

In Situ Analysis and Visualization with Catalyst and Ascent

Jean M. Favre (Swiss National Supercomputing Center), François Mazen (Kitware Europe)

ISC-2022 half-day tutorial

May 29, 2022

Thanks to different teams

- The ISC Tutorial Review Committee
- Many actors in the visualization and in-situ dev teams:
 - Berkeley Lab, ANL, LLNL, Los Alamos, Sandia, UofO, Kitware, and many others (in particular Cyrus Harrison)

Agenda

- 09:00 Welcome, Overview and Motivation
 - Agenda and technical details for demonstrations
- 09:15 Introduction to in-situ visualization, workflows and terminology
- 09:30 Conduit, an API to describe hierarchical scientific data
 - The Mesh Blueprint, usage conventions, examples
- 10:00 Ascent, an in-situ visualization and analysis library using Conduit
 - Making images
 - Transforming data, extracting data
 - Queries and Conditional triggers
- 10:30 Instrumentation of different simulation codes with Ascent
 - LULESH: an open-source parallel unstructured flow solver
 - Supplementary code examples (SPH-EXA, Jacobi Python)
- 11:00 Coffee break

Agenda

- 11:30 ParaView Catalyst v2, an in-situ visualization and analysis library using Conduit
- The ParaView interactive application, introduction
 - The Paraview parallel server architecture
 - The Catalyst API
 - The ParaView Catalyst Blueprint
 - Python scripting, Data Extractors
- 12:00 Instrumentation of simulation codes with Catalyst
- SPH-EXA: an open-source parallel particle simulation code
 - Supplementary code examples (LULESH, Jacobi C++)
 - ParaView Cinema: An Image-Based Approach to Extreme-Scale Data Analysis
- 12:25 Ascent executing ParaView Python code
- 12:35 Future developments, alternative workflows (in-transit visualization)
- 12:45-13:00 Wrap-up, Q&A

Technical resources

- If you have Docker installed on your desktop you can obtain a Docker image with a ready-to-use ascent install from Docker Hub. We will use the image and demonstrations presented here:
https://ascent.readthedocs.io/en/latest/Tutorial_Setup.html
- ParaView Catalyst (see <https://catalyst-in-situ.readthedocs.io/en/latest>)
- ParaView discussion forum <https://discourse.paraview.org/c/in-situ-support/8>
- Ascent discussion forum <https://github.com/Alpine-DAV/ascent/discussions>
- Slides and examples:
git clone <https://github.com/jfavre/InSitu-Vis-Tutorial2022>

Overview

- What is in-situ visualization, why do we need it? What solutions are available to implement it?
- See recent book “[In Situ Visualization for Computational Science](#)”
- Reflect on our past experience with other libraries and motivate the use of two new frameworks: Catalyst and Ascent.
- Replay some of the presentations from the most recent Ascent tutorial at SC21
- Detail the ParaView-Catalyst and Ascent solutions, with practical examples.

The past

- For decades, the dominant paradigm has been *post-hoc* visualization
- Simulation codes iterate, and save data at regular time intervals.
 - Visualization and domain scientists can then read the data back from storage and interactively explore the data without time constraints

“Without I/O, no visualization is possible”

The true cost of doing I/O is an aggregate of the solver's I/O phase and the many iterations of visualization sessions.

Post-hoc visualization

Even if scientists could afford to keep most of the data for analysis, they must transfer the data to a machine with sufficient capacity and processing power:

Very high data transfer:

- Visualization machine needs to be almost as powerful as the supercomputer

The alternative:

- use smaller temporal and spatial subsets

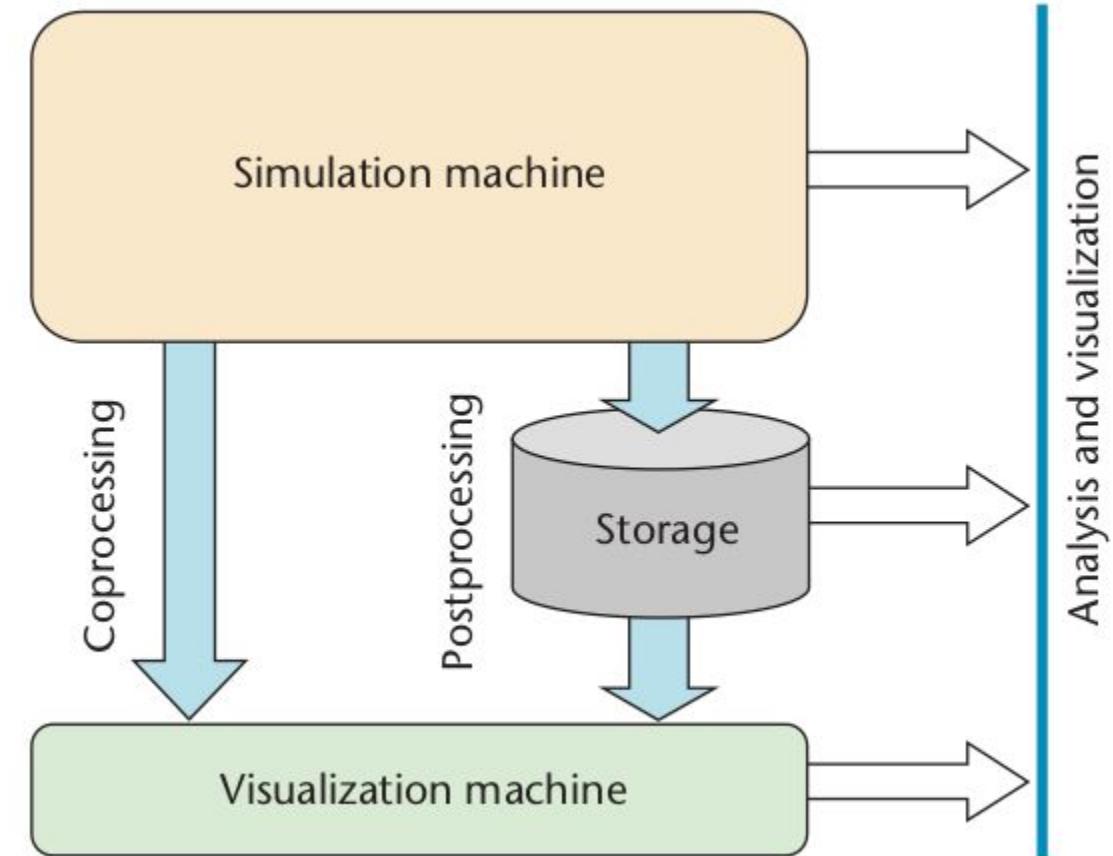


Figure taken from “*In Situ Visualization at Extreme Scale: Challenges and Opportunities*”, Kwan-Liu Ma, IEEE CG&A, nov/dec 2009

in situ visualization

Instrument the code such that both the simulation and visualization calculations run on the same hardware

This runtime co-processing can render images directly or extract features -- *which are much smaller than the original raw data*

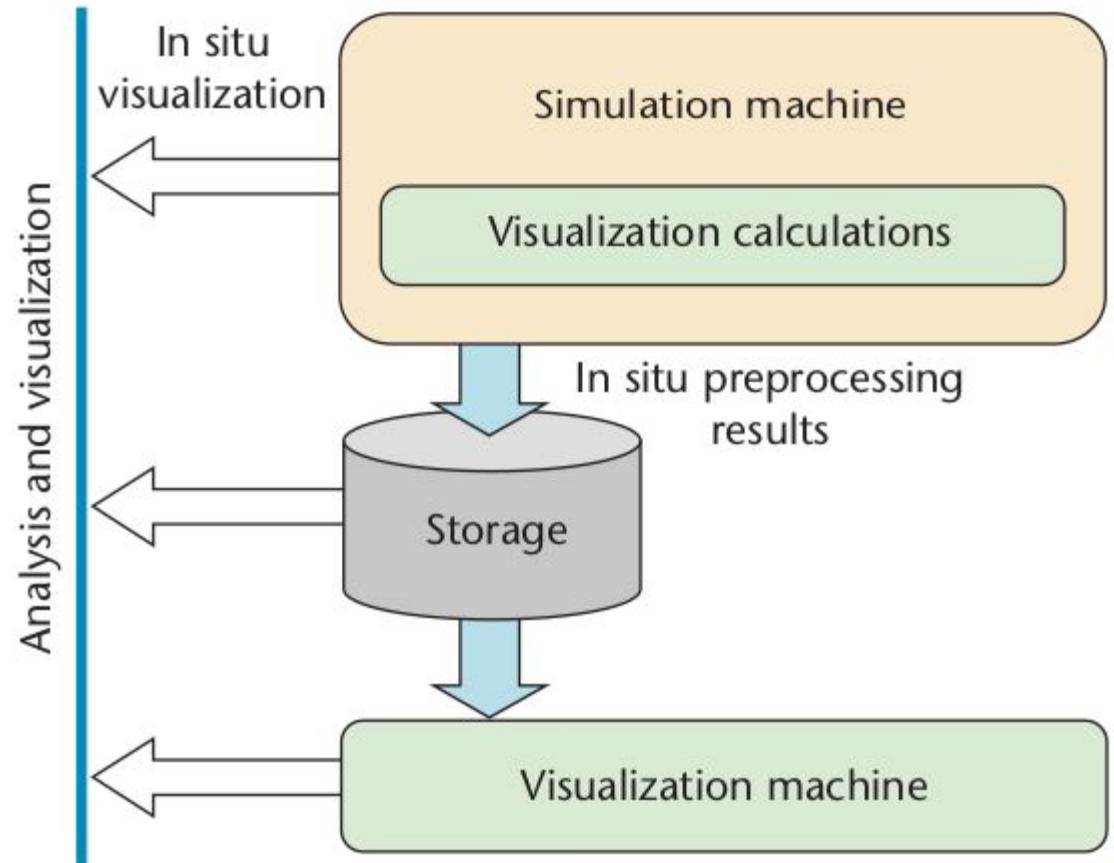


Figure taken from “*In Situ Visualization at Extreme Scale: Challenges and Opportunities*”, Kwan-Liu Ma, IEEE CG&A, nov/dec 2009

In-situ visualization has raised quite a few questions

- Sharing physical resources and domain decomposition?
- What % of time can we afford to “do visualization” vs. “advance the solver”?
- Which feature extraction and visualization tasks are best suited for on-the-fly processing?
- Since less data would be effectively stored to disk, should we augment it with ancillary data?
- Can we provide a generic abstraction to describe the data and mesh structures?

