In Situ Analysis and Visualization with Ascent and ParaView Catalyst

[Tutorial Introduction]

SC23 Tutorial
Monday November 13th, 2023

Cyrus Harrison, Lawrence Livermore National Laboratory (LLNL)

Jean M. Favre, Swiss National supercomputing Centre (CSCS)

Corey Wetterer-Nelson, Kitware Inc.

Nicole Marsaglia, Lawrence Livermore National Laboratory (LLNL)

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LLNL-PRES-856413
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

Lawrence Livermore National Laboratory

Welcome! Today you will learn:

- About in situ scientific visualization paradigms and use cases
- How to use ***Conduit***, a shared interface for describing in-memory mesh-based data
- How to use two in situ HPC scientific visualization tools:

  Ascent, ParaView Catalyst 2

http://software.llnl.gov/conduit

http://ascent-dav.org

https://catalyst-in-situ.readthedocs.io/en/latest/

Tutorial Outline

- **Introduction** [Lecture, 30 minutes]
  - Scientific Visualization and In Situ Processing Concepts
  - Ascent and Catalyst Project Overviews
- **Hands-on Cloud Environment Setup** [Hands-on, 10 minutes]
- **Using Conduit to Describe Mesh Data** [Hands-on, 50 minutes]
- ***Break*** [30 minutes]
- **Learning Ascent** [Hands-on, 40 minutes]
- **Learning Catalyst** [Hands-on, 40 minutes]
- **Closing Remarks and Questions** [10 minutes]

Introduction:
Scientific visualization and In Situ Processing Concepts

Scientific visualization tools transform, analyze, and render mesh-based data from HPC simulations

Mesh Data

```
coordsets:
  coords:
    type: "explicit"
    values:
      x: [-1.0, 0.0, 0.0, 0.0, 1.0]
      y: [0.0, -1.0, 0.0, 1.0, 0.0]
      z: [0.0, 0.0, 1.0, 0.0, 0.0]
topologies:
  topo:
    type: "unstructured"
    coordset: "coords"
    elements:
      shape: "tet"
      connectivity: [0, 1, 3, 2, 4, 3, 1, 2]
fields:
  density:
    association: "element”
    topology: ”topo"
    values: [1.0, 2.0]
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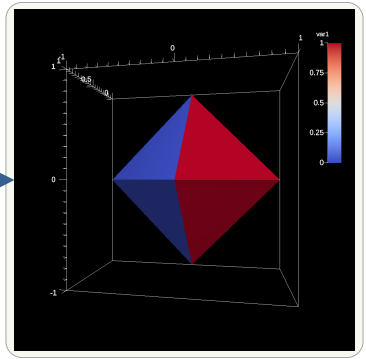
Actions

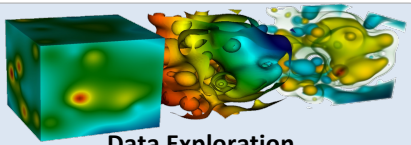
```
-
  action: "add_scenes"
  scenes:
    my_scene:
      plots:
        my_plot:
          type: "pseudocolor"
          field: "var1"
```

Visualization Tool

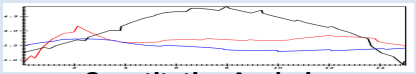
Transform, Analyze, Render



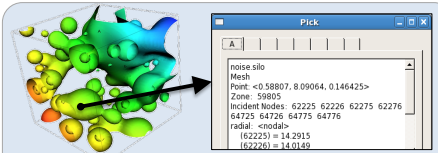
Scientific visualization tools support a wide range of use cases



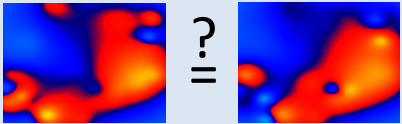
Data Exploration



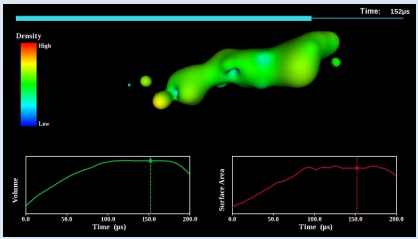
Quantitative Analysis



Visual Debugging

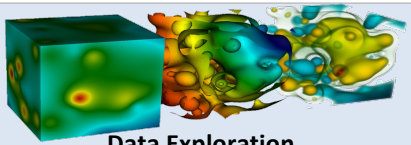


Comparative Analysis

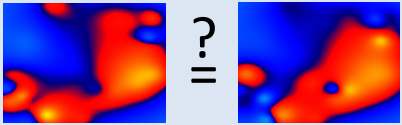


Presentation Graphics

Scientific visualization tools support a wide range of use cases

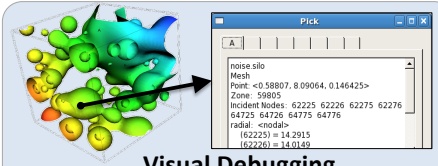


Data Exploration

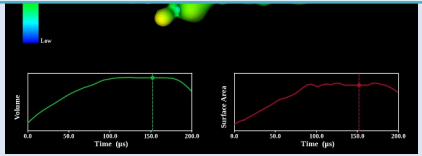


Comparative Analysis

These tools are used daily by scientists to digest and understand HPC simulation results



Visual Debugging



Presentation Graphics

Scientific visualization tools are used both *post hoc* and *in situ*

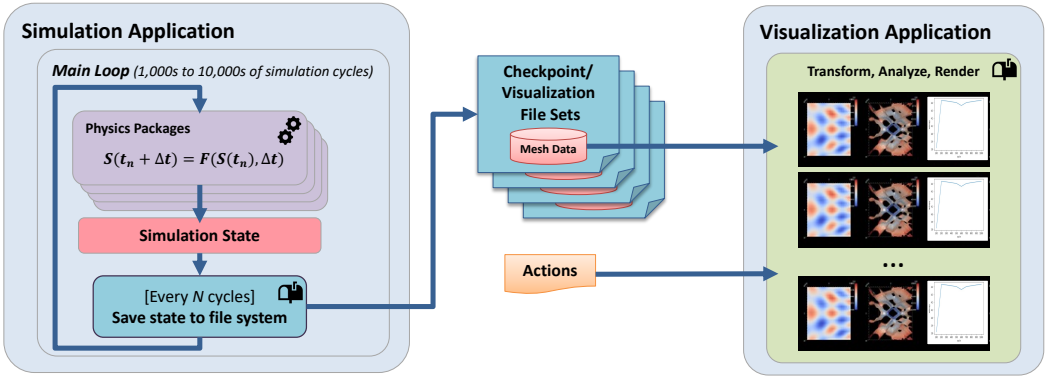
Post Hoc

Simulation data is processed after the simulation is run using distinct compute resources.

In Situ

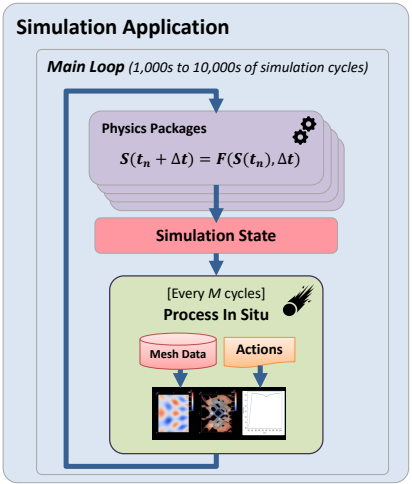
Simulation data is processed while it is generated, sharing compute resources with the simulation application.

Post Hoc visualization is the most widely used paradigm to process simulation results



In situ processing expands the data we can access

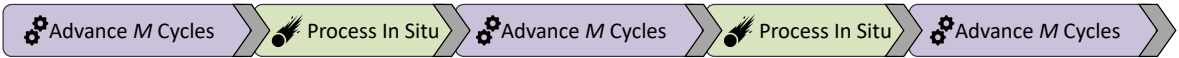
- In situ tools couple visualization and analysis routines with the simulation application (avoiding file system I/O)
- Pros:
  - No or greatly reduced I/O vs post hoc processing
  - Can access all simulation data
  - Computational power is readily available
  - Results are ready after simulation completes
- Cons:
  - More difficult when lacking a priori knowledge of what to visualize/analyze
  - Increasing complexity
  - Constraints (memory, network)



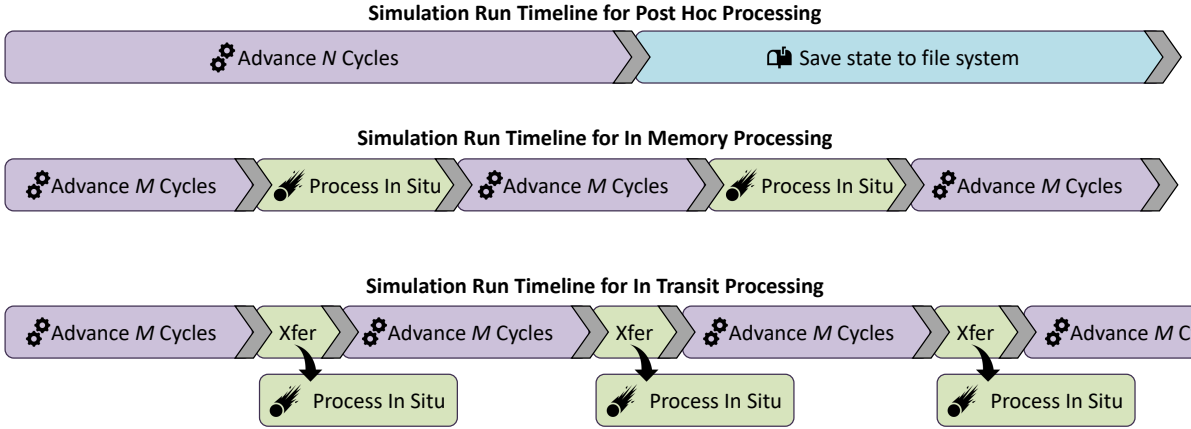
HPC Compute vs I/O speed ratios can favor in situ processing

Simulation Run Timeline for Post Hoc Processing

Simulation Run Timeline for In Memory Processing

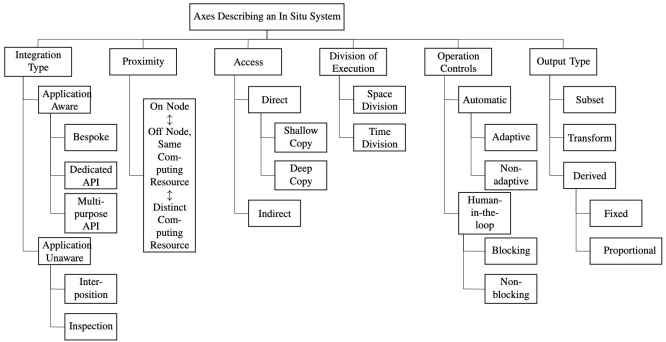


In transit is a flavor of in situ processing that can use additional resources to improve runtime



There are many considerations and flavors of in situ processing

Question: How deep does the rabbit hole go?



Answer: "A Terminology for In Situ Visualization and Analysis Systems", H. Childs, et al.
https://cdux.cs.uoregon.edu/pubs/ChildsIJHPCA.pdf

We need to pass simulation mesh data and user actions to our in situ visualization tools

Mesh Data

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coordsets:
  coords:
    type: "explicit"
    values:
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    elements:
      shape: "tet"
      connectivity: [0, 1, 3, 2, 4, 3, 1, 2]
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Actions

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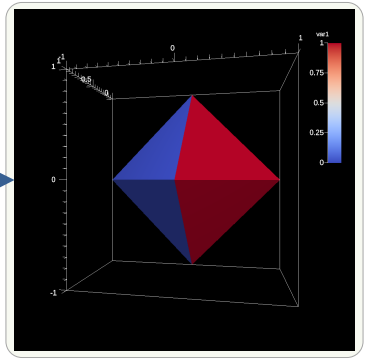
In Situ Visualization Tools

Transform, Analyze, Render

Ascent

ParaView Catalyst



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Question 1: How do we pass simulation meshes to these tools?

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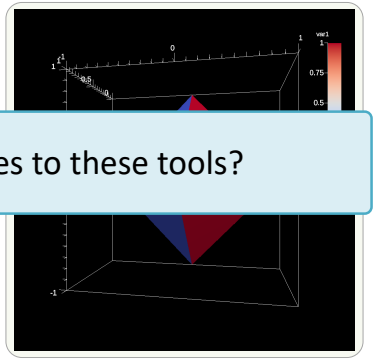
In Situ Visualization Tools

Ascent

ParaView Catalyst



HPC simulation applications implement and leverage a wide range of mesh data structures and APIs

- A variety of simulation codes leverage their own bespoke in-memory mesh data models.
- Other tools leverage a range of mesh-focused toolkits, frameworks, and APIs including: VTK, VTK-m, MFEM, SAMRAI, AMReX, (and many more …)
- A wide set of powerful analysis tools are mesh agnostic (NumPy, PyTorch, etc) and recasting mesh data into these tools is a challenge
- *A single full-fledged API will never cover all use cases across the ecosystem*

HPC simulation applications implement and leverage a wide range of mesh data structures and APIs

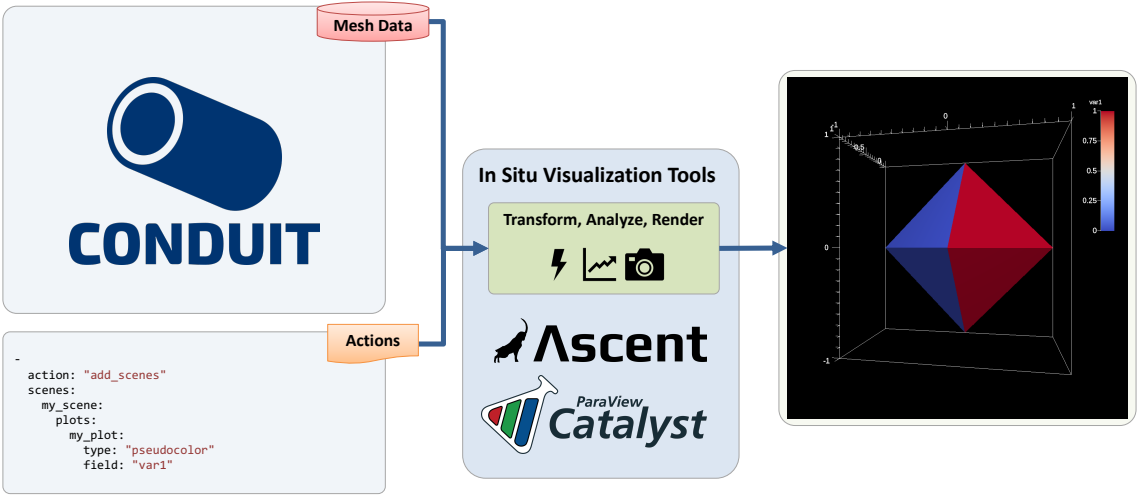
- A variety of simulation codes leverage their own bespoke in-memory mesh data models.
- Other tools leverage a range of mesh-focused toolkits, frameworks, and APIs

Conduit Mesh Blueprint provides a strategy to describe and adapt mesh data between a wide range of APIs

and recasting mesh data into these tools is a challenge

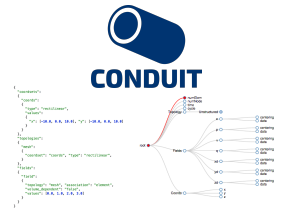
- *A single full-fledged API will never cover all use cases across the ecosystem*

Both Ascent and Catalyst use *Conduit* as a shared interface to describe and accept simulation mesh data

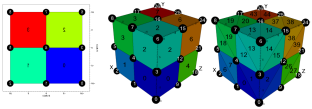


Conduit provides intuitive APIs for in-memory data description and exchange

- **Provides an intuitive API for in-memory data description**
  - Enables *human-friendly* hierarchical data organization
  - Can describe in-memory arrays without copying
  - Provides C++, C, Python, and Fortran APIs
- **Provides common conventions for exchanging complex data**
  - Shared conventions for passing complex data (e.g. *Simulation Meshes*) enable modular interfaces across software libraries and simulation applications
- **Provides easy to use I/O interfaces for moving and storing data**
  - Enables use cases like binary checkpoint restart
  - Supports moving complex data with MPI (serialization)



Hierarchical in-memory data description



Conventions for sharing in-memory mesh data

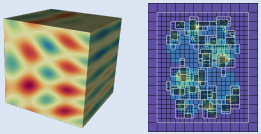
http://software.llnl.gov/conduit
http://github.com/llnl/conduit

Website and GitHub Repo

The Conduit Blueprint library provides tools to share common flavors of data with Conduit

Blueprint

Supports shared higher-level conventions for using Conduit to represent data



- Computational Meshes
- Multi-component Arrays
- One-to-many Relations
- Example Meshes
- Mesh Transforms

We will share several examples of Conduit “Blueprint” meshes in this tutorial

