VisWeek 09
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ParaView

In Situ Post-Processing and Visualization

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Outline

- Motivation & Teaser
- Example
  - Part I: Creating a script and source — David
  - Part II: Gluing it all together — Nathan
- Conclusion

Motivation & Teaser

Motivation

- Want to allow direct access to simulation state
  - To avoid writing to disk when possible
  - To perform analysis not otherwise possible
- Avoid rewriting glue code
- Allow quick reconfiguration for exploration
- Provide but don't require parallel rendering
- Hmmm... why not take advantage of ParaView Scripting from this morning's tutorial?

Solution

- A small utility library available to simulations via a simple interface:

  Initialize Start up pvbatch Python interp, provide script, provide information about state variables

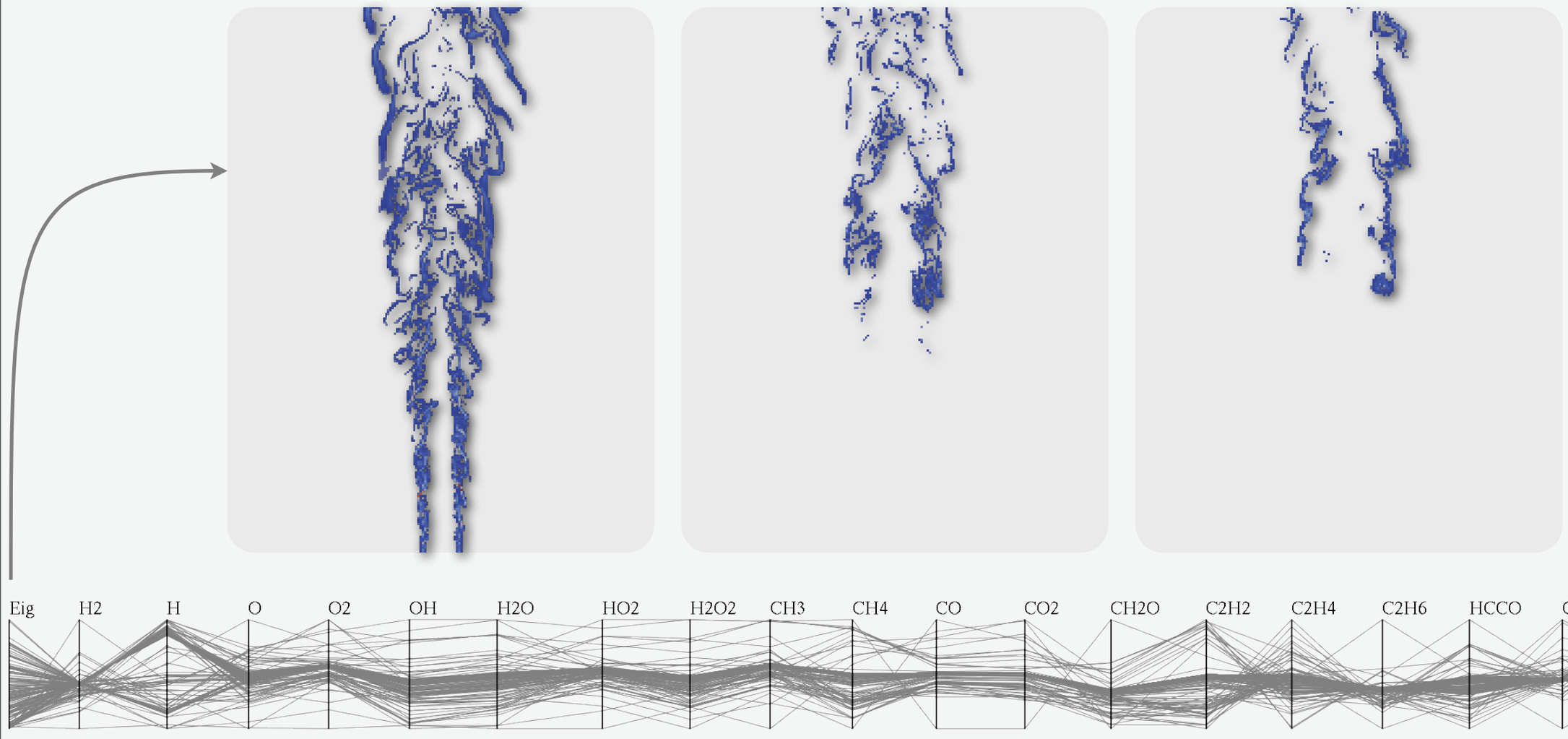
  Update Evaluate Python function to update pipeline