A third paradigm also emerged: in-transit visualization

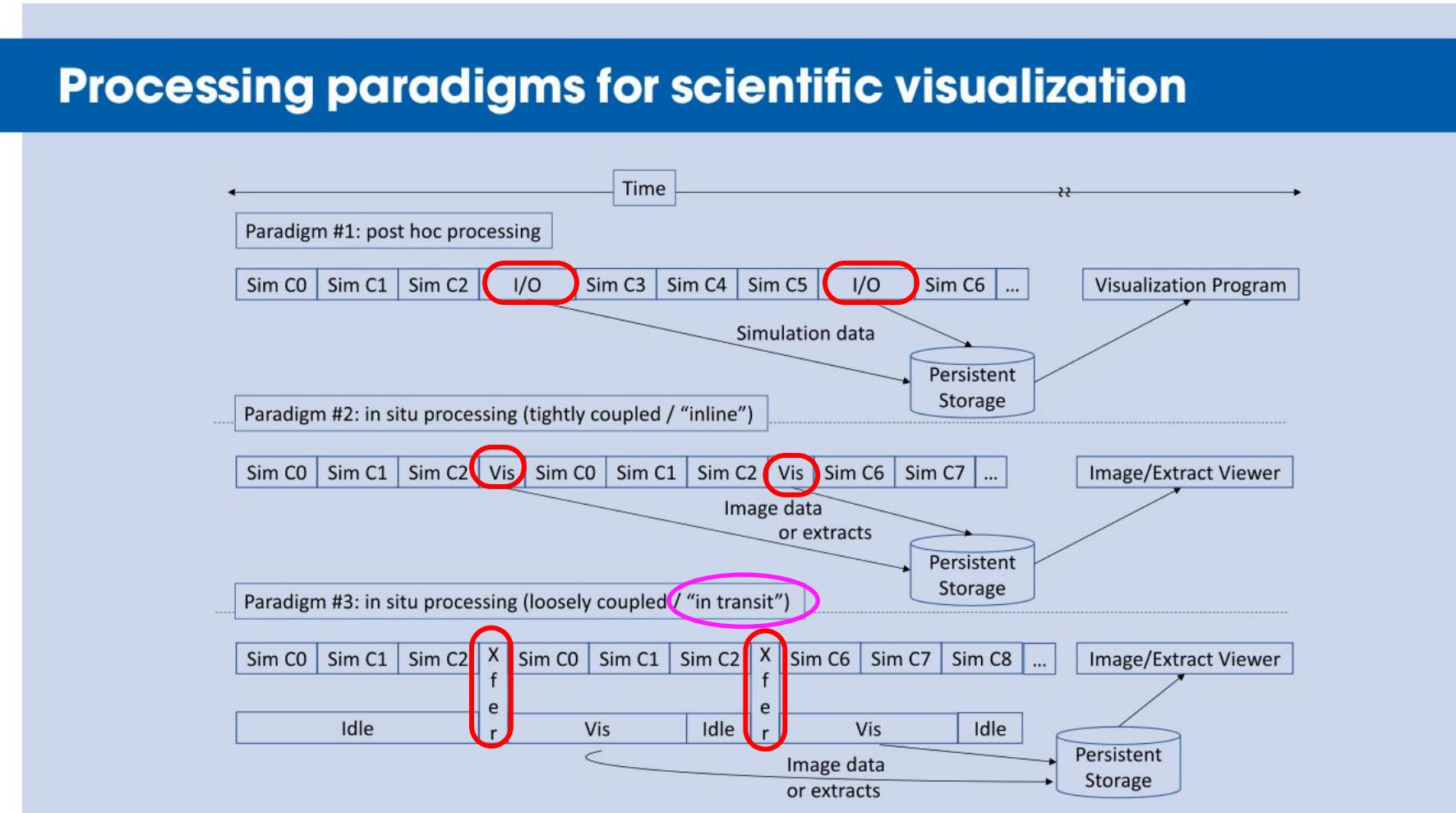


Figure taken from “*In Situ Visualization for Computational Science*”, Hank Childs et al., IEEE CG&A, nov/dec 2019

Does “in-situ” mean “in place”?

- The data is already in the processor’s memory space, without touching the disks
- If simulation data is moved to a distinct set of resources (nodes dedicated to visualization), we are still analysing data “in place”, but is it “in-situ”?
- There has been quite a few variants on the terminology:
 - Co-processing, concurrent processing, run-time visualization

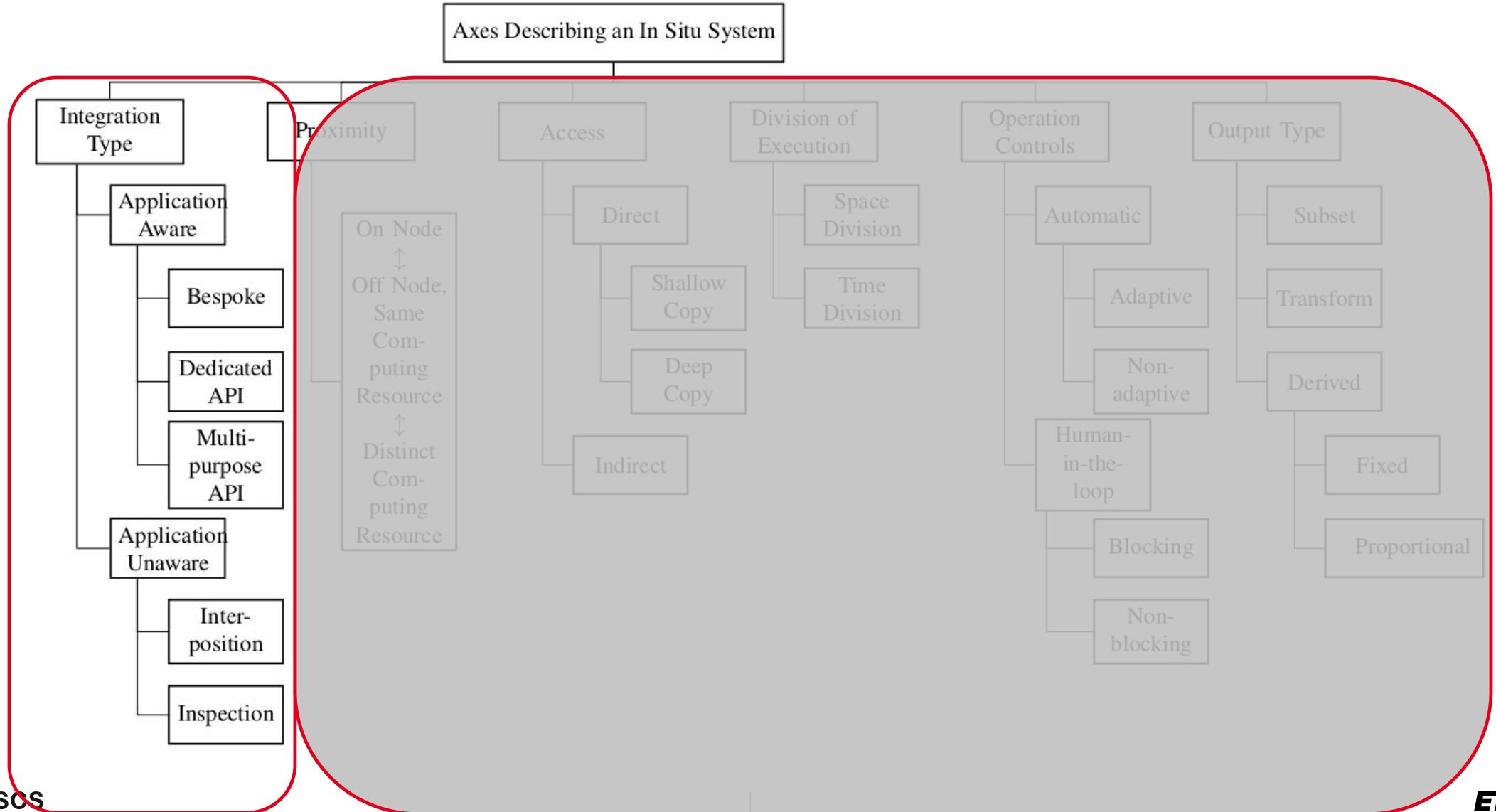
Many definitions and colloquial use for “in-situ”

- An exhaustive panorama of the different systems in use was created
- "A Terminology for In Situ Visualization and Analysis Systems", Hank Childs et al, International Journal of High Performance Computing Applications, 34(6):676–691
- <http://cdux.cs.uoregon.edu/pubs/ChildsIJHPCA.pdf>
- For the scope of this paper, “in situ processing” was defined to be:
“processing data as it is generated”

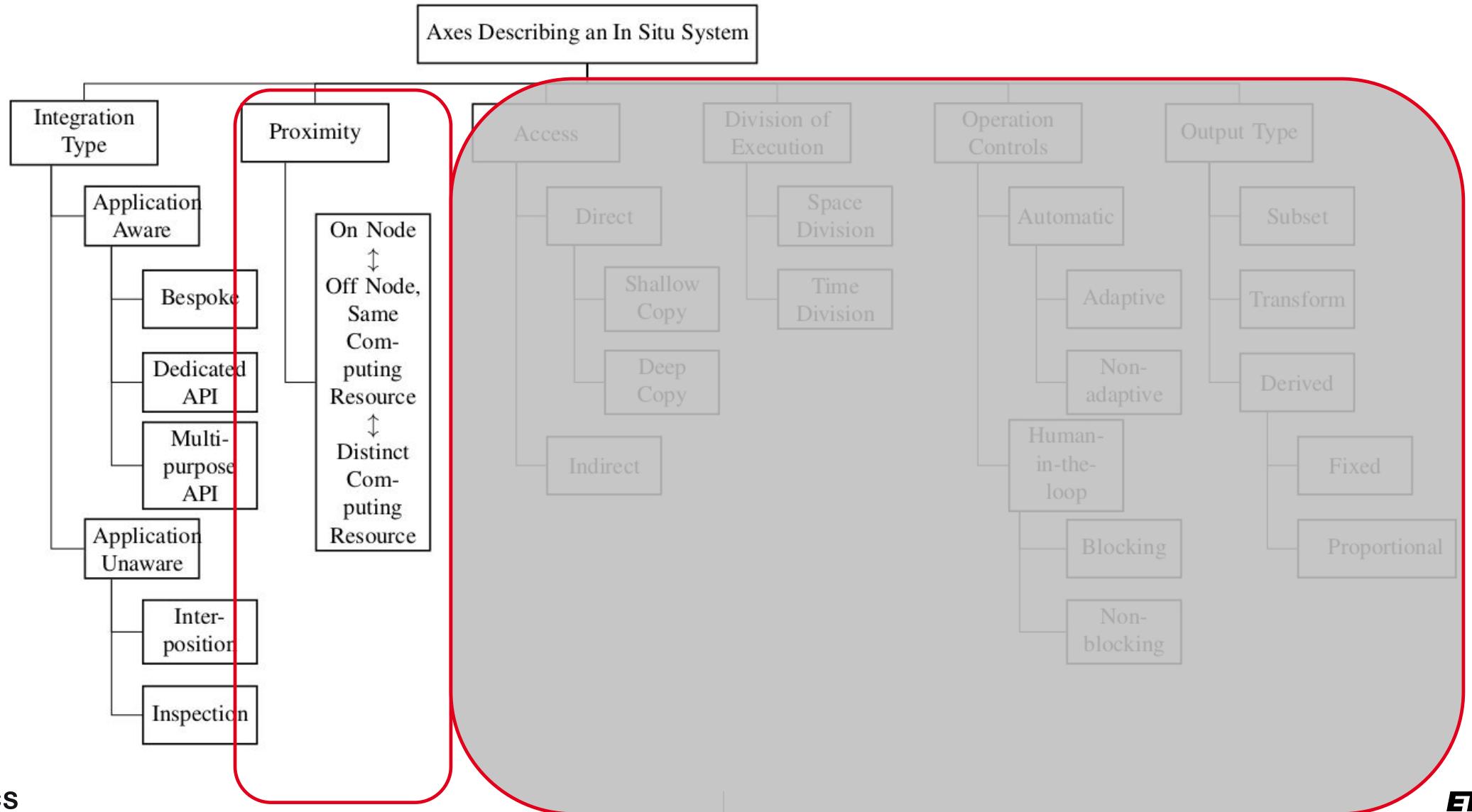
in situ systems were best described via multiple, distinct axes

- integration type
 - How visualization and analysis code is integrated with the simulation code?
- proximity
 - How close is the visualization code from the data?
- Access
 - How does the simulation give access to the data?
- division of execution:
 - how compute resources are shared between simulation and in situ routines.
- operation controls:
 - the mechanism for selecting which operations are executed during run-time
- output type
 - which types of operations are performed on the simulation data before it is output.

