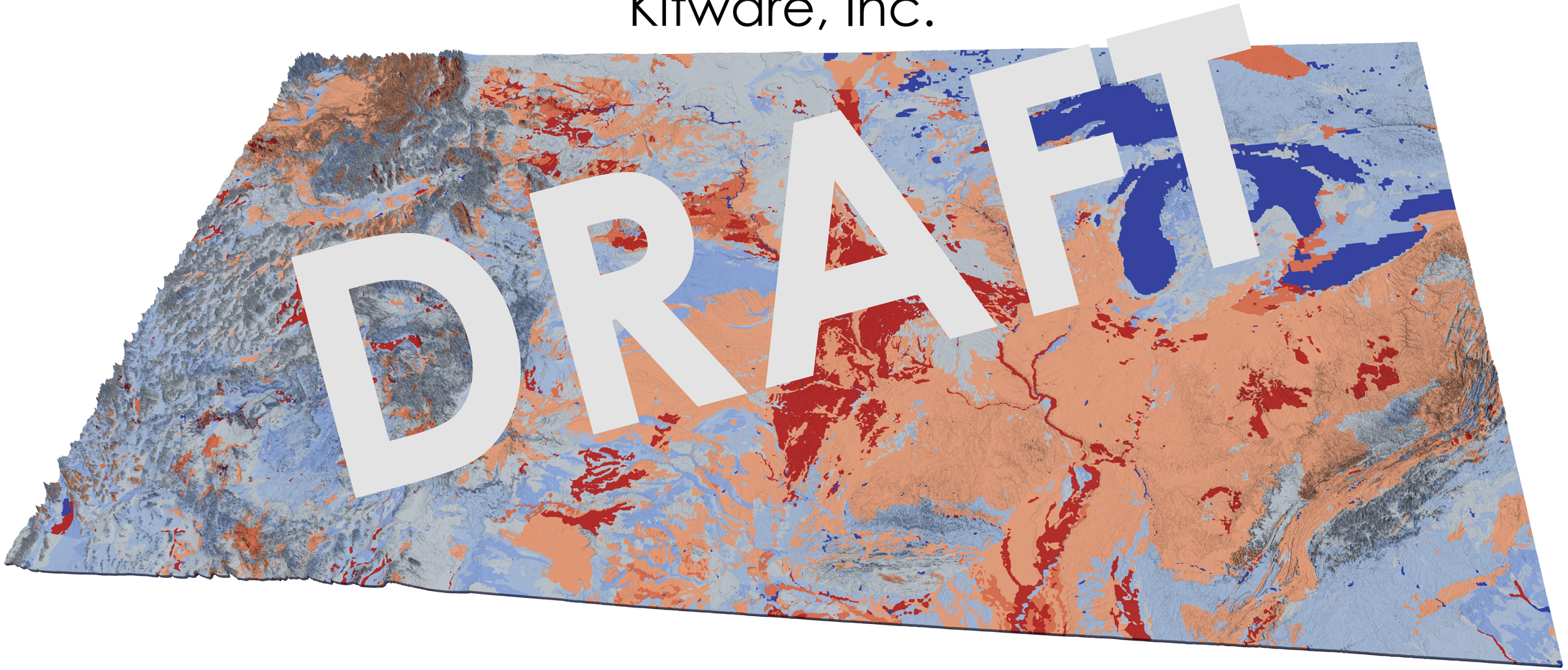
ParFlow Visualization with ParaView

Kitware, Inc.



Overview

- Data types & filter pipelines in VTK & ParaView **20 min**
- Visualization is composition **20 min**
- Tools for ParFlow **45 min**
- Going further with Python and NumPy **45 min**
- Catalyst and web demonstrations **20 min**

What are VTK & ParaView

- The Visualization Tool Kit (VTK)[1] is a set of libraries.
- ParaView[2] is an application built using VTK.
- Both are freely licensed (modified BSD) and maintained by Kitware via government grants and some of our commercial customers.
- C++, Python, and JavaScript.
- ParaView Guide: `https://paraview.org/paraview-guide/`

1. https://vtk.org/
2. https://paraview.org ⟵ If you are following along on your own computer, download ParaView from here now.

Data Types & Filter Pipelines

- Data type refers to how it is stored:
  - The underlying primitive types (string, int, float, ...)
  - The structure of the values and the corresponding geometric interpretation.
- The basic unit of data in VTK is an ***array***.
- The basic unit of structure in VTK is ***field data***.

Data Arrays

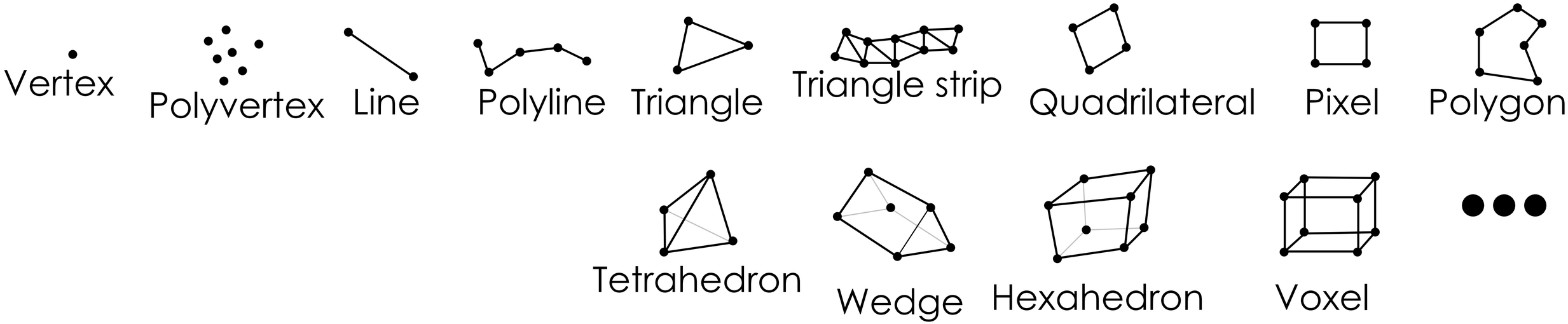
- An array in VTK is
  - an ordered collection of ***tuples***;
  - each *tuple* has the same number of ***components***;
  - each component is a number or string of the same primitive type.
- VTK arrays may also be interpreted as matrices.

Data Types & Filter Pipelines

- Field data holds any number of arrays.
- A ***data object*** holds a single field data. It has no geometric interpretation; it is up to the application or user to add meaning.
- A ***data set*** has a concept of *points* and *cells* defined by those points. Each concept has associated field data (arrays corresponding to points and cells), plus the unassociated field data inherited from data object above.

Points & Cells

- Cells are defined by points that serve as corners or shape controls.
- Multiple cells can reference the same point along shared boundaries.

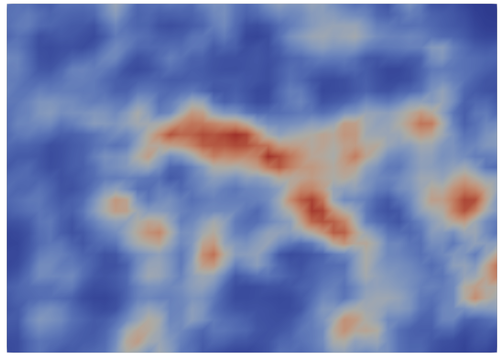


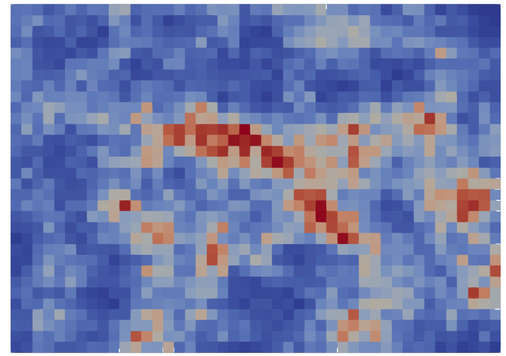
Data Types & Filter Pipelines

- Points and cells may be implicitly or explicitly represented.
  - Implicit points & cells: ***image data***.
  - Explicit points, implicit cells: ***rectilinear data*** and ***structured (curvilinear) data***.
  - Explicit points & cells: ***polydata*** and ***unstructured grids***.

Data Types & Pipelines

- Field data defined on points and cells is treated differently:
  - point data is interpolated,
  - cell data is constant.
- Nearly all ParFlow data is cell-centered.





Data Types & Filter Pipelines

- A ***filter*** constructs, transforms, or consumes data.
- Filters may be *chained* together: one filter's output can serve as another filter's input.
- Asking a filter for its output may cause the filter's upstream source filters to run, followed by the filter itself running.
- This lazy execution avoids unnecessary work.

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source **filter** **sink**

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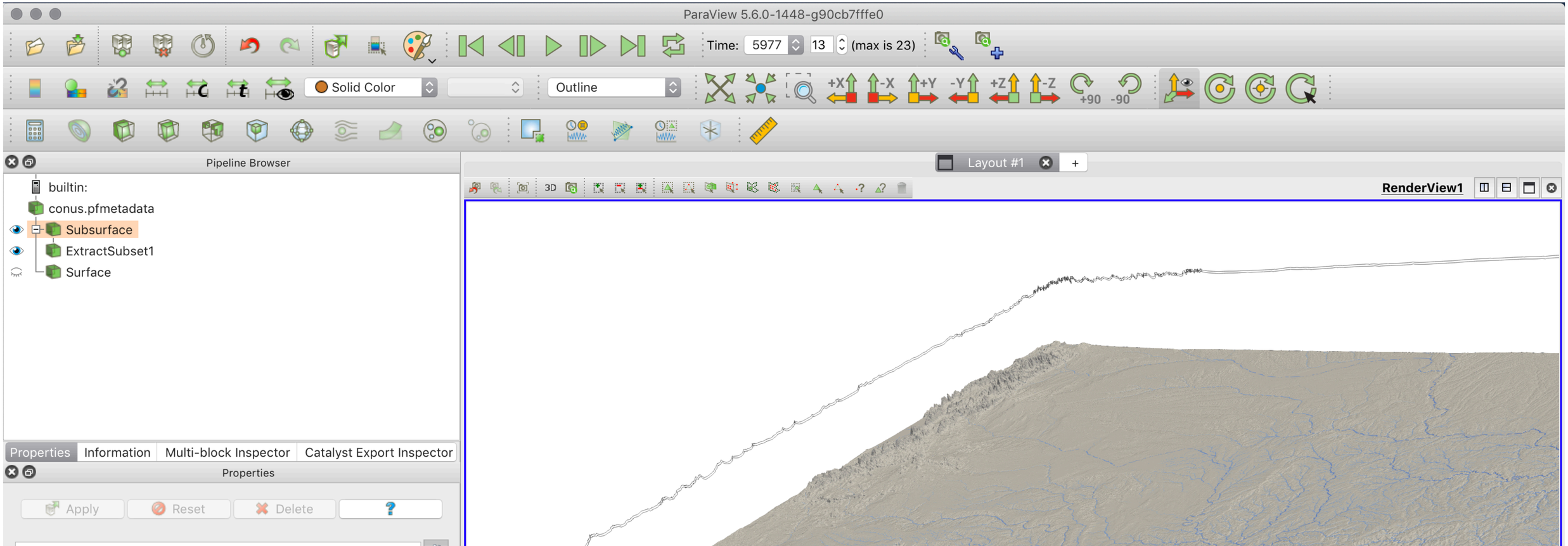
ParaView

- ParaView shows you sources, filters, sinks, and their connections in the Pipeline Browser.



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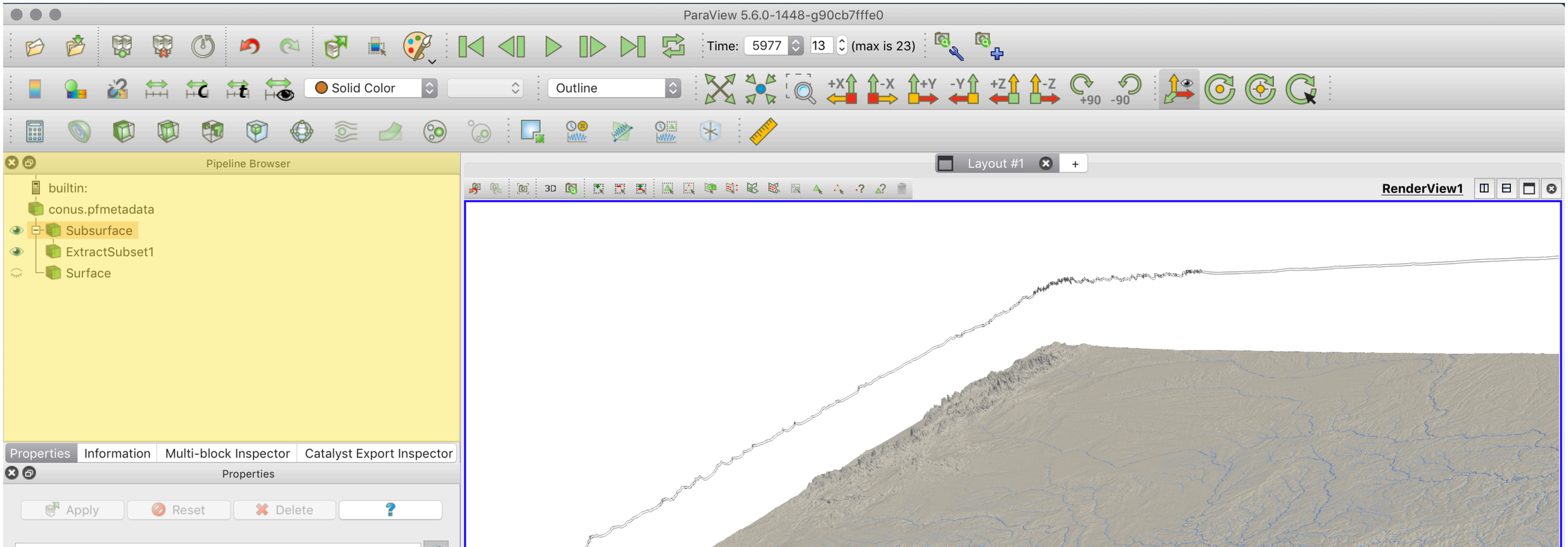
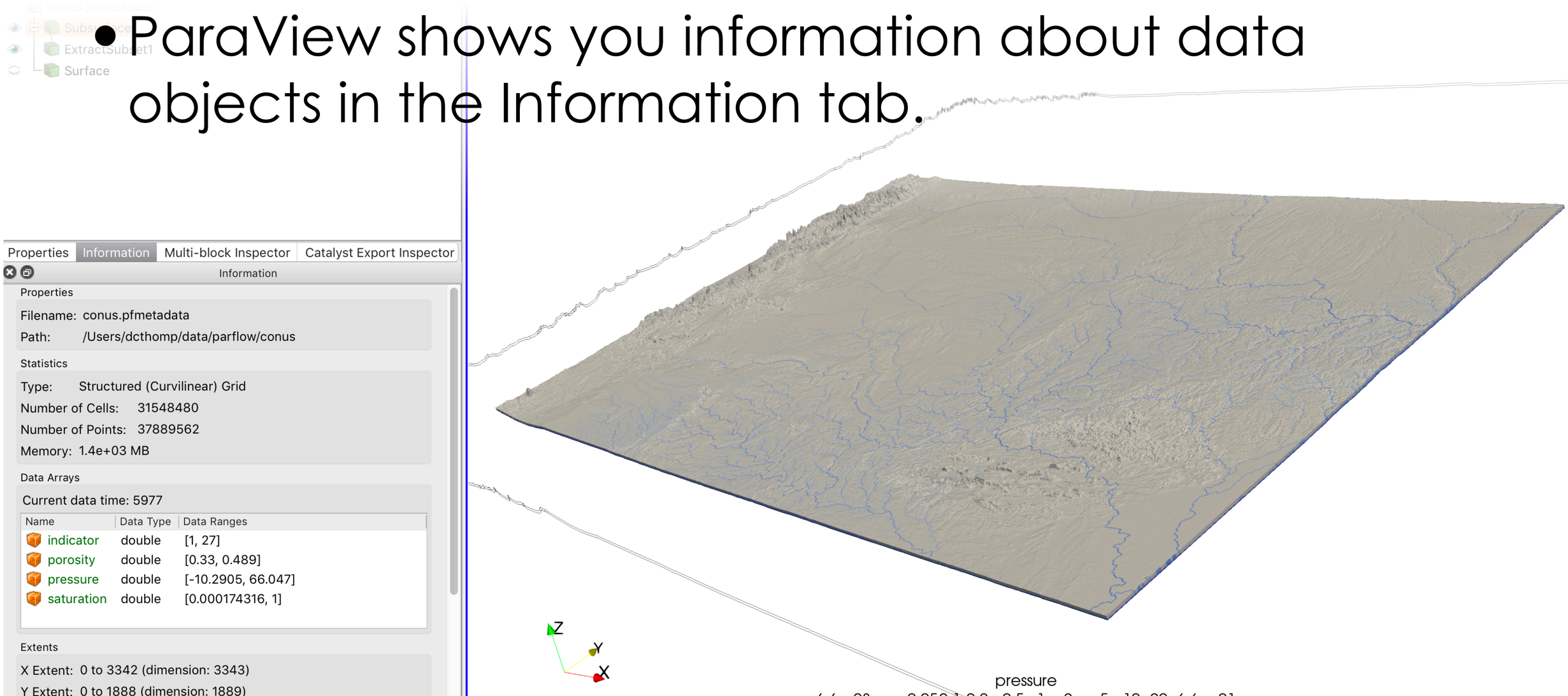


