Kitware

VTK + ParaView Using NetCDF & VTK

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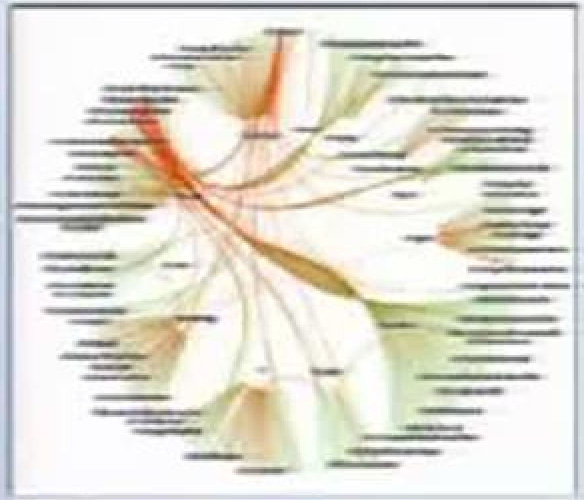
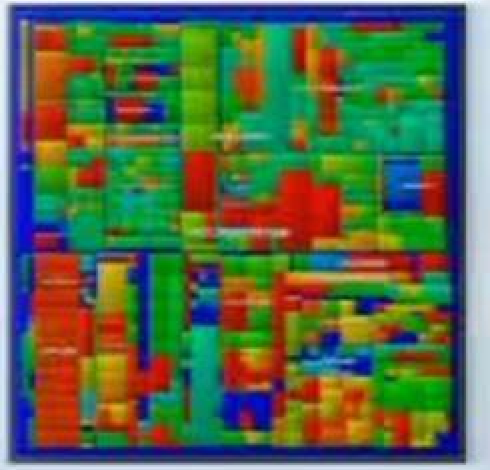
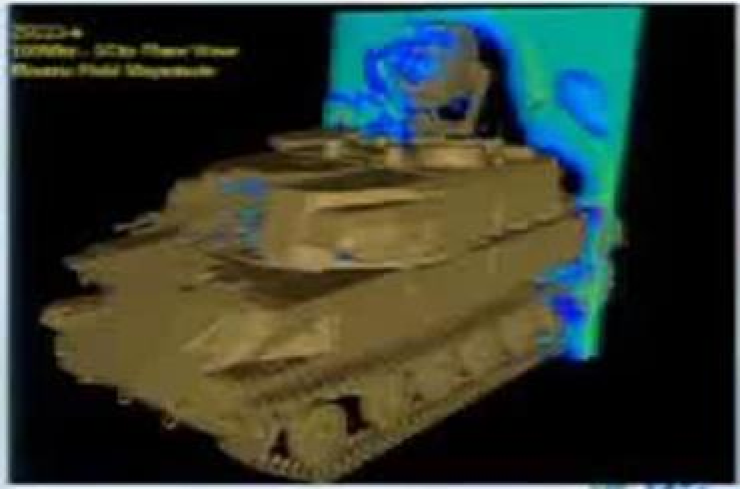
The Visualization Toolkit (VTK)

- www.vtk.org
- Started in 1993 at GE
- Visualization Library
  - Written in C++ (+8.2 million LOC) – BSD License
  - Automatic binding for Java, TCL, Python
  - Portable by design: Linux, Windows, Mac OSX, Solaris…
- Very active community: 4000+ users on the mailing list







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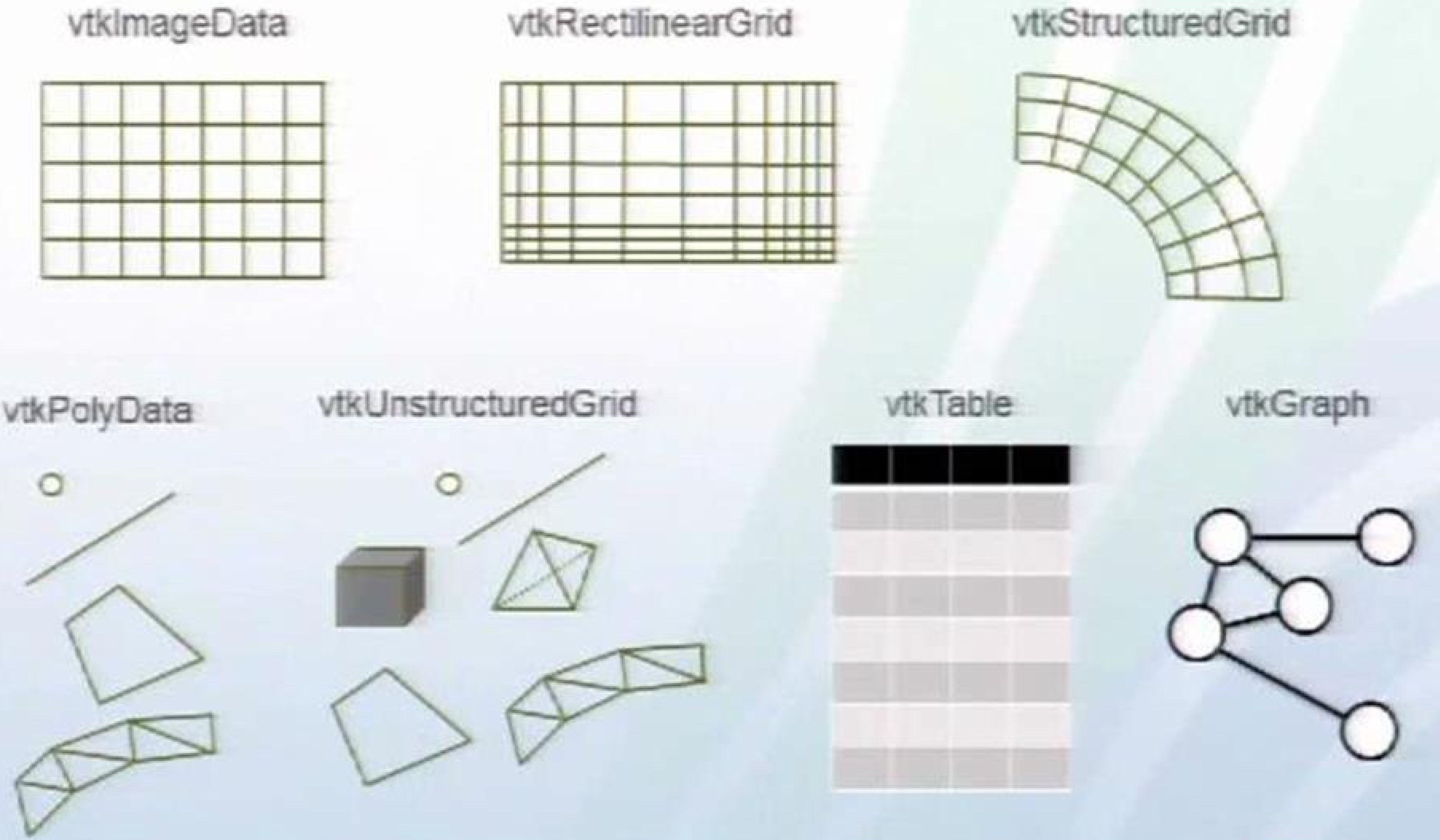
VTK Data Types



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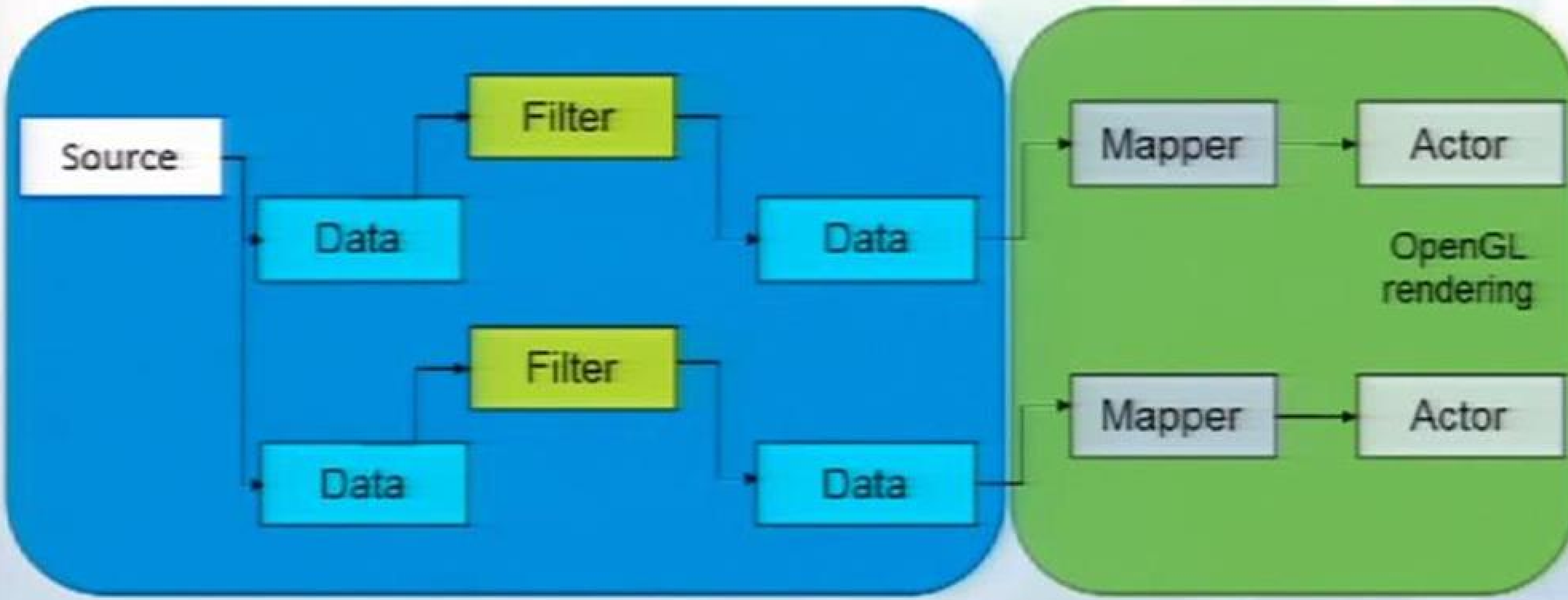
VTK Pipeline Architecture

- A sequence of algorithms that operate on data objects to generate geometry that can be rendered by the graphics engine or written to a file