```
coordsets:
  coords:
    type: "explicit"
    values:
      x: [-1.0, 0.0, 0.0, 0.0, 1.0]
      y: [0.0, -1.0, 0.0, 1.0, 0.0]
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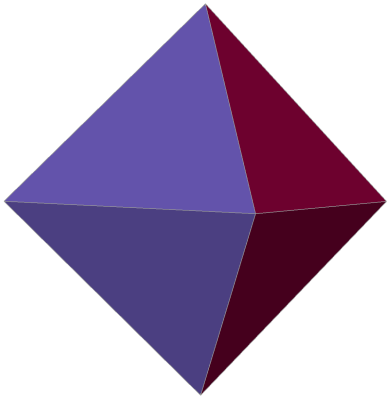
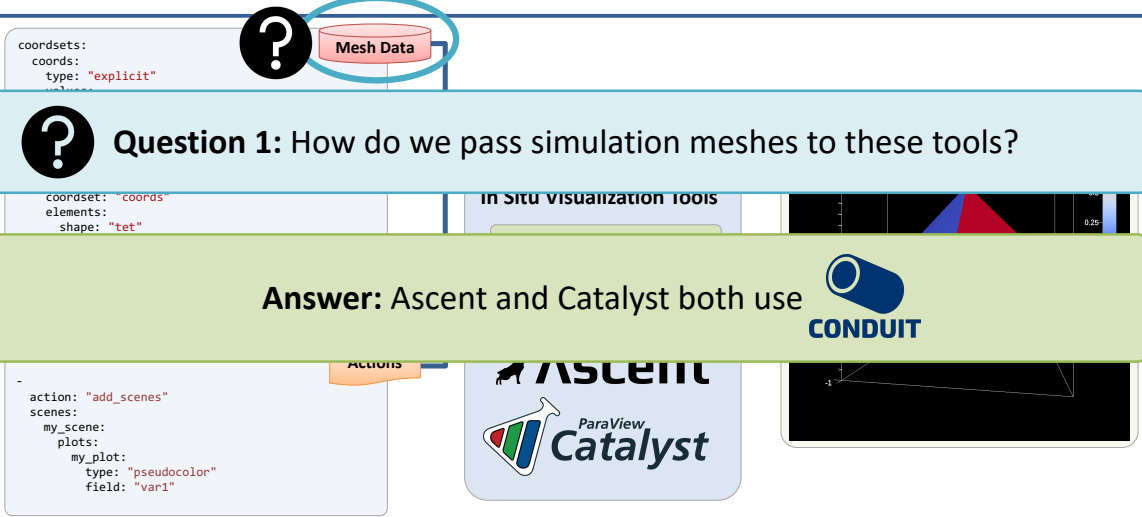
Example YAML Output



An unstructured tet mesh

We need to pass simulation mesh data and user actions to our in situ visualization tools



Question 1: How do we pass simulation meshes to these tools?