ParaView

- ParaView shows you information about data objects in the Information tab.



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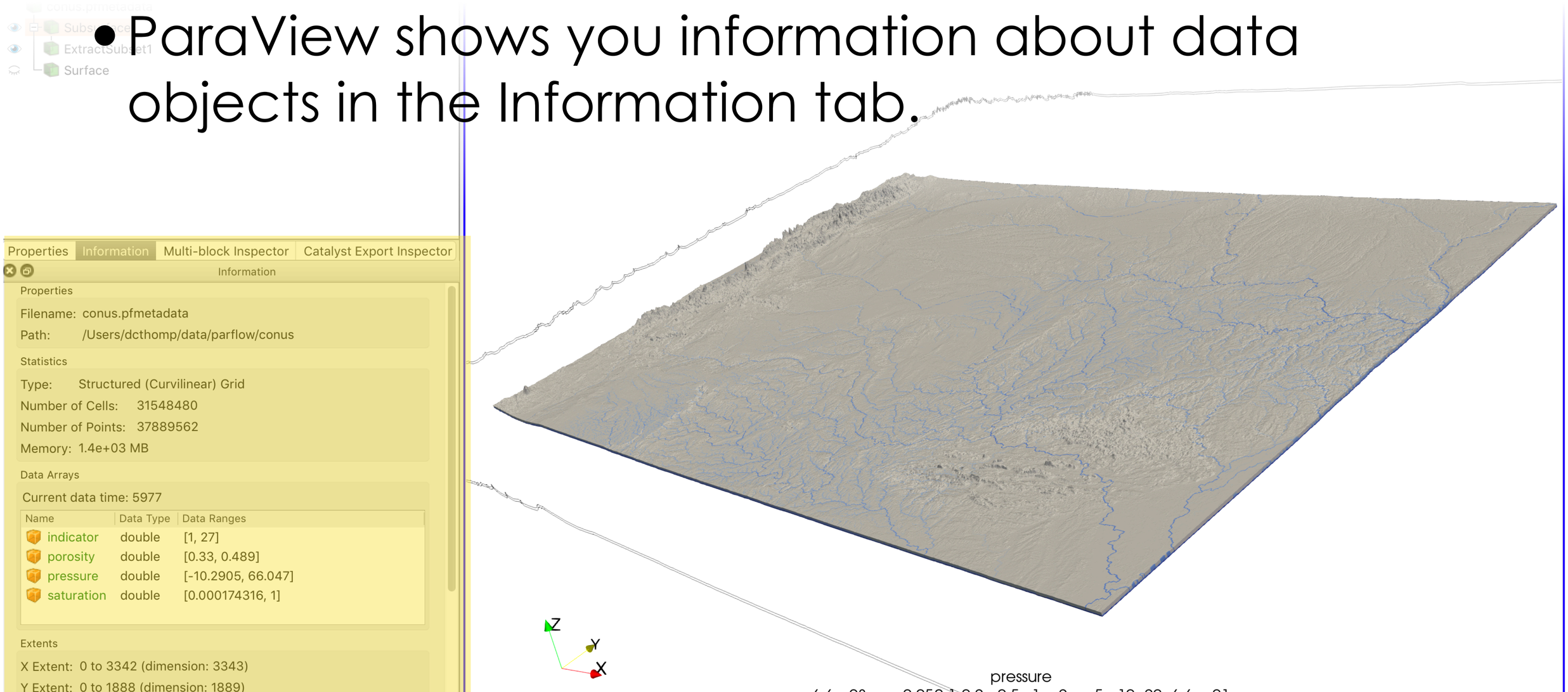
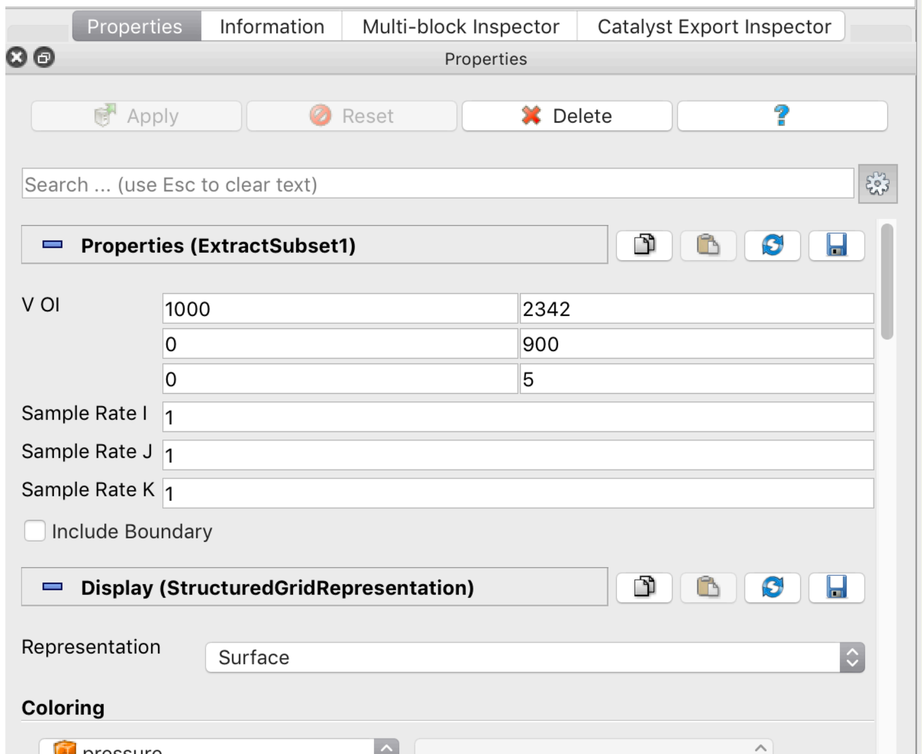
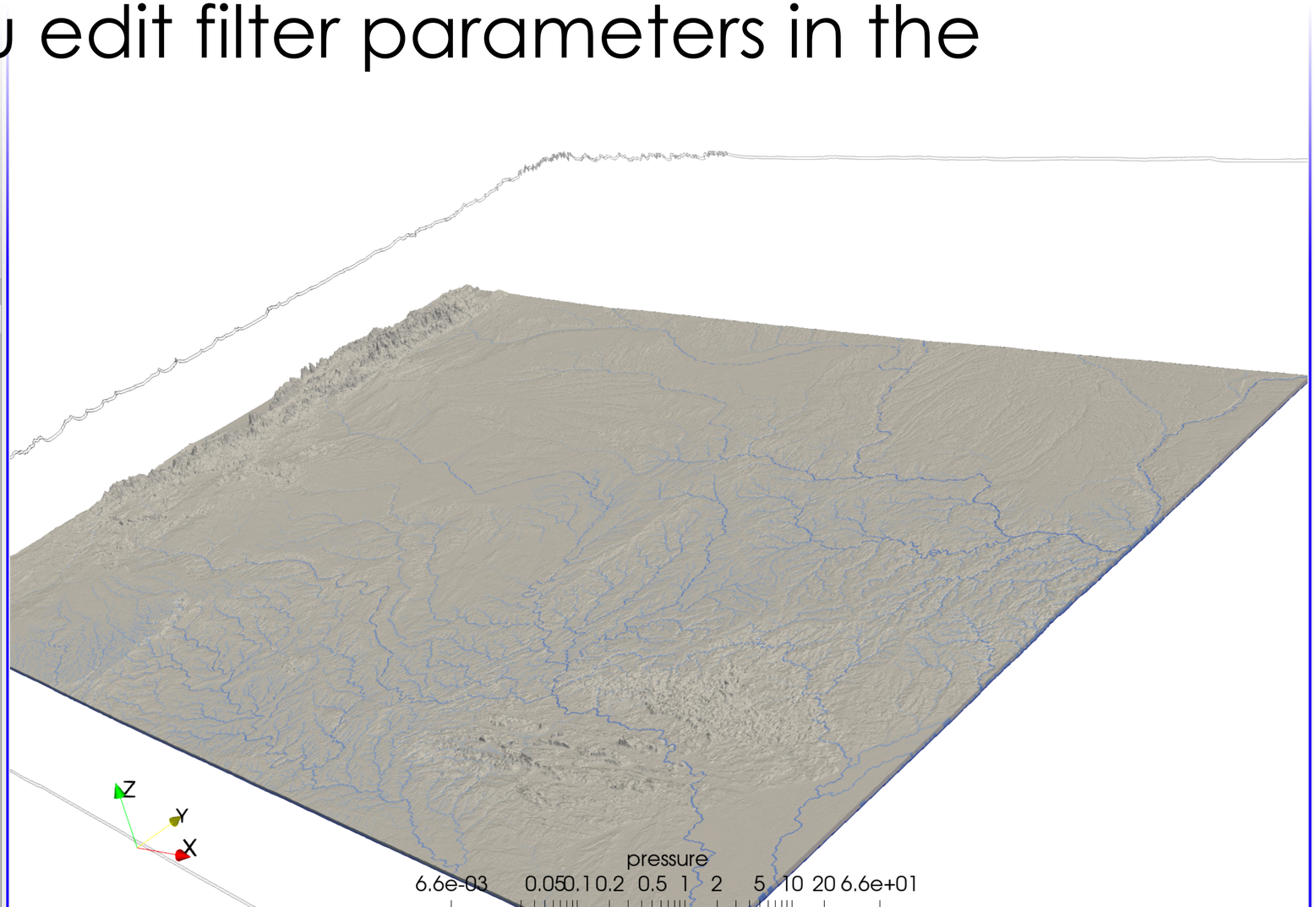


ParaView

- ParaView lets you edit filter parameters in the Properties tab.





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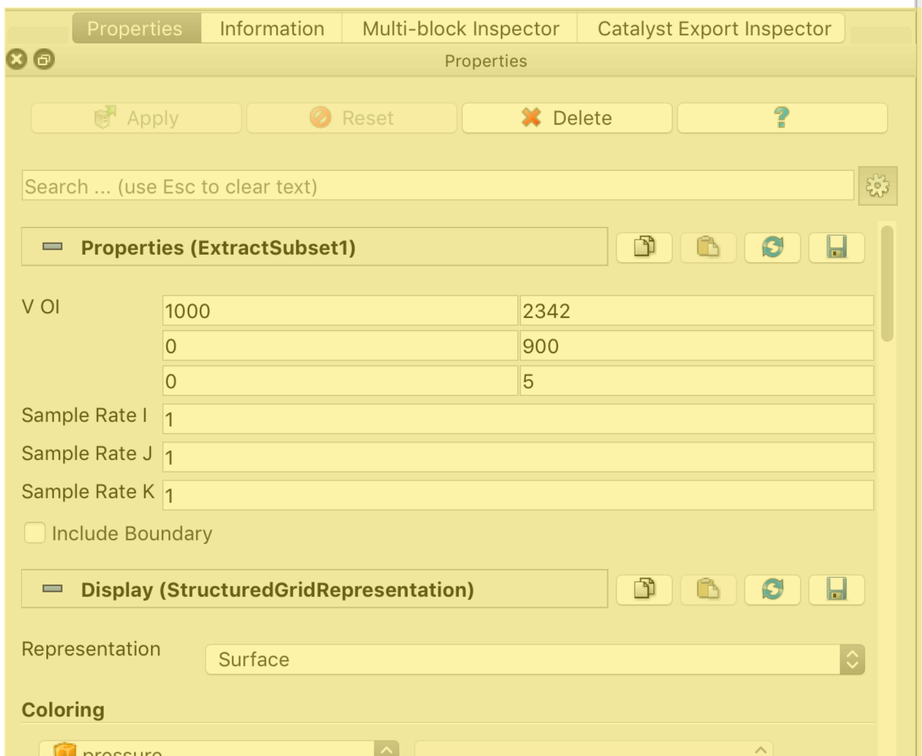