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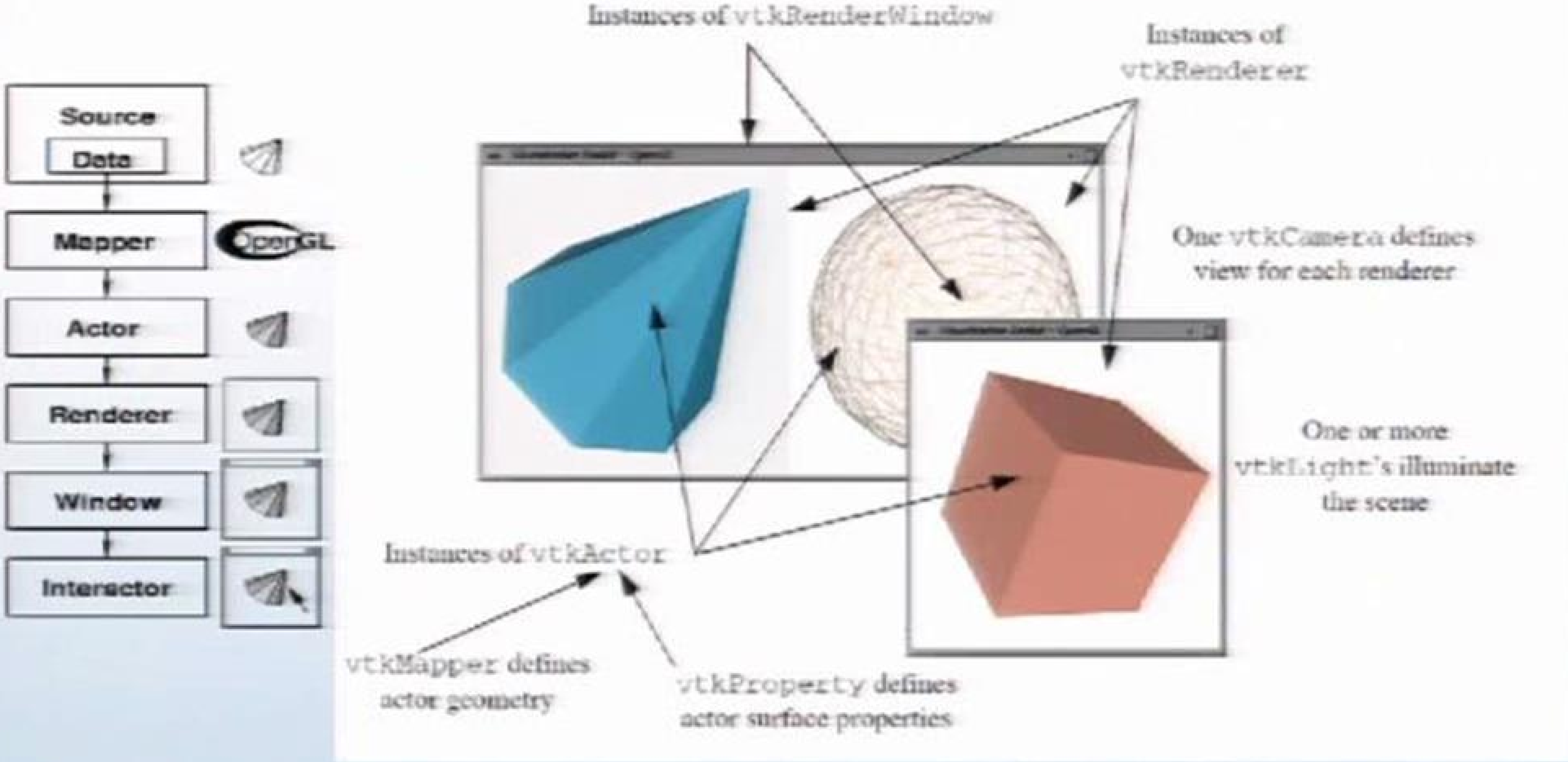
The VTK Graphics Subsystem



VTK with Python

- VTK distribution
  - www.vtk.org
  - vtkpython standalone Python interface (Python 2.7)
  - Active work to support Python 3
- Anaconda
  - https://store.continuum.io/cshop/anaconda/
- Compilation from source
  - www.vtk.org (via CMake)

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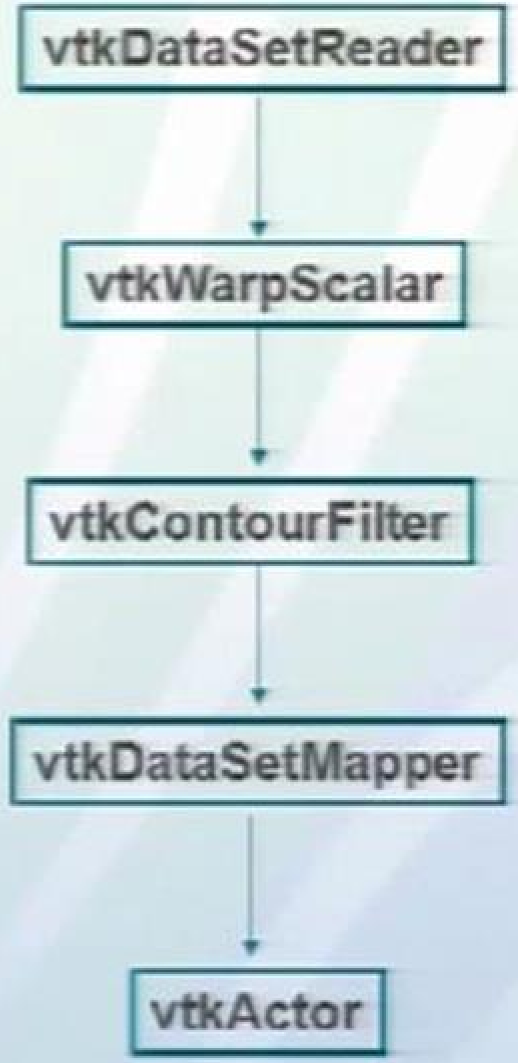
Why Use VTK with Python

- Get direct access to VTK objects
  - Can inspect data objects and values
  - Can set data objects and values
- Access to VTK's filters
  - Read data
  - Operate on data
  - Write data
  - View data
- Fine level control of rendering

Tutorial – Display and Interact with DEM Data

- Input Data
  - Digital Elevation model
  - Standard Geospatial File Format
  - SaintHelens.vtk
  - Structured Grid with an elevation scalar field
- We want to be able to
  - Load data
  - Represent the elevation → 3D
  - Represent isolines of elevation
  - Clip the data
- Source code at /home/pyvis/tutorial/Section4_vtk_pv/vtk_dem.py
  - Can run with vtkpython or pvpython



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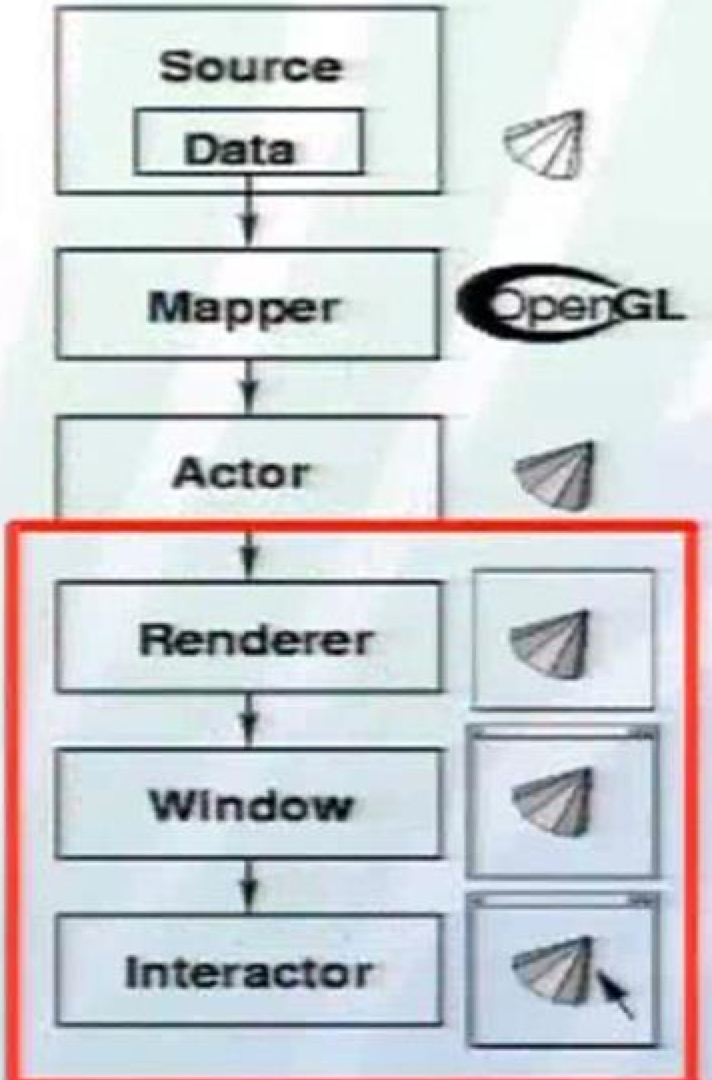
Step 1 – Creating the Display

```
# First thing first
import vtk

# Make a window on our display
renwin = vtk.vtkRenderWindow()
# Define the size of the initial window
renwin.SetSize(500,500)
# Create a renderer
renderer = vtk.vtkRenderer()
renderer.SetBackground2(1,1,1)
renderer.SetGradientBackground(1)
# Create an interactor
iren = vtk.vtkRenderWindowInteractor()
# Add the renderer to the render window
renwin.AddRenderer(renderer)
# Set the interactor to the render window
renwin.SetInteractor(iren)
# Show the (empty) window
windowrenwin.Render()
```