  Finalize Shut down Python interpreter

- Minimal work on analysis side:
  - Write a data source
  - Create/modify a ParaView Python script

Results

PCA run on subgrids of a 2025x1600x400 combustion simulation:



Thanks to Chunsang Yoo, Jacqueline H. Chen, and Ray Grout
for providing combustion data, compute time, and expertise.

Overview of Interface

- View from simulation side:
  - Calls to initialize/finalize a utility library
  - One call per timestep for updates
- View from analysis script side:
  - Simulation is source of a pipeline set up by script.
  - One script function called each timestep to possibly modify and definitely re-run the pipeline

Source Class

- Inherits vtkAlgorithm subclass based on type of data (e.g. vtkPolyDataAlgorithm)
- Will usually own a data object to shallow-copy into RequestData() output
- Provides methods for simulation to prepare data object with simulation state. You must decide:
  - whether to copy or grant direct access
  - whether to use barriers/fences and threads or not
  - whether to provide derived state or direct state

Example: Simulation

```
CALL in_situ_init( rank, comm, &
 num_species, species, &
 ni, nj, nk, mi, mj, mk, neighbors )
```

```
10 CALL advance_simulation( time, dt )
   CALL in_situ_step( time, dt )
   IF ( .NOT. evaluate_exit_condition() ) GOTO 10

   CALL in_situ_fini( rank, comm )
```

