Scientific Visualization

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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://w3.pppl.gov/~efeibush/movies/m3_720.mov
Visualization of 1 Particle Path

\( f(x, y, \text{time}) \) in one picture

Vis of time axis in 3D
Time Step Simulation

Render each time step to a JPEG image.

Combine images to create animation.

http://w3.pppl.gov/~efeibush/movies
tfden.mov
Complex Compute Grid – Concentric Rings

Gaining insight ...
Time Step Simulation

Render overview + Region of Interest

Combine images into movie.

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

Simulations generate data
Acquire data from experiments

Biology
Chemistry
Physics
Engineering

...
Vis Plot Types

( Based on graphics primitives )

Points
Lines
Vectors
Contour lines & isosurfaces
Polygons, mesh
Volume
Molecule
Designing a Visualization

I want a visualization of my climate model.

Map your data to a plot type.

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

\[ f(x) \]
\[ f(x, \text{time}) \]
\[ f(x, y) \]
\[ f(x, y, \text{time}) \]
\[ f(x, y, z) \]
\[ f(x, y, z, \text{time}) \]

Time dependent data is a good candidate for animation.
Implementation

Vis GUI – VisIt, ParaView

VTK – Visualization ToolKit

Graphics Primitives

Pixels
VisIt Can Read Data Files

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

Database reader plug-ins can be developed for new formats

Variable types
- Scalar
- Vector
- Tensor
- Arrays
- Label
- Material
- Species
- X,Y pairs
Install VisIt on Your Computer

[https://visit-dav.github.io/visit-website](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
Start
All Programs
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.
Open File  strpts3d.vtk

Add Mesh
Add Pseudocolor $\rightarrow$ density

VTK:
STRUCTURED_POINTS
3 x 2 x 2 = 12 points
SCALARS density double

Download Data File:
https://www.princeton.edu/~efeibush/viscourse/visit_data/
Structured Points

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
Open File  strpts3d.vtk

Add Pseudocolor → density

Operators

Slicing

ThreeSlice

X = 6
Y = 7.5
Z = 9.5
Different color maps for different variables.
Lighting – off.
Gray background.
Density labels at mesh points.
Color Maps

Divergent color maps

+100.
0.
-100.
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

mpeg2encode in VisIt software distribution

mpeg1 format only – MPEG

Click the arrow to apply your config
Combine Images into Movies

ffmpeg

Most comprehensive
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

Non-Uniform Axis Spacing

```
# 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
```
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

vtk DataFile Version 3.0
vtk output
ASCII
DATASET STRUCTURED_GRID
DIMENSIONS 2 2 2
POINTS 8 float
0 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 0.0287671 0 0 0.0287671
0 0.0258604 0 0 0.0258604 0 0 0.0258604
0 0.0287671 0 0 0.0258604
Unstructured Grid

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

Paraview wiki: Users Guide VTK_Data_Model

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](image1)
![Plots clipped with 2 planes](image2)
![Plots clipped with a sphere](image3)

Sphere slice movie
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
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://w3.pppl.gov/~efeibush/movies
teiso015.mov
Operators on Structured Points

https://w3.pppl.gov/~efeibush/vis/rt_vis.mp4
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:

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
<th>density</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5</td>
<td>0.5</td>
<td>-0.1</td>
<td>0.003</td>
</tr>
</tbody>
</table>

Example: rho2.Point3D
Polygons vs. Grid

Data defined by discrete points connected with polygons.

Surface data only.
Not a sliceable solid!
Transforms

Relocate geometry
Translate
Rotate
Scale
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
Open File  crotamine.pdb
Type:  ProteinDataBank
Add Molecule → element
attributes
Molecular Dynamics Example

Draw points as spheres

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
jpeg, png files → QuickTime .mov

Complex python scripting

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
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
Web search for: “visit visualization”

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 HPC /projects or scratch.

Display without transferring data.

Render on tigressdata GPU instead of laptop.
TurboVNC Remote Visualization

Knowledge Base

Below is a list of guides for popular subjects. It is not comprehensive so please search our site if you do not find what you are looking for.

- **checkquota** is a command for checking your storage quota and requesting quota increases.
- **Connect by SSH** provides instruction on how to access the clusters through a command line interface.
- **Connect by Web** provides instruction on how to access the clusters through a web browser.
- **Data storage** is available on all clusters via various filesystems.
- **Environment modules** and **custom environment modules** make it easy to use software.
- **Gaussian** is software package for quantum chemistry calculations.
- **Globus** can be used to transfer large amounts of data.
- **GPU Computing** covers the hardware at Princeton and related tools.
- **Graphical applications using X11 forwarding** can be used as described on this page.
- **GROMACS** is a biomolecular simulation package.
- **JAX** is a flexible Python library for machine learning research.
- **Jenkins** provides automatic testing typically for continuous integration.
- **Job Priority** of Slurm jobs is explained on this page.
- **Job Stats** or `stats.rc` provides detailed metrics about running and completed jobs.
- **Julia** is a programming language for scientific and numerical computing.
- **Jupyter notebooks** can be run in various ways on the HPC clusters.
- **LAMMPS** is a molecular dynamics simulation package.
- **MAP** is performance profiler for parallel and GPU codes.
- **Mathematica** is an integrated environment for numerical computing.
- **MATLAB** is a popular environment for scientific computing.
- **Memory allocation for Slurm script** is explained on this page.
ssh tigressdata

Off-Campus Considerations

How to ssh to tigressdata

VPN

OIT web page - search for VPN

How do I connect to University online resources from off-campus?
File System

df command shows:

/tigress

/tiger/scratch/gpfs

/projects
tigressdata Remote Vis

TurboVNC remote desktop, Client - Server architecture

3 Step Process

1. Start vncserver on tigressdata

2. Establish tunnel from your computer to tigressdata

3. Run vncviewer on your computer (client)

search: turbovnc
Install from
sourceforge.net/projects/turbovnc
1. Start VNC Server

ssh tigressdata

$ module load turbovnc

$ vncserver

$ vncserver -list

note X Display # such as :2

First time: create password, stored in
~/.vnc/passwd (delete file to reset)
2. Establish Tunnel

*(because turbovnc is not encrypted)*

```
ssh -A -L 5902:localhost:5902 efeibush@tigressdata
```

5900 + X Display #  *(hence step 2 is after step 1)*

- **A** Enables authentication forwarding.

- **L** Enables client-server port-to-port connection.
3. Run turbovnc locally

Enter your .vnc/passwd
client: turbovnc viewer
module load virtualgl
Contact

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www.princeton.edu/~efeibush/viscourse

Visualization Help:
visrc@princeton.edu

Computing Help:
researchcomputing.princeton.edu

Support --> Submit a ticket
Open File interplines.vtk
Add Pseudocolor temperature
Add Label temperature

Example of data defined by discrete points connected with lines.