Kitware

ParaView Catalyst:
Scalable *In Situ* processing

Andrew Bauer (Kitware, Inc.)
Jeffrey Mauldin (Sandia National Laboratories)

Agenda

- Introduction to ParaView Catalyst
- Catalyst for Developers
- Catalyst for Users
- Building ParaView Catalyst

Goals

- Understand the flow of control and data when using ParaView Catalyst with a simulation code
  - Understand efficiency trade-offs
- Hands-on exercises for:
  - Interfacing a simulation code with Catalyst
  - Creating VTK data structures to represent grid and field information from simulation data structures
  - Creating a Python script to extract data and screenshots through ParaView Catalyst
- Running a simulation with all of the parts put together

Online Materials

- This presentation and VM virtual appliance at:
  - http://www.paraview.org/Wiki/ParaView/Catalyst/PETTT_Tutorial
- Install ParaView 4.1
  - www.paraview.org/download
- Install VirtualBox
  - www.virtualbox.org

Kitware

VirtualBox

- Run VirtualBox and go to “File→Import Appliance…”
- Click on “Open appliance…” and select catalysttutorial1.ova, click on “Next >”
- Can adjust appliance settings as needed and click on “Import”
  - Suggest keeping defaults
- Click on “Start” to run VirtualBox with Catalyst tutorial examples
  - Can click on “OK” for warning messages

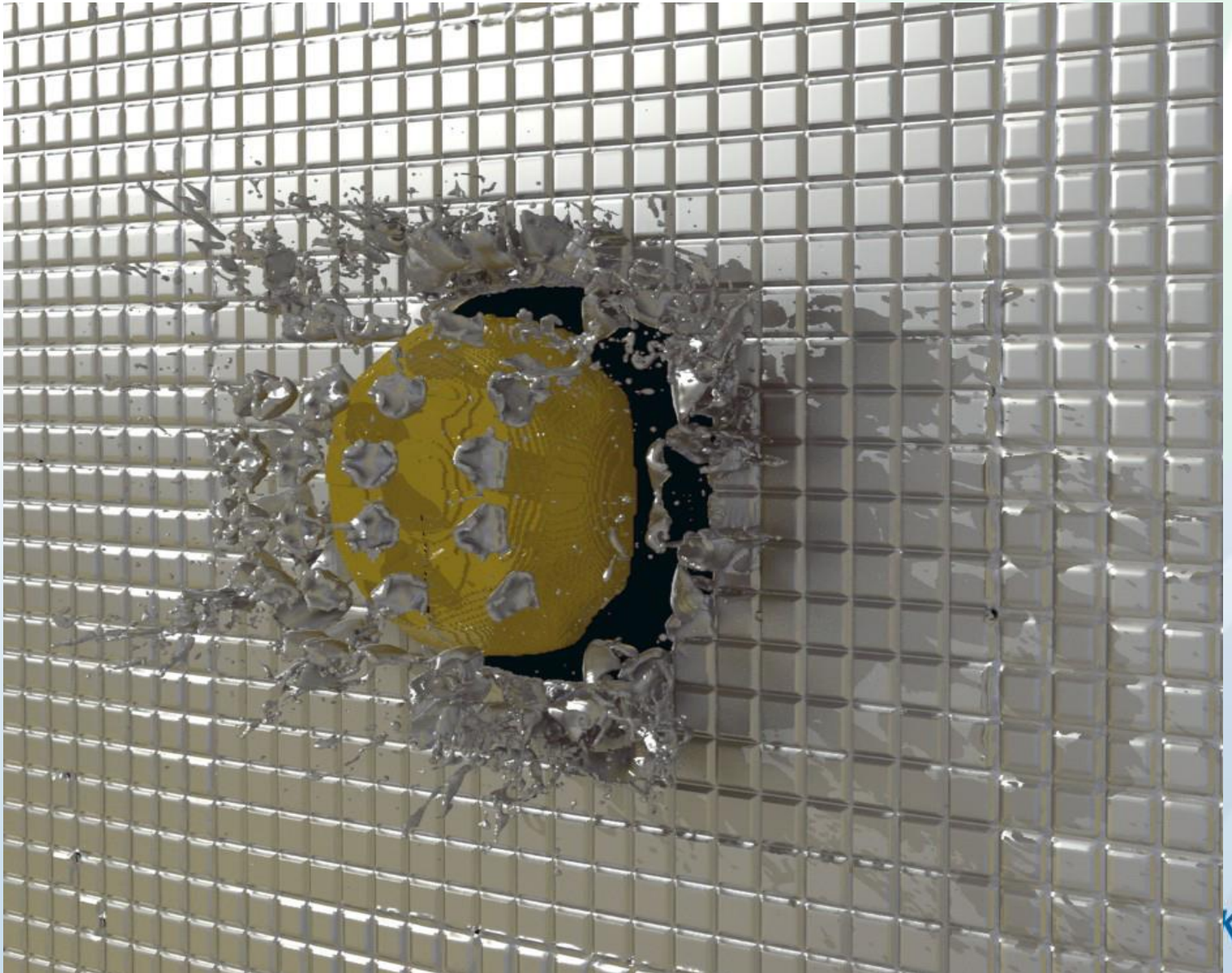
VirtualBox

- Use Jeff Mauldin account
  - Password is “l7oleW-r” (el seven oh el ee double-u dash are)
- Get terminal by clicking in upper-left and typing terminal
- Get examples with “wget https://github.com/acbauer/miniFE-2.0_ref_Catalyst/archive/tutorial.zip”
- May want to install emacs/vim
  - sudo apt-get install [emacs23,vim]

Online Help

- Catalyst User's Guide:
  - http://paraview.org/Wiki/images/4/48/CatalystUsersGuide.pdf
- Email list:
  - paraview@paraview.org
- Doxygen:
  - http://www.vtk.org/doc/nightly/html/classes.html
  - http://www.paraview.org/ParaView3/Doc/Nightly/html/classes.html
- Sphinx:
  - http://www.paraview.org/ParaView3/Doc/Nightly/www/py-doc/index.html
- Websites:
  - http://www.paraview.org
  - http://catalyst.paraview.org
- Examples:
  - https://github.com/acbauer/CatalystExampleCode

What is Catalyst?



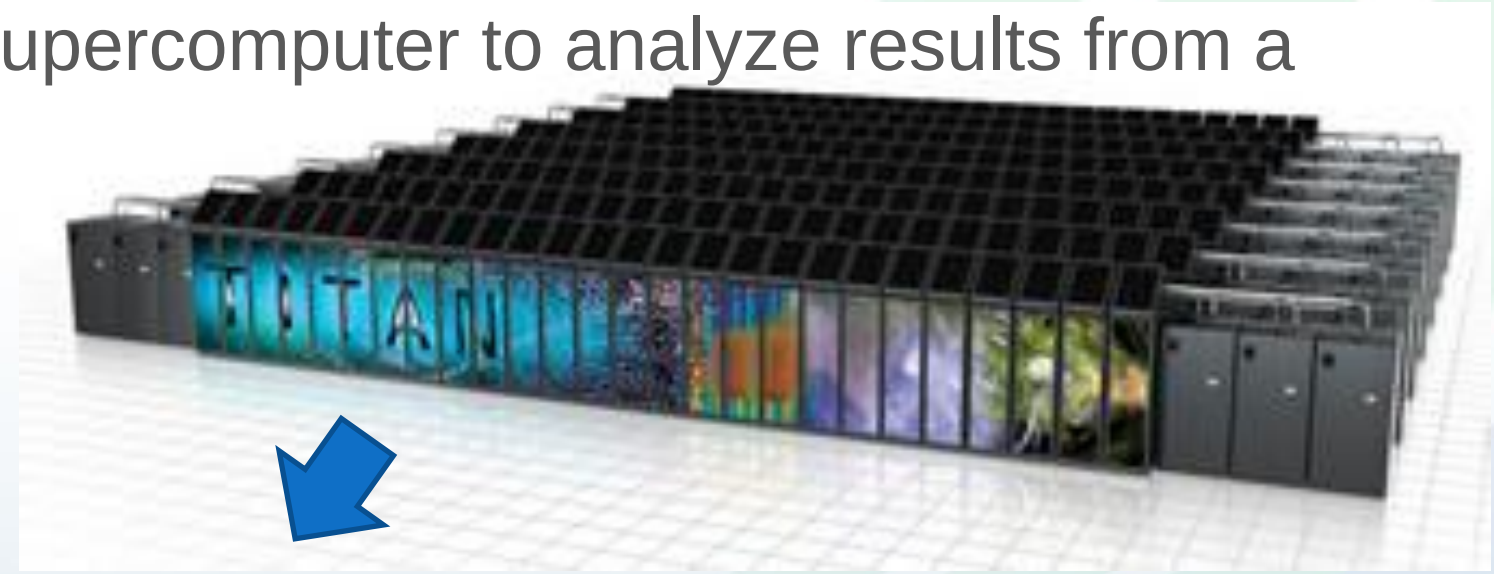
Why *In Situ*?

	2010	2018	Factor Change
System peak	2 Pf/s	1 Ef/s	500
Power	6 MW	20 MW	3
System Memory	0.3 PB	10 PB	33
Node Performance	0.125 Tf/s	10 Tf/s	80
Node Memory BW	25 GB/s	400 GB/s	16
Node Concurrency	12 cpus	1,000 cpus	83
Interconnect BW	1.5 GB/s	50 GB/s	33
System size (nodes)	20 K nodes	1 M nodes	50
Total Concurrency	225 K	1 B	4,444
Storage	15 PB	300 PB	20
Input/Output Bandwidth	0.2 TB/s	20 TB/s	100

DOE Exascale Initiative Roadmap, Architecture and Technology Workshop, San Diego, December, 2009.

Why *In Situ*?

Need a supercomputer to analyze results from a hero run

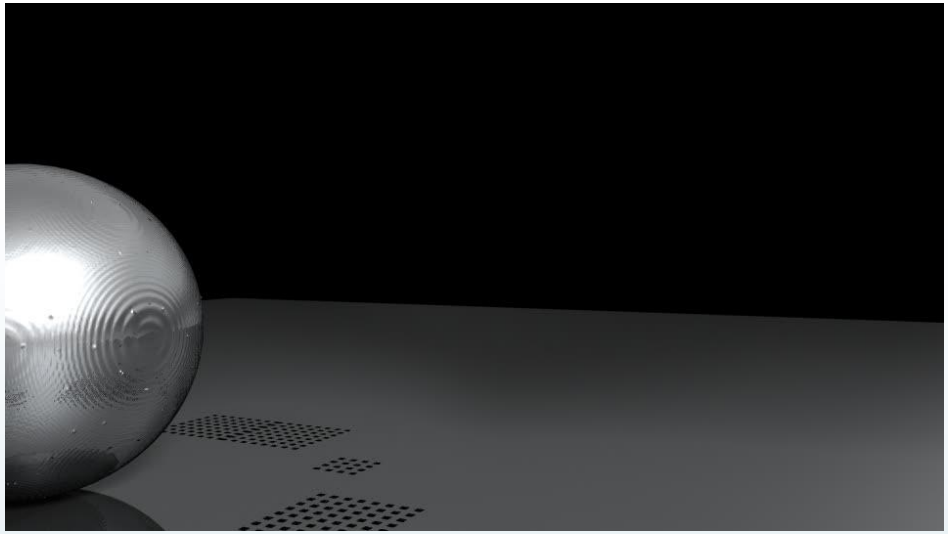


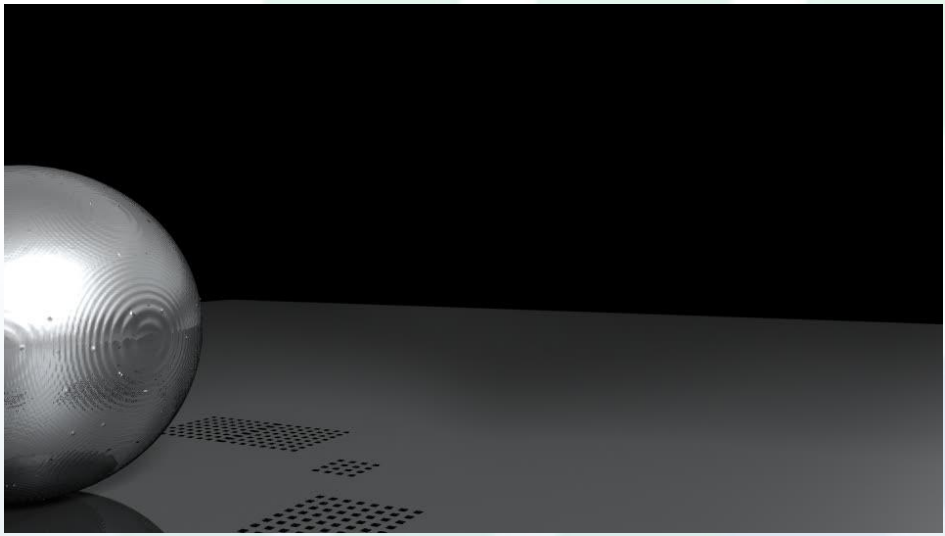
RHEA

2 orders of magnitude difference between each level

Kitware

Access to More Data





Post-processing

In situ processing

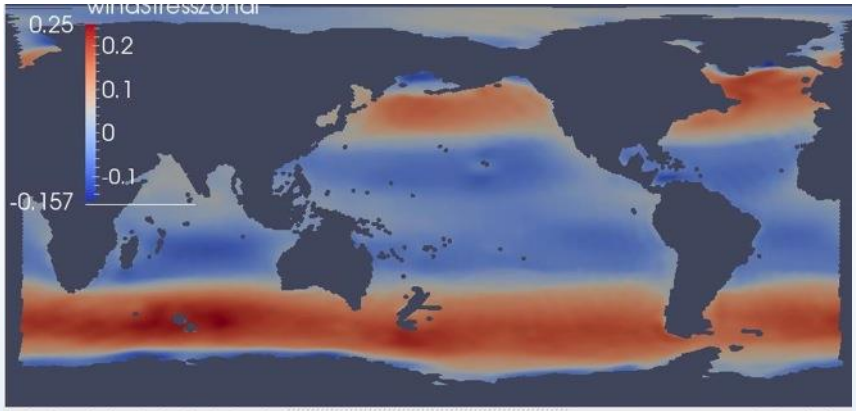
CTH (Sandia) simulation with roughly equal data stored at simulation time

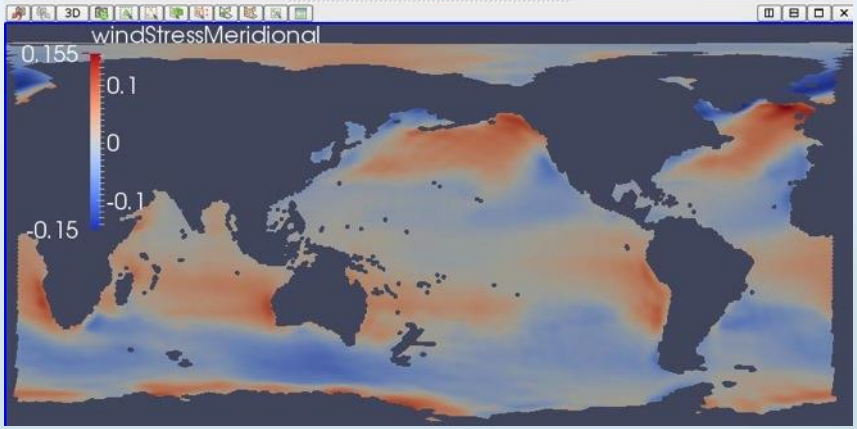
Reflections and shadows added in post-processing for both examples

Kitware

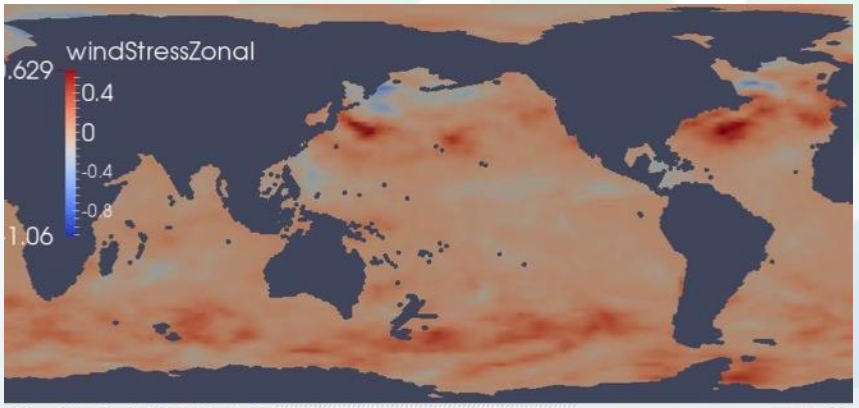
Quick and Easy Run-Time Checks

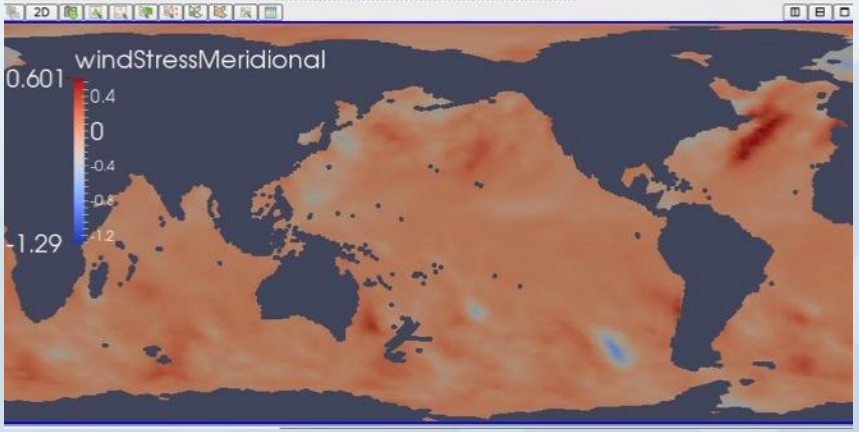
Expected wind stress field at the surface of the ocean