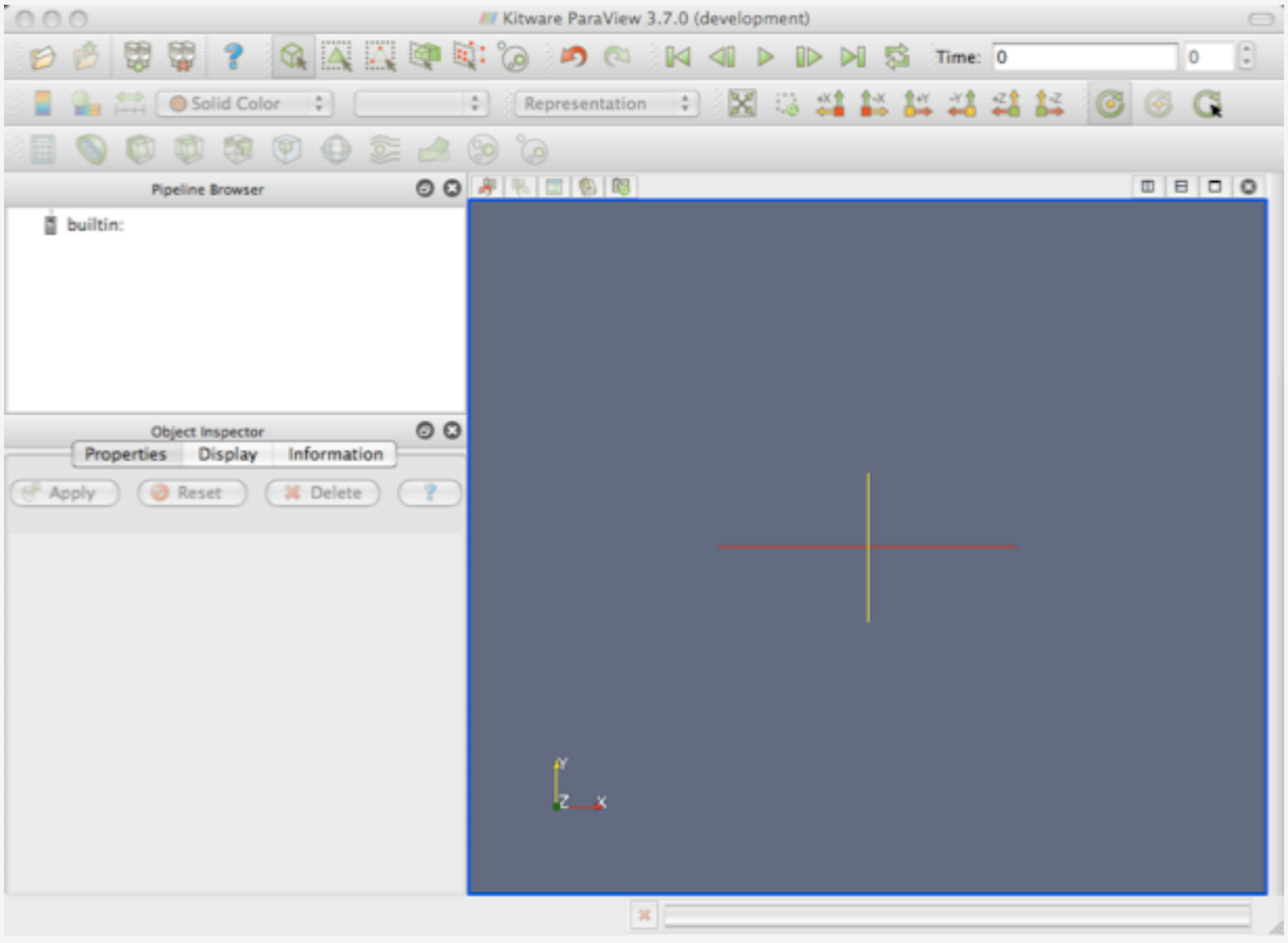
Example: Script

```
from paraview import *
s3dData = S3DSource()
pca = GridPCA()
pca.Input = s3dData
km = PKMeans()
km.Input = pca
wr = TableWriter()
def update( p, ti, time, dt ):
  wr.SetFileName( ‘kmeans-%d-%d.vtk’ % (p,ti) )
  wr.Write()
```

Example, Part 1

Creating a Script

- No need to write script from start...
- ... use ParaView to prototype.



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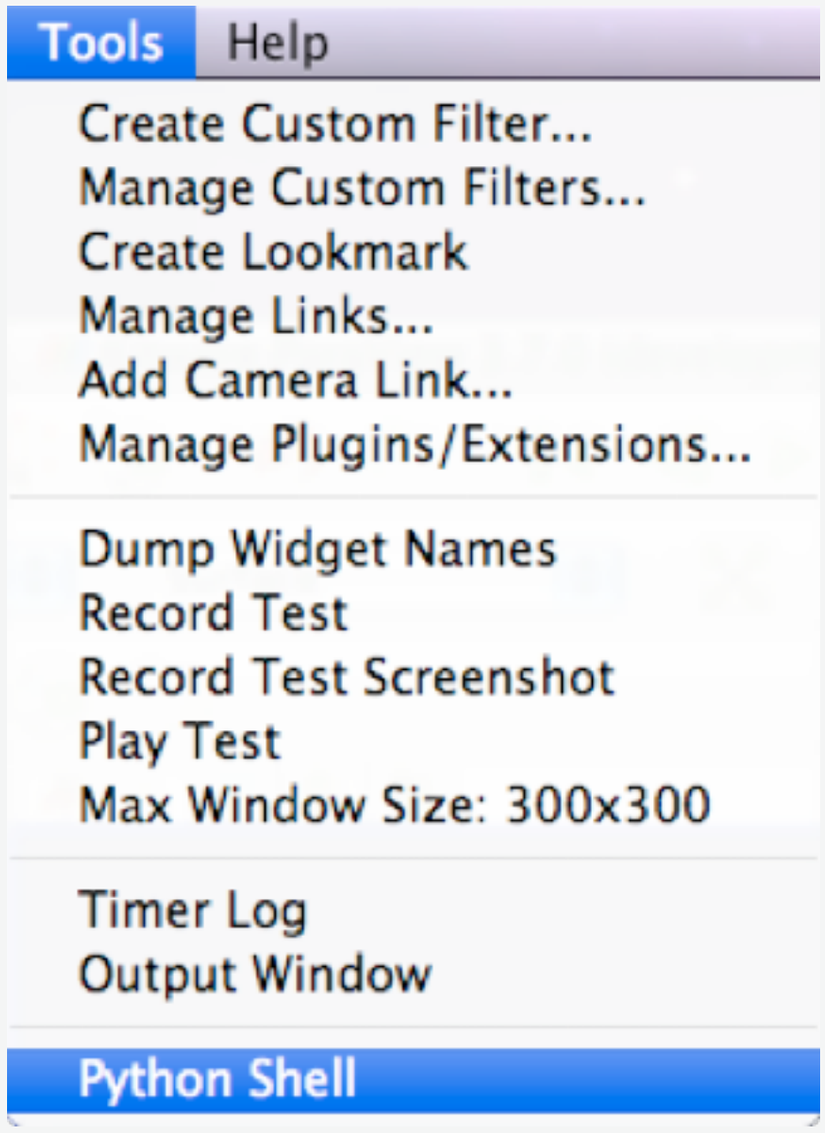

