Scientific Visualization

Tools & Techniques

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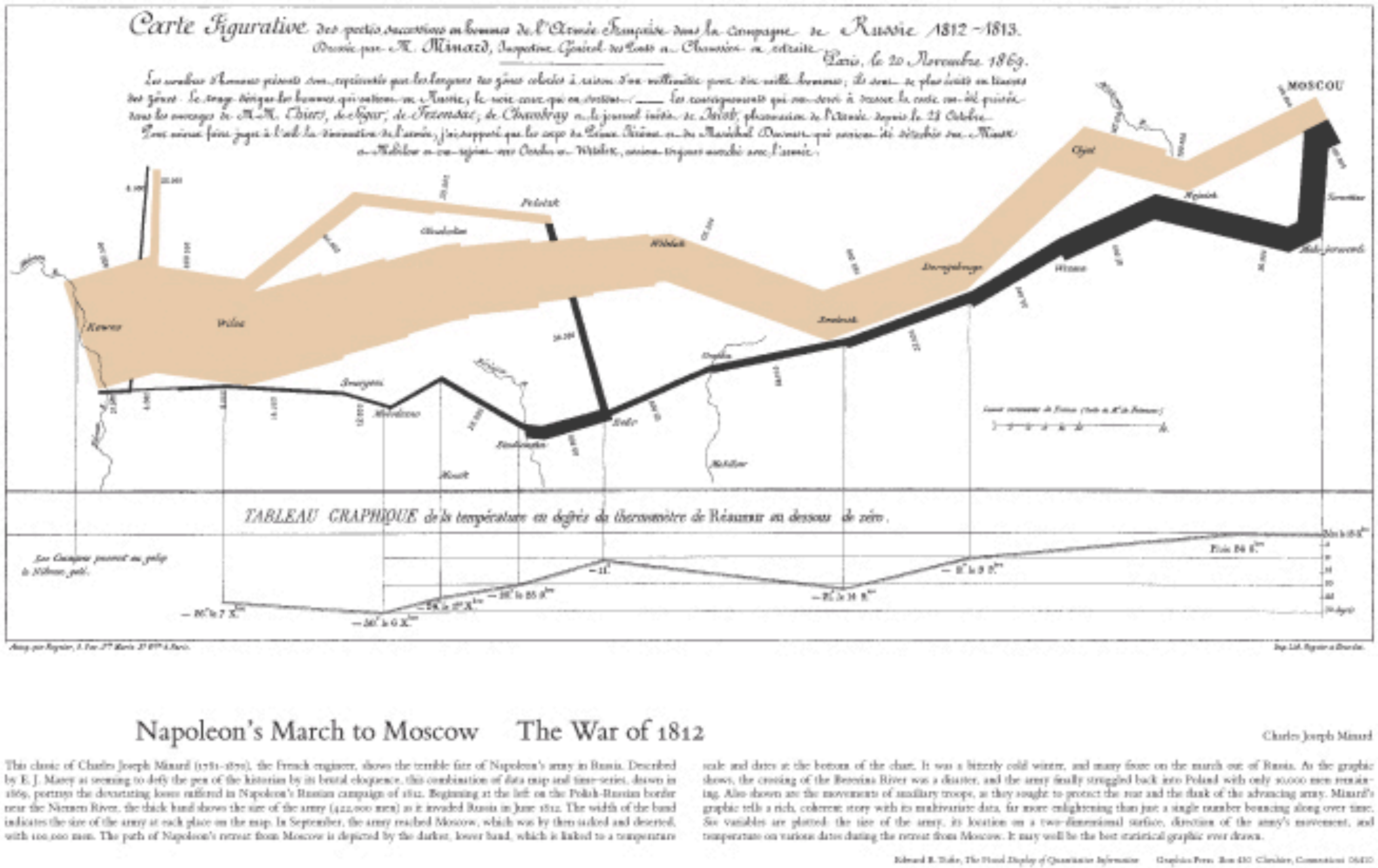
CPPG Seminar

September 26, 2018

Early Multivariate Data Vis

Not so good for Napoleon in 1812



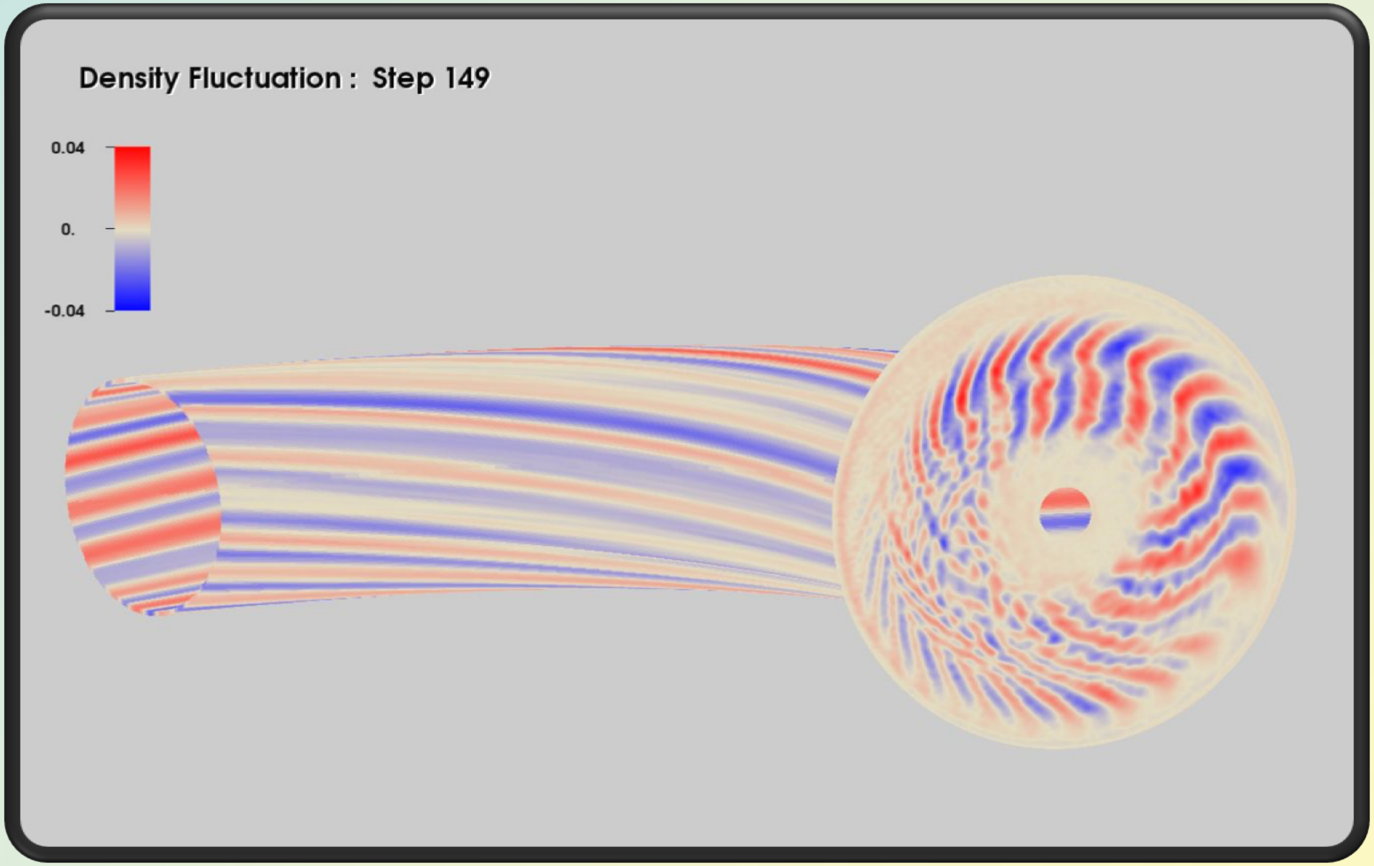
Credit: Edward Tufte via Charles Minard 1869

Modern Scientific Data Vis

Simulate

or

Acquire



Analyse **Visualize**

Scientific Visualization

Simulations generate data.

Acquire data from experiments.

- GTS
- XGC
- M3D-C1
- MDSplus
    - ...

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

Designing a Visualization

I want a visualization of my Phase Space model.

Physicist

Map your data to a plot type.

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)

Presentation

Dimensionality 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.

Python

Very convenient for converting data to vis formats.

Analyze & extract.

Good economy for programmer/user.

matplotlib

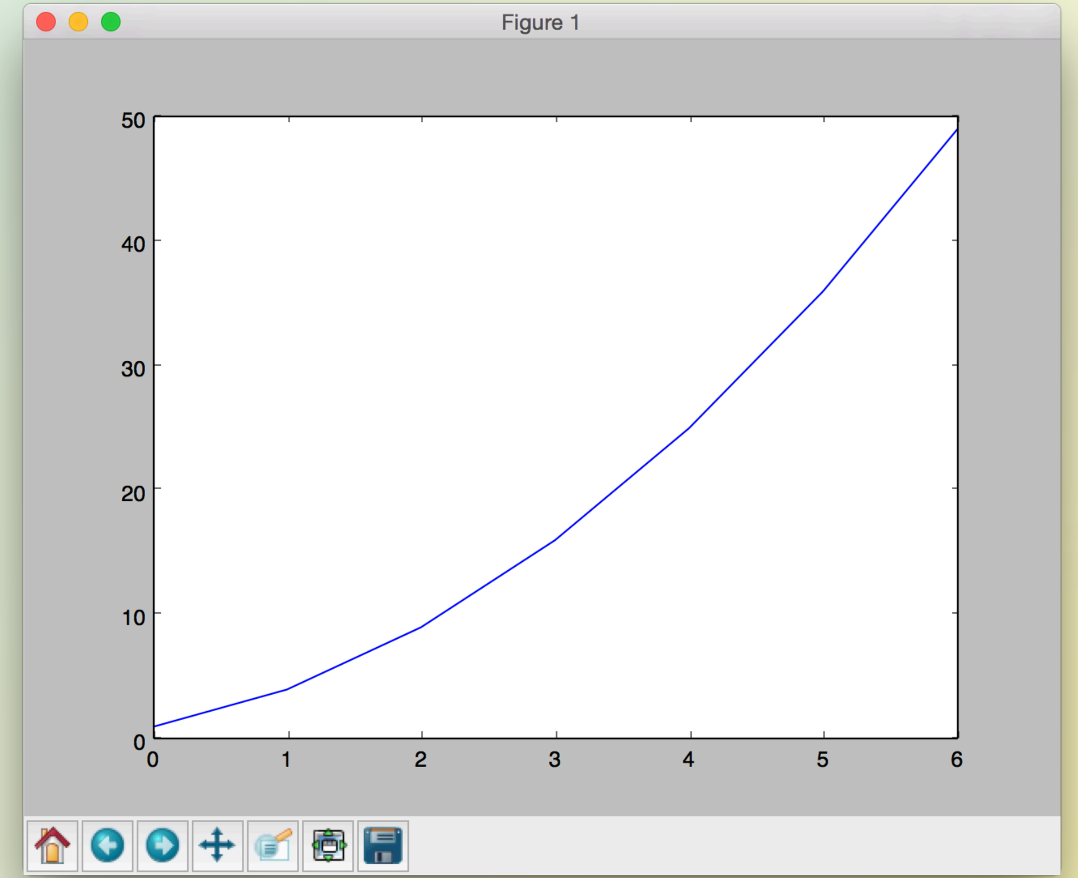
Examples: *f(x), f(x,y), f(x,y,t)*

numpy, scipy, PIL

tkinter

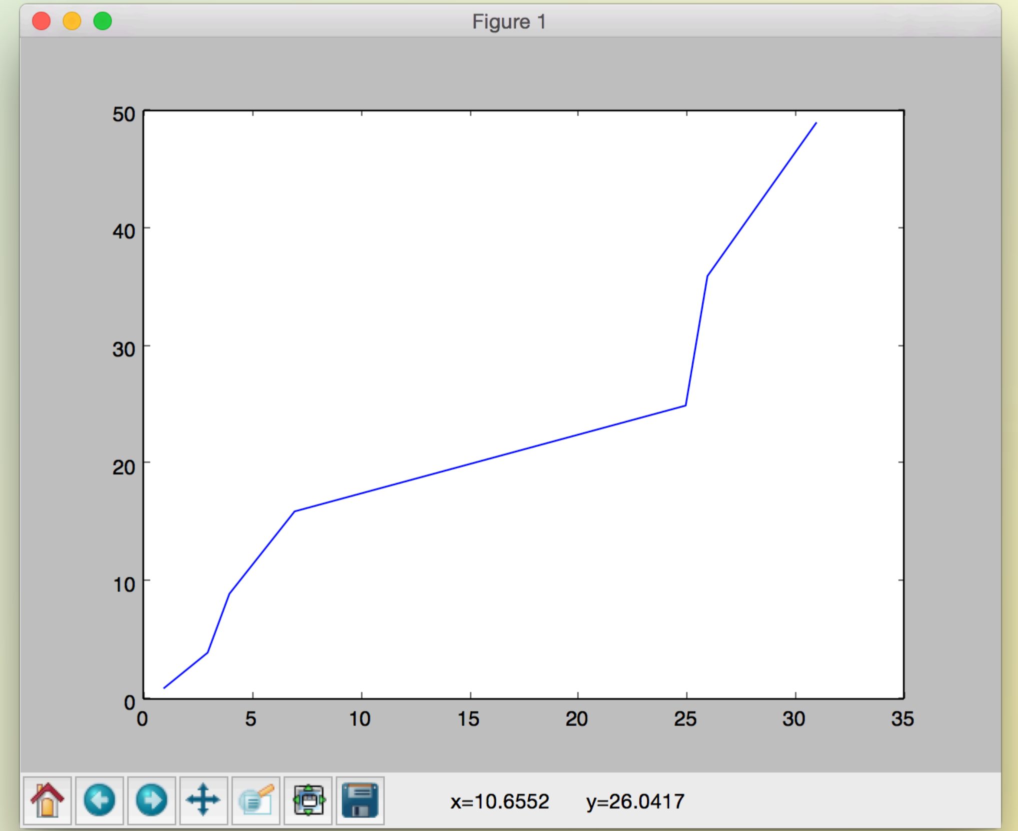
matplotlib *f(x)*

```
import matplotlib.pyplot as plt
y = [1, 4, 9, 16, 25, 36, 49]
plt.plot(y)
plt.show()
```



matplotlib *f(x)*

```
import matplotlib.pyplot as plt
y = [1, 4, 9, 16, 25, 36, 49]
x = [1, 3, 4, 7, 25, 26, 31]
plt.plot(x,y)
plt.show()
```



---

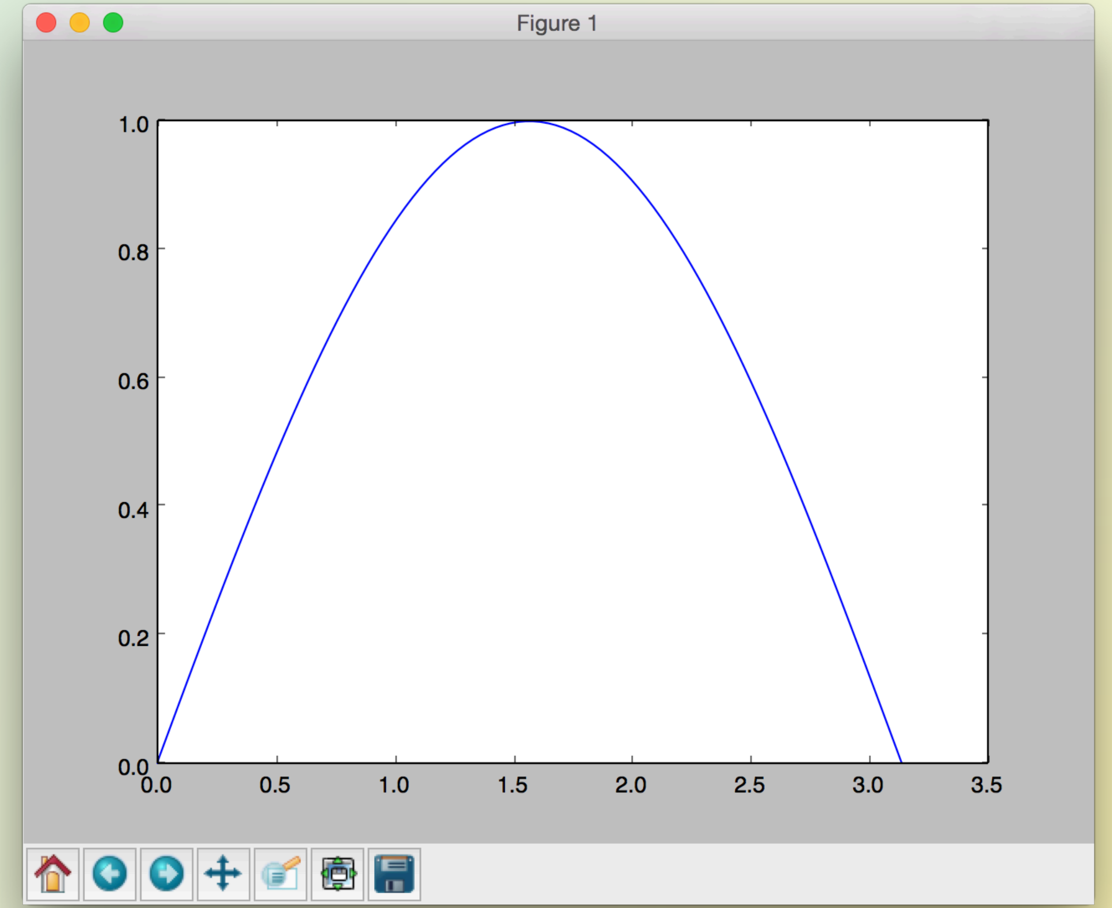
matplotlib.org

docs, API

Examples, Tutorials

matplotlib + numpy *f(x)*

```
import matplotlib.pyplot as plt
import numpy
x = numpy.arange(0., numpy.pi, .01)    # loop with floats
y = numpy.sin(x)
plt.plot(x,y)
plt.show()
```



x and y are
1D numpy.ndarray

arange takes floats

Anaconda Python

Very good distribution of Python.