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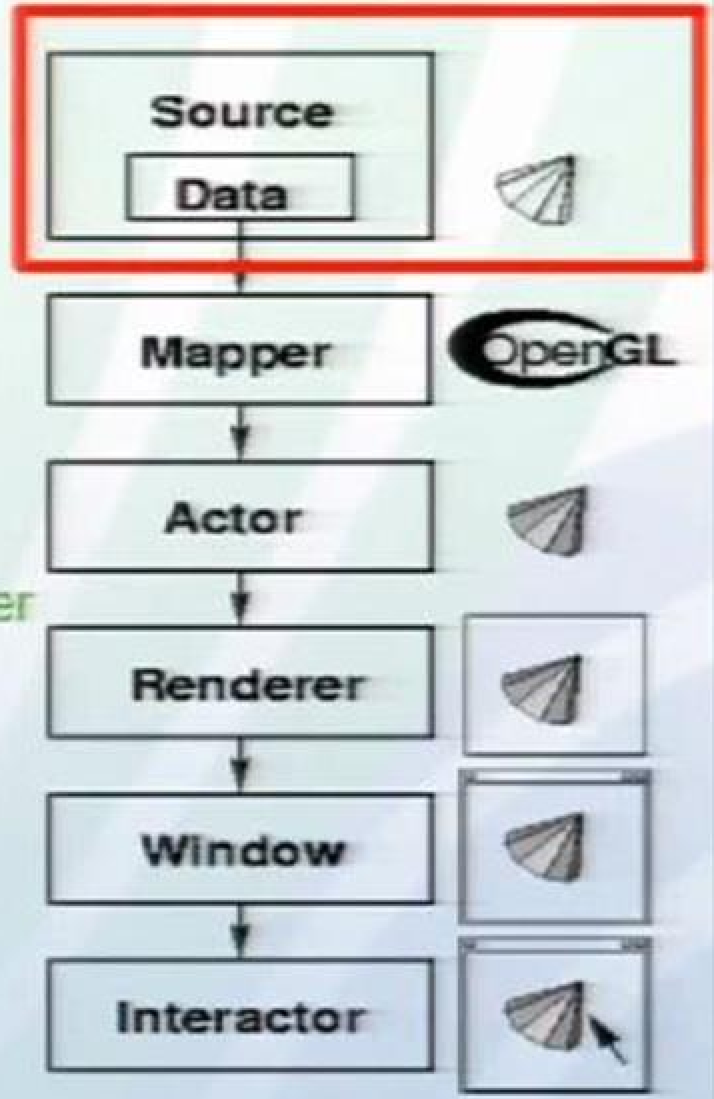
Step 1b – Enabling interactions

```
# Initialize the interactor
iren.Initialize()
# Update the rendering pipeline
renwin.Render()
# Start the UI event loop
iren.Start()
```

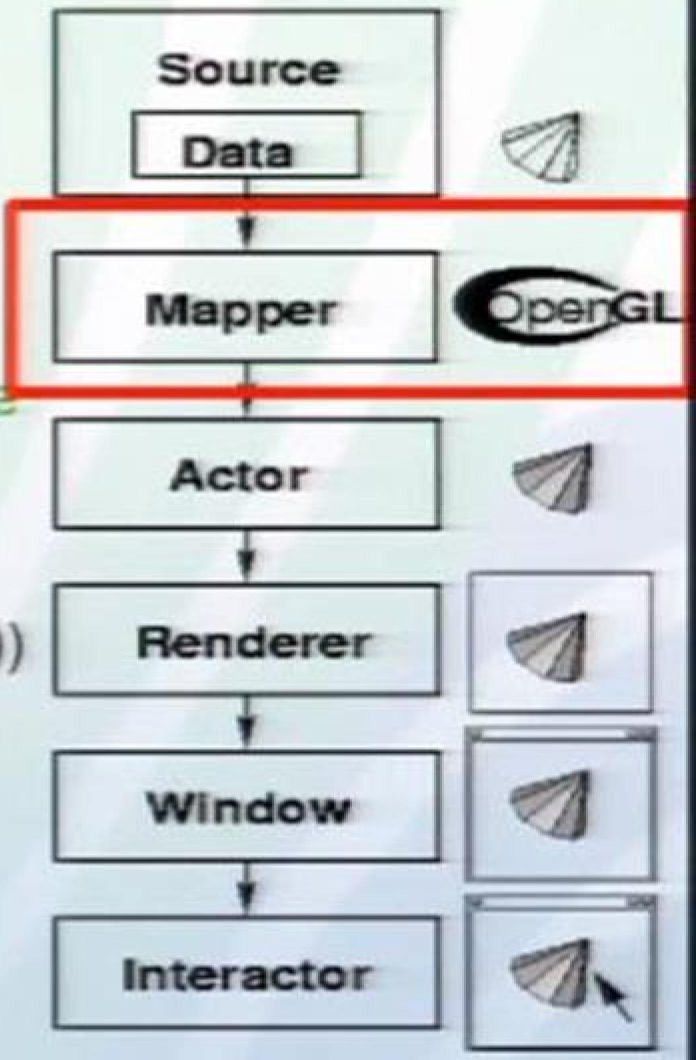
Step 2 – Read the DEM file

```
# Creating a reader
reader = vtk.vtkDataSetReader()
filename = "SaintHelens.vtk"
reader.SetFileName(filename)
# Updating the pipeline
reader.Update()
# Printing information about the output of the reader
id = reader.GetOutput()
print(id.GetClassName())
print(id.GetBounds())
print id.GetPointData().GetArray(0).GetRange()
```



Step 3 – Creating the mapper

```
# Create the mapper
mapper = vtk.vtkDataSetMapper()
# Set the visibility on the scalar
mapper.ScalarVisibilityOn()
# Set the scalar range to have a nice blue-red range
mapper.SetScalarRange(682.0, 2543.0)
# Connect the mapper to the reader
mapper.SetInputConnection(reader.GetOutputPort())
```



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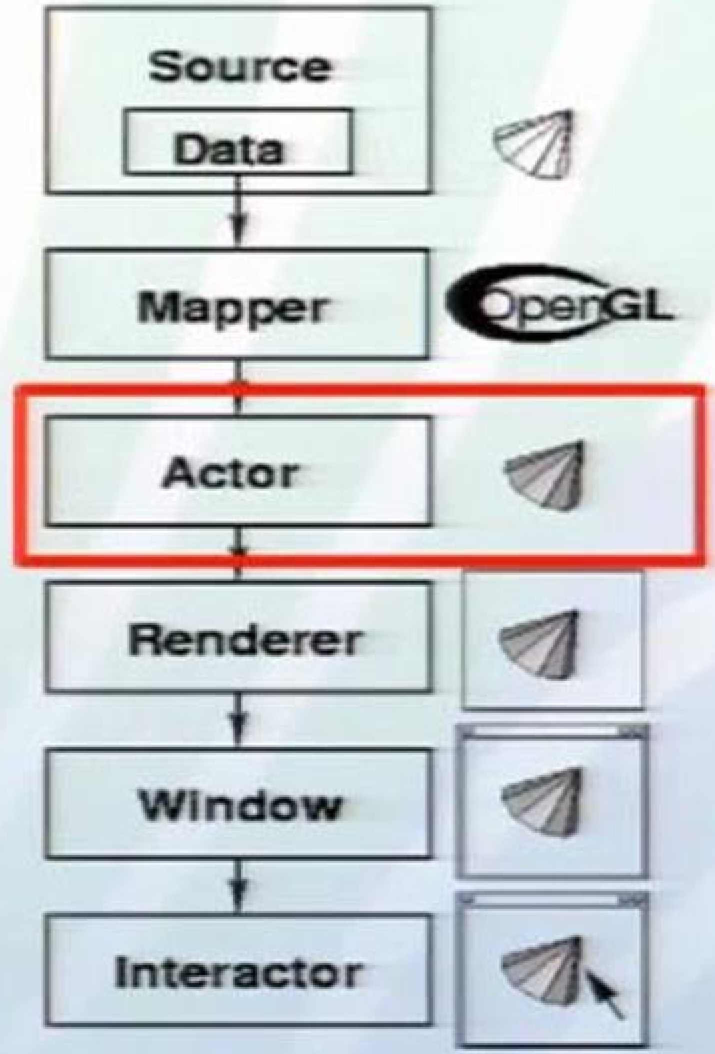
Step 4 – Creating the Actor

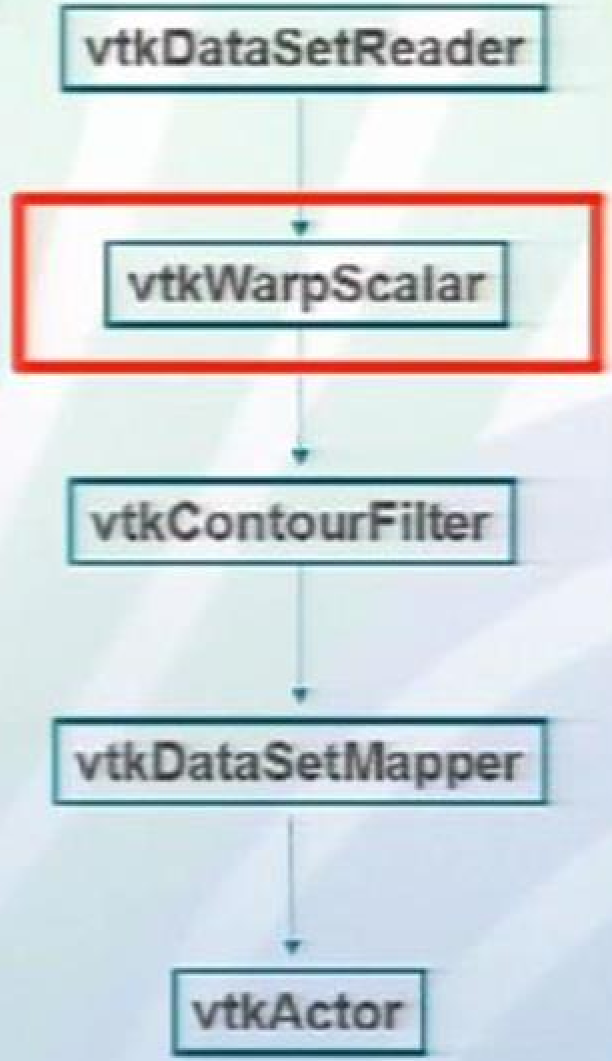
```
# Create the actor
actor = vtk.vtkActor()
# Sets the mapper to the actor
actor.SetMapper(mapper)
# Add the actor to the renderer
renderer.AddViewProp(actor)
# Perform rendering
renwin.Render()
# Center the camera to see the full scene
renderer.ResetCamera()
# Final rendering
renwin.Render()
```