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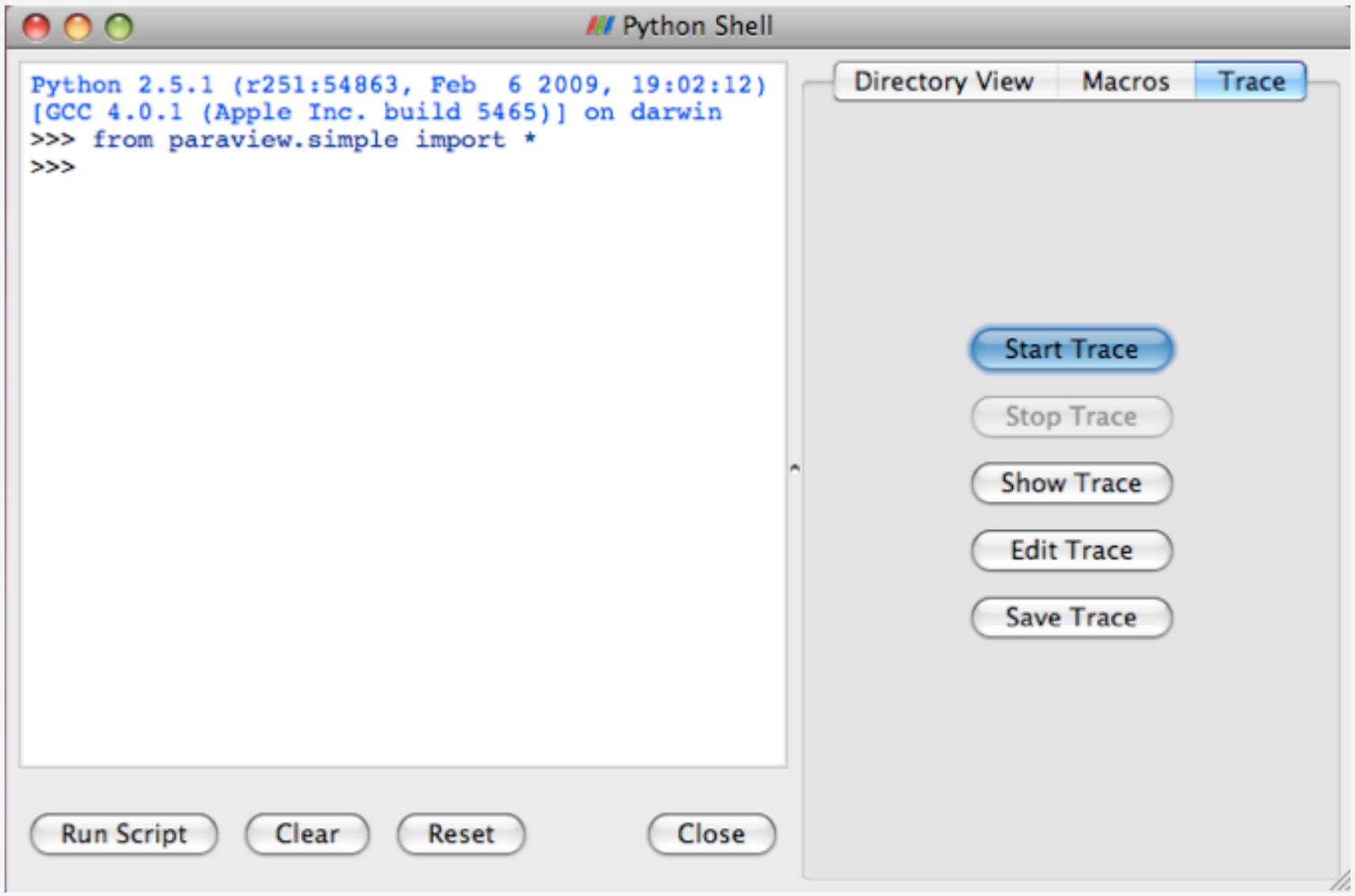