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

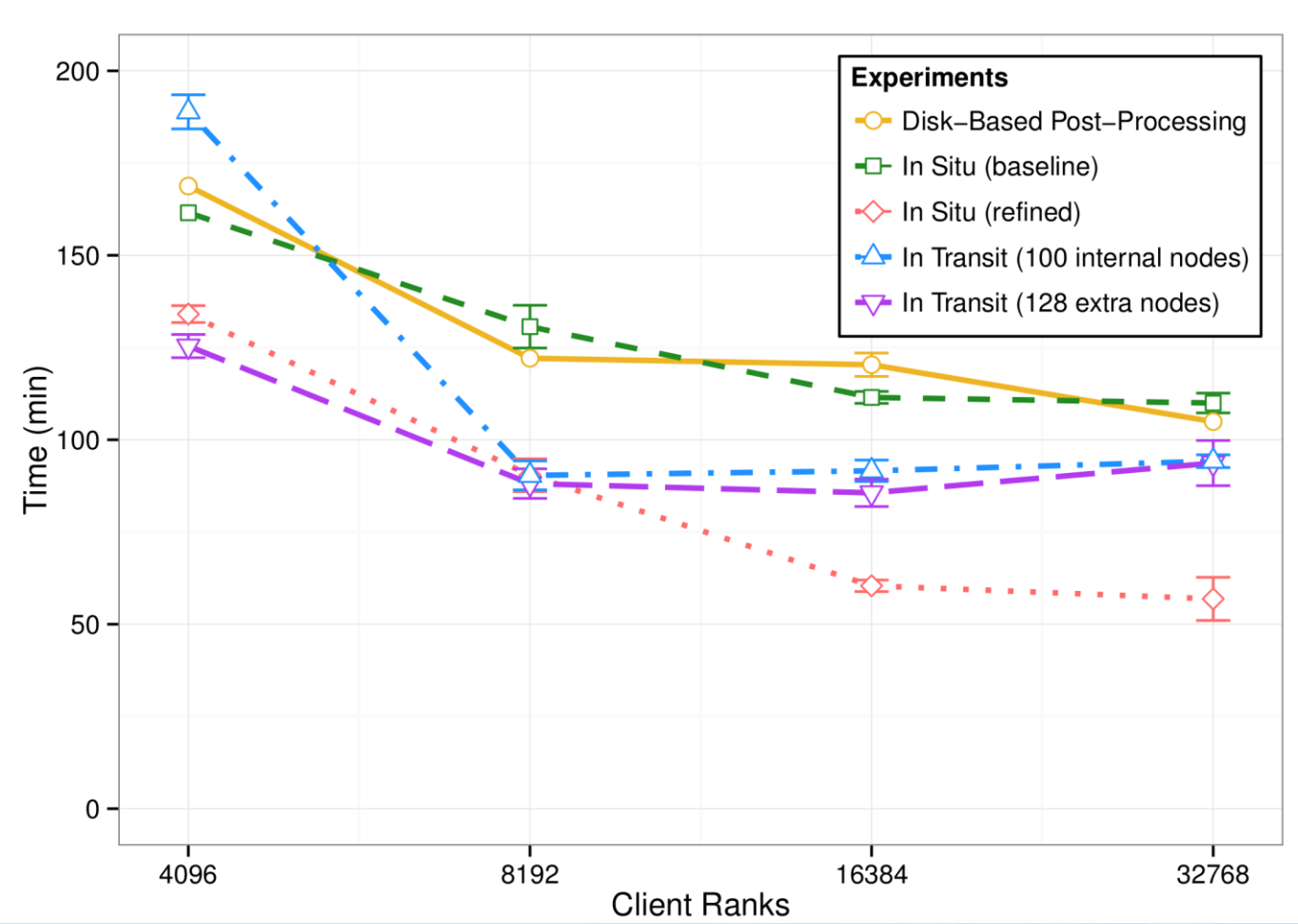




MPAS-O (LANL) simulation

Kitware

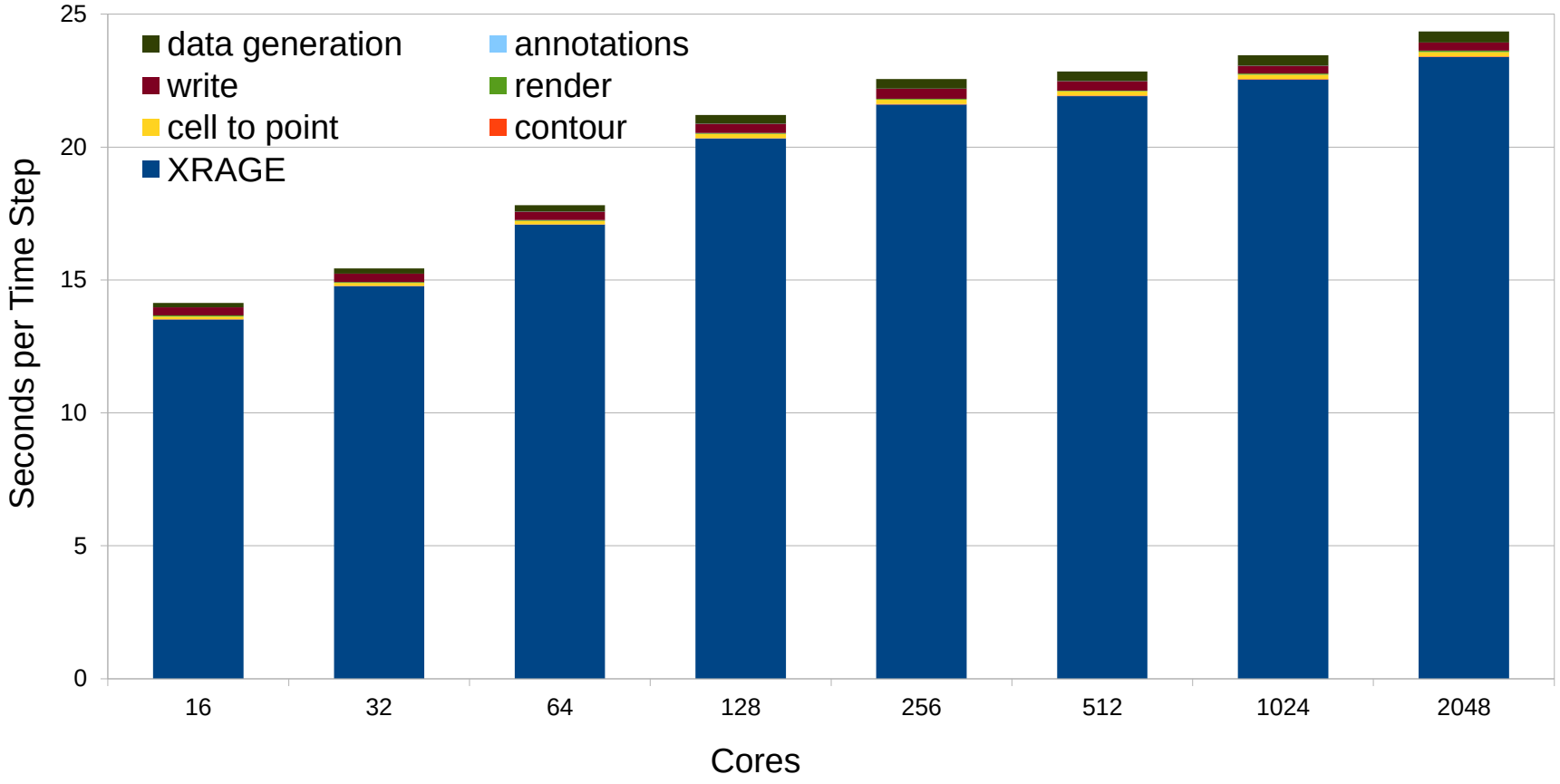
Faster Time to Solution



CTH (Sandia) simulations comparing different workflows

Kitware

Small Run-Time Overhead



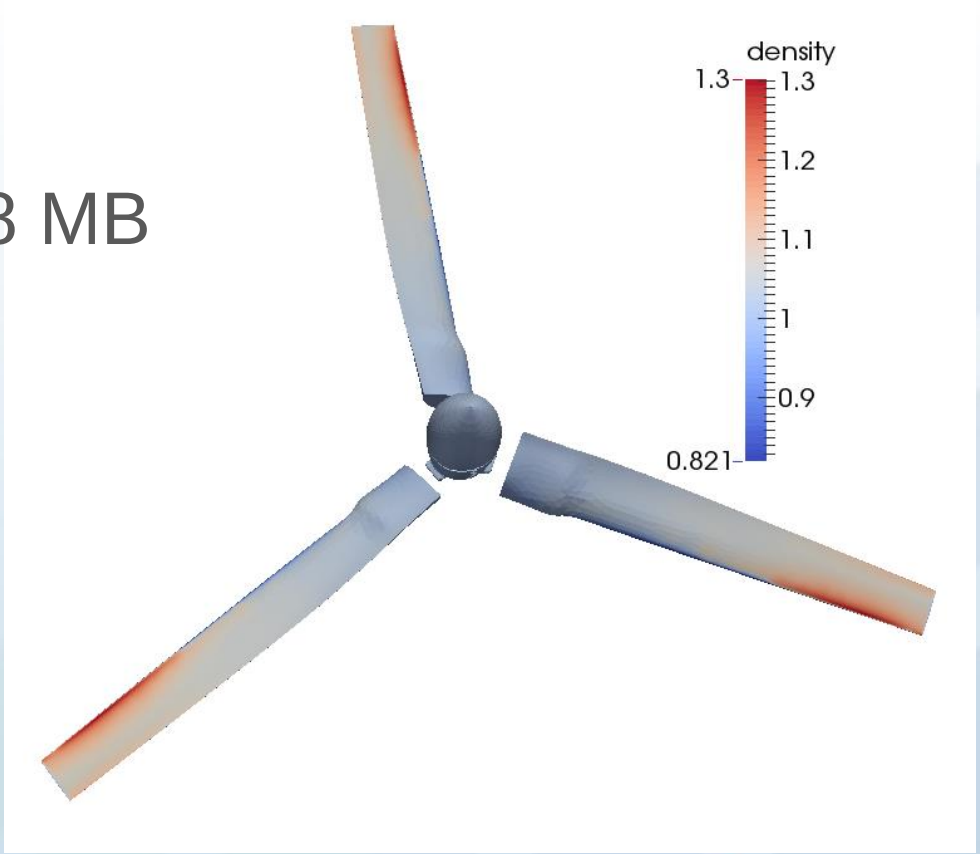
XRAGE (LANL) simulation

Kitware

Reduced File Size

Rotorcraft simulation output size for a single time step

- Full data set – 448 MB
- Surface of blades – 2.8 MB
- Image – 71 KB



Helios (Army AFDD/AMRDEC) simulation

Kitware

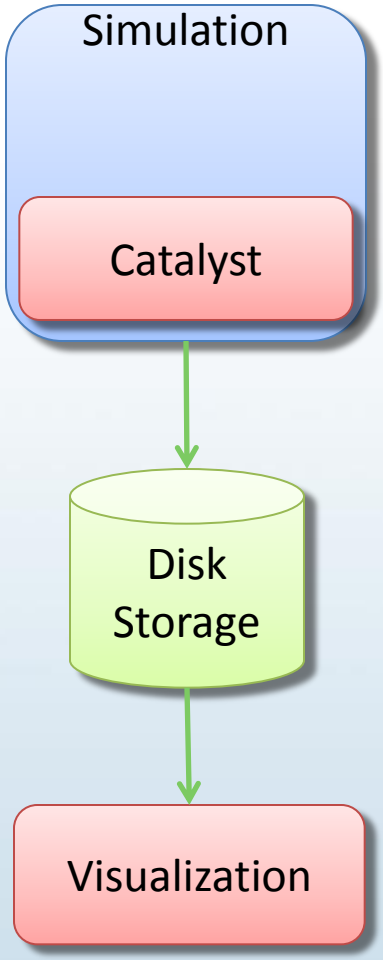
Reduced File IO Costs

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

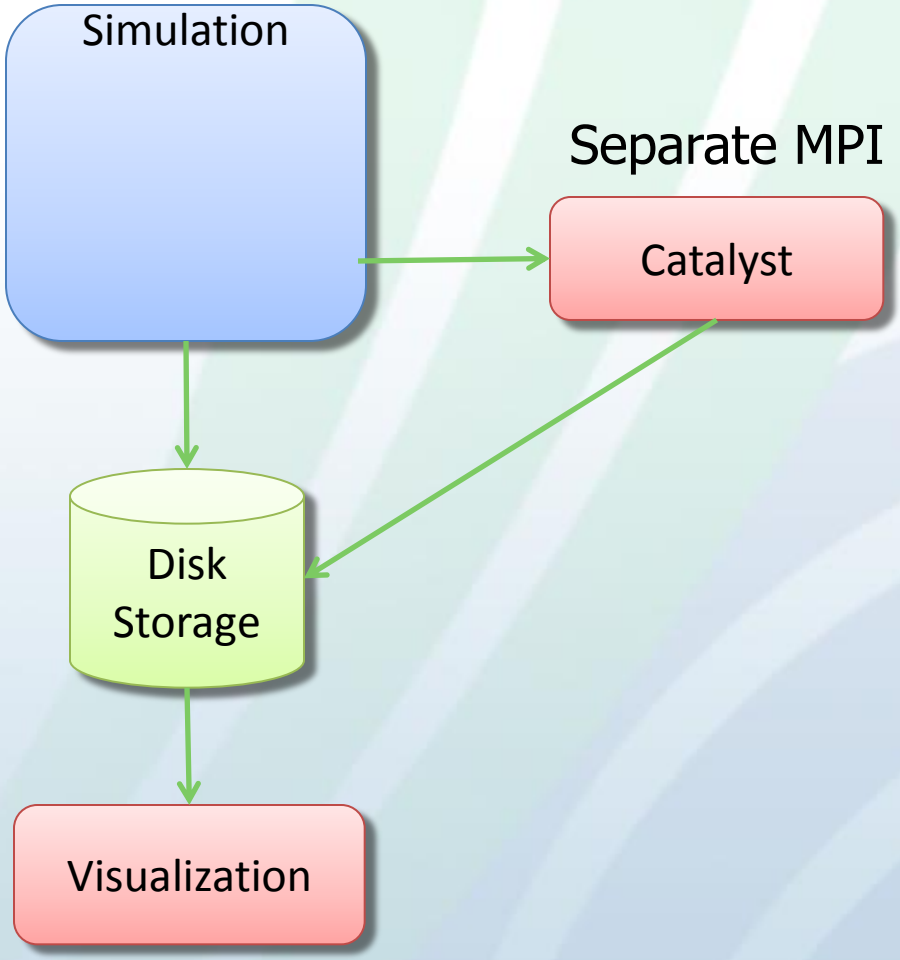
XRAGE (LANL) simulation

Kitware

Two Ways to Run in Batch



In Situ

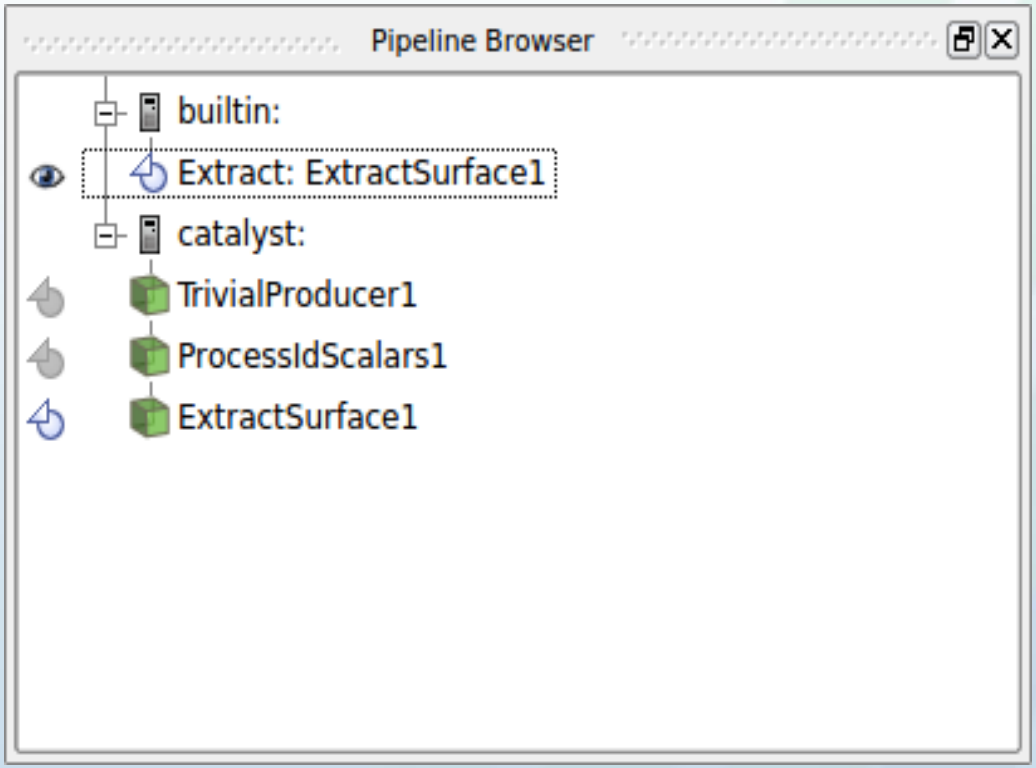


In Transit

Kitware

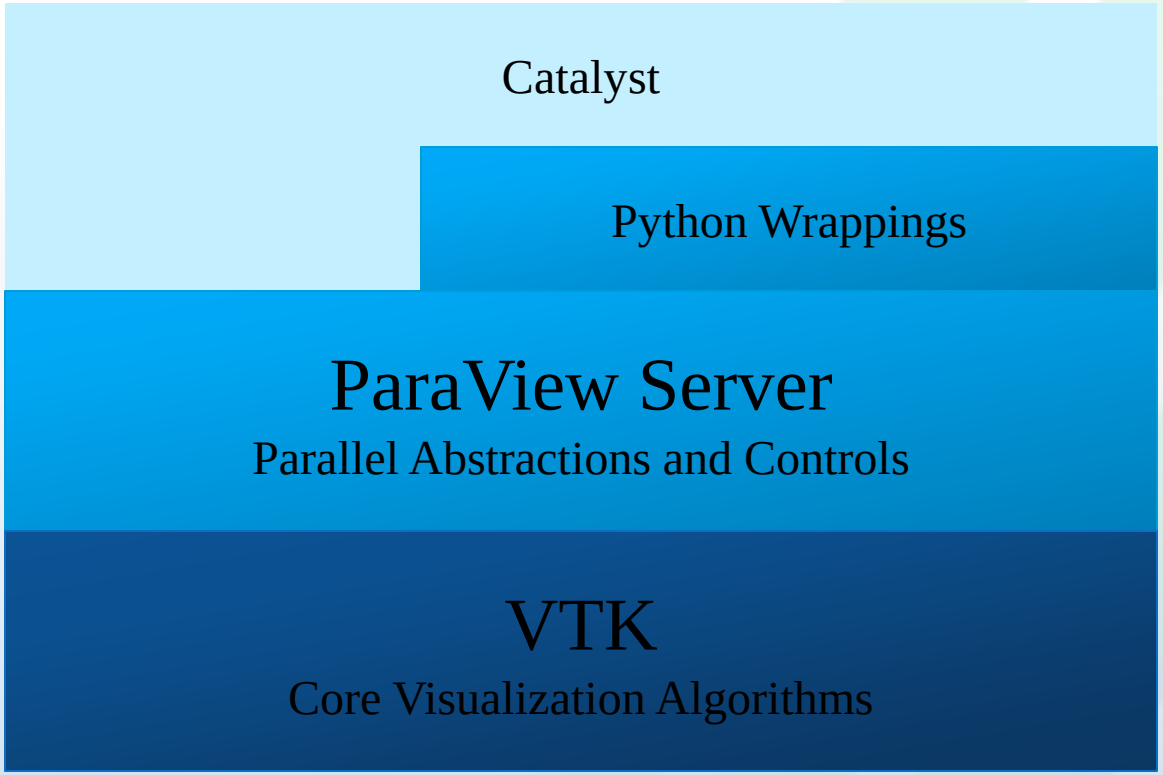
Run Interactively

- Interactive to see current results from simulation
- Access to pipeline on Catalyst server and client



Kitware

Catalyst Architecture



High Level View

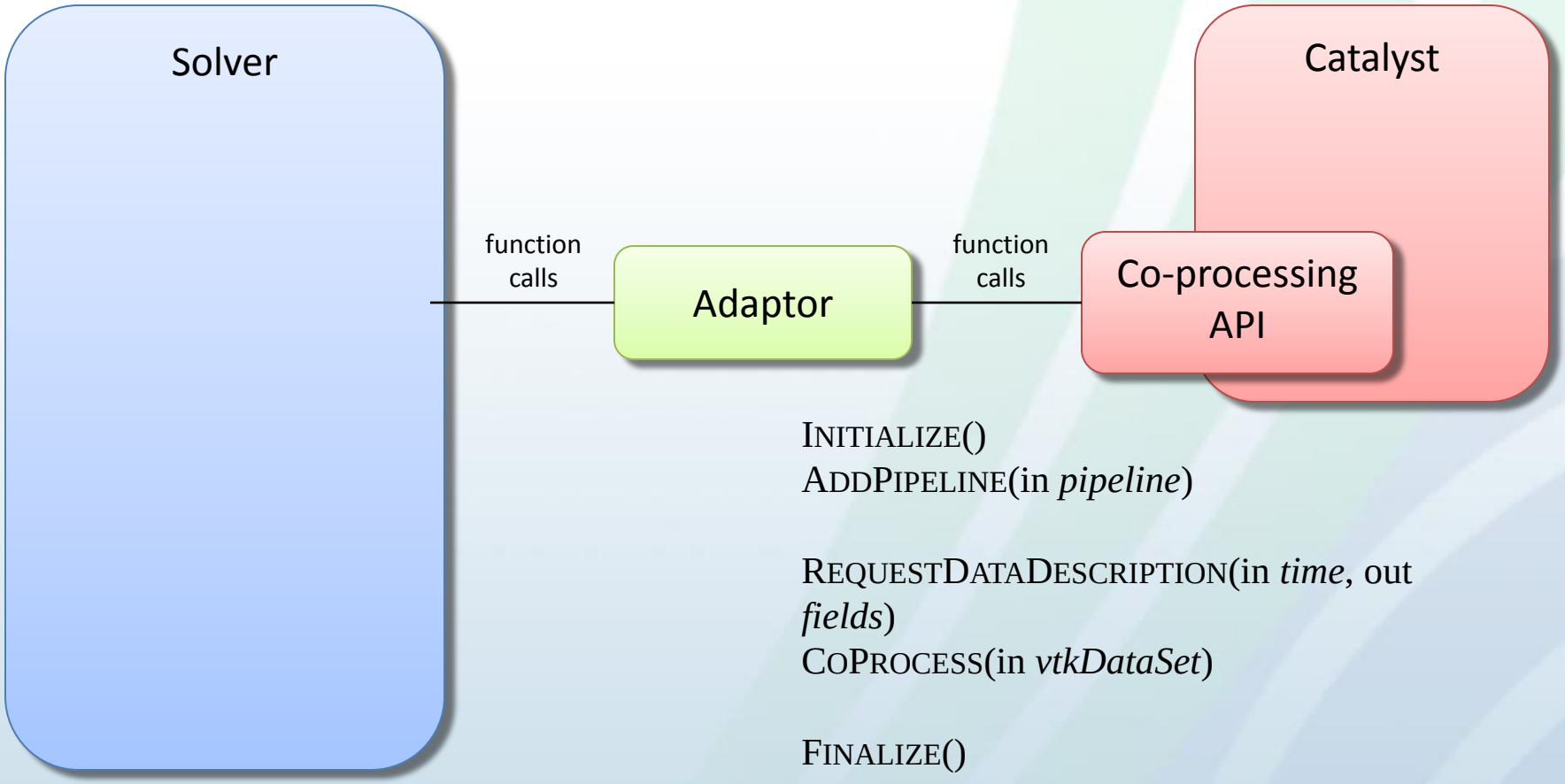
Simulation Developers

- Pass necessary simulation data to ParaView
- Need sufficient knowledge of both codes
  - VTK for grids and field data
  - ParaView Catalyst libraries
- Transparent to simulation users
- Extensible

Simulation Users

- Knowledge of ParaView as a post-processing/analysis tool
  - Basic interaction with GUI co-processing script generator plugin
  - Incremental knowledge increase to use the co-processing tools from basic ParaView use
- Programming knowledge can be useful to extend the tools

Developer Perspective



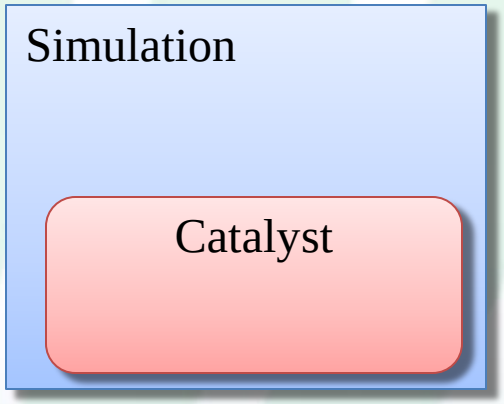
INITIALIZE()
ADDPIPELINE(in *pipeline*)

REQUESTDATADESCRIPTION(in *time*, out *fields*)
COPROCESS(in *vtkDataSet*)

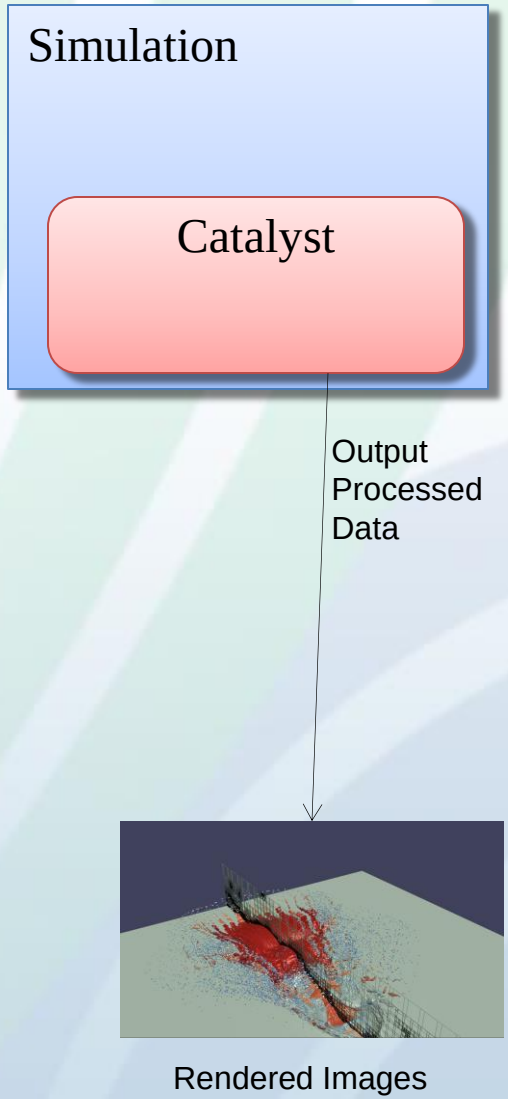
FINALIZE()