Step 5 – Elevating our surface to 3D

```
# We elevate the surface with the vtkWarpScalarFilter
warp = vtk.vtkWarpScalar()
# Connect the filter to the reader
warp.SetInputConnection(reader.GetOutputPort())
# Update the pipeline
warp.Update()
print(warp.GetOutput().GetBounds())

# Show the elevated surface
mapper.SetInputConnection(warp.GetOutputPort())
renwin.Render()
renderer.ResetCamera()
renwin.Render()
```



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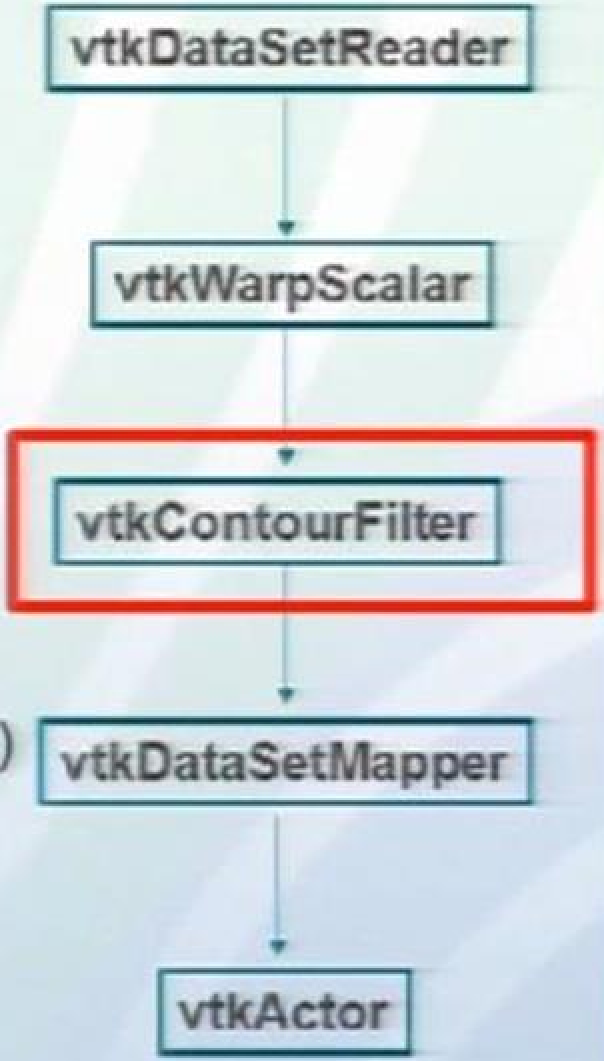
Step 5b – Drawing iso-surfaces

```
# Draw the iso-surface
isosurface = vtk.vtkContourFilter()
# Generate 10 iso-surfaces along the elevation
isosurface.GenerateValues(10,682.0,2543.0);
# Connect the filter to the reader
isosurface.SetInputConnection(warp.GetOutputPort())
# Update the pipeline
isosurface.Update()

mapper.SetInputConnection(isosurface.GetOutputPort())
renwin.Render()
renderer.ResetCamera()
renwin.Render()
```



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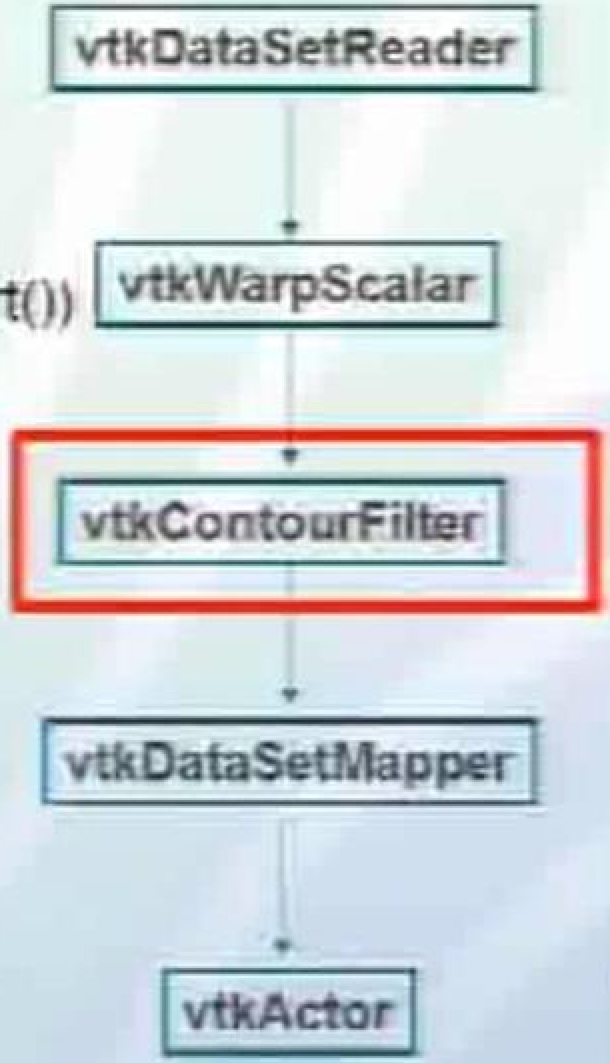
Step 6 – Exercise - Display iso-surface and data

```
# Render everything into one
mapper.SetInputConnection(warp.GetOutputPort())
# Create a new mapper
mapperiso = vtk.vtkDataSetMapper()
mapperiso.SetInputConnection(isosurface.GetOutputPort())
# Create the actor
actoriso = vtk.vtkActor()
actoriso.SetMapper(mapperiso)
# Disable the scalar coloring
mapperiso.ScalarVisibilityOff()
# Set the color to black
actoriso.GetProperty().SetColor(0,0,0)
# Set the line width larger
actoriso.GetProperty().SetLineWidth(2)
# add the actor to the rendering
renderer.AddViewProp(actoriso)
```



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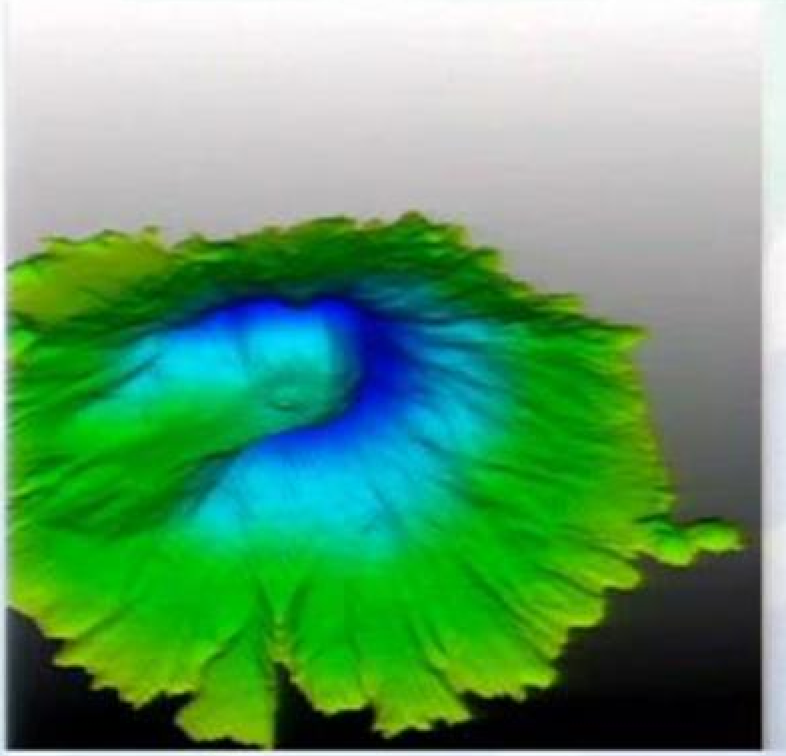
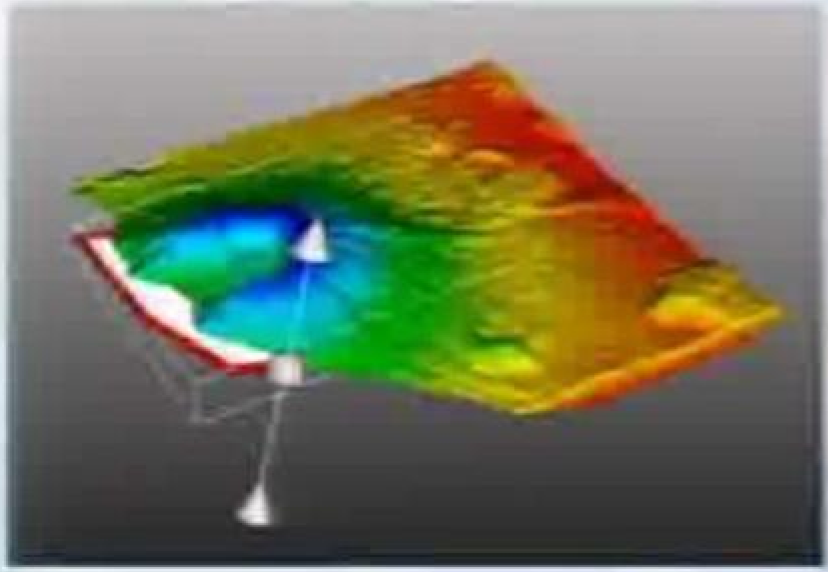
Step 7 – Clipping the data

```
# Remove first the iso actor
renderer.RemoveViewProp(actoriso)

# Clip the data
cf = vtk.vtkClipDataSet()
# Set the clipping plane
plane = vtk.vtkPlane()
cf.SetClipFunction(plane)
print plane
# Set the plane origin
plane.SetOrigin(560000,5120000,2000)
# Connect the pipeline
cf.SetInputConnection(warp.GetOutputPort())
mapper.SetInputConnection(cf.GetOutputPort())
```



Step 8 – Clipping Widget interaction

```
# Creates an implicit plane widget
widget = vtk.vtkImplicitPlaneWidget()
widget.PlaceWidget(warp.GetOutput().GetBounds())
widget.SetOrigin([plane.GetOrigin()[x] for x in 0,1,2])
widget.SetNormal([plane.GetNormal()[x] for x in 0,1,2])
widget.SetInteractor(iren)

# Connects the interaction event to the plane
def cb(obj,event):
    global plane
    obj.GetPlane(plane)
widget.AddObserver("InteractionEvent", cb)
widget.SetEnabled(1)
widget.DrawPlaneOn()
widget.TubingOn()
renwin.Render()
```



