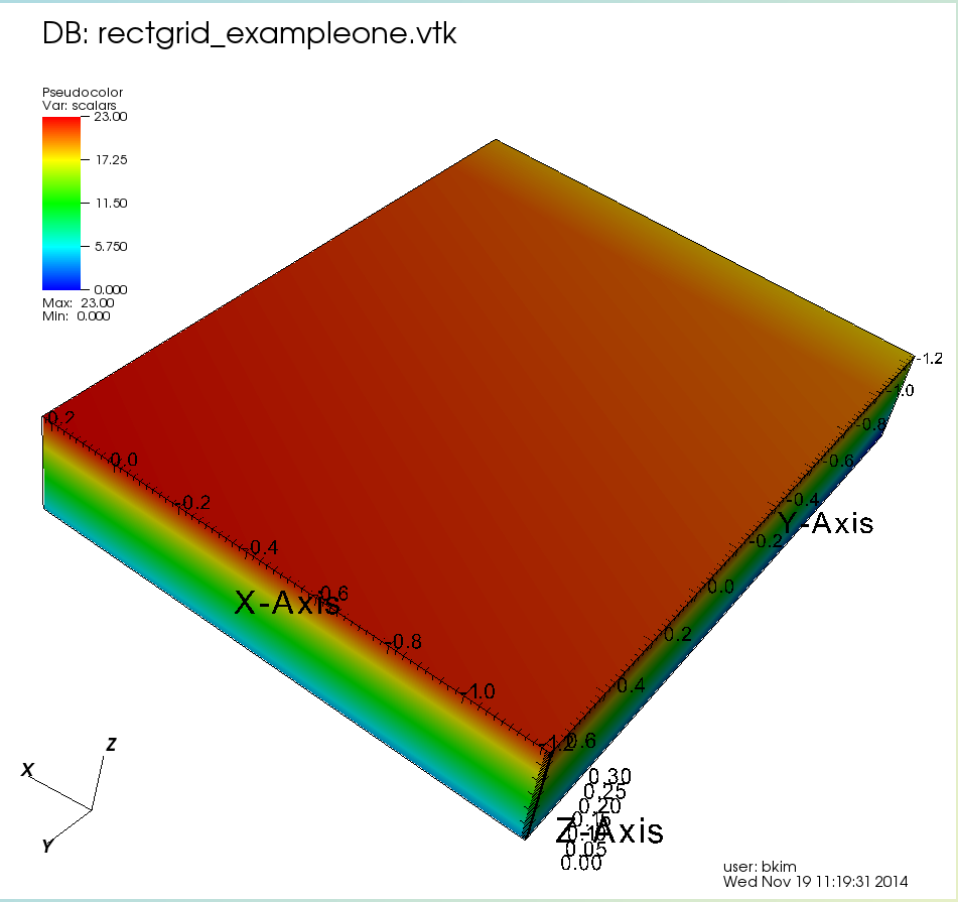




Continuous volume of data defined at specific points.

Non-Uniform spacing per axis.

Rectilinear Grids

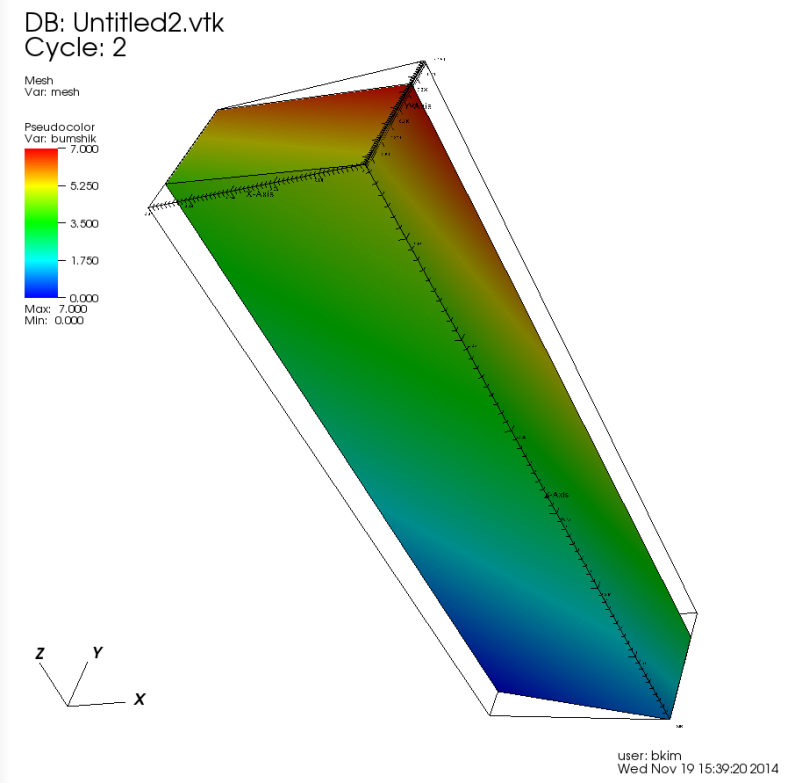


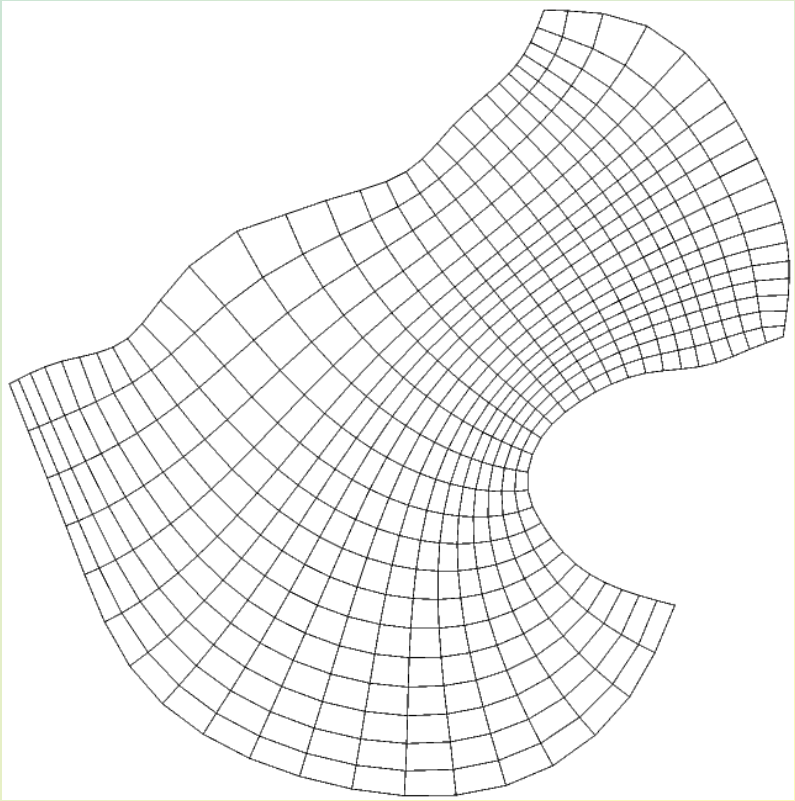
rectgrid_exampleone

```
# vtk DataFile Version 3.0
VTK format
ASCII
DATASET RECTILINEAR_GRID
DIMENSIONS 2 3 4
X_COORDINATES 2 float
-1.22 0.23
Y_COORDINATES 3 float
-1.25 -1.01 0.6125
Z_COORDINATES 4 float
0 0.1 0.2 0.3
POINT_DATA 24
SCALARS scalars float
LOOKUP_TABLE default
0 1 2 3 4 5 6 7 8 9 10
11 12 13 14 15 16 17 18 19
20 21 22 23
```

Non-Uniform Axis Spacing

Structured Grids





Continuous volume (or surface) of data defined at specific points.

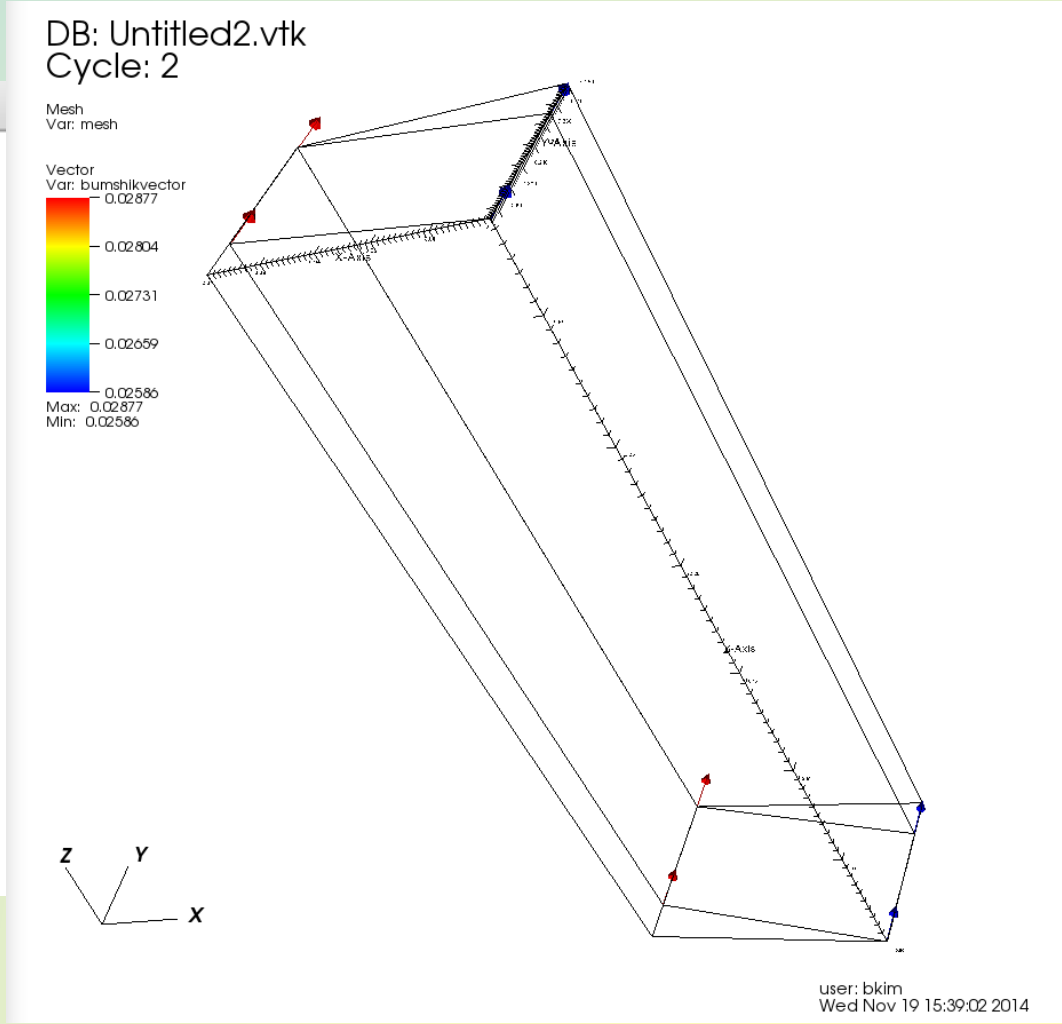
Non-Uniform, Non-Orthogonal, any spacing per axis.
Quadrilateral cell faces. Can be curvilinear.