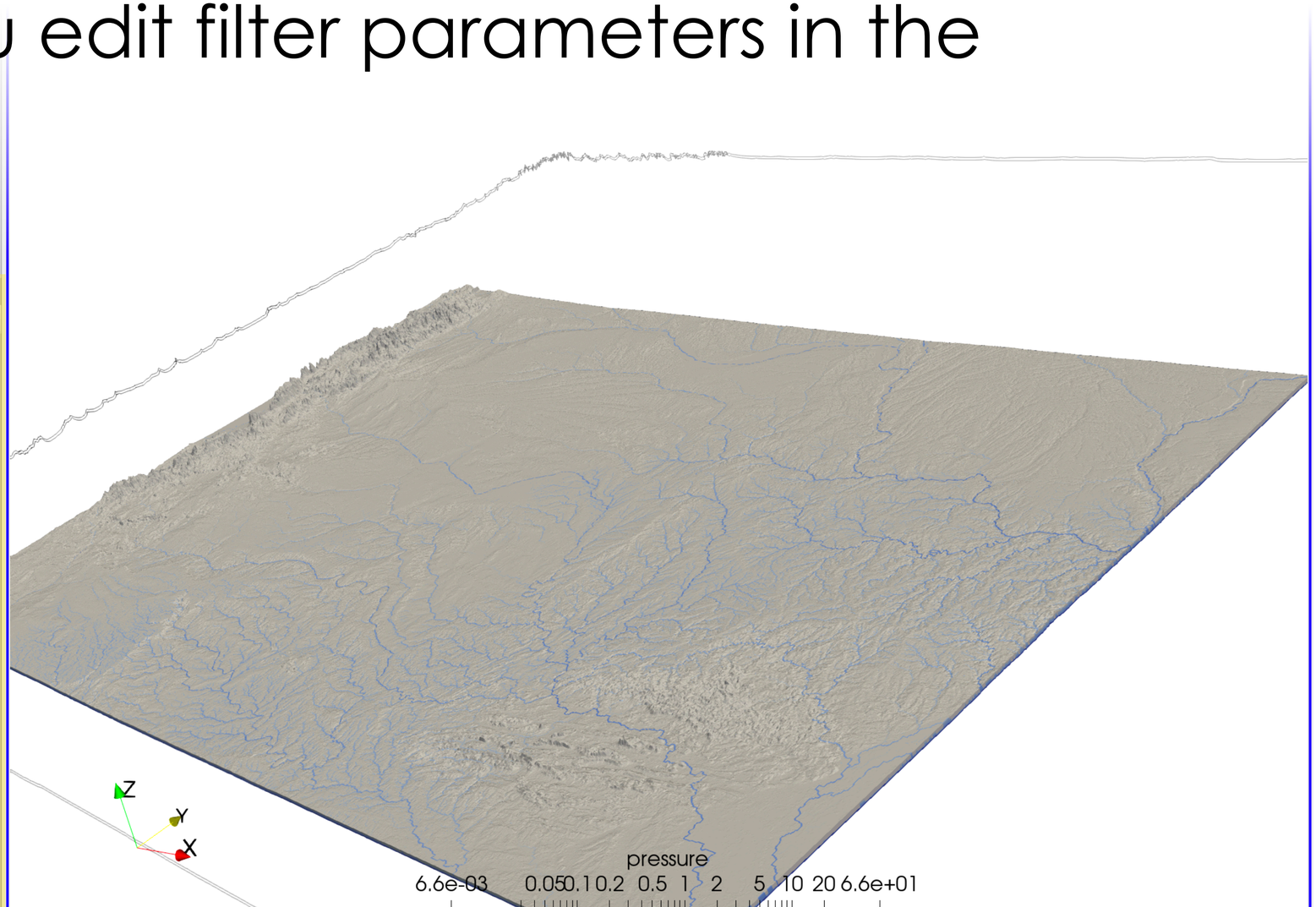

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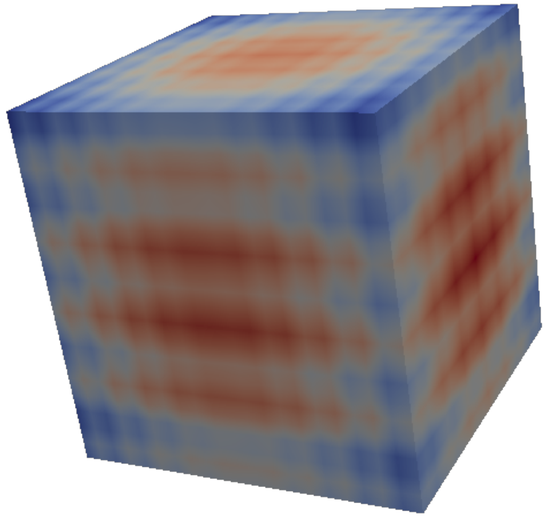
Visualization is Composition

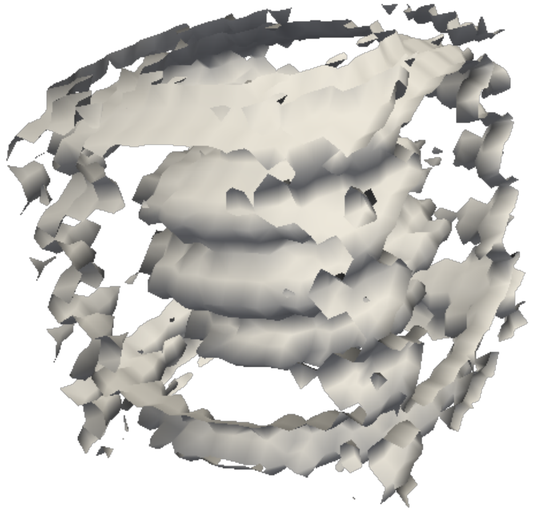
- There are relatively few fundamental visualization operations: color-by-value, cut, clip, threshold, isocontour, streamline/streakline, glyphs, volume rendering, deformation, legends/keys, parallel coordinates, focus+context, small multiples, ...
- Most compelling visualizations are compositions of these that convey information by using human perception while avoiding clutter.

Color by value



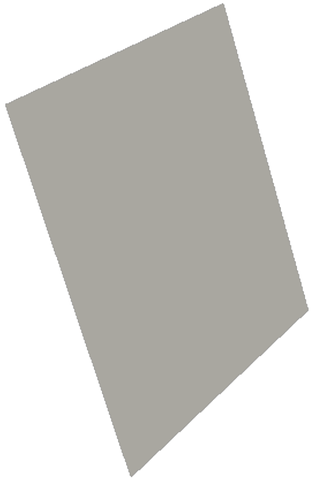
- Color each point by simulated value.
- Interpolate between points (or not, depending on simulation).
- Only shows surface values.
- Color scale and palette induce psychological bias.

Isocontour



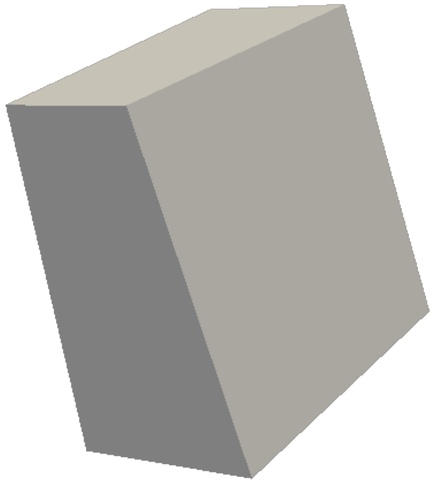
- Find locus of points with a given value at time t.
- Shows interesting shapes, but ...
- ... shapes may not be stable and may miss features.
- Multiple isocontours behave like onion layers.

Cutting Surfaces



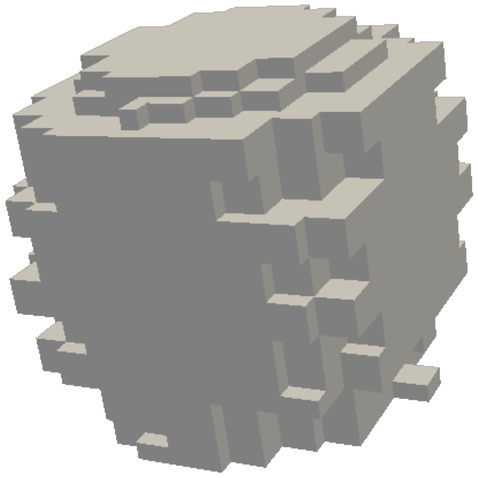
- Slice domain of simulation with a plane or other surface.
- Useful when domain changes shape over time.
- Only shows a small region of domain; features may be missed.

Clipping



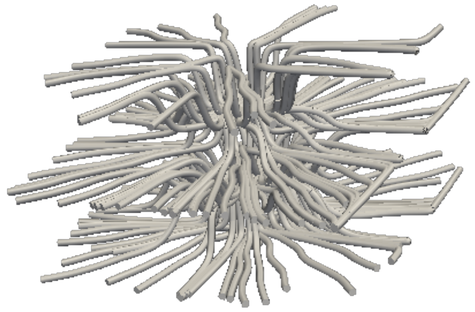
- Slice domain of simulation with a halfspace.
- Like a cutting plane, but provides more context.
- Clipped dataset often used as input for other visualizations.

Threshold



- Subset of grid cells whose values are in a given range.
- Like clipping plane, but preserves shape of grid cells.
- Good for showing effect of discretization of domain.

Streamlines/Streaklines



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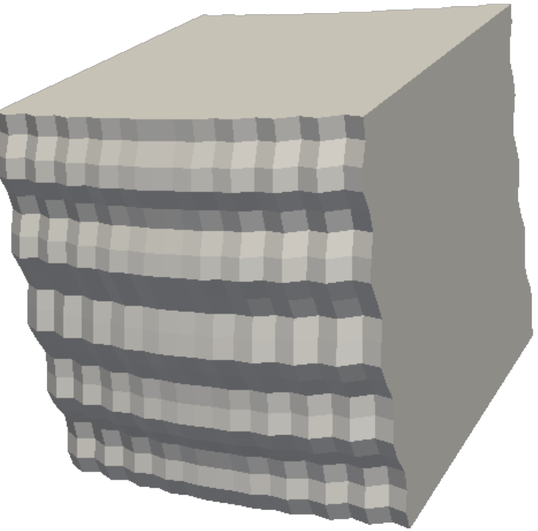
- Like a clipping plane, but provides more context.
- Clipped dataset often used as input for other visualizations.

Volume Rendering

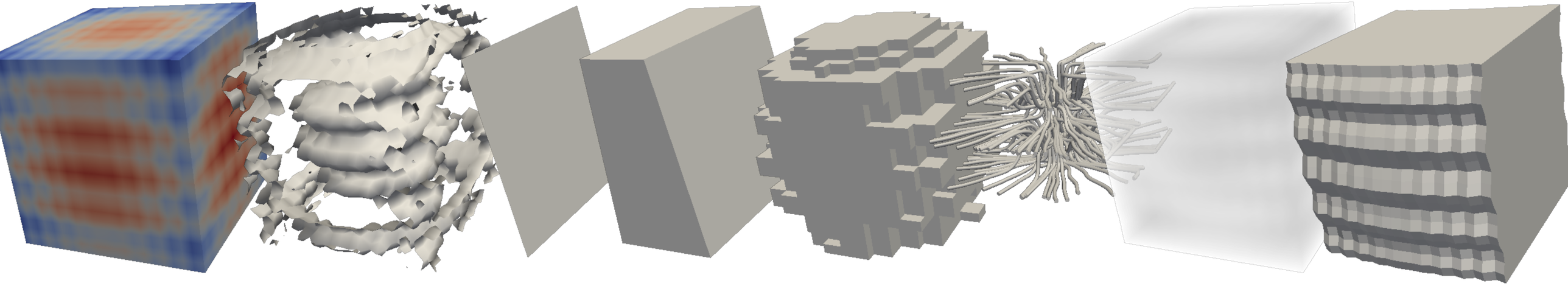
- Values are semitransparent according to a transfer function.
- See features inside volume.
- Often fuzzy, so it can be hard to discern feature shape.
- Occlusion can still be a problem.

Deformation



- Displace each point by a vector to change shape of grid.
- Often used in solid mechanics.
- Displacement can be exaggerated to make features clear.
- Occlusion can be a problem.

Visualizations Are Compositions!



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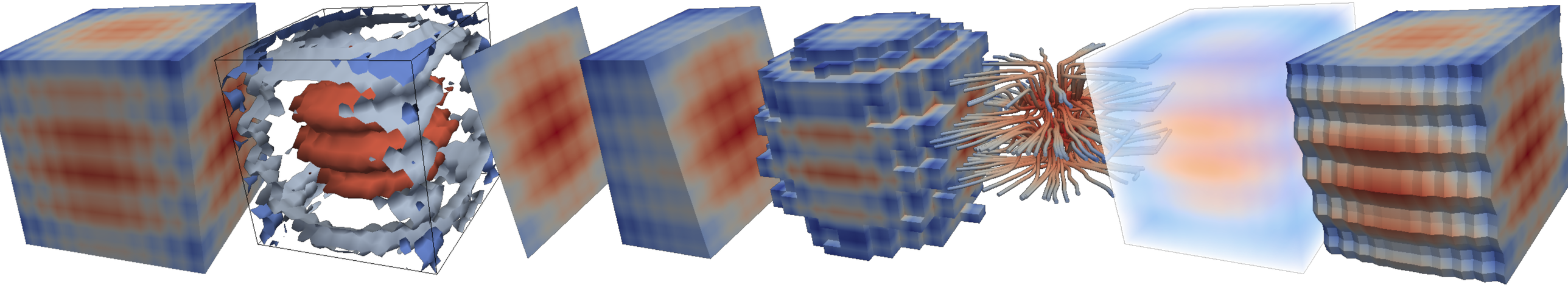


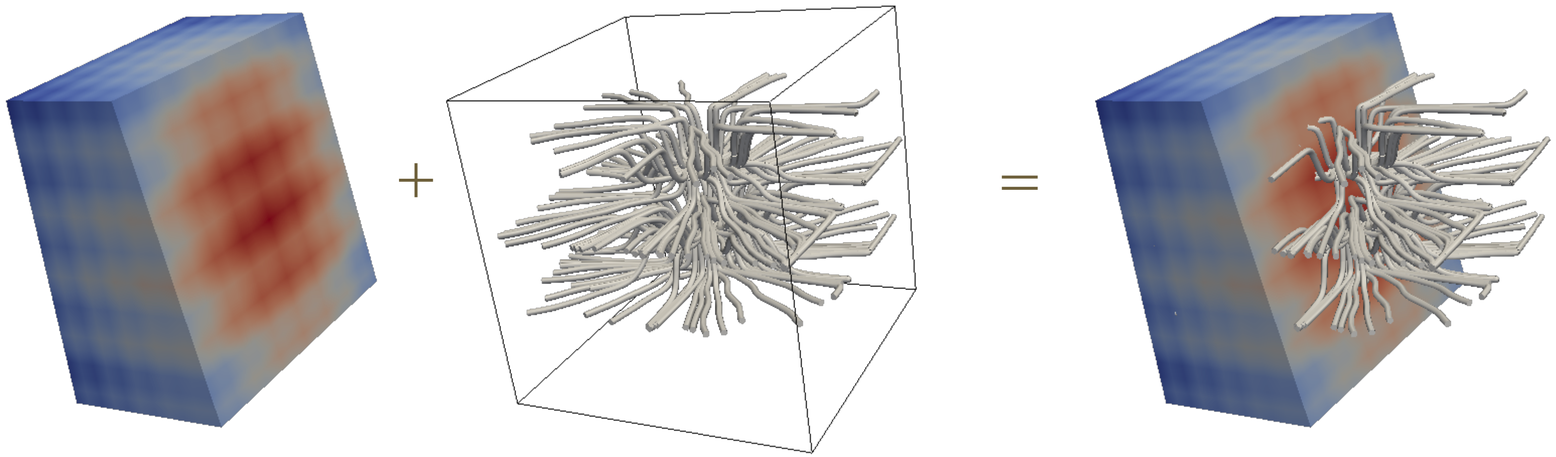
Visualization

- Traditionally, visualization performed after a simulation (hence *post*-processing); until recently, adjusting the composition has been simple.
- Heterogenous nature of computers and communication provides an opportunity for visualization/analysis with higher fidelity, but at the expense of some flexibility in composition.