Kitware

User Perspective

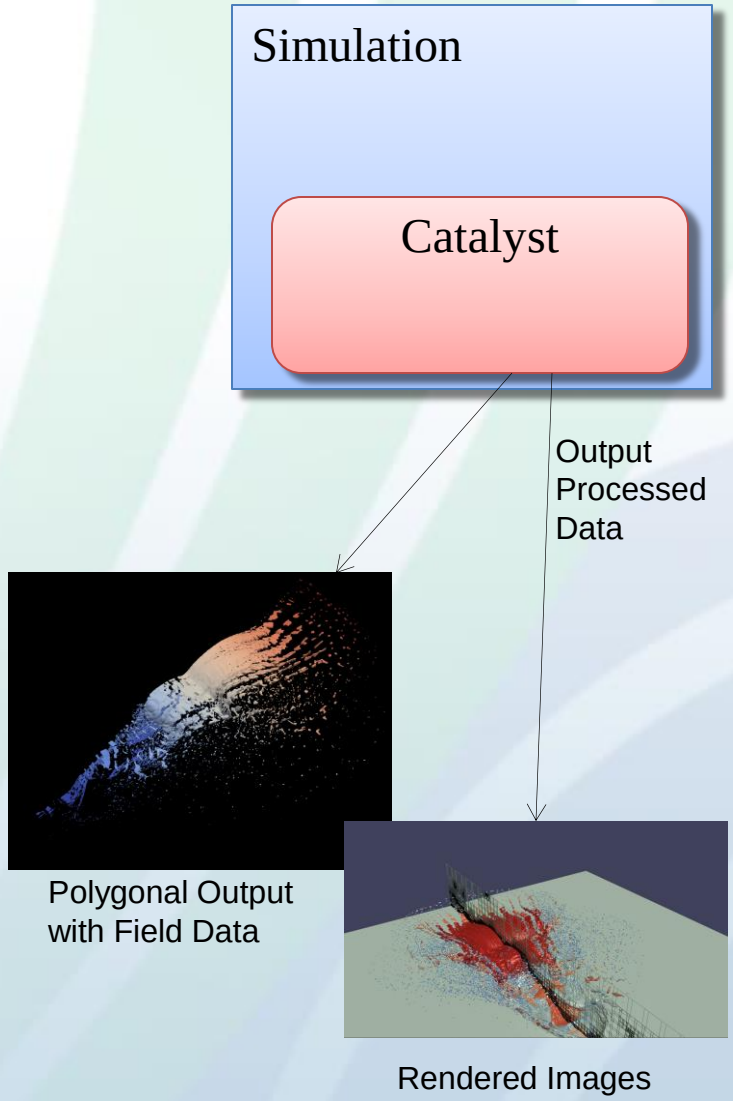


User Perspective



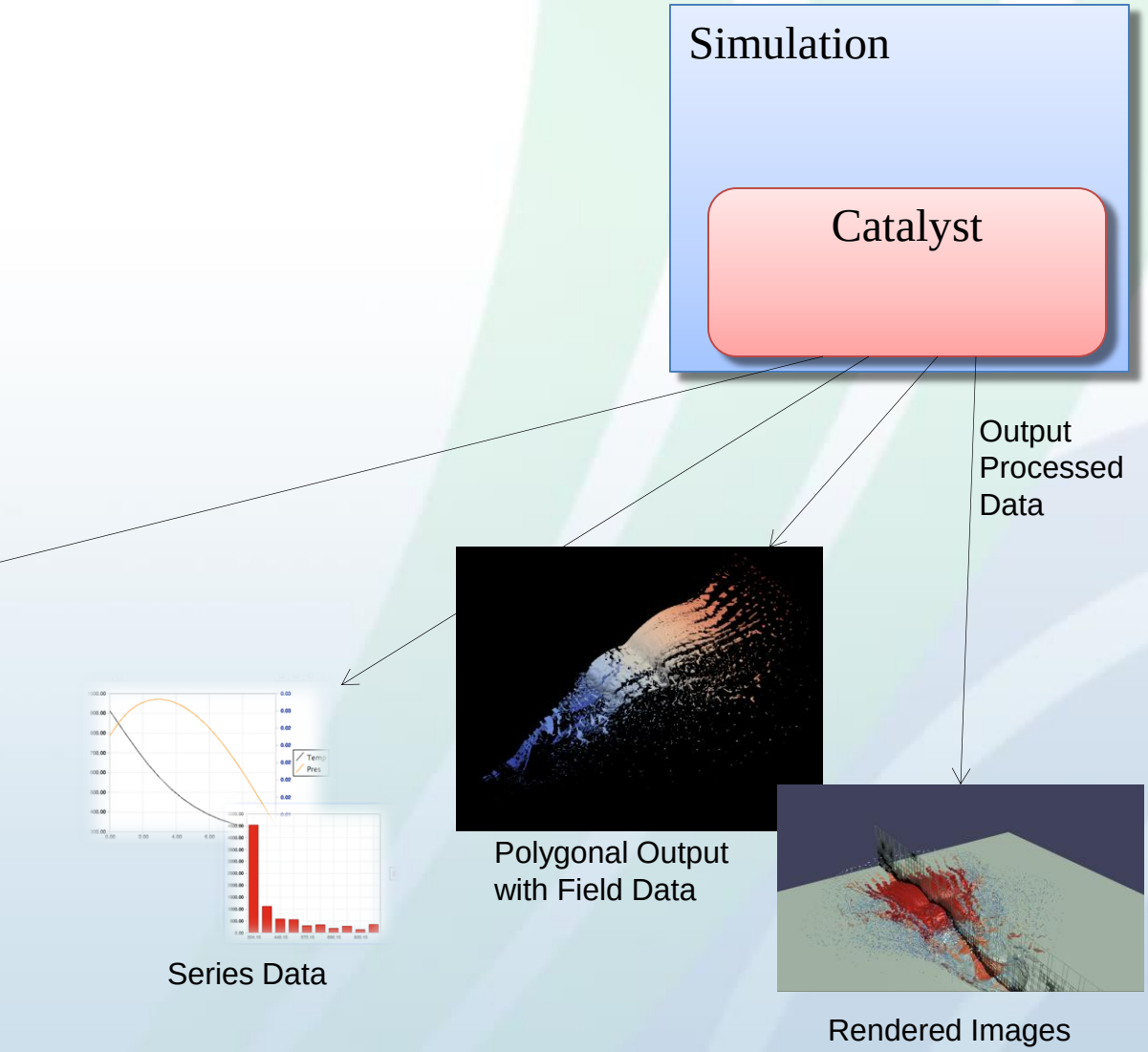
Kitware

User Perspective



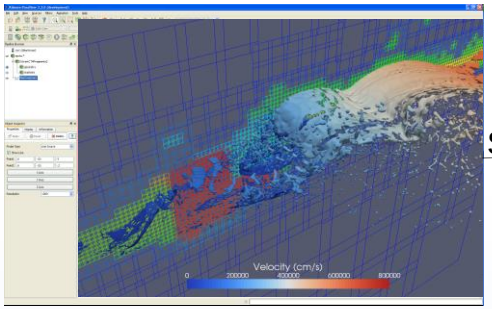
Kitware

User Perspective



Kitware

User Perspective



Script Export

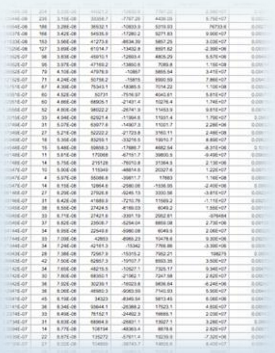
```
# Create the reader and set the filename.
reader = servermanager.sources.Reader(FileNames=path)
view = servermanager.CreateRenderView()
repr = servermanager.CreateRepresentation(reader, view)
reader.UpdatePipeline()
dataInfo = reader.GetDataInformation()
pDinfo = dataInfo.GetPointDataInformation()
arrayInfo = pDInfo.GetArrayInformation("displacement9")
if arrayInfo:
  # get the range for the magnitude of displacement9
  range = arrayInfo.GetComponentRange(-1)
  lut = servermanager.rendering.PVLookupTable()
  lut.RGBPoints  = [range[0], 0.0, 0.0, 1.0,
                    range[1], 1.0, 0.0, 0.0]
  lut.VectorMode = "Magnitude"
  repr.LookupTable = lut
  repr.ColorArrayName = "displacement9"
  repr.ColorAttributeType = "POINT_DATA"
```

Augmented script in input deck.

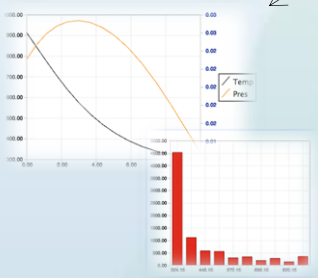
Simulation

Catalyst

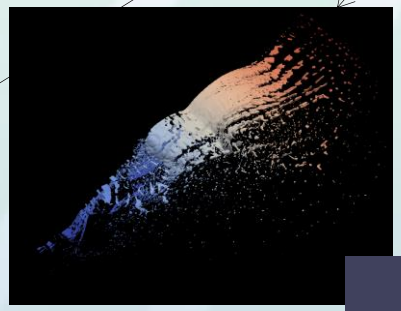
Output Processed Data



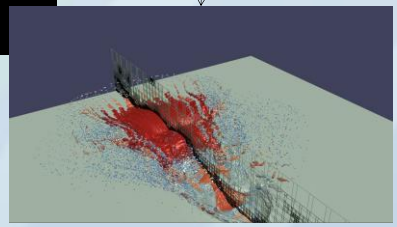
Statistics



Series Data



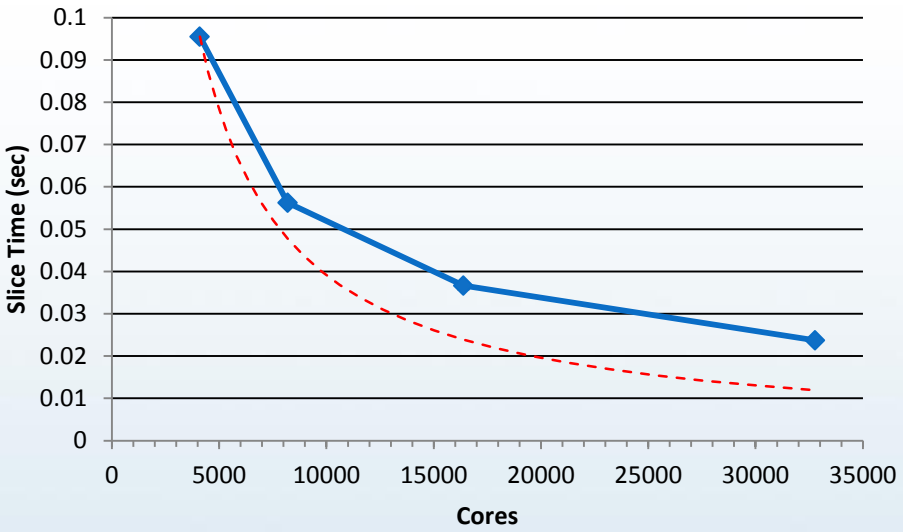
Polygonal Output with Field Data

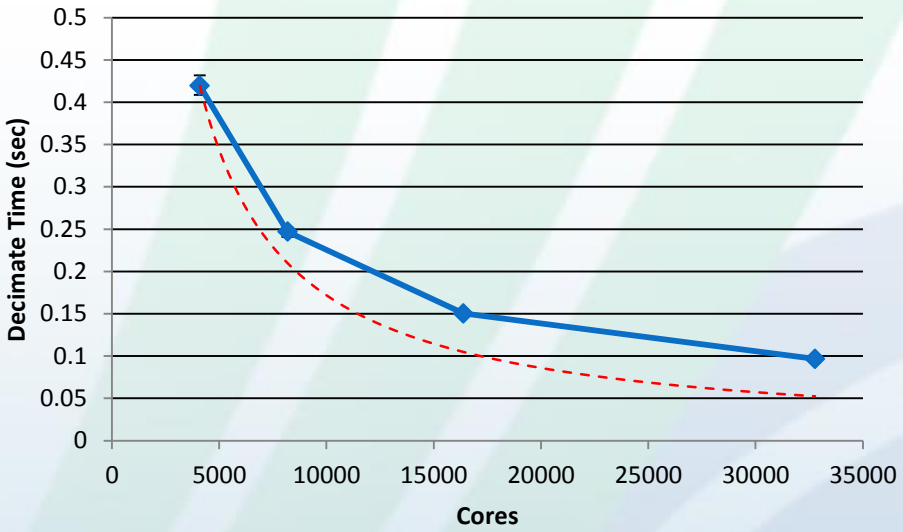


Rendered Images

Kitware

User & Developer Perspective





Kitware

Kitware

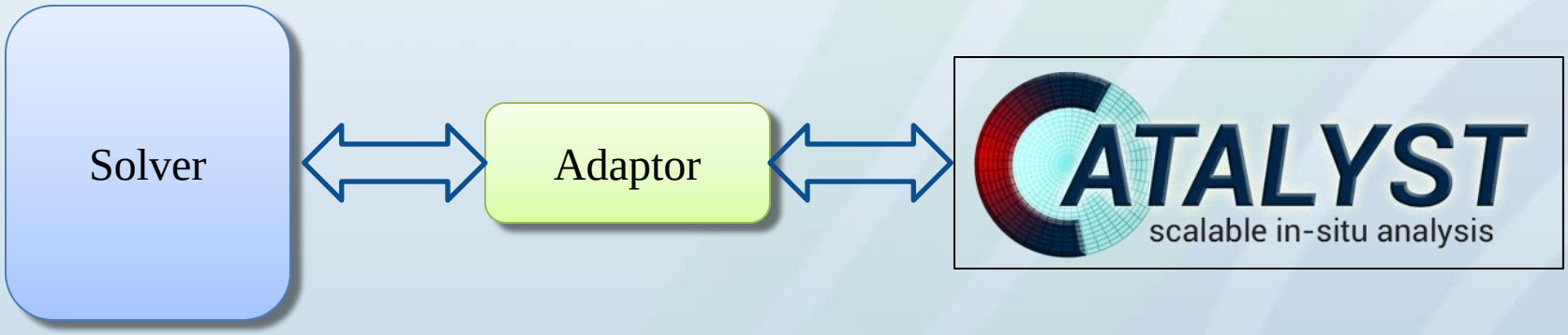
ParaView Catalyst for Simulation Developers

Developers Section Overview

- Most work is done in creating the adaptor between the simulation code and Catalyst
- Small footprint in main simulation code base
- Needs to be efficient both in memory and computationally
- Will work with examples based on miniFE-2.0 from set of Mantevo's mini-apps (mantevo.org)
  - Steady-state Poisson equation solver – instead of time stepping we'll examine CG iterative convergence of the field
  - Uses a Cartesian grid with nodal partitioning of the point data field

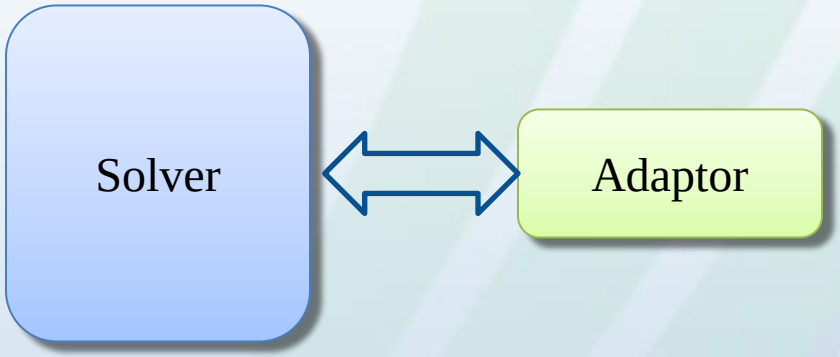
Interaction Overview

- Simulation has separate data structures from VTK data structures
- User an adaptor to bridge the gap
  - Try to reuse existing memory
  - Also responsible for other interactions between simulation code and Catalyst



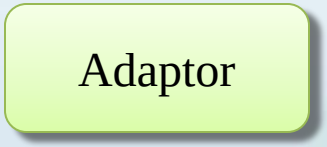
Interaction Overview

- Functional interface – typically 3 calls between simulation code and adaptor
  - Initialize
  - CoProcess
  - Finalize



Adaptor Overview

- Creates VTK data objects representing simulation data
- Creates Catalyst pipelines
  - Information on how to process VTK data objects to get desired output



Finalize Overview

- Last chance to do something
- Clean up any allocated memory

Information Needed By Adaptor During Initialization

- What pipelines to use?
  - Canned pipelines – pre-built pipelines that take in a few parameters (e.g. slice output with output file name, frequency and slice normal and origin)
  - Python pipelines – generated in the ParaView GUI and potentially edited
- Optionally
  - Information to construct grids and fields

Information Needed By Adaptor During CoProcess

- Time, time step
- Optionally
  - Information to construct grids and fields if not passed in during initialization step
  - Force all pipelines to execute (simulation may know something important has happened)
  - Other information to add in extra logic to pipelines

VTK Preliminaries

- Many objects in VTK are reused so we use reference counting to keep track of how many other objects are keeping track of them
  - New() – creates a new object in dynamic memory and sets reference count to 1
  - Delete() – reduces reference count by 1 and if reference count goes to 0 then object gets deleted
  - a->Set*(b), a->Add*(b) – b's reference count gets increased by 1

```
vtkDoubleArray* a = vtkDoubleArray::New(); // a's ref count = 1
vtkPointData* pd = vtkPointData::New() ; // pd's ref count = 1
pd->AddArray(a); // a's ref count = 2
a->Delete(); // a's ref count = 1
a->SetName("an array"); // valid as a hasn't been deleted
pd->Delete(); // deletes both pd and a
```

Helpful VTK Objects

- vtkSmartPointer<vtkObject*>
  - Deals with creating and deleting vtkObjects
  - Increases reference count when set
  - Reduces reference count when it gets deleted

```
vtkPointData* pd = vtkPointData::New() ; // pd's ref count = 1
{
  vtkSmartPointer<vtkDoubleArray> a =
    vtkSmartPointer<vtkDoubleArray>::New();
  pd->AddArray(a);
}
// a no longer exists but the generated vtkDoubleArray does
vtkSmartPointer<vtkPointData> pd2 = pd; // pd's ref count = 2
```

http://www.vtk.org/doc/nightly/html/classvtkSmartPointer.html

Helpful VTK Objects (2)

- vtkNew<vtkObject*>
  - Deals with creating and deleting vtkObjects
  - Increases reference count when set
  - Reduces reference count when it gets deleted

```
vtkPointData* pd = vtkPointData::New() ; // pd's ref count = 1
{
  vtkSmartPointer<vtkDoubleArray> a =
    vtkSmartPointer<vtkDoubleArray>::New();
  pd->AddArray(a);
}
// a no longer exists but the generated vtkDoubleArray does
```

http://www.vtk.org/doc/nightly/html/classvtkNew.html

Writing the Initialization Method

- Assuming we will pass in data to create VTK grid and field data objects during CoProcess call
- ParaView classes to look at:
  - vtkCPProcessor – main manager object
  - vtkCPPipeline/vtkCPPythonScriptPipeline – object to control Catalyst pipeline (typically one object per pipeline)

http://www.paraview.org/ParaView3/Doc/Nightly/html/classvtkCPProcessor.html

http://www.paraview.org/ParaView3/Doc/Nightly/html/classvtkCPPythonScriptPipeline.html

vtkCPProcessor Initialization Step

- vtkCPProcessor
  - vtkCPProcessor* New()
    - Static constructor method that sets reference count to 1
  - void Delete()
    - Reduce reference count by 1 (not necessarily delete though)
  - int Initialize()
    - Returns 1 for success and 0 for failure
  - int AddPipeline(vtkCPPipeline* pipeline)
    - Pass in a vtkCPPipeline object, vtkCPProcessor will keep reference to pipeline so it won't get deleted
    - Returns 1 for success and 0 for failure
- Will go through other important vtkCPProcessor methods later

vtkCPProcessor Initialization Step

For ParaView 4.2, can initialize Catalyst with a separate MPI communicator

- Use “int Initialize(vtkMPICommunicatorOpaqueComm*)” instead of “int Initialize()”
- vtkMPICommunicatorOpaqueComm defined in vtkMPI.h
- Use constructor vtkMPICommunicatorOpaqueComm(MPI_Comm*)

vtkCPPipeline Initialization Step

- vtkCPPipeline
  - Abstract class – methods are usually only called by vtkCPProcessor
- vtkCPPythonScriptPipeline
  - vtkCPPythonScriptPipeline* New()
    - Static constructor method that sets reference count to 1
  - int Initialize(const char *fileName)
    - fileName is the Python script pipeline which can include a relative or absolute path
    - Returns 1 for success and 0 for failure

vtkCPProcessor Finalize Step

- vtkCPProcessor
  - int Finalize()
  - Delete the vtkCPProcessor object
- If ParaView was built with DEBUG_LEAKS_ON, will get messages that VTK objects were not deleted before exiting.
  - Most likely from not deleting vtkCPProcessor, vtkCPipeline or VTK objects created in the adaptor.

Configuring with CMake

- Configuring the build is simplified by using CMake
  - Determines dependencies automatically for compiling (location of header files) and linking (location of libraries)
- Typically use ccmake for terminal-based interface
  - Often building on a remote machine
  - Command: ccmake <path to source dir> <preset configuration options>
- Create build directory at <miniFE-2.0_ref>/adaptor_build

Example 1 – Write It!

- Assume all Python scripts for pipeline specifications
- Starting file:
  - <miniFE-2.0_ref>/adaptor/catalyst_adapter.cpp
  - Function signatures:
    - int initialize(miniFE::Parameters& params)
      - Python script names in params.script_names which is type std::vector<std::string>
      - Processor in anonymous namespace
    - int Finalize()
- CMake configuration step in adapter_build:
  - ccmake ../adapter -DParaView_DIR:PATH=<location of ParaView build>

Kitware

Example 1 – A Solution

```
void initialize(miniFE::Parameters& params)
{
   Processor = vtkCPProcessor::New();
   Processor->Initialize();
   for(std::vector<std::string>::const iterator
      it=params.script_names.begin();
      it!=params.script_names.end();it++) {
     vtkCPPythonScriptPipeline* pipeline =
      vtkCPPythonScriptPipeline::New();
     pipeline->Initialize(it->c_str());
     Processor->AddPipeline(pipeline);
     pipeline->Delete();
     }
  }
```

```
void finalize()
  {
    if(Processor)
      Processor->Finalize();
      Processor->Delete();
      Processor = NULL;
      }
  }
```

Kitware

Writing the CoProcess Method

- Assuming we will pass in data to create VTK grid and field data objects during CoProcess call
- ParaView classes to look at:
  - vtkCPProcessor – main manager object
  - vtkCPDataDescription

http://www.paraview.org/ParaView3/Doc/Nightly/html/classvtkCPDataDescription.html

Writing the CoProcess Method

Main stage with 2 stages

- First stage
  - Check with Catalyst pipelines to see if there is anything to do
  - Should check after every time step
  - Should be very fast
- Second stage
  - Only done if at least one Catalyst pipeline wants to do something this time step
  - Construct needed input (i.e. VTK grids and fields)
  - Execute the pipelines that need to do something

Writing the CoProcess Method: First Stage

- ParaView classes to look at:
  - vtkCPProcessor – main manager object
  - vtkCPDataDescription – meta-description of what simulation is able to provide

vtkCPProcessor CoProcess Step: First Stage

- vtkCPProcessor
  - int RequestDataDescription(vtkCPDataDescription*)
    - Have the processor check if any Catalyst pipelines need to execute this time step
    - Returns 1 for success and 0 for failure
- vtkCPDataDescription
  - void AddInput(const char* name)
    - Specify source of pipelines
    - Convention for single input is name="input"
  - void SetTimeData(double time, vtkIdType timeStep)
    - Set the current simulation time and time step
  - void ForceOutputOn()/SetForceOutput() – optional
    - Specify that all Catalyst pipelines should execute

Example 2 – Write It!