Answer: Ascent and Catalyst both use CONDUIT

We need to pass simulation mesh data and user actions to our in situ visualization tools

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Mesh Data

Question 2: How do we pass user actions to these tools?

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In Situ Visualization Tools

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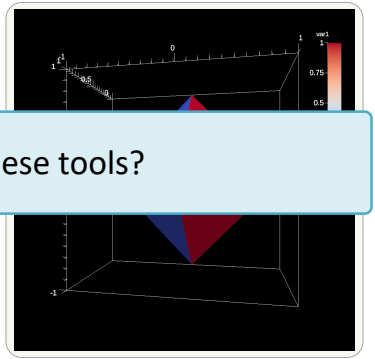

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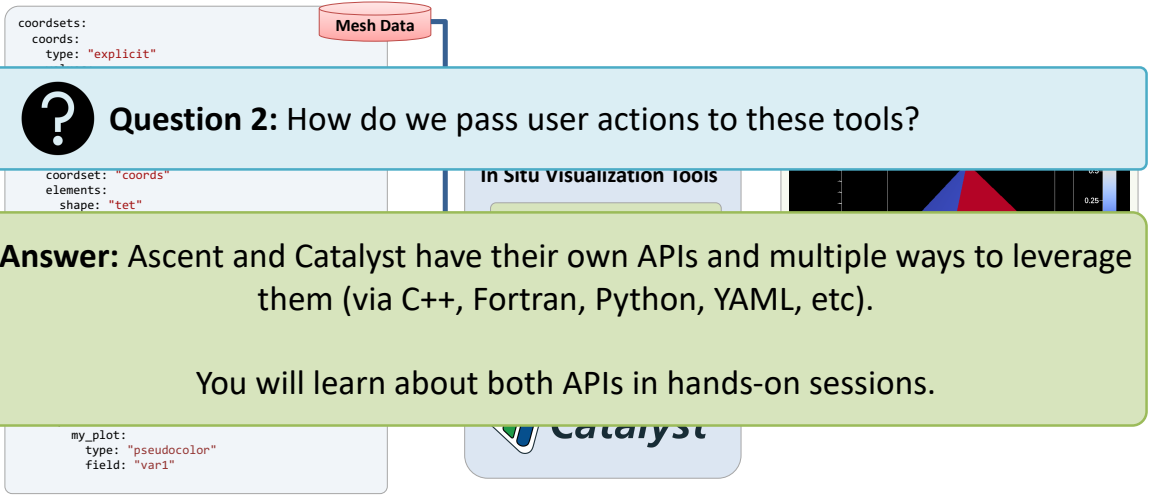

Question 2: How do we pass user actions to these tools?

Answer: Ascent and Catalyst have their own APIs and multiple ways to leverage them (via C++, Fortran, Python, YAML, etc).

You will learn about both APIs in hands-on sessions.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344.
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In Situ Analysis and Visualization with Ascent and ParaView Catalyst

[Ascent Project Overview]

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Denver, CO | i am hpc.

Ascent: Flyweight In Situ Visualization and Analysis for HPC Simulations

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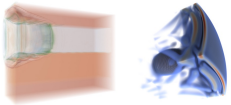
Ascent is an easy-to-use flyweight in situ visualization and analysis library for HPC simulations

- **Easy to use in-memory visualization and analysis**
  - Use cases: ***Making Pictures, Transforming Data,*** and ***Capturing Data***
  - Young effort, yet already supports most common visualization operations
  - Provides a simple infrastructure to integrate custom analysis
  - Provides C++, C, Python, and Fortran APIs
- **Uses a flyweight design targeted at next-generation HPC platforms**
  - Efficient distributed-memory (MPI) and many-core (CUDA, HIP, OpenMP) execution
    - Demonstrated scaling: In situ filtering and ray tracing across ***16,384 GPUs*** on LLNL's Sierra Cluster
  - Has lower memory requirements than current tools
  - Requires less dependencies than current tools (ex: no OpenGL)
    - Builds with Spack https://spack.io/

Ascent



Visualizations created using Ascent

python™ HDF CINEMA

Extracts supported by Ascent

http://ascent-dav.org
https://github.com/Alpine-DAV/ascent

Website and GitHub Repo

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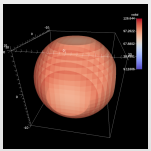
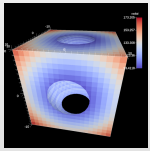
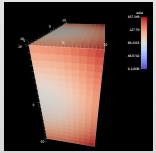
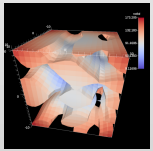
Ascent supports common visualization use cases









Clips

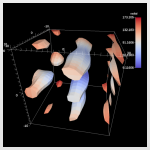
[powered by]

VTK-m

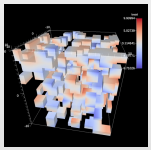
RAJA

mfem

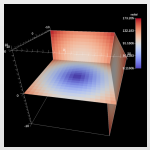
Devil Ray



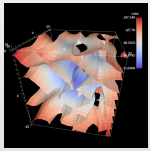
Iso-Volume



Threshold

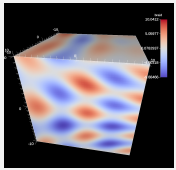


Slice

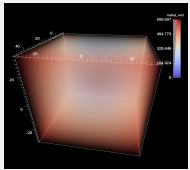


Contour

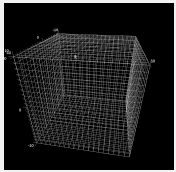
Rendering



Pseudocolor



Volume

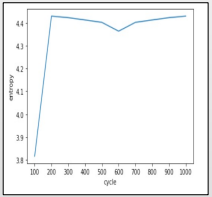


Mesh

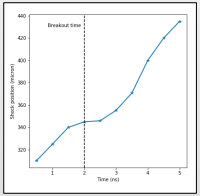
Ascent supports common analysis use cases

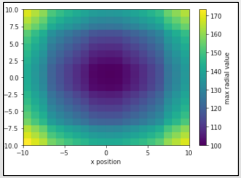
```
expression: |
  du = gradient(field('velocity','u'))
  dv = gradient(field('velocity','v'))
  dw = gradient(field('velocity','w'))
  w_x = dw.y - dv.z
  w_y = dw.z - dv.x
  w_z = dw.x - dv.y
  vector(w_x,w_y,w_z)
name: vorticity
```

Derived Fields



Time Histories





Lineouts and Spatial Binning

```
condition:
  entropy - history(entropy,
            relative_index = 1) > 0.5
```

Triggers

Extracts

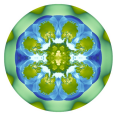
Scalar Images

HDF5 Files

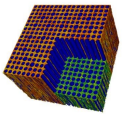
Cinema Databases

We are working to integrate and deploy Ascent with HPC simulation codes (ECP and beyond)

CEED
EXASCALE DISCRETIZATIONS

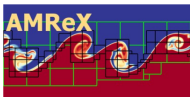


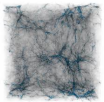
MARBL



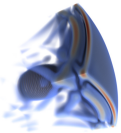
NekRS

AMReX

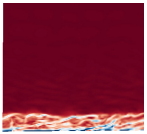




Nyx



WarpX



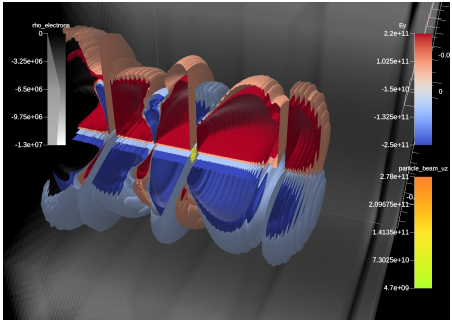
AMRWind

Pele

Ascent

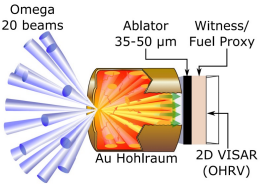
Science Enabling Results: WarpX Simulations on ORNL Frontier (2023)

- The ***578.8 million*** element simulation ran across ***552 GPUs*** on ***69 Nodes***
- The simulation application used **HIP** to run on the GPUs and passed device pointers to Ascent, providing **zero-copy** in situ processing of the time-varying data
- Ascent leveraged **RAJA** to create derived fields and **VTK-m** to run visualization algorithms on the GPUs

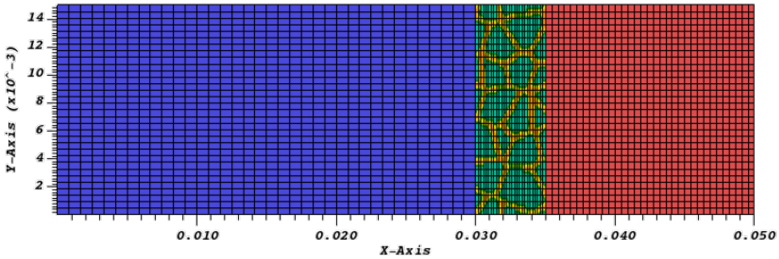


Visualization of a staged laser-wakefield accelerator simulation. Shown is the strong traversal focusing fields (red-blue) in the first plasma stage (gray) and injected into this structure is an electron beam (orange-green) that is accelerated to the right to high energies.