Structured Grids + Vectors

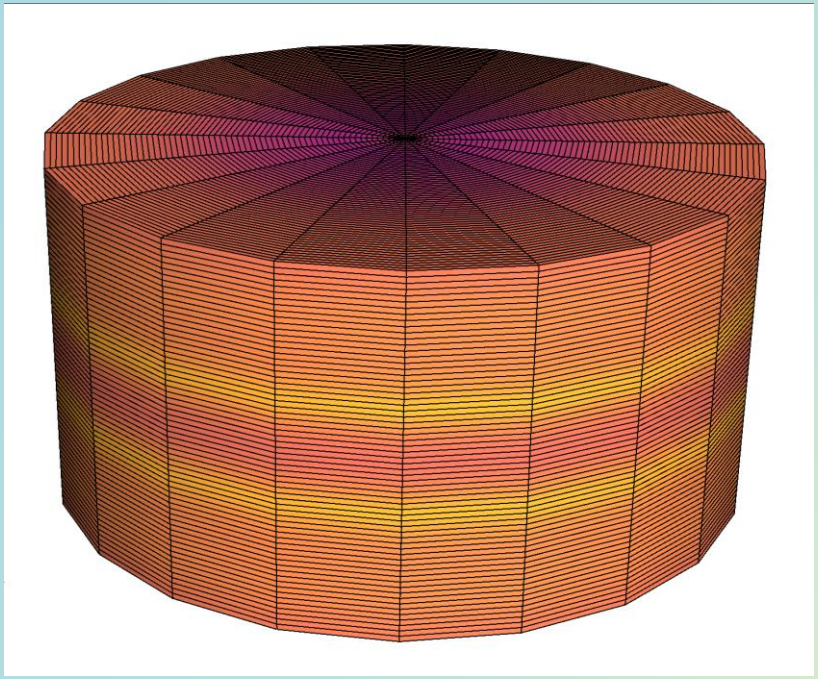
Untitled2.vtk

```
# vtk DataFile Version 3.0
vtk output
ASCII
DATASET STRUCTURED_GRID
DIMENSIONS 2 2 2
POINTS 8 float
0 0.2 0 0.1 0.184843 0 0 0.25 0
0.1 0.234843 0 0 0.2 0.333333 0.1 0.184843 0.333333
0 0.25 0.333333 0.1 0.234843 0.333333

POINT_DATA 8
SCALARS bumshik float
LOOKUP_TABLE default
0 1 2 3 4 5 6 7
VECTORS bumshikvector float
0 0.0287671 0 0 0.0258604 0 0 0.0287671 0
0 0.0258604 0 0 0.0287671 0 0 0.0258604 0
0 0.0287671 0 0 0.0258604 0
```



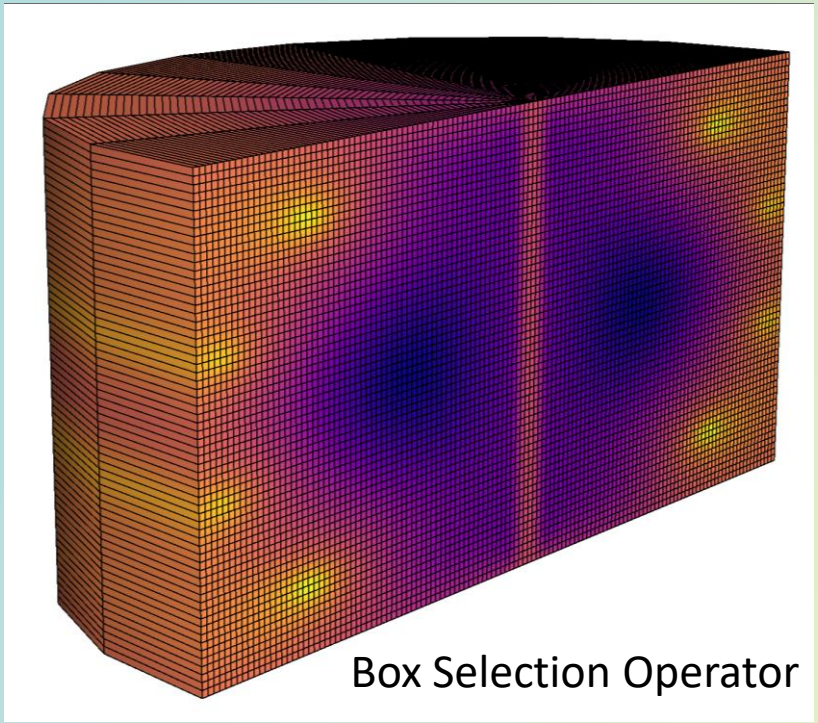
If 3D grid is not aligned to XYZ axes.



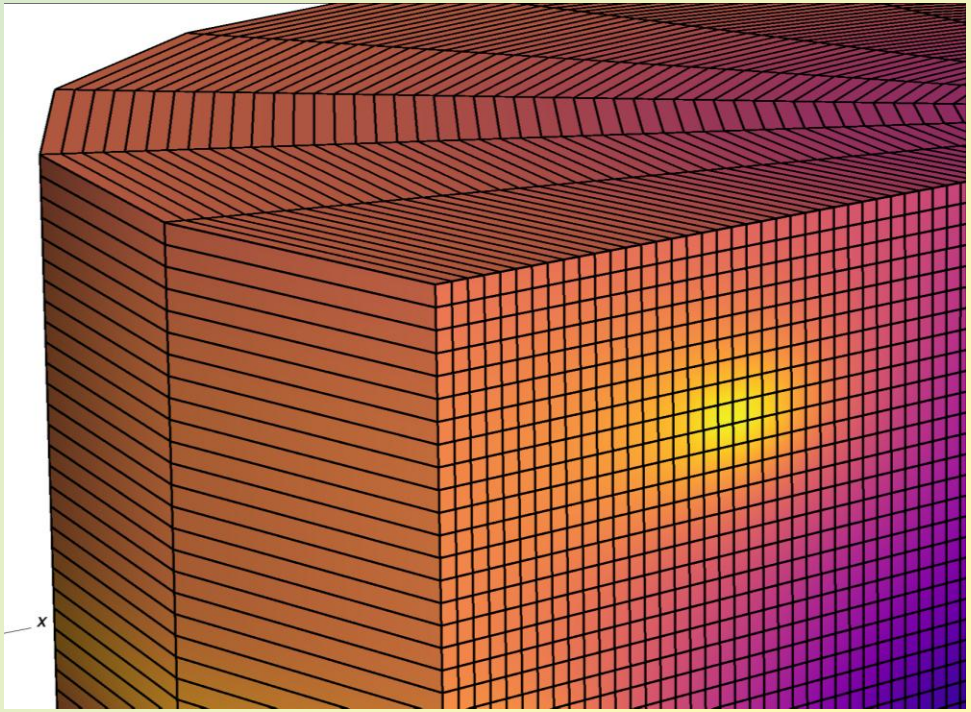
Unstructured Grid

Hexahedron element example

Magnetic field data



Box Selection Operator



Grid Summary

Structured Points – uniform spacing, orthogonal

Rectilinear Grid – non-uniform spacing, orthogonal

Structured Grid – non-orthogonal quads

Unstructured Grid – any combination of elements

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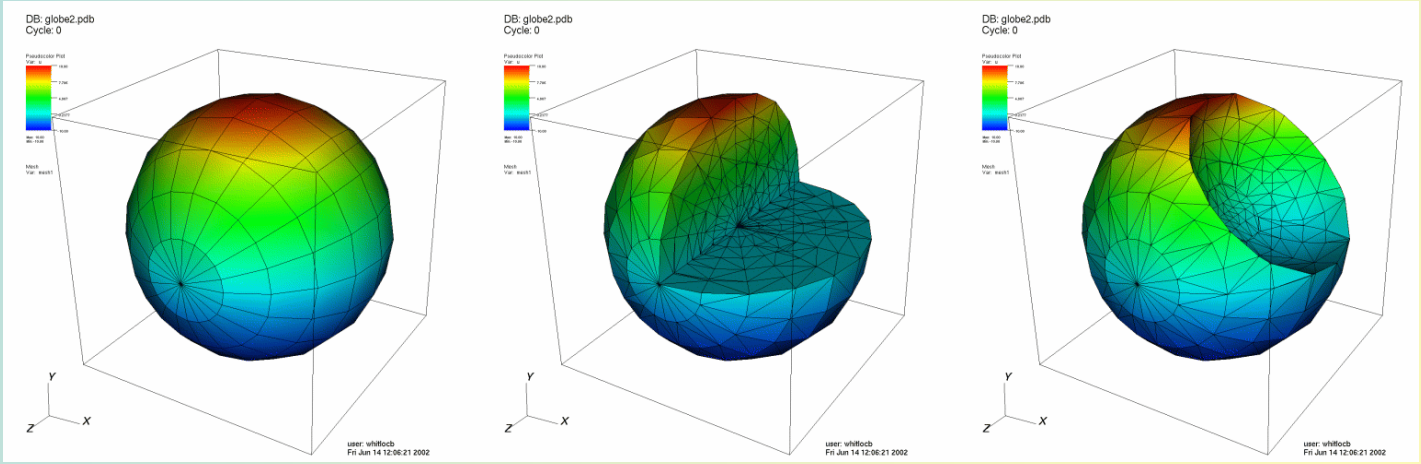
docs.vtk.org: file formats

www.princeton.edu/~efeibush/viscourse/vtk.pdf

Geometric Selection - Clip Operator

- The Clip operator clips 2D or 3D plots against planes or a sphere to remove sections of the plots
- Use this operator when you want to see a cross section of a 3D plot, while still leaving the plot in 3D