Integration of packages: numpy, scipy, PIL, many others

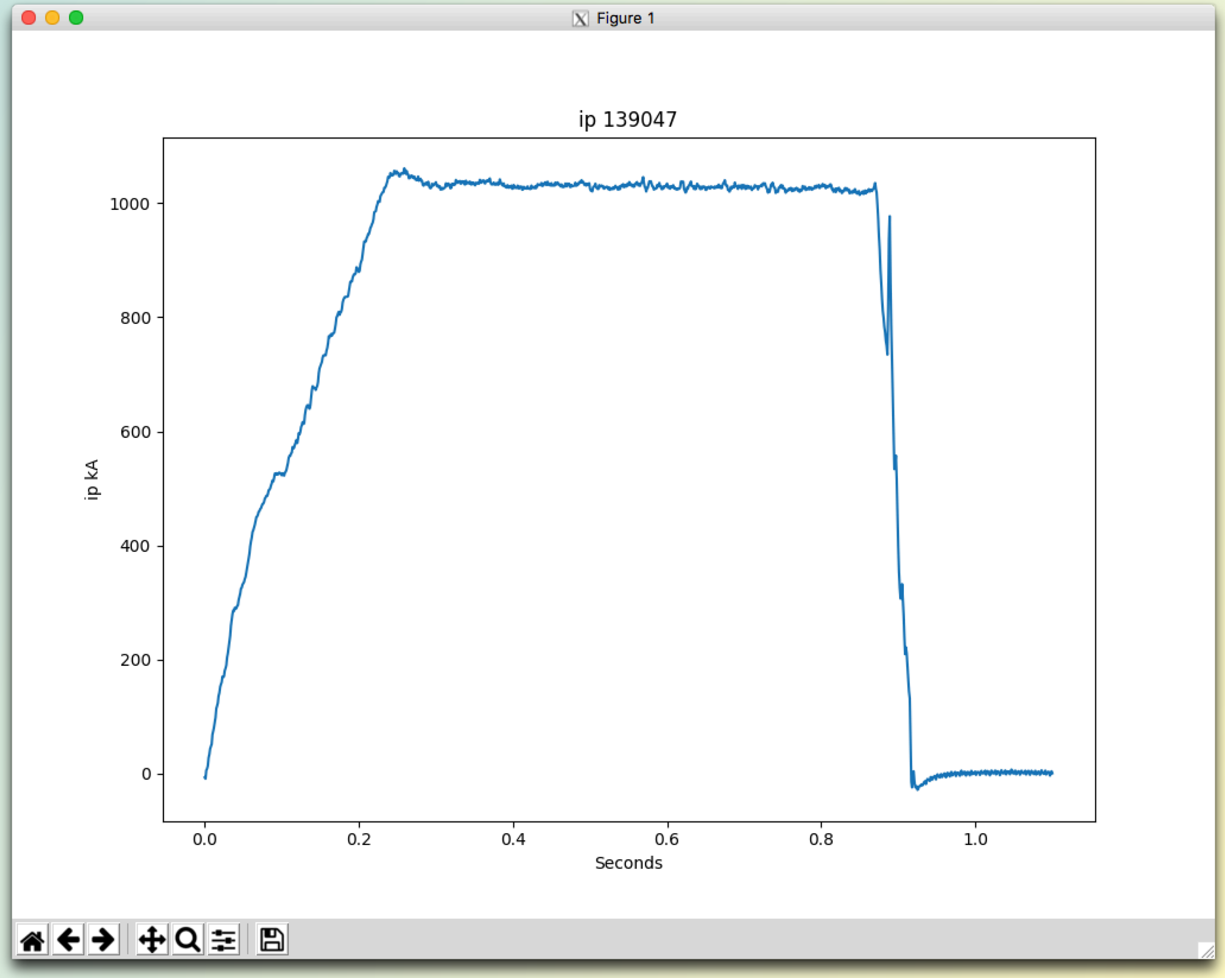
- Free
- Mac, Windows, Linux
  - /usr/pppl - module avail anaconda

Mac – do not change your original python

- *Used by OS, Safari, etc.*

Python – Read from MDSplus

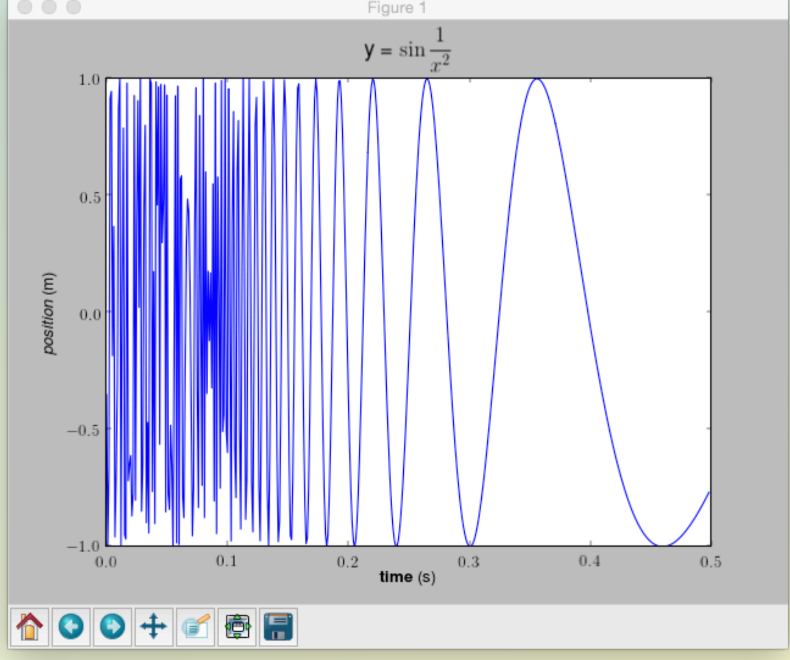
```
module load nstx
module load anaconda2/4.4.0
```



```
import MDSplus

shot = 139047
tree = MDSplus.Tree("nstx", shot, "Readonly")       # MDSplus.tree.Tree

ipNode = tree.getNode("\\ip")      # MDSplus.treenode.TreeNode   "\\ip" becomes \ip
tree.setDefault(ipNode)

signal = ipNode.getData()          # MDSplus.compound.Signal
                                   #   can also access by ipNode.record
print signal.units                 # MDSplus String type, not just str

ipA = signal.data()                # numpy.ndarray is data to plot
xAxis = signal.dim_of()            # MDSplus.compound.Dimension
axis = xAxis.getAxis()             # MDSplus.compound.Range
print axis.units                   # MDSplus.mdsscalar.String
descs = axis.getDescs()            # tuple NoneType, NoneType, MDSplus.mdsscalar.Float32
xIncr = descs[2].value

x = 0.
xL = []   # x axis values

for i in range(len(ipA)):
    xL.append(x)
    x += xIncr
```

```
import matplotlib.pyplot as g

g.plot(xL, ipA)
g.title("ip " + str(shot))
g.xlabel(str(axis.units))
g.ylabel("ip " + str(signal.units))

g.show()

# /u/efeibush/python/mdsplus/ipPlot.py
```

Latex in Graphs



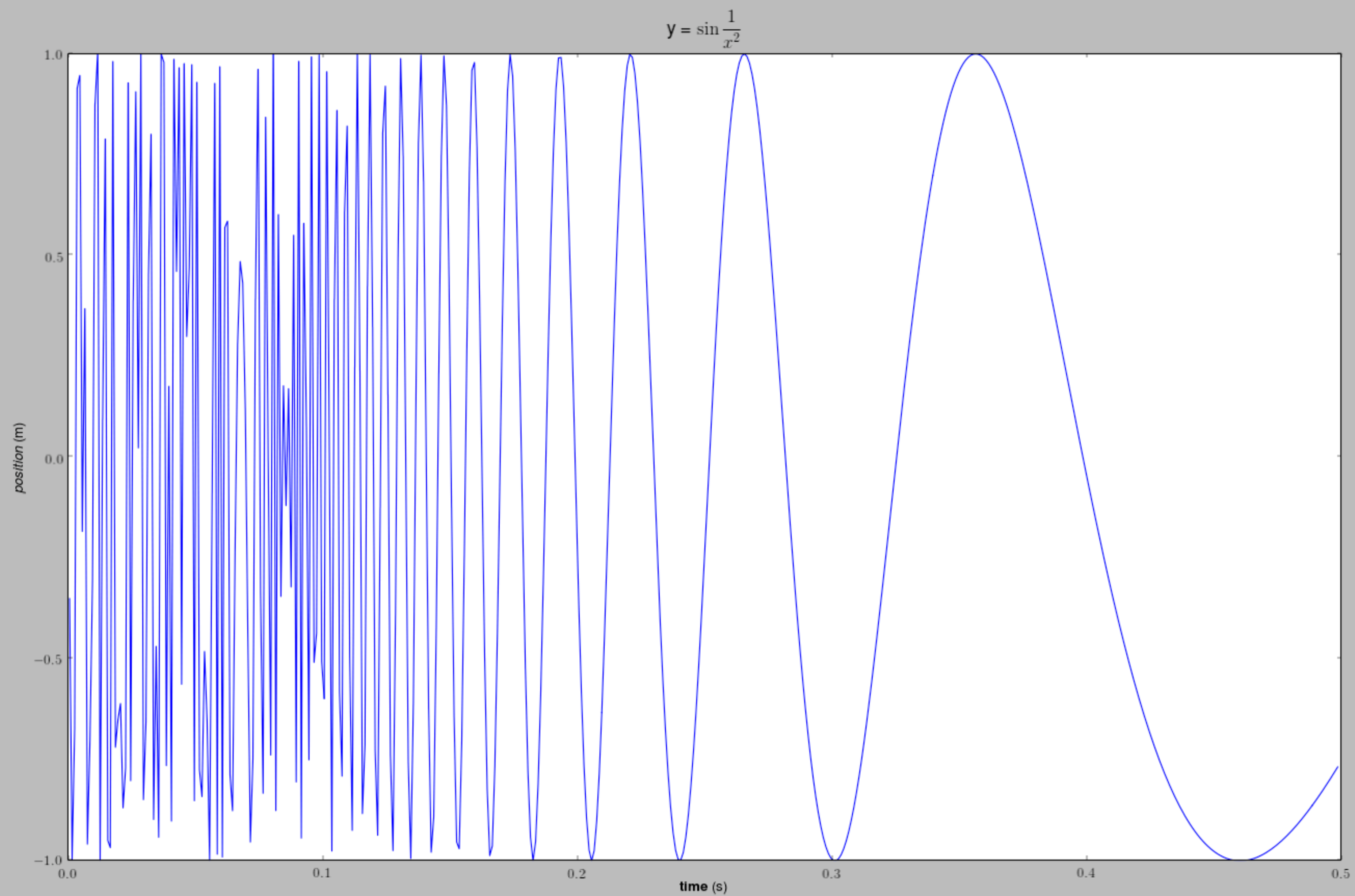
export PATH=$PATH:/Library/TeX/texbin

```
plt.rc(“text”, usetex=True)
plt.plot(x,y)
plt.xlabel(r"\textbf{time} (s)")
plt.ylabel(r"\textit{position} (m)")
```

raw string r before quotes *escapes* tex format instead of \t becoming a tab character

```
plt.title(r"y = "
   r"$\displaystyle\sin\frac{1}{x^2}$",
   fontsize=16)

plt.show()
```

Python system call to /usr/bin/latex on portal is OK.



y = $\sin\frac{1}{x^2}$
1.0
0.5
0.0
−0.5
−1.0
position (m)
0.0
0.1
0.2
0.3
0.4
0.5
time (s)

matplotlib – Save to PDF File

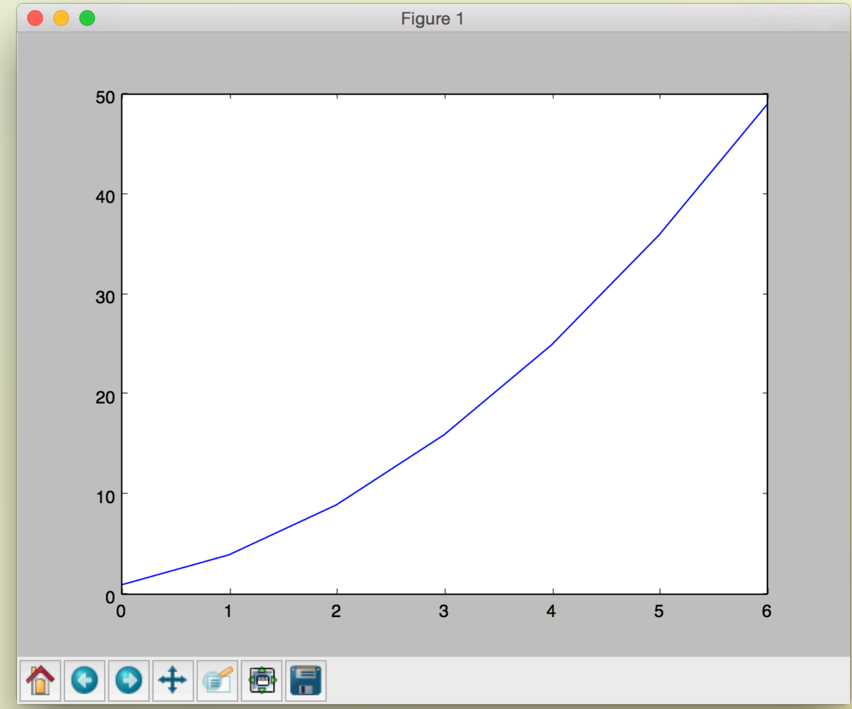
```
import matplotlib.pyplot as plt
```

```
from matplotlib.backends.backend_pdf import PdfPages
pdfp = PdfPages('multipage.pdf')    # starts pdf file, 1 plot per page
```

```
y = [1, 4, 9, 16, 25, 36, 49]
plt.plot(y)
```

```
plt.savefig(pdfp, format='pdf')
          # save fig to file before showing
pdfp.close()      # after last save fig
```

```
plt.show()
```

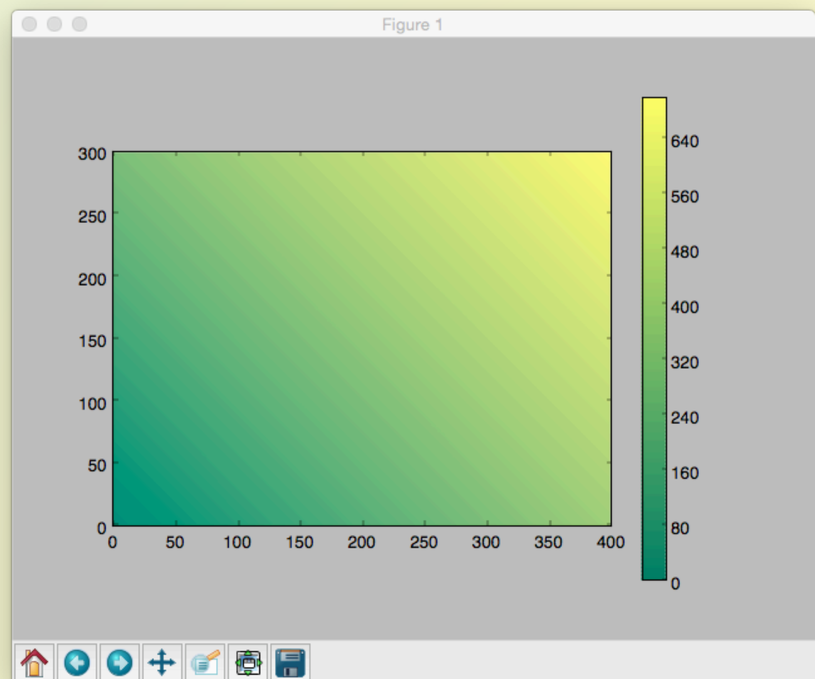


Save Multiple Graphs to 1 PDF File

```
import matplotlib.pyplot as plt
from matplotlib.backends.backend_pdf import PdfPages
pdfp = PdfPages('multipage.pdf')    # starts pdf file, 1 plot per page

plt.plot( … )       # Figure 1, page 1
plt.savefig(pdfp, format='pdf')
plt.show()

plt.plot( … )       # Figure 2, page 2
plt.savefig(pdfp, format='pdf')
plt.show()

plt.plot( … )       # Figure 3, page 3
plt.savefig(pdfp, format='pdf')
plt.show()

pdfp.close()     # after last save fig
```

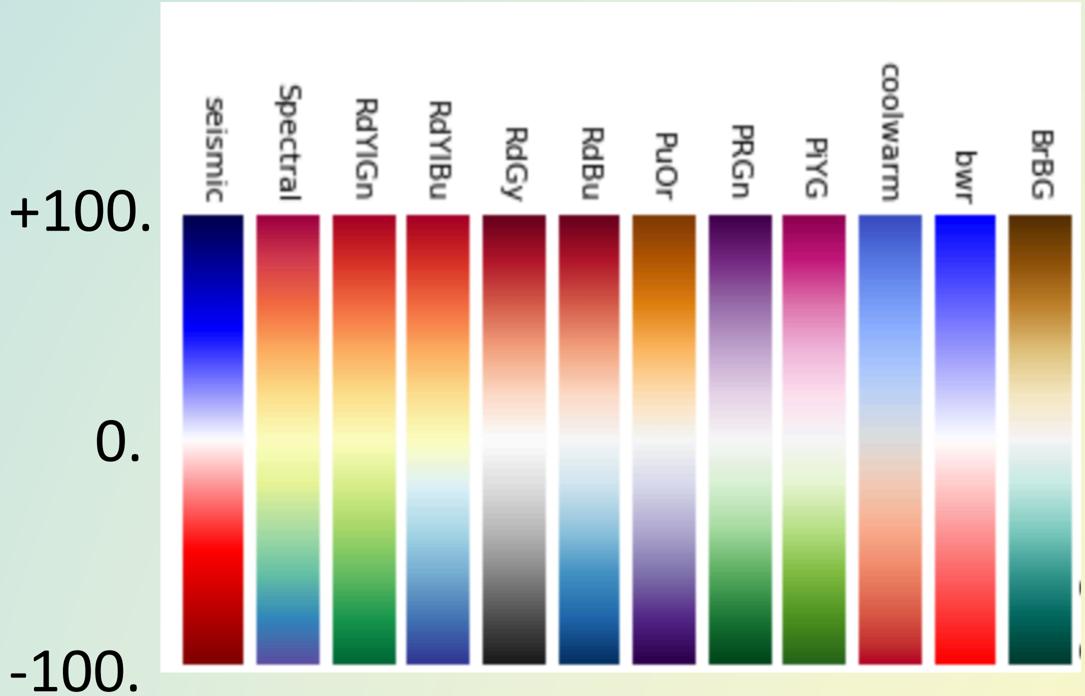
matplotlib + numpy *f(x,y)*

```
import matplotlib.pyplot as plt
import numpy
a = numpy.zeros( (300,400) )     # 2D ndarray

for i in range(300):
    for j in range(400):
        a[i,j] = i + j

plt.imshow(a, origin=“lower”, map=plt.cm.summer)
plt.colorbar()
plt.show()

# show names of colormaps
dir(plt.cm)

    # summer is a “sequential” colormap
    # summer_r to reverse order
```