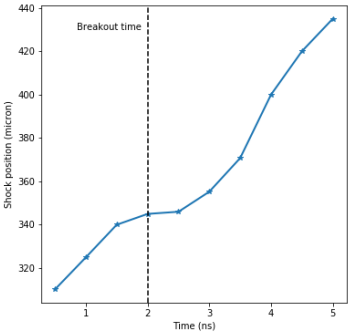
Science Enabling Results: Shock Front Tracking (VISAR)



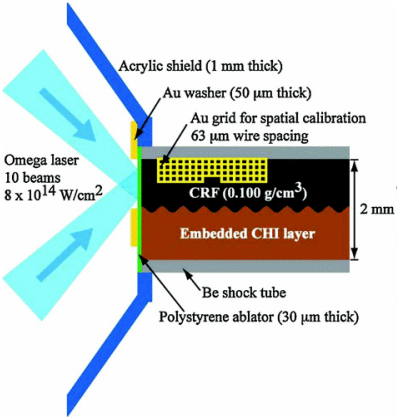
Velocity interferometer system for any reflector (VISAR)



Shock position tracked in Ascent

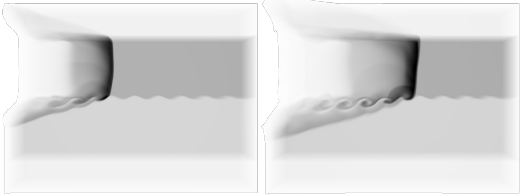


Science Enabling Results: Simulation Validation

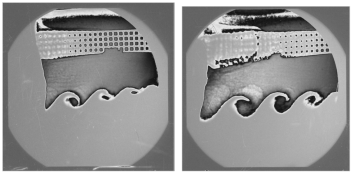


Radiographs

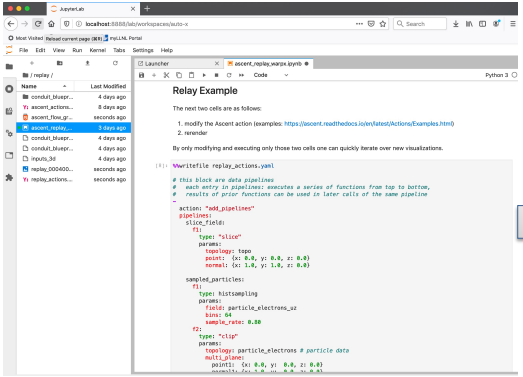
Simulated



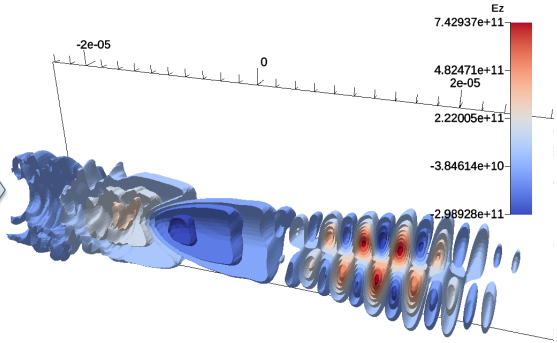
Experimental



Science Enabling Results: WarpX Workflow Tools (Jupyter Lab)



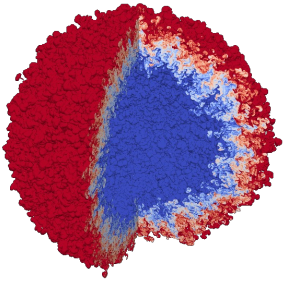
Jupyter Lab Interface



Resulting Image

Science Enabling Results: Rendering At Scale (2018)

- The ***97.8 billion*** element simulation ran across ***16,384 GPUs*** on ***4,096 Nodes***
- The simulation application used **CUDA** via **RAJA** to run on the GPUs
- Time-varying evolution of the mixing was visualized in-situ using **Ascent**, also leveraging 16,384 GPUs
- Ascent leveraged **VTK-m** to run visualization algorithms on the GPUs



Visualization of an idealized Inertial Confinement Fusion (ICF) simulation of Rayleigh-Taylor instability with two fluids mixing in a spherical geometry.

Ascent Project Resources and Contacts

Ascent Resources:

- Github: https://github.com/alpine-dav/ascent
- Docs: http://ascent-dav.org/
- Tutorial Landing Page: https://www.ascent-dav.org/tutorial/

Contact Info:

Cyrus Harrison: cyrush@llnl.gov
Nicole Marsaglia: marsaglia1@llnl.gov

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344.
Lawrence Livermore National Security, LLC

This research was supported by the Exascale Computing Project (17-SC-20-SC), a joint project of the U.S. Department of Energy's Office of Science and National Nuclear Security Administration, responsible for delivering a capable exascale ecosystem, including software, applications, and hardware technology, to support the nation's exascale computing imperative.

In Situ Analysis and Visualization with Ascent and ParaView Catalyst

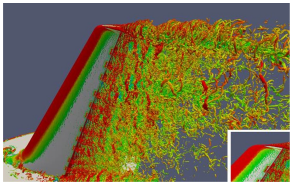
[Catalyst Project Overview]

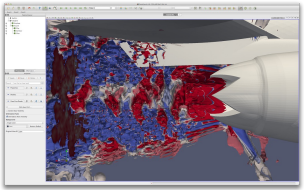
SC23 Tutorial
Monday November 13th, 2023

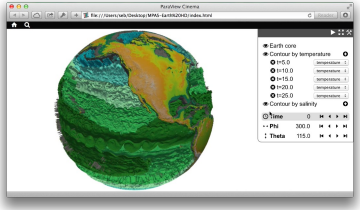
Corey Wetterer-Nelson, Kitware Inc.

Catalyst

ParaView Catalyst is an **in situ library**, with an adaptable application programming interface (API), that orchestrates the delicate alliance between simulation and analysis and/or visualization tasks.





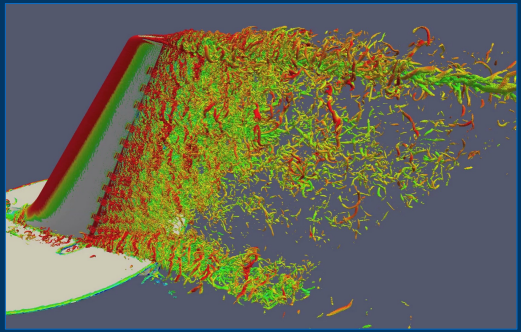


kitware

ParaView Catalyst background

- Initial work started in 2008 from an Army SBIR
- Sep 2010 First ParaView release with CoProcessing (renamed to Catalyst in 2012)
- Sep 2014 Catalyst Live released
- Sep 2014 ParaView Cinema released
- Scaled to 1Mi MPI ranks on ALCF's Mira BG/Q
- SC16 visualization showcase winner generated animation using Catalyst
- Based on the ParaView libraries – full access to ParaView capabilities
- Batch and interactive in situ analysis and visualization
- In transit workflows done with standalone ParaView and ADIOS

>1M MPI ranks on Mira@ANL



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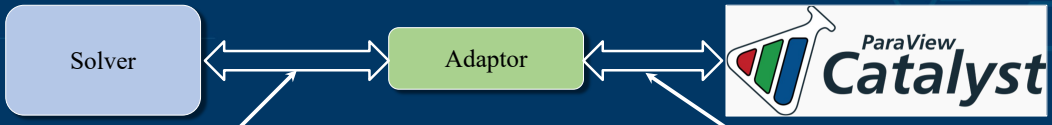
Simulation, Adaptor and Catalyst Interactions



- Typically 3 calls between simulation code and adaptor
  - **catalyst_initialize()**
    - MPI communicator (optional)
    - Add analysis scripts
  - **catalyst_execute()**
    - Does the work
  - **catalyst_finalize()**

- Information provided by solver to adaptor
  - Time, time step, force output
  - Grids and fields

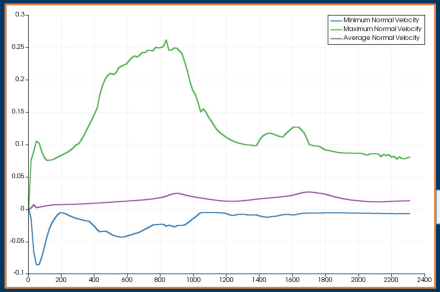
- **Information provided by adaptor**
  - Pipelines to execute
  - Time, time step, force output
  - Grid and fields when needed
  - MPI communicator
- **Information provided by Catalyst**
  - If co-processing needs to be done
  - What grids and fields are needed
- **User data can be shared both ways**

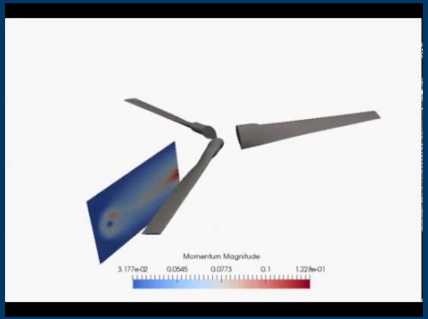
Performing In Situ Efficiently with Catalyst

- Small run-time overhead
  - Small initialization and finalization times
  - Scalable analysis and visualization algorithms
  - Reduced amount of IO (possibly at expense of more complex IO patterns)
- Small code footprint
  - Typically ~3 calls from simulation code to Catalyst (initialize, execute, finalize)
- Efficiency in computing and memory-management
  - On demand compute
  - Request only needed information
  - Flexible ways to represent different pieces of information
  - Zero-copy use of simulation data structures

Configurability

- Allow simulation specific output customization
- Edit Python scripts for Catalyst
  - Can change in situ output without any recompilation