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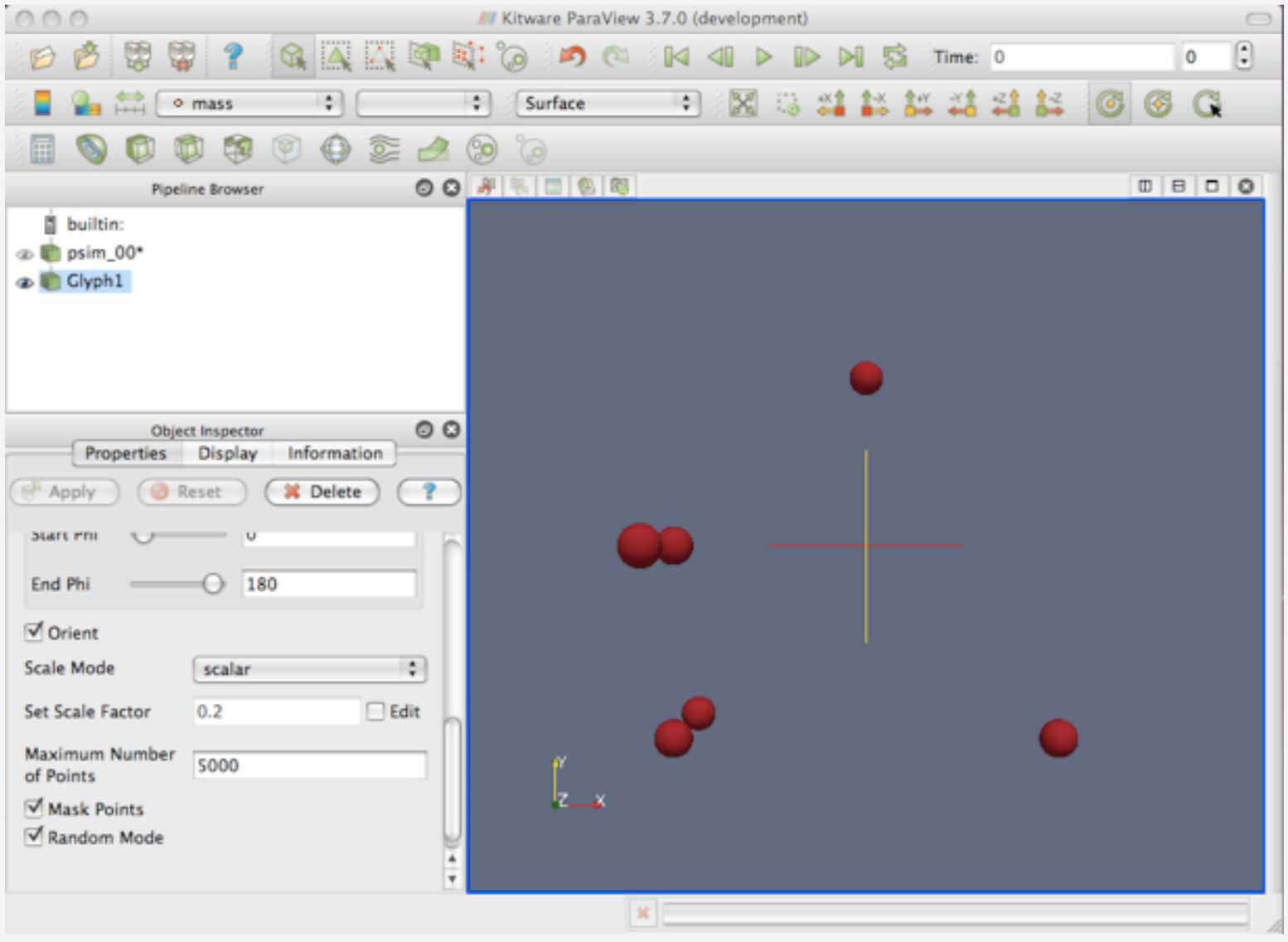