Visualization Strategies

- Perform analysis during simulation to determine when to save results and which results to save.
- Generate visualizations using a script prepared with results of smaller runs where traditional post-processing tools can be used.
- Generate visualization artifacts which allow post-simulation composition.

Visualization Strategies



Visualization is Composition

- For further study:
  - Edward Tufte, *The Visual Display of Quantitative Information*. Graphics Press, 2001.
  - Colin Ware, *Information Visualization*. Morgan Kaufmann, 2012.

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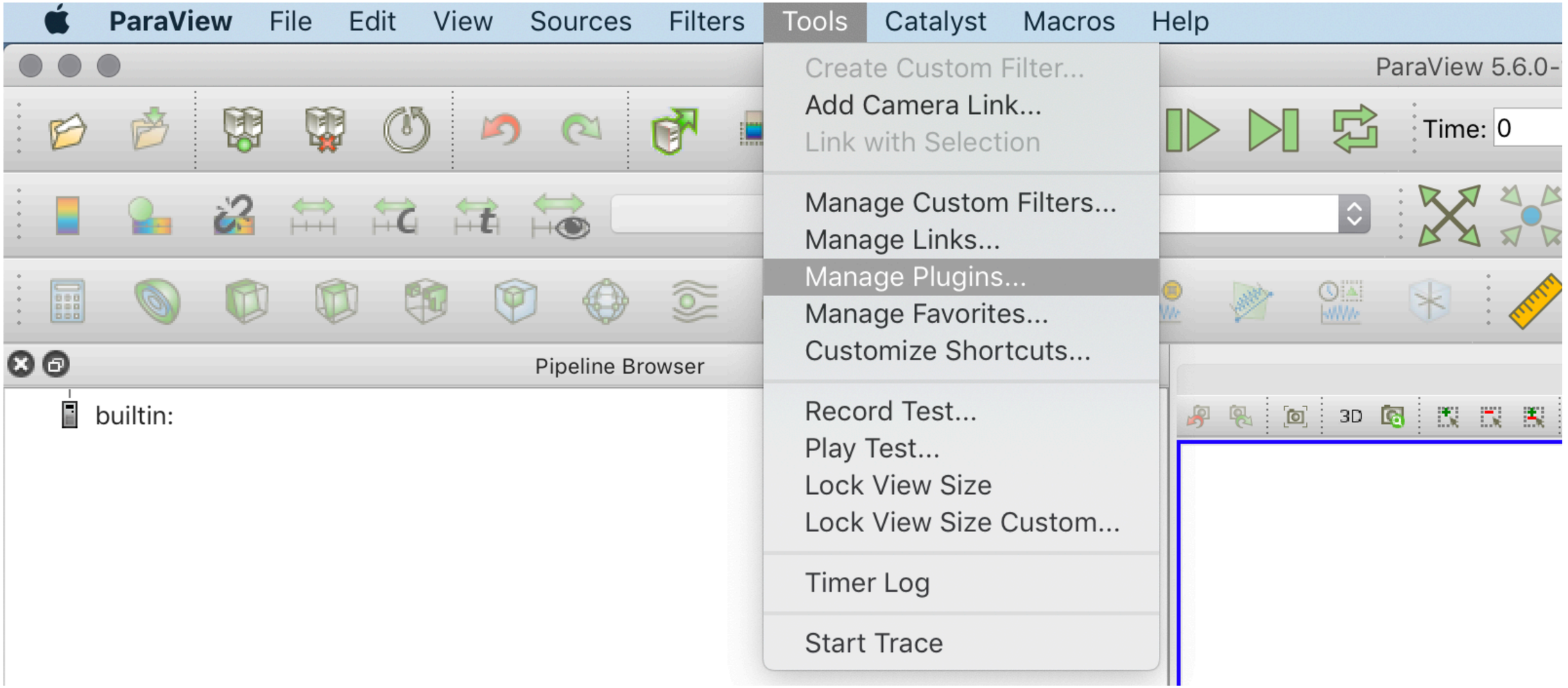
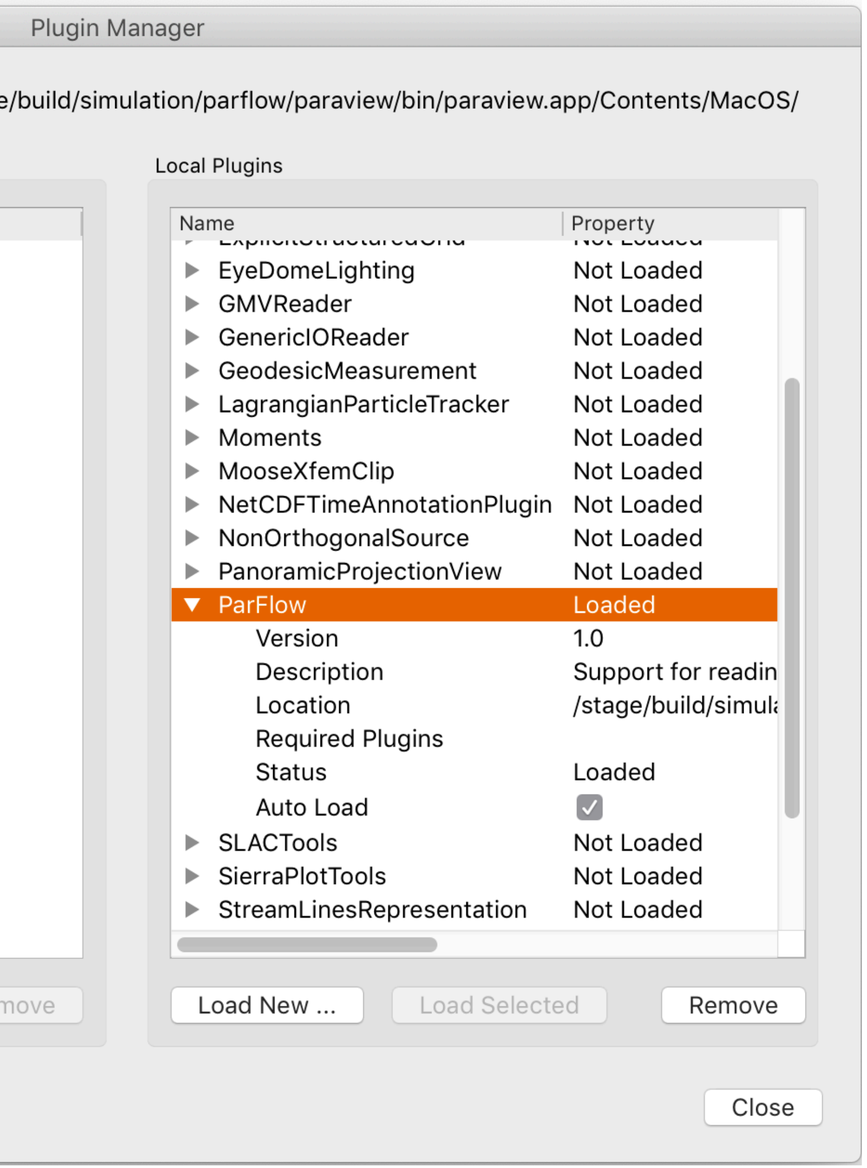
Tools for ParFlow

- Loading plugins
- Reading and animating data
- Plotting selections over time
- Colormaps for stream flow
- Simple calculations

Tools for ParFlow



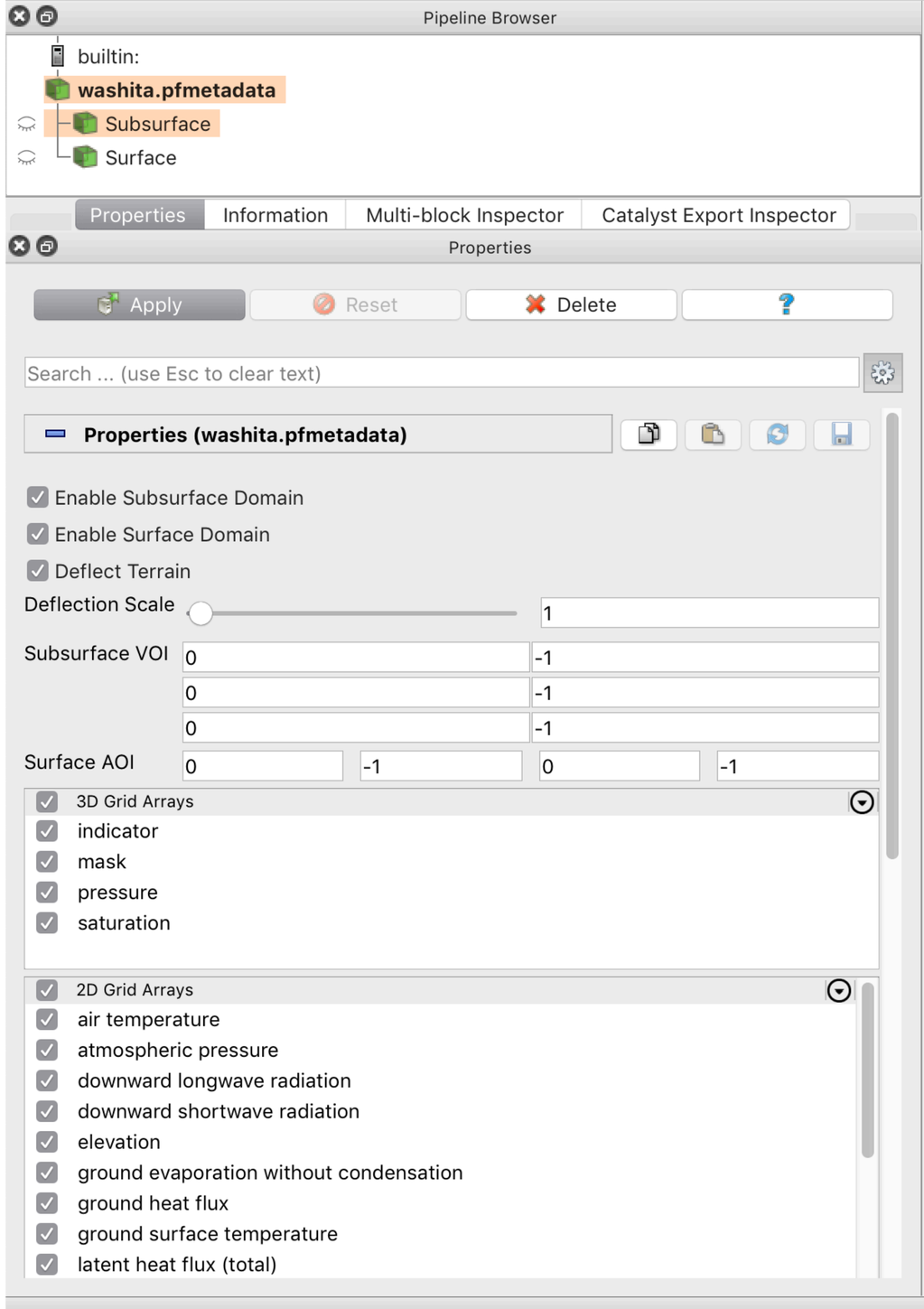
Tools for ParFlow



- Expand "ParFlow" plugin
- Click "Auto Load"
- Quit ParaView and restart (this saves the autoload preference)
- Now `.pfb`, `.C.pfb`, `.pfmetadata` are recognized file formats.