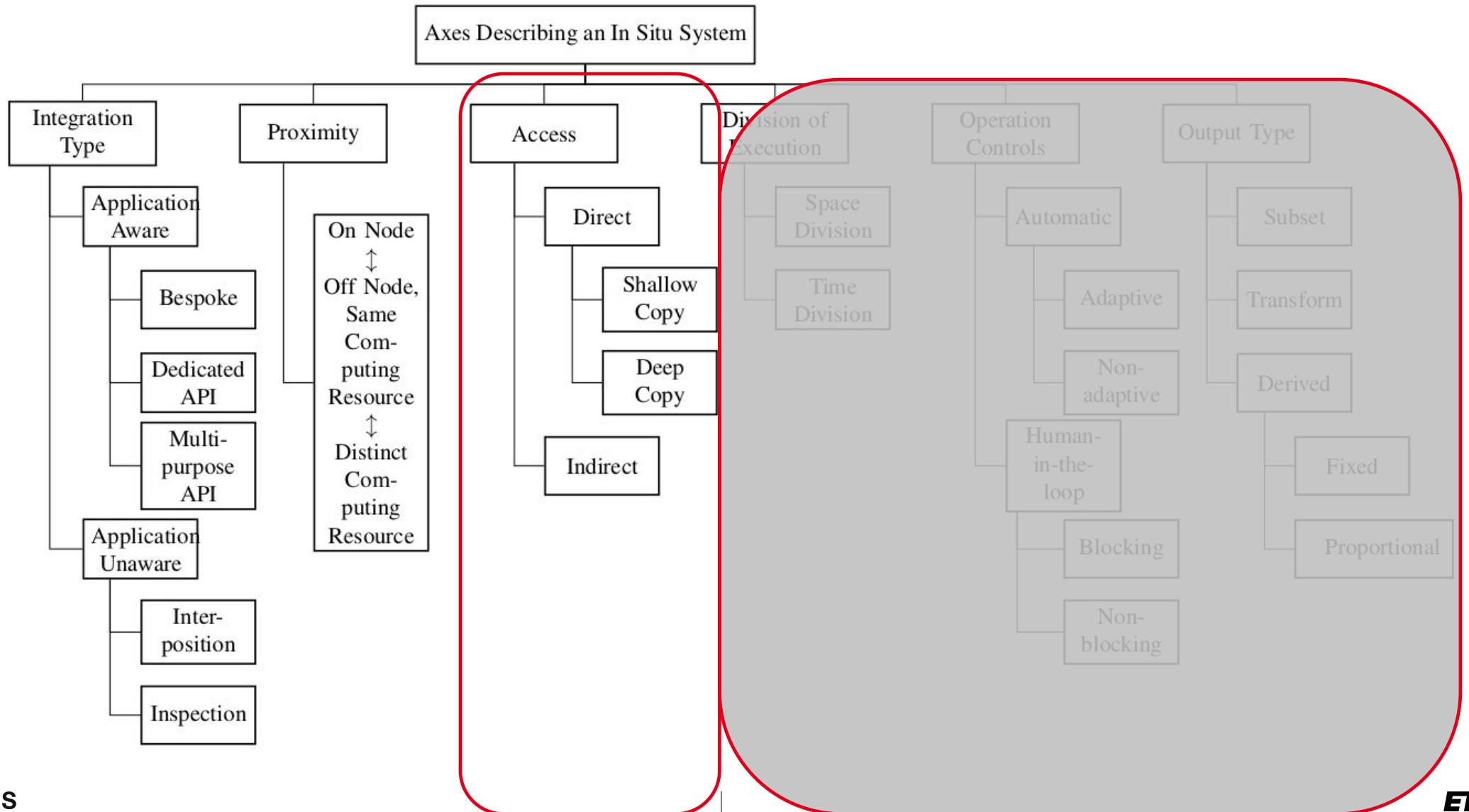
Integration Type



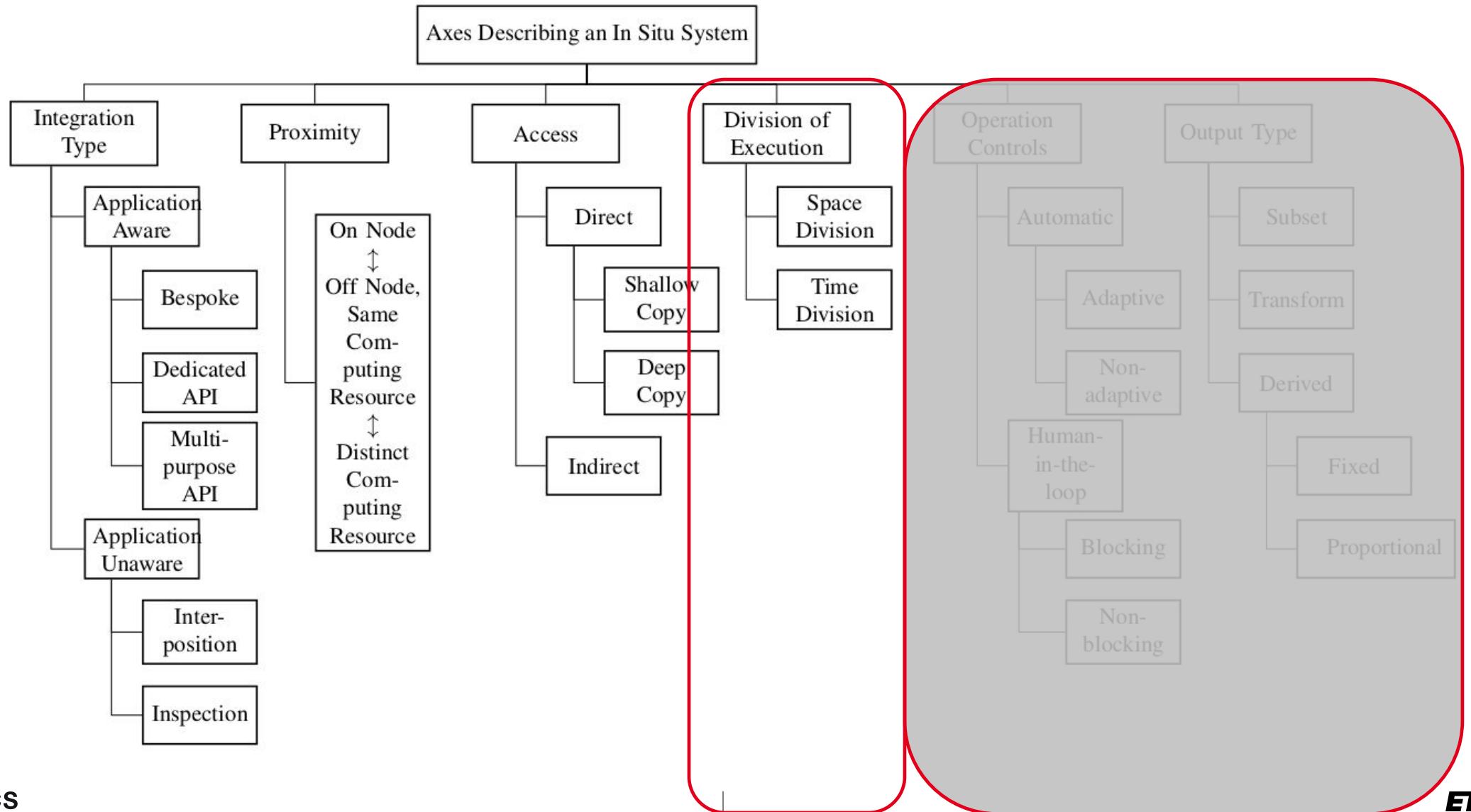
Proximity



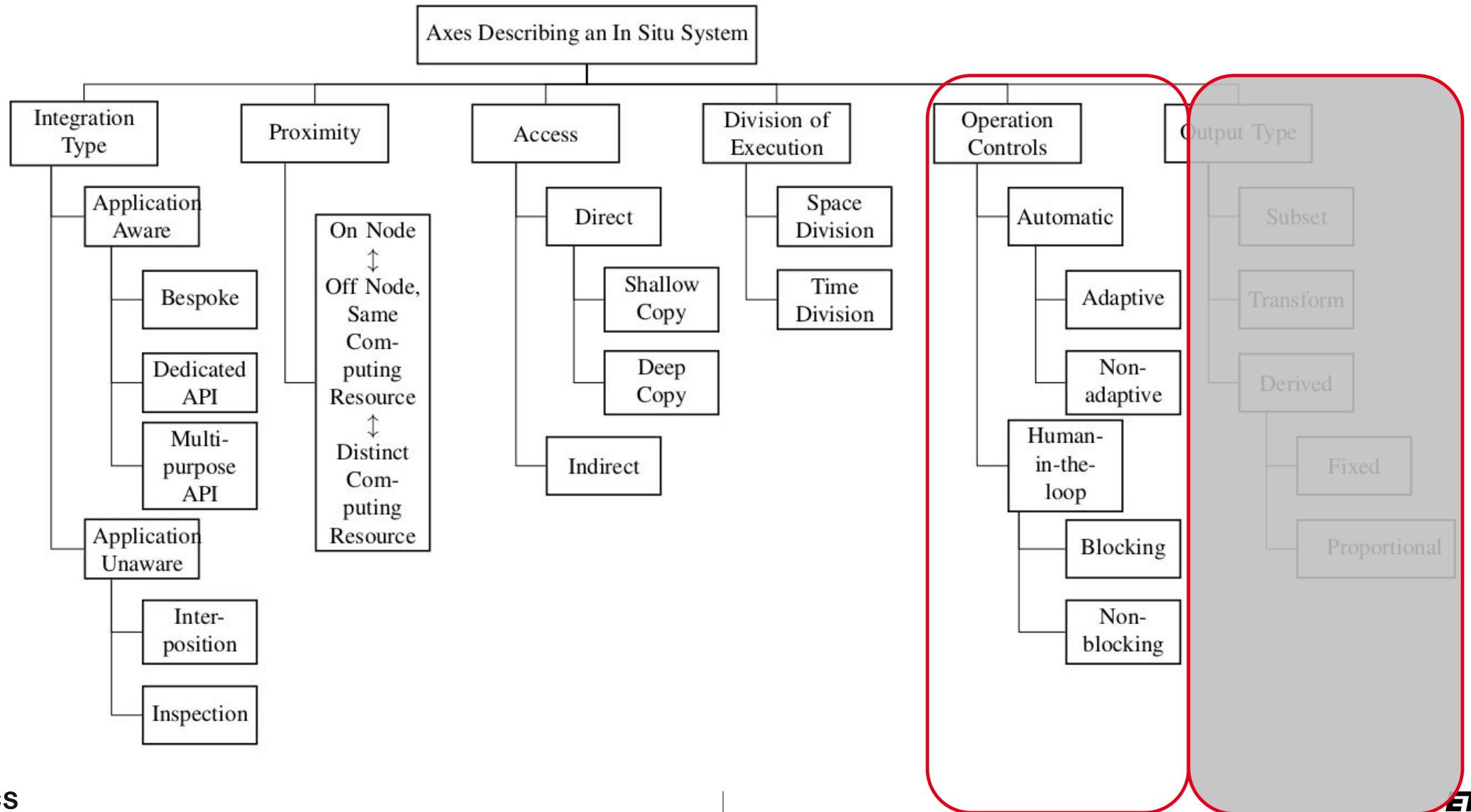
Access



Division of Execution

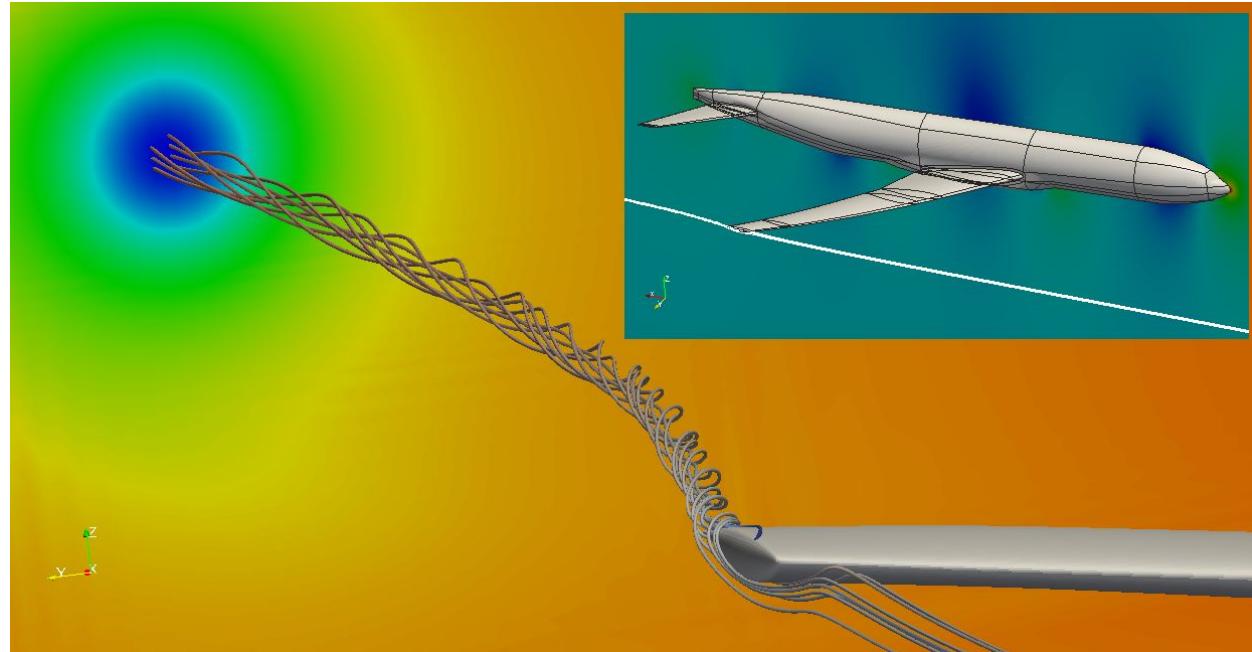


Operation Controls



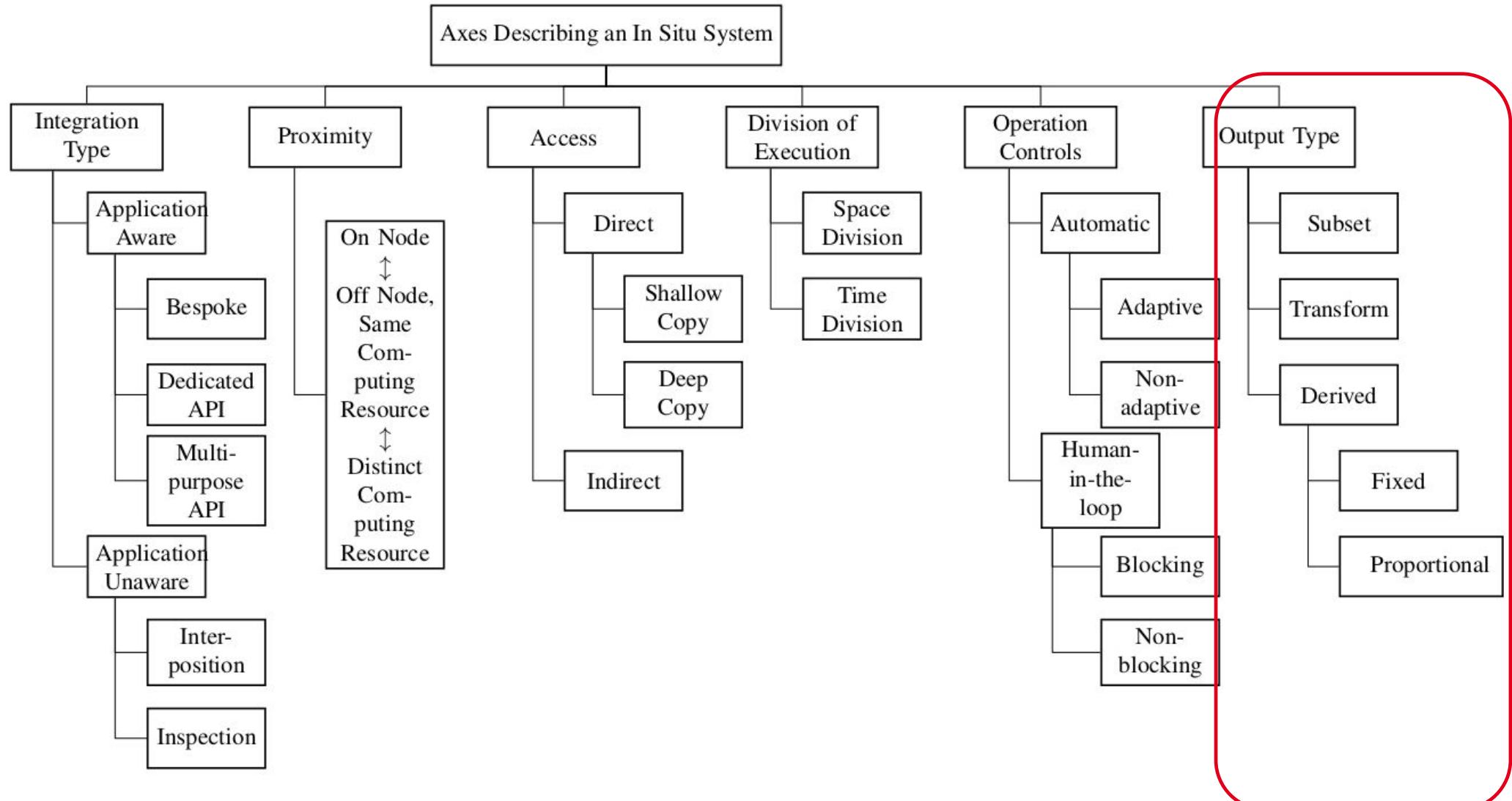
Feature extraction

- What's a feature?
- Some small[er] data worth of interest because of domain knowledge



- Without “interactive” data exploration, it can be difficult to know a-priori which features to extract, or how to tune parameters.
- Knowing when to trigger a potentially expensive calculation would also be handy.

Output types



Outcome of this survey

- In that paper, 15 existing systems were reviewed. Half of them implement a Time Division, with On Node proximity.
 - The simulation advances, then pauses and hands control to the in situ system which completes its operations, hands control back, and so on
 - For example: Ascent, ParaView-Catalyst, Visit/Libsim
- Other examples, ADIOS, SENSEI, which can operate in different modes, sending also their data to distinct vis resources
- ADIOS, for example, can integrate with other workflow or data analytics systems without detailed knowledge of the underlying software and hardware stack
- ADIOS allows users to combine data storage, data staging, data compression, and/or data reduction (ZFP, SZ, BZip2 (compression), FlexPath, Dataspace (data staging), and coupling with ParaView, Visit, Ascent)

SENSEI

SENSEI provides a generic API to enable a “write-once, run-anywhere” environment. This approach focuses on data proximity and portability, runtime selection between running On Node or Off Node