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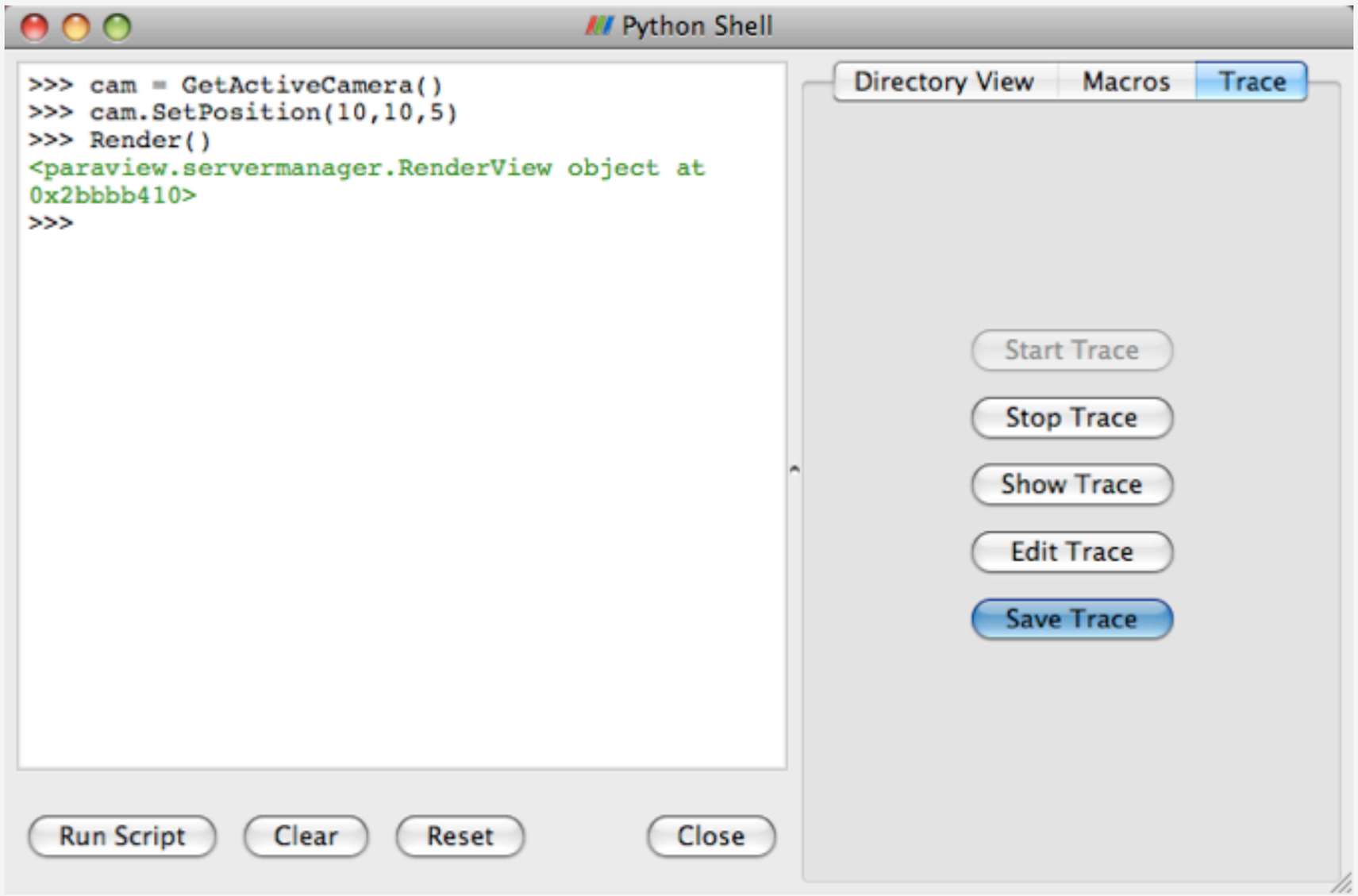