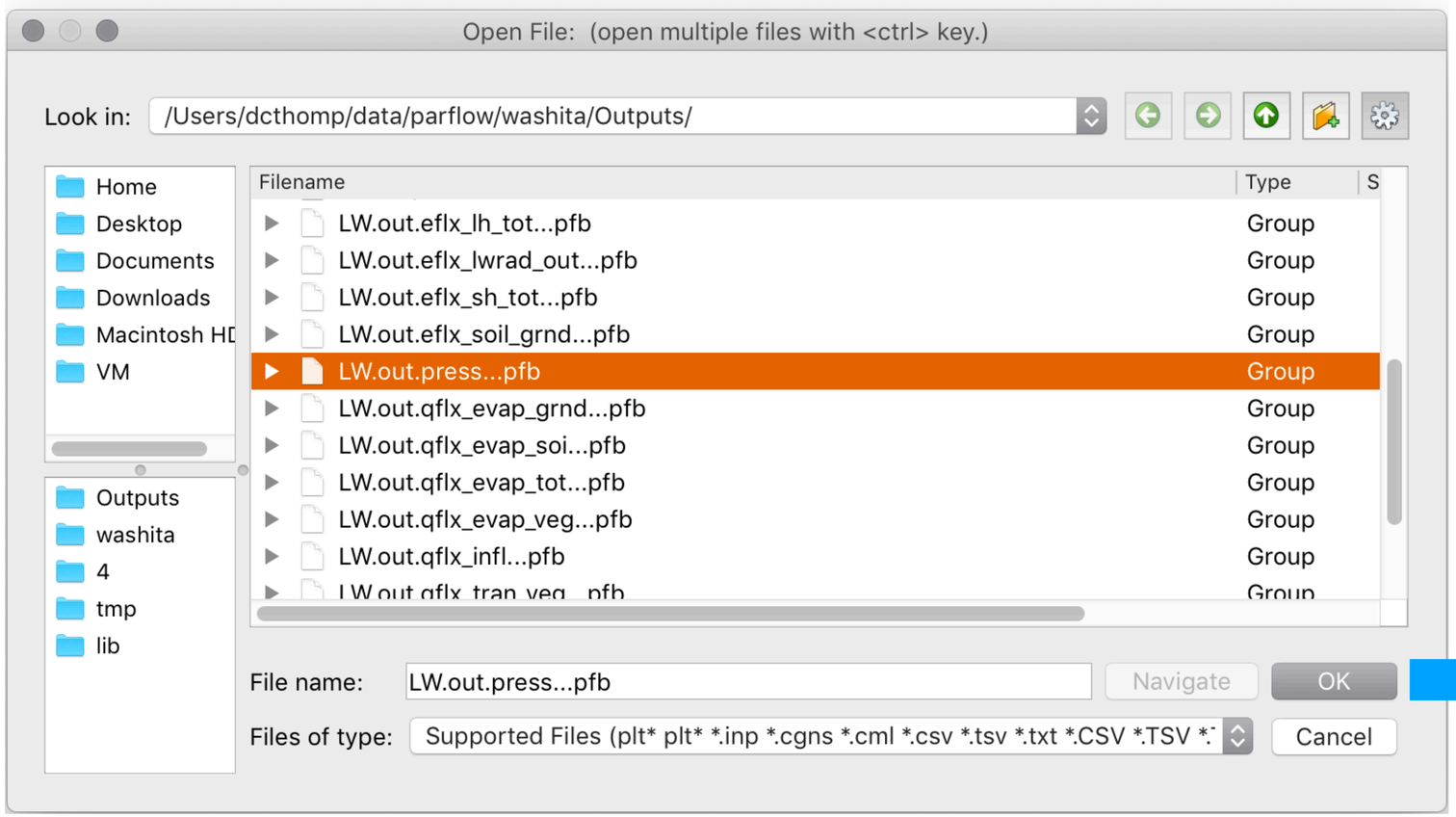
Tools for ParFlow

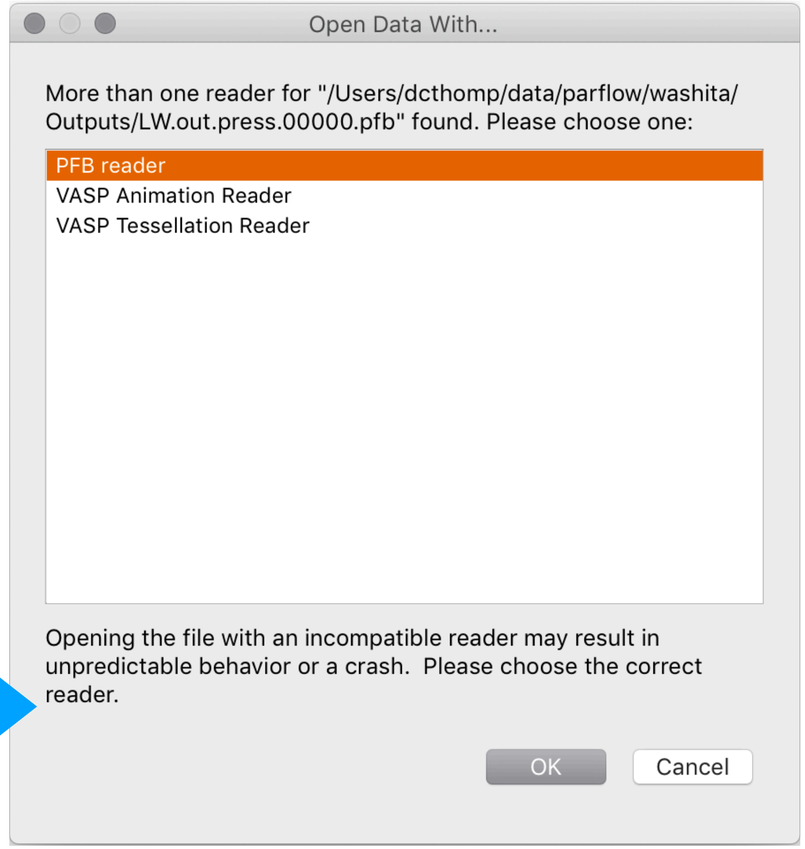
- Open a `.pfmetadata` file.
- Nothing is actually loaded until you click *Apply* since the data may be large; this can load many PFB files at once.
- VOI/AOI use "-1" to indicate the full extent should be used.



Tools for ParFlow

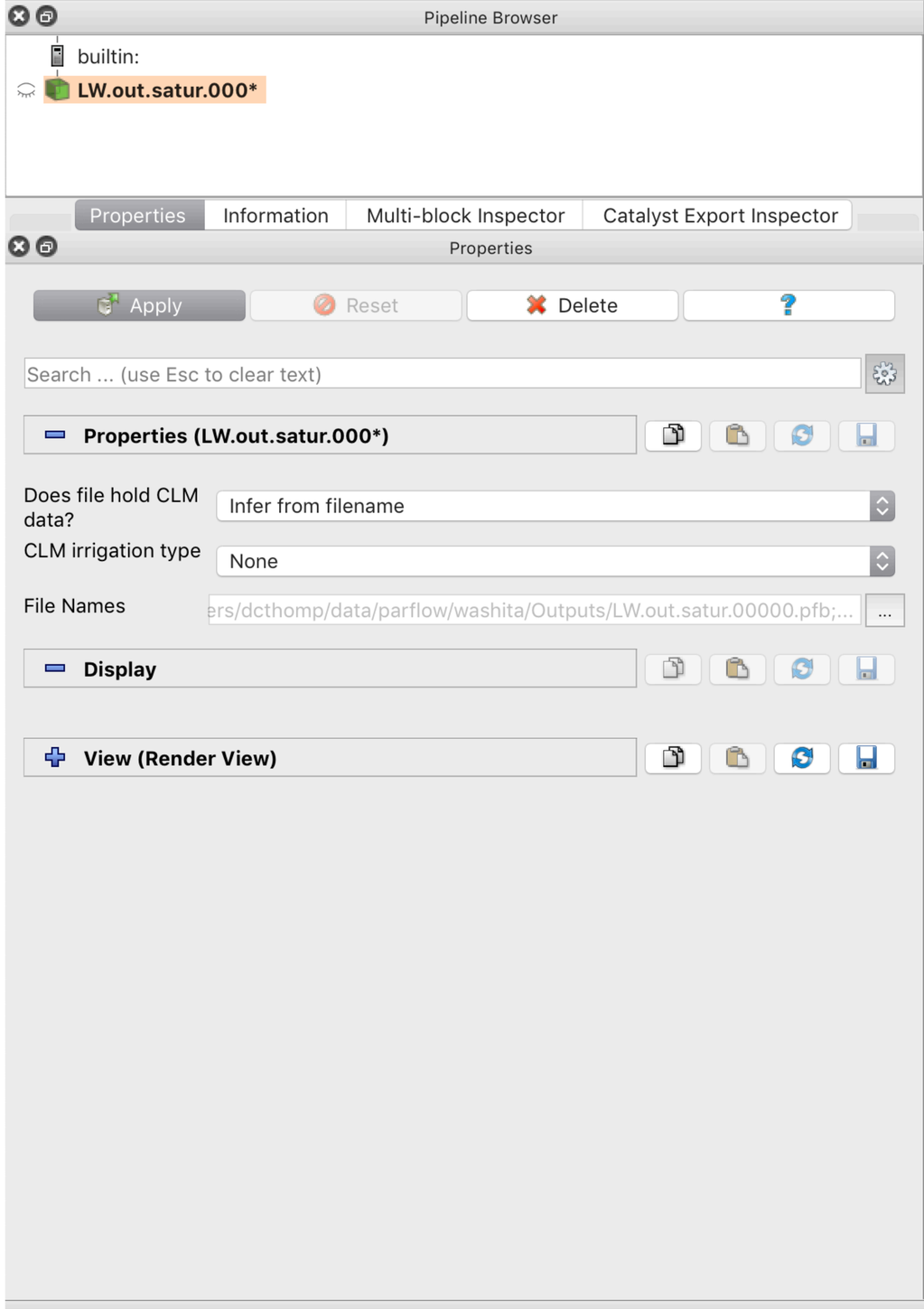
When opening `.pfb`, `.C.pfb` files, you need to tell ParaView the files are ParFlow data, not VASP data.





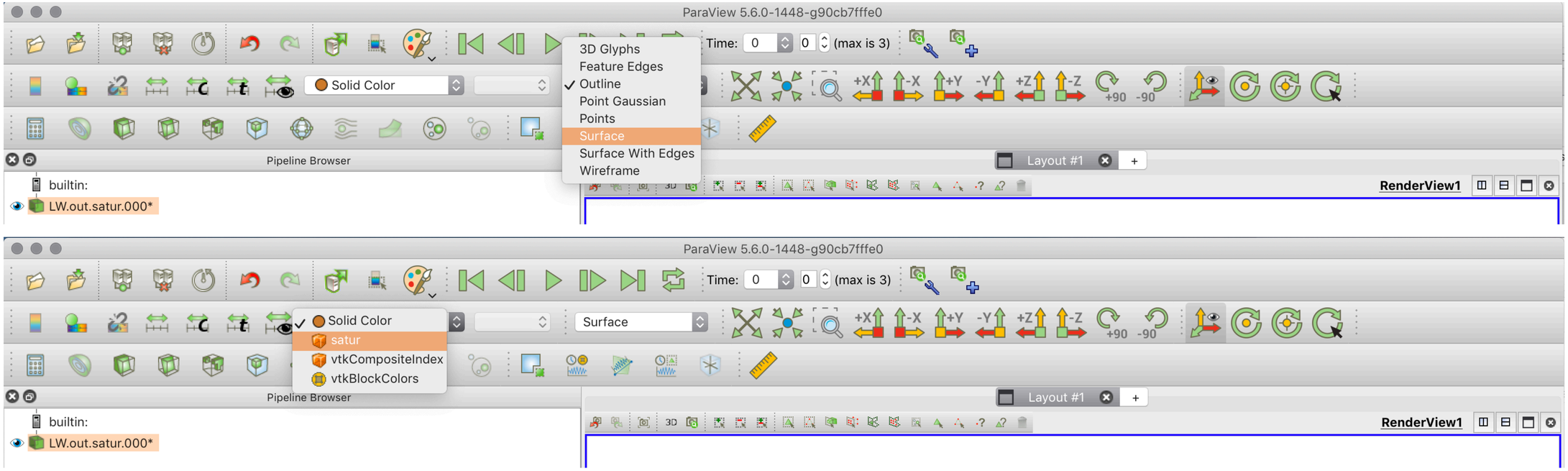
Tools for ParFlow

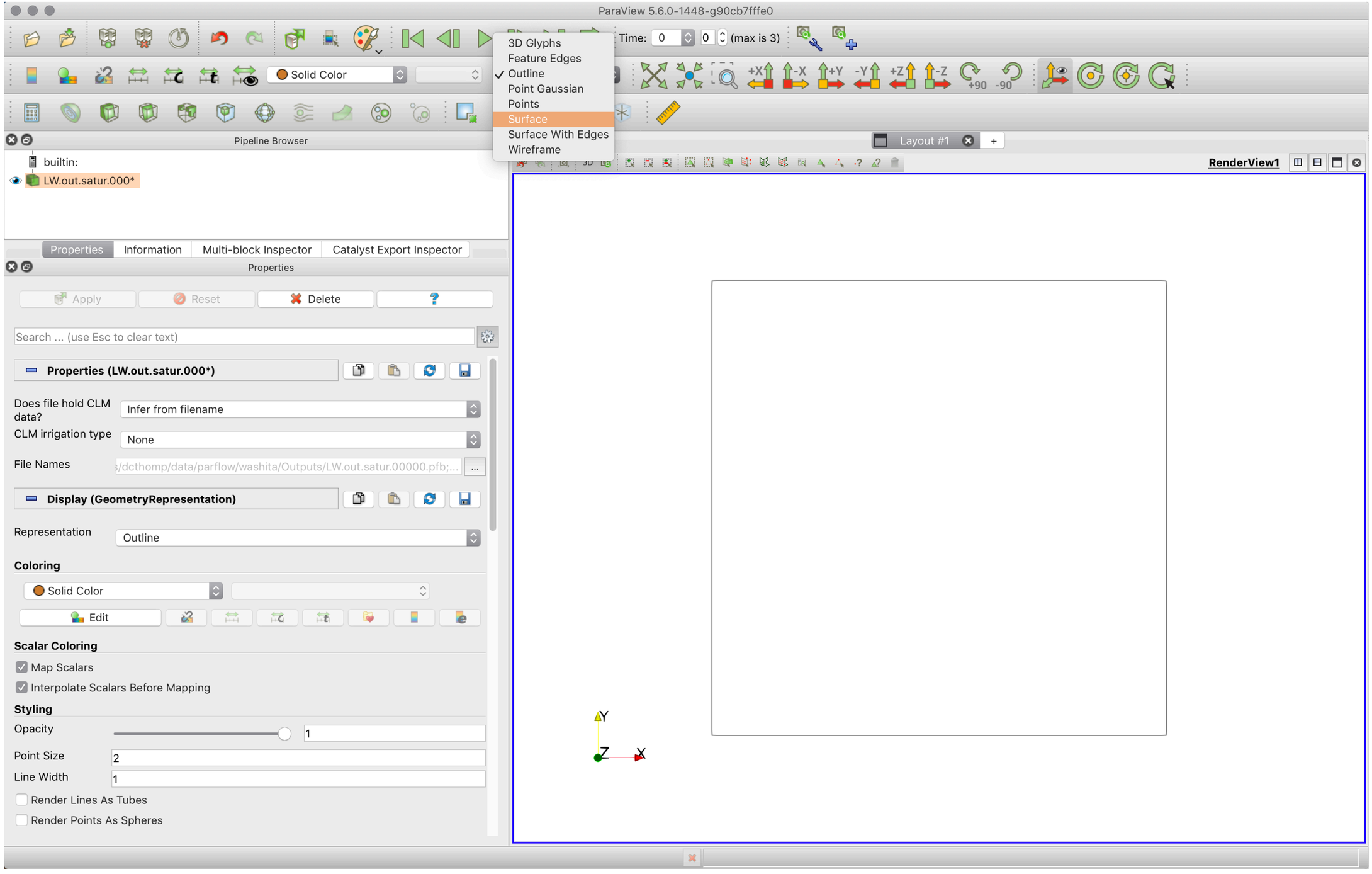
- Open a `.pfb` file.
- Nothing is actually loaded until you click *Apply*.
- If loading CLM PFB files (`.C.pfb`), you need to specify the irrigate type since the file does not indicate it.



ParaView Tip: Representations

- The toolbar controls the active filter's visual properties (how it is drawn and colored).