SENSEI provides access to a diverse set of in situ analysis back-ends and transport layers such as ADIOS, Libsim, Ascent, Catalyst etc , through a simple API and data model.

Simulations instrumented with the SENSEI API can process data using any of these back-ends interchangeably. The back-ends are selected and configured at run-time via an XML configuration file.

For more details, refer to the SC2021 tutorial notes

What about our [the solver] internal data model?

- Do the standard visualization applications support all the data structures I use in my code?
 - => Use Data Adaptors
- Are our standard visualization applications ready to handle new alternate data representations?
 - => Use Data Converters
- In recent years, we have seen new ways of thinking about data simulations (run multiphysics code, run ensembles, use ML).
- => new data, perhaps quite different from the traditional "mesh of gridded points"



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Conduit: introduction

Conduit: Simplified Data Exchange for HPC Simulations

- [Conduit](#) is an open source project from Lawrence Livermore National Laboratory that provides an intuitive model for describing hierarchical scientific data in C++, C, Fortran, and Python. It is used for data coupling between packages in-core, serialization, and I/O tasks.
- Conduit provides a convention to describe computational simulation meshes. This is called the [Mesh Blueprint](#).
- [Illustration](#) of Mesh Blueprint examples
- [Ascent](#) and [Catalyst](#) use [Conduit](#) for describing data and other parameters which can be communicated between a simulation and the visualization apps.