Color Maps

Divergent color maps

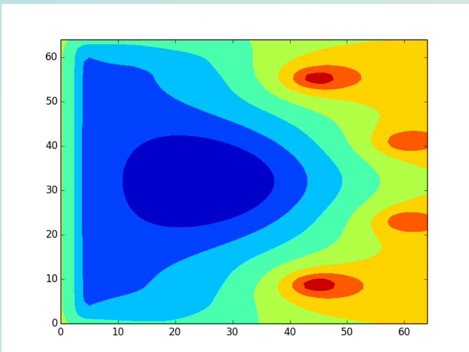


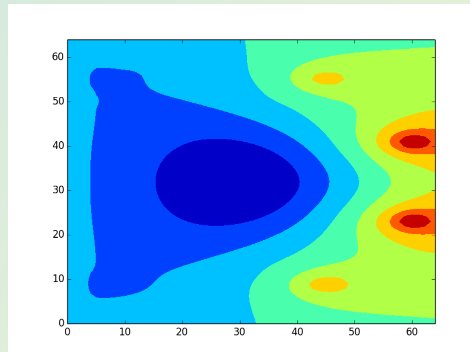
See also: Sequential & Qualitative colormaps discussion

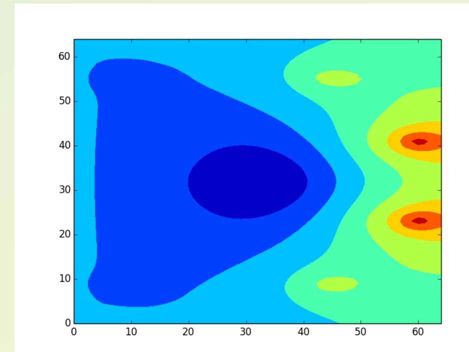
matplotlib.org/users/colormaps.html

f(x,y,t)

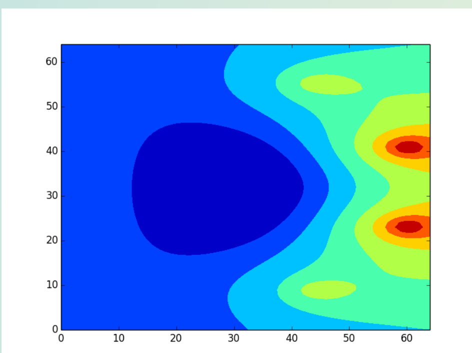
2D Magnetic Field for 84 time steps

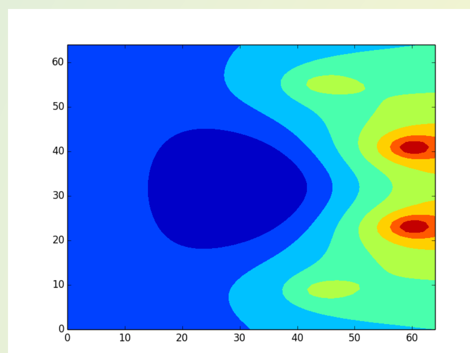


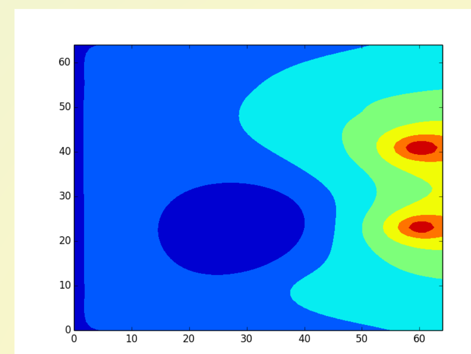




84 Image Files ...







Combine with ffmpeg into .mov or .mp4 movie file

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

matplotlib + numpy *f(x,y,t)* + netCDF

```
import matplotlib.pyplot as plt
from scipy.io import netcdf
```

from netCDF4 import Dataset

```
f = netcdf.netcdf_file("psiRZ.cdf", "r")
for v in f.variables:                  # f.variables is a dictionary
    print v                            # print keys, name of variable

rz = f.variables["pout_psiRZ"].data        # get the data
shape = rz.shape      # (84, 65, 65) tuple:  84 steps,  65 x 65 magnetic field
for i in range(shape[0]):              # for each time step
    rzt = rz[i][:][:]                  # get the time slice
    plt.contour(rzt)                   # make a contour plot
    plt.draw()                         # draw on screen for .1 second
    plt.pause(.1)
    fname = "figs/" + str(i).zfill(3) + ".png"  # 001.png ...
    plt.savefig(fname)                 # save each plot to a PNG file
```

Movie Maker Program

`ffmpeg`

- Most comprehensive
- Downloads for Mac & Windows; build for Linux*
- Command line Linux - module load ffmpeg/4.0.1

```
ffmpeg
   –y –f image2
   –framerate 8
   –pattern_type glob –I ‘*.png’
   –b:v 4000k
   –pix_fmt yuv420p
   psiRZ.mov
```

ImageMagick - Resize all images in directory

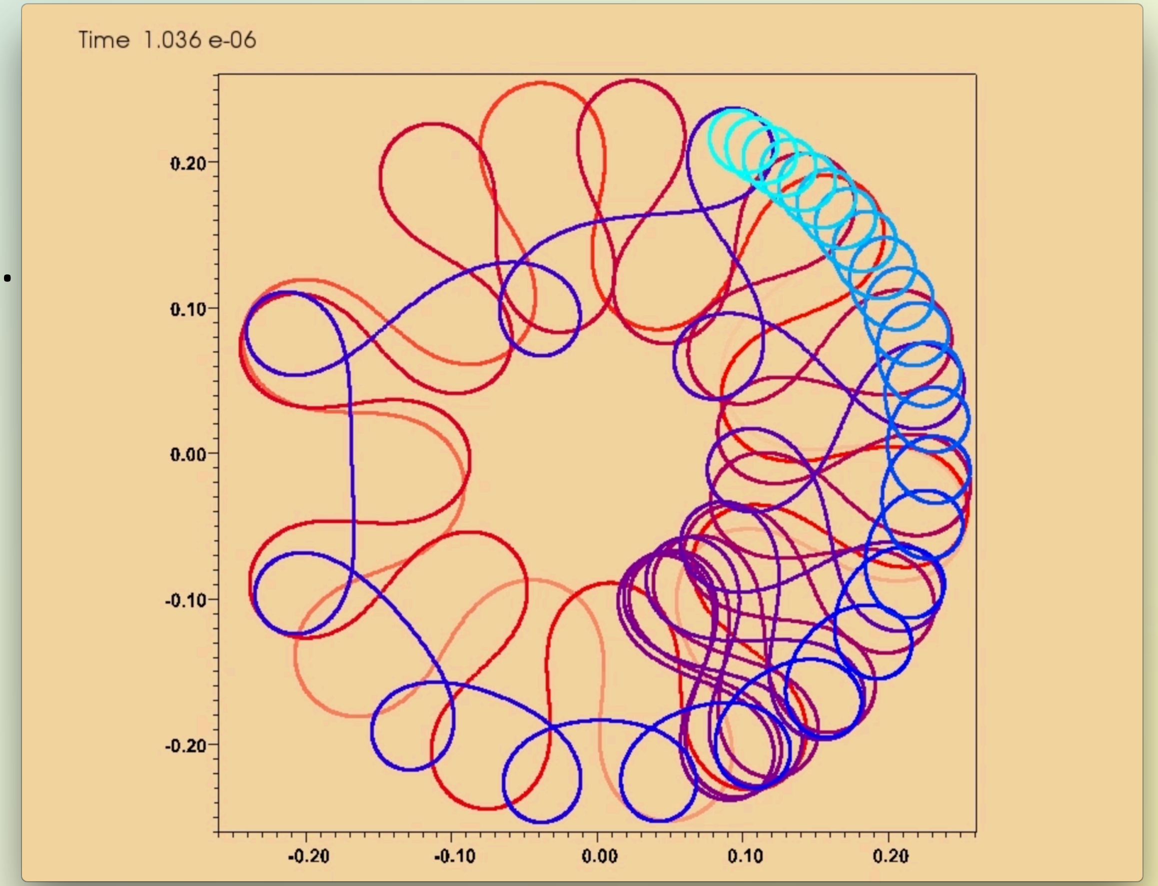
mogrify -resize 90% *.jpeg

Implementation

- Vis GUI – VisIt, ParaView
- VTK – Visualization ToolKit
- Graphics Primitives
- Pixels

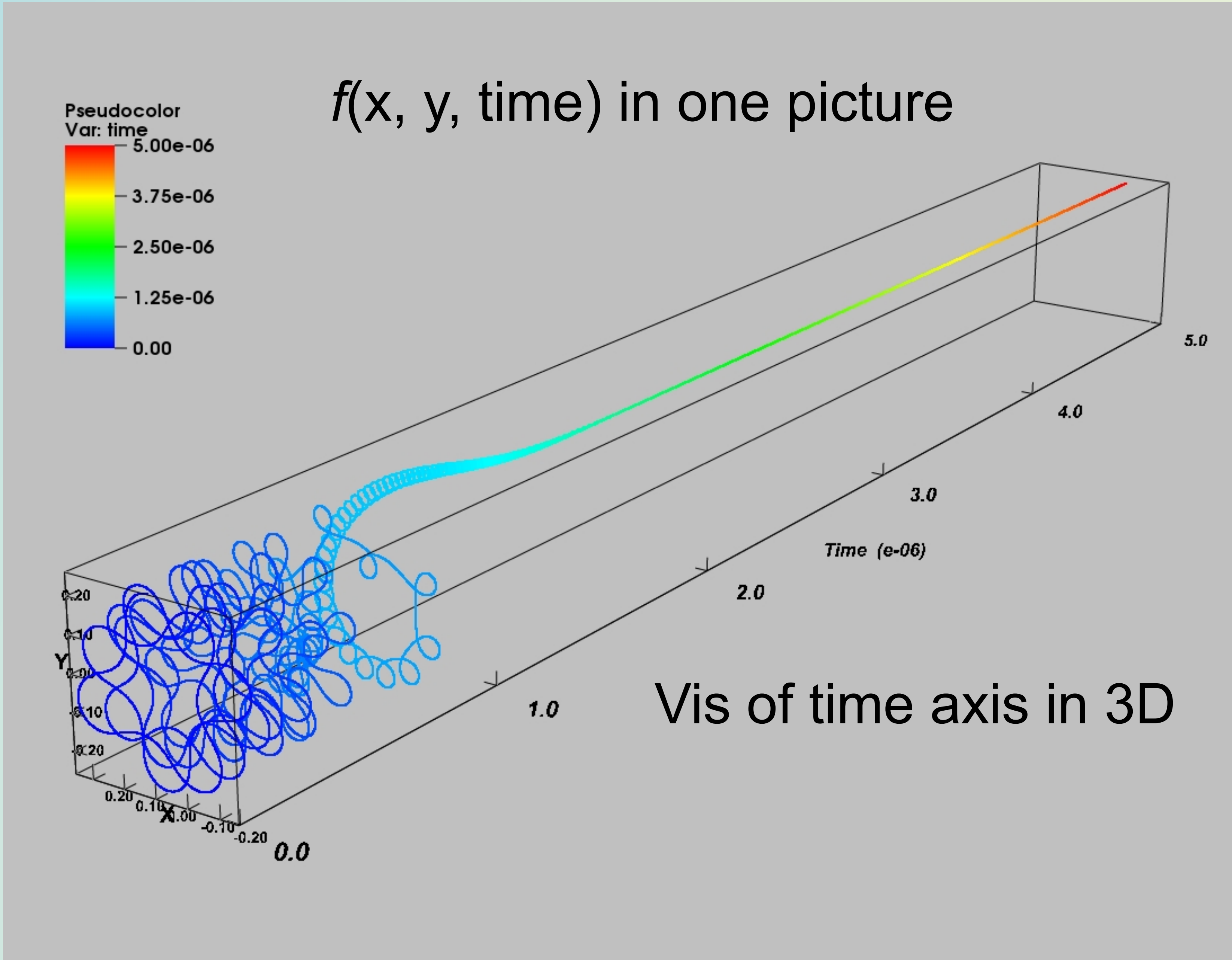
Visualization of 1 Particle Can Be Interesting: *Simulation of Ion Path as Energy Decreases*

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



http://w3.pppl.gov/~efeibush/movies/m3_720.mov

Visualization in 1 Picture



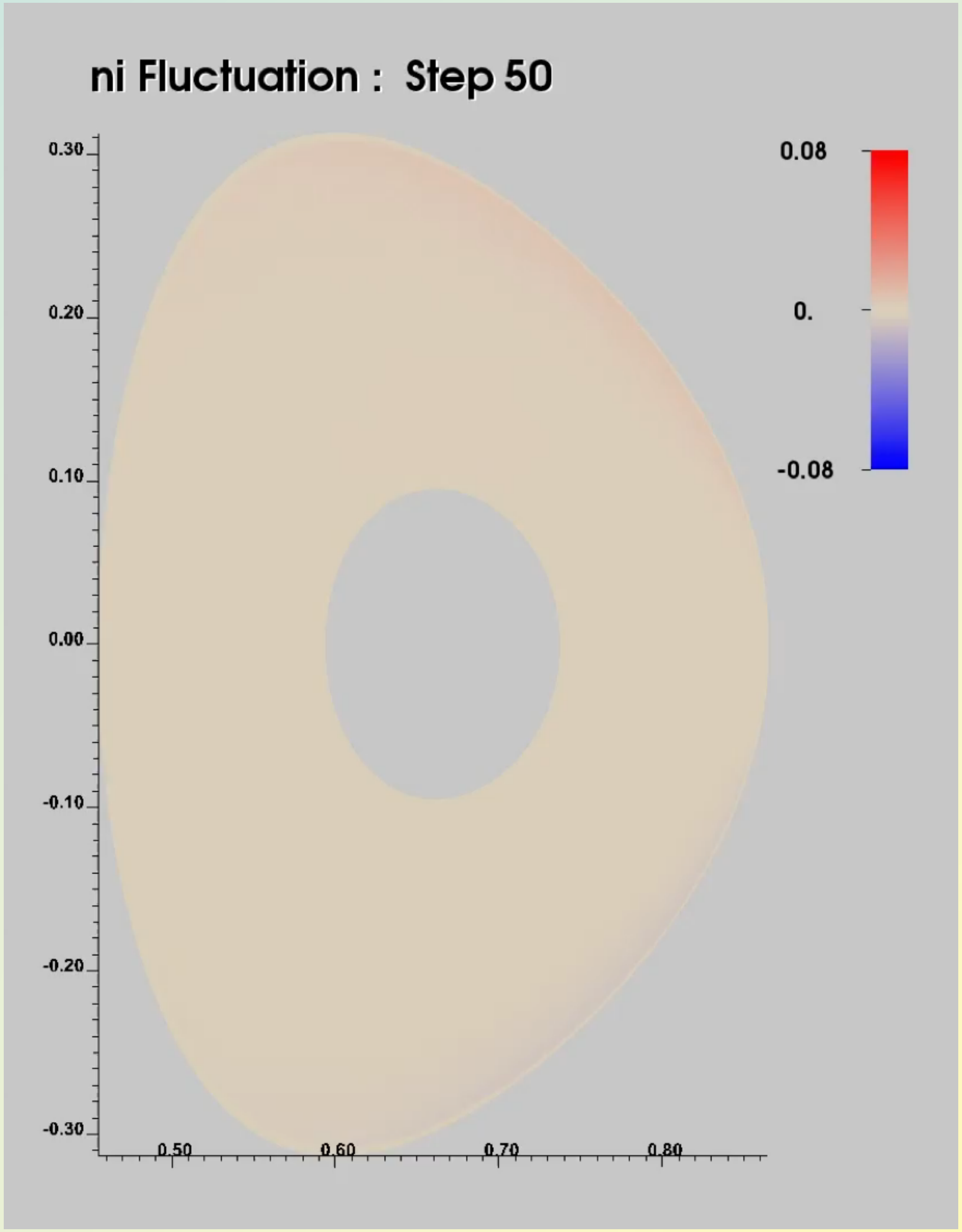
Time Step Simulation

GTS

f(x,y,t)
Ion Density Fluctuation

Direction
Magnitude
Structure

Divergent color map.

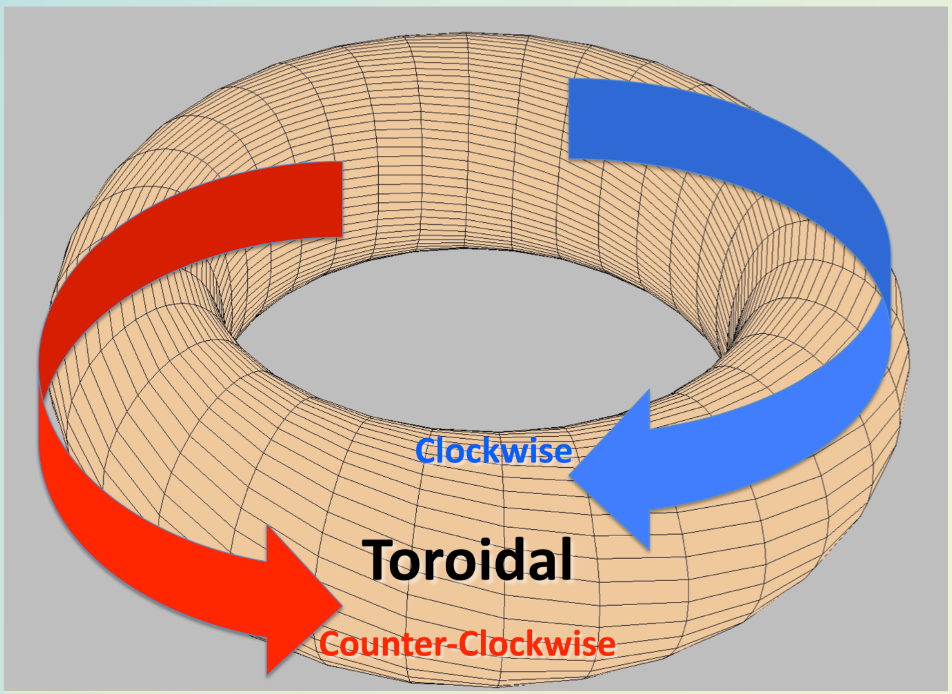


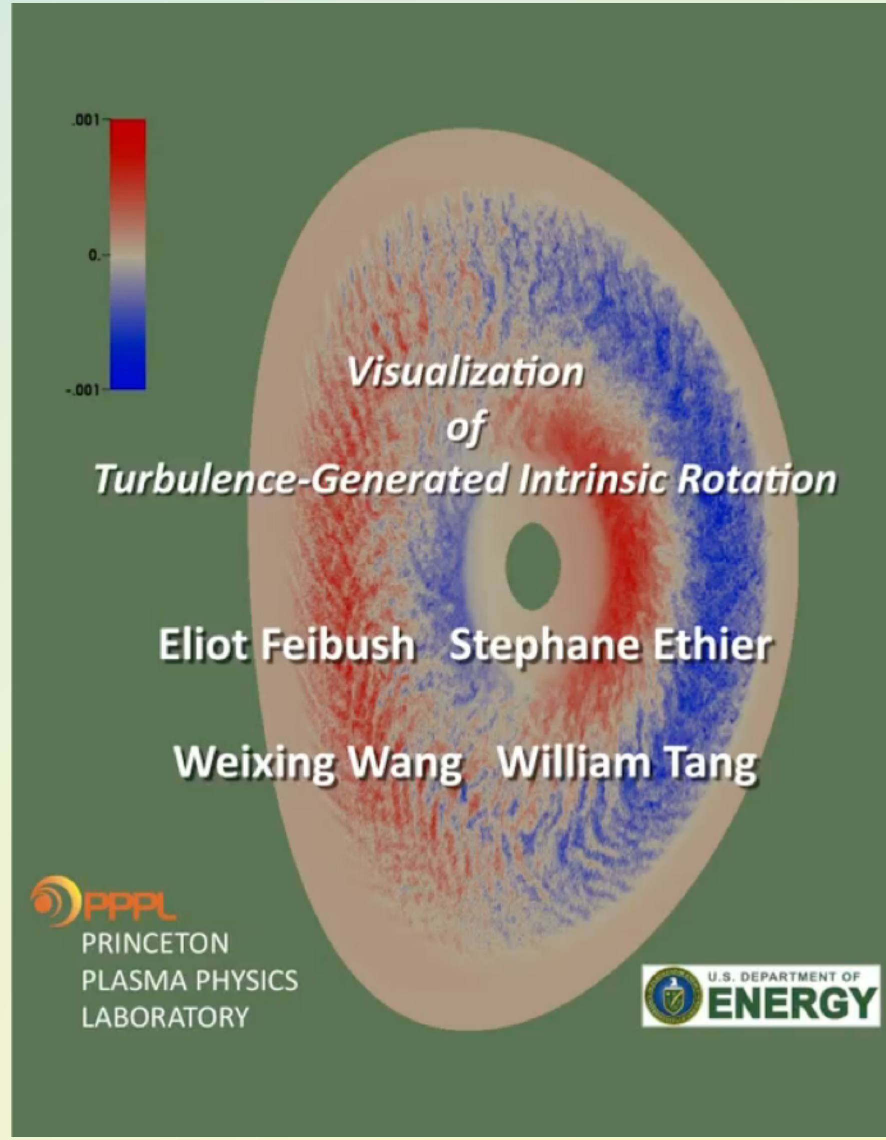
http://www.princeton.edu/~efeibush/movies/ni1080.mov

Time Step Simulation

GTS

Plasma Flow around torus.