Original plots | Plots clipped with 2 planes | Plots clipped with a sphere



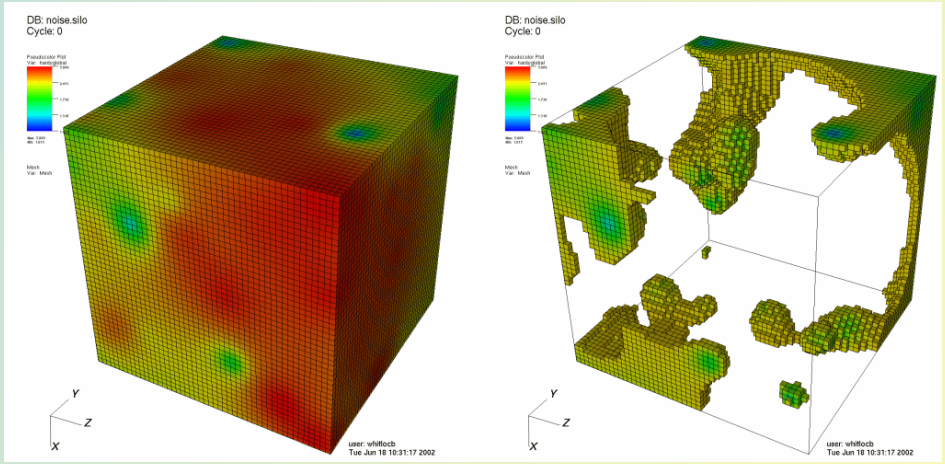
http://www.princeton.edu/~efeibush/movies

sphslice.mp4

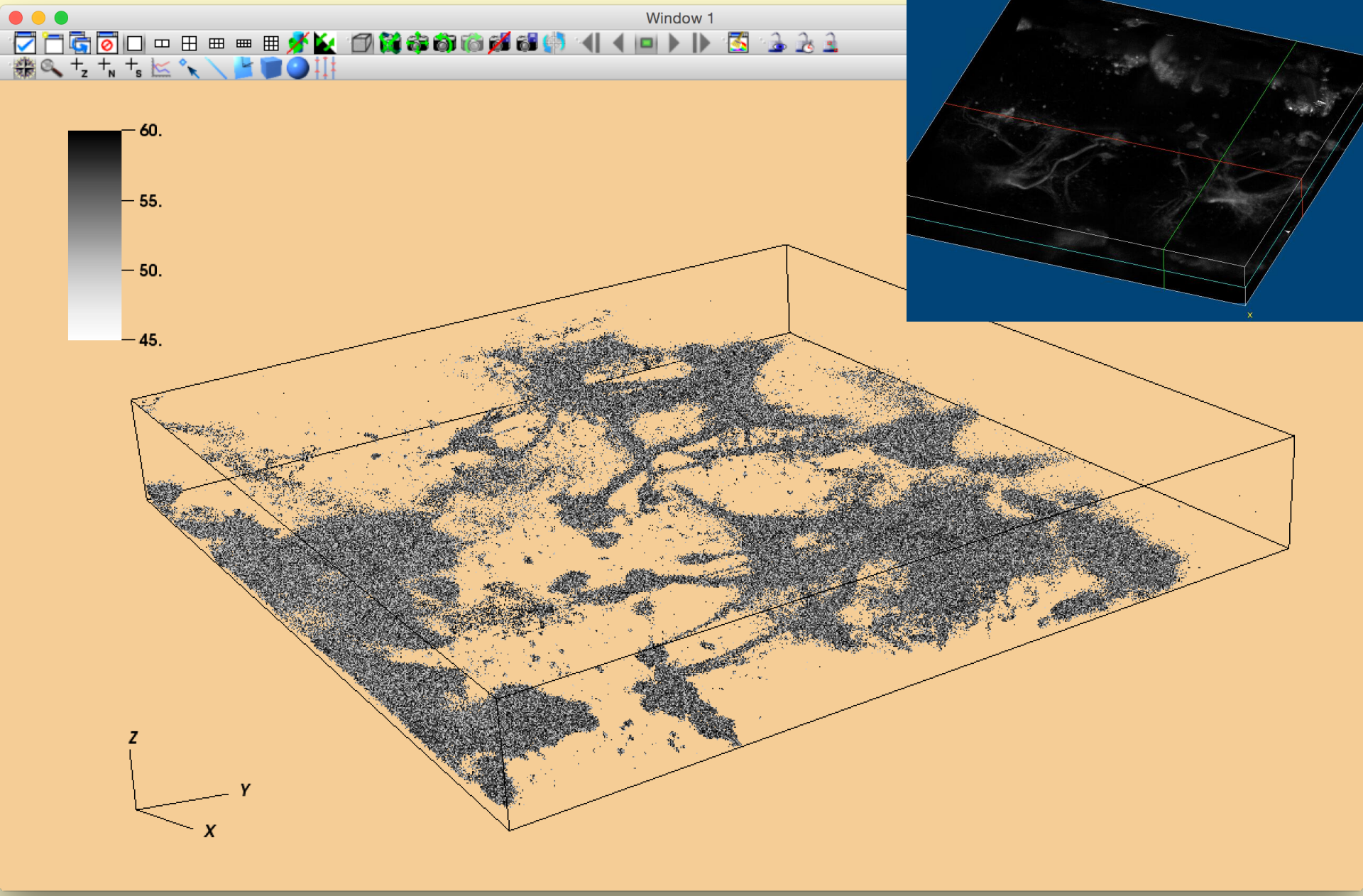
Data Value Selection - Threshold Operator

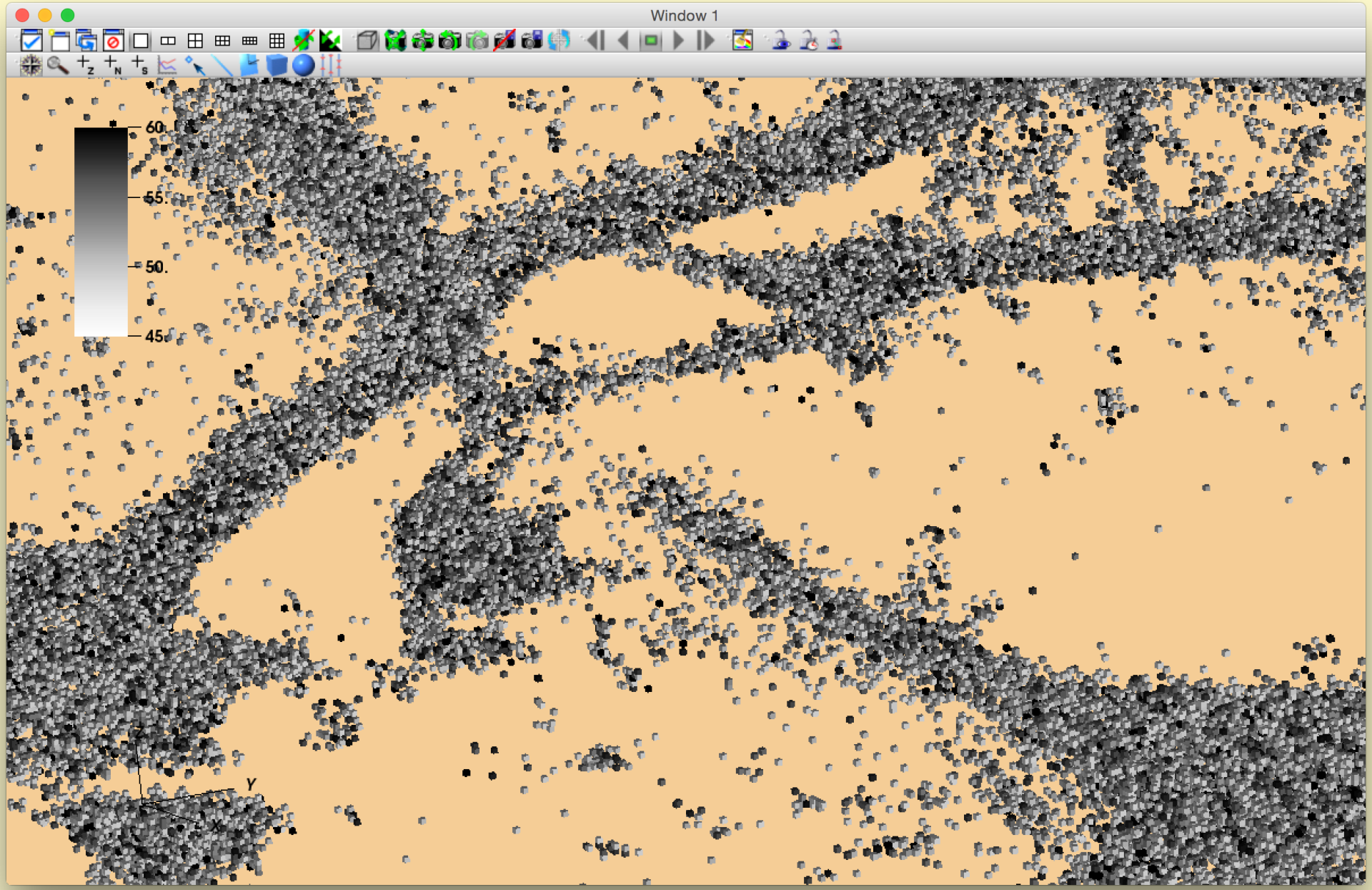
Use this operator to look only at cells that have values within a numerical range.

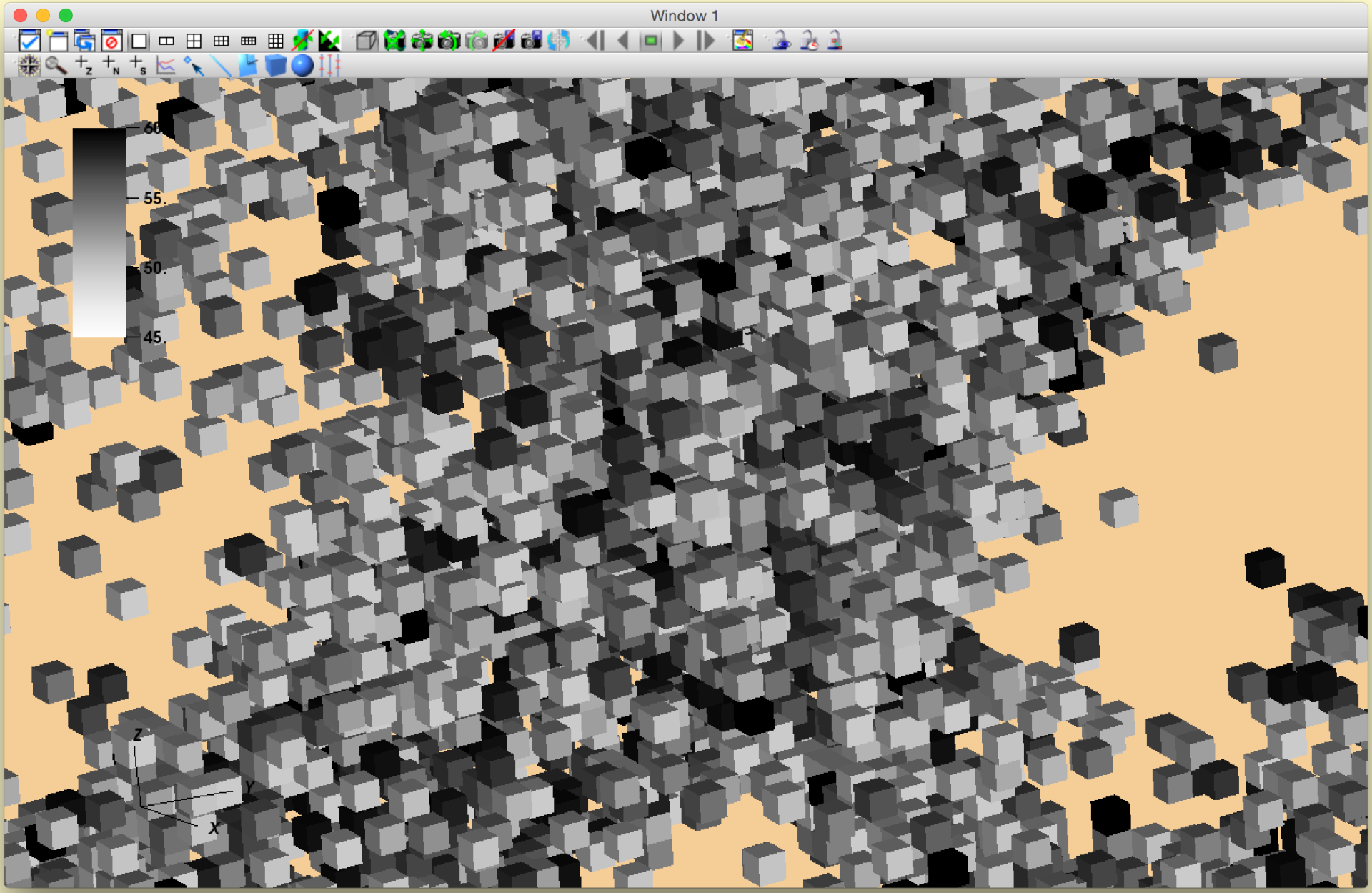
Removes cells whose value is not in the specified range.