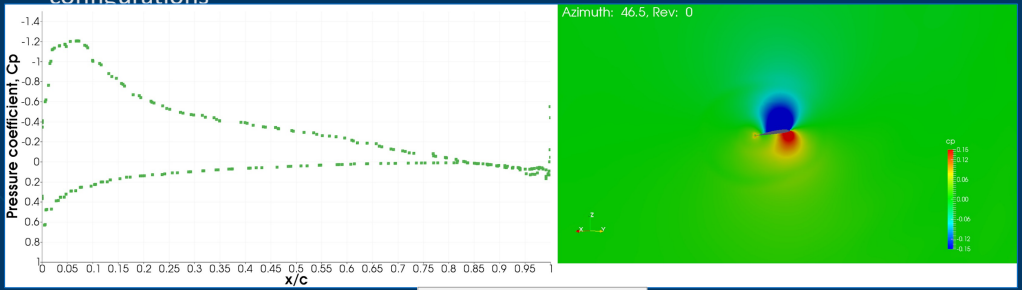


Results courtesy Rajneesh Singh & Ben Jimenez (ARL)

kitware

Combined Viz & Analysis

- Constructing relatively complex in situ pipelines requires both domain and viz experts
  - Increased interactions
  - Viz experts can help guide work early on
- Conceptually complex in situ output can be done through parameterized input configurations



Singh & Jimenez (ARL)

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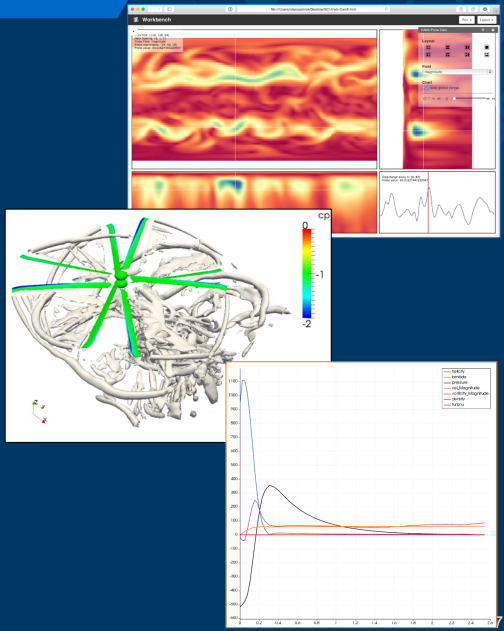
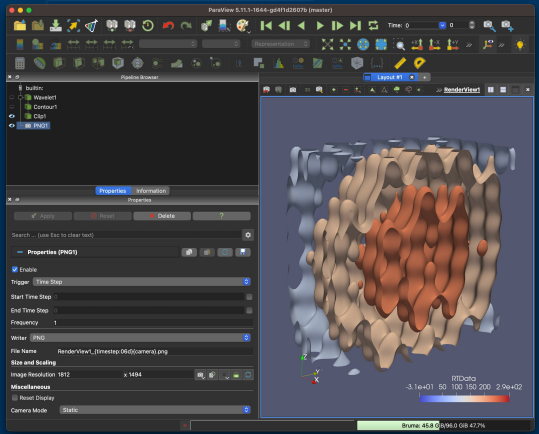
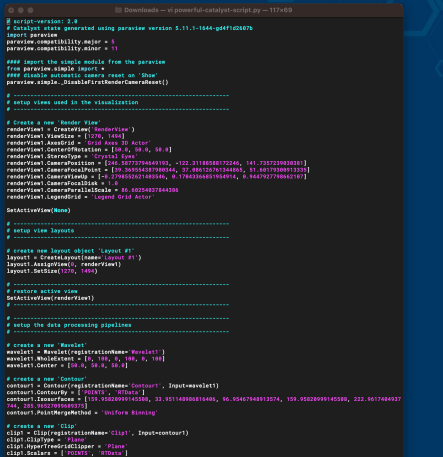
Multiple Output Types

- Images
  - Size is independent of grid size
  - Explorable through Cinema output (cinemascience.org)
  - Charts
- Data extracts
  - Large collection of file formats supported including VTK, ADIOS, HDF5 (in progress)
- ASCII output
  - Single quantities (e.g. field values at a point)
  - Statistics
  - Custom (e.g. value and location of highest temperature value)



Automated Pipeline Generation in ParaView





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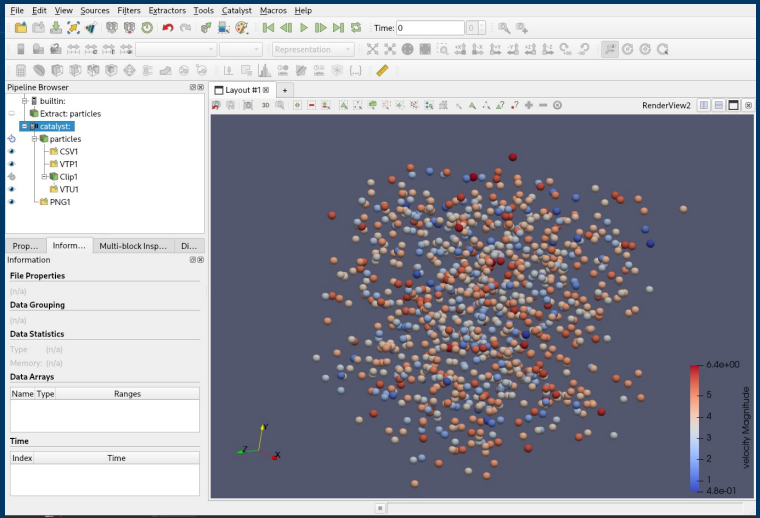
ParaView Enables Live Visualization



kitware

Catalyst Runtime Selectable Backends

- **catalyst-stub**: no external dependencies, suitable for building
- **catalyst-paraview**: full in situ access to ParaView and VTK
- **catalyst-adios:** in transit workflows for asynchronous interactive analysis and visualization
- **catalyst-ascent** (you read that right!): Catalyst passthrough to Ascent platform
- Debug, replay, etc.
- your implementation!

In Situ Analysis and Visualization with Ascent and ParaView Catalyst

[Conduit Mesh Representation Introduction and Hands-on]

SC23 Tutorial
Monday November 13th, 2023

Cyrus Harrison, Lawrence Livermore National Laboratory (LLNL)

Jean M. Favre, Swiss National supercomputing Centre (CSCS)

A heat-diffusion mini-app to demonstrate in-situ visualization with Ascent and Catalyst

Jean M. Favre

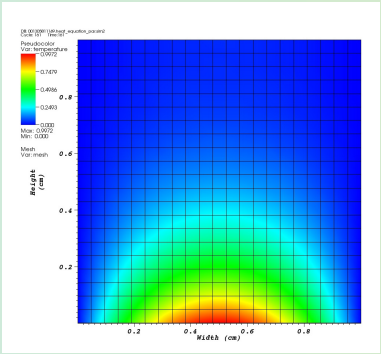
Swiss National supercomputing Centre (CSCS)

Motivations

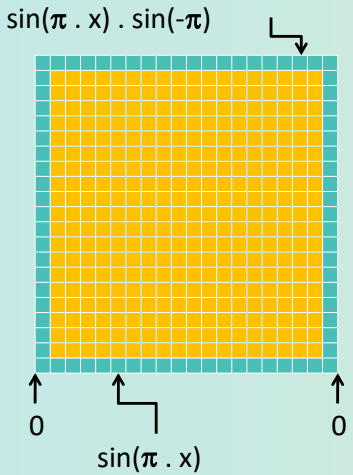
- A simple demonstrator for in-situ couplings based on Conduit + {Ascent, Catalyst}
  - in C++ and Python
  - with MPI (optional)
  - with four different grid types (uniform, rectilinear, structured and unstructured)

Assumptions

- This 2D heat-diffusion solver relies on a very simple 5-point stencil to update the nodes of a mesh.
- No focus on computational performance
- A very simple partitioning grid for parallel runs
- The underlying grid points form a uniform, Cartesian grid, defined solely with an **origin**, a fixed **spacing** between points (in X and Y), and a grid **resolution**
- For didactic purposes only, the same grid can also be viewed as:
  - a rectilinear grid (special case with equally spaced grid points along both axis)
  - A structured grid (special case with the points' coordinates explicitly given)
  - An unstructured grid of quadrilateral cells (with an explicit connectivity list)
- The physical global domain is [0.,0.]->[1.,1.]



The domain fixed boundary conditions



Update grid with solver

Fixed boundary conditions

Laplace equation: $\Delta u = 0$

Generic run-time options

usage: heat_diffusion_insitu_*.py [-h] [-t TIMESTEPS] [--res RES] [-m {uniform,rectilinear,structured,unstructured} [-n] [-v]

-h, --help show this help message and exit

-t TIMESTEPS, --timesteps TIMESTEPS

number of timesteps to run the miniapp (default: 1000)

--res RES resolution in each coordinate direction (default: 64)

-m {uniform,rectilinear,structured,unstructured}, --mesh {uniform,rectilinear,structured,unstructured}

mesh type (default: uniform)

-n, --noinsitu toggle the use of the in-situ vis coupling

-v, --verbose toggle printing of the conduit nodes

API-specific run-time options

With Ascent

-f FREQUENCY, --frequency FREQUENCY

How often should the Ascent script be executed

-d DIR, --dir DIR path to a directory where to dump the Blueprint output (final step)

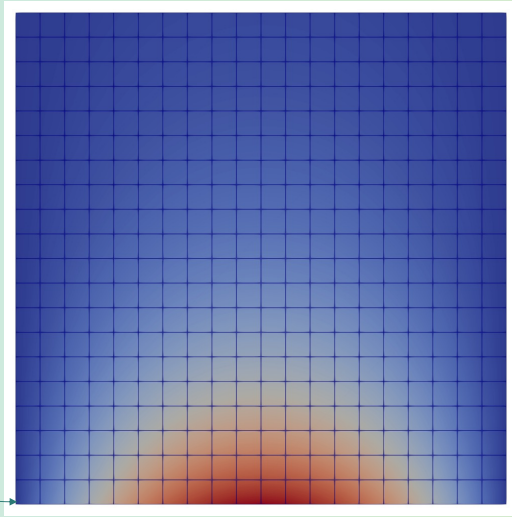
With Catalyst

-s SCRIPT, --script SCRIPT

path to the Catalyst script to use for in situ processing.