Conduit by examples

https://ascent.readthedocs.io/en/latest/Tutorial_Setup.html

```
docker run -p 8888:8888 -t -i alpinedav/ascent-jupyter
```

Run 02_conduit_basics.ipynb



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Conduit + Ascent

Ascent

[Ascent](#) is an easy-to-use flyweight in situ visualization and analysis library for HPC simulations:

- Supports: Making Pictures, Transforming Data, and Capturing Data for use outside of Ascent
- Young effort, yet already includes most common visualization operations
- Provides a simple infrastructure to integrate custom analysis
- Provides C++, C, Python, and Fortran APIs
- [Ref](#)

“The ALPINE in situ infrastructure: Ascending from the ashes of strawman”, M. Larsen et al., Proc. 3rd Workshop In Situ Infrastructures Enabling Extreme Scale Anal. Vis. Denver, CO, USA, Nov. 12–17, 2017

Ascent

Ascent is based on several components:

- The Conduit Mesh Blueprint!
- Runtimes providing analysis, rendering and I/O
 - Runtimes will execute a number of *actions*, defined by Conduit Nodes
- Data Adaptors (internal)

Ascent tutorial pages (from LLNL)

- [Tutorial link](#)
- [SC2021](#) tutorial !!! Big thanks go to Cyrus Harrison and co-developers!!!
- docker run -p 8888:8888 -t -i alpinedav/ascent-jupyter

Ascent tutorial first example

run 01_ascent_first_light.ipynb

Ascent tutorial examples,

Generating time dependent data

- Run 03_conduit_blueprint_mesh_examples.ipynb

Rendering images with Scenes

- Run 04_ascent_scene_examples.ipynb

Transforming data with Pipelines

- Run 05_ascent_pipeline_examples.ipynb

Running with different visualization pipelines

In its basic form, we have a default scene description in the Ascent bridge code

- At run-time, we can supply different scenes, with additional pipelines
- If present, a file called "ascent_actions.{json,yaml}" will be read, overriding the actions previously set
- <http://www.yamllint.com/> is your friend
- Example will be given later...
Examples/LULESH/{ascent_actions.yaml,trigger_ascent_actions.yaml}

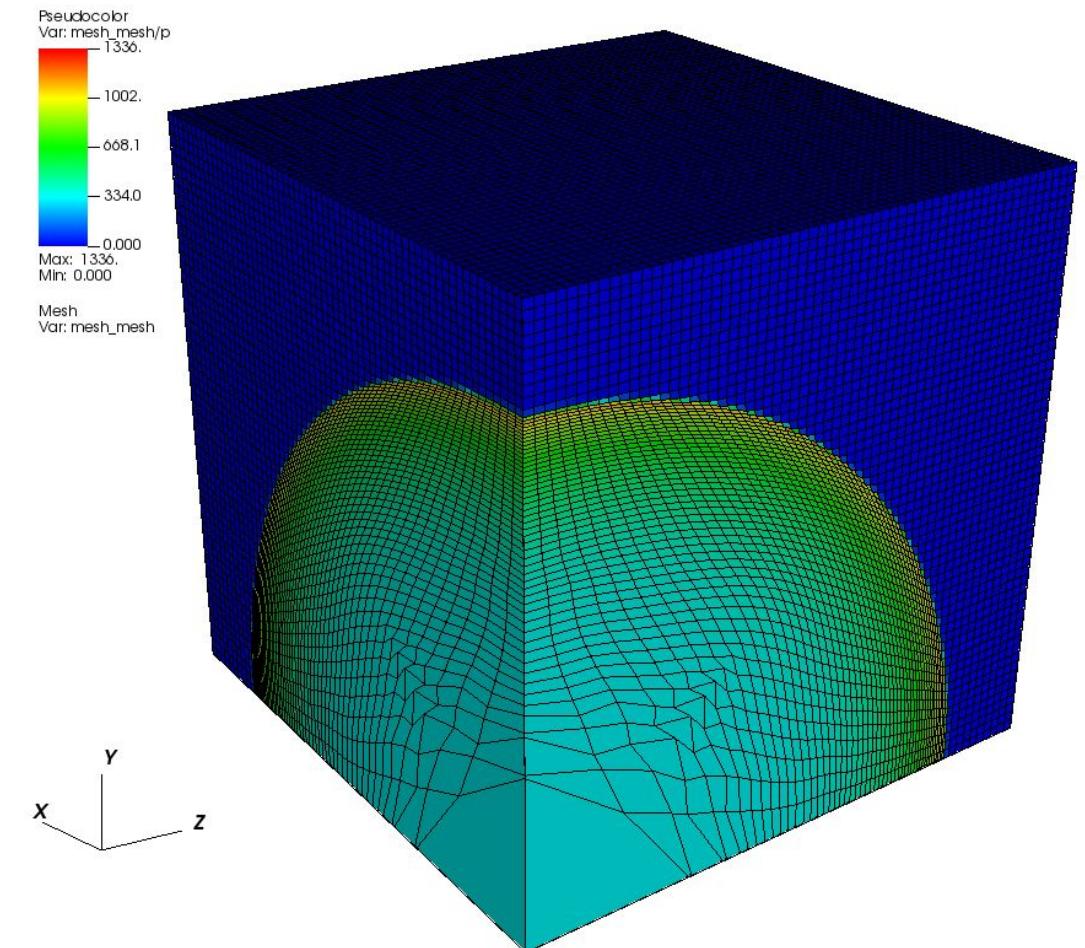
scene descriptions (JSON or YAML)

```
[  
 {  
   "action": "add_scenes",  
   "renders":  
   {  
     "r1":  
     {  
       "camera":  
       {  
         "azimuth": 30,  
         "elevation": 11  
       },  
       "image_prefix": "PressureImage.%05d"  
     } [text cut off because it is too long....]
```

```
-  
   action: "add_scenes"  
   renders:  
     r1:  
       camera:  
         azimuth: 30  
         elevation: 11  
         image_prefix: "PressureImage.%05d"  
       scenes:  
         s1:  
           plots:  
             p1:  
               field: "p"  
               type: "pseudocolor"
```

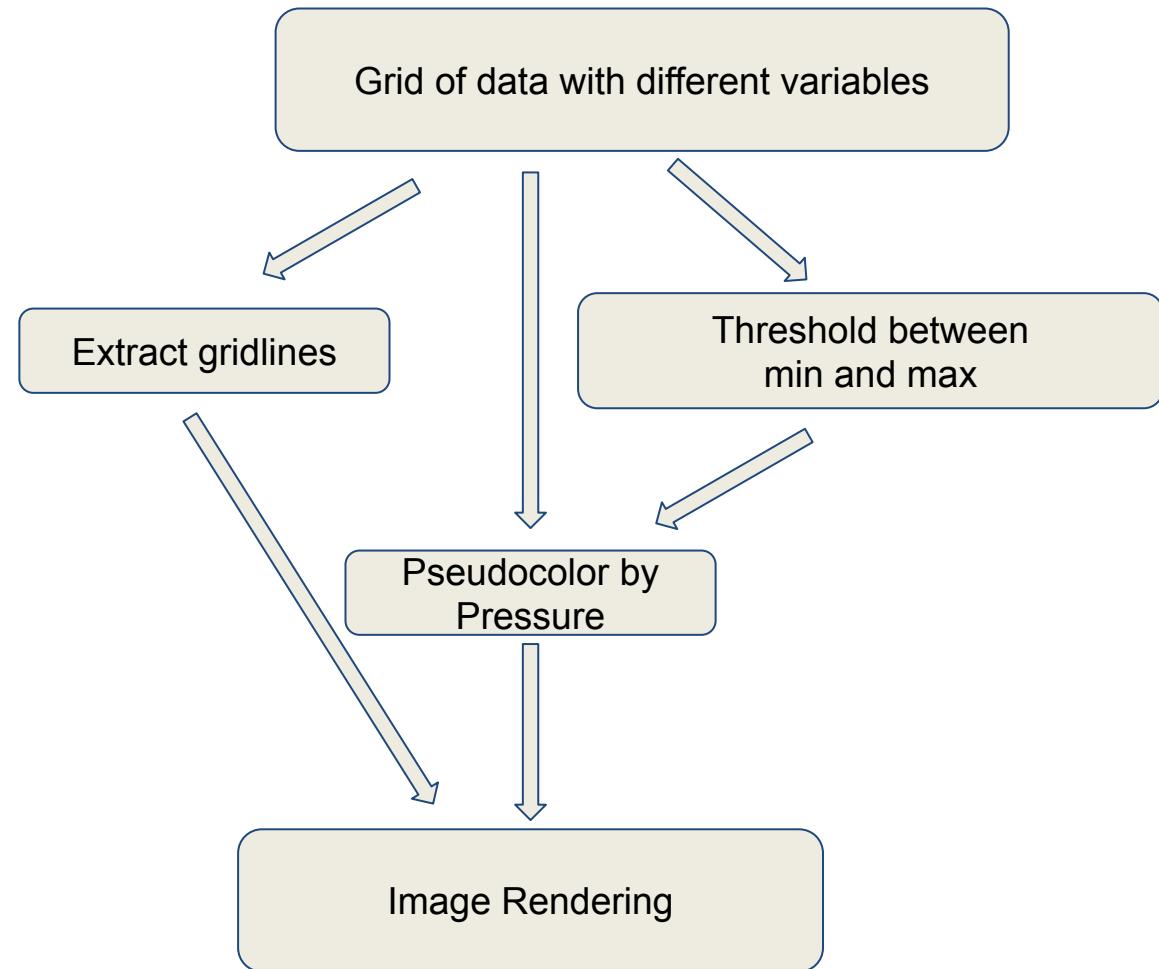
A simple color plot of Pressure (p)

```
action: "add_scenes"  
renders:  
r1:  
camera:  
azimuth: 30  
elevation: 11  
image_prefix: "PressureImage.%05d"  
scenes:  
s1:  
plots:  
p1:  
field: "p"  
type: "pseudocolor"
```



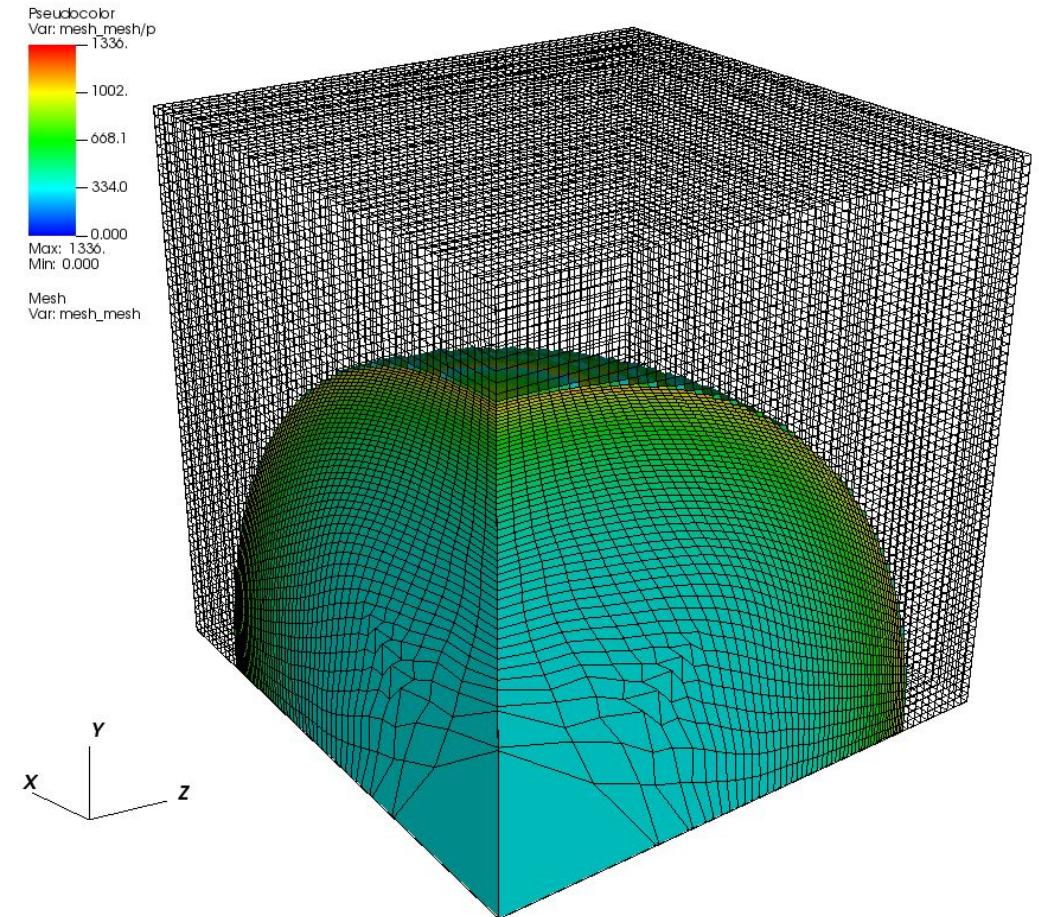
Let's add a “pipeline” description

```
- action: "add_pipelines"  
  pipelines:  
    pl1:  
      f1:  
        type: "threshold"  
        params:  
          field: "p"  
          min_value: 300  
          max_value: 2000
```