VTK and NumPy – Step 1: VTK to NumPy

Source code at
/home/pyvis/tutorial/Section4_vtk_pv/vtk_to_numpy.py

- Run with pvpython (vtkpython doesn't have support for NumPy)

```
# Example of VTK array to NumPy
import vtk
vtkarray = vtk.vtkDoubleArray()
vtkarray.InsertNextValue(1)
vtkarray.InsertNextValue(2)
from vtk.util.numpy_support import vtk_to_numpy
numpyarray = vtk_to_numpy(vtkarray)
```

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Improved VTK - NumPy Integration

Source code at /home/pyvis/tutorial/Section4_vtk_pv/improved_vtk_numpy_integration.py

- Run with pvpython (vtkpython doesn't have support for NumPy)

```
import vtk
from vtk.numpy_interface import dataset_adapter as dsa
from vtk.numpy_interface import algorithms as algs
reader = vtk.vtkMPASReader()
reader.SetFileName('MPASReader.nc')
# Have reader examine what information is available
reader.UpdateInformation()
# Print out available arrays
for i in range(reader.GetNumberOfCellArrays()):
   print reader.GetCellArrayName(i)
```

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Improved VTK - NumPy Integration (continued)

```
# Don't read in the ke cell data array
reader.SetCellArrayStatus('ke', 0)
reader.Update()
# Wrap the reader output to simplify access
wrappedreader = dsa.WrapDataObject(reader.GetOutput())
print wrappedreader.PointData.keys()
print wrappedreader.CellData['vorticity']
vorticity = wrappedreader.CellData['vorticity']
# Perform some operations on the data
wrappedreader.CellData.append(vorticity + 1, 'vorticity plus one')
print algs.max(vorticity)
print algs.max(wrappedreader.CellData['vorticity plus one'])
```

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Grid Aware Algorithms

Source code at /home/pyvis/tutorial/Section4_vtk_pv/grid_aware_algorithms.py

- Run with pvpython (vtkpython doesn't have support for NumPy)

```
import vtk
from vtk.numpy_interface import dataset_adapter as dsa
from vtk.numpy_interface import algorithms as algs
# Create a dataset
w = vtk.vtkRTAnalyticSource()
t = vtk.vtkDataSetTriangleFilter()
t.SetInputConnection(w.GetOutputPort())
t.Update()
# Compute gradient of RTData array
ugrid = dsa.WrapDataObject(t.GetOutput())
print algs.gradient(ugrid.PointData['RTData'])
```

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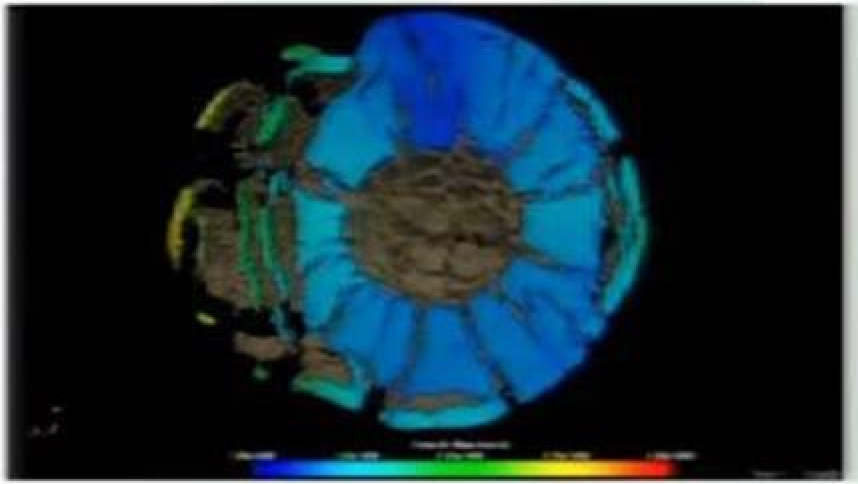
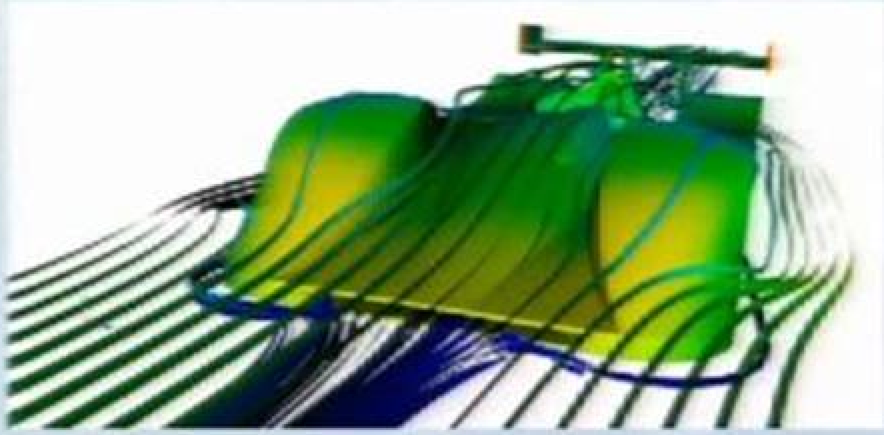
ParaView

- www.paraview.org
- Open source (BSD)
- Based on VTK
- C++/Qt
- Python support
- Very active community (HPC Wire award)
- Multi-core support (MPI)
- Co-processing (*in situ*)
- More than 50 data readers



1 billion cell asteroid detonation simulation



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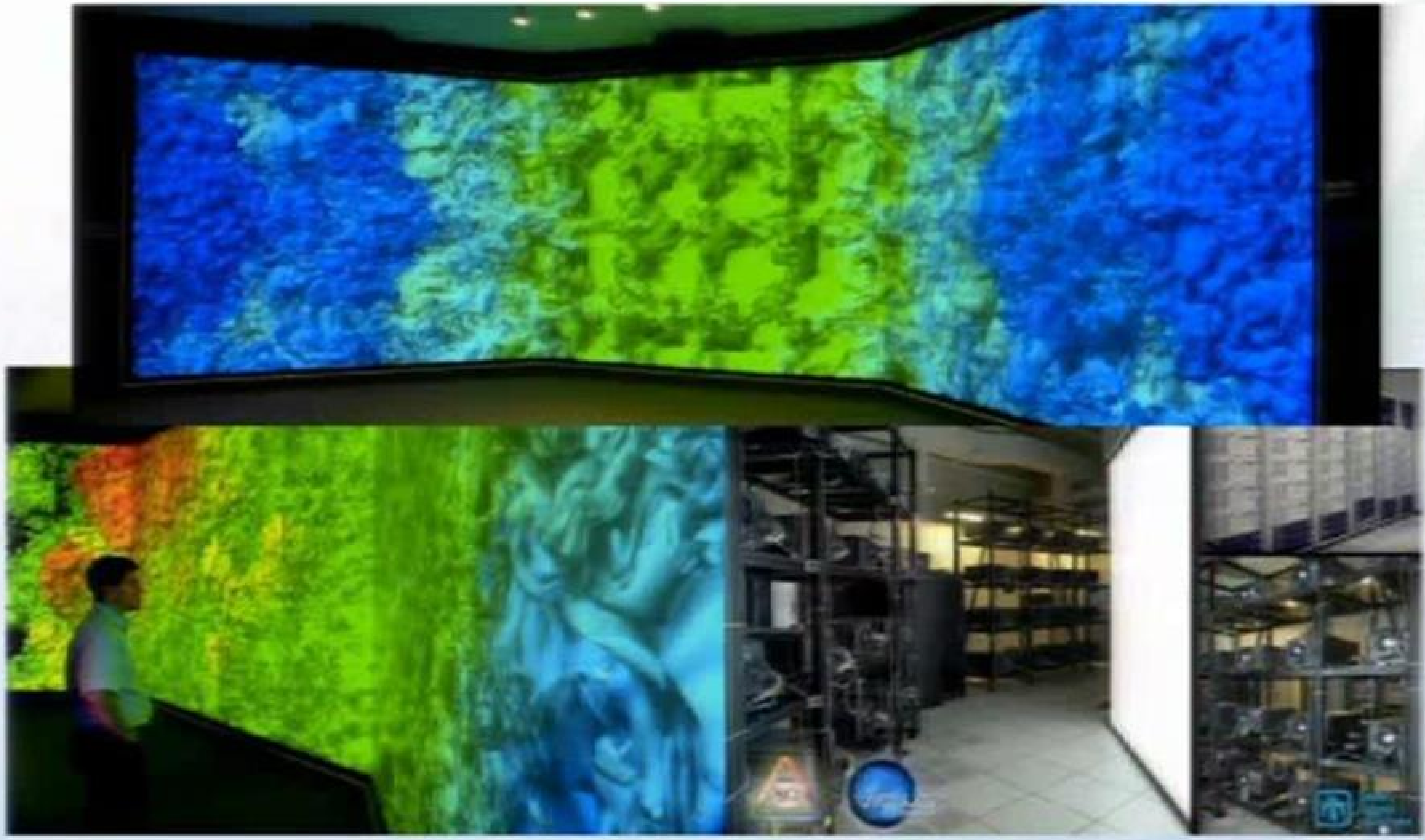
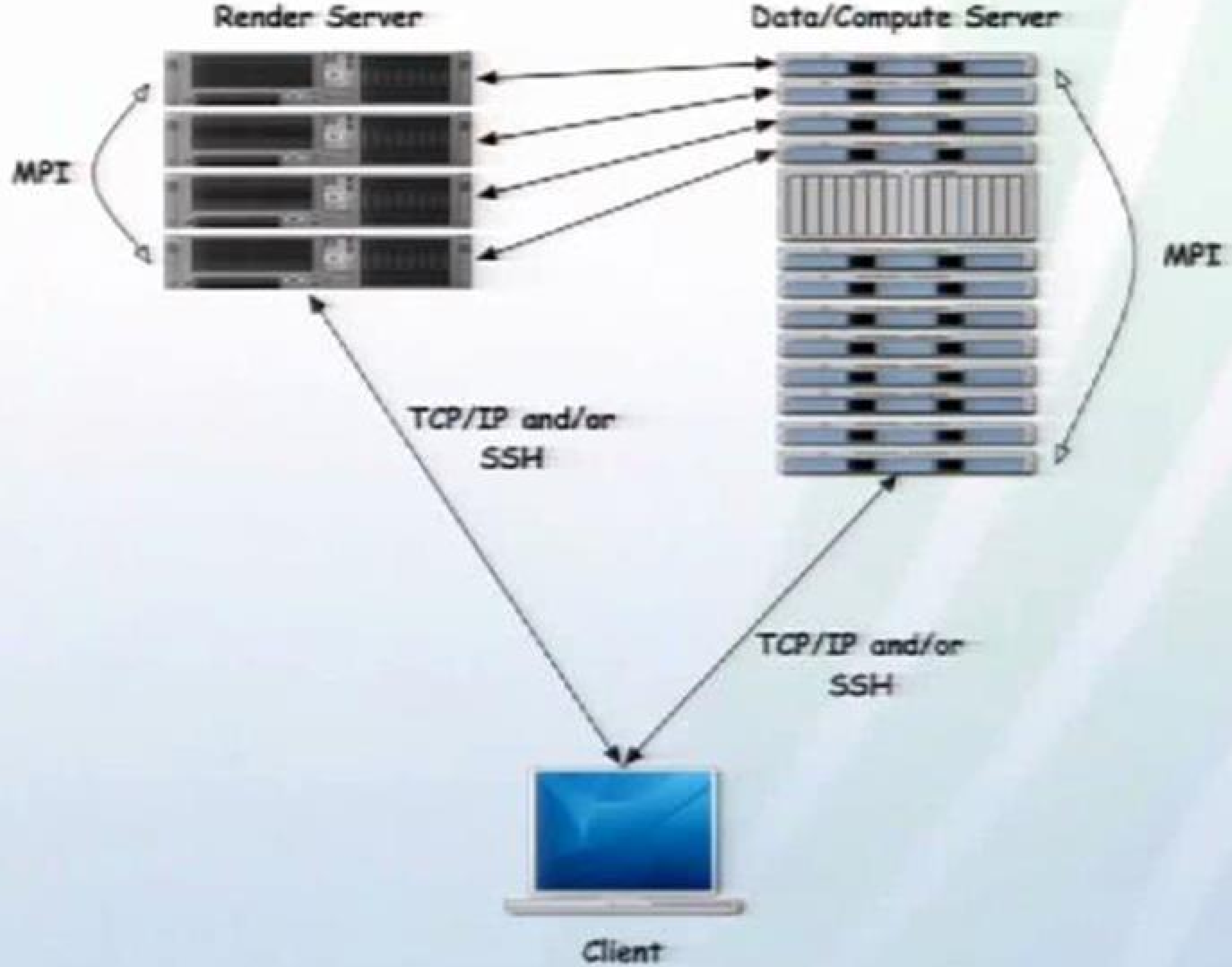
ParaView in Use – Immersive Visualization