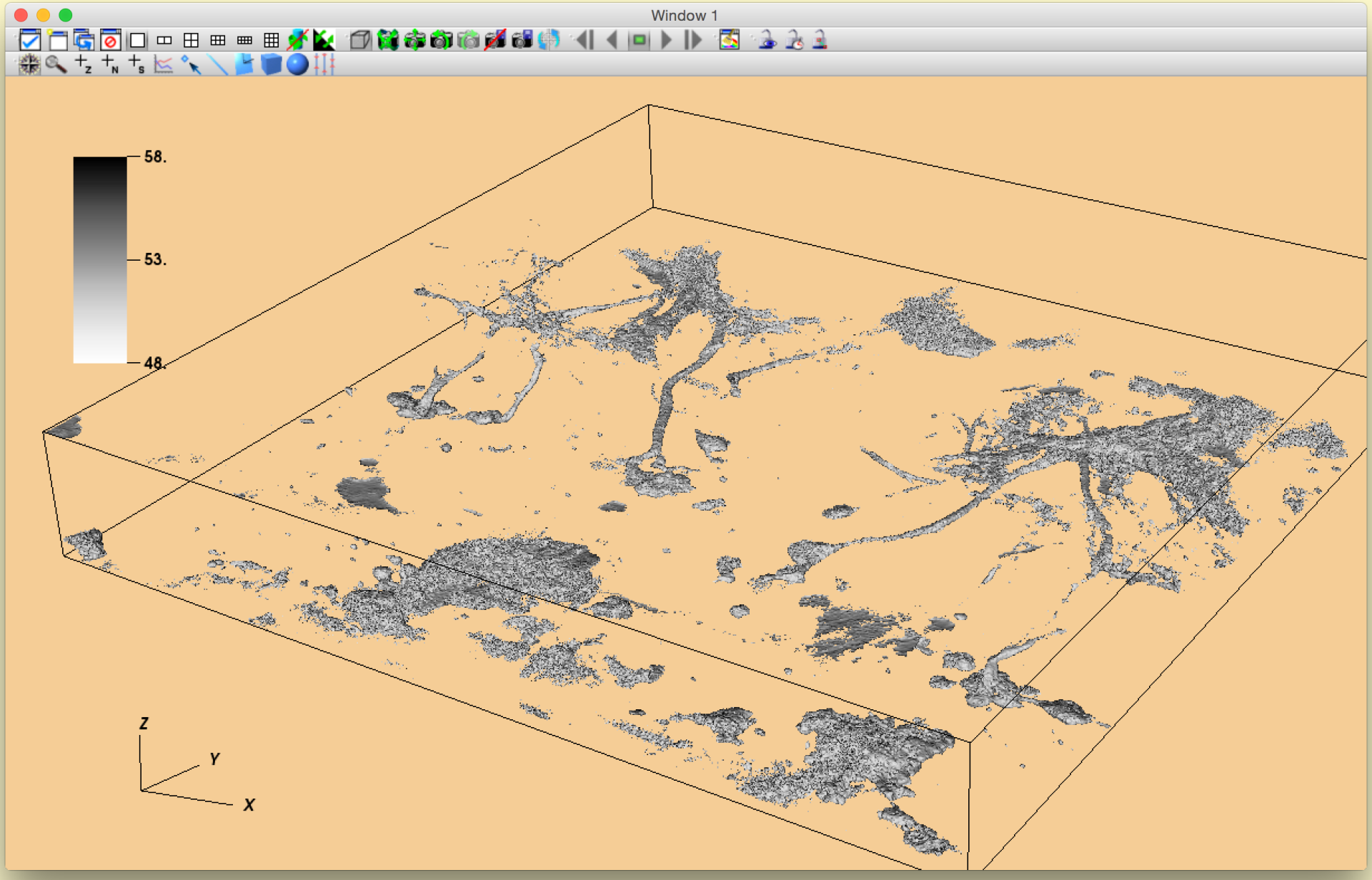
Threshold Operator

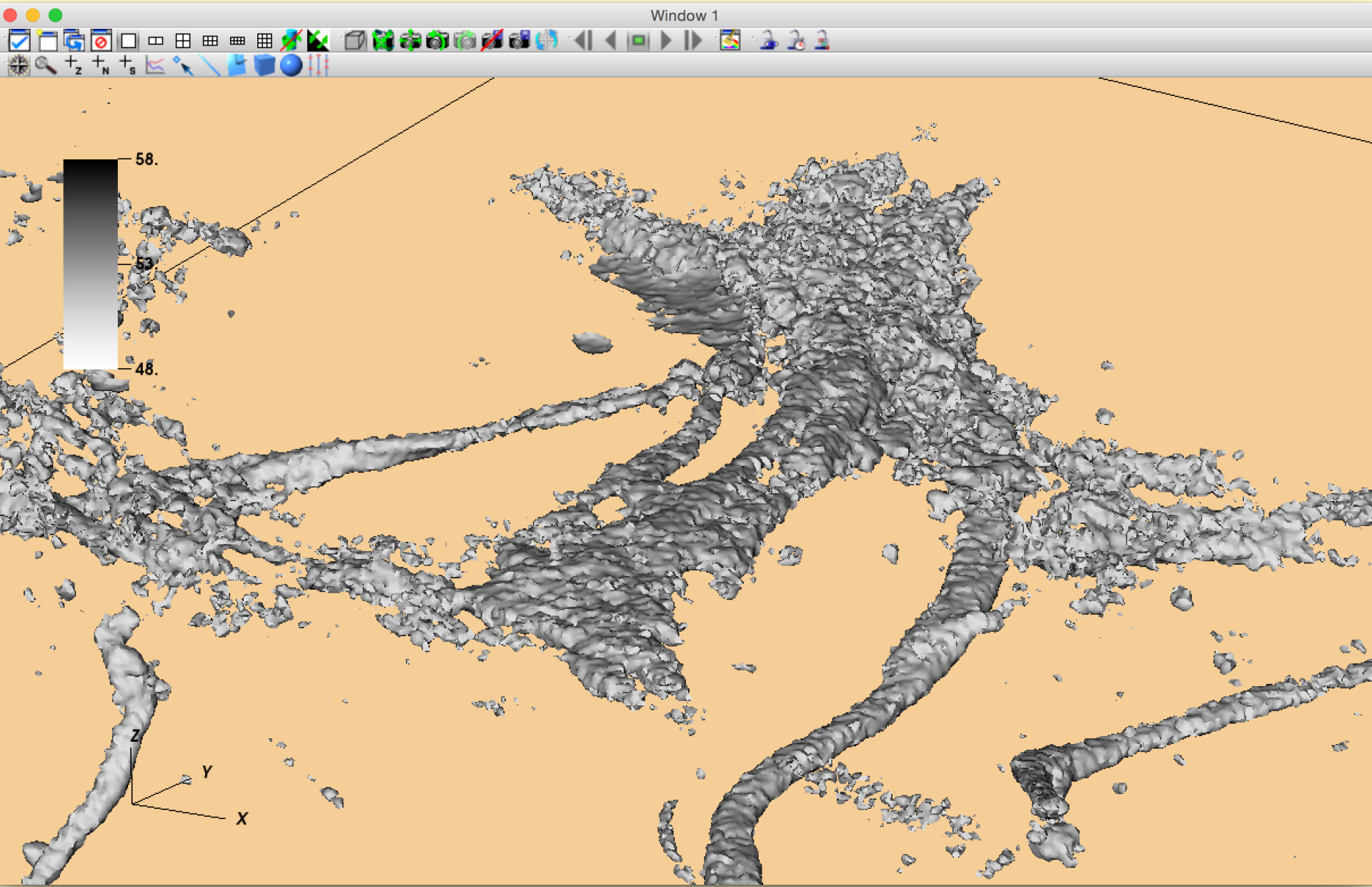



Window 1
60.
55.
50.
45.
Y
X


Window 1
60.
55.
50.
45.
Z
Y
X

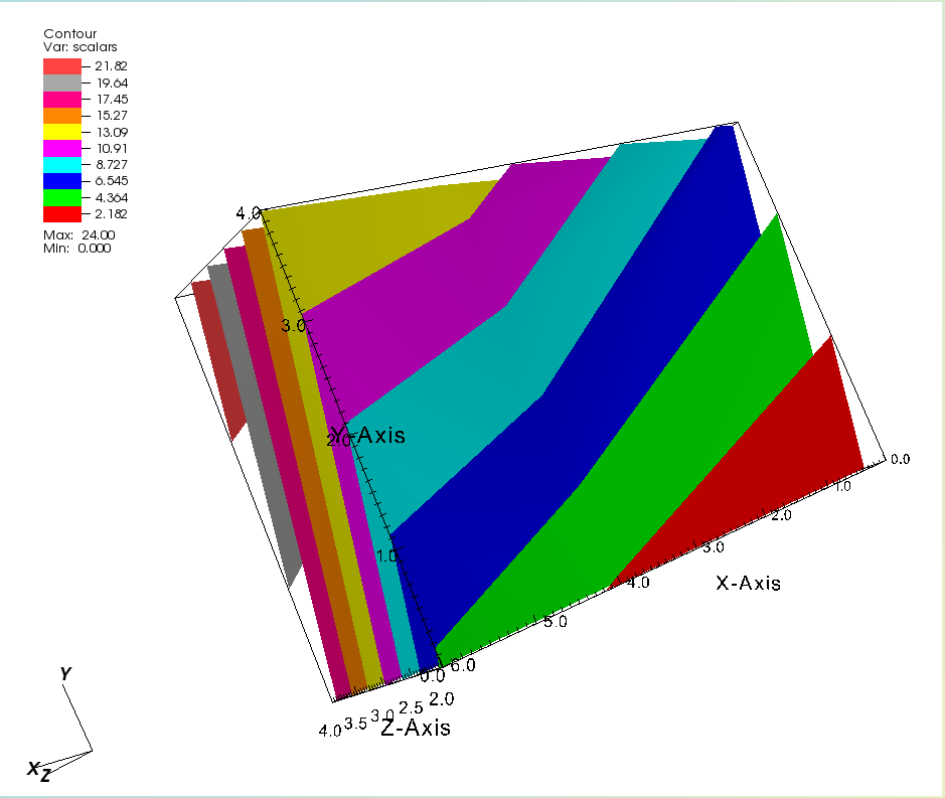
Isovolume Operator

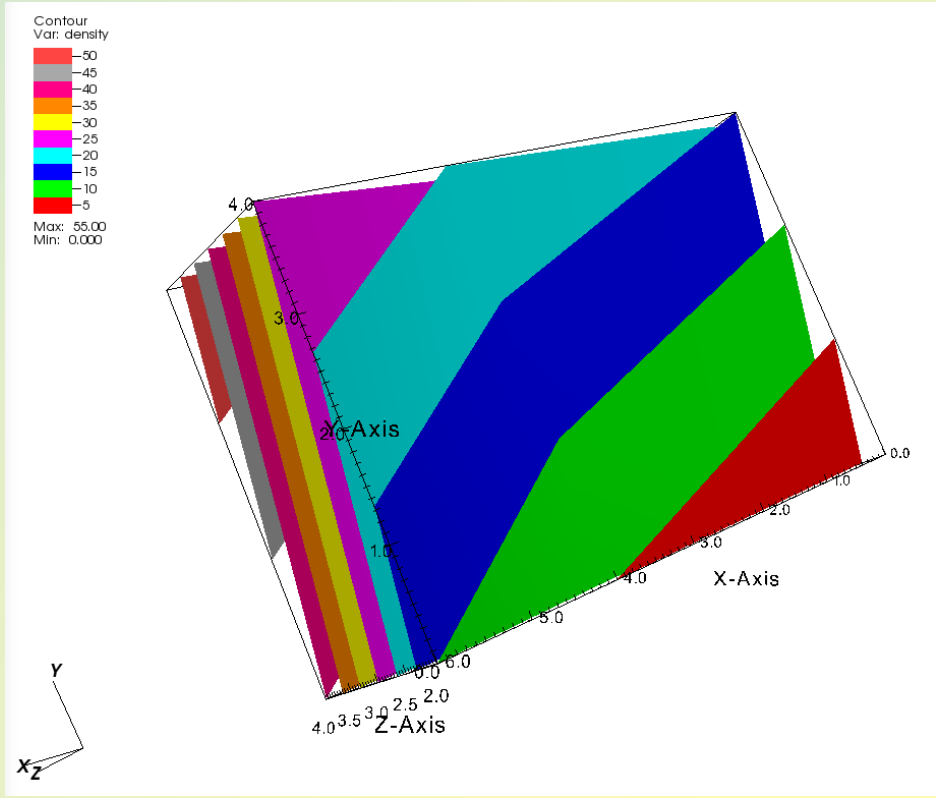


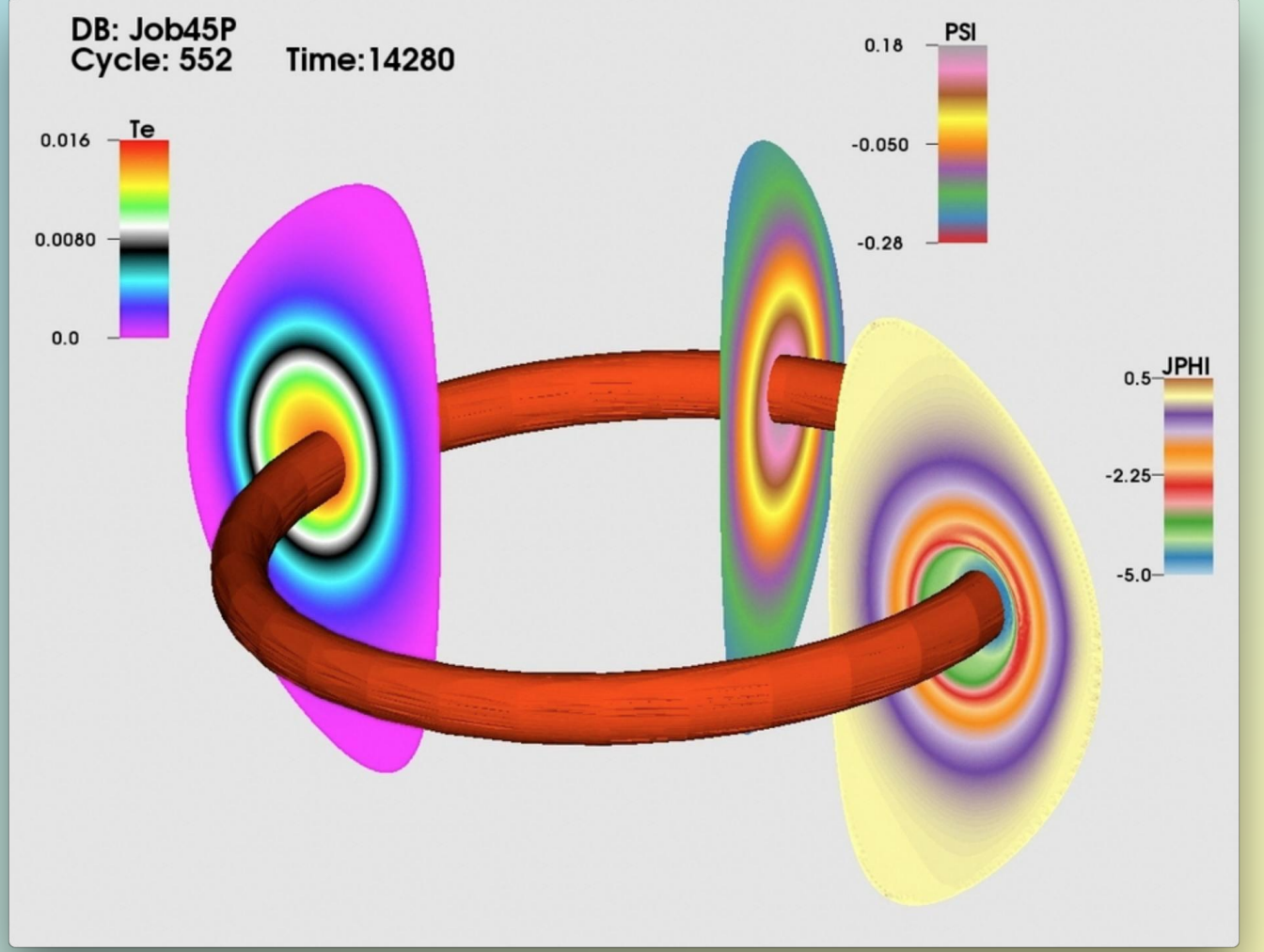

Window 1
58.
53.
48.
Z
Y
X

Data Value Selection – Isosurface Operator

Series of isosurfaces between data min-max.