Plasma Flow through 1 poloidal plane

http://w3.pppl.gov/~efeibush/gts/intrinsicvphi720.mov

Time Step Simulation

XGC

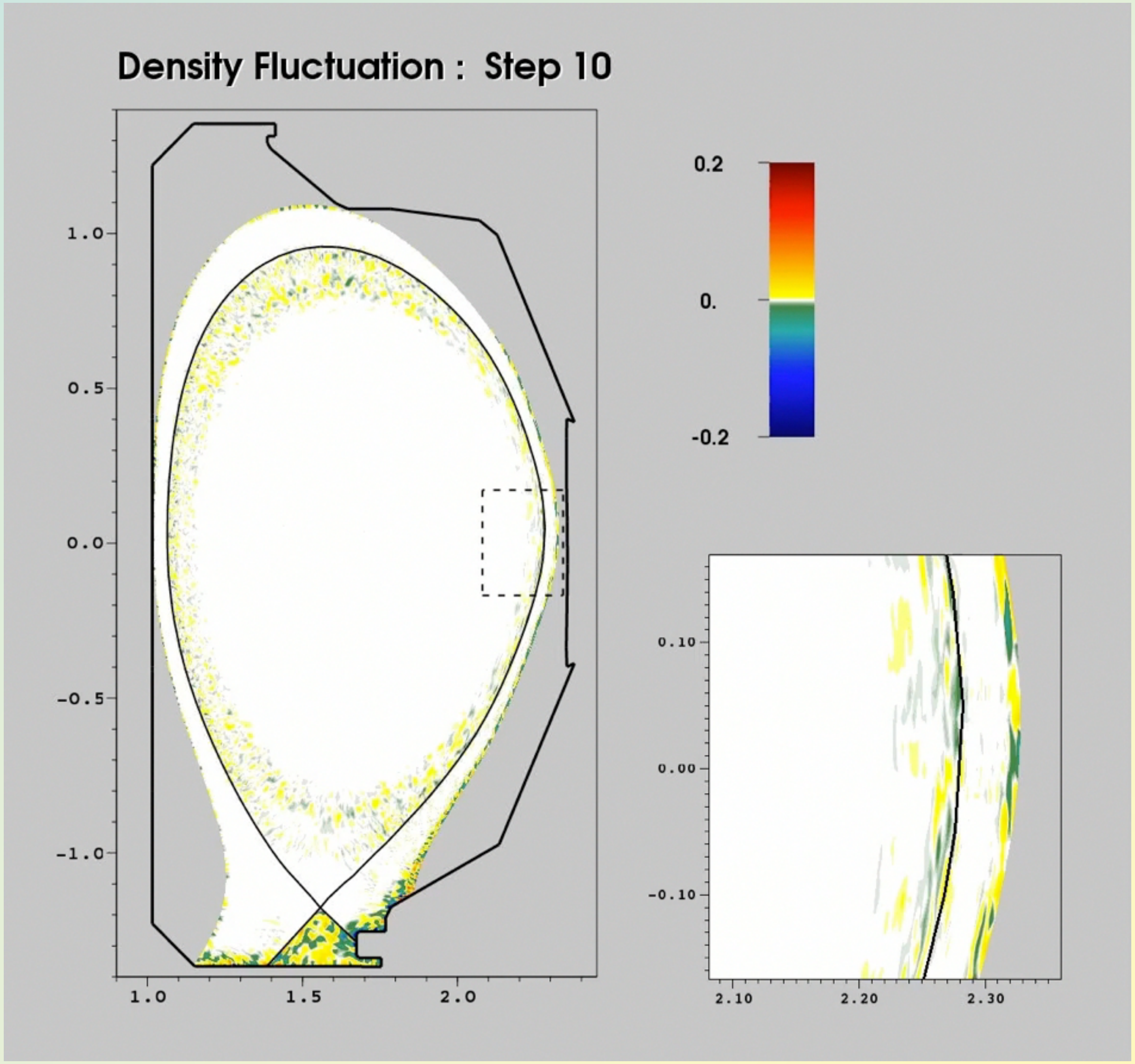
Render overview

\+

Region of Interest.

Merge images.

Custom color map.



http://w3.pppl.gov/~efeibush/movies/deninsetb1080.mov

VisIt Can Read Data Files

- Silo
- Chombo, AMR
- GTC
- M3D, M3DC1
- H5Nimrod
- POINT3D
- S3D
- OpenFOAM
- ITAPS
- XDMF
- Adios
- FLASH
- EnSight
- VTK **VTK is Internal Format**
- NetCDF
- CGNS
- NASTRAN, ANSYS
- 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

Getting Data into VisIt

Discrete Point Data

Define and display data at specific points in 3D.

Each point is a unique, independent sample.

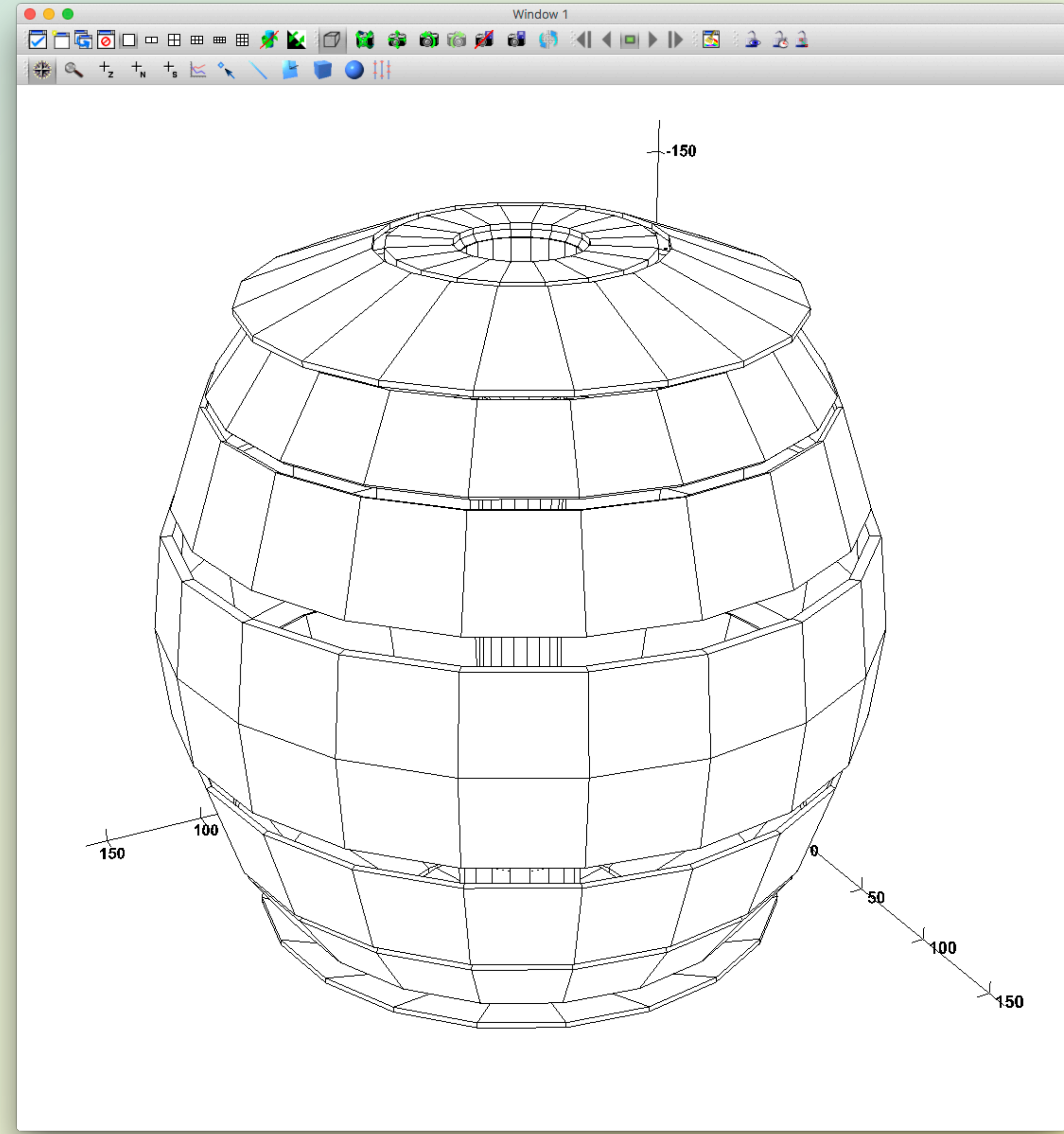
Taken from simulation grid (perhaps).

Look at Point3D data file:

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

Connecting Points → Polygons

```
DATASET POLYDATA
POINTS 48
90. -140. 100.
80. -140. 100.
...
POLYGONS 24
4 0 1 24 25
4 1 2 25 26
...
```



Structured 3D Grids

3D volume of data – sampled at grid points

f(x,y,z)

VisIt interpolates among grid points in all 3 directions for continous display.

Specify data at grid locations.

Apply Operators to explore & examine data.

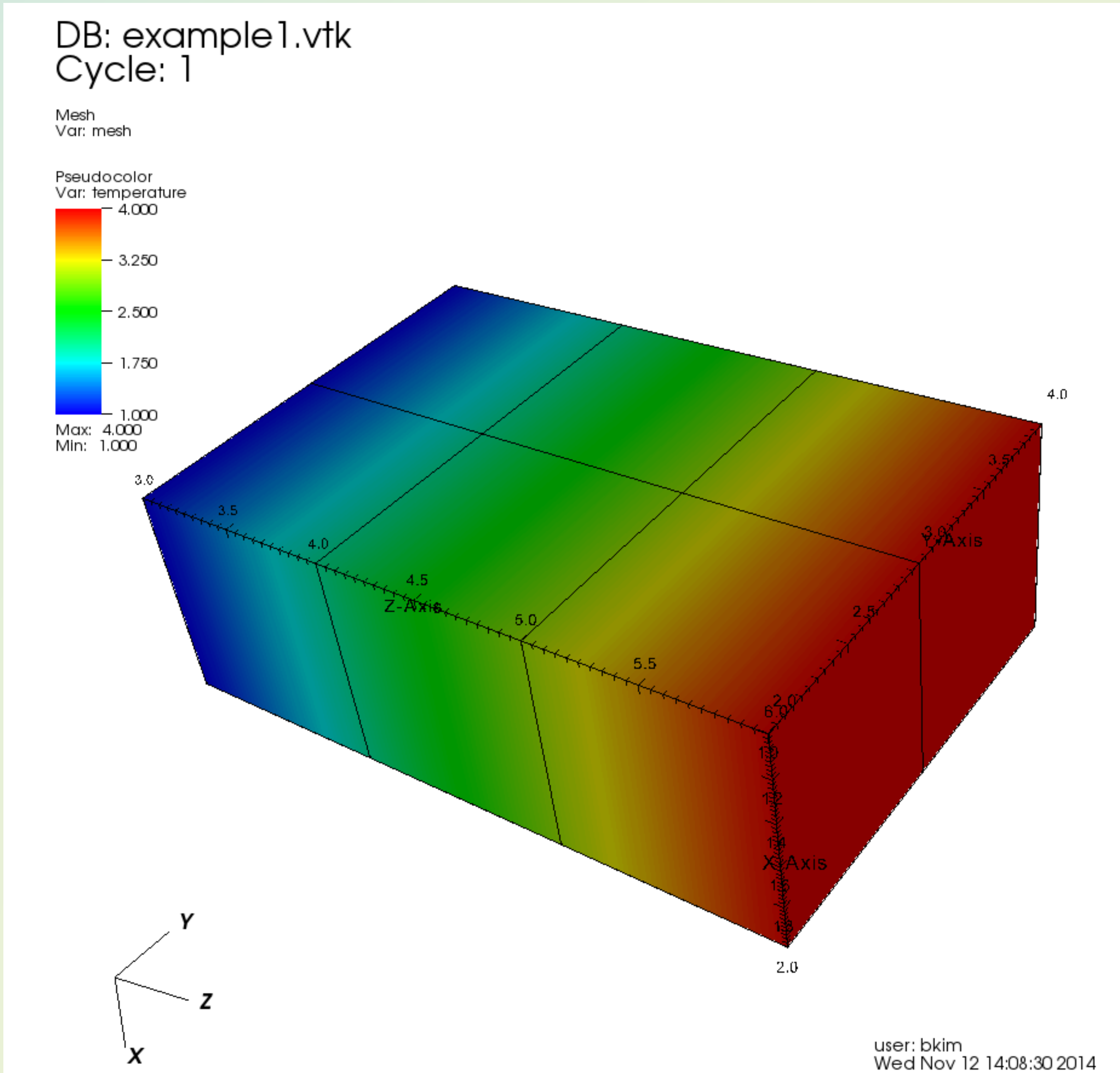
Structured Points *f(x,y,z)*

```
# 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
2
2
2
2
2
2
3
3
3
3
3
3
4
4
```

Uniform spacing per axis.

Value at each point.

Interpolates into continuous volume of data.



Structured Points Ordering

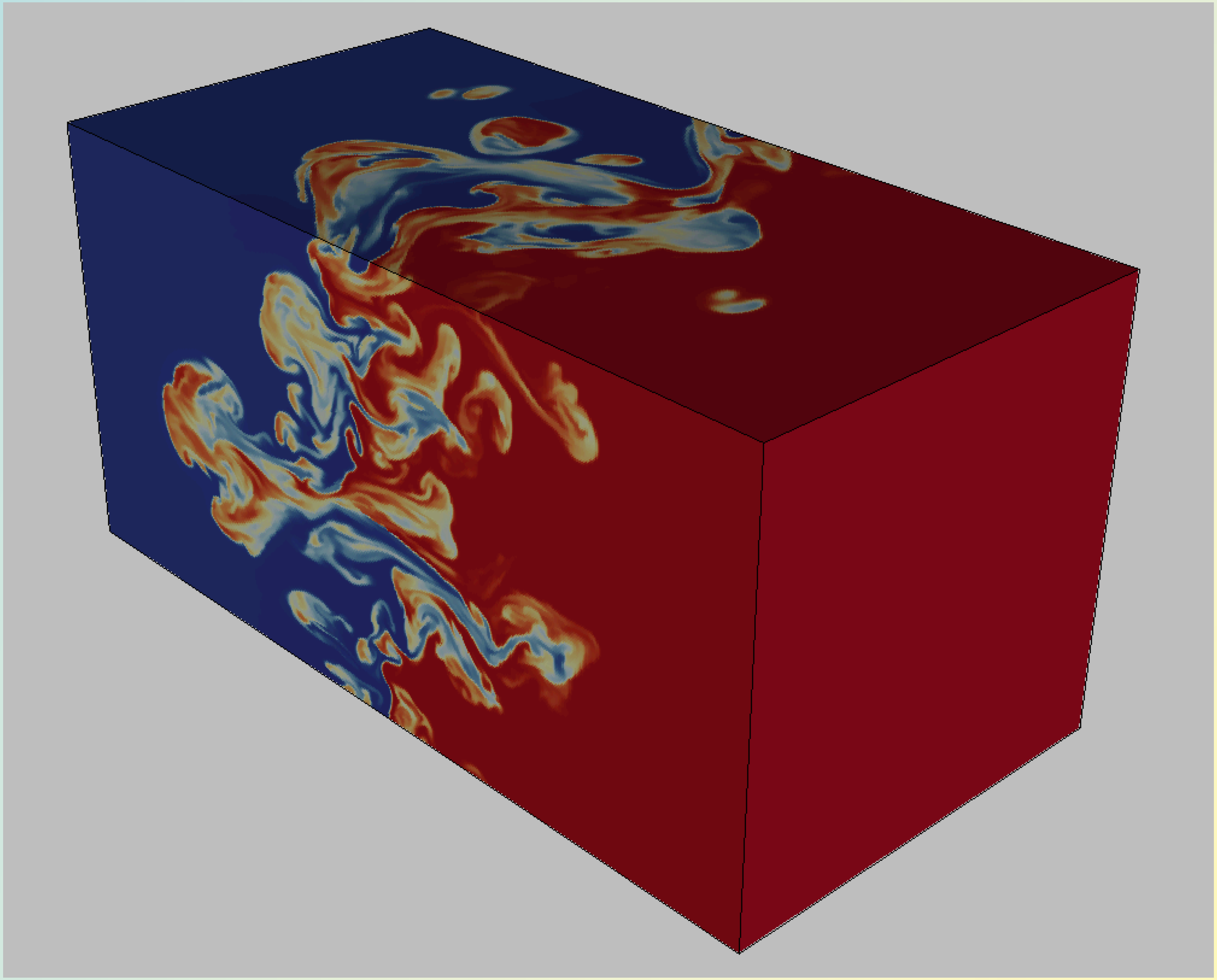
Example python loop to write values to vtk file

```
for z in range(4):
    for y in range(3):
        for x in range(2):
```