- Function signature:
  - void coprocess(const double spacing[3], const Box& global_box, const Box& local_box, std::vector<double>& minifepointdata, int time_step, double time, bool force_output);
- Starting file:
  - <miniFE-2.0_ref>/adaptor/catalyst_adapter.cpp
  - Only need to use time_step, time and force_output for this part

Example 2 – A Solution

```
void coprocess(const double spacing[3], const Box& global_box,
  const Box& local_box, std::vector<double>& minifepointdata,
  int time_step, double time, bool force_output)
{
  vtkSmartPointer<vtkCPDataDescription> dataDescription =
      vtkSmartPointer<vtkCPDataDescription>::New();
  dataDescription->AddInput("input");
    dataDescription->SetTimeData(time, time_step);
  dataDescription->SetForceOutput(force_output);
  if(Processor->RequestDataDescription(dataDescription) == 0)
    {
     return;
     }
…
```

Writing the CoProcess Method: Second Stage

- ParaView classes to look at:
  - vtkCPProcessor – main manager object
  - vtkCPDataDescription – meta-description of what simulation is able to provide
  - vtkCPInputDataDescription – Catalyst description of what it needs in order to execute a pipeline

http://www.paraview.org/ParaView3/Doc/Nightly/html/classvtkCPInputDataDescription.html

vtkCPProcessor CoProcess Step: Stage Two

- vtkCPProcessor
  - int CoProcess(vtkCPDataDescription*)
    - Have the coprocessor execute the desired Catalyst pipelines
    - Returns 1 for success and 0 for failure
- vtkCPDataDescription
  - vtkCPInputDataDescription* GetInputDescriptionByName(const char* name)
    - Given an input name (“input”), get the input description object to determine what is needed
- vtkCPInputDataDescription
  - void SetGrid(vtkDataObject*)
    - Set the VTK data source object for a Catalyst pipeline

Example 3 – Write It!

- Still using function signature:
  - void coprocess(const double spacing[3], const Box& global_box, const Box& local_box, std::vector<double>& minifepointdata, int time_step, double time, bool force_output);
  - Create a vtkImageData object that we'll set up later

Example 3 – A Solution

```
void coprocess(const double spacing[3], const Box& global_box,
  const Box& local_box, std::vector<double>& minifepointdata,
  int time_step, double time, bool force_output)
{
  vtkSmartPointer<vtkCPDataDescription> dataDescription =
      vtkSmartPointer<vtkCPDataDescription>::New();
  dataDescription->AddInput("input");
    dataDescription->SetTimeData(time, time_step);
  dataDescription->SetForceOutput(force_output);
  if(Processor->RequestDataDescription(dataDescription) == 0)
    {
     return;
     }
  vtkNew<vtkImageData> grid;
  dataDescription->GetInputDescriptionByName("input")->SetGrid(grid.GetPointer());
…
```

Writing the CoProcess Method: Second Stage

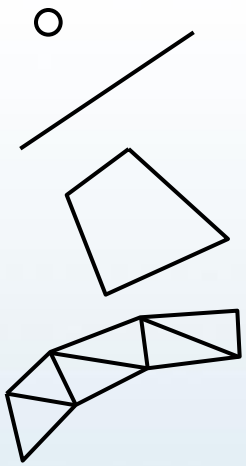
- VTK classes to look at:
  - Depends on simulation's grid type
  - Classes that derive from:
    - vtkDataObject for grids
    - vtkAbstractArray for fields
    - vtkFieldData for managing vtkAbstractArrays
  - Other useful classes:
    - vtkCellType – types of cells for unstructured grids (vtkPolyData and vtkUnstructuredGrid)
- Can look at readers or sources that provide the same type of VTK data object

Getting Data Into Catalyst

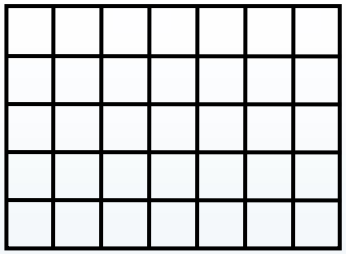
- Main object will derive from vtkDataObject
  - Grids that derive from vtkDataSet
  - Multiblock grids that contain multiple vtkDataSets
- Field (aka attribute) information
  - Point data – information specified for each point in a grid
  - Cell data – information specified for each cell in a grid
  - Field data – meta-data not associated with either points or cells
- All object groups are 0-based/C/C++ indexing

vtkDataSet Subclasses

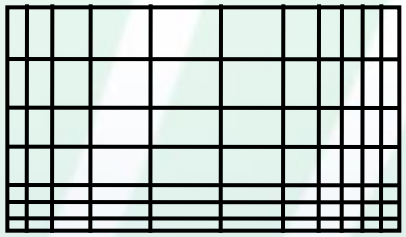
vtkPolyData



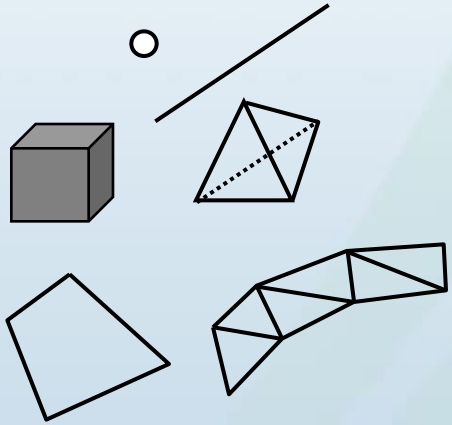
vtkImageData
vtkUniformGrid



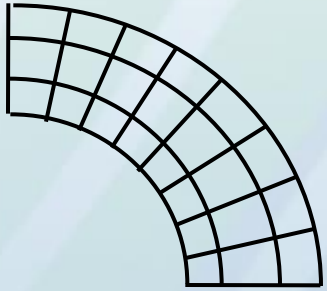
vtkRectilinearGrid



vtkUnstructuredGrid



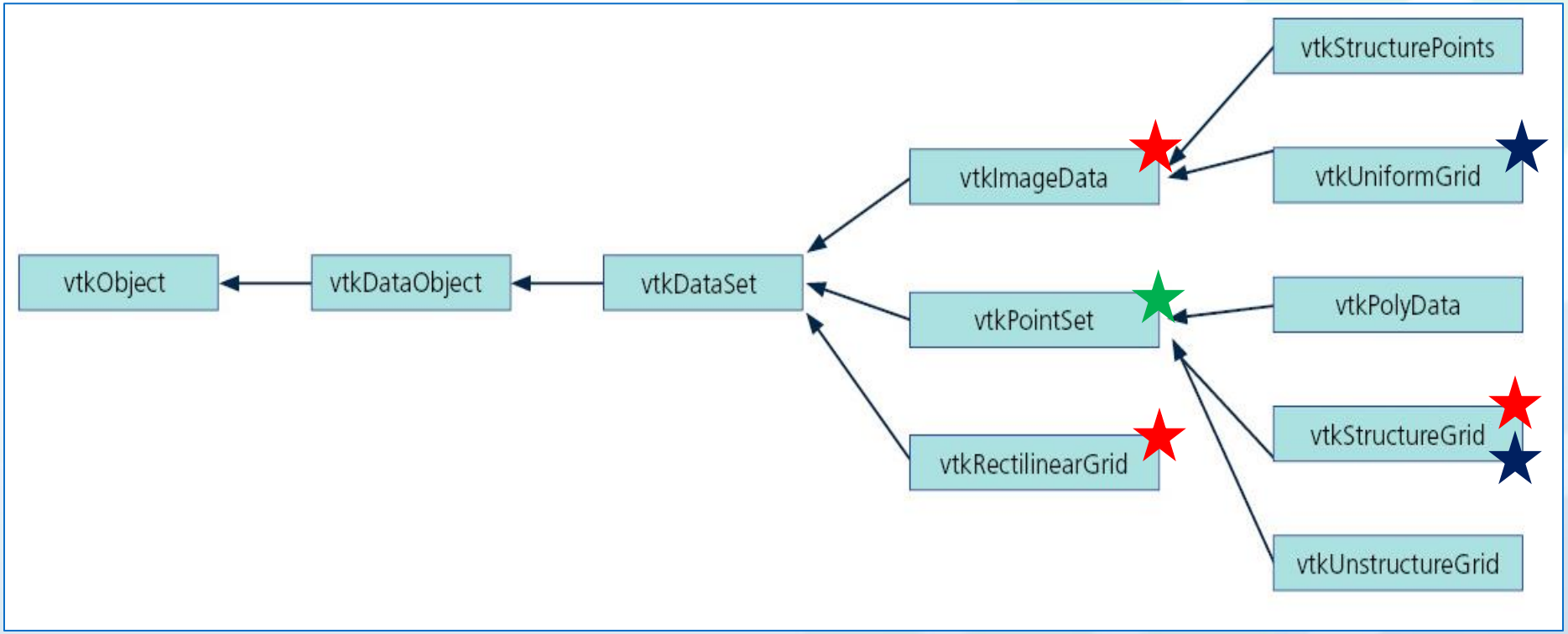
vtkStructuredGrid



http://www.vtk.org/doc/nightly/html/classvtkDataSet.html

Kitware

vtkDataSet Class Hierarchy



★ Topologically regular grid

★ Irregular geometry

★ Supports blanking

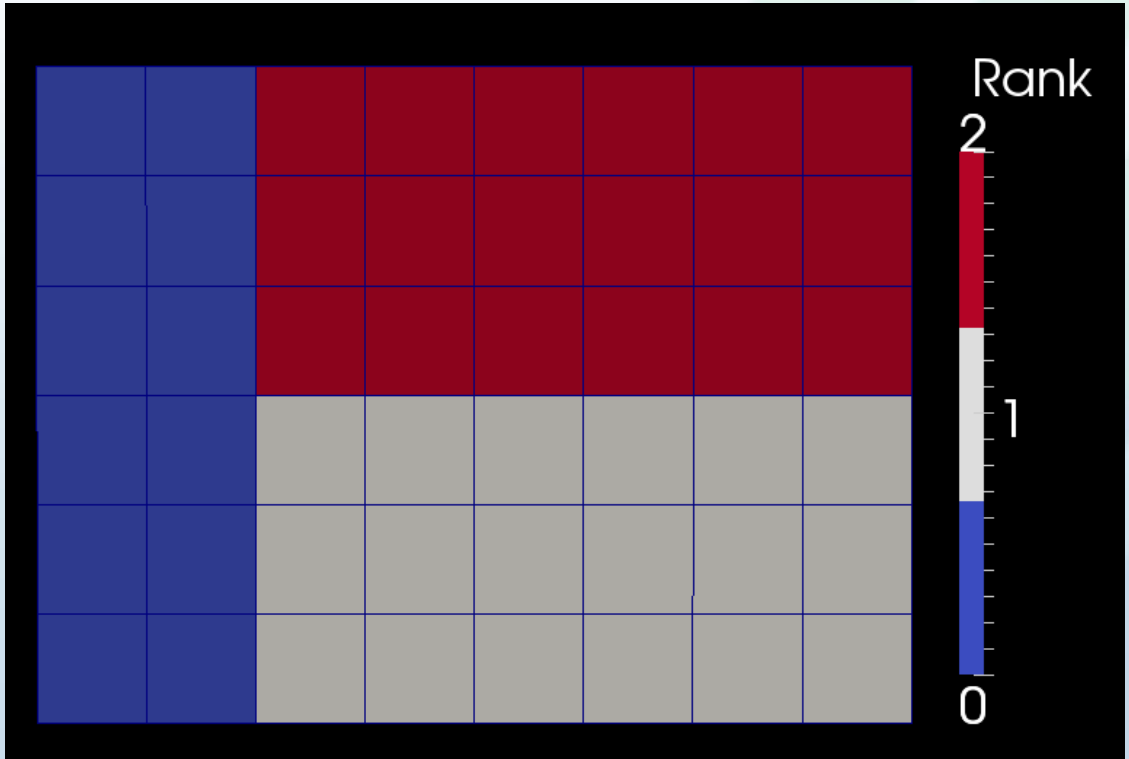
Kitware

Topologically Regular Grids

- vtkImageData/vtkUnstructuredGrid, vtkRectilinearGrid and vtkStructuredGrid
- Topological structure defined by whole extent
  - Gives first and last point in each logical direction
  - Not required to start at 0
- Partitioning defined by extents
  - First and last point in each logical direction of part of the entire grid
- Ordering of points and cells is fastest in logical x-direction, then y-direction and slowest in z-direction

Extents

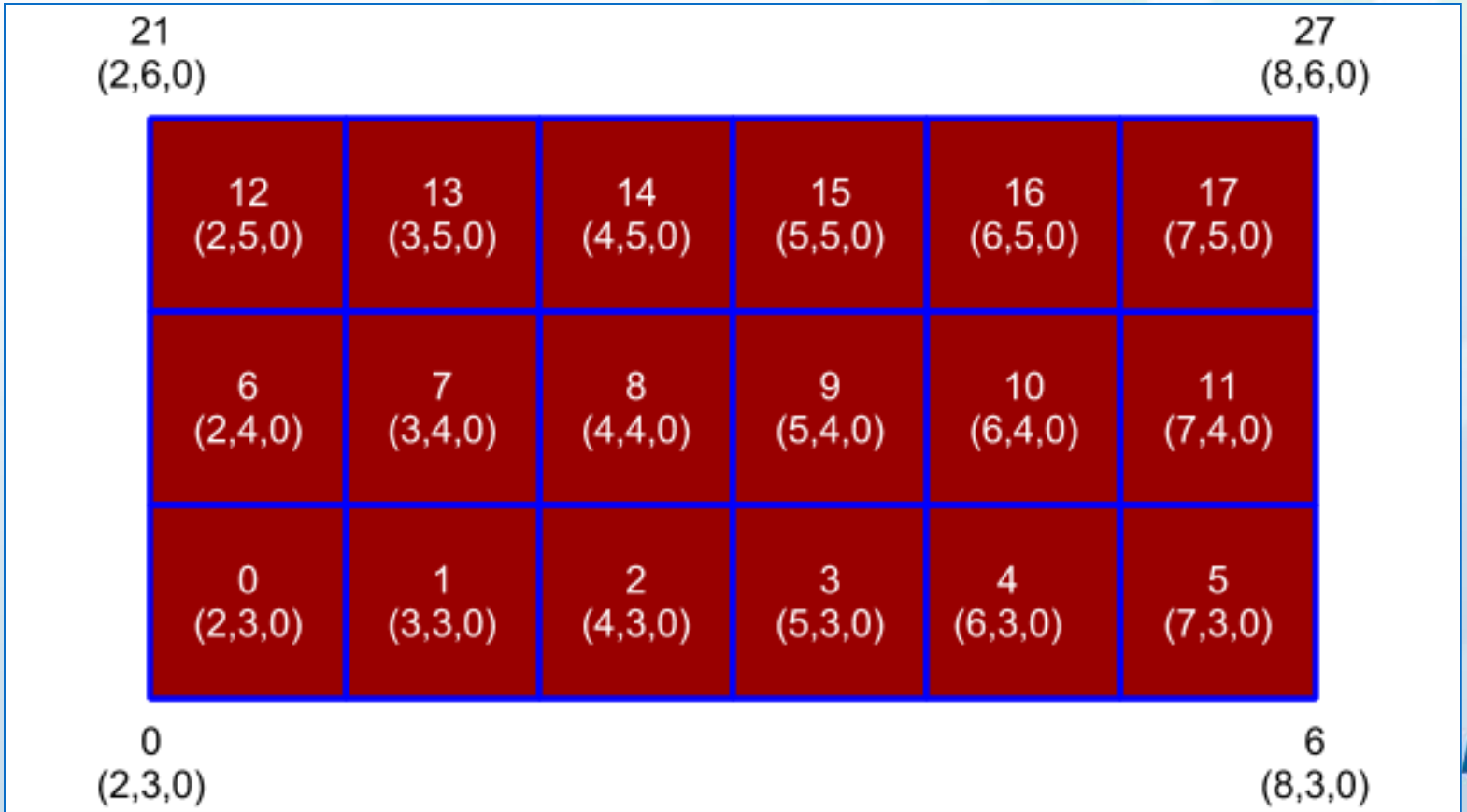
- Whole extent for all processes (0, 8, 0, 6, 0, 0)
- Extents different for each process
  - Rank 0: (0, 2, 0, 6, 0, 0), 21 points, 12 cells
  - Rank 1: (2, 8, 0, 3, 0, 0), 28 points, 18 cells
  - Rank 2: (2, 8, 3, 6, 0, 0), 28 points, 18 cells



Kitware

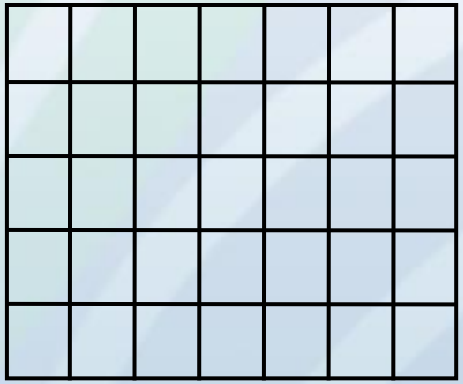
Extents

- Point and cell indices for extent of (2, 8, 3, 6, 0, 0)
  - From rank 2 in previous slide
  - 28 points and 18 cells



vtkImageData/vtkUniformGrid

- vtkCPInputDataDescription::SetWholeExtent() – total number of points in each direction
- SetExtent() – a process's part of the whole extent
- SetSpacing() – cell lengths in each direction (same for all processes)
- SetOrigin() – location of point at i=0, j=0, k=0 (same for all processes)



- vtkUniformGrid
  - Supports cell blanking
  - Currently written to file as vtkImageData

http://www.vtk.org/doc/nightly/html/classvtkUniformGrid.html

Example 4 – Write It!

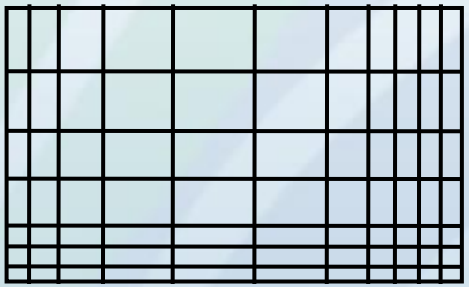
- Still using function signature:
  - void coprocess(const double spacing[3], const Box& global_box, const Box& local_box, std::vector<double>& minifepointdata, int time_step, double time, bool force_output);
  - Local extent is contained in local_box:
    - Points range from local_box[0][0] to local_box[0][1] in X-direction, local_box[1][0] to local_box[1][1] in Y-direction, local_box[2][0] to local_box[2][1] in Z-direction
  - Global extent is contained in global_box:
    - Points range from global_box[0][0] to global_box[0][1] in X-direction, global_box[1][0] to global_box[1][1] in Y-direction, global_box[2][0] to global_box[2][1] in Z-direction

Example 4 – A Solution

```
…
  vtkNew<vtkImageData> grid;
  int extent[6] = {local_box[0][0], local_box[0][1], local_box[1][0],
                   local_box[1][1], local_box[2][0], local_box[2][1]};
  grid->SetExtent(extent);
  grid->SetSpacing(spacing[0], spacing[1], spacing[2]);
  grid->SetOrigin(0, 0, 0);
  dataDescription->GetInputDescriptionByName("input")->SetGrid(grid.GetPointer());
  int wholeExtent[6] = {global_box[0][0], global_box[0][1], global_box[1][0],
                        global_box[1][1], global_box[2][0], global_box[2][1]};
  dataDescription->GetInputDescriptionByName("input")->
     SetWholeExtent(wholeExtent);
…
```

vtkRectilinearGrid

- vtkCPInputDataDescription::SetWholeExtent() – total number of points in each direction
- SetExtents() – a process's part of the whole extent
- Set<X,Y,Z>Coordinates() – point coordinates in each direction
  - Only values for process's extents
  - Index starting at 0



http://www.vtk.org/doc/nightly/html/classvtkRectilinearGrid.html

vtkPointSet

- Abstract class for grids with arbitrary point locations
  - Derived classes: vtkStructuredGrid, vtkPolyData, vtkUnstructuredGrid
- SetPoints(vtkPoints*) – set the number and coordinates of a process's points
- vtkPoints
  - Class used to store actual point location array
  - C/C++ indexing
  - SetDataTypeTo<Int,Float,Double>()
  - SetNumberOfPoints() – allocation
  - SetPoint() – fast but doesn't do bounds checking
  - InsertPoint()/InsertNextPoint() – safe but does bounds checking and reallocation as needed

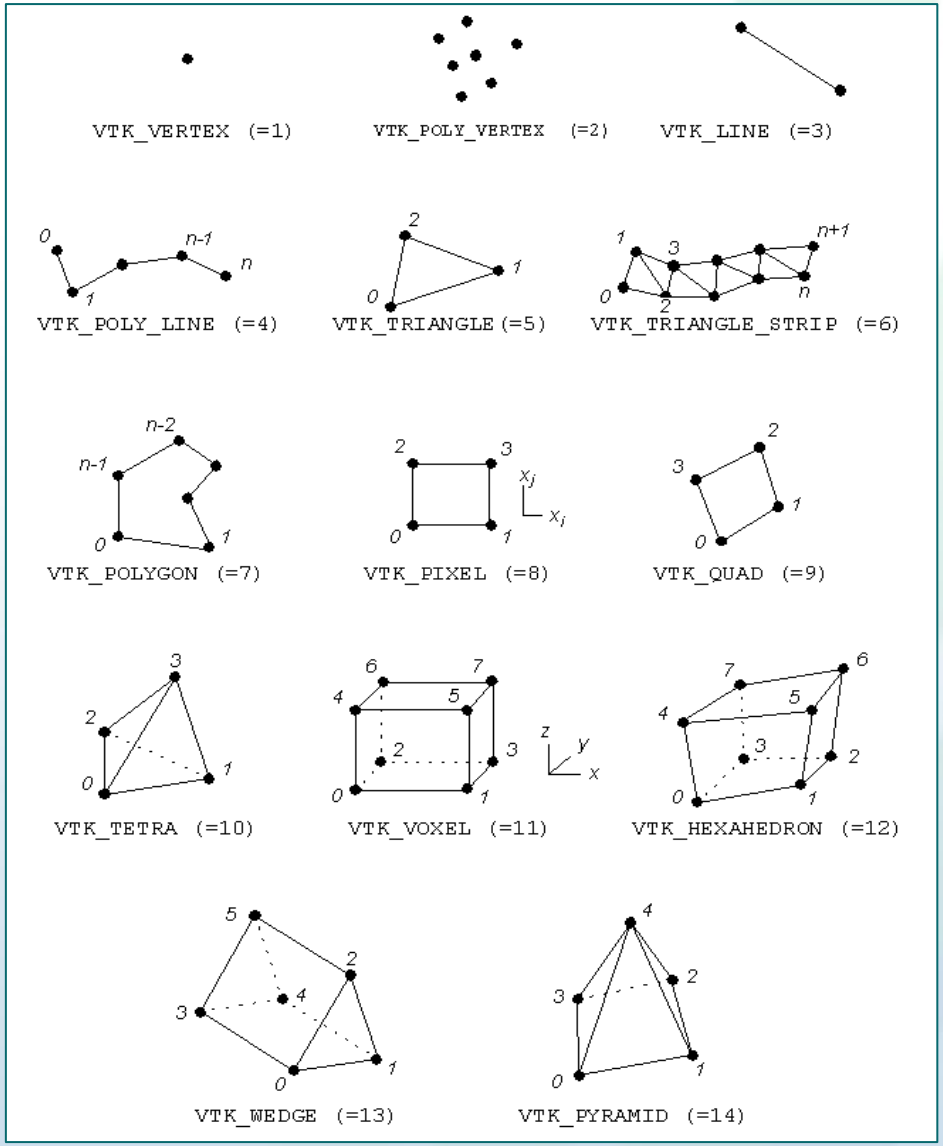
http://www.vtk.org/doc/nightly/html/classvtkPointSet.html

vtkStructuredGrid

- vtkCPInputDataDescription::SetWholeExtent() – total number of points in each direction
- SetExtents() – a process's part of the whole extent
- Ordering for points and cells
  - Fastest in x-direction
  - Next in y-direction
  - Slowest in z-direction
  - vtkPoints must be ordered in same manner

http://www.vtk.org/doc/nightly/html/classvtkStructuredGrid.html

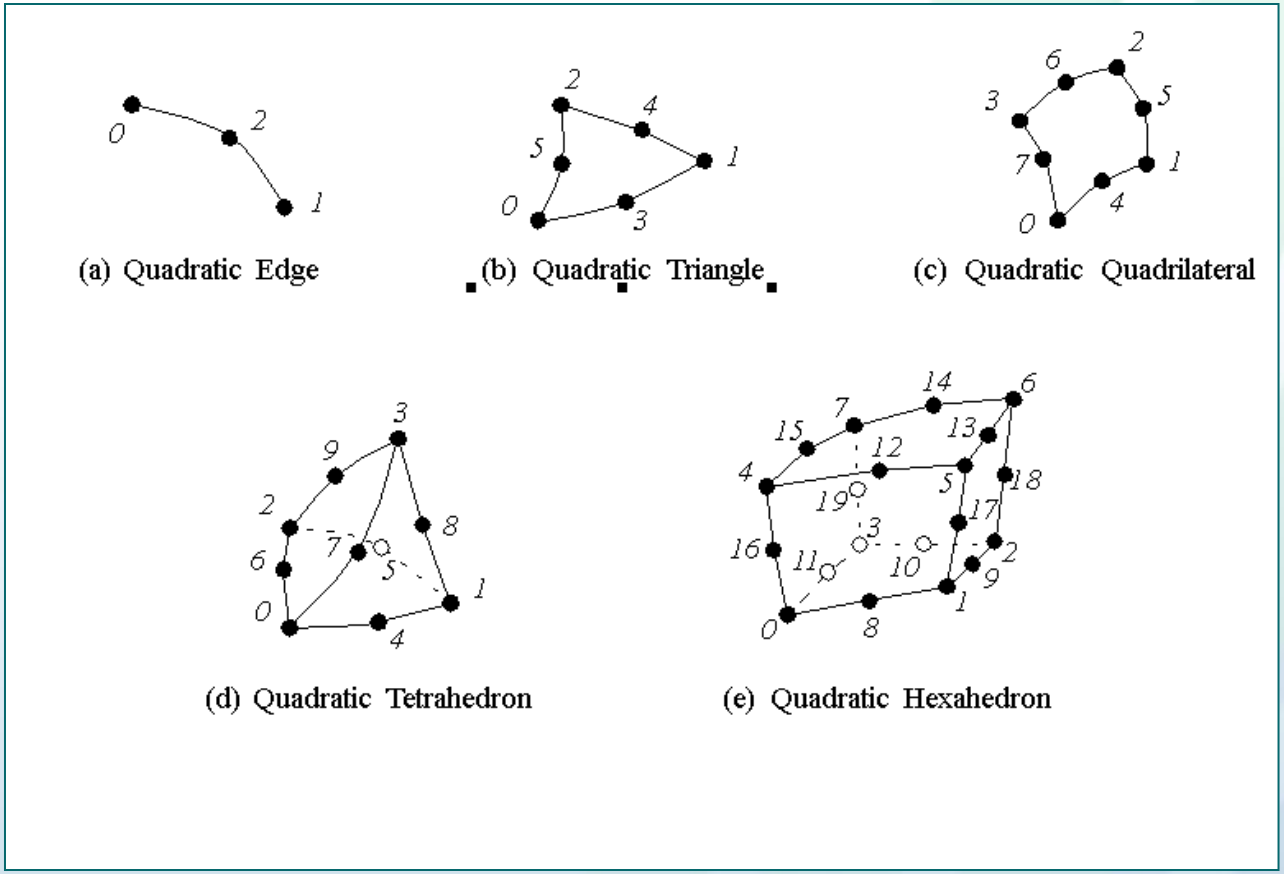
vtkCell Straight-Edged Types



http://www.vtk.org/doc/nightly/html/classvtkCell.html

Kitware

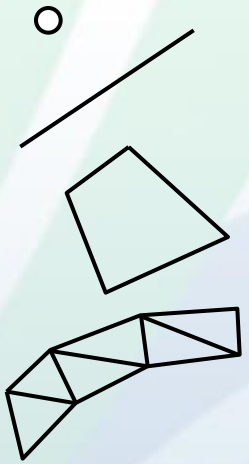
vtkCell Curvilinear-Edge Types



Kitware

vtkPolyData Cells

- Efficient way – build through vtkCellArray
  - vtkCellArray::SetNumberOfCells()
  - Done for verts, lines, polys, triangle strips



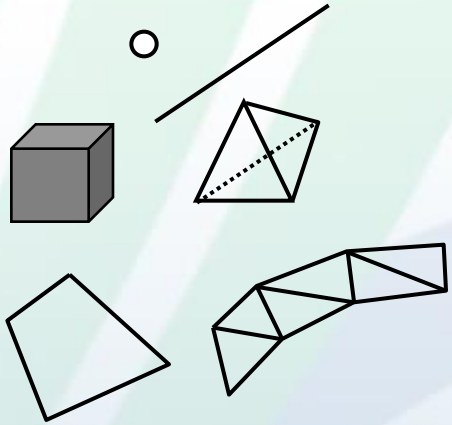
- Simple way – build through poly data API
  - Allocate()
  - InsertNextCell()
  - Squeeze() – reclaim unused memory

- WARNING – Order that cells are added may be different than they are accessed
  - Ordered by verts, lines, polys, triangle strips
  - Need to match with cell data

http://www.vtk.org/doc/nightly/html/classvtkPolyData.html

vtkUnstructuredGrid Cells

- Order of cells is order of insertion
  - 0-based indexing
- Allocate()
- InsertNextCell()
- SetCells()
- Squeeze()
- Inserted points of cells are 0-based indexing



http://www.vtk.org/doc/nightly/html/classvtkUnstructuredGrid.html

Example 5 – Write It!

- Still using function signature:
  - void coprocess(const double spacing[3], const Box& global_box, const Box& local_box, std::vector<double>& minifepointdata, int time_step, double time, bool force_output);
- Hint: example5_catalyst_adaptor.cpp
  - void getpointcoordinate(const int indices[3], const double spacing[3], double coord[3]);
  - void getcellpointids(const Box& local_box, const int indices[3], vtkIdType pointids[8]);

Example 5 – A Solution

```
…
 vtkNew<vtkUnstructuredGrid> grid;
 grid->Initialize();
 vtkNew<vtkPoints> points;
 points->SetNumberOfPoints( (local_box[0][1]-local_box[0][0]+1) *
   (local_box[1][1]-local_box[1][0]+1)*(local_box[2][1]-local_box[2][0]+1) );
 double coord[3]; int indices[3]; vtkIdType id=0;
 for(int iz=local_box[2][0]; iz<=local_box[2][1]; ++iz)
    for(int iy=local_box[1][0]; iy<=local_box[1][1]; ++iy)
      for(int ix=local_box[0][0]; ix<=local_box[0][1]; ++ix) {
        int indices[3] = {ix, iy, iz};
        getpointcoordinate(indices, spacing, coord);
        points->SetPoint(id++, coord);
        }
   grid->SetPoints(points.GetPointer());
…
```

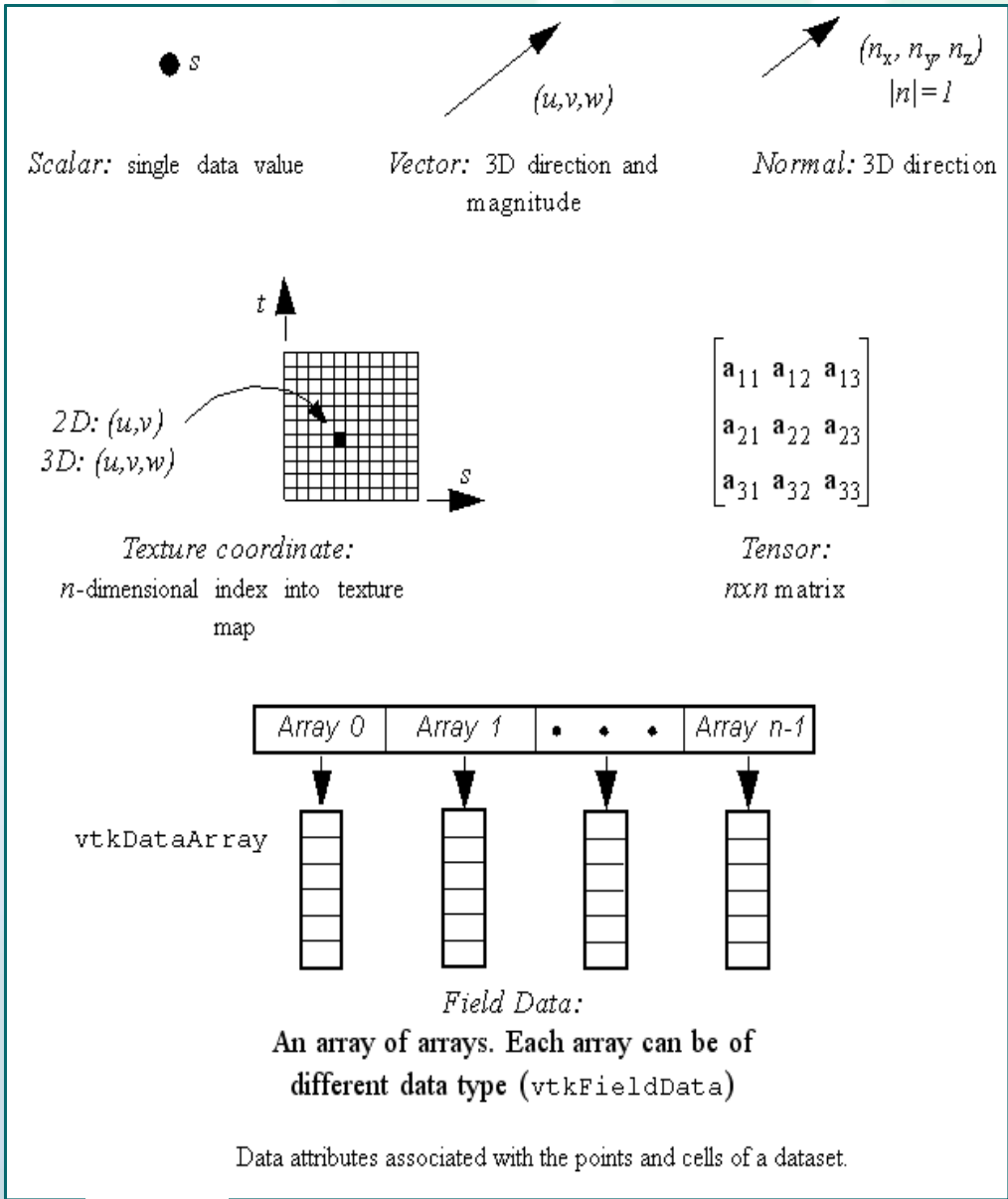
Kitware

Example 5 – A Solution (2)

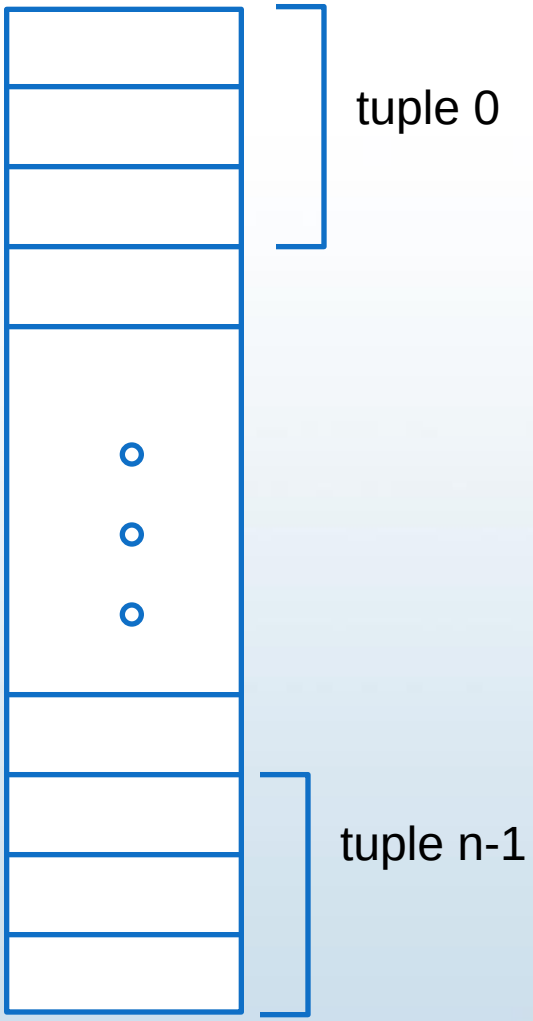
```
…
  grid->Allocate( (local_box[0][1]-local_box[0][0]) *
      (local_box[1][1]-local_box[1][0])*(local_box[2][1]-local_box[2][0]) );
    vtkIdType pointids[8];
    for(int iz=local_box[2][0]; iz<local_box[2][1]; ++iz)
      for(int iy=local_box[1][0]; iy<local_box[1][1]; ++iy)
        for(int ix=local_box[0][0]; ix<local_box[0][1]; ++ix) {
          int indices[3] = {ix, iy, iz};
          getcellpointids(local_box, indices, pointids);
          grid->InsertNextCell(VTK_HEXAHEDRON, 8, pointids);
        }
…
```

Field Information

- Store information defined over grids
- Stored in concrete classes that derive from vtkDataArray
  - vtkFloatArray
  - vtkIntArray
  - vtkDoubleArray
  - vtkUnsignedCharArray
  - …



vtkDataArray – Basis for vtkDataObject Contents



- An array of *n* tuples
- Each tuple has *m* components which are logically grouped together
- Internal implementation is a pointer to an n x m block of memory
- Data type determined by class

- Two APIs : generic and data type specific

http://www.vtk.org/doc/nightly/html/classvtkDataArray.html

vtkDataArray

- SetNumberOfComponents() – call first
- SetNumberOfTuples()
  - For point data must be set to number of points
  - For cell data must be set to number of cells
- SetArray()
  - If flat array has proper component & tuple ordering use existing simulation memory – most efficient
  - Can specify who should delete
  - VTK uses pipeline architecture so Catalyst libraries will NOT modify array values
- SetTupleValue() – uses native data type
- SetValue() – uses native data type
- SetName() – array descriptor, e.g. velocity, density

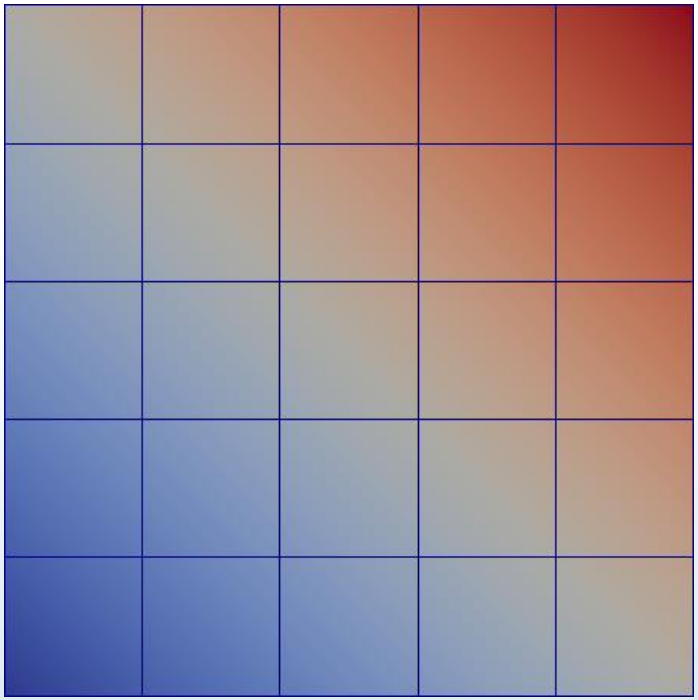
http://www.vtk.org/doc/nightly/html/classvtkDataArray.html

vtkFieldData

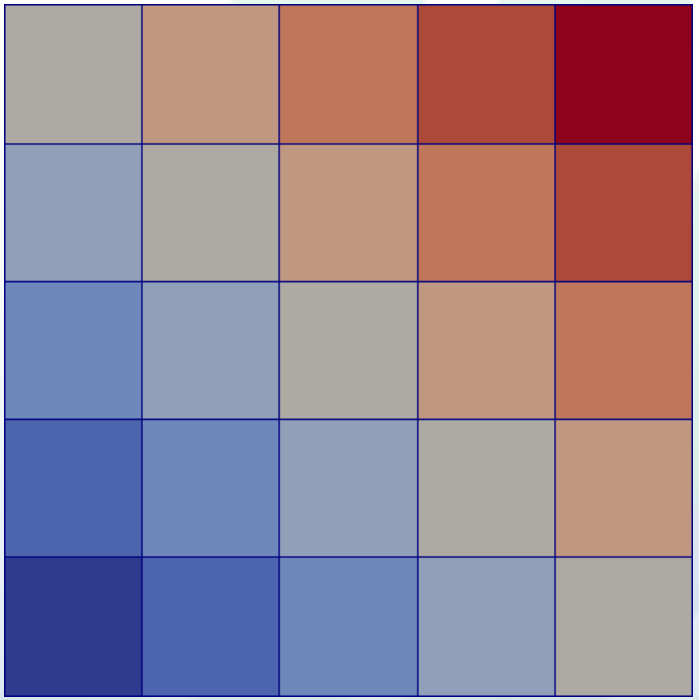
- Object for storing vtkDataArrays
- vtkDataSet::GetFieldData() – non-grid associated arrays
- Derived classes
  - vtkPointData – vtkDataSet::GetPointData()
  - vtkCellData – vtkDataSet::GetCellData()
- vtkFieldData::AddArray(vtkDataArray*)
- Specific arrays are normally retrieved by name from vtkFieldData
  - Uniqueness is not required but can cause unexpected results

http://www.vtk.org/doc/nightly/html/classvtkFieldData.html

Point Data and Cell Data



Point data – 36 values



Cell data – 25 values

Example 6 – Write It!

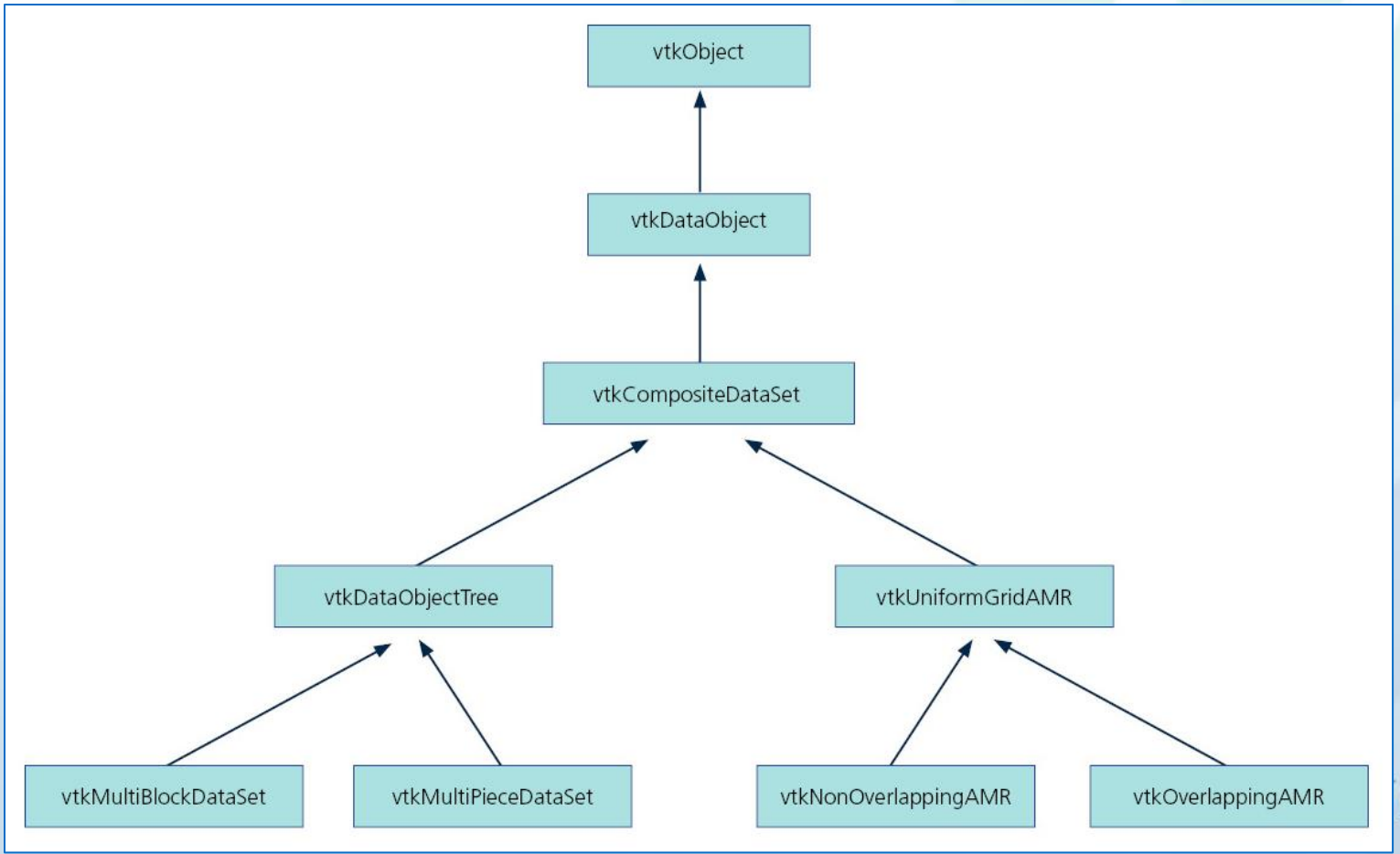
- Still using function signature:
  - void coprocess(const double spacing[3], const Box& global_box, const Box& local_box, std::vector<double>& minifepointdata, int time_step, double time, bool force_output);
- Use vtkpointdata vector for source
  - Already ordered for our grid's points

Example 6 – A Solution

```
…
  std::vector<double> vtkpointdata;
  getlocalpointarray(global_box, local_box, minifepointdata, vtkpointdata);
  vtkSmartPointer<vtkDoubleArray> myDataArray =
      vtkSmartPointer<vtkDoubleArray>::New();
  myDataArray->SetNumberOfComponents(1);
  myDataArray->SetName("myData");
  myDataArray->SetArray(&(vtkpointdata[0]), vtkpointdata.size(), 1);
  grid->GetPointData()->AddArray(myDataArray);
…
```

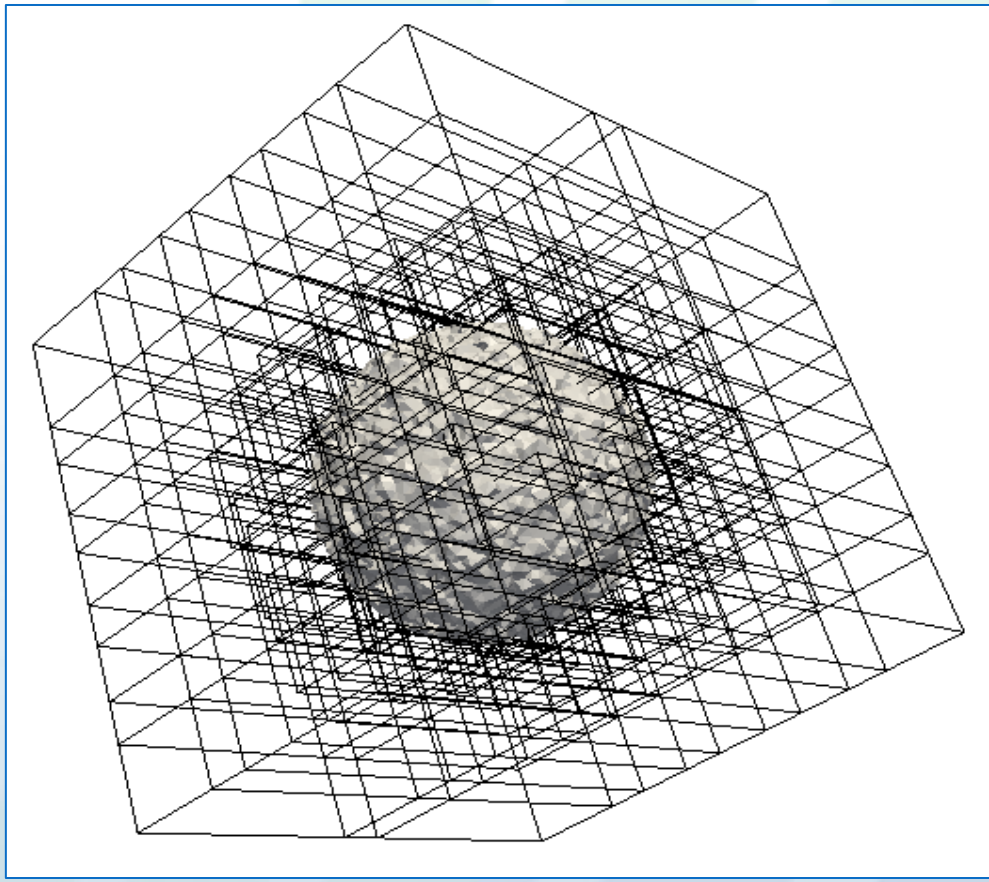
Multiple Grids

- Use something that derives from vtkCompositeDataSet to group multiple vtkDataSets together



vtkMultiBlockDataSet

- Most general way of storing vtkDataSets and other vtkCompositeDataSets
- Block structure must be the same on each process
- Block is null if data set is on a different process
- SetNumberOfBlocks()
- SetBlock()



http://www.vtk.org/doc/nightly/html/classvtkMultiBlockDataSet.html

Kitware

vtkMultiPieceDataSet

- Way to combine multiple vtkDataSets of the same type into a single logical object
  - Useful when the amount of pieces is unknown *a priori*
- Must be contained in a vtkMultiBlockDataSet
- SetNumberOfPieces()
- SetPiece()

http://www.vtk.org/doc/nightly/html/classvtkMultiPieceDataSet.html

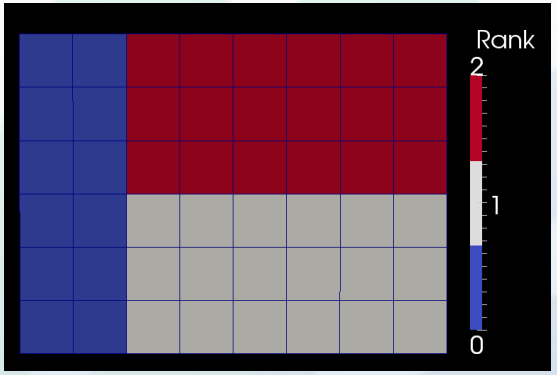
AMR Data Sets

- Classes derive from vtkUniformGridAMR
- Concept of grid levels for changing cell size locally
- Uses only vtkUniformGrids
  - vtkNonOverlappingAMR – no blanking used since no data sets overlap
  - vtkOverlappingAMR – vtkUniformGrids overlap and use blanking

http://www.vtk.org/doc/nightly/html/classvtkUniformGridAMR.html

Grid Partitioning

- For unstructured grids and polydatas
  - Single data set per process – use as is
  - Multiple data sets per process – choice of combining or not depends on memory layout

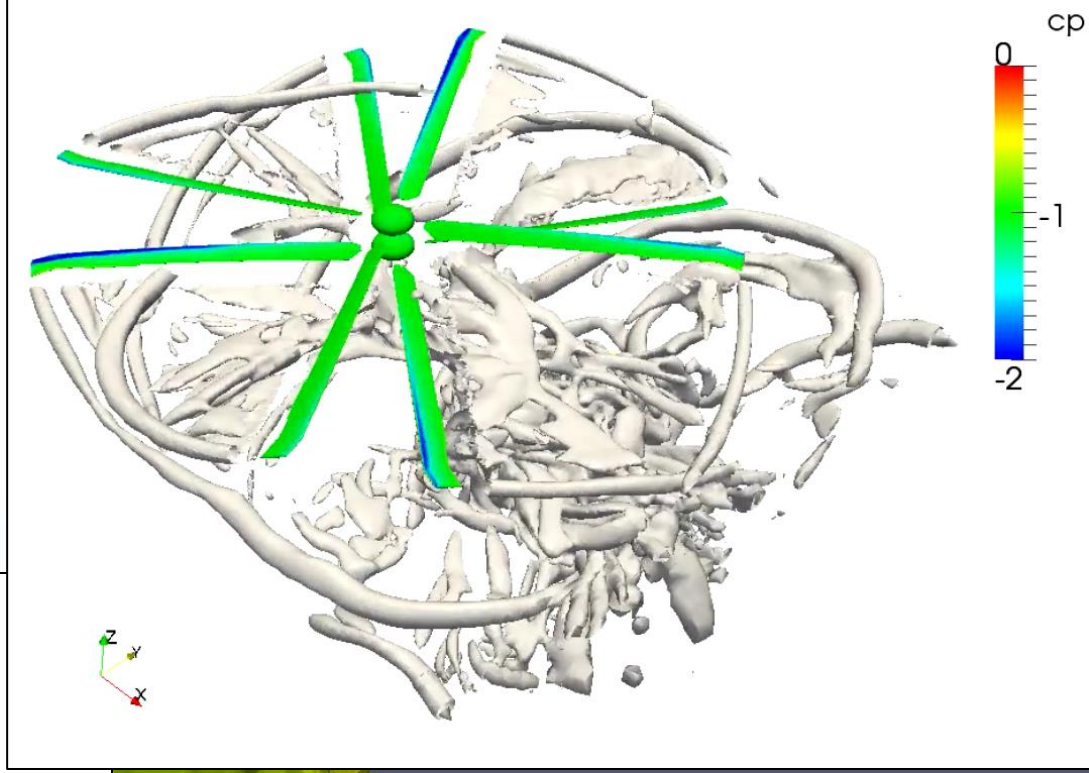


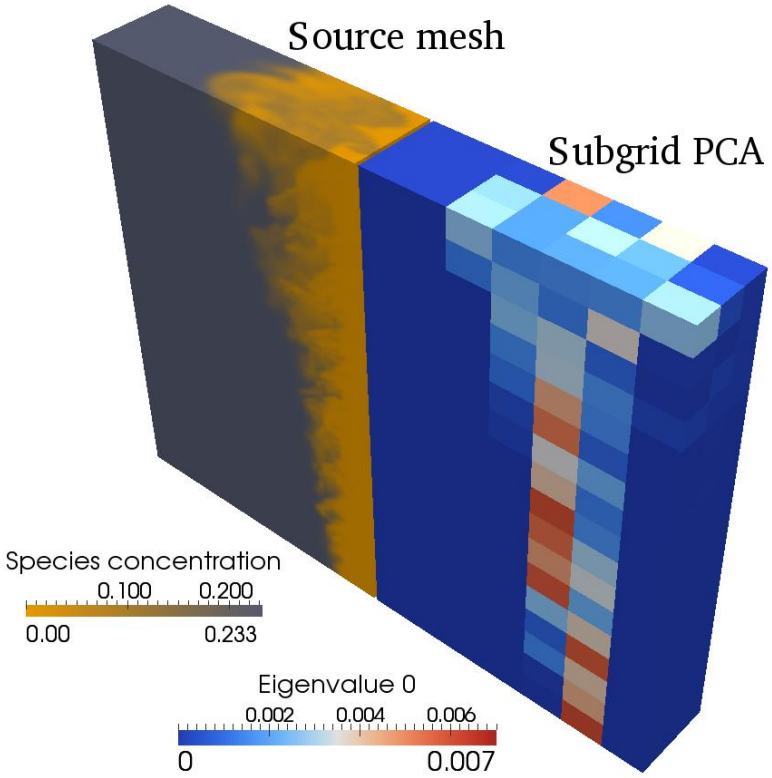
- For topologically structured grids
  - Must be partitioned into logical blocks
  - SetExtent()
    - Index of first and last point in each direction
    - Will be different on each process
  - vtkCPInputDataDescription::SetWholeExtent() – same on each process

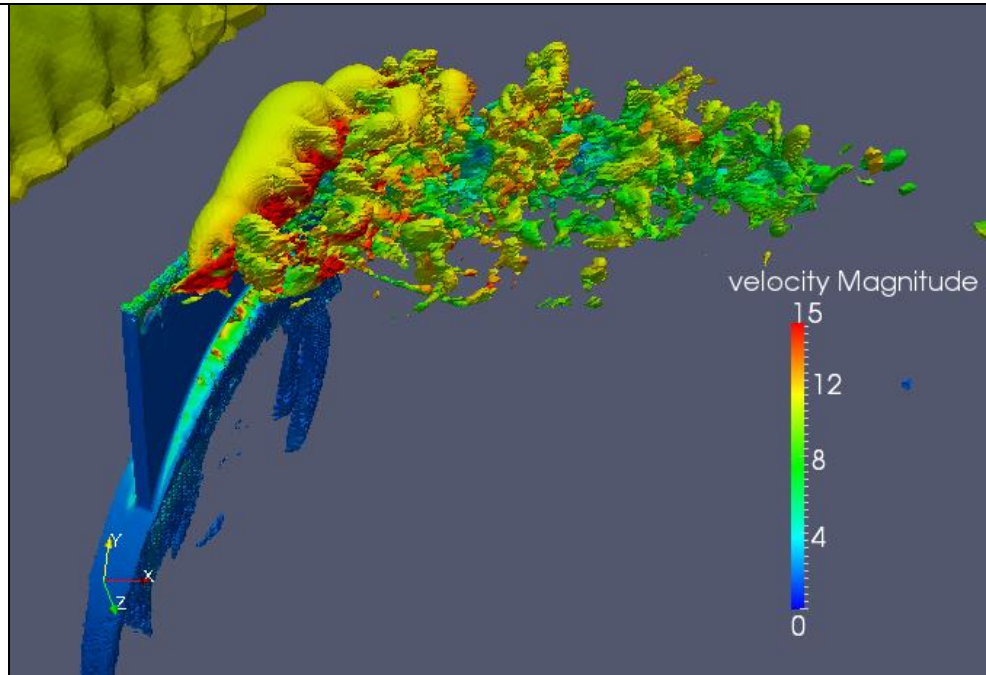
Advanced Topics

- Zero-copy for VTK arrays
  - Reuse existing memory in layout different than standard VTK arrays
- Hard-coded C++ pipelines
  - Removes dependency on Python
  - Use simulation input parameters to remove requirement that users create pipelines in ParaView
- Ghost information
- CMake for automatic C++ and Fortran function name mangling

Gratuitous Catalyst Images







ParaView Catalyst for Simulation Users

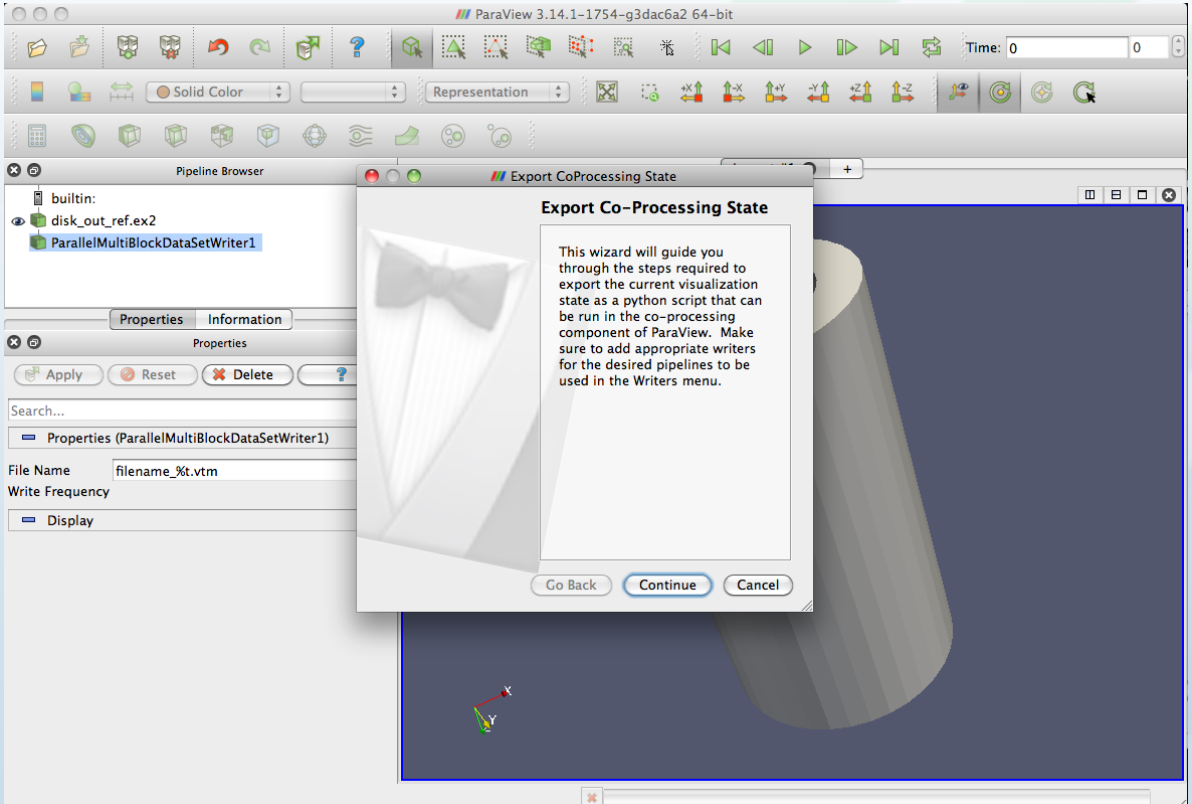
Creating Catalyst Output

Two main ways:

- Create and/or modify Python scripts
  - ParaView GUI plugin to create Python scripts
  - Modification with knowledge of ParaView Python API
- Developer generated “canned” scripts
  - User provides parameters for already created Catalyst pipelines
  - User may not even need to know ParaView
  - See ParaView Catalyst User’s Guide

Create Python Scripts from ParaView

- Interact with ParaView normally
- Export a script that mimics that interaction
- Queries during each co-processing step
  - (one frame at a time)



Kitware

ParaView GUI Plugin

- Similar to using ParaView interactively
  - Setup desired pipelines
  - Ideally, start with a representative data set from the simulation
- Extra pipeline information to tell what to output during simulation run
  - Add in data extract writers
  - Create screenshots to output
  - Both require file name and write frequency

In Situ Demo

- Create a ParaView Catalyst Python pipeline script
  - Specify desired outputs from run
  - Export the script
- Run the script with a fictitious input
  - Time dependent grid and field data come from a file instead of from an actual simulation
- Examine results

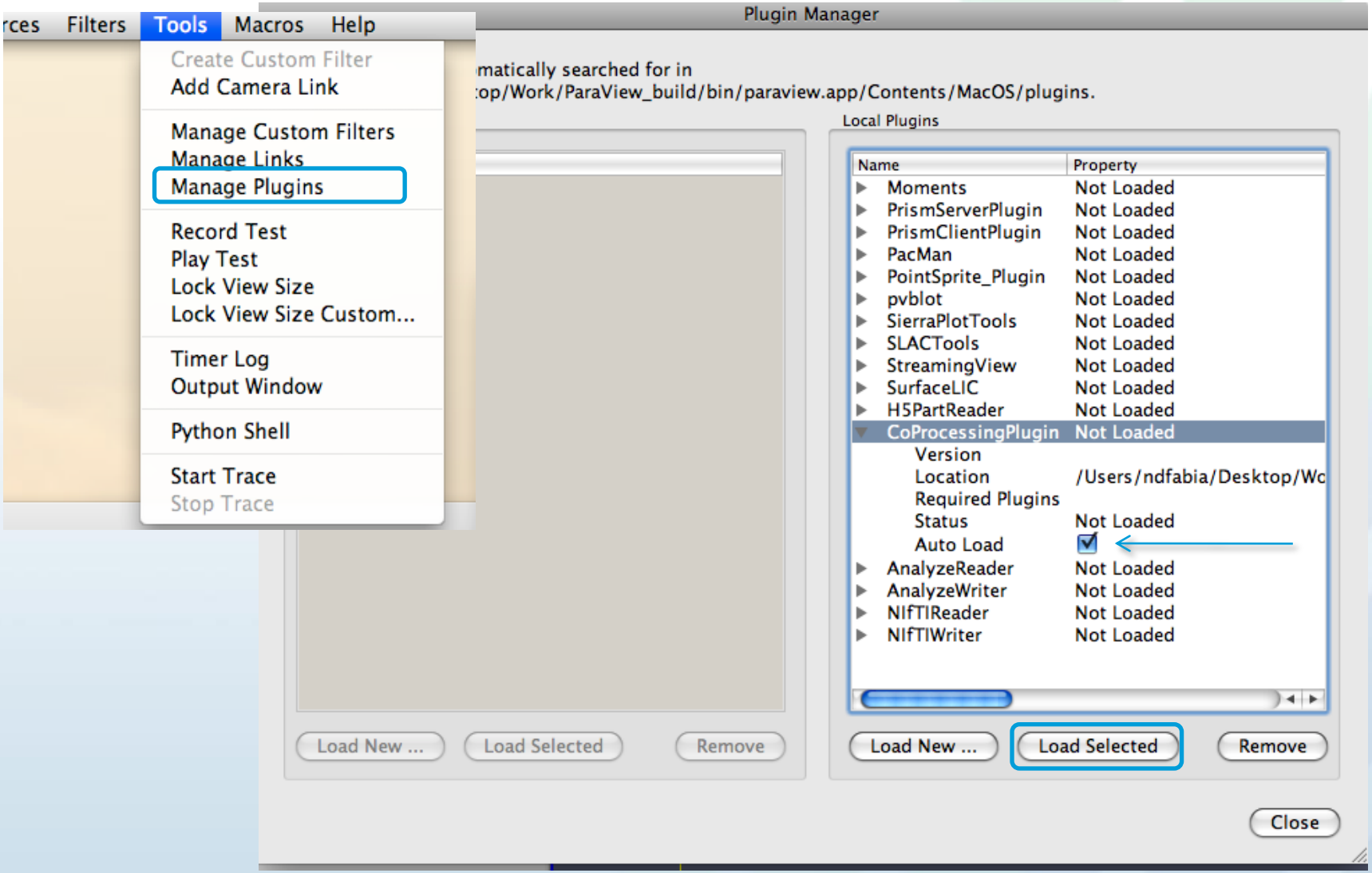
Use Catalyst to Write Out Grid

- Need something to start with
- Grid of the same type
- Fields of the same type
- The closer to the actual simulation the better

Run It!

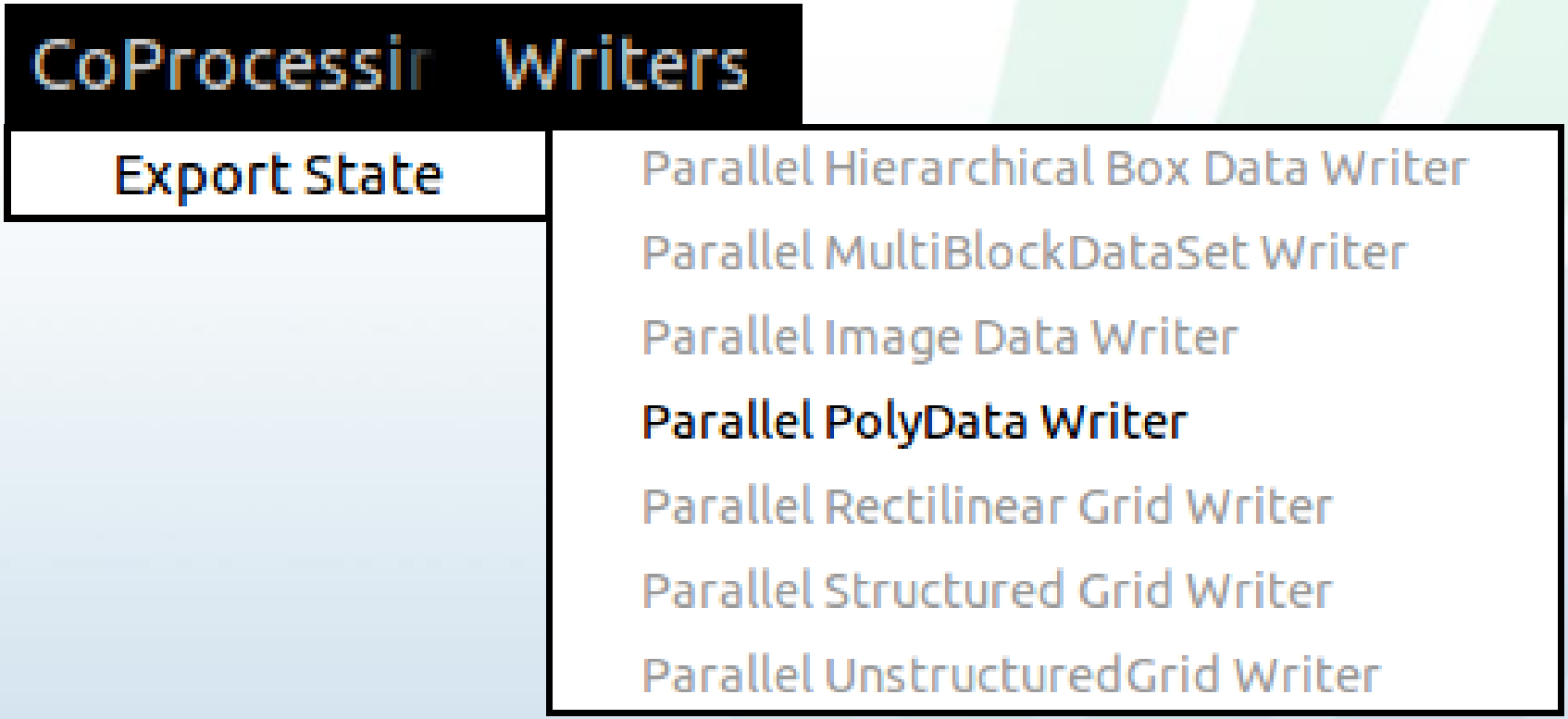
- Go to <miniFE-2.0_ref>/src and finish building miniFE, i.e. “make”
- Make sure gridwriter.py is there
  - Simple Catalyst Python pipeline to write out the full grid and fields every time step
  - Run with “./miniFE.x script_names=gridwriter.py”
  - Output file will be:
    - filename_*.pvtu for unstructured grid case
    - filename_*.pvti for image data (i.e. Cartesian grid) case

In Situ Demo – Load Plugin Step



Kitware

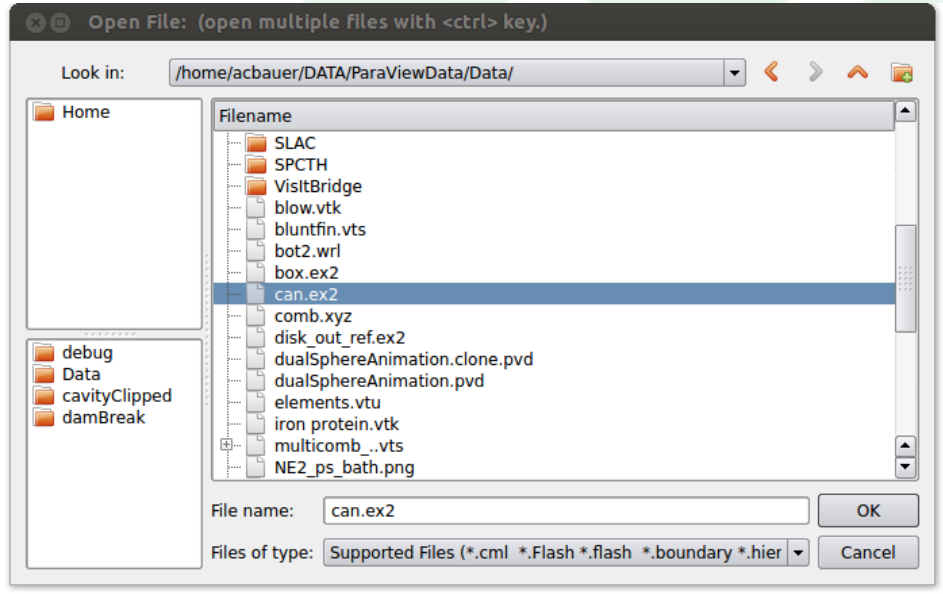
In Situ Demo – New Plugin Menus



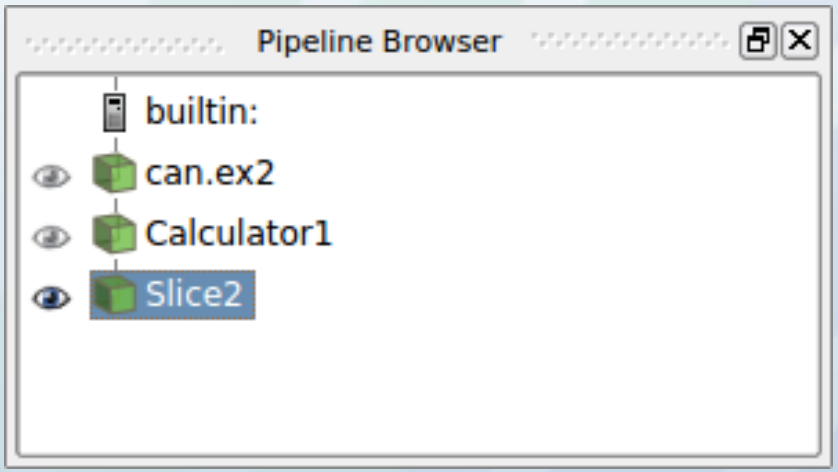
Kitware

In Situ Demo – Creating a Catalyst Python Script

- Load output file filename_*.{pvti,pvtu} from previous run



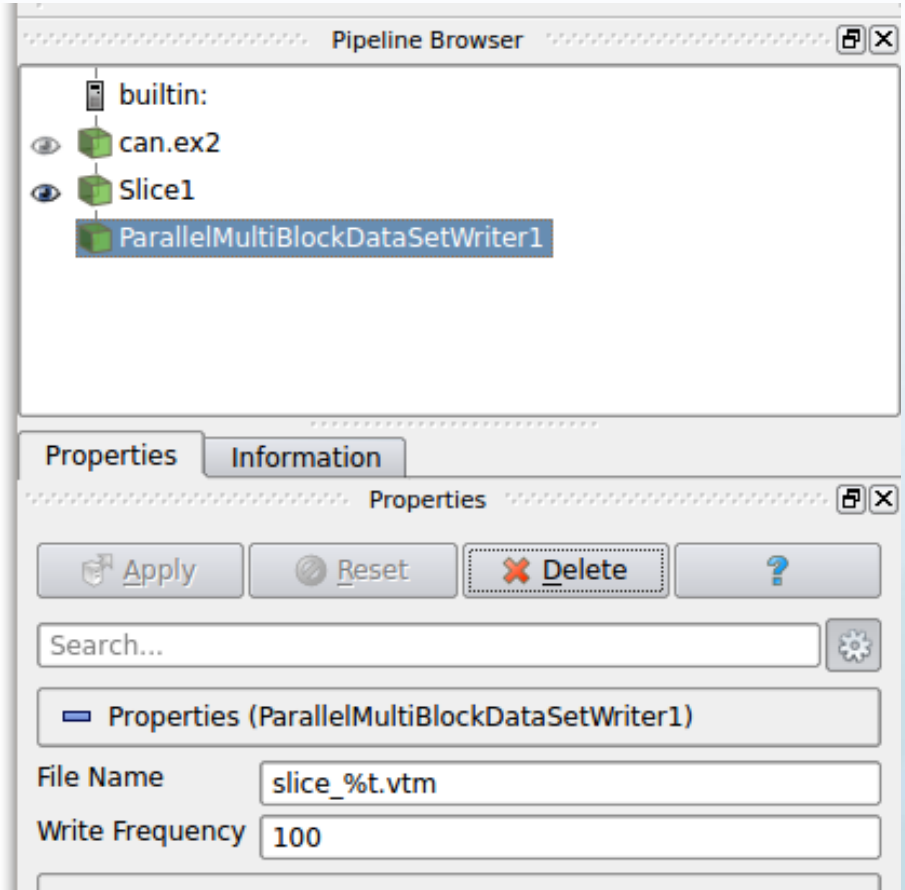
- Create desired pipeline

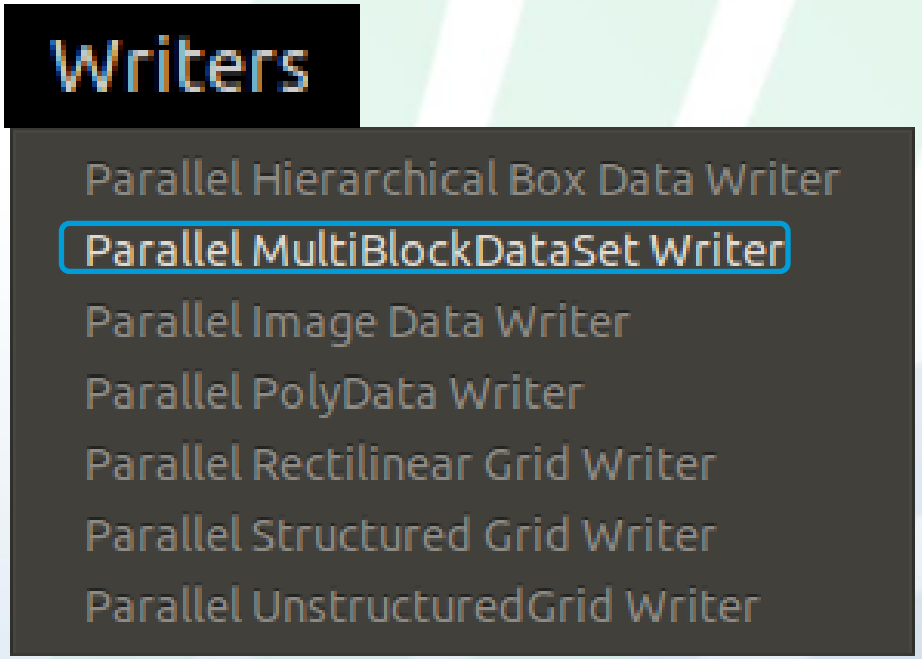


Kitware

In Situ Demo – Adding in Writers

- Parameters:
  - File Name – %t gets replaced with time step
  - Write Frequency





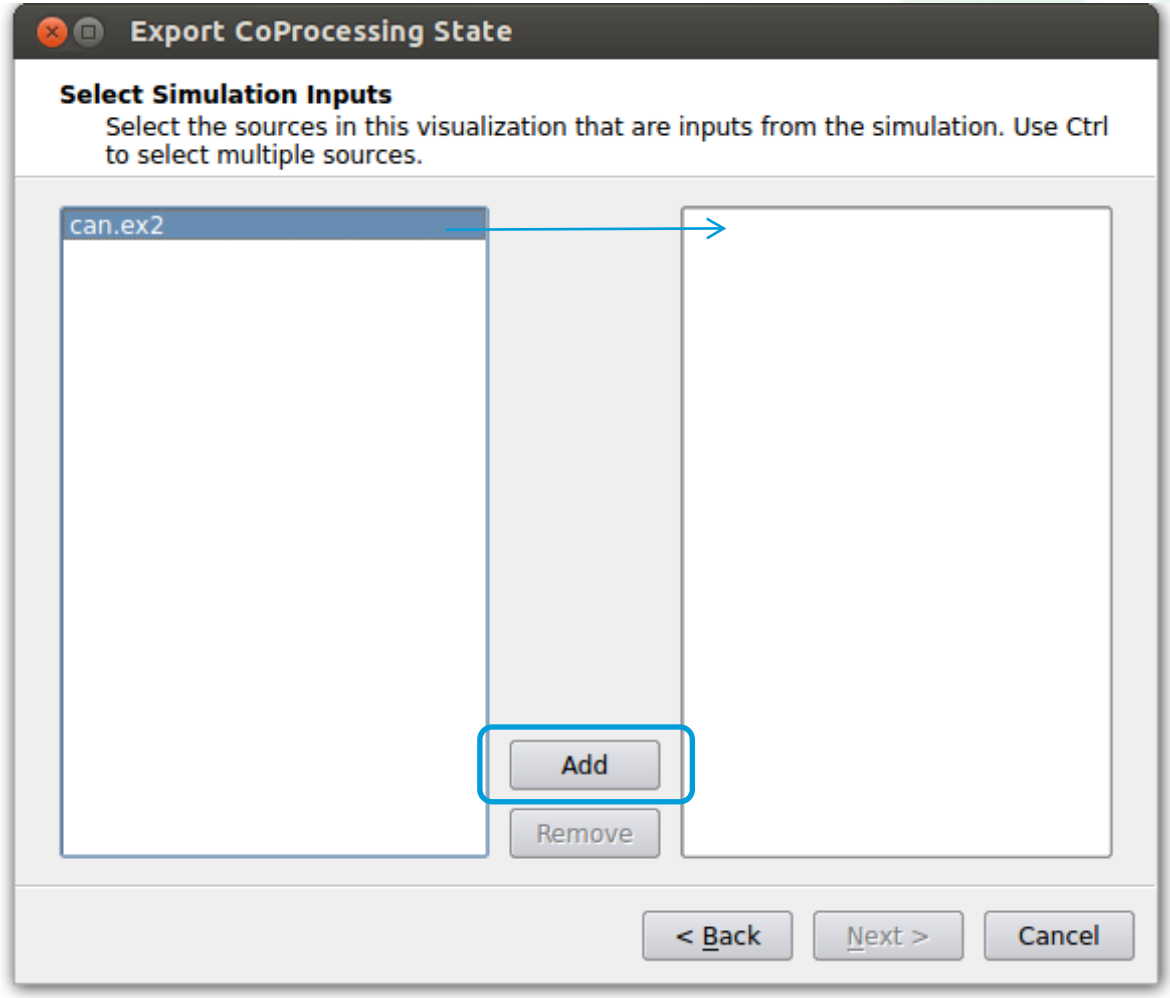
Kitware

In Situ Demo – Exporting the Script

Kitware

In Situ Demo – Select Inputs

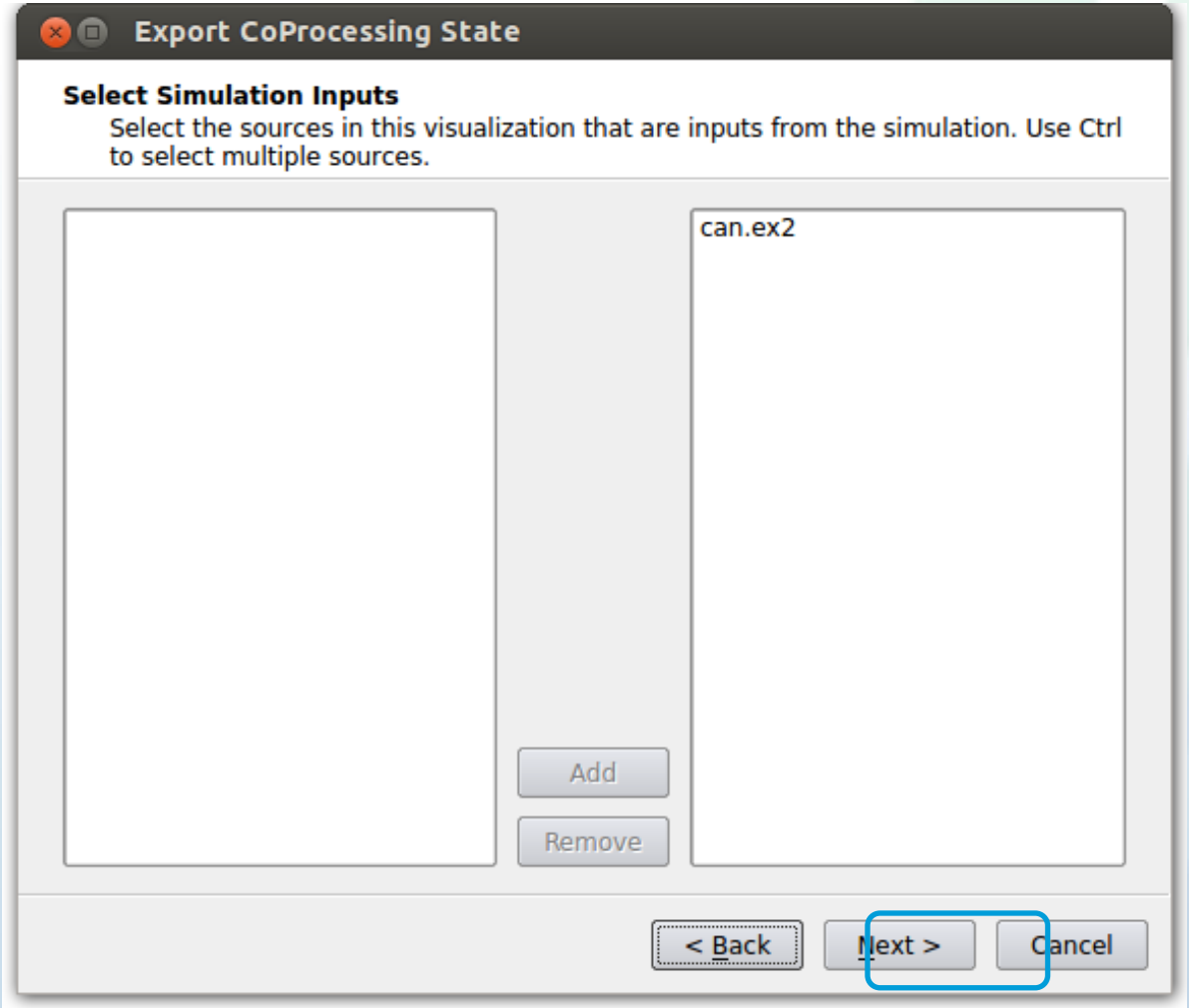
- Usually only a single input but can have multiple inputs



Kitware

In Situ Demo – Select Inputs

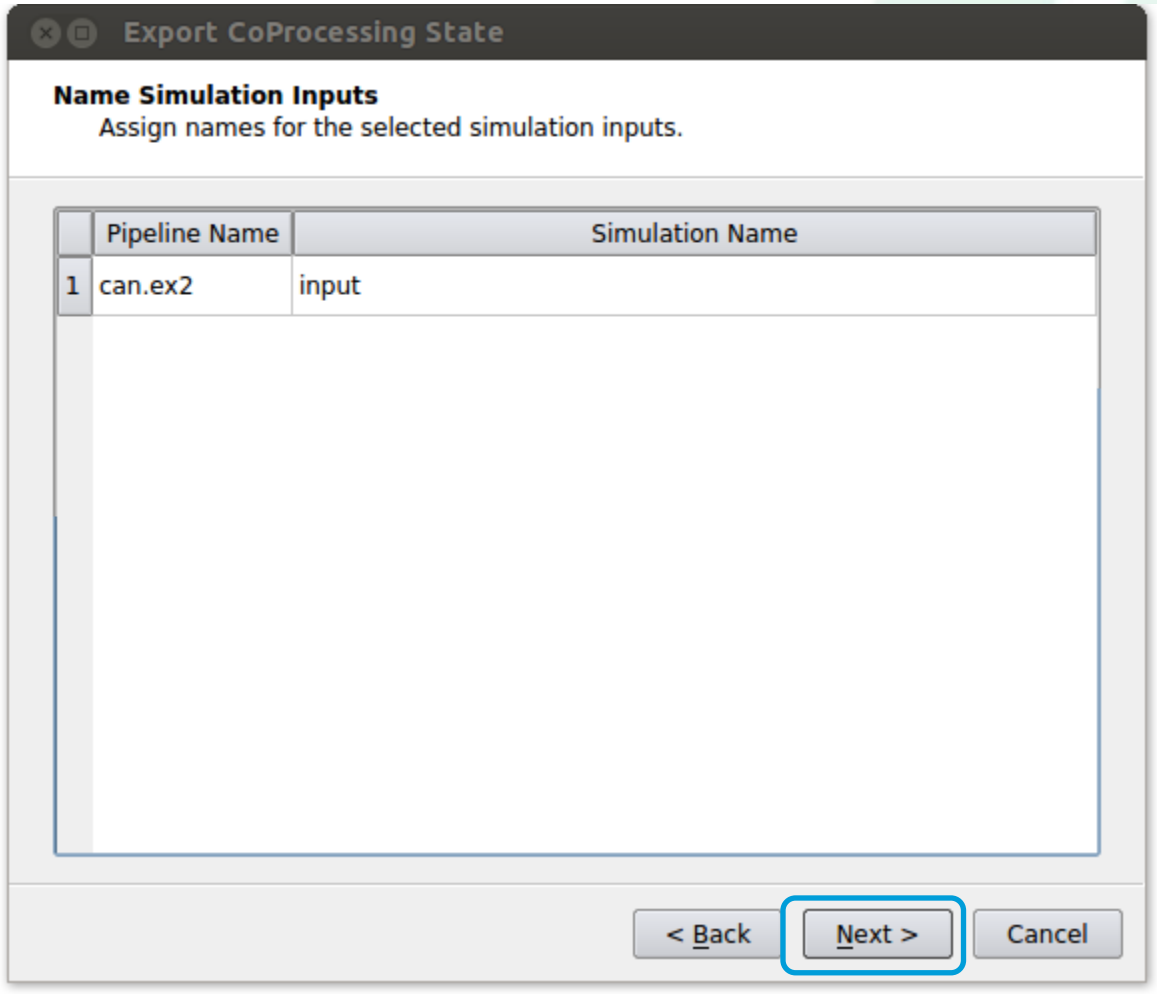
- Each pipeline source is a potential input



Kitware

In Situ Demo – Match Up Inputs

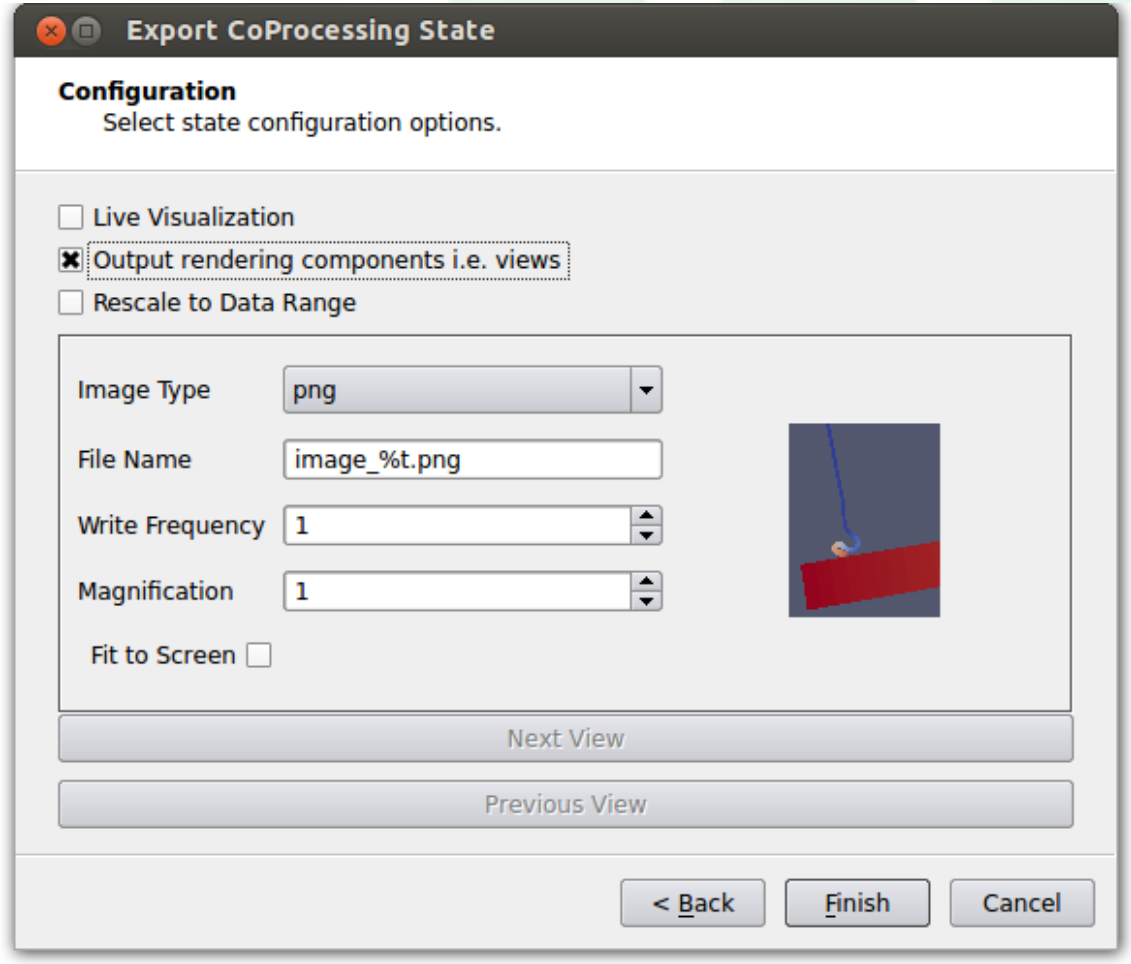
- Source name (e.g. “can.ex2”) needs to be matched with string key in adaptor (e.g. “input”)



Kitware

In Situ Demo – Generating an Image

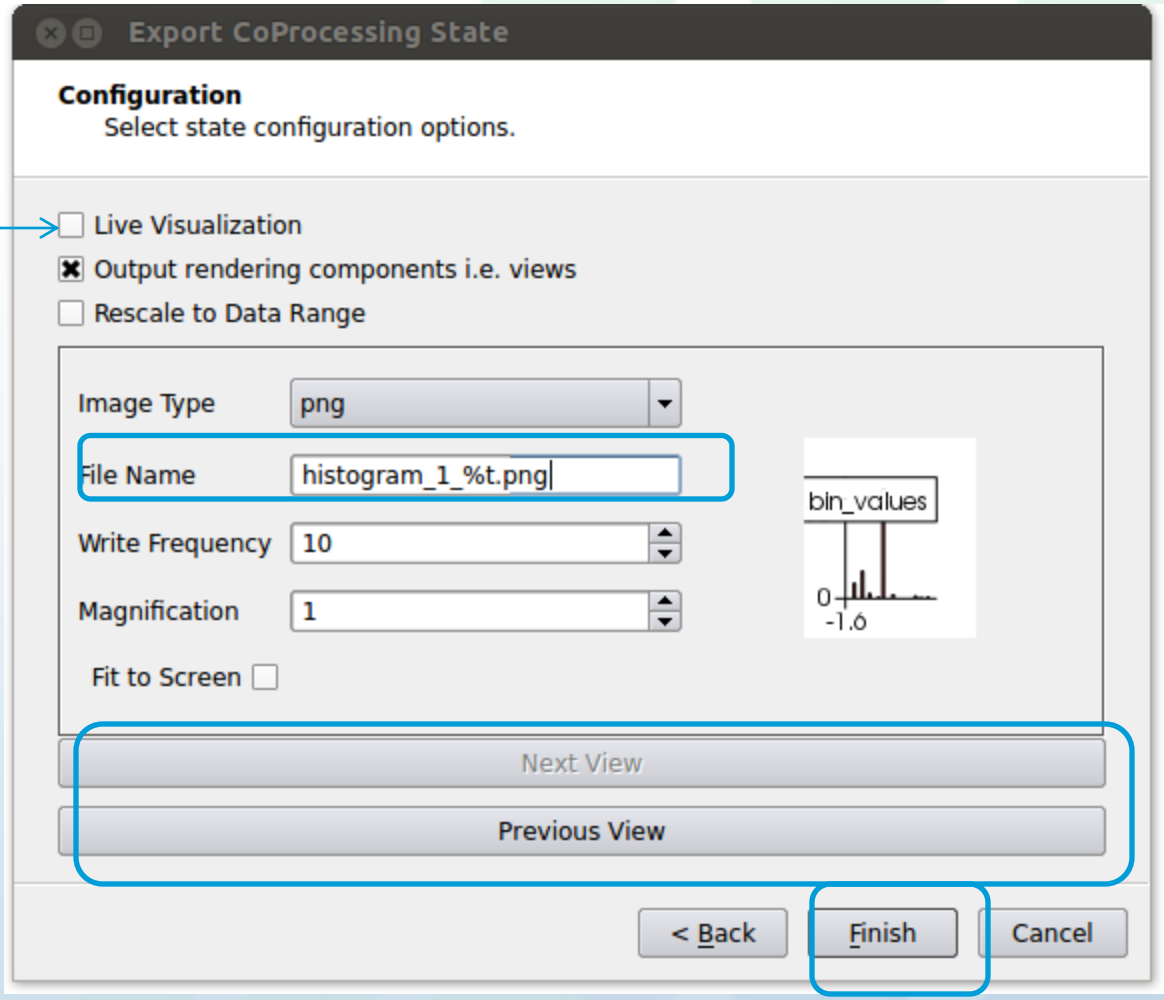
- Parameters/Options:
  - Live visualization
  - Rescale to Data Range (all images)
  - Individual images
    - Image Type
    - File Name
    - Write Frequency
    - Magnification
    - Fit to Screen
- %t gets replaced with time step



Kitware

In Situ Demo – Generating Two Images

- Parameters/Options:
  - Live visualization
    - Check this as we will use this later
  - Rescale to Data Range (all images)
  - Individual images
    - Image Type
    - File Name
    - Write Frequency
    - Magnification
    - Fit to Screen



Kitware

In Situ Demo – Write Out the Script

- Generated script will look something like this

```
def DoCoProcessing(datadescription):

   input = CreateProducer( datadescription, "input" )

   ParallelMultiBlockDataSetWriter1 = CreateWriter(
XMLMultiBlockDataWriter, "filename_%t.vtm", 1 )
```

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

cp_writers = []

def RequestDataDescription(datadescription):
    "Callback to populate the request for current timestep"
    timestep = datadescription.GetTimeStep()


    input_name = 'input'
    if (timestep % 1 == 0) :
        datadescription.GetInputDescriptionByName(input_name).AllFieldsOn()
        datadescription.GetInputDescriptionByName(input_name).GenerateMeshOn()
    else:
        datadescription.GetInputDescriptionByName(input_name).AllFieldsOff()
        datadescription.GetInputDescriptionByName(input_name).GenerateMeshOff()


def DoCoProcessing(datadescription):
    "Callback to do co-processing for current timestep"
    global cp_writers
    cp_writers = []
    timestep = datadescription.GetTimeStep()

    input = CreateProducer( datadescription, "input" )

    ParallelMultiBlockDataSetWriter1 = CreateWriter( XMLMultiBlockDataWriter, "filename_%t.vtm", 1 )



    for writer in cp_writers:
        if timestep % writer.cpFrequency == 0:
            writer.FileName = writer.cpFileName.replace("%t", str(timestep))
                                ine()


                                nager.GetRenderViews()

                                renderviews)):
                                ame.replace("%v", str(view))
                                ace("%t", str(timestep))
                                renderviews[view])

                                oxies -- we do it this way to avoid problems with prototypes
                                Delete()
                                :

                                esToDelete()


    iter = servermanager.vtkSMProxyIterator()
    iter.Begin()
    tobedeleted = []
    while not iter.IsAtEnd():
      if iter.GetGroup().find("prototypes") != -1:
         iter.Next()
         continue
      proxy = servermanager._getPyProxy(iter.GetProxy())
      proxygroup = iter.GetGroup()
      iter.Next()
      if proxygroup != 'timekeeper' and proxy != None and proxygroup.find("pq_helper_proxies") == -1 :
          tobedeleted.append(proxy)

    return tobedeleted

def CreateProducer(datadescription, gridname):
  "Creates a producer proxy for the grid"
  if not datadescription.GetInputDescriptionByName(gridname):
    raise RuntimeError, "Simulation input name '%s' does not exist" % gridname
  grid = datadescription.GetInputDescriptionByName(gridname).GetGrid()
  producer = TrivialProducer()
  producer.GetClientSideObject().SetOutput(grid)
  producer.UpdatePipeline()
  return producer


def CreateWriter(proxy_ctor, filename, freq):
    global cp_writers
    writer = proxy_ctor()
    writer.FileName = filename
    writer.add_attribute("cpFrequency", freq)
    writer.add_attribute("cpFileName", filename)
    cp_writers.append(writer)
    return writer
```

In Situ Demo – Run the Script

- Put the generated Python script in <miniFE-2.0_ref>/src directory

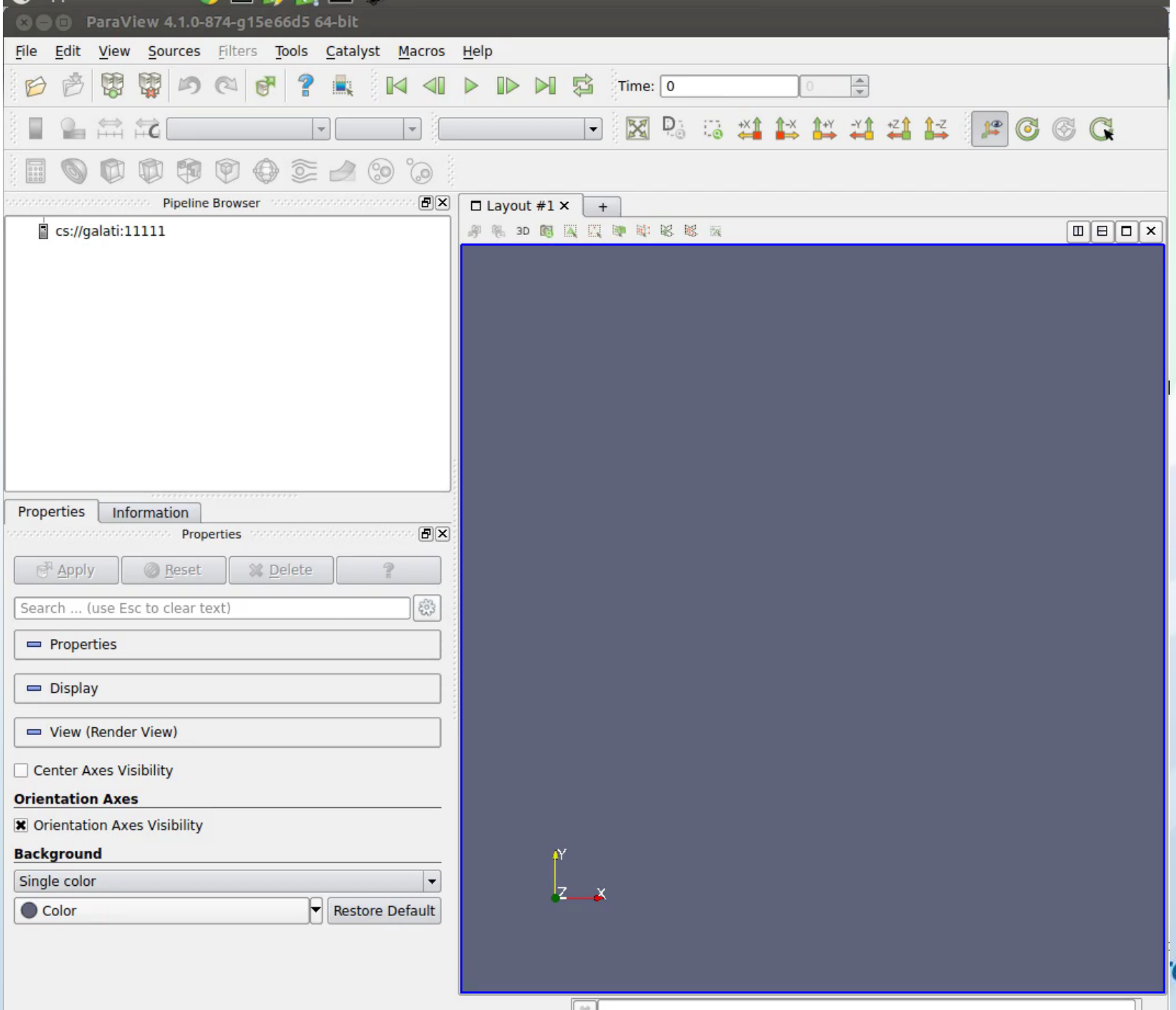
- Run with "./miniFE.x script_names=<outputscript>"
  - Can use MPI to run with more processes
  - Change grid size with nx=, ny=, nz= command line arguments
  - Run multiple scripts with comma separated list script_names=<script1>,<script2>,<script3>

Live *In Situ* Analysis and Visualization

- Everything before this was “batch”
  - Preset information with possible logic
- Functionality for interacting with simulation data during simulation run
  - When exporting a Python script, select “Live Visualization”
  - During simulation run choose the “Tools→Connect to Catalyst” GUI menu item

Two Ways for Live *In Situ* Analysis and Visualization

- Without blocking
  - Simulation proceeds while the user interacts with the data from a specific time step
  - “At scale” mode
- With blocking
  - Simulation is blocked while the user interacts with the data
  - “Debugging” mode
  - Work in progress
- Can switch between interactive and batch during run


ParaView 4.1.0-874-g15e66d5 64-bit
File Edit View Sources Filters Tools Catalyst Macros Help
Time: 0
Pipeline Browser
cs://galati:11111
Properties Information
Properties
Apply Reset Delete
Search ... (use Esc to clear text)
Properties
Display
View (Render View)
Center Axes Visibility
Orientation Axes
Orientation Axes Visibility
Background
Single color
Color
Restore Default
Layout #1
3D
Y
Z
X

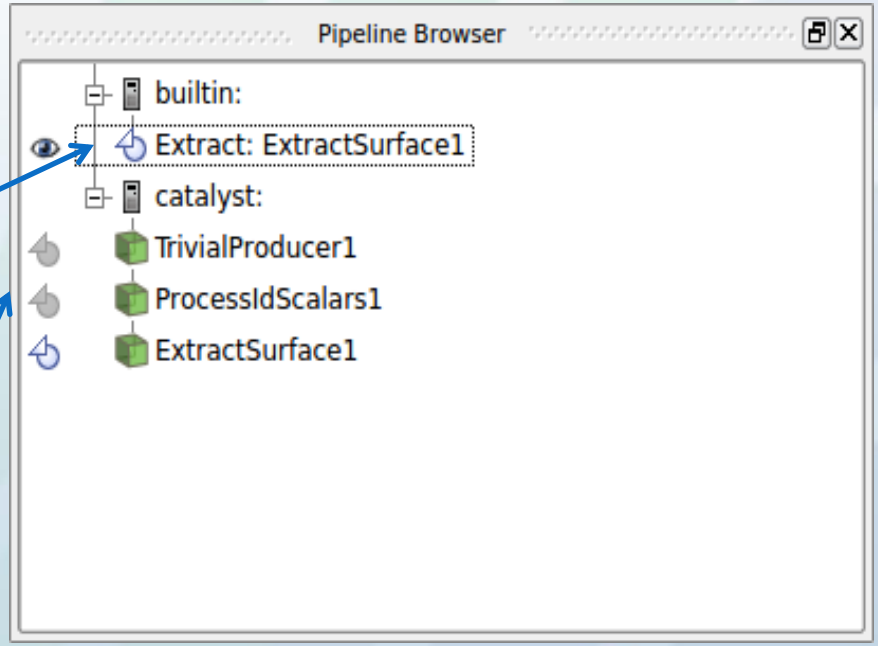
Live *In Situ* Example

- Need to “lengthen” the simulation time
  - Increase nx, ny and nz
  - Add in “sleep(5);” at the end of coprocess() method in catalyst_adapter.cpp
- Run as before with “./miniFE.x script_names=<outputscript>”
  - Must have Catalyst “Live Visualization” enabled
- Start ParaView and select Tools→Connect to Catalyst
  - Select port (22222 is default)

Live *In Situ* Example

- Only transfer requested data from server (simulation run) to client
  - ExtractSurface1 is already getting extracted
- Use 

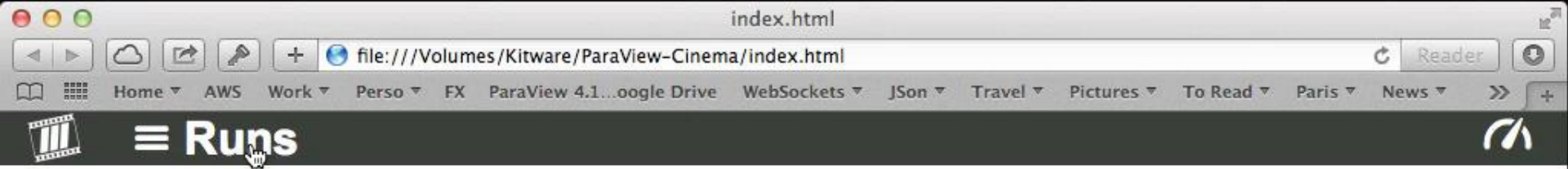
on client to stop transferring to client
- Click on  to transfer to client from Catalyst



Kitware

ParaView Cinema + Catalyst

- Image output is orders magnitude less than an entire data set
  - Helios: full data set – 448 MB, surface of blades – 2.8 MB, image – 71 KB
- Use Catalyst to make a set of images at each time step with small output changes (rotations, slice planes locations, iso-surfaced variables & values, etc.)
- Use a web-browser to view images later
- Should be in ParaView 4.2 as beta functionality



An Image-based approach to Extreme Scale In Situ Visualization and Analysis

James Ahrens*, Sebastien Jourdain**, Patrick O'Leary**, John Patchett*, David H. Rogers*

* Los Alamos National Laboratory ** Kitware Inc.

ADIOS Writer

- Improved IO for at scale HPC runs
  - https://www.olcf.ornl.gov/center-projects/adios/
- Still in development but should be in ParaView 4.2
- Separate PETTT project to study scaling IO on Garnet & Copper DSRCs

Building ParaView Catalyst

Build Considerations Overview

- Shared library build
  - Easier for development but can kill the IO system on HPC machines for large scale runs
- Static library build
  - Freezing Python allows it to be built statically into the executable instead of having it behave similar to shared libraries
- Mesa
  - When window manager isn't available or don't want render windows popping up for image generation

Catalyst Editions

- Doing a full ParaView build gives full Catalyst functionality
  - Also can add 150 MB or more to the executable size depending on ParaView configuration
- Most people use a small subset of VTK and ParaView filters for analysis and visualization
- Catalyst editions allow simpler ways to remove unneeded functionality
  - Can get Catalyst library size down to 15 to 30 MB depending on configuration

Preconfigured Catalyst Editions

- Base – a minimal set of functionality to build other editions from but not meant for use on its own
- Essentials – base + several of the most popular filters
- Extras – base + essentials + parallel XML writers and a couple more filters
- Rendering – coming soon…
- Python version of each available as well
- Available at www.paraview.org/download

Acknowledgements

- Funding through PETTT project PP-ACE-KY05-009-P3
- Tutorial facilities setup by Michael Stephens & John Mason

Kitware

Online Help

- Catalyst User's Guide:
  - http://paraview.org/Wiki/images/4/48/CatalystUsersGuide.pdf
- Email list:
  - paraview@paraview.org
- Doxygen:
  - http://www.vtk.org/doc/nightly/html/classes.html
  - http://www.paraview.org/ParaView3/Doc/Nightly/html/classes.html
- Sphinx:
  - http://www.paraview.org/ParaView3/Doc/Nightly/www/py-doc/index.html
- Websites:
  - http://www.paraview.org
  - http://catalyst.paraview.org
- Examples:
  - https://github.com/acbauer/CatalystExampleCode