ParaView 5.6.0-1448-g90cb7fffe0
Time: 0 0 (max is 3)
3D Glyphs
Feature Edges
Outline
Point Gaussian
Points
Surface
Surface With Edges
Wireframe
Solid Color
Pipeline Browser
builtin:
LW.out.satur.000*
Layout #1
RenderView1
Properties
Information
Multi-block Inspector
Catalyst Export Inspector
Properties
Apply
Reset
Delete
Search ... (use Esc to clear text)
Properties (LW.out.satur.000*)
Does file hold CLM data?
Infer from filename
CLM irrigation type
None
File Names
/dcthomp/data/parflow/washita/Outputs/LW.out.satur.00000.pfb;...
Display (GeometryRepresentation)
Representation
Outline
Coloring
Solid Color
Edit
Scalar Coloring
Map Scalars
Interpolate Scalars Before Mapping
Styling
Opacity
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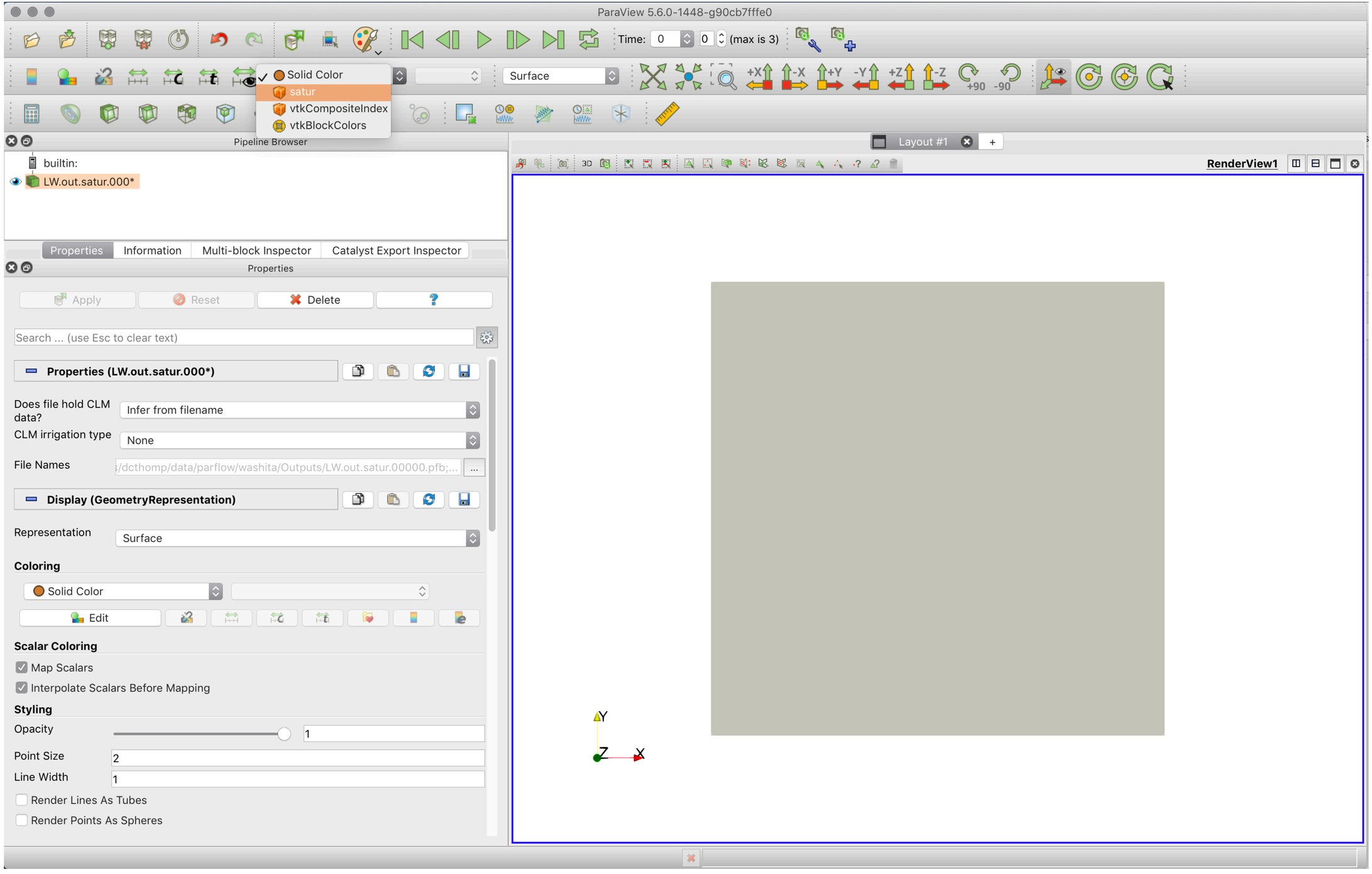
Point Size
2
Line Width
1
Render Lines As Tubes
Render Points As Spheres
Y
Z
X


ParaView 5.6.0-1448-g90cb7fffe0
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Information
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Catalyst Export Inspector
Properties
Apply
Reset
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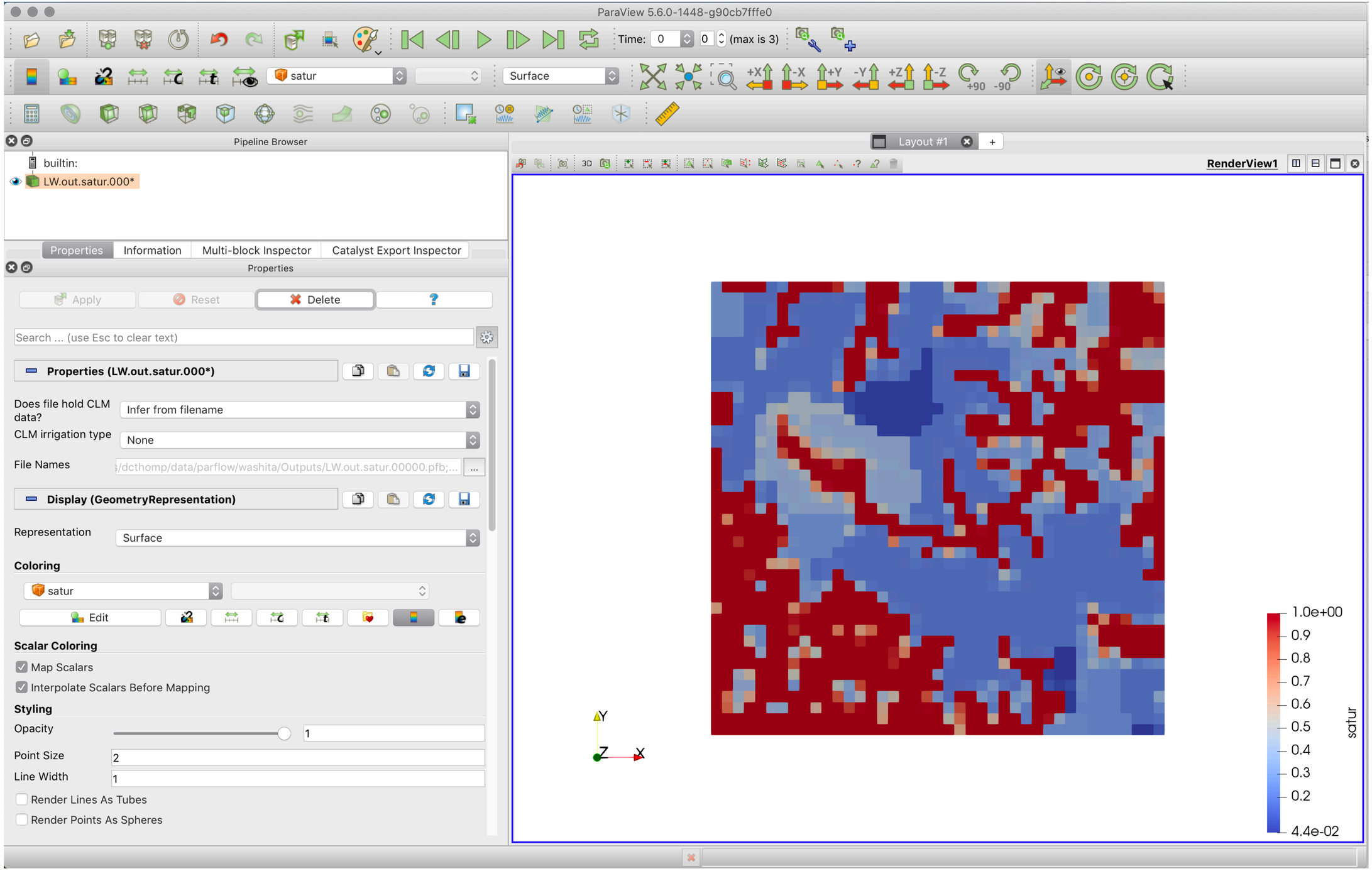
ParaView 5.6.0-1448-g90cb7fffe0
Time: 0 0 (max is 3)
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1
Point Size
2
Line Width
1
Render Lines As Tubes
Render Points As Spheres
Layout #1
RenderView1
1.0e+00
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
4.4e-02
satur
Y
Z
X

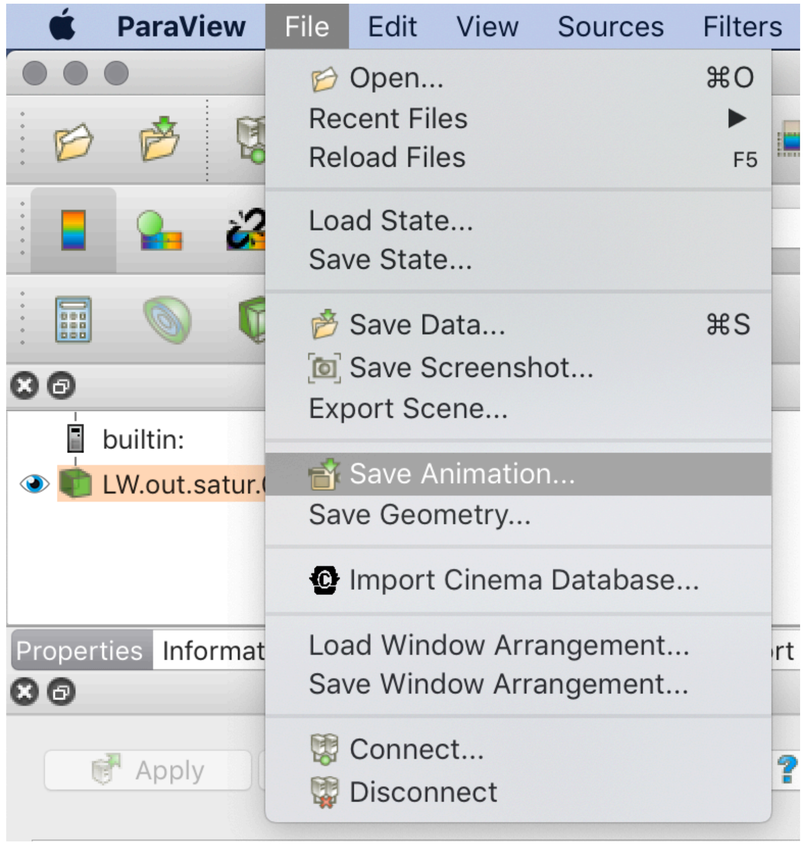
Tools for ParFlow

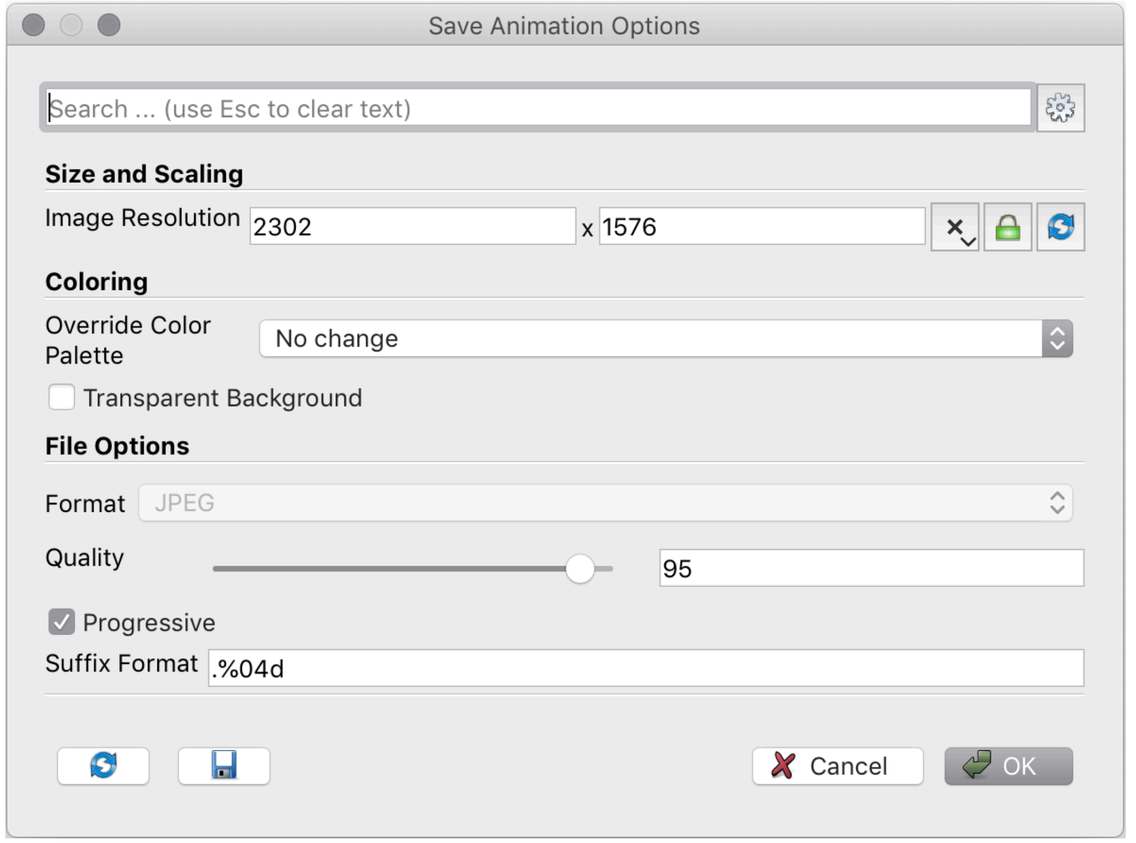
- Both the `.pfb` and `.pfmetadata` readers can read timeseries data. Neither provide the actual time value yet, only an integer timestep.

- This toolbar controls the current timestep being displayed in ParaView.

Tools for ParFlow

ParaView can also create image sequences (and movies directly on some platforms) for animation.

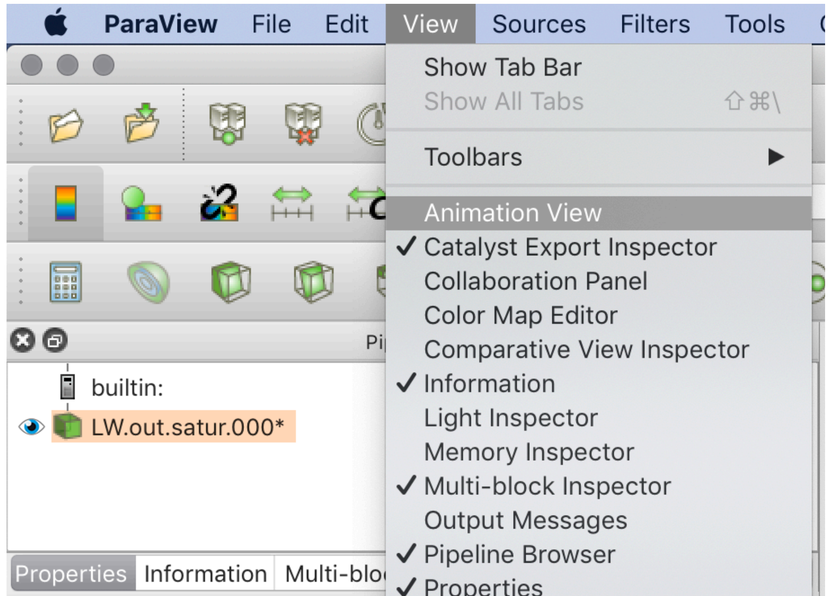


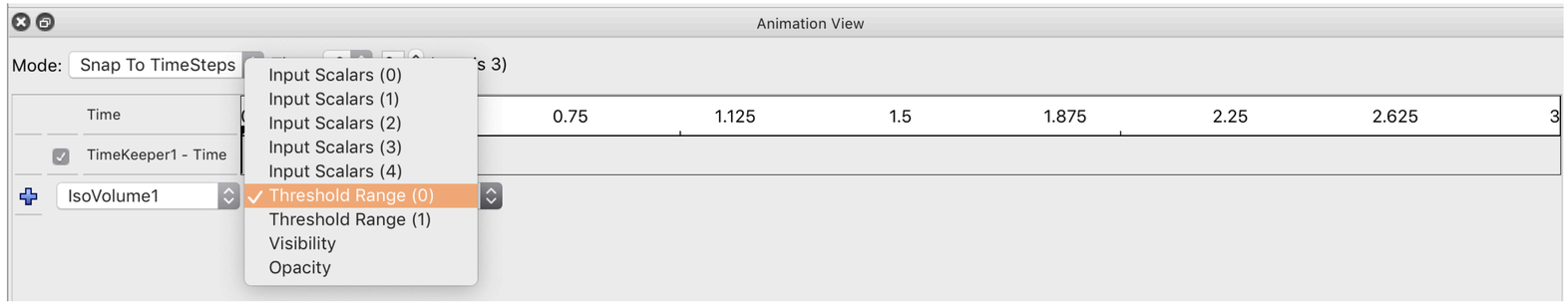


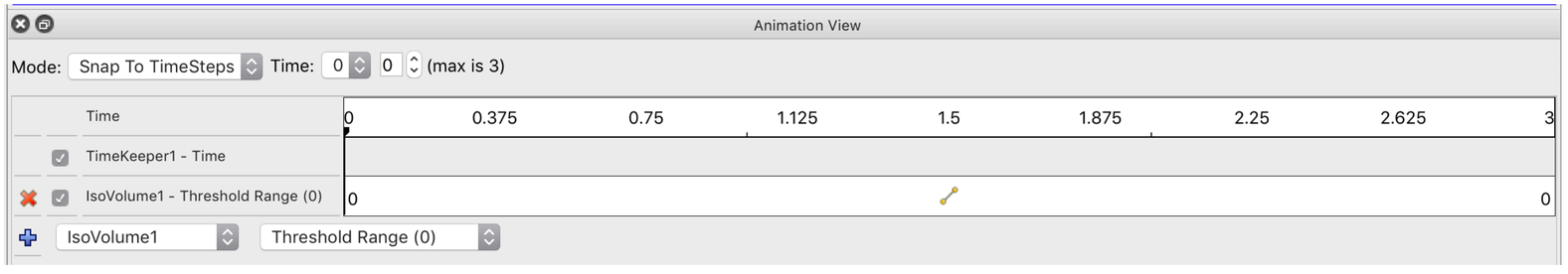
Tools for ParFlow

- In addition to playing timeseries data, ParaView can adjust (1) filter parameters like isovalue and (2) camera position and focus during animation.