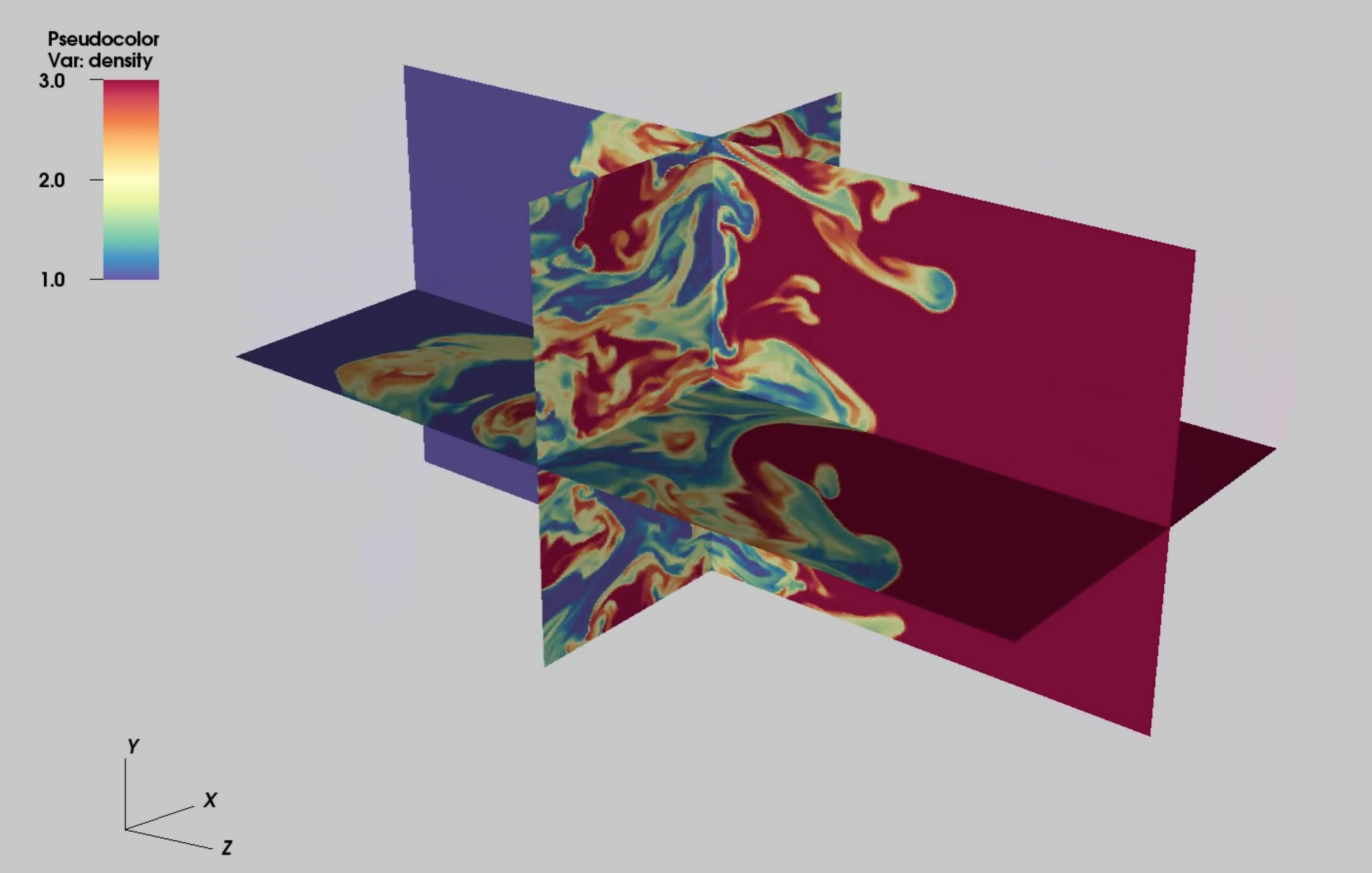
write *f(x,y,z)* value to file

VTK - text or binary (byte representation of ASCII file)
(large text files are OK)

Structured Points *$f(x,y,z)$*



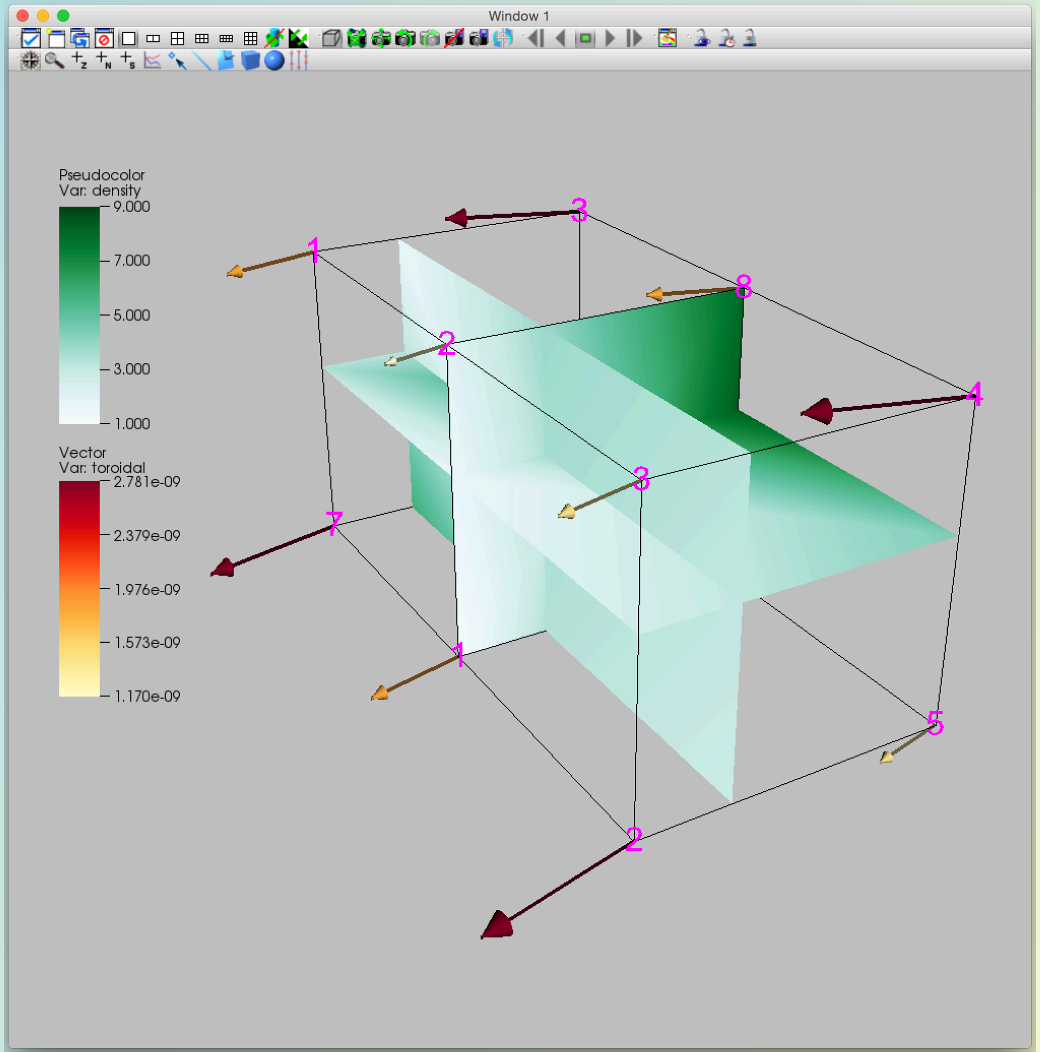
Continuous Volume of Data: Slicable



Geometric Operator: 3-Slice

Examine data throughout the volume …

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



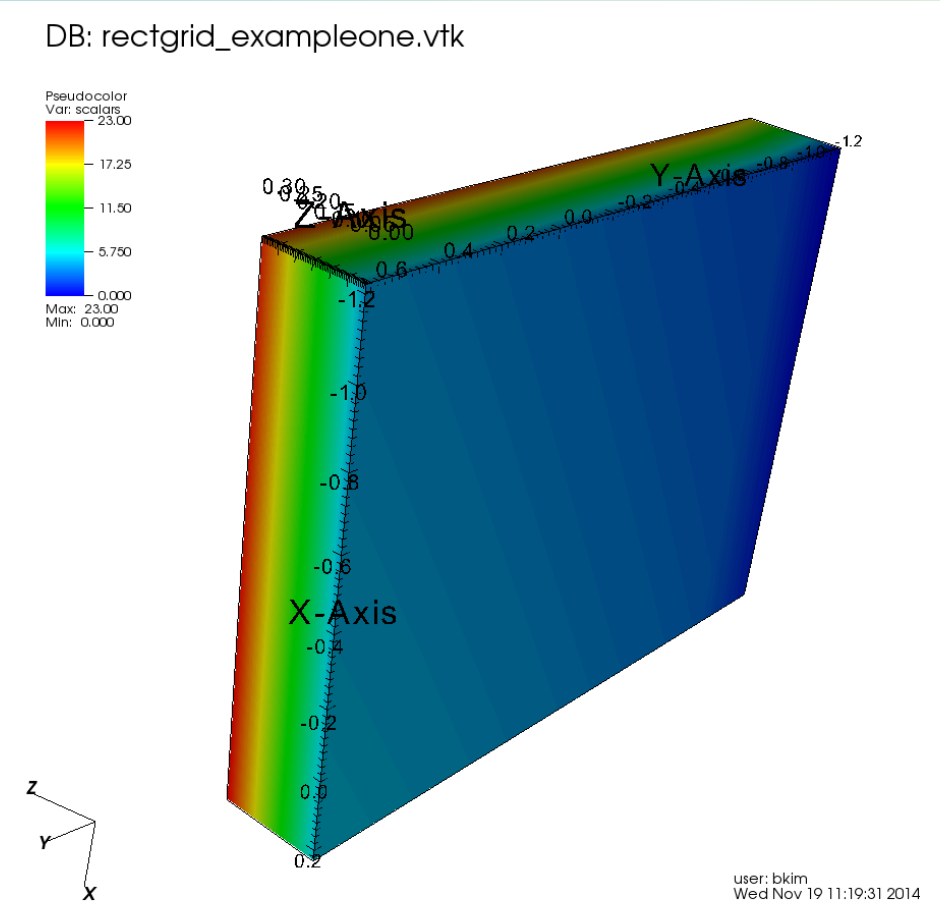
Different color maps for different variables.

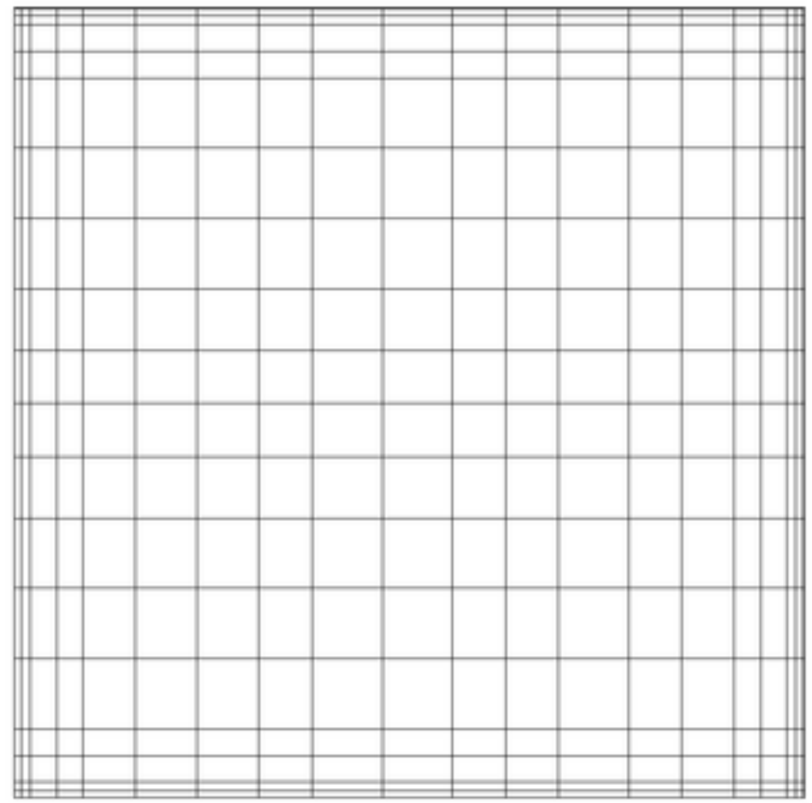
Scalars

Vectors

Density labels at grid points.

Rectilinear Grid

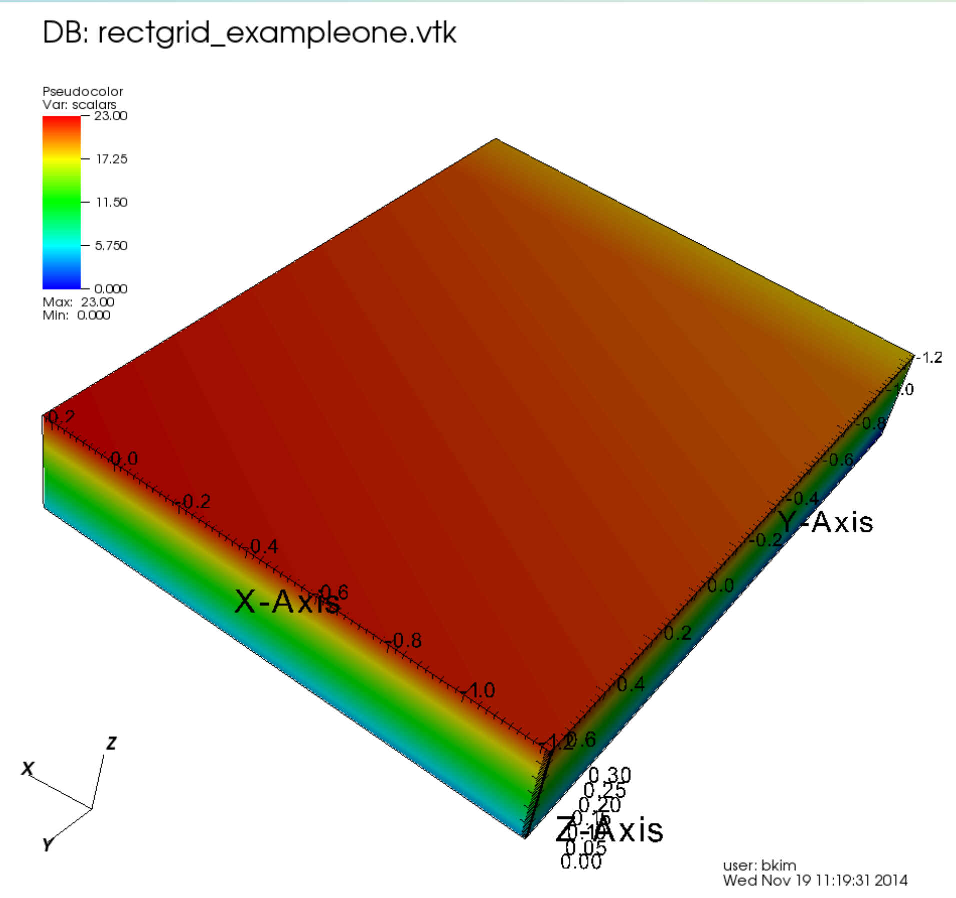




Continuous volume of data defined at specific points.

Non-Uniform spacing per axis.