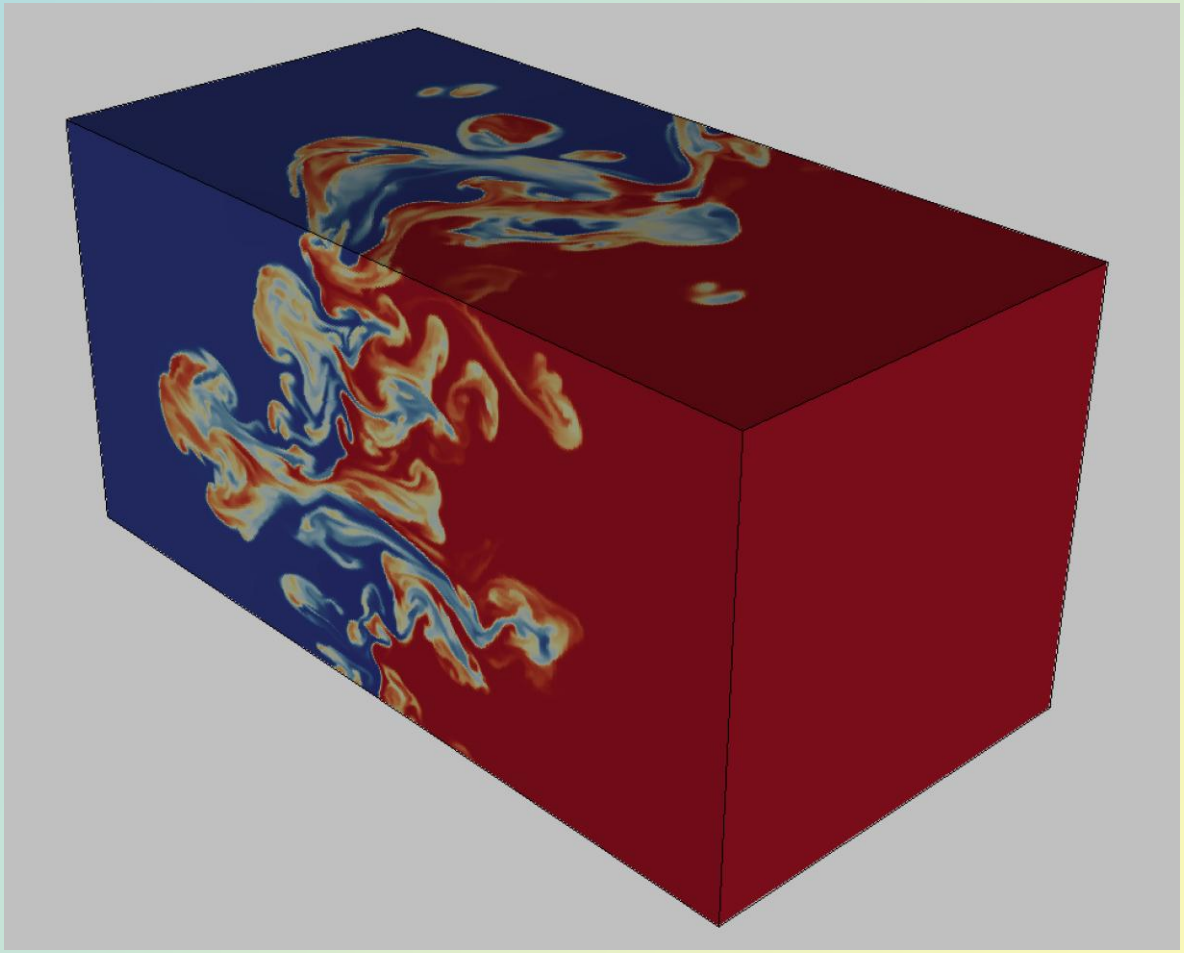


Isosurface of Te = 0.015 at each time step.
Shows Te, PSI, and JPHI concurrently.

http://www.princeton.edu/~efeibush/movies

teiso015.mp4

Operators on Structured Points



https://www.princeton.edu/~efeibush/movies/rt_vis.mp4

Discrete Point Data

Define and display data at specific points in 3D.

Each point is a unique, independent sample.

Taken from compute grid (perhaps).