The scene description is refined with the new pipeline

```
- action: "add_scenes"  
renders:  
r1:  
camera:  
azimuth: 30  
elevation: 11  
image_prefix: "PressureImage.%05d"  
scenes:  
s1:  
plots:  
p1:  
field: "p"  
pipeline: "pl1"  
type: "pseudocolor"
```

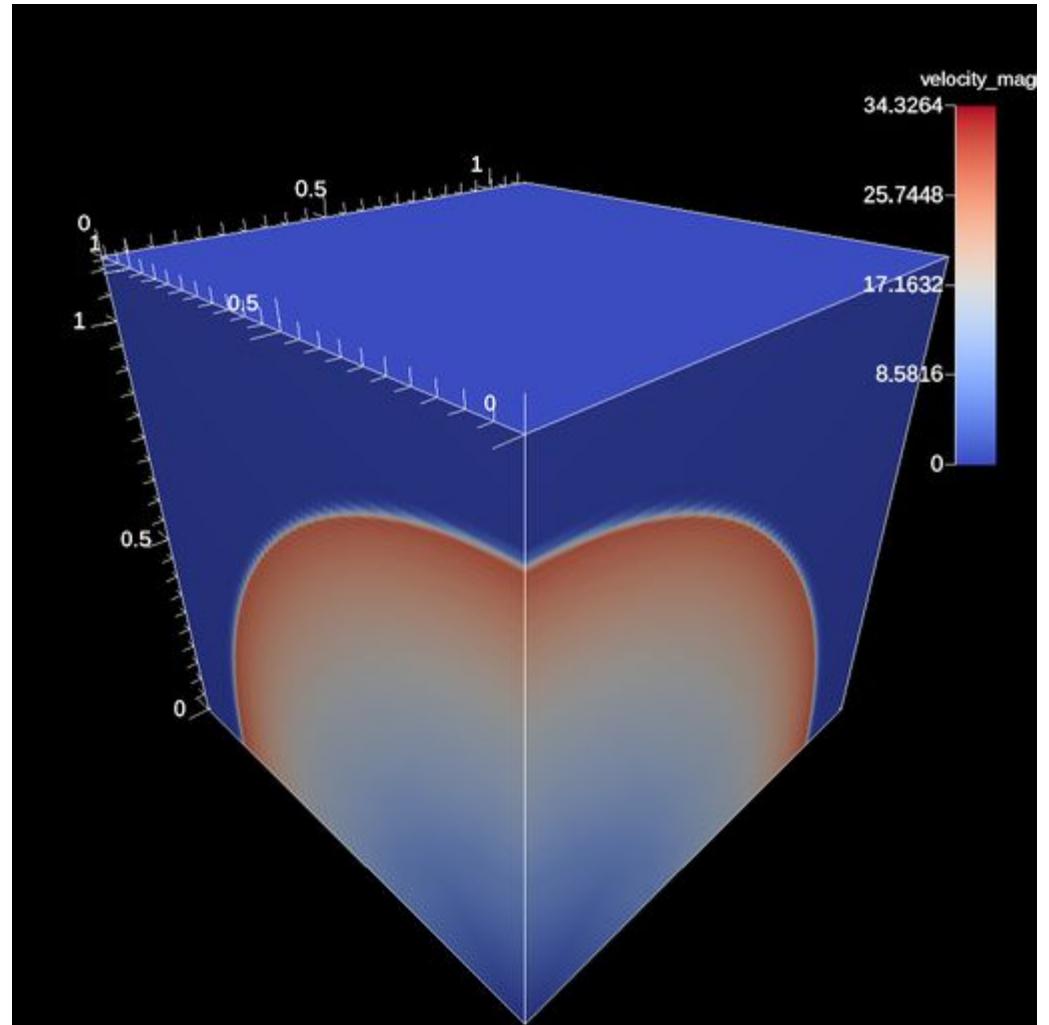


LULESH

- <https://ascent.readthedocs.io/en/latest/ExampleIntegrations.html>
- LULESH is one of 5 proxy application examples
- We added some content to the source to enable compilation of the same code with our two frameworks (Ascent and Catalyst)
- <https://github.com/jfavre/InSitu-Vis-Tutorial2022/tree/main/Examples/LULESH>

Instrument the LULESH example with Ascent

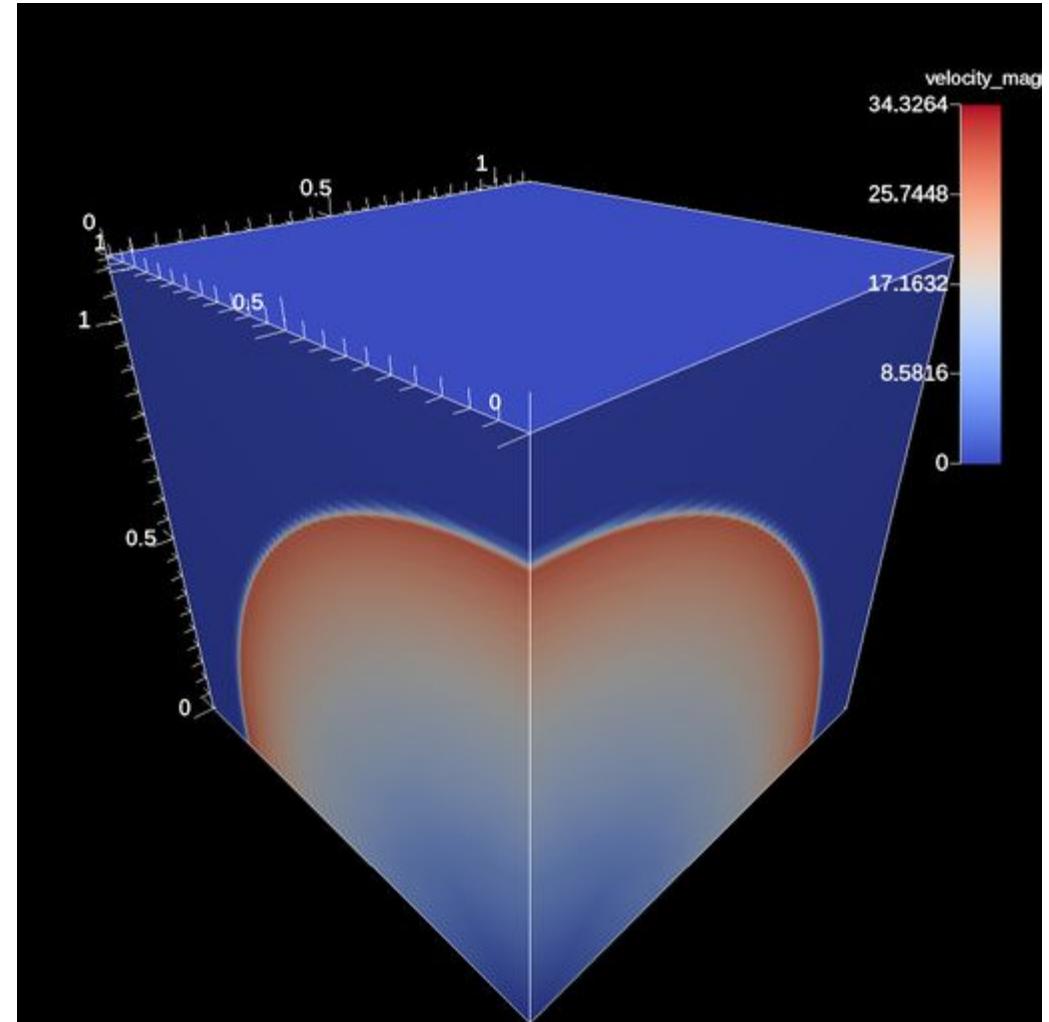
- Define a Conduit [mesh](#) definition
- Define a Conduit [scene](#) definition



Run-time visualization examples

Re-define the basic visualization script
in ascent_action.yaml

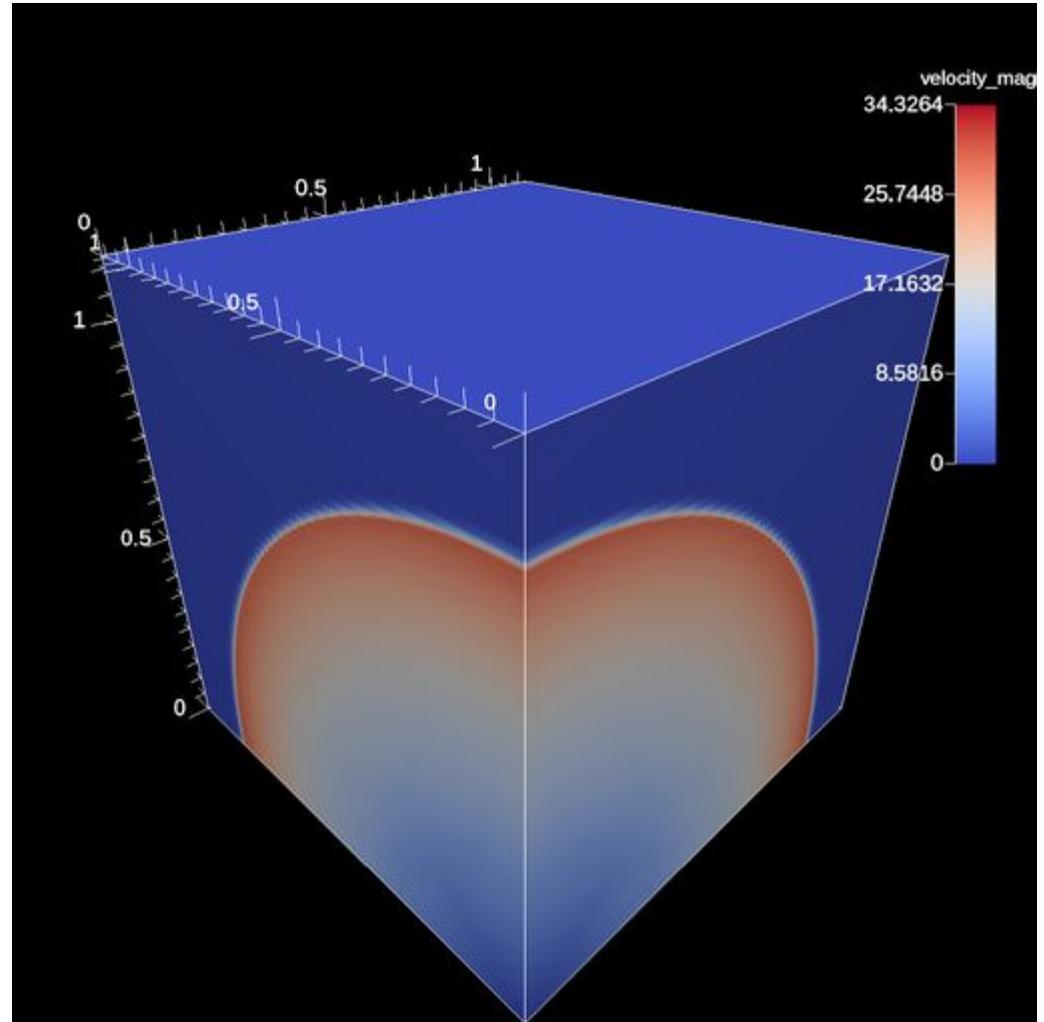
```
- action: "add_triggers"
  triggers:
    t1:
      params:
        condition: "cycle() % 100 == 0"
        actions_file: "trigger_ascent_actions.yaml"
```