Rectilinear Grid

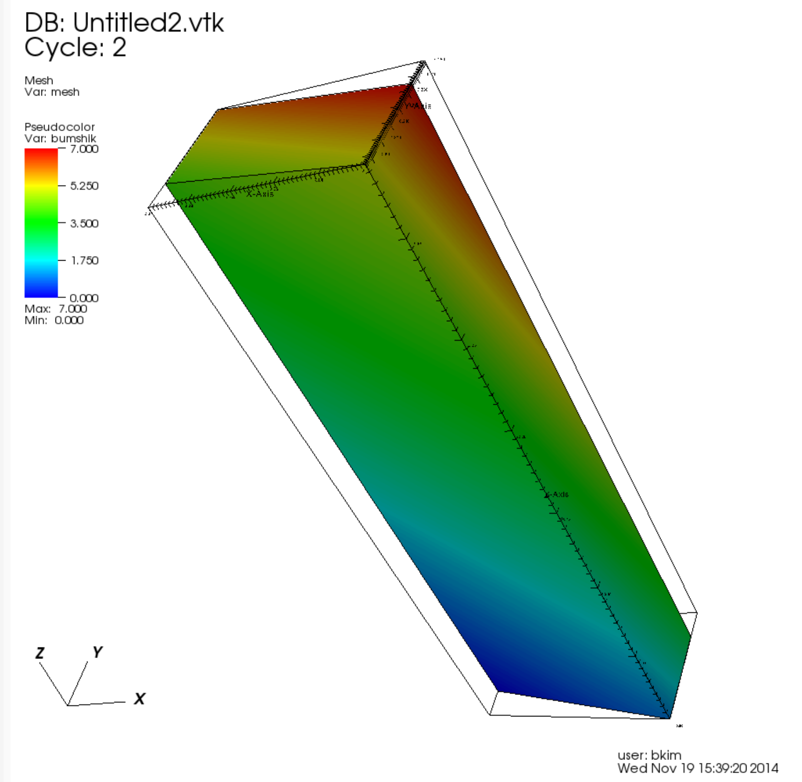


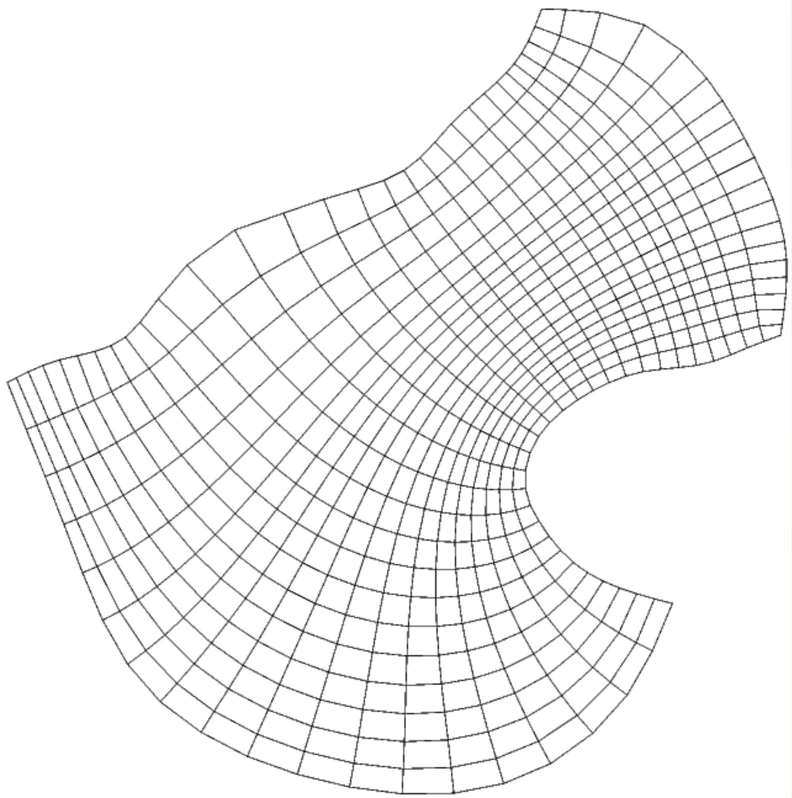
rectgrid_exampleone

```
# 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 Grid





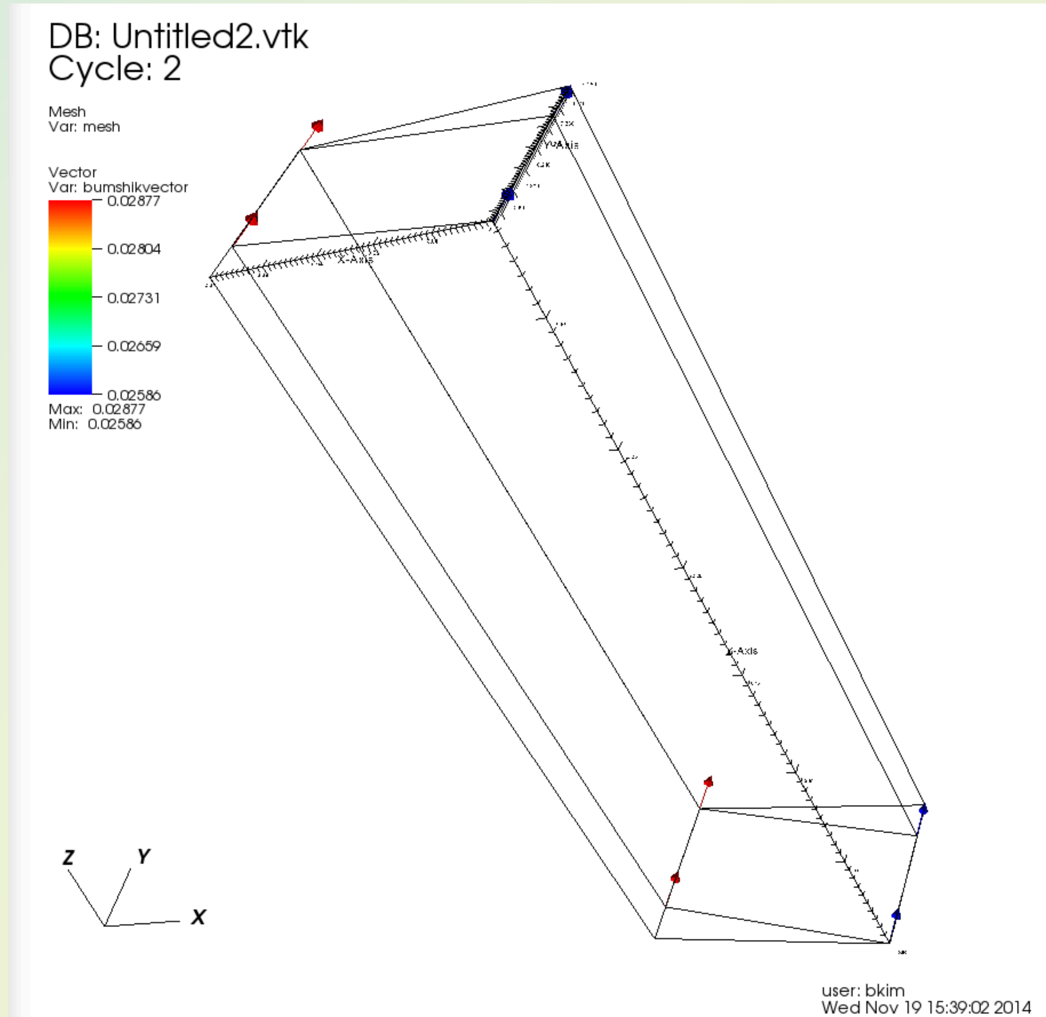
Continuous volume (or surface) of data defined at specific points.

Regular topology, non-orthogonal, specify each point location. Quadrilateral cell faces.

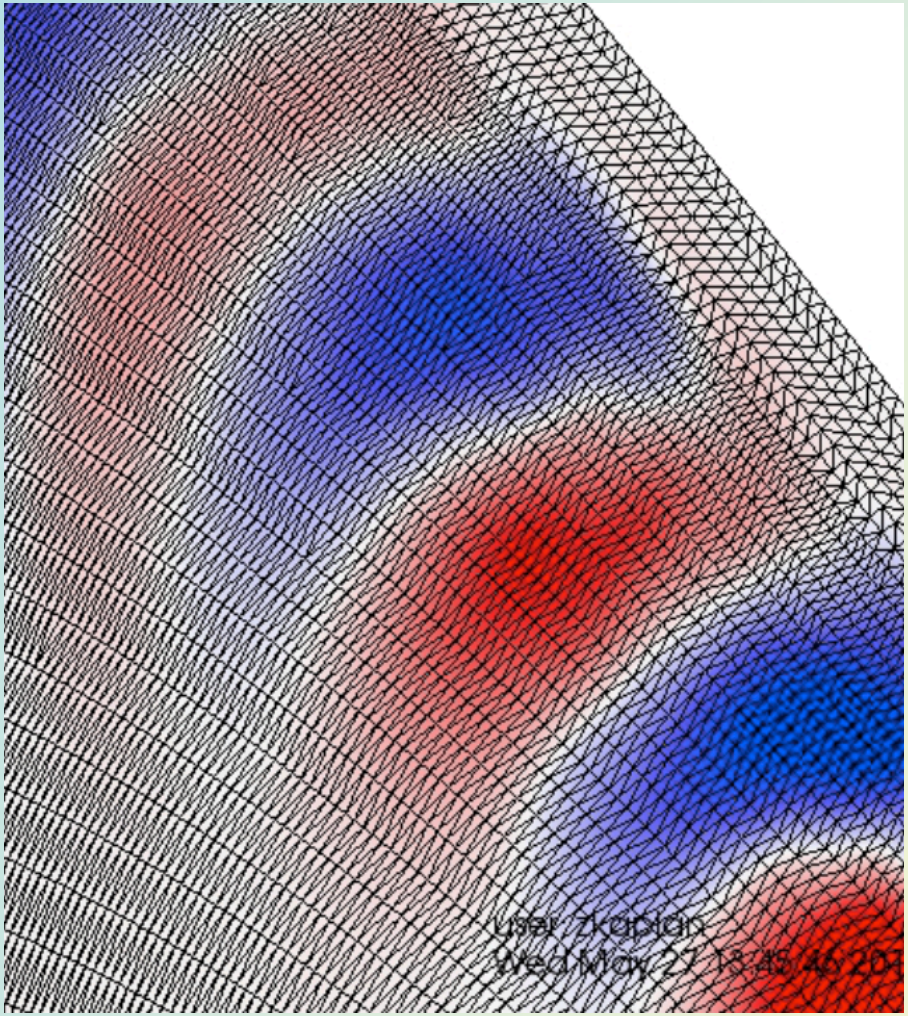
Structured Grids + Vectors

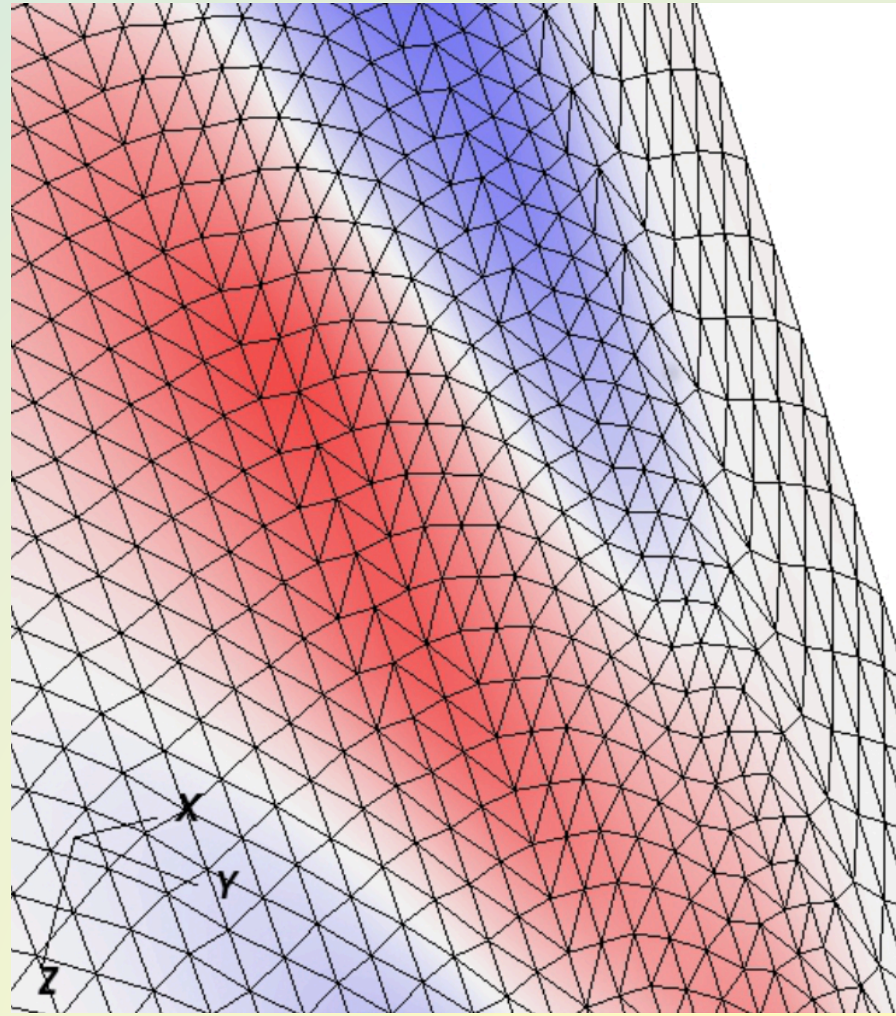
Untitled2.vtk