Look at data file:

```
x y z density
2.5  0.5  -0.1  .003
...
```

Example: `rho2.Point3D`

Polygons vs. Grid

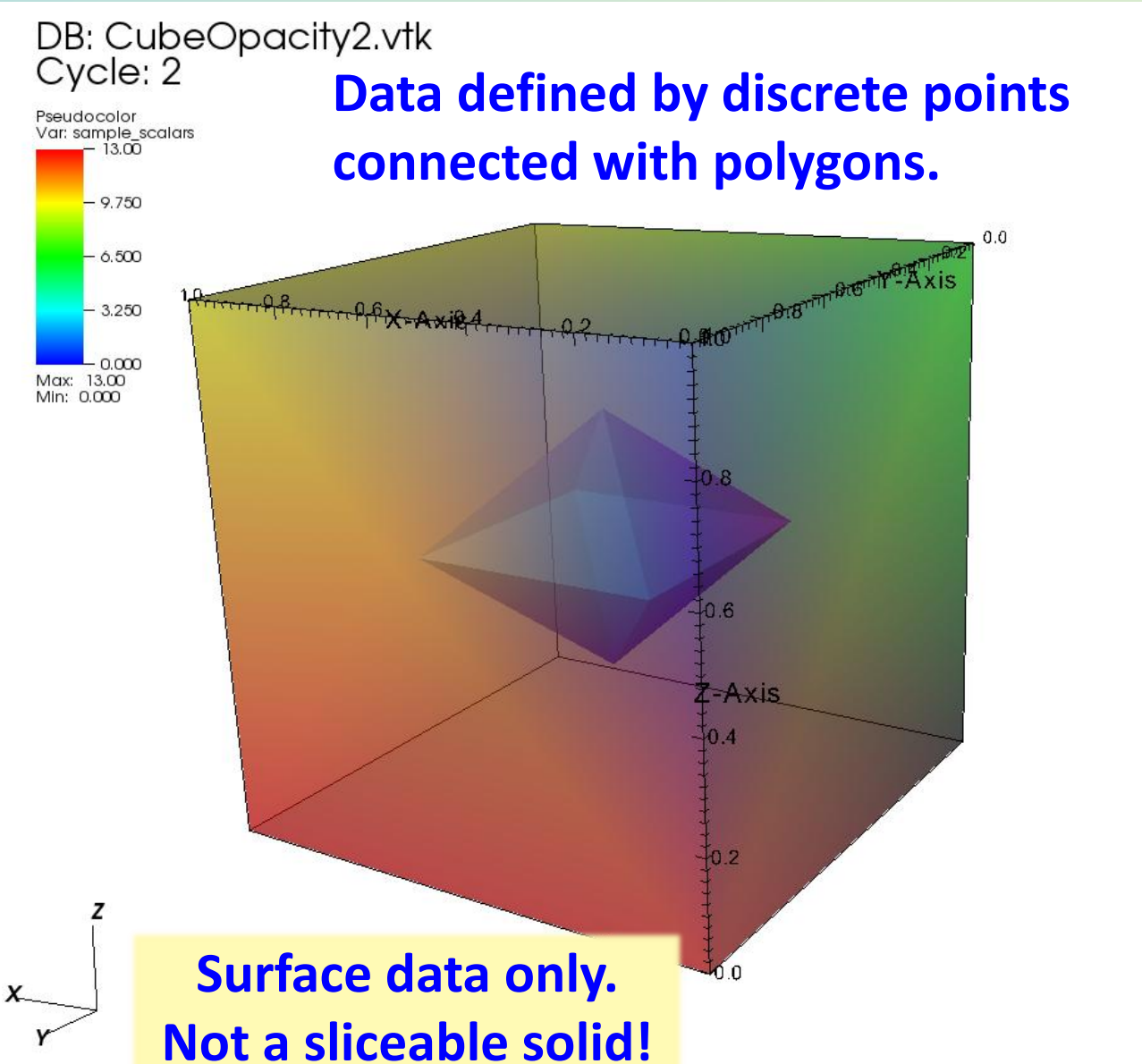
CubeOpacity2

```
# vtk DataFile Version 2.0
Cube example
ASCII
DATASET POLYDATA
POINTS 14 float
0.0 0.0 0.0
1.0 0.0 0.0
1.0 1.0 0.0
0.0 1.0 0.0
0.0 0.0 1.0
1.0 0.0 1.0
1.0 1.0 1.0
0.0 1.0 1.0
0.5 0.5 0.25
0.25 0.25 0.5
0.25 0.75 0.5
0.75 0.25 0.5
0.75 0.75 0.5
0.5 0.5 0.75

POLYGONS 14 62
4 0 1 2 3
4 4 5 6 7
4 0 1 5 4
4 2 3 7 6
4 0 4 7 3
4 1 2 6 5
3 8 9 10
3 8 9 11
3 8 10 12
3 8 11 12
3 11 12 13
3 9 11 13
3 10 12 13
3 9 10 13

POINT_DATA 14
SCALARS sample_scalars float 1
LOOKUP_TABLE my_table
 0.0
 1.0
 2.0
 3.0
 4.0
 5.0
 6.0
 7.0
8 9 10 11 12 13
```

POINTS

POLYGONS

VALUES



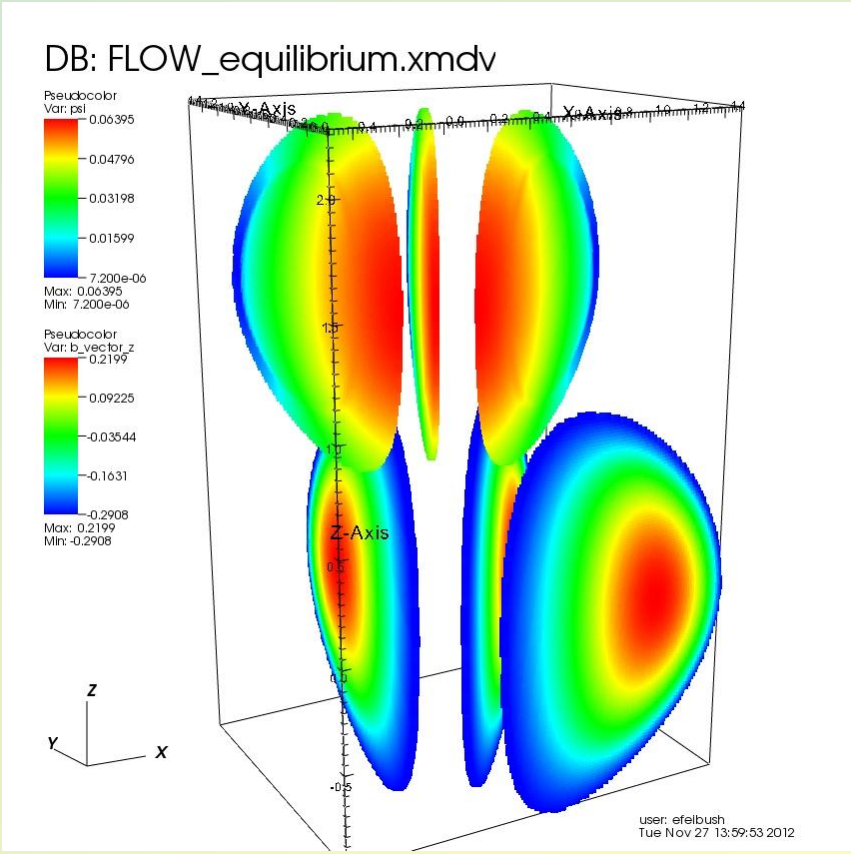
Data defined by discrete points connected with polygons.

Surface data only.
Not a sliceable solid!