Run-time visualization examples

1 every N iterations, execute
trigger_ascent_action.yaml

```
-  
action: add_pipelines  
  
pipelines:  
    pl1:  
        f1:  
            params:  
                field: velocity  
                type: vector_magnitude  
  
-  
action: add_scenes  
  
scenes:  
    s1:  
        plots:  
            p1:  
                field: velocity_magnitude  
                pipeline: pl1  
                type: pseudocolor
```



A comprehensive set of code snippets to learn Ascent by Examples

You'll ask...

How do I do ...this...and that?

[Ascent Actions Examples — Ascent 0.8.0 documentation](#)

How do I compile and run LULESH+Ascent?

Default compilation:

```
cd <source_code>; mkdir build; cd build  
cmake -DINSITU=None -DWITH_MPI:BOOL=ON -DWITH_OPENMP:BOOL=ON ..
```

With Ascent:

```
module load daint-gpu Ascent  
cmake -DINSITU=Ascent -DWITH_MPI:BOOL=ON -DWITH_OPENMP:BOOL=ON ..
```

Execute (for example on CSCS' Cray supercomputer):

```
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK
```

```
mkdir $SCRATCH/Lulesh  
cp buildAscent/bin/lulesh2.0 $SCRATCH/Lulesh  
cp ascent_actions.yaml trigger_ascent_actions.yaml $SCRATCH/Lulesh  
pushd $SCRATCH/Lulesh  
srun ./lulesh2.0 -s 30 -p
```

Compilation on my laptop:

```
cmake -DINSITU=Ascent  
-DAscent_DIR=/local/apps/ascent-install/lib  
/cmake/ascent
```

Execute on my laptop)

```
mpiexec -n 8 --use-hwthread-cpus  
.bin/lulesh2.0 -p -i 10
```



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Supplementary material

Instrumentation of different simulation codes with Ascent

- An SPH solver (C++)
 - git clone <https://github.com/unibas-dmi-hpc/SPH-EXA.git>
- A 2D heat equation solver (Python) (C++ coming soon)
 - git clone <https://github.com/jfavre/InSitu-Vis-Tutorial2022.git>

Ex1: Instrument the SPH-EXA simulation package with Ascent

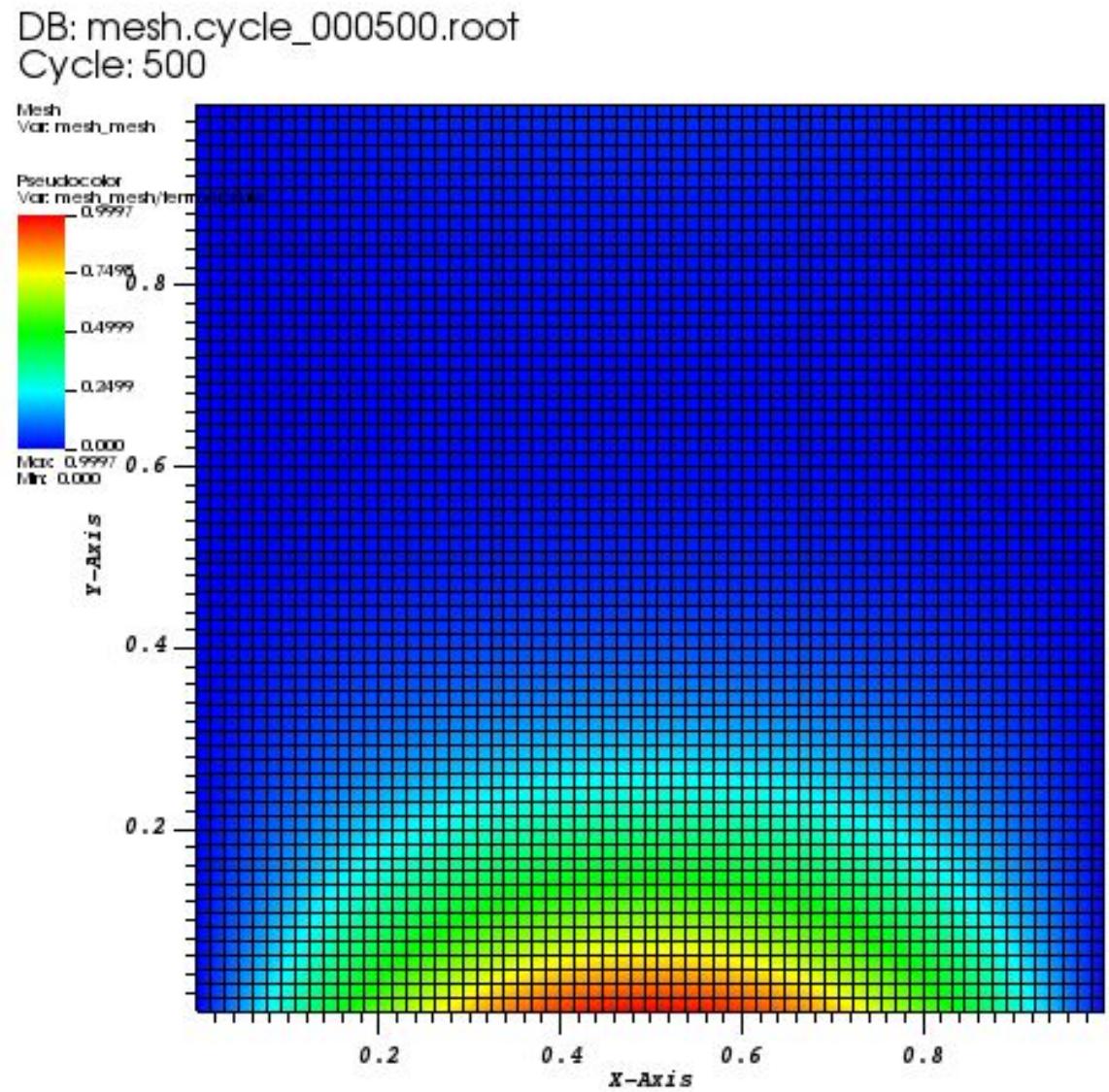
- Define a Conduit [mesh](#) definition
- Define a Conduit [scene](#) definition

About 150 lines of code. Total!

Ex2: Instrument a simple Python 2D heat equation solver with Ascent

Source code

- Define a Conduit [mesh](#) definition
- Define a Conduit [scene](#) definition





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Coffee Break



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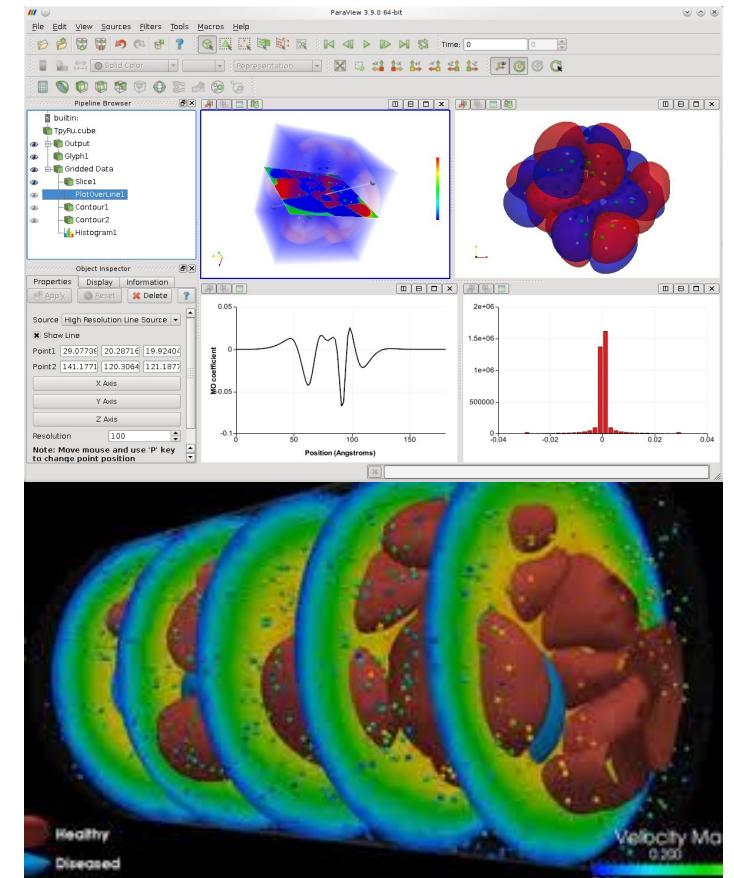
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Before jumping to ParaView Catalyst, let's first introduce ParaView

ParaView / High-Performance Post-Processing

- Open-source, multi-platform, data analysis and visualization application
- Analysis of extremely large datasets using distributed memory computing resources
- Over 20 years of development
- Contributions from over 270 developers
- Over 1.6 million lines of code
- Over 150k yearly downloads
- www.paraview.org