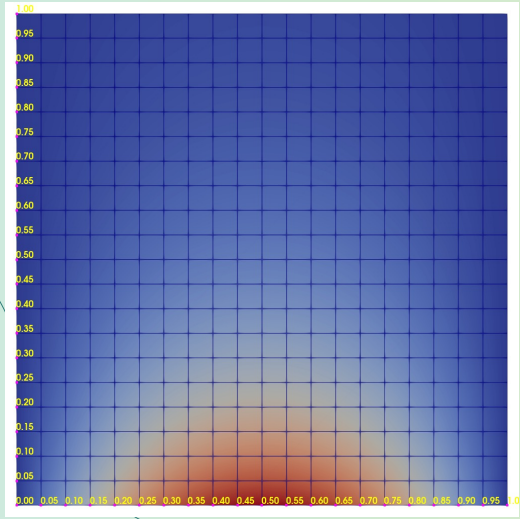
The default case: a uniform grid

```
coordsets:
  coords:
    type: "uniform"
    dims:
      i: 21
      j: 21
    origin:
      x: 0.0
      y: 0.0
    spacing:
      dx: 0.05
      dy: 0.05
topologies:
  mesh:
    type: "uniform"
    coordset: "coords"
fields:
  temperature:
    association: "vertex"
    topology: "mesh"
    Values: [0.0, 0.156, 0.309, ..., 0.006, 5.29e-18]
```



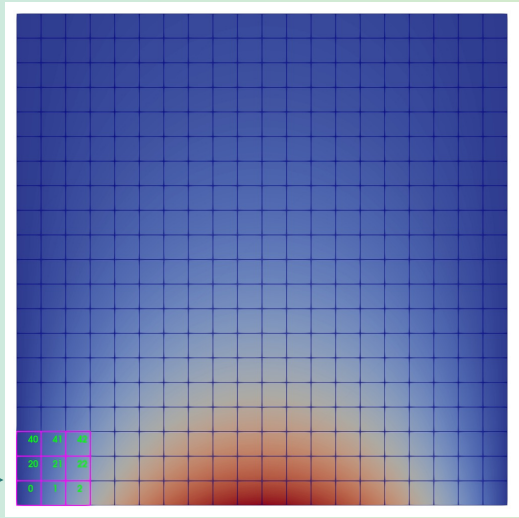
The rectilinear grid

```
coordsets:
  coords:
    type: “rectilinear"
    values:
      x: [0.0, 0.05, 0.1, ..., 0.95, 1.0]
      y: [0.0, 0.05, 0.1, ..., 0.95, 1.0]
topologies:
  mesh:
    type: " rectilinear "
    coordset: "coords"
fields:
  temperature:
    association: "vertex"
    topology: "mesh"
    values: [0.0, 0.156, 0.309, ..., 0.006,
5.29e-18]
```



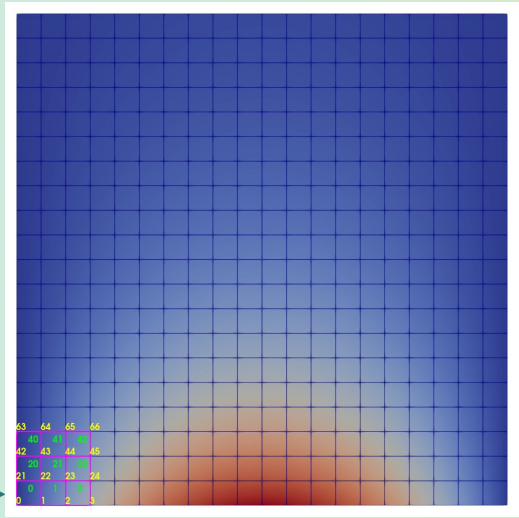
The structured grid

```
coordsets:
  coords:
    type: "explicit"
    values:
      x: [0.0, 0.05, 0.1, ..., 0.95, 1.0]
      y: [0.0, 0.0, 0.0, ..., 1.0, 1.0]
topologies:
  mesh:
    type: "structured"
    coordset: "coords"
     elements:
      dims:
        i: 20
        j: 20
fields:
  temperature:
    association: "vertex"
    topology: "mesh"
    values: [0.0, 0.149, 0.294, ..., 0.006,
5.29e-18]
```



The unstructured grid

```
coordsets:
  coords:
    type: "explicit"
    values:
      x: [0.0, 0.05, 0.1, ..., 0.95, 1.0]
      y: [0.0, 0.0, 0.0, ..., 1.0, 1.0]
topologies:
  mesh:
    type: "unstructured"
    coordset: "coords"
    elements:
      shape: "quad"
      connectivity: [0, 21, 22, 1,..., 440, 419]
fields:
  temperature:
    association: "vertex"
    topology: "mesh"
    values: [0.0, 0.156, 0.309, ..., 0.006,
5.29e-18]
```



Actions need to be defined

Ascent

```
actions = conduit.Node()
add_act = actions.append()
add_act["action"] = "add_scenes"

# declare a scene (s1) to render the dataset
scenes = add_act["scenes"]
scenes["s1/plots/p1/type"] = "pseudocolor"
scenes["s1/plots/p1/field"] = "temperature“
# add a second plot to draw the grid lines
scenes["s1/plots/p2/type"] = "mesh"
```

ParaView Catalyst (can be written by the ParaView client)

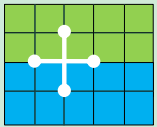
```
renderView1 = GetRenderView()
reader = TrivialProducer(registrationName='grid')

rep = Show(reader, renderView1)
rep.Representation = 'Outline'
ColorBy(rep, ['POINTS', 'temperature'])
temperatureLUT = GetColorTransferFunction('temperature')
temperatureLUT.RescaleTransferFunction(0.0, 1.0)

contour1 = Contour(Input=reader)
contour1.ContourBy = ['POINTS', 'temperature']
contour1.ComputeScalars = 1
contour1.Isosurfaces = [i*0.1 for i in range(11)]

png1 = CreateExtractor('PNG', renderView1)
png1.Trigger = 'TimeStep'
png1.Trigger.Frequency = 100
png1.Writer.FileName = 'view-{timestep:06d}{camera}.png'
```

Going parallel

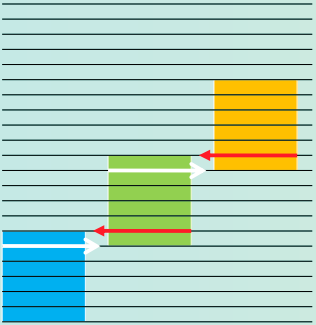
MPI-BASED EXECUTION

The Python example uses a 1D grid partitioning

- The grid is partitioned along the Y direction
- Boundary conditions are set
- A single line of ghost-nodes insure that the 5-point stencil is continuous across MPI task boundaries



Ghost data exchange for N MPI tasks



Overlap Send and Receive

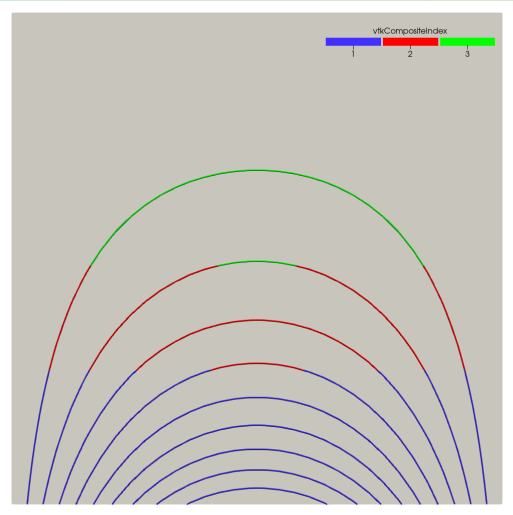
Proc. 0 does not receive data from “below”

Proc. (N-1) does not send data “above”

Conduit nodes:
What's new in parallel?

```
coordsets:
  coords:
    type: "uniform"
    dims:
      i: 21
      j: … => new for each MPI task
    origin:
      x: 0.0
      y: … => new for each MPI task
```

```
coordsets:
  coords:
    type: "rectilinear"
    values:
      x: [0.0, 0.05, 0.1, ..., 0.95, 1.0]
      y: … => new for each MPI task
```



Iso-contour lines, colored by their process-id

Conduit nodes:
What's new in parallel?

```
coordsets:
  coords:
    type: "explicit"
    values:
      x: [0.0, 0.05, 0.1, ..., 0.95, 1.0]
      y: … => new for each MPI task
topologies:
  mesh:
    type: "structured"
    coordset: "coords"
     elements:
       dims:
         i: 20
         j: … => new for each MPI task
```

```
coordsets:
  coords:
    type: "explicit"
    values:
      x: [0.0, 0.05, 0.1, ..., 0.95, 1.0]
      y: … => new for each MPI task topologies
  mesh:
    type: "unstructured"
    coordset: "coords"
    elements:
      shape: "quad"
      connectivity: … => new for each MPI task
```

N.B. the connectivity list can use local point ids (starting at 0)

The Blueprint output

- It is common for Blueprint data files to represent meshes that have been partitioned and must later be treated as a whole.
- Blueprint root files contain an index that facilitates reading in many individual Blueprint files => metadata about the overall contents of individual files
- The root file is a hierarchical index dataset created with Conduit that has been saved to a file using Relay
- https://llnl-conduit.readthedocs.io/en/latest/blueprint_mesh.html#mesh-index-protocol