ParaView Architecture



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Why Use ParaView with Python

- Client-server architecture
- Easy to use in parallel
  - Image compositing & rendering
  - Avoid common VTK mistakes (e.g. parallel XML formats need process 0 to have field data arrays for meta-data file)
- All of VTK filters plus more
- Meta-data instead of data
  - Bounds, ranges, sizes
- GUI shortcuts
  - Trace option to mirror GUI operations in Python
  - GUI widgets to execute Python scripts

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Creating a simple visualization

Source code at
/home/pyvis/tutorial/Section4_vtk_pv/simple_visualization.py
- Run with pvpython

- Create a cone
```
>>> myCone = Cone()
```
- Get documentation on cone and its properties
```
>>> help(myCone)
```
- Examine a property
```
>>> myCone.Center
```
- Change a property
```
>>> myCone.Center = [0,0,1]
```
- Show the result
```
>>> Show(myCone)
>>> Render()
```

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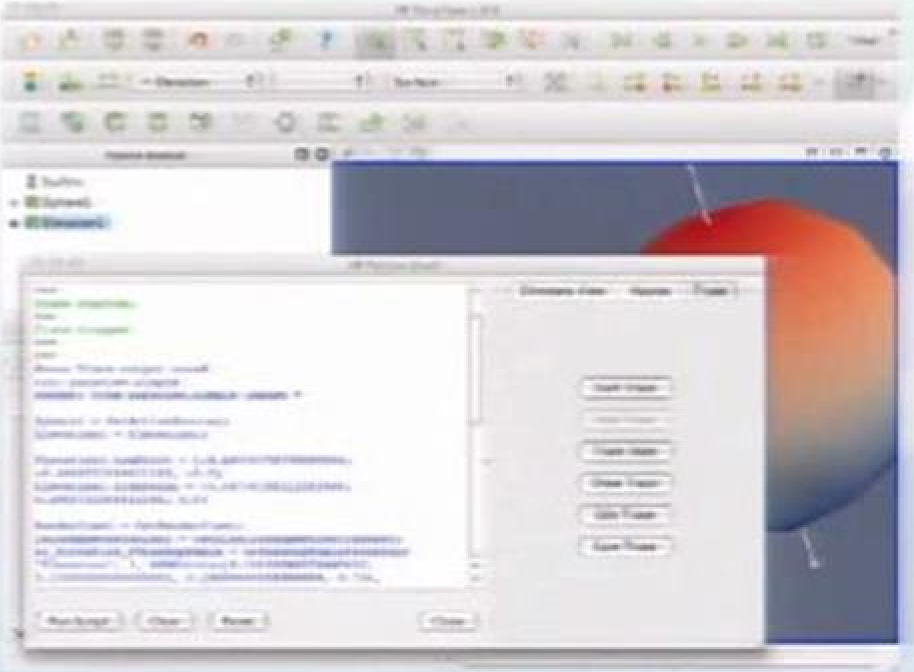
Trace – record python script from GUI

- Tools → Start Trace
  - Starts recording GUI actions
- Tools → Stop Trace
  - Finishes recording
  - Brings up script editor
- File → Save
  - Writes script to file
- File → Save as Macro…
  - Saves script and adds button to menu that calls it
- Macros
  - Execute and manage macros you've created



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NetCDF with ParaView

- Source code at /home/pyvis/tutorial/Section4_vtk_pv/netcdf_with_paraview.py
- Run pvpython

```
>>> from paraview.simple import *
>>> reader = NetCDFMPASreader(FileName='MPASReader.nc')
>>> # Get information about what's in the file
>>> reader.UpdatePipelineInformation()
>>> print reader.PointArrayStatus
>>> print reader.TimestepValues
>>> # Read in only some of the arrays
>>> reader.PointArrayStatus = ['latCell', 'lonCell', 'xCell', 'nEdgesOnCell', 'areaCell']
>>> # Read in the requested data
>>> reader.UpdatePipeline()
>>> # Change time steps
>>> animation = GetAnimationScene()
>>> animation.GoToLast()
>>> animation.GoToPrevious()
```

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ParaView Catalyst

- Goals:
  - Provide flexible *in situ* analysis and visualization options in addition to traditional post-processing options
    - Integrated workflow with widely used tool set
    - Traditional options still available
  - Increase the value of data saved to permanent storage
    - Increased fidelity in time/space
  - Create framework for sampling and visualization R&D
    - Large scale sampling
    - Novel visualization options (ParaView Cinema, etc.)
  - Optimize I/O
    - Will continue to be under heavy constraints ...

Why *In Situ*?

System Parameter	2011	"2018"		Factor Change
System peak	2 PF	1 EF		500
Power	6 MW	≤20 MW		3
System Memory	0.3 PB	32-64 PB		33
Node Performance	0.125 TF	1 TF	10 TF	8-80
Node Concurrency	12	1,000	10,000	83-830
Network BW	1.5 GB/s	100 GB/s	1,000 GB/s	66-660
System Size (nodes)	18,700	1M	100k	50
Total Concurrency	225 K	10 B	100 B	40k-400k
Storage Capacity	15 PB	300-1,000 PB		20-67
I/O BW	0.2 TB/s	20-60 TB/s		100-300

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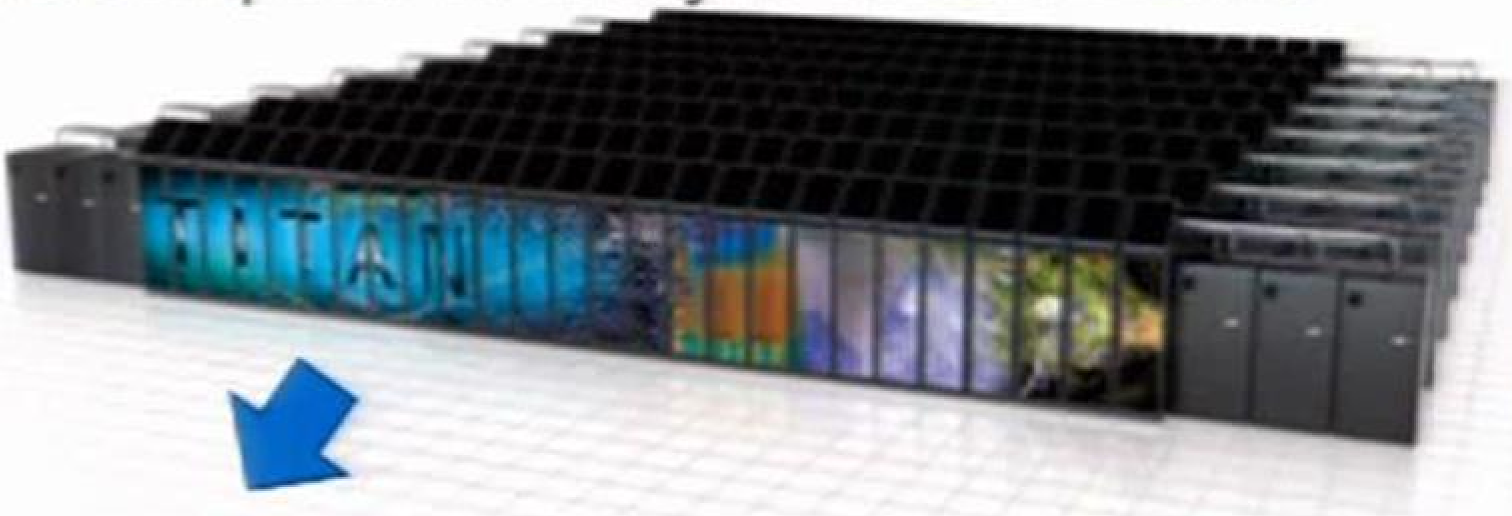
Why *In Situ*?