Creating a Script

Now remove the reader and add an *in situ* source...

```
try: paraview.simple
except: from paraview.simple import *

psim_0001 = XMLPolyDataReader( FileName=['psim_0001.vtp'] )
psim_0001.PointArrayStatus = ['pmom', 'pfrc', 'mass']

RenderView1 = GetRenderView()
...
```

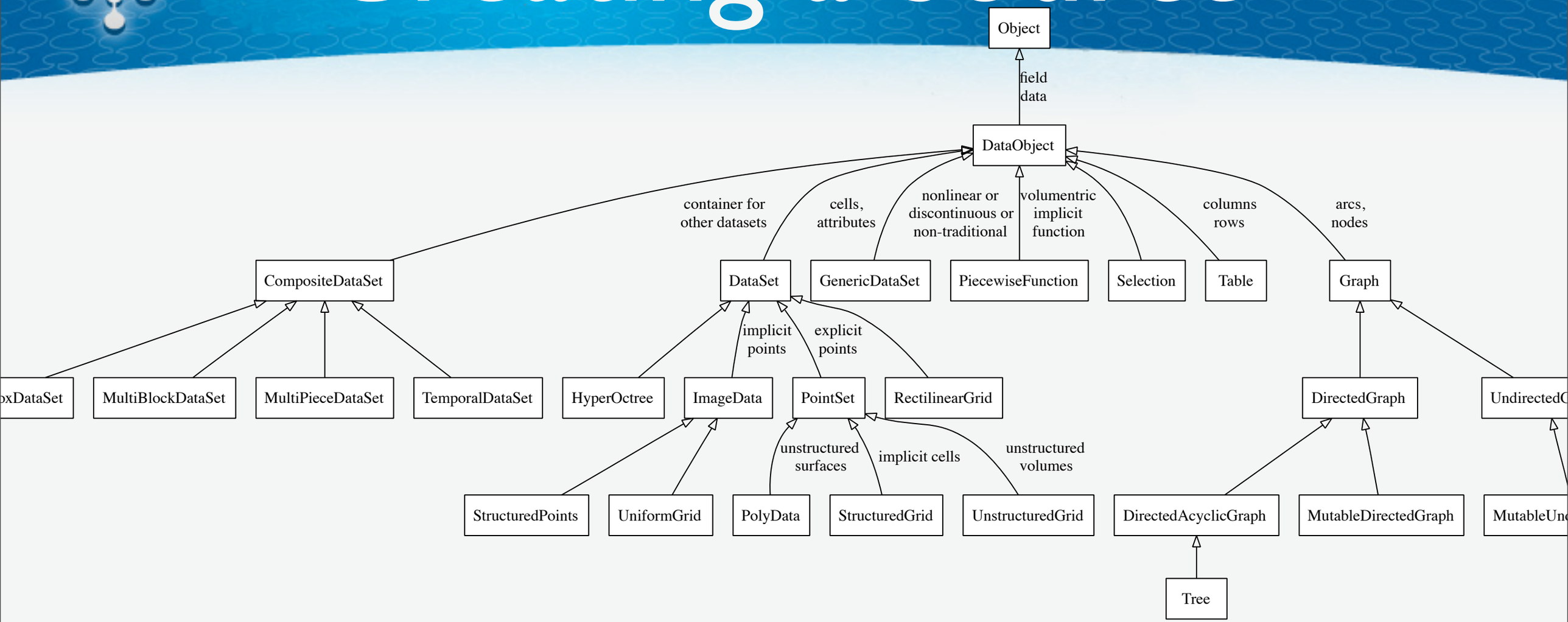
```
try: paraview.simple
except: from paraview.simple import *

psim_0001 = servermanager.server.DotSource()

RenderView1 = GetRenderView()
...
```