```
# 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
```



VTK *Unstructured* Grid

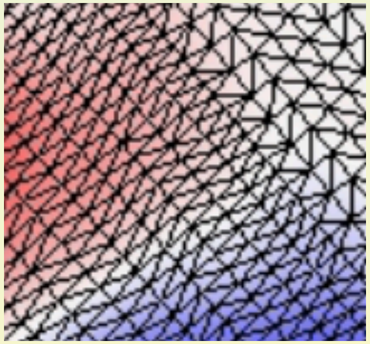




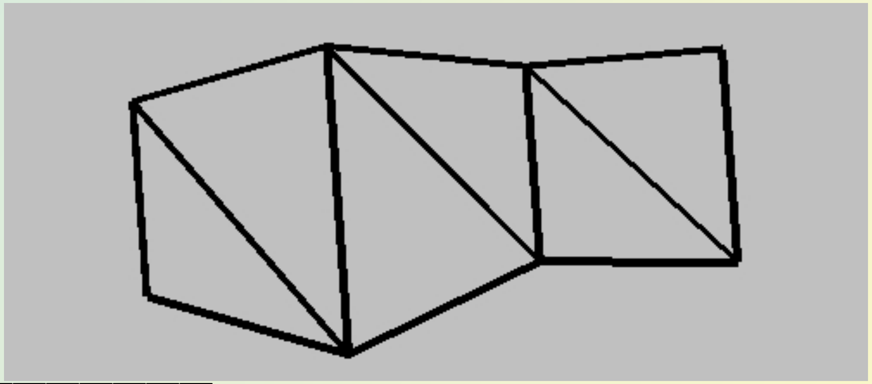
GTS Complex Mesh – Poloidal Rings
Delaunay Triangulation Algorithm

VTK Grid Summary

Structured Points – uniform spacing, orthogonal
Rectilinear Grid – non-uniform spacing, orthogonal
Structured Grid – non-orthogonal quads
Unstructured Grid – any combination of polygons:



Triangle Strip



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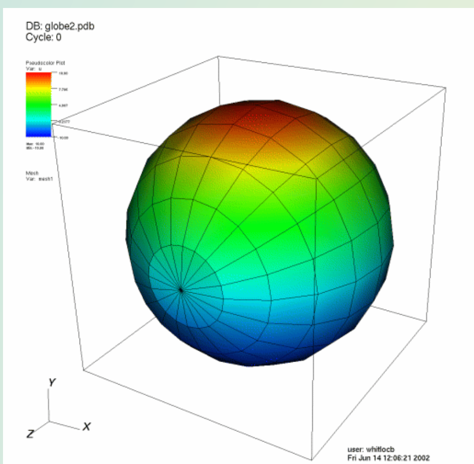
Paraview wiki: Users Guide VTK_Data_Model

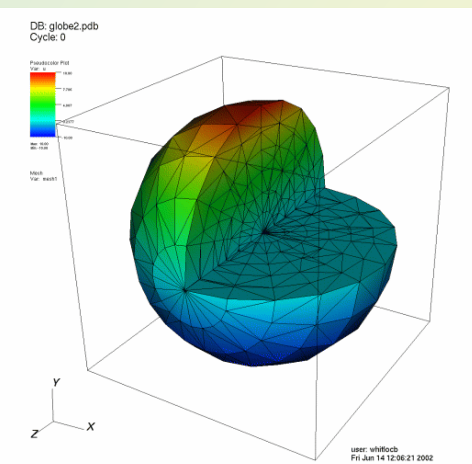
Geometric Selection - *Clip* Operator

- 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

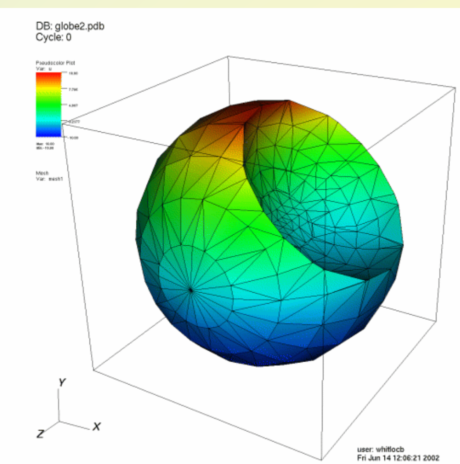
Original plots



Plots clipped with 2 planes



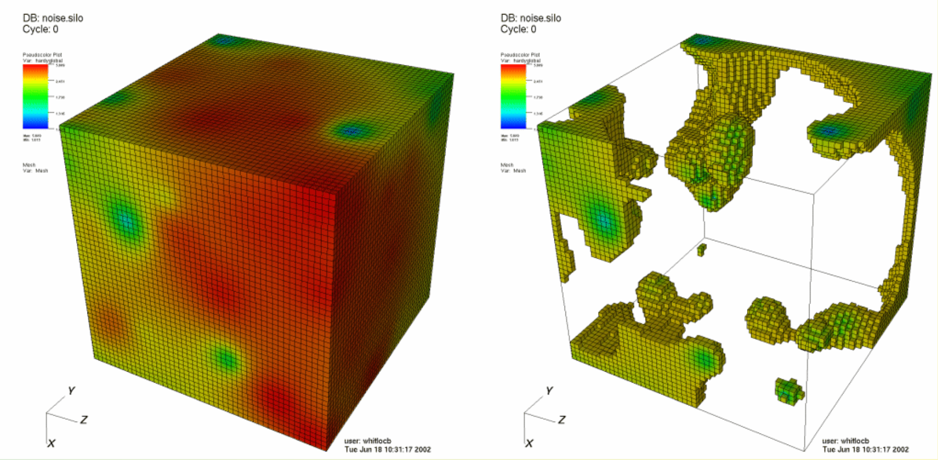
Plots clipped with a sphere



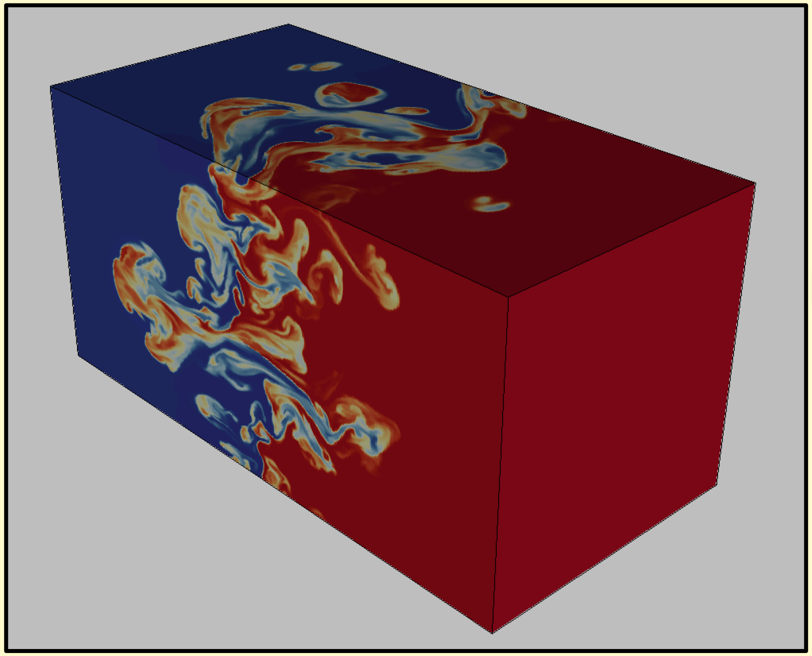
Data Value Selection - *Threshold* Operator

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

Removes cells whose value is not in the specified range.

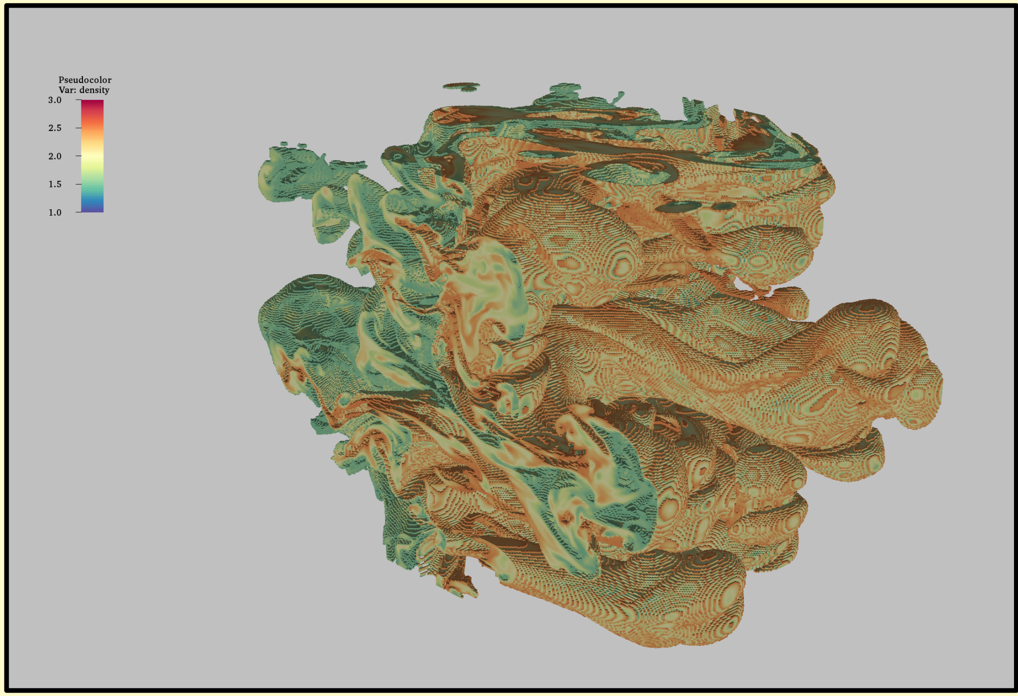


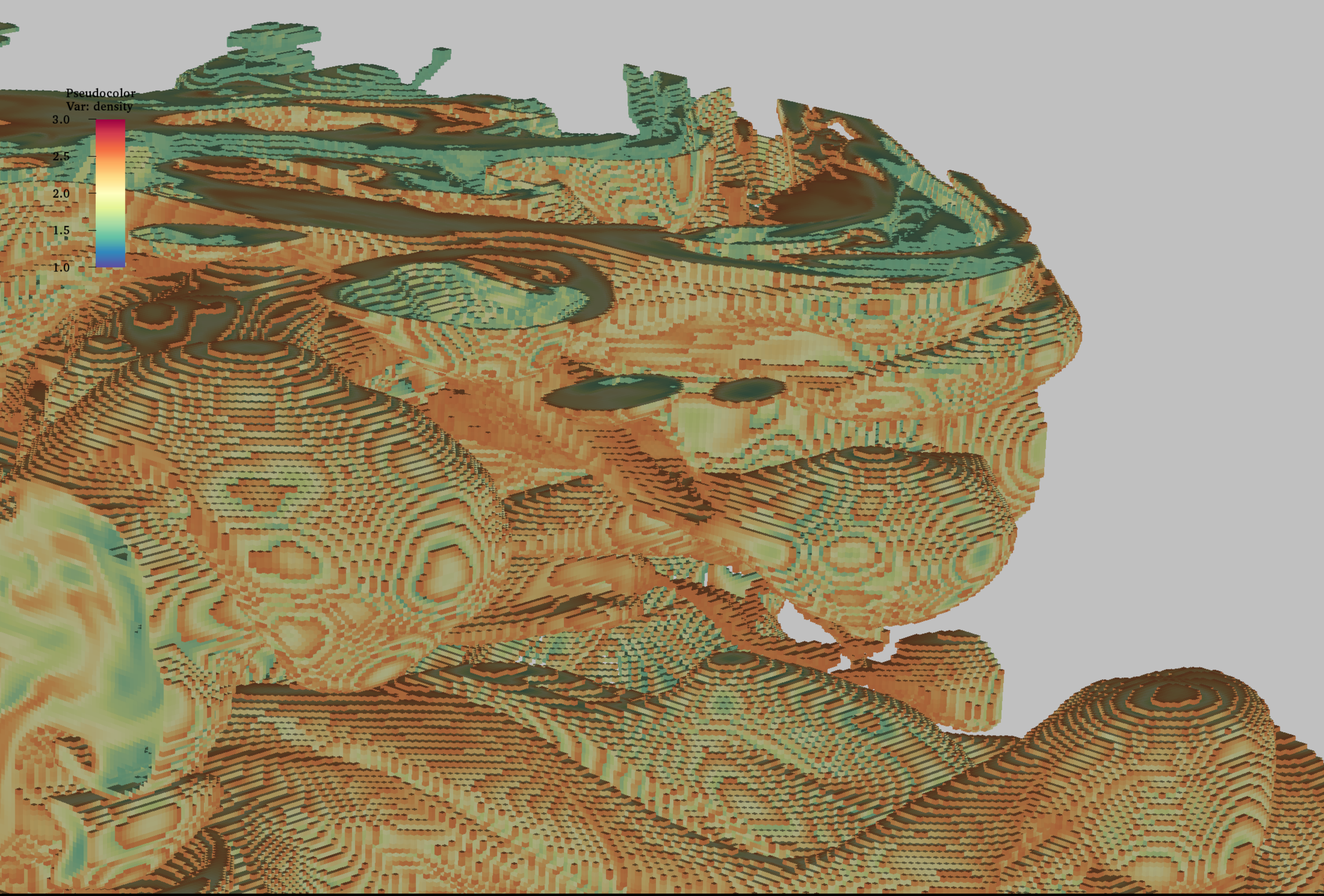
Data Value Selection



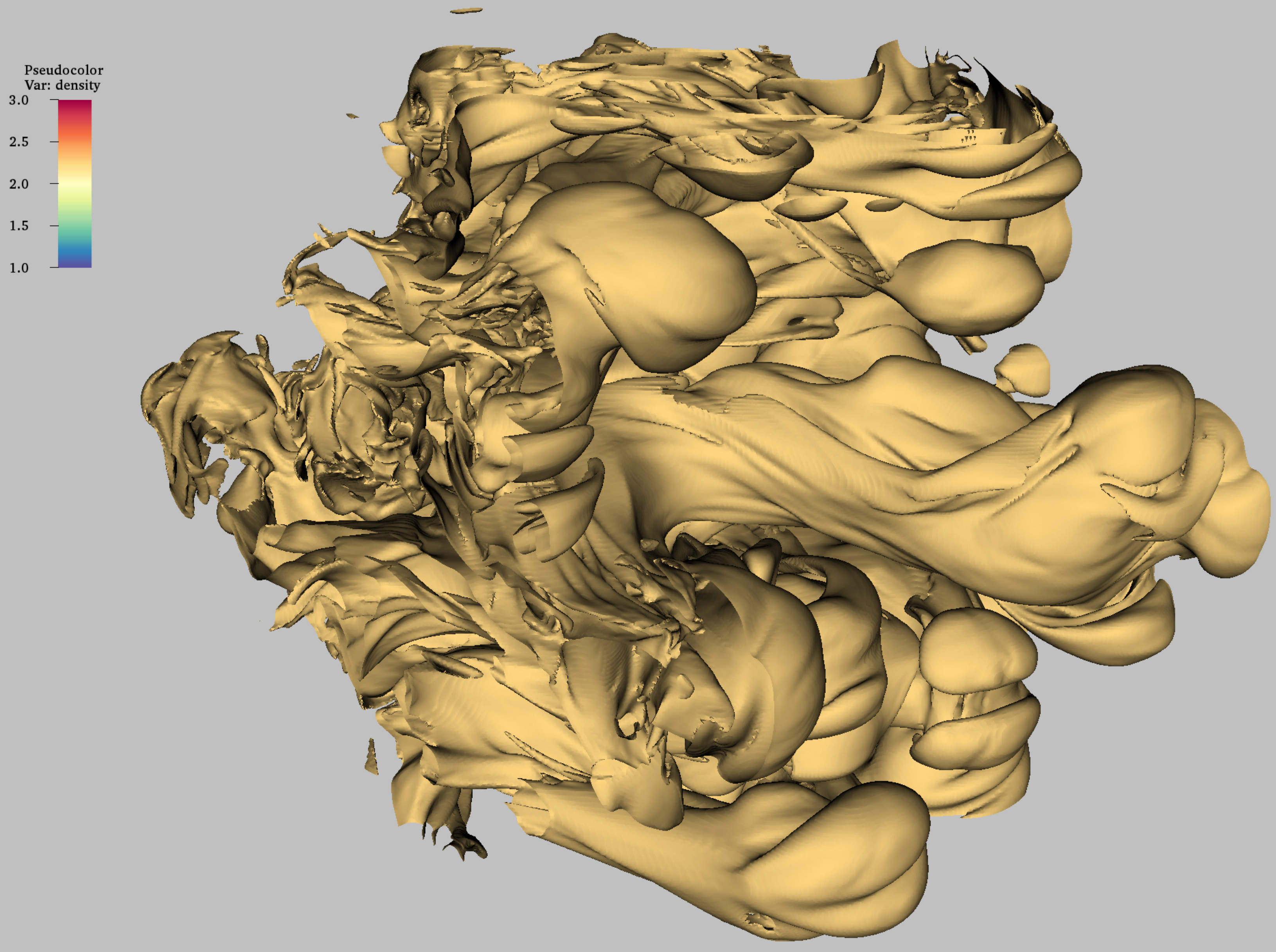
257 x 257 x 51 grid
Scalar value per grid point

Threshold Operator
Range 1.5 to 2.5

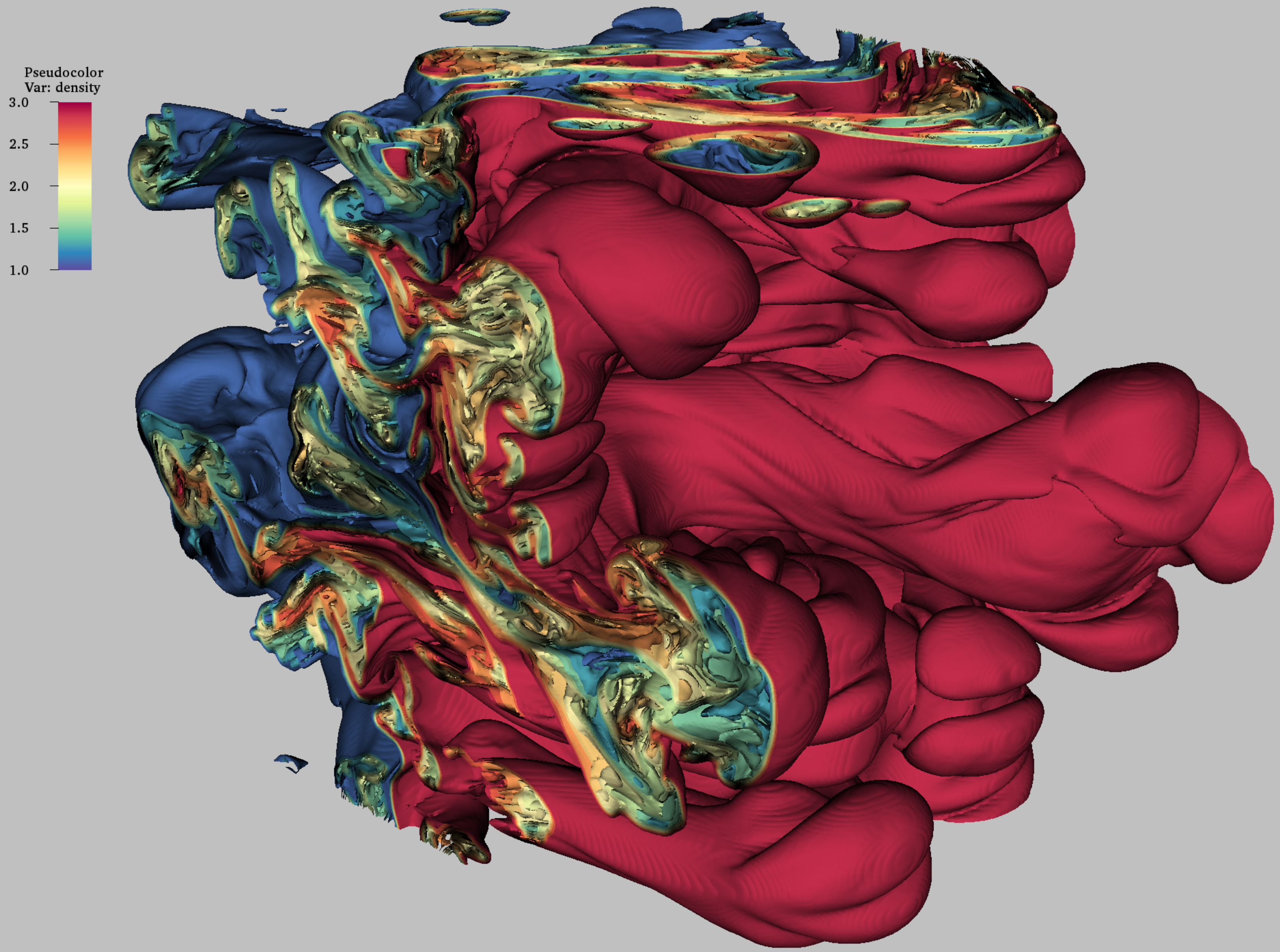


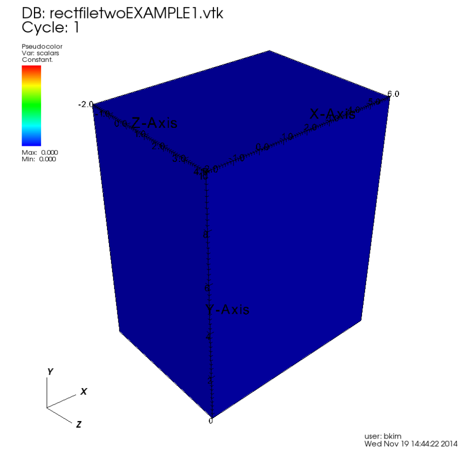

Pseudocolor
Var: density
3.0
2.5
2.0
1.5
1.0

Data Value Selection - *Isosurface*



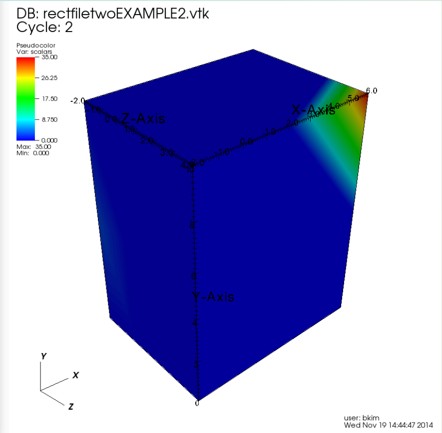
10 Isosurfaces Between Data min - max

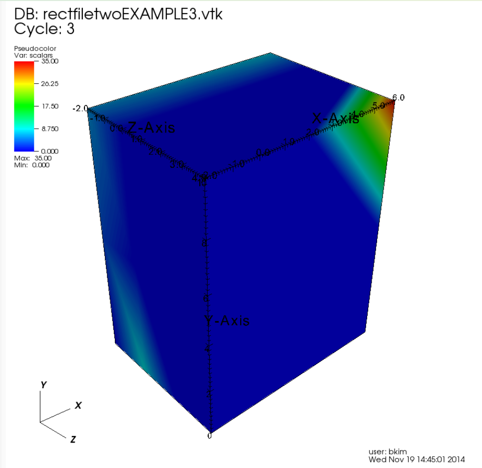


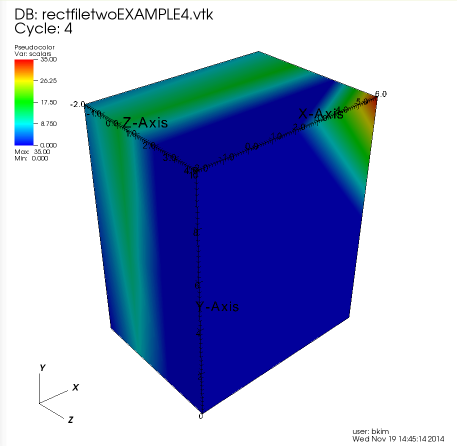


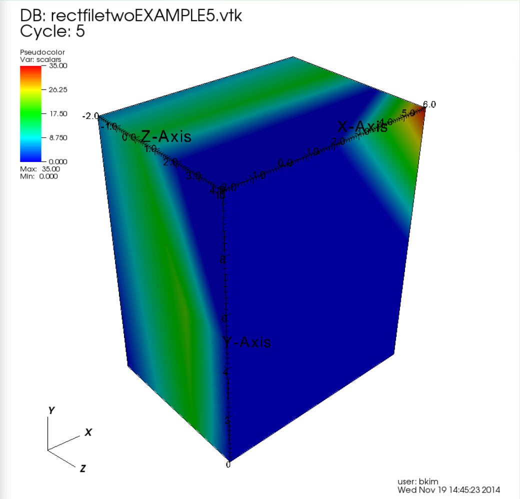
Time Steps *f(x,y,z,t)*

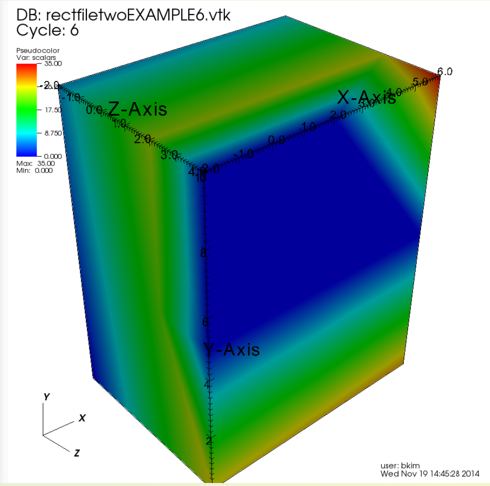
VisIt automatically reads files named in numerical order for time step visualization.

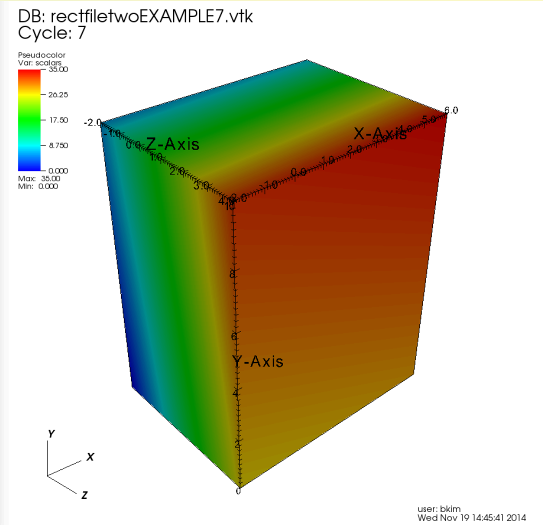


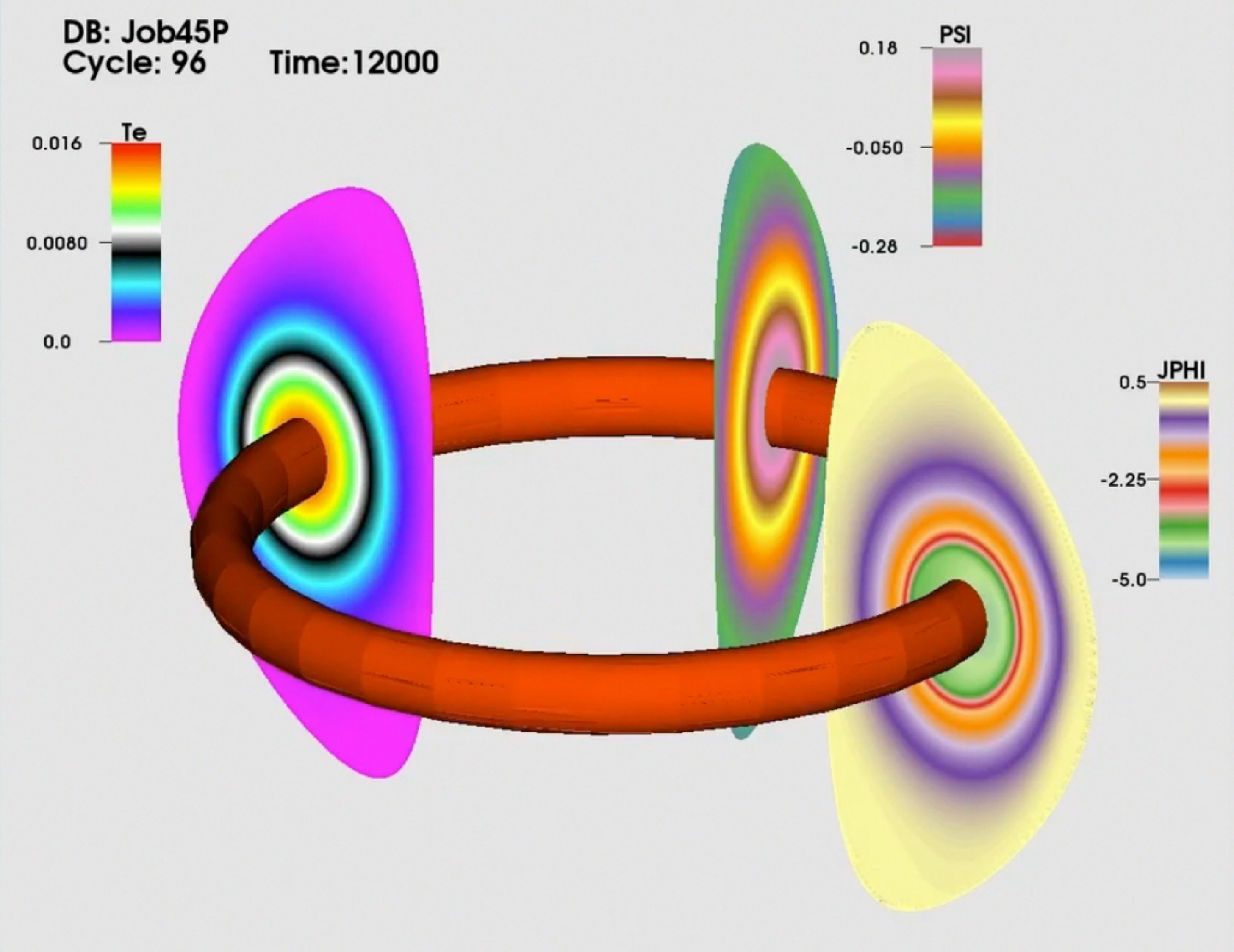












Isosurface of Te = 0.015 at each time step.

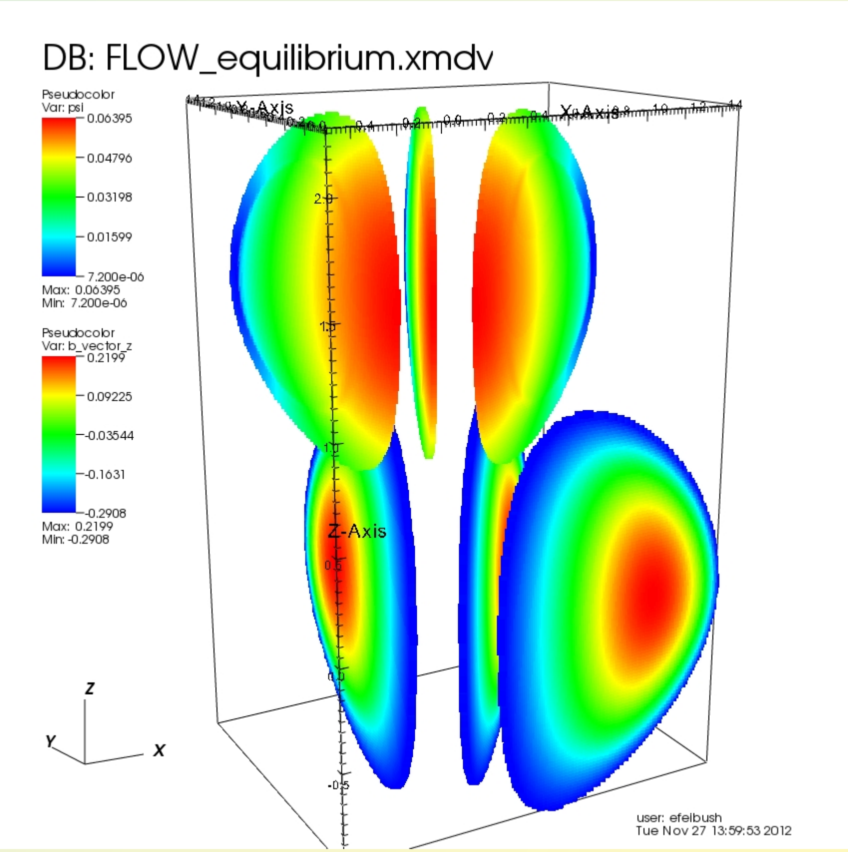
Shows Te, PSI, and JPHI concurrently.

http://w3.pppl.gov/~efeibush/movies/teiso015.mov

Transforms

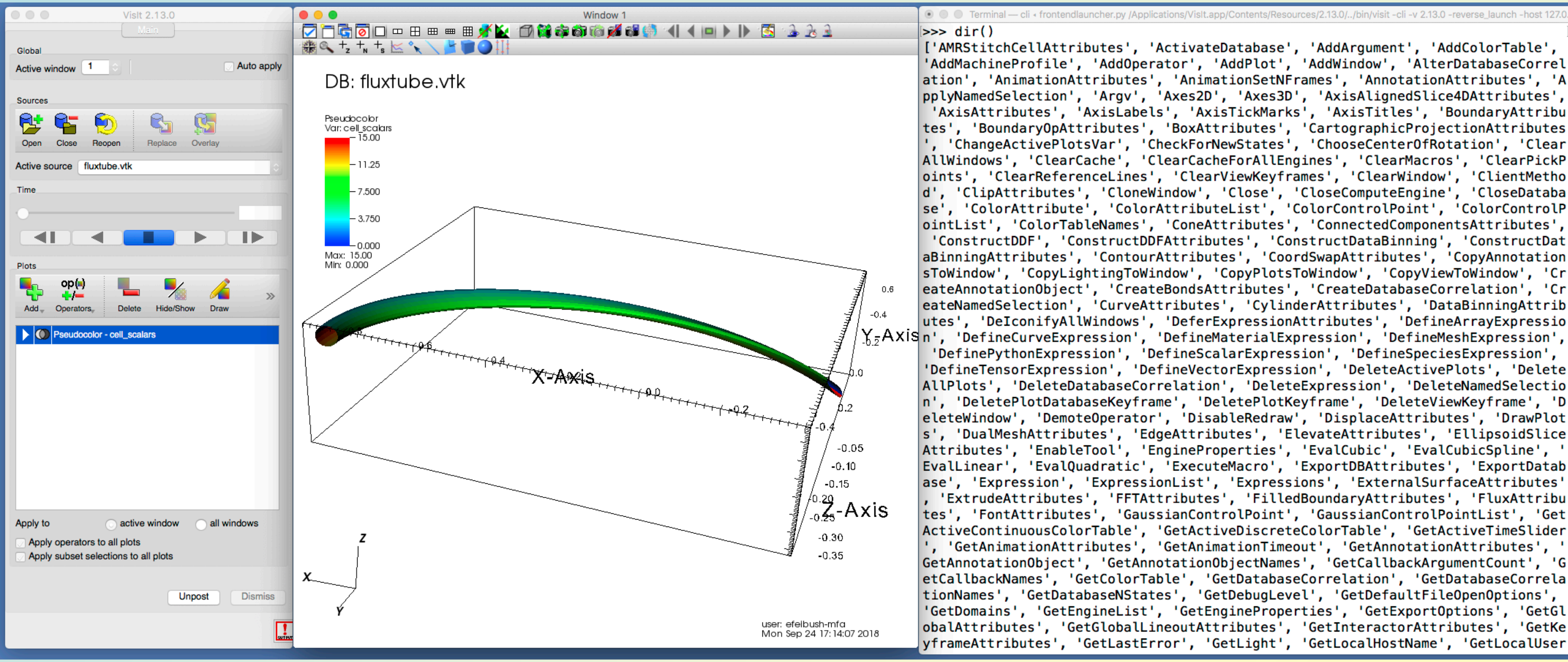
Relocate geometry

- Translate
- Rotate
- Scale



VisIt Python Interpreter

Anything from the GUI + loops, file I/O, numpy …



VisIt Python Interpreter

Anything from the GUI + loops, file I/O, numpy …