Paraview Gallery

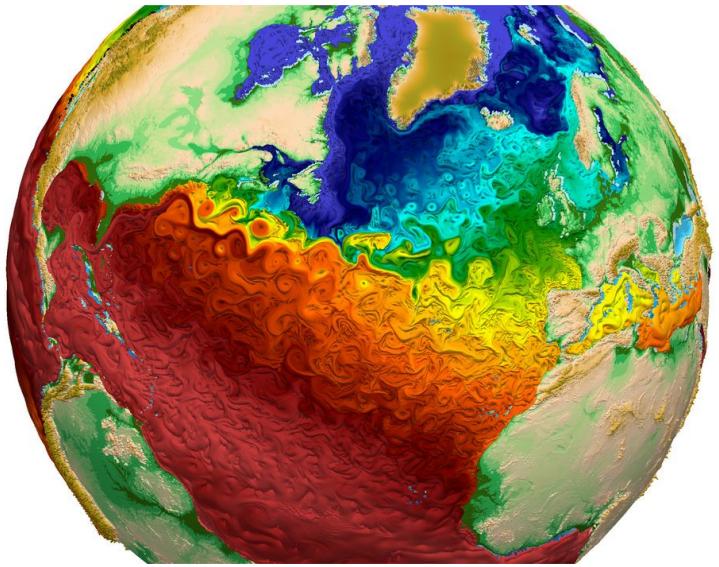
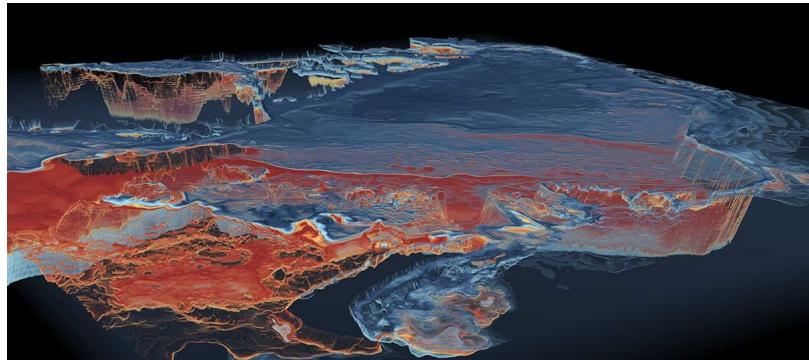
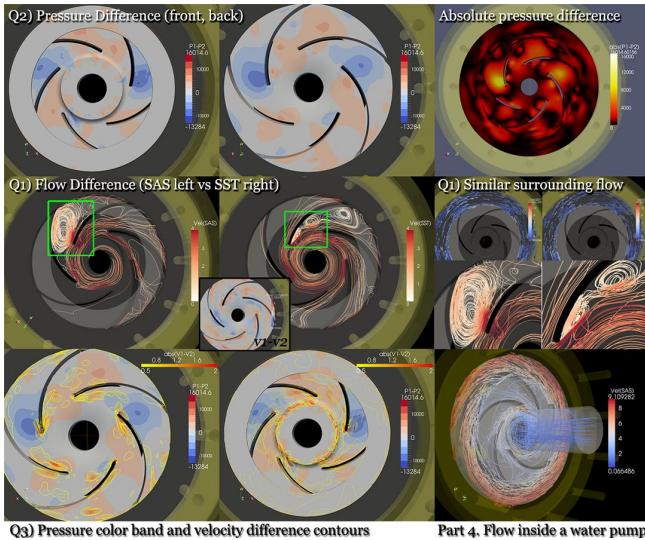


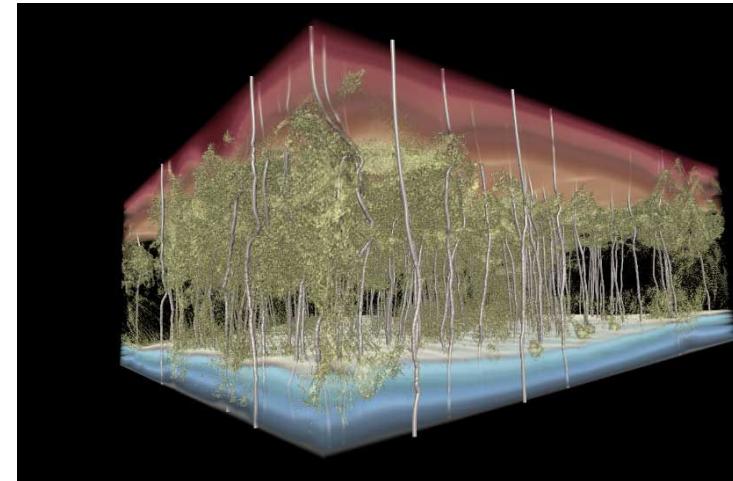
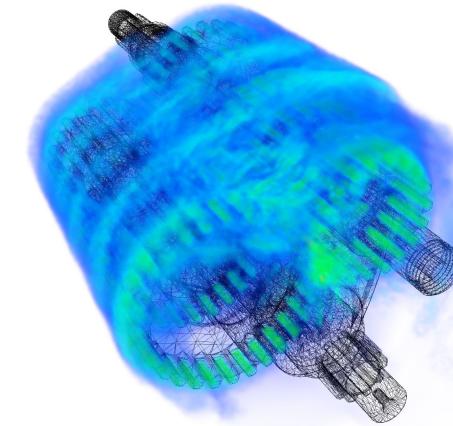
Image Courtesy of Los Alamos National Laboratory



Greg Foss, Texas Advanced Computing Center Science: Nguyen, An T., Heimbach, P. and Vocanía, V., Institute for Computational Engineering and Sciences, The University of Texas at Austin.



Data courtesy of the 2011 IEEE Visualization Contest

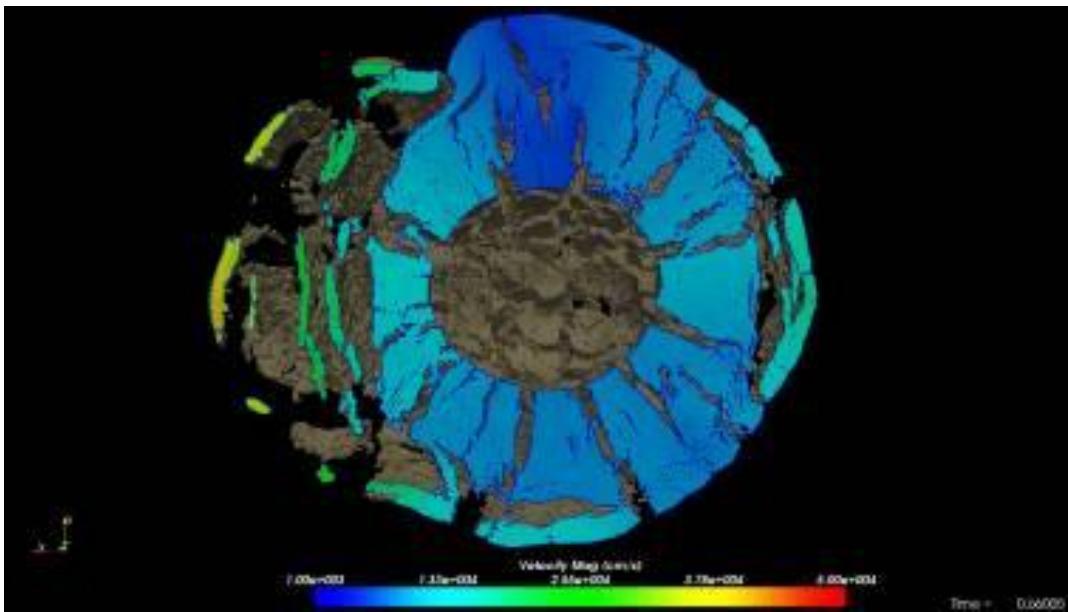


Baskar Ganapathysubramanian Research Group/Iowa State University; Greg Foss/Texas Advanced Computing Center (TACC).

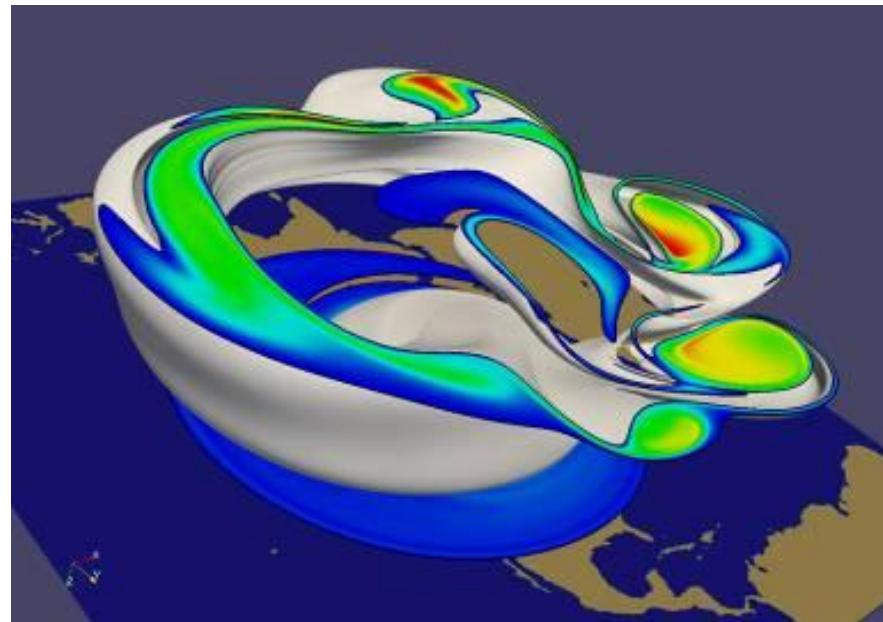


Extremely Large Data

1 billion cell asteroid detonation simulation



½ billion cell weather simulation

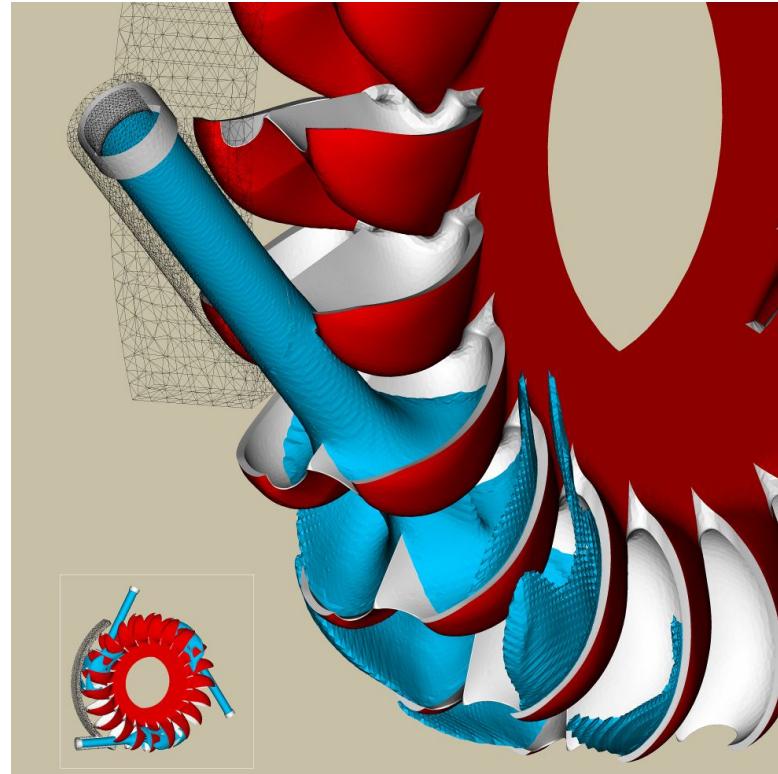