- Can be read by VisIt out-of-the-box
- Currently developing a reader for ParaView (WIP)

The Blueprint output

```
>>> import conduit

>>> import conduit.relay.io

>>> import numpy as np

>>> mesh = conduit.Node()

>>> conduit.relay.io.load(mesh,
"/dev/shm/mesh.cycle_001000.root", "hdf5")

>>> mesh
```

```
blueprint_index:
  mesh:
    state:
      number_of_domains: 4
      partition_pattern:
"mesh.cycle_001000/domain_{domain:06d}.hdf5:/"
      partition_map:
        file: [0, 1, 2, 3]
        domain: [0, 1, 2, 3]
    coordsets:
      coords:
        type: "uniform"
        coord_system:
          type: "cartesian"
      path: "mesh/coordsets/coords"
    topologies:
      mesh:
        type: "uniform"
        coordset: "coords"
        path: "mesh/topologies/mesh"
    fields:
      temperature:
        number_of_components: 1
        topology: "mesh"
        association: "vertex"
```

Demonstrations / exercises

```
python3 heat_diffusion_insitu_parallel_Ascent.py --help
python3 heat_diffusion_insitu_parallel_Ascent.py -v --mesh=uniform --res=64

mpiexec –n 4 python3 heat_diffusion_insitu_parallel_Ascent.py -v --mesh=uniform --res=64
```

```
python3 heat_diffusion_insitu_parallel_Catalyst.py --help
python3 heat_diffusion_insitu_parallel_Catalyst.py -v --mesh=uniform --res=64

mpiexec –n 4 python3 heat_diffusion_insitu_parallel_Catalyst.py -v --script=pvPythonScript.py
```

In Situ Analysis and Visualization with Ascent and ParaView Catalyst

[Ascent Hands-on]

SC23 Tutorial
Monday November 13th, 2023

Cyrus Harrison, Lawrence Livermore National Laboratory (LLNL)

Nicole Marsaglia, Lawrence Livermore National Laboratory (LLNL)

SC23
Denver, CO | i am hpc.

Ascent Hands-on Session

SC23 Tutorial

Monday November 13th, 2023

Cyrus Harrison (LLNL)
Nicole Marsaglia (LLNL)

LLNL-PRES-856413
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

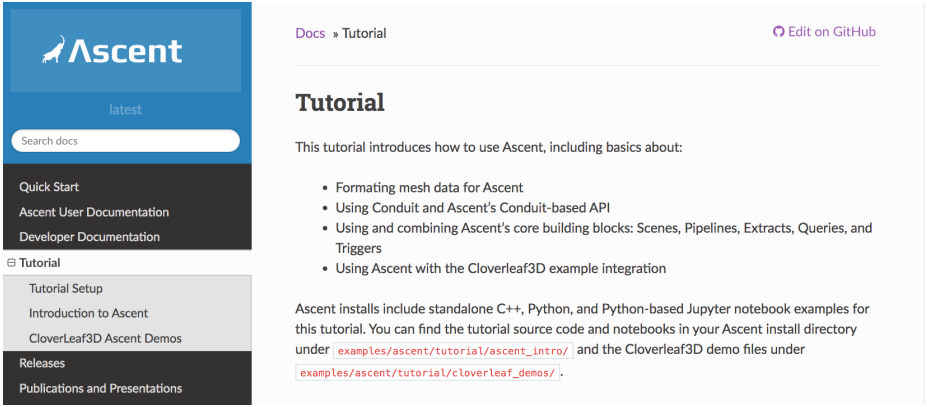
Lawrence Livermore National Laboratory

Today we will teach you about Ascent's API and capabilities

You will learn:

- How to use Conduit, the foundation of Ascent's API
- How to get your simulation data into Ascent
- How to tell Ascent what pictures to render and what analysis to execute

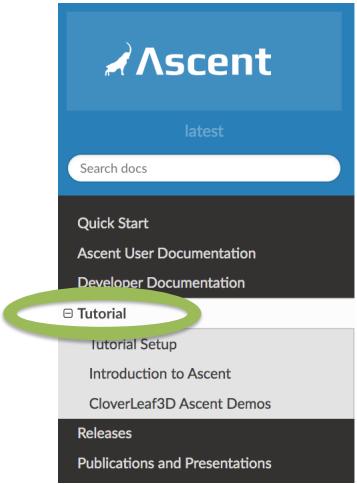
Ascent tutorial examples are outlined in our documentation and included ready to run in Ascent installs



http://ascent-dav.org

Ascent tutorial examples are outlined in our documentation and included ready to run in Ascent installs

- http://ascent-dav.org
- Click on “Tutorial”



Ascent's interface provides five top-level functions

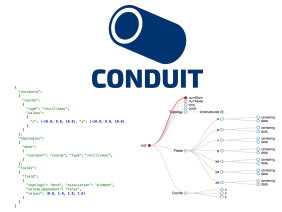
- **open() / close()**
  - Initialize and finalize an Ascent instance
- **publish()**
  - Pass your simulation data to Ascent
- **execute()**
  - Tell Ascent what to do
- **info()**
  - Ask for details about Ascent's last operation

```
//
// Run Ascent
//

Ascent ascent;
ascent.open();

ascent.publish(data);
ascent.execute(actions);
ascent.info(details);

ascent.close();
```

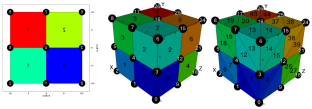
The *publish(), execute(),* and *info()* methods take Conduit trees as an argument.
What is a Conduit tree?

Conduit provides intuitive APIs for in-memory data description and exchange

- **Provides an intuitive API for in-memory data description**
  - Enables *human-friendly* hierarchical data organization
  - Can describe in-memory arrays without copying
  - Provides C++, C, Python, and Fortran APIs
- **Provides common conventions for exchanging complex data**
  - Shared conventions for passing complex data (e.g. *Simulation Meshes*) enable modular interfaces across software libraries and simulation applications
- **Provides easy to use I/O interfaces for moving and storing data**
  - Enables use cases like binary checkpoint restart
  - Supports moving complex data with MPI (serialization)



Hierarchical in-memory data description



Conventions for sharing in-memory mesh data

http://software.llnl.gov/conduit
http://github.com/llnl/conduit

Website and GitHub Repo

Ascent uses Conduit to provide a flexible and extendable API

- Conduit underpins Ascent's support for C++, C, Python, and Fortran interfaces
- Conduit also enables using YAML to specify Ascent actions
- Conduit's zero-copy features help couple existing simulation data structures
- Conduit Blueprint provides a standard for how to present simulation meshes

Learning Ascent equates to learning how to construct and pass Conduit trees that encode your data and your expectations.

To start, let's look at the Ascent "First Light" Example in C++

- https://ascent.readthedocs.io/en/latest/Tutorial_Intro_First_Light.html

```
#include <iostream>

#include "ascent.hpp"
#include "conduit_blueprint.hpp"

using namespace ascent;
using namespace conduit;

int main(int argc, char **argv)
{
    // print info about how ascent was configured
    std::cout << ascent::about() << std::endl;

    // create conduit node with an example mesh using
    // conduit blueprint's braid function
    // ref: https://llnl-conduit.readthedocs.io/en/latest/blueprint_mesh.html#braid

    // things to explore:
    //  changing the mesh resolution

    Node mesh;
    conduit::blueprint::mesh::examples::braid("hexs",
                                              50,
                                              50,
                                              50,
                                              mesh);
```

Instrument your "main" loop or similar function with access to evolving simulation state

This code generates an example mesh

To start, let's look at the Ascent "First Light" Example in C++

- https://ascent.readthedocs.io/en/latest/Tutorial_Intro_First_Light.html

```
// create an Ascent instance
Ascent a;

// open ascent
a.open();
```

Create an Ascent instance and set it up

```
// publish mesh data to ascent
a.publish(mesh);
```

Now Ascent has access to our mesh data

To start, let's look at the Ascent "First Light" Example in C++

- https://ascent.readthedocs.io/en/latest/Tutorial_Intro_First_Light.html

```
//
// Ascent's interface accepts "actions"
// that to tell Ascent what to execute
//
Node actions;
Node &add_act = actions.append();
add_act["action"] = "add_scenes";

// Create an action that tells Ascent to:
// add a scene (s1) with one plot (p1)
// that will render a pseudocolor of
// the mesh field `braid`
Node & scenes = add_act["scenes"];

// things to explore:
//  changing plot type (mesh)
//  changing field name (for this dataset: radial)
scenes["s1/plots/p1/type"] = "pseudocolor";
scenes["s1/plots/p1/field"] = "braid";
// set the output file name (ascent will add ".png")
scenes["s1/image_name"] = "out_first_light_render_3d";
```

Create a tree that describes the actions we want Ascent to do

```
-
  action: "add_scenes"
  scenes:
    s1:
      plots:
        p1:
          type: "pseudocolor"
          field: "braid"
      image_name: "out_first_light_render_3d"
```

```
// view our full actions tree
std::cout << actions.to_yaml() << std::endl;
```

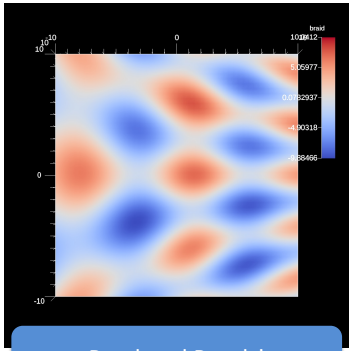
Equivalent YAML Description

To start, let's look at the Ascent "First Light" Example in C++

- https://ascent.readthedocs.io/en/latest/Tutorial_Intro_First_Light.html

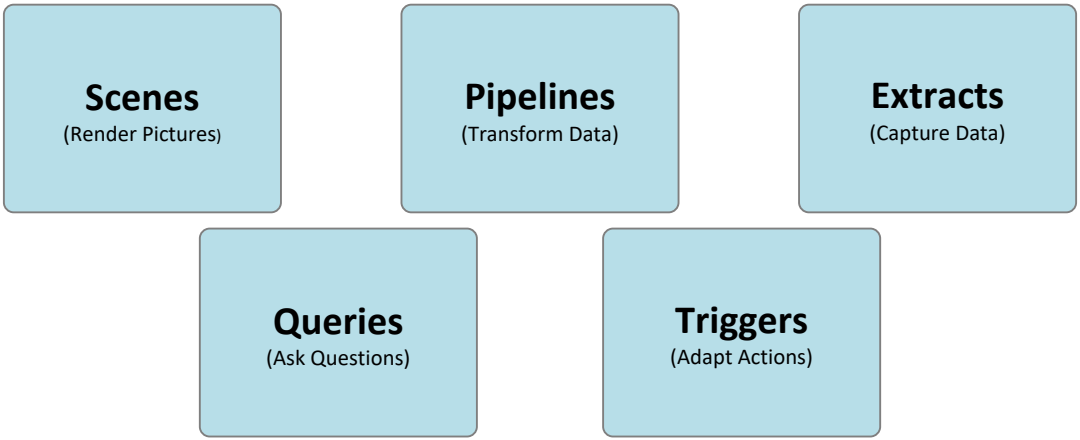
```
// execute the actions
a.execute(actions);
```

Tell Ascent to execute these actions



Rendered Result!