```
for k in range(3000):                          # time steps
    filename = "densityData/den" + str(k) + ".Point3D"
    print "opening database file:  " + filename
    OpenDatabase(filename, 0, "Point3D”)
    AddPlot("Pseudocolor", "value")
    DrawPlots()
    SaveWindow()        # auto increments image file name number
```

```
SetPlotOptions                    # range,  log,  geometry
   colorTableName = “CS_Chang”
Legend.numTicks = 3               # also position,  title,  font
SaveWindowAttributes()            # width,  height,  filename
```

Paraview also has a python interpreter!

Summary of Features in VisIt

Plots + Attributes
- Mesh
  - Points, Lines
- Pseudocolor
  - Polygons
  - Color Maps
- Vectors

Data Files
- VTK - grids
- Point3D

Transform Operators
- Scale, Rotate, Translate

Selection Operators
- Clip (geometric)
- Box
- Threshold (data)

Slicing Operators
- Slice, ThreeSlice
- Isosurface

Viewing

Lighting, Shadow, Depth-Cue

Annotation

Animation
- Simple Time Slider movie
- Python scripting

Images to QuickTime movie

Animation

Time step

Variable index

Geometry change

View

Operators (slice, clip, etc.)

Simple VTK file time steps

or

Complex python scripting

jpeg, png files → QuickTime .mov or .mp4

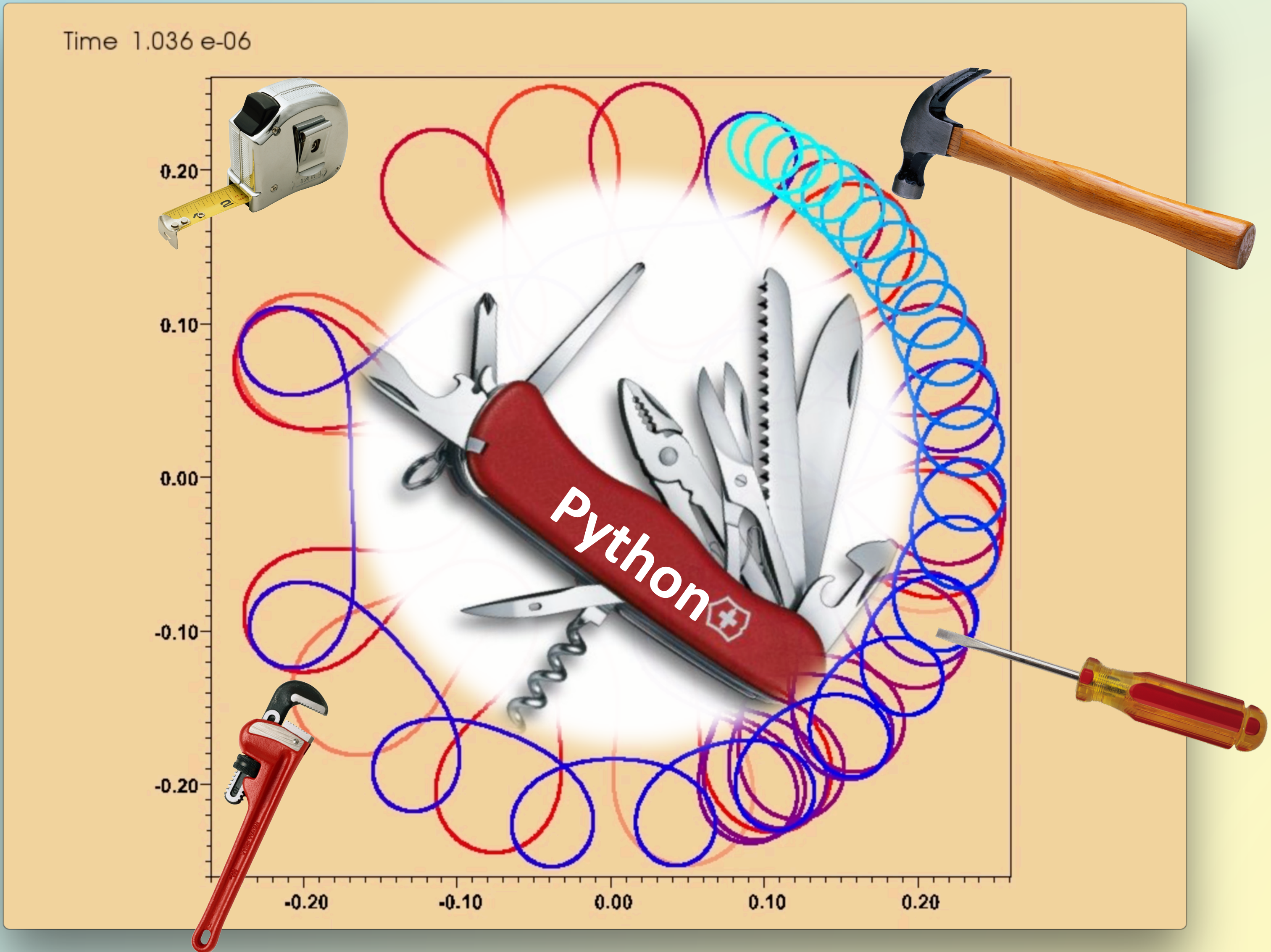
Python interpreter -

```
import myscript
```

[edit, retry]

```
reload(myscript)
```

Include Vis in Workflow



matplotlib
numpy
scipy
Imaging

VisIt
Paraview
VTK
ffmpeg

netCDF

https://wci.llnl.gov/simulation/computer-codes/visit

Downloads

Just search for: "visit visualization"

visitusers.org search ...

paraview.org

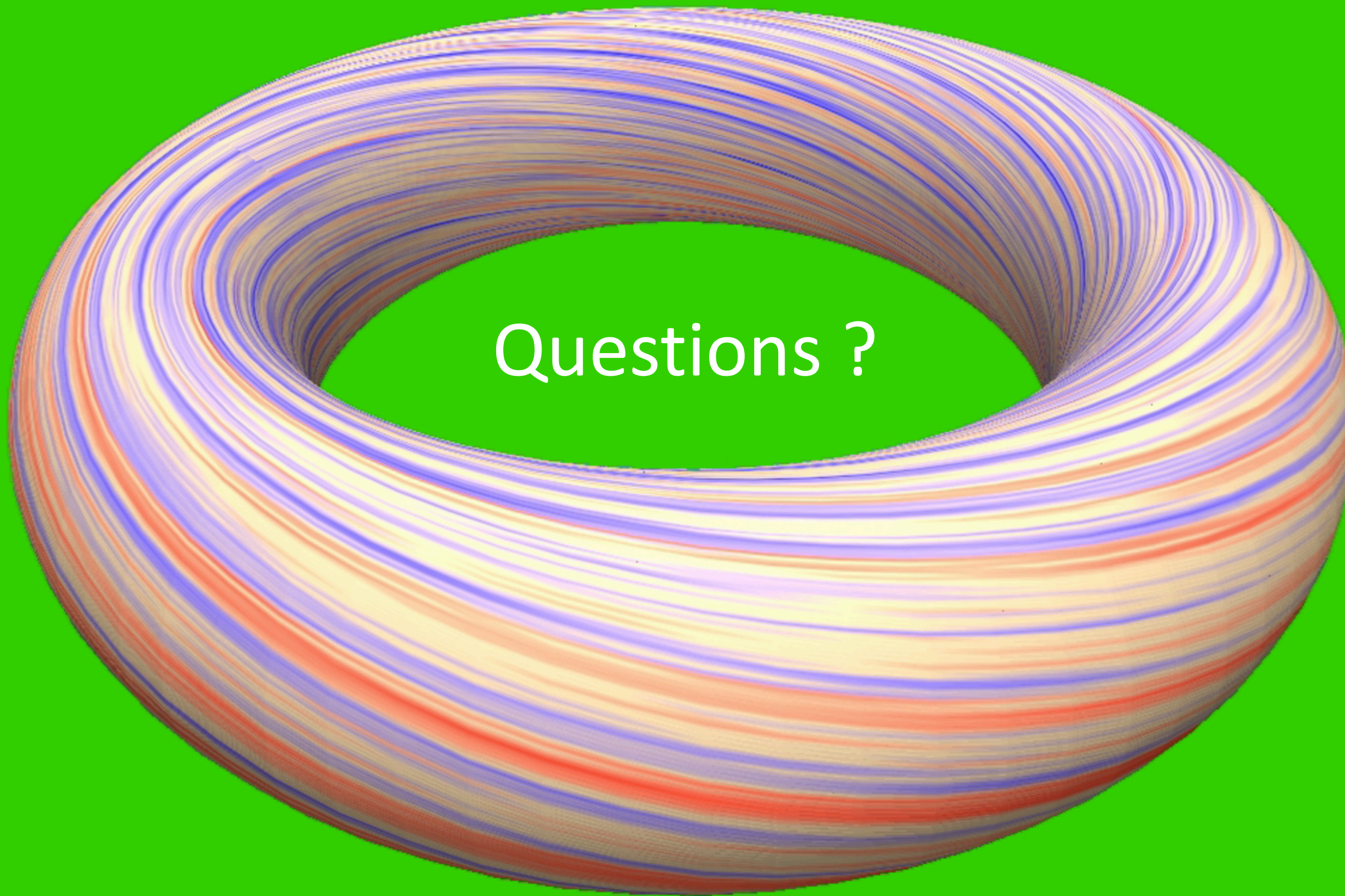
Getting Data Into VisIt - document (& your goal)

VTK File Formats - vtk.pdf on my website

www.princeton.edu/~efeibush

Visualization with VisIt mini-course 11/30

Python Programming Techniques 11/16


Questions ?