Transforms

Relocate geometry

- Translate
- Rotate
- Scale



Try It

Open File

FLOW_equilibrium.xmdv

Add Pseudocolor→psi

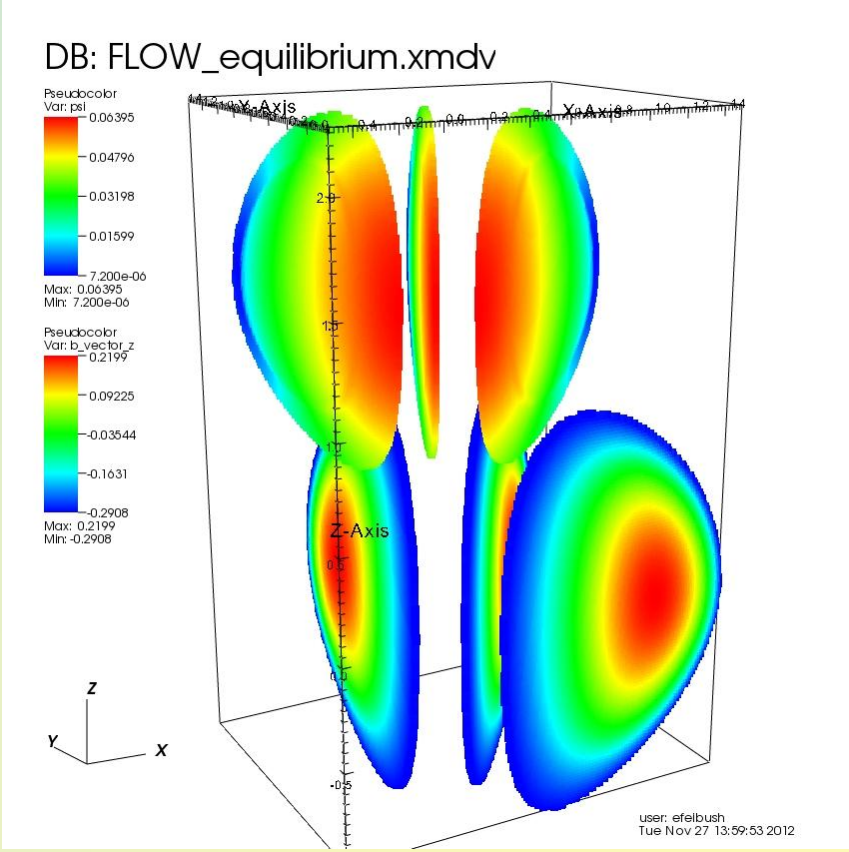
Turn off Apply operators to all plots

Add Pseudocolor→b_vector_z

Operators→Transforms→Transform

Rotate 25 degrees

Translate Z 1.5



xmdv – multiple scalar variables per point

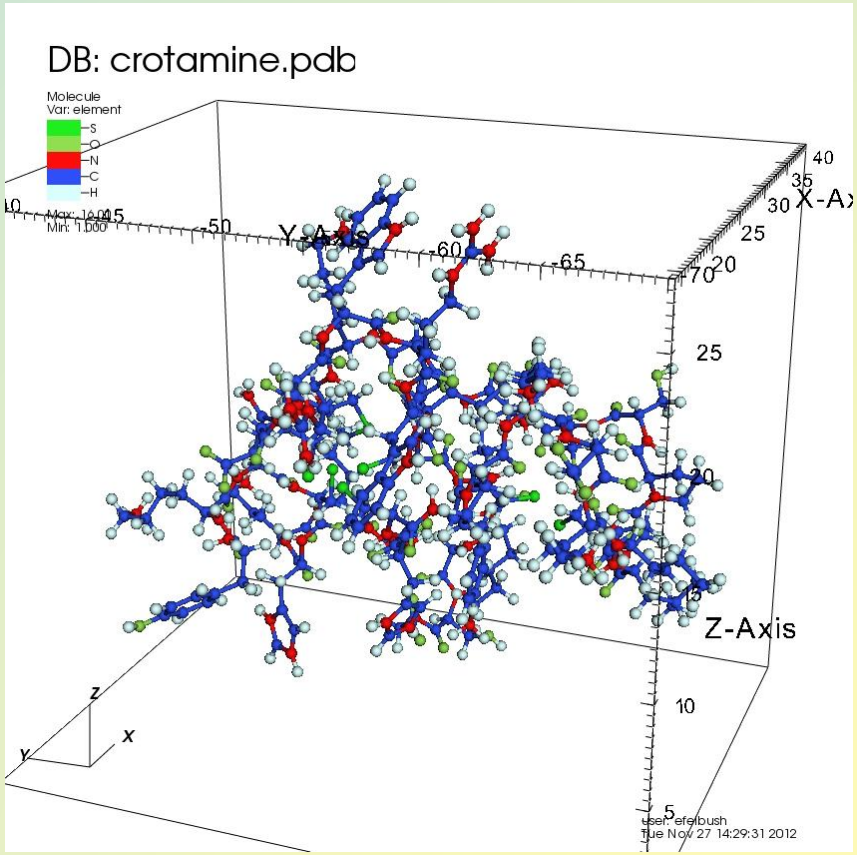
Try It

Open File crotamine.pdb

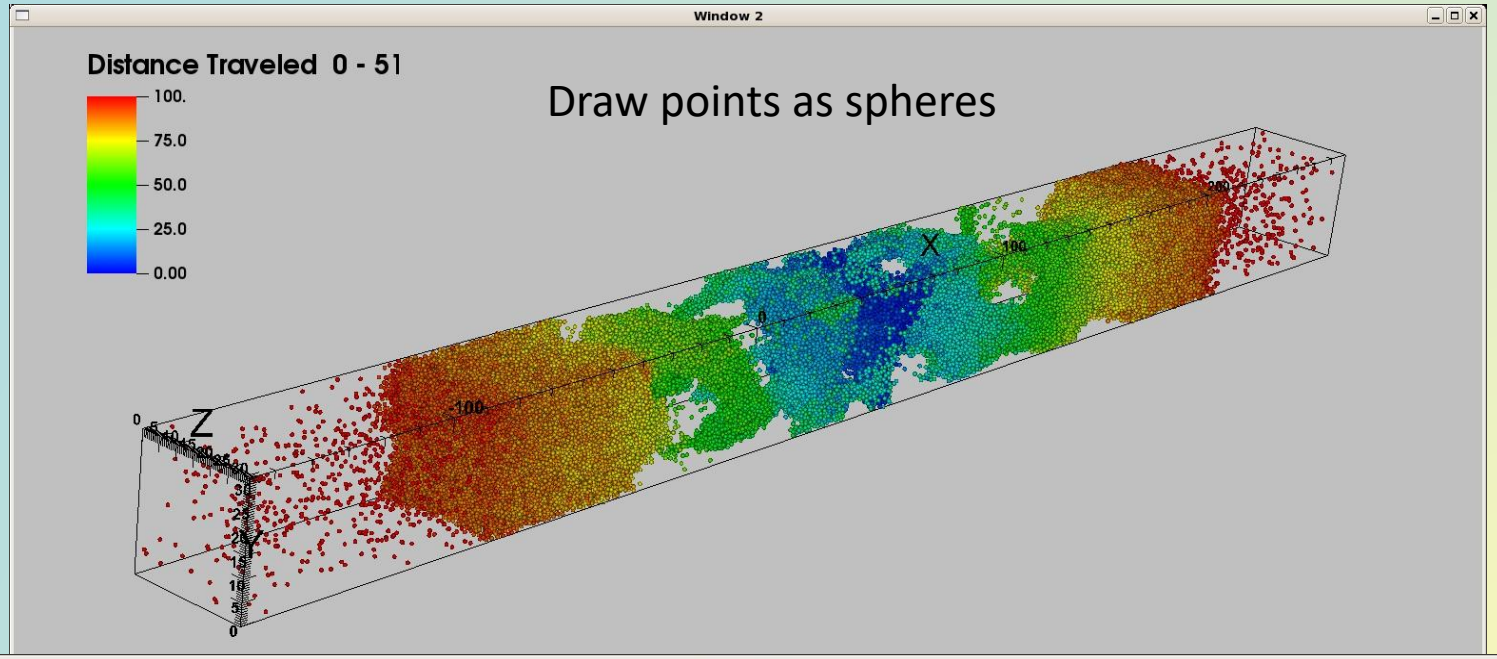
Type: ProteinDataBank

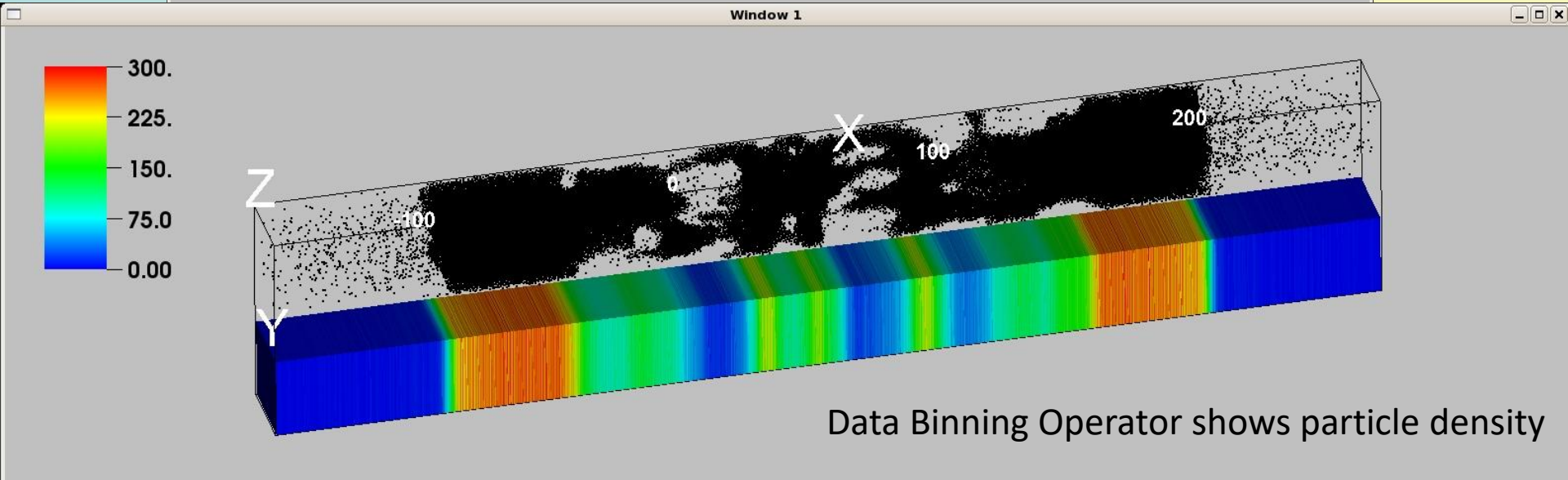
Add Molecule→element

attributes



Molecular Dynamics Example





Data Binning Operator shows particle density

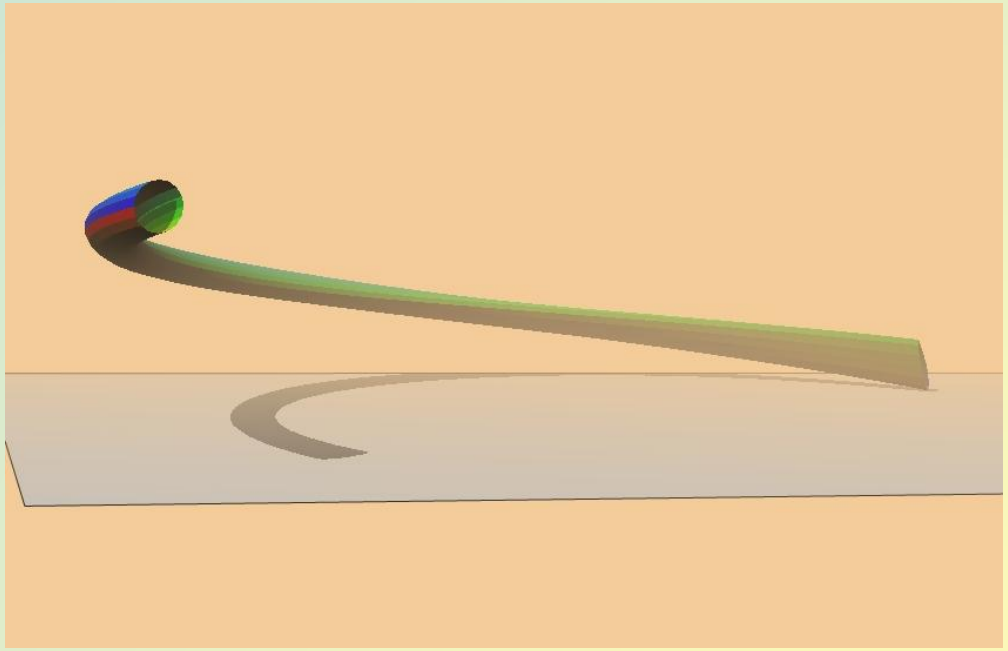
Try It

Open File base.vtk

Open File fluxtube.vtk

Options→Rendering ...

Controls→Lighting



Animation

Time step
Variable index
Geometry change

View
    Operators (slice, clip, etc.)

Simple VTK file time steps
        or
Complex python scripting

jpeg, png files → .mp4 movie

    Python interpreter: Controls → Launch CLI ...

```
>>> Source("rt3slice.py")
```

[edit, retry]