- The Animation panel lets you choose what to vary.





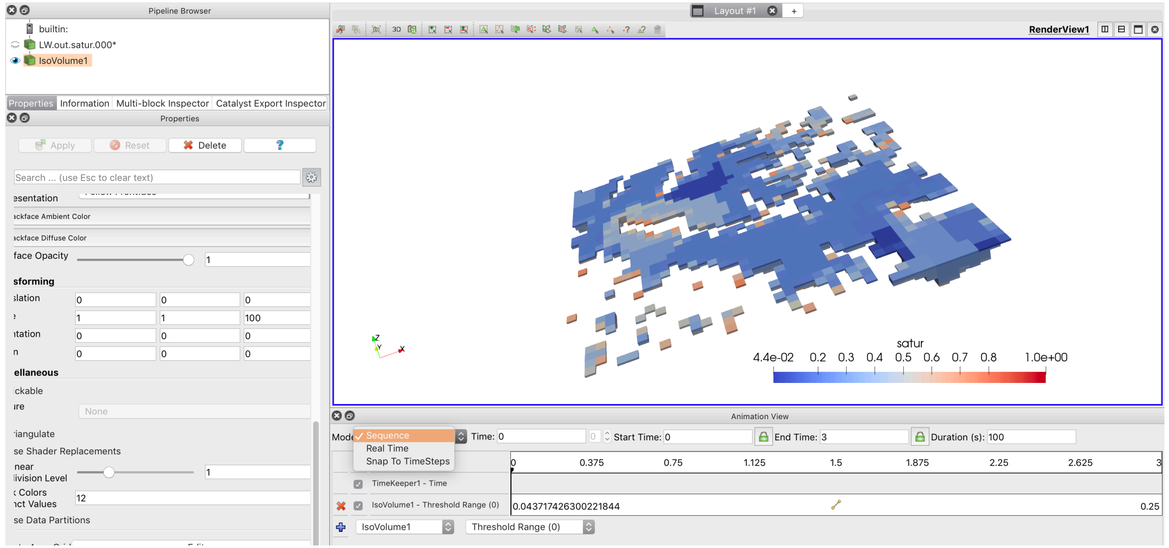


Tools for ParFlow

- In addi aView
  can ac e and
  (2) car nation.
- The An t to vary.

Tools for ParFlow

- By default, ParaView snaps animation timesteps to times available from sources (readers).
- If you want a movie that has more frames, you can change the animation mode in the panel.



Pipeline Browser

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Properties

Reset | Delete | ?

Esc to clear text)

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Layout #1 | +

RenderView1

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Animation View

Mode: Sequence | Real Time | Snap To TimeSteps

Time: 0 | Start Time: 0 | End Time: 3 | Duration (s): 100

0 0.375 0.75 1.125 1.5 1.875 2.25 2.625

TimeKeeper1 - Time

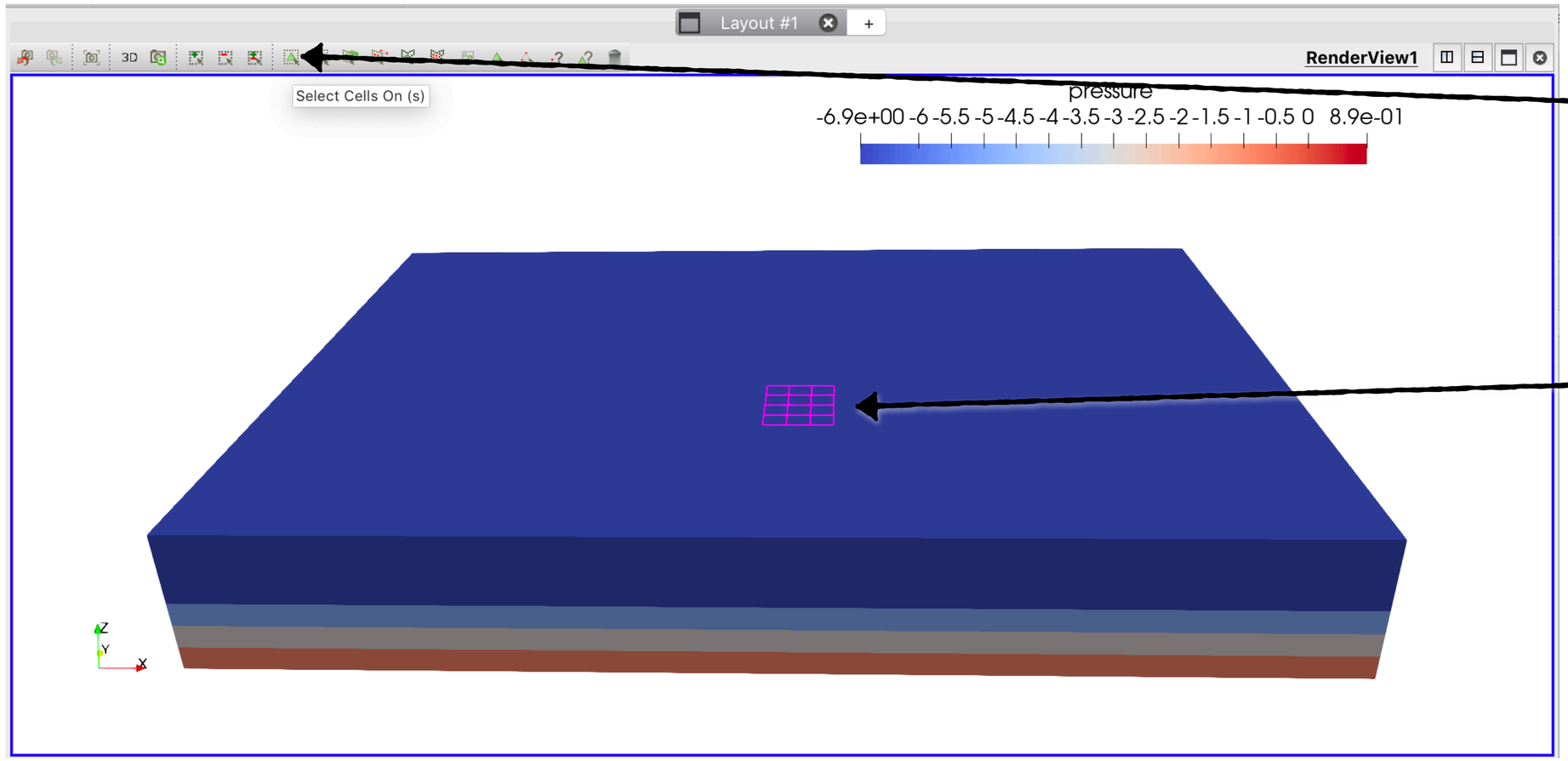
IsoVolume1 - Threshold Range (0)

0.043717426300221844

IsoVolume1 | Threshold Range (0)

Tools for ParFlow

- Now let's plot values of a selection over time.

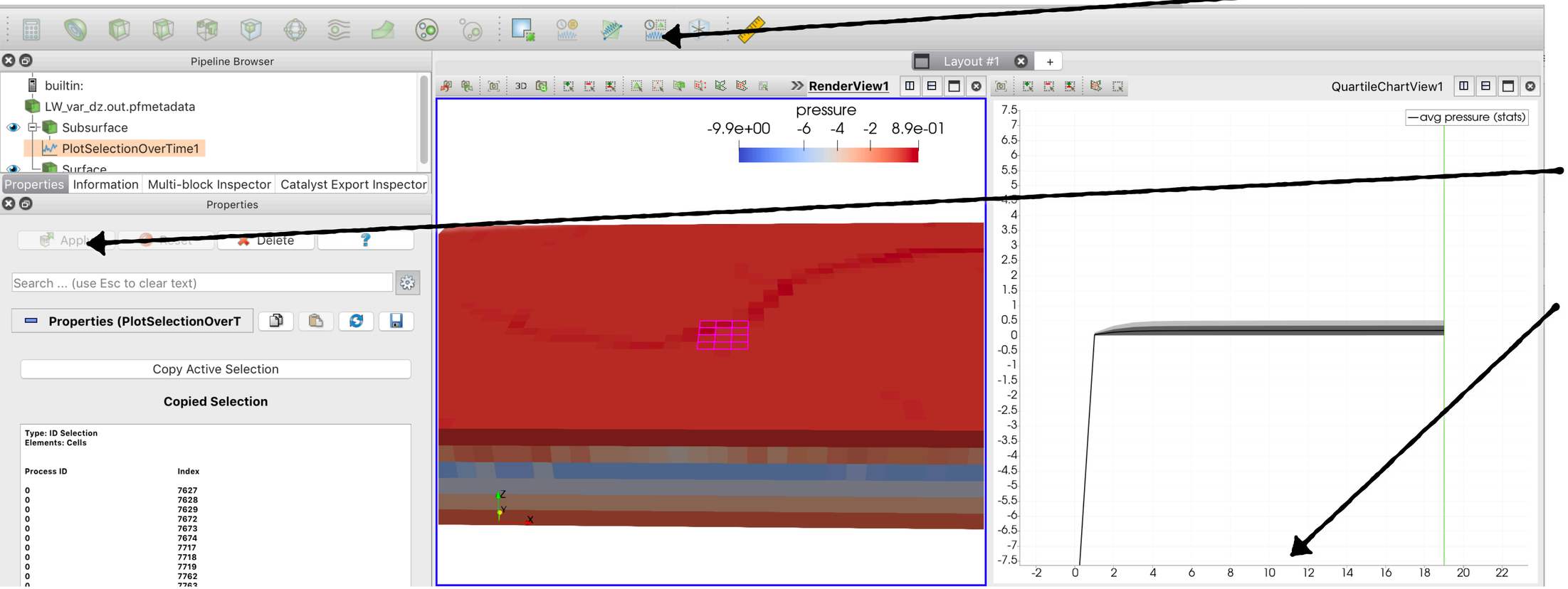


Type 's' or click the Select Cells On button.

Click-drag on the dataset to choose cells. They will be highlighted in magenta.

Tools for ParFlow

- Now let's plot values of a selection over time.



Click on the "Plot Selection Over Time" toobar button.

Click Apply in the Properties panel.

New chart view appears with timestep on the horizontal axis.

Tools for ParFlow

- Loading plugins
- Reading and animating data
- Plotting selections over time
- Colormaps for stream flow
- Simple calculations

TODO

Overview

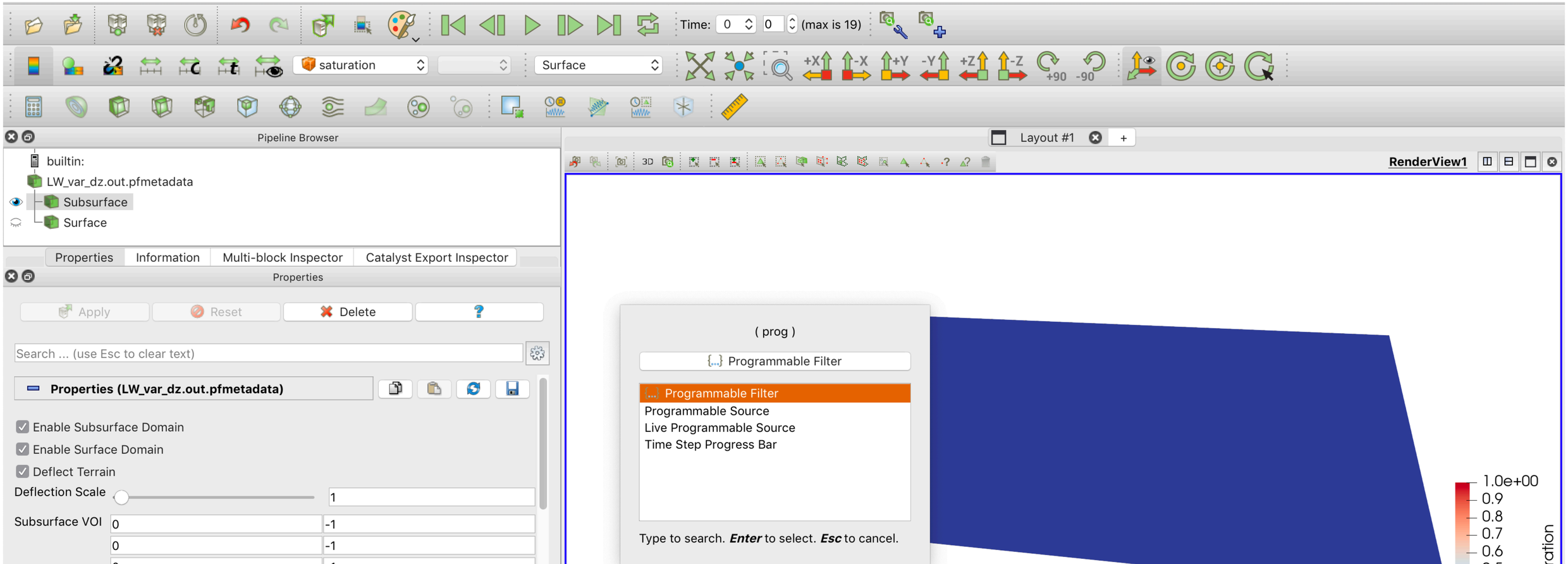
- Data types & filter pipelines in VTK & ParaView **20 min**
- Visualization is composition **20 min**
- Tools for ParFlow **45 min**
- Going further with Python and NumPy **45 min**
- Catalyst and web demonstrations **20 min**