Need a supercomputer to analyze results from a hero run



2 orders of magnitude difference between each level

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Access to More Data

Post-processing

In situ processing

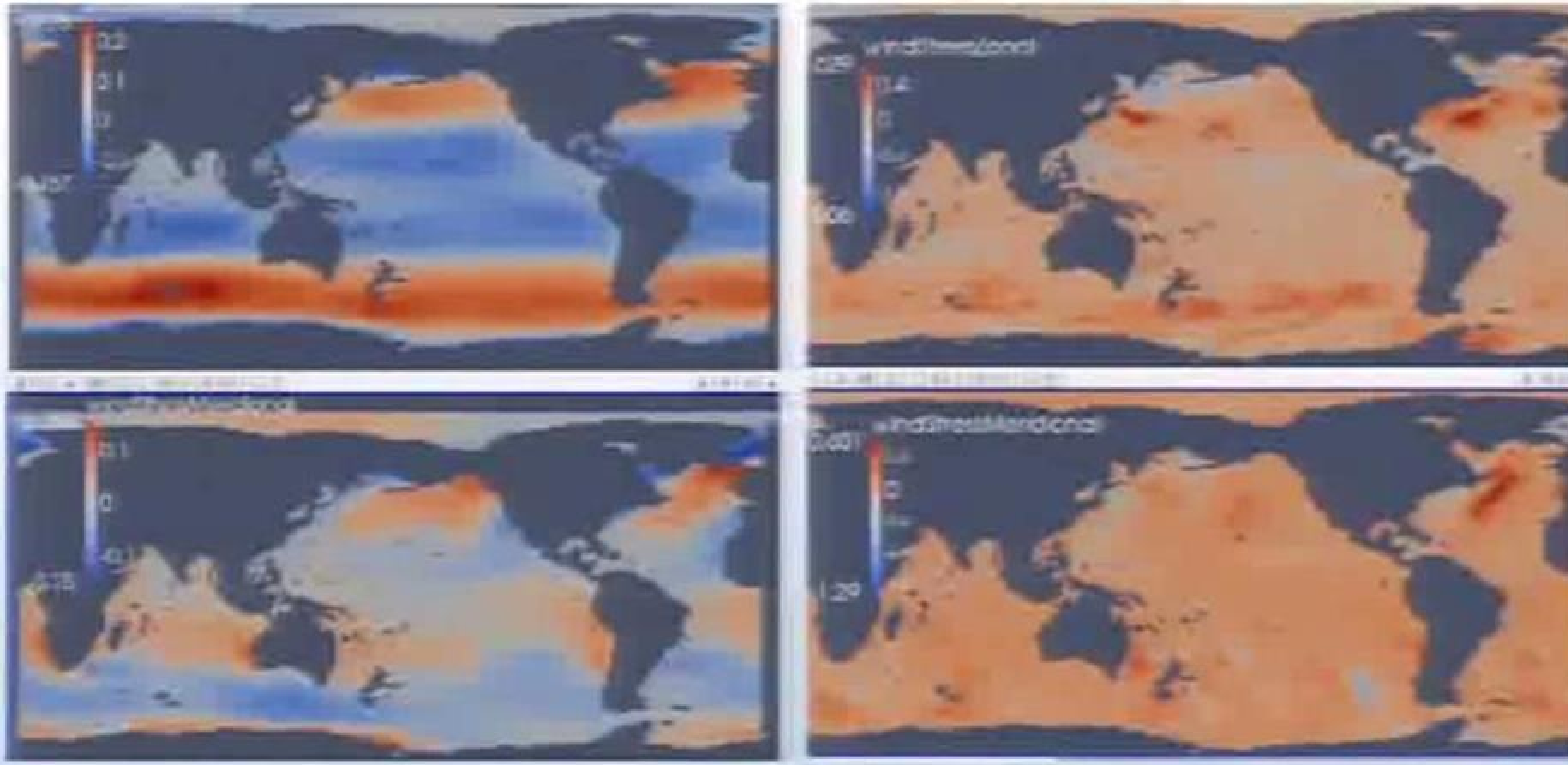
CTH (Sandia) simulation with roughly equal data stored at simulation time

Reflections and shadows added in post-processing for both examples

Quick and Easy Run-Time Checks

Expected wind stress field at the surface of the ocean

Wind stress in new run, quick glance indicates we are using wrong wind stress



MPAS-O (LANL) simulation

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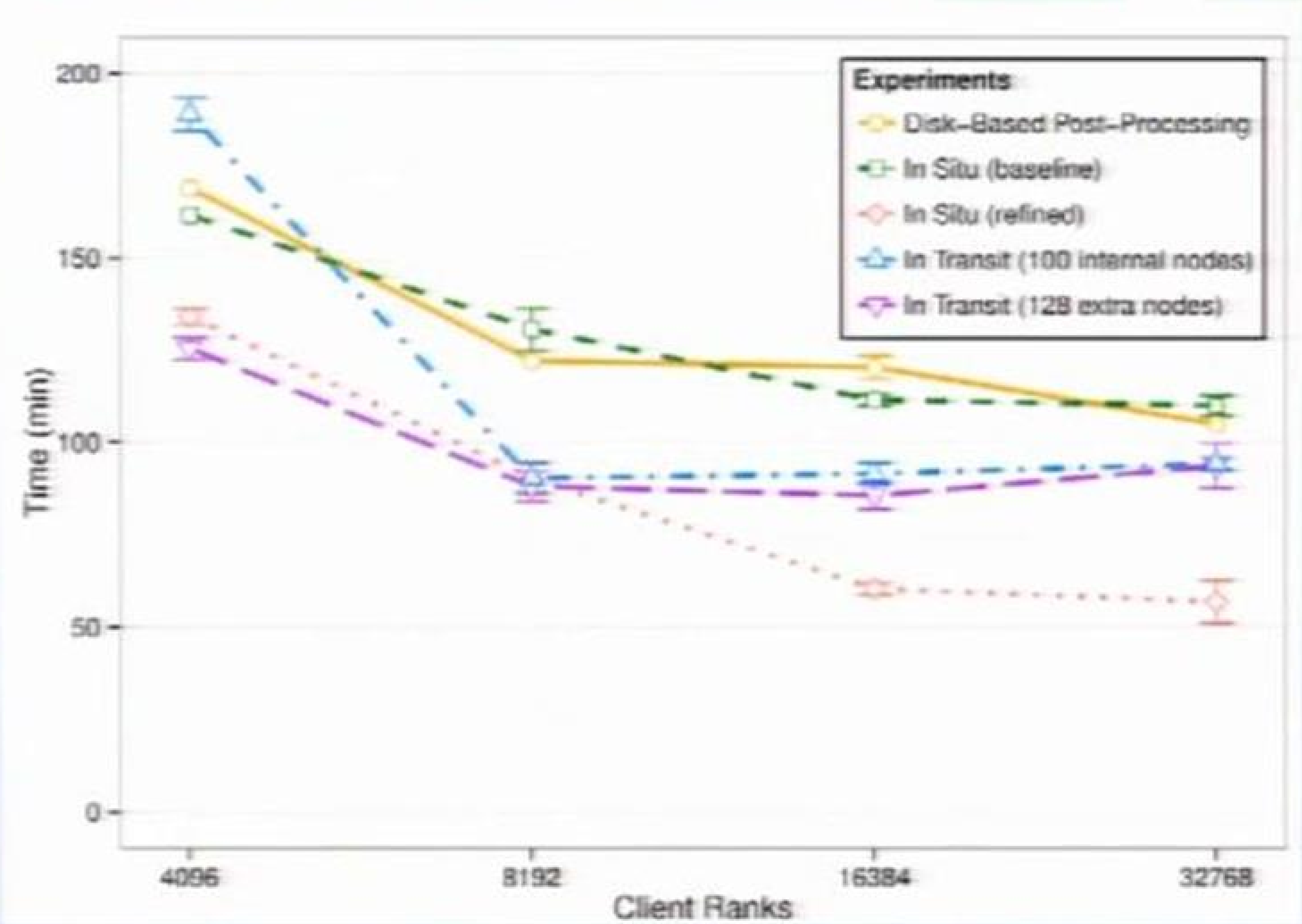
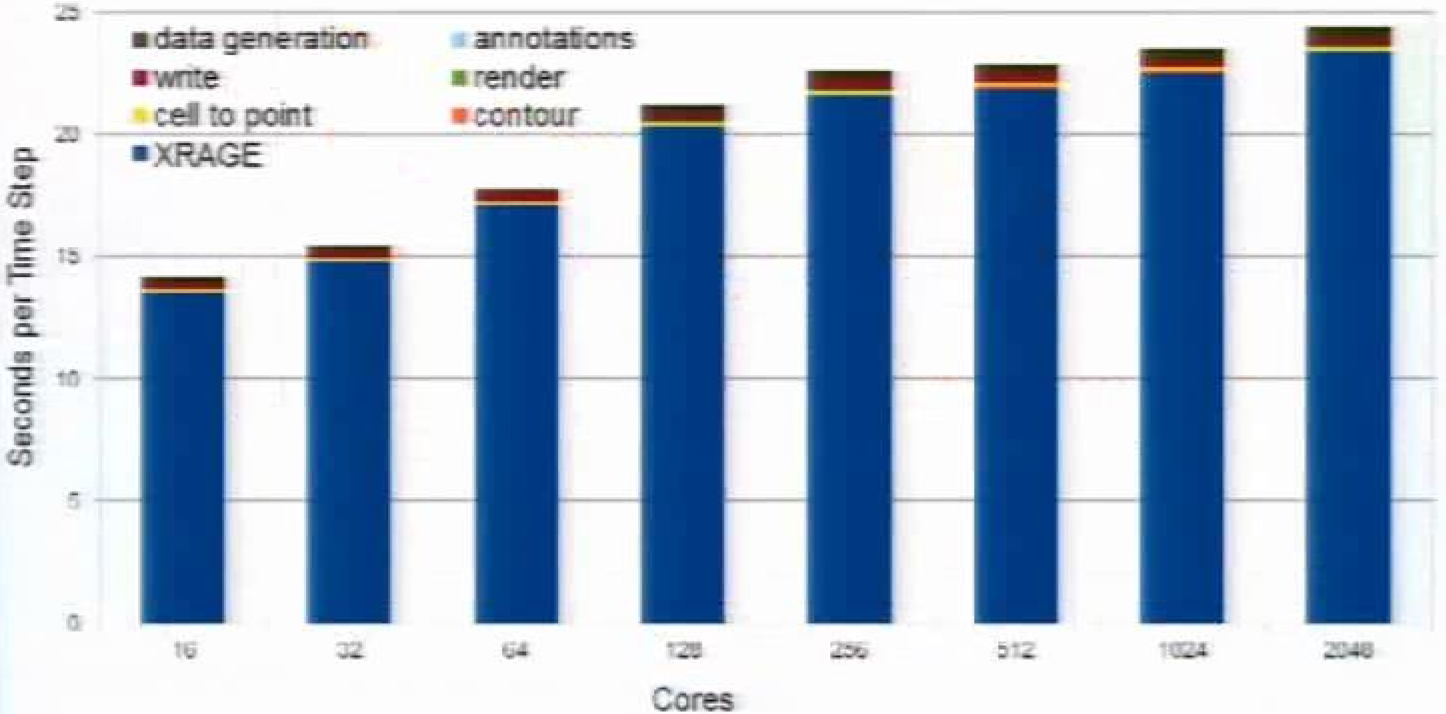
Faster Time to Solution