Movie Enhancements

Titles - iMovie, Adobe Premier

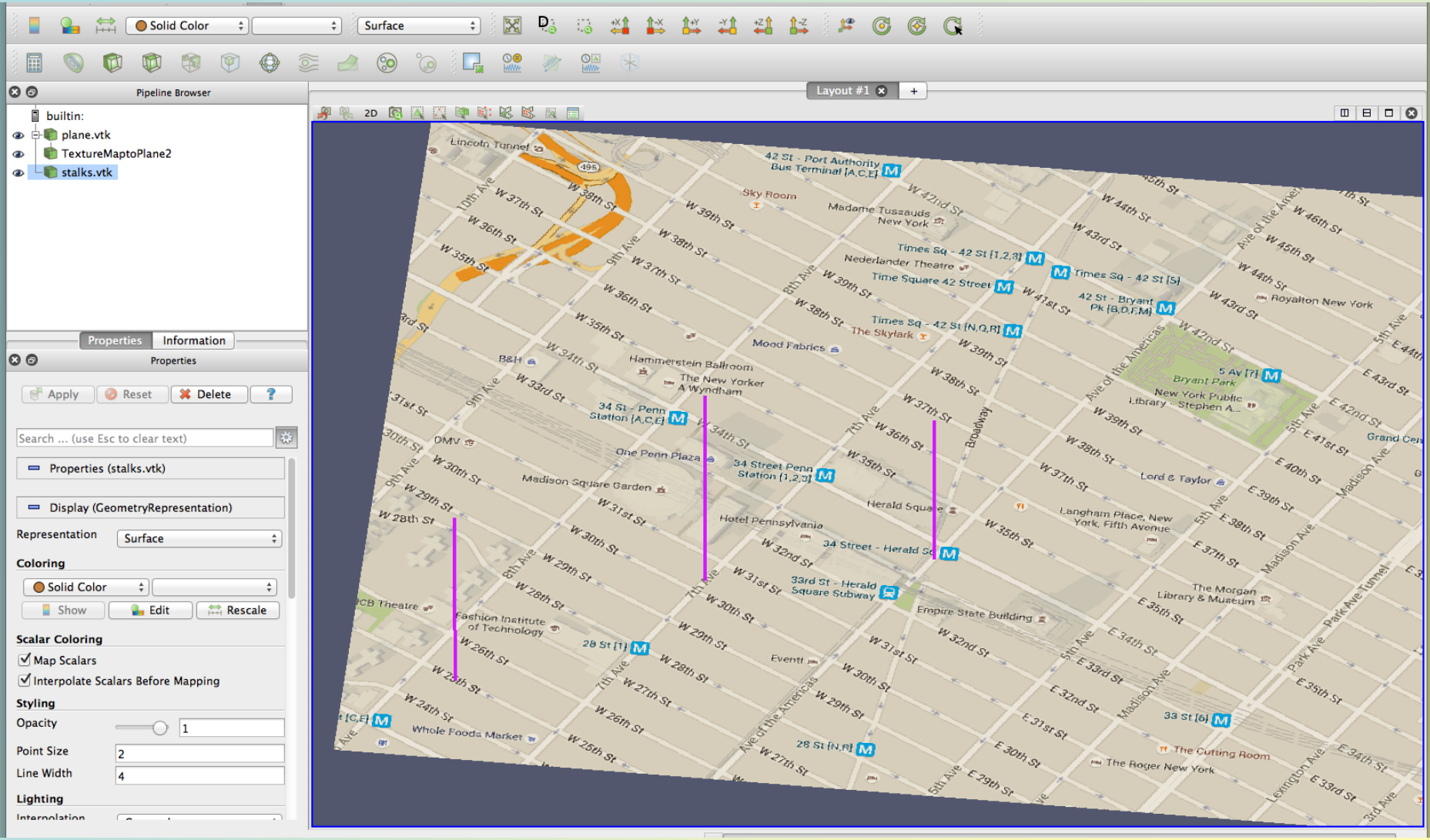
Video

Audio

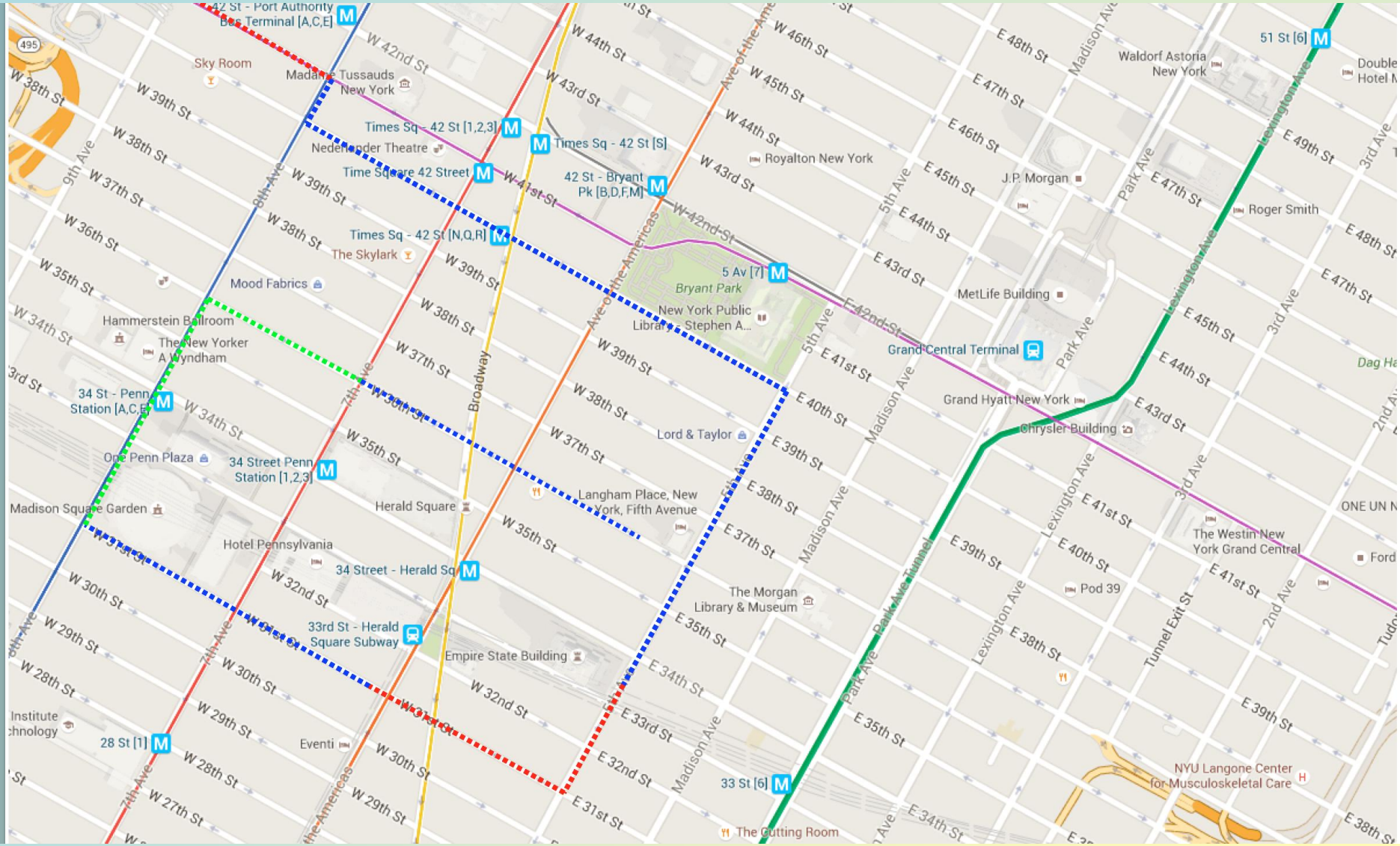
Digital Learning Lab resources

Paraview

Texture Rendering + VTK → 3D View



Geo-Locate with Maps



Summary of Today's Features

Plots + Attributes
- Mesh
- Pseudocolor
  - Points, Lines, Vectors, Polygons, Mesh – Color Tables
- Contour
- Molecule
- Volume

Data files
- VTK
- Point3D, xmdv

Transform operators
- Scale, Rotate, Translate

Selection operators
- Clip
- Box
- Threshold

Slicing operators
- Slice, ThreeSlice
- Isosurface

Viewing

Lighting, Shadow, Depth-Cue

Annotation

Animation
- Simple Time Slider movie
- Python scripting

Images to QuickTime movie

https://visit-dav.github.io/visit-website

Downloads

Releases

Web search for: “visit visualization”

visitusers.org search …

Getting Data Into VisIt - document (& your project)

VTK - text or binary

VTK File Formats - vtk.pdf on my website
www.princeton.edu/~efeibush

Visualization with VisIt mini-course

paraview.org

Remote Vis at Princeton

Large amount of data on Princeton cluster.

Display without transferring data.

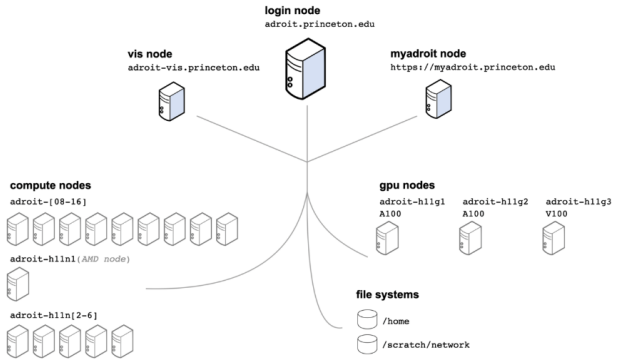
Render on vis node GPU instead of laptop.

Adroit

Overview

The Adroit cluster is intended for running smaller jobs, as well as developing, debugging, and testing codes. Despite being one of our smaller clusters, Adroit is built like our larger clusters (such as **Della** or **Tiger**), and is therefore ideal to use as training for eventual work on the larger clusters.

Some Technical Specifications:
Adroit is a Beowulf cluster acquired through a partnership between Dell Computer Corporation and OIT. The compute nodes on the "all" partition have 64 CPU-cores and 512 GB of memory while those on the "class" partition have 32 CPU-cores and 384 GB RAM. There is one AMD node with 128 CPU-cores. Run the "snodes" command for more information. There are also three nodes with GPUs and a visualization node. For more details, see the Hardware Configuration section below.



Schematic diagram of the Adroit cluster.

myadroit.princeton.edu

How to Access the Adroit Cluster

To use the Adroit cluster you have to request an account on Adroit and then log in through SSH.

Requesting Access to Adroit

If you would like an account on Adroit, please fill out the **Adroit Registration** form to request an account.

Logging into Adroit

Once you have been granted access to Adroit, you can connect by opening an **SSH client** and typing the following SSH command (**VPN** required from off-campus):

```
$ ssh <YourNetID>@adroit.princeton.edu
```

For more on how to SSH, see the Knowledge Base article **Secure Shell (SSH)**. If you have trouble connecting then see **SSH troubleshooting**.

MyAdroit Web Portal

If you prefer to navigate Adroit through a graphical user interface rather than the Linux command line, Adroit has a web portal option called MyAdroit (**VPN** required from off-campus):

https://myadroit.princeton.edu

Contact

Eliot Feibush ---- efeibush@princeton.edu

www.princeton.edu/~efeibush/viscourse

Visualization Help:

visrc@princeton.edu

Computing Help:

researchcomputing.princeton.edu

Support --> Submit a ticket

Try It

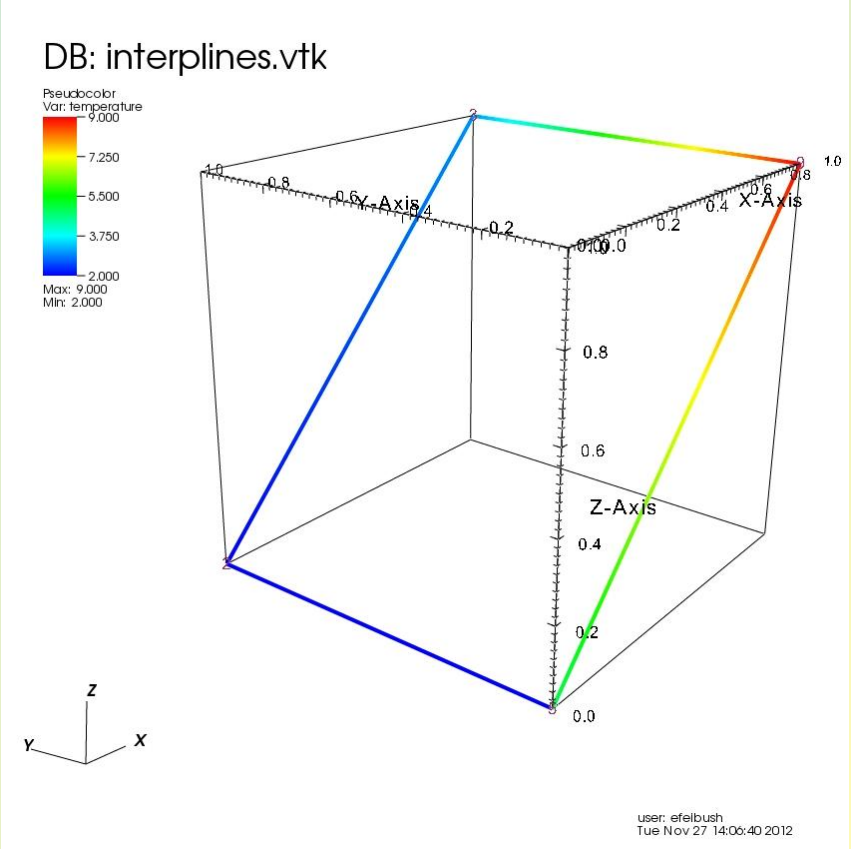
Open File interplines.vtk

Add Pseudocolor

temperature

Add Label

temperature



Example of data defined by discrete points connected with lines.