Python and NumPy

- ParaView makes it easy to write filters in Python and use them interactively.
- Step 1: Python Programmable Filter
- Step 2: Python filter plugins
- Step 3: Fancier computations

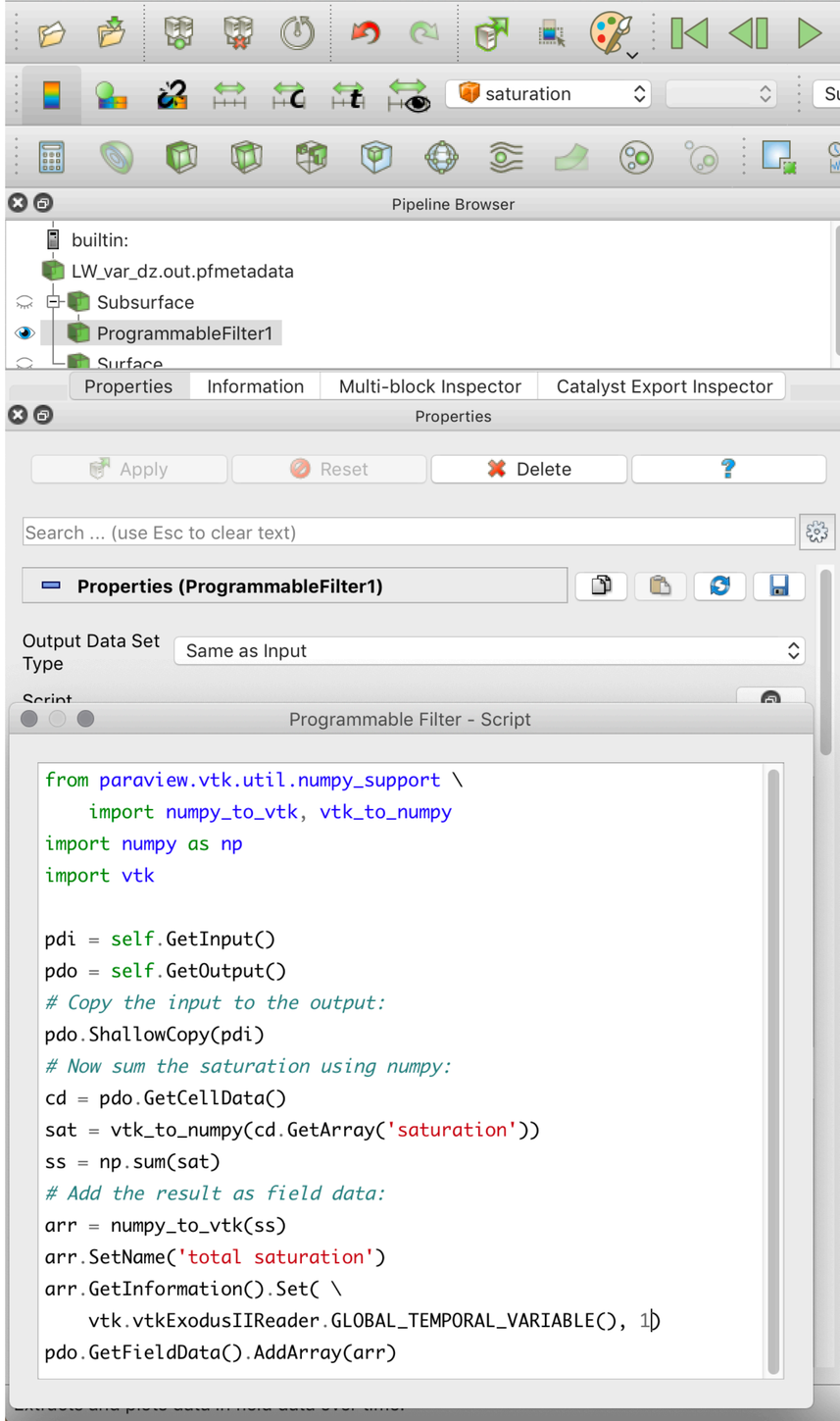
Programmable Filter

- Let's sum the saturation over the entire volume so we can plot the total saturation sum over time.



Programmable Filter

- Enter a script into the programmable filter's editor, which can be detached from the panel.
- Click apply, then look at the information panel to confirm that the filter added a new array.



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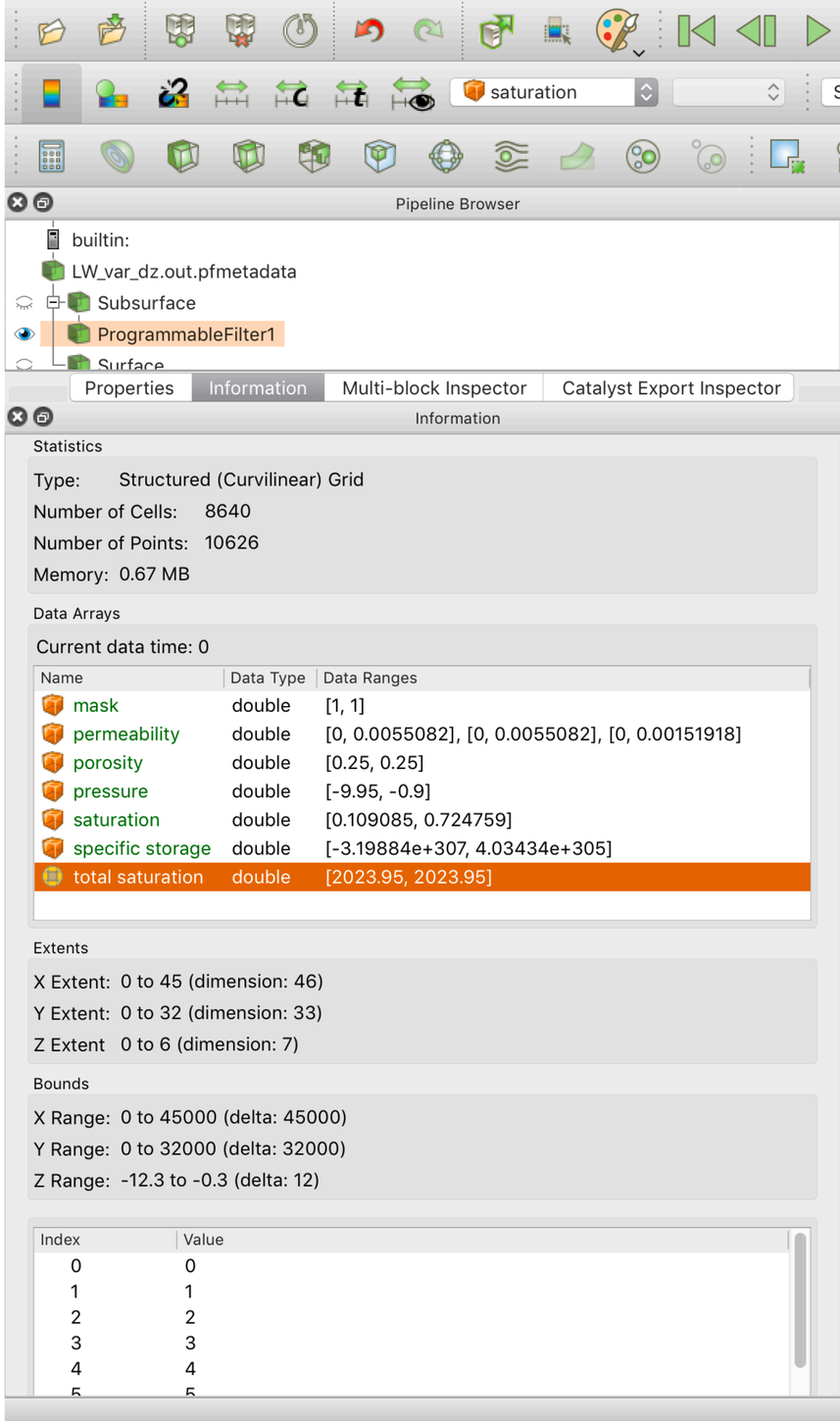


Programmable Filter

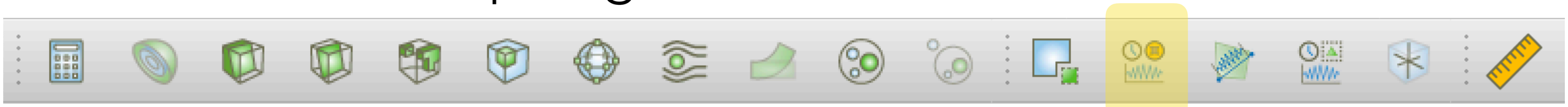
This marks the new array as a time-varying array so that the filter will attempt to plot it.


```
from paraview.vtk.util.numpy_support \
    import numpy_to_vtk, vtk_to_numpy
import numpy as np
import vtk

pdi = self.GetInput()
pdo = self.GetOutput()
# Copy the input to the output:
pdo.ShallowCopy(pdi)
# Now sum the saturation using numpy:
cd = pdo.GetCellData()
sat = vtk_to_numpy(cd.GetArray('saturation'))
ss = np.sum(sat)
# Add the result as field data:
arr = numpy_to_vtk(ss)
arr.SetName('total saturation')
arr.GetInformation().Set( \
    vtk.vtkExodusIIReader.GLOBAL_TEMPORAL_VARIABLE(), 1)
pdo.GetFieldData().AddArray(arr)
```

Programmable Filter

- Now we can plot global data over time.



Pipeline Browser

LW_var_dz.out.pfmetadata
Subsurface
ProgrammableFilter1
PlotGlobalVariablesOverTime1
Surface

Properties | Information | Multi-block Inspector | Catalyst Export Inspector

Properties

Apply | Reset | Delete | ?

Search ... (use Esc to clear text)

Properties (PlotGlobalVariablesOverTime1)

Display (XYChartRepresentation)

Attribute Type: Row Data

X Axis Parameters

Use Index For XAxis

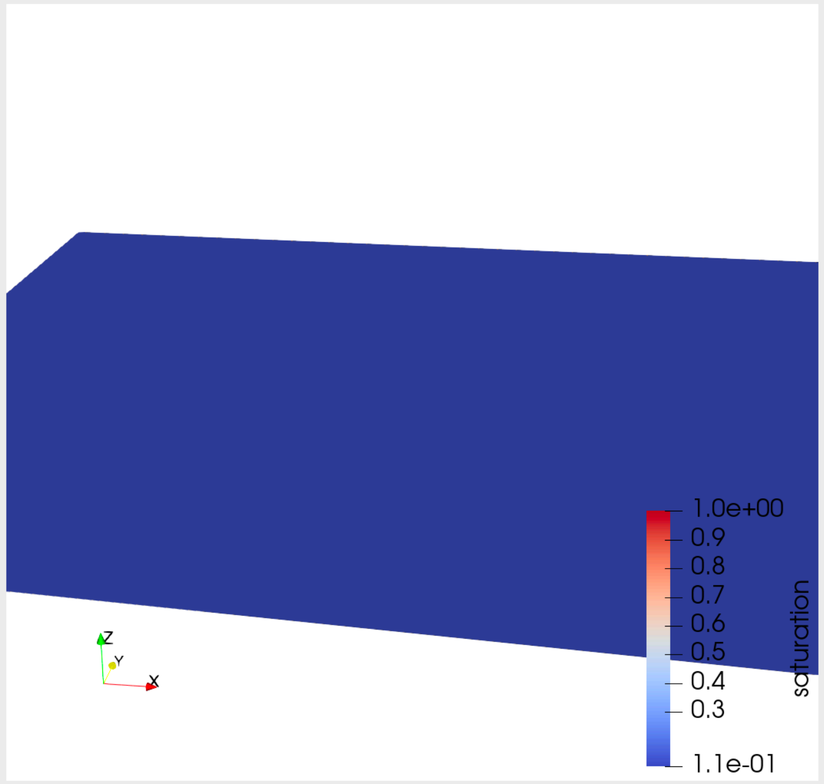
X Array Name: Time

Series Parameters

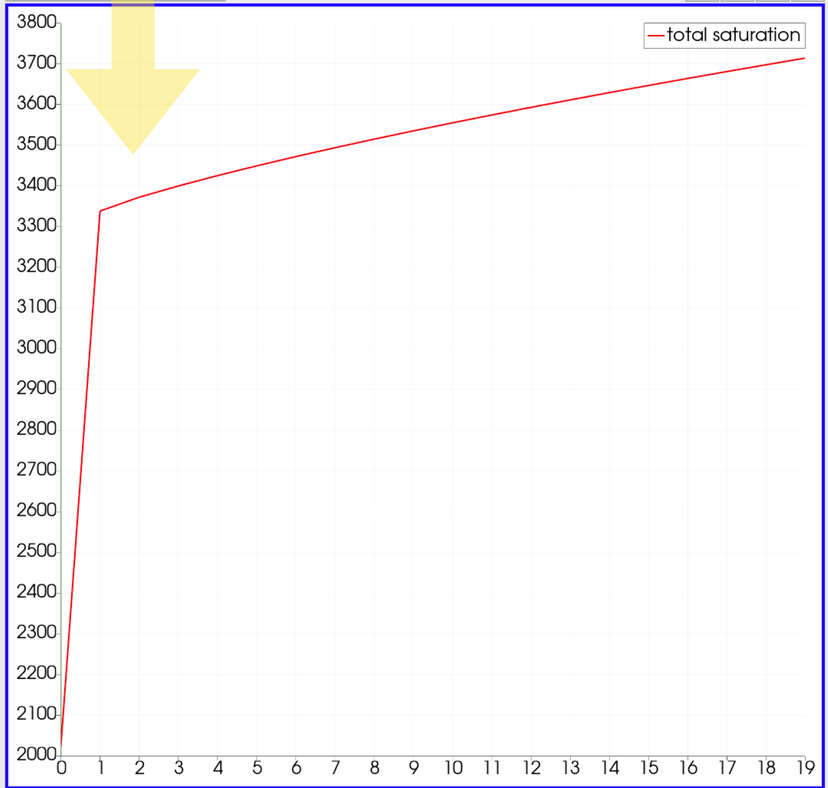
Variable	Legend Name
Time	Time

Layout #1

RenderView1



LineChartView1



Python Filter Plugins

- To reuse a Python programmable filter, encapsulate it into a custom plugin.
- Plugins can be autoloaded and filters added to a toolbar, so access to the filter is easy.

Python and NumPy

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Catalyst, Cinema, ParaViewWeb

Acknowledgments

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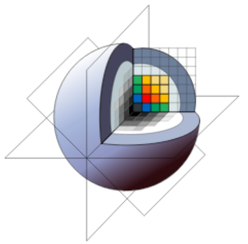
Kitware

- Software process
- Scientific visualization & HPC
- Cloud data & analytics
- Medical computing
- Computer vision

Kitware






- Collaborative R&D
- Custom software
- Support
- Training