CTH (Sandia) simulations comparing different workflows

Small Run-Time Overhead



XRAGE (LANL) simulation

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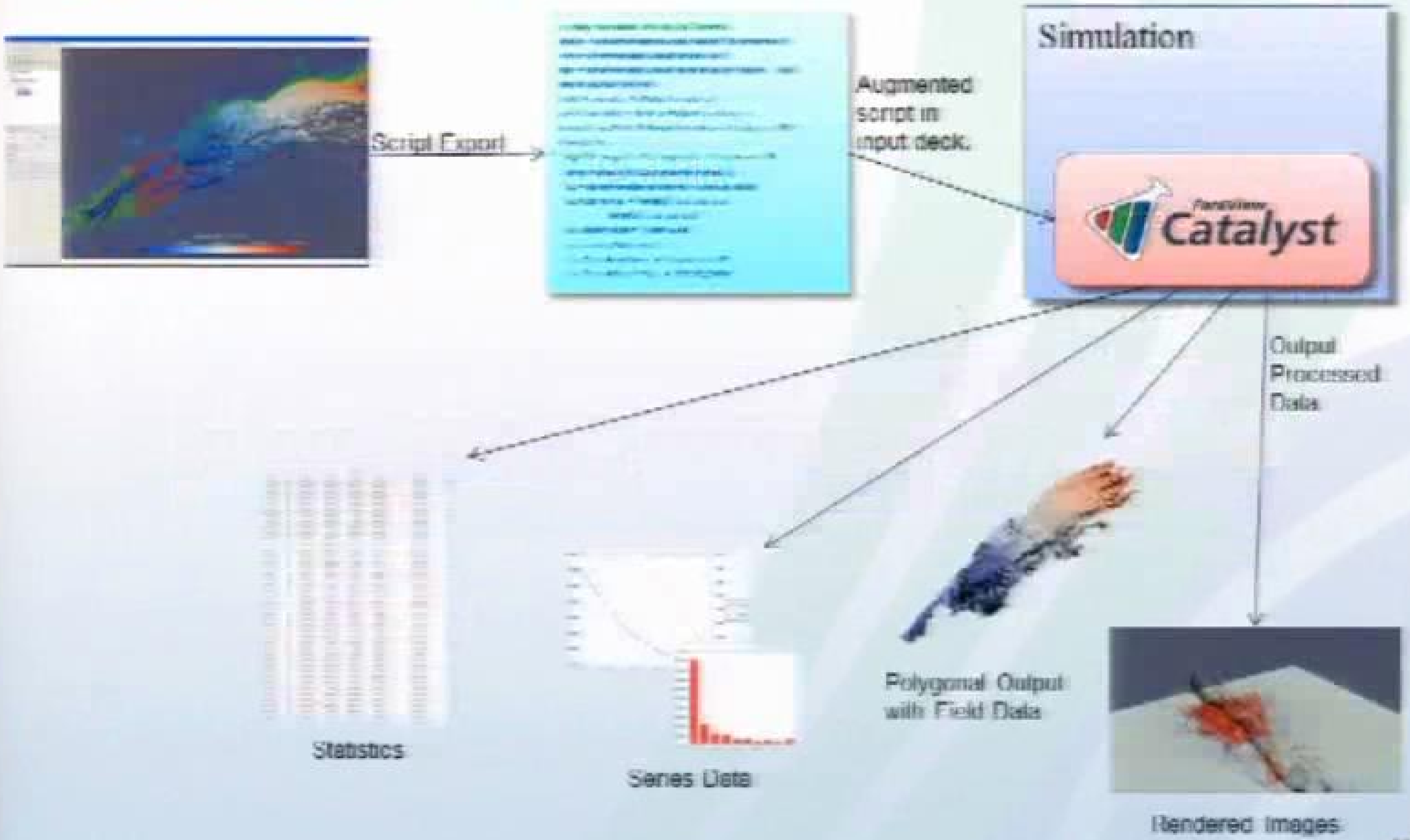
Reduced File IO Costs

Time of Processing	Type of File	Size per File	Size per 1000 time steps	Time per File to Write at Simulation
Post	Restart	1,300 MB	1,300,000 MB	1-20 seconds
Post	Ensight Dump	200 MB	200,000 MB	> 10 seconds
In Situ	PNG	.25 MB	250 MB	< 1 second

XRAGE (LANL) simulation

Workflow


Script Export
Augmented script in input deck.
Simulation
Catalyst
Output Processed Data
Statistics
Series Data
Polygonal Output with Field Data
Rendered Images

ParaView Catalyst with PHASTA

- Parallel Hierarchic Adaptive Stabilized Transient Analysis (PHASTA)
  - Joint development at UC Boulder, RPI, Argonne
  - Fully-implicit, stabilized, semi-discrete finite element method for the transient, incompressible Navier-Stokes partial differential equation (PDE)
- 1.3 billion element unstructured mesh
- 256K MPI processes run on 128K cores
  - Argonne BG/Q (Mira)
  - Using 2 of 4 hardware threads per core
- Python driven output from Catalyst

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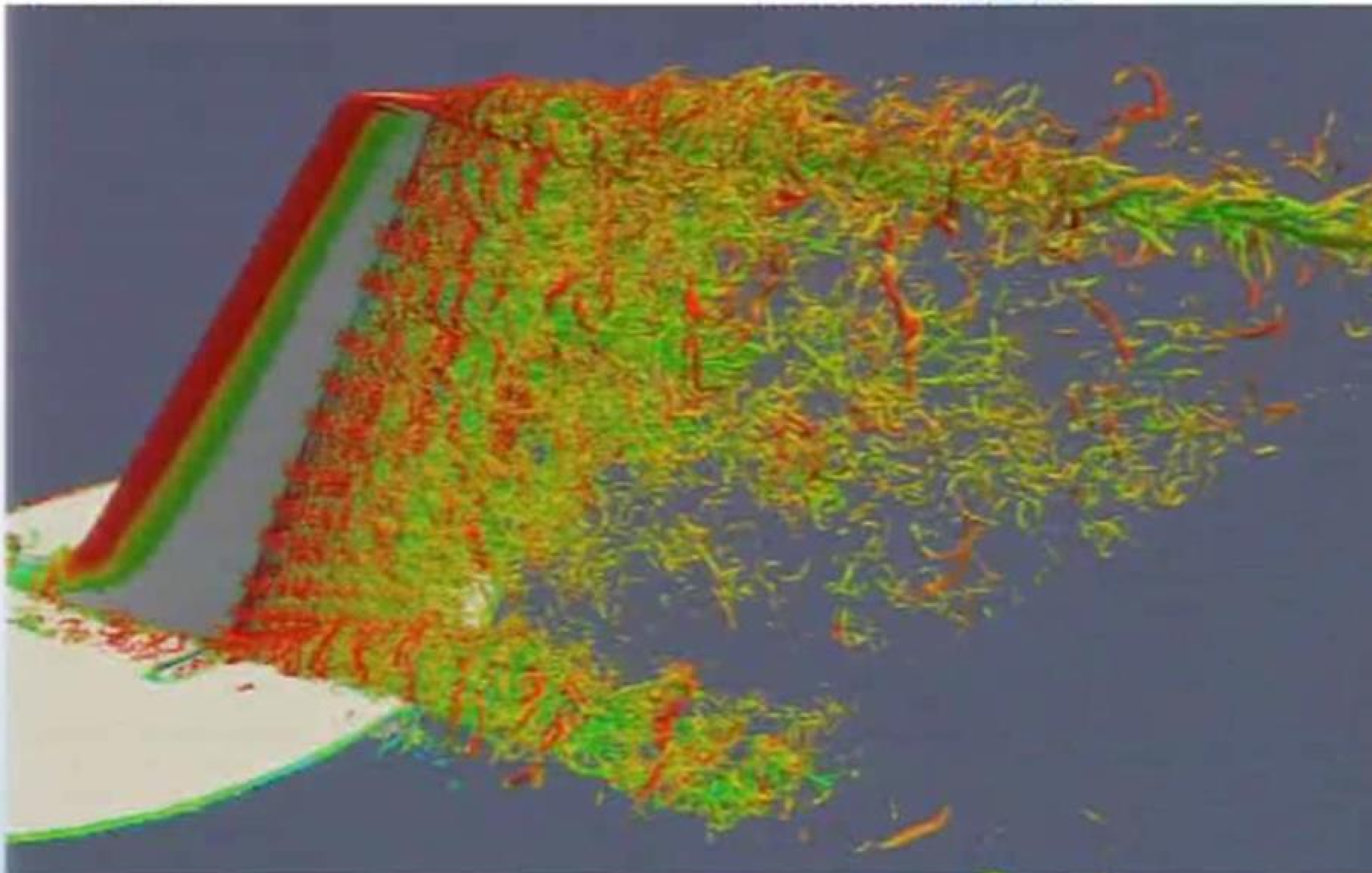
Flow Visualization: Full Span and Wake



Credit: Michel Rasquin (ANL) and Ken Jansen (UC Boulder)

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Thank You!

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