... which we'll write next.

Creating a Source



- Find state you wish to expose in simulation.
- Determine appropriate subclass of vtkDataObject and thus vtkAlgorithm for your source.
- Add methods to populate dataset from simulation.

Creating a Source

From the Fortran module `simulation/particle_m.f90` we identify some state to expose:

```
! ----------------------------------------------------------------------
! PARTICLE STATE
! ----------------------------------------------------------------------
module particle_m
use parallel_m

! ----------------------------------------------------------------------
integer num_particles ! number of particles in the simulation
integer num_neighbors ! number of nearest neighbors to track
real terminal_force ! the smallest inter-particle force we'll allow.
real terminal_velocity ! the smallest particle velocity we'll allow.
integer min_steps ! the smallest number of time steps we'll allow.
integer simstep  ! the number of steps we've simulated
real,    allocatable, target, public :: pxyz(:,:) ! particle coordinates
real,    allocatable, target, public :: pmom(:,:) ! particle momenta
real,    allocatable, target, public :: pfrc(:,:) ! particle forces
real,    allocatable, target, public :: mass(:)   ! particle masses
```

Creating a Source

Now create a vtkAlgorithm subclass and add an initialization method to `insitu/vtkDotSource.h`:

```
#include "vtkPolyDataAlgorithm.h"
class VTK_EXPORT vtkDotSource : public vtkPolyDataAlgorithm
{
public:
  static vtkDotSource* New();
  ...
  /// Prepare SimulationData using arrays from the simulation.
  virtual void Initialize( int num_particles, double* pxyz, double* mass,
                double* pmom, double* pfrc, int local_id, int num_procs );
protected:
  virtual int RequestData( vtkInformation*, vtkInformationVector**, ...
  vtkPolyData* SimulationData; // References arrays owned by simulation.
};
```

Creating a Source

Implementing the source simply involves a shallow copy of the initialized object in `insitu/vtkDotSource.cxx`:

```
int vtkDotSource::RequestData( vtkInformation*,
     vtkInformationVector** inInfoVec, vtkInformationVector* ouInfoVec )
{
  if ( this->SimulationData ) {
    vtkInformation* ouInfo0 = ouInfoVec->GetInformationObject( 0 );
    if ( ! ouInfo0 ) return 0;
    vtkDataObject* ouData0 = ouInfo0->Get(vtkDataObject::DATA_OBJECT());
    if ( ouData0 ) {
      ouData0->ShallowCopy( this->SimulationData );
      ouData0->GetInformation()->Set( vtkDataObject::DATA_TIME_STEPS(),
        &this->SimulationTime, 1 );
    }
  }
  return 1;
}
```