Ascent's interface provides five composable building blocks

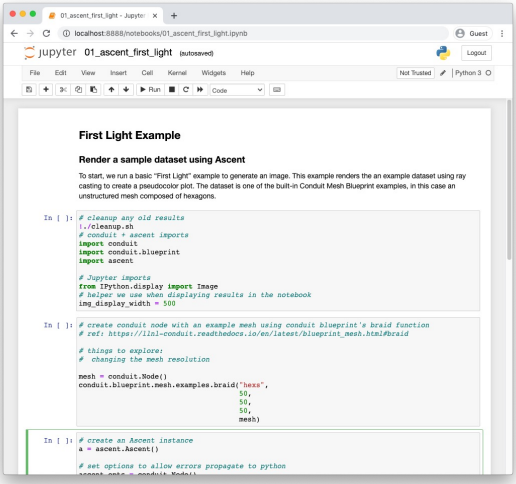


The tutorial provides examples for all of these.

For the reminder of the tutorial, we will run the Ascent Tutorial examples using Jupyter Notebooks

NOTE:

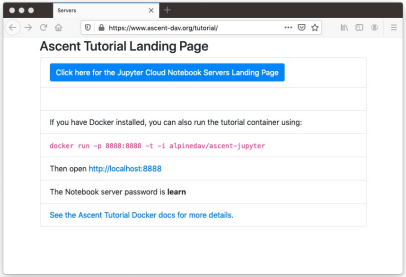
- VPNs or firewalls may block access to general AWS IP addresses and ports
- You may need to disconnect from VPN or request a firewall exemption
- LLNL attendees, you can use the EOR process: https://cspservices.llnl.gov/eor/



You can run our tutorial examples using cloud hosted Jupyter Lab servers

Start here:

https://www.ascent-dav.org/tutorial/



Thanks!

Ascent Resources:

- Github: https://github.com/alpine-dav/ascent
- Docs: http://ascent-dav.org/
- Tutorial Landing Page: https://www.ascent-dav.org/tutorial/

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Nicole Marsaglia: marsaglia1@llnl.gov

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Lawrence Livermore National Security, LLC

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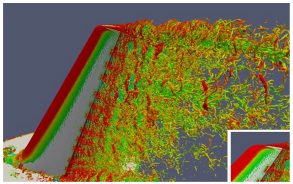
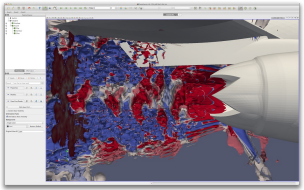
[Catalyst Hands-on]

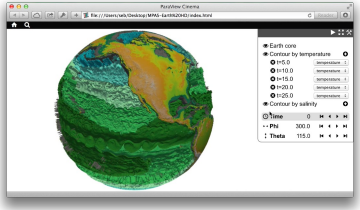
SC23 Tutorial
Monday November 13th, 2023

Corey Wetterer-Nelson, Kitware Inc.

Catalyst







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Anatomy of a Catalyst Adaptor

https://gitlab.kitware.com/paraview/paraview/-/tree/master/Examples/Catalyst2

- Image Data
- Polygonal
- Polyhedra
- Multimesh
- Multi Channel

Anatomy of a Catalyst Adaptor

Initialize

CxxFullExample — vi CatalystAdaptor.h — 84×16

```
void Initialize(int argc, char* argv[])
{
  conduit_cpp::Node node;
  for (int cc = 1; cc < argc; ++cc)
  {
    node["catalyst/scripts/script" + std::to_string(cc - 1)].set_string(argv[cc]);
  }
  node["catalyst_load/implementation"] = "paraview";
  node["catalyst_load/search_paths/paraview"] = PARAVIEW_IMPL_DIR;
  catalyst_status err = catalyst_initialize(conduit_cpp::c_node(&node));
  if (err != catalyst_status_ok)
  {
    std::cerr << "Failed to initialize Catalyst: " << err << std::endl;
  }
}
```

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Anatomy of a Catalyst Adaptor

Execute

CxxFullExample — vi CatalystAdaptor.h — 70×12

```
void Execute(int cycle, double time, Grid& grid, Attributes& attribs)
{
  conduit_cpp::Node exec_params;

  // add time/cycle information
  auto state = exec_params["catalyst/state"];
  state["timestep"].set(cycle);
  state["time"].set(time);
  state["multiblock"].set(1);
```

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Anatomy of a Catalyst Adaptor

Execute

CxxFullExample — vi CatalystAdaptor.h — 99×29

```
// Add channels.
// We only have 1 channel here. Let's name it 'grid'.
auto channel = exec_params["catalyst/channels/grid"];

// Since this example is using Conduit Mesh Blueprint to define the mesh,
// we set the channel's type to "mesh".
channel["type"].set("mesh");

// now create the mesh.
auto mesh = channel["data"];

// start with coordsets (of course, the sequence is not important, just make
// it easier to think in this order).
mesh["coordsets/coords/type"].set("explicit");

mesh["coordsets/coords/values/x"].set_external(
  grid.GetPointsArray(), grid.GetNumberOfPoints(), /*offset=*/0, /*stride=*/3 * sizeof(double));
mesh["coordsets/coords/values/y"].set_external(grid.GetPointsArray(), grid.GetNumberOfPoints(),
  /*offset=*/sizeof(double), /*stride=*/3 * sizeof(double));
mesh["coordsets/coords/values/z"].set_external(grid.GetPointsArray(), grid.GetNumberOfPoints(),
  /*offset=*/2 * sizeof(double), /*stride=*/3 * sizeof(double));

// Next, add topology
mesh["topologies/mesh/type"].set("unstructured");
mesh["topologies/mesh/coordset"].set("coords");
mesh["topologies/mesh/elements/shape"].set("hex");
mesh["topologies/mesh/elements/connectivity"].set_external(
  grid.GetCellPoints(0), grid.GetNumberOfCells() * 8);
```

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Anatomy of a Catalyst Adaptor

Execute

CxxFullExample — vi CatalystAdaptor.h — 111×27

```
  // Finally, add fields.
  auto fields = mesh["fields"];
  fields["velocity/association"].set("vertex");
  fields["velocity/topology"].set("mesh");
  fields["velocity/volume_dependent"].set("false");

  // velocity is stored in non-interlaced form (unlike points).
  fields["velocity/values/x"].set_external(
    attribs.GetVelocityArray(), grid.GetNumberOfPoints(), /*offset=*/0);
  fields["velocity/values/y"].set_external(attribs.GetVelocityArray(), grid.GetNumberOfPoints(),
    /*offset=*/grid.GetNumberOfPoints() * sizeof(double));
  fields["velocity/values/z"].set_external(attribs.GetVelocityArray(), grid.GetNumberOfPoints(),
    /*offset=*/grid.GetNumberOfPoints() * sizeof(double) * 2);

  // pressure is cell-data.
  fields["pressure/association"].set("element");
  fields["pressure/topology"].set("mesh");
  fields["pressure/volume_dependent"].set("false");
  fields["pressure/values"].set_external(attribs.GetPressureArray(), grid.GetNumberOfCells());

  catalyst_status err = catalyst_execute(conduit_cpp::c_node(&exec_params));
  if (err != catalyst_status_ok)
  {
    std::cerr << "Failed to execute Catalyst: " << err << std::endl;
  }
}
```

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Anatomy of a Catalyst Adaptor

Finalize

CxxFullExample — vi CatalystAdaptor.h — 71×11

```
void Finalize()
{
  conduit_cpp::Node node;
  catalyst_status err = catalyst_finalize(conduit_cpp::c_node(&node));
  if (err != catalyst_status_ok)
  {
    std::cerr << "Failed to finalize Catalyst: " << err << std::endl;
  }
}
```

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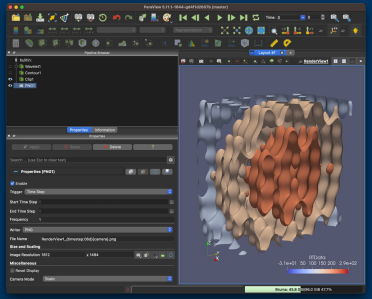
Customizing Catalyst Pipelines

- Build example with Catalyst enabled
- Run example with sample pipeline script
- Modify the script to manipulate the pipeline
- Rerun the example with your new script

ParaView Show & Tell

Follow along!

https://www.paraview.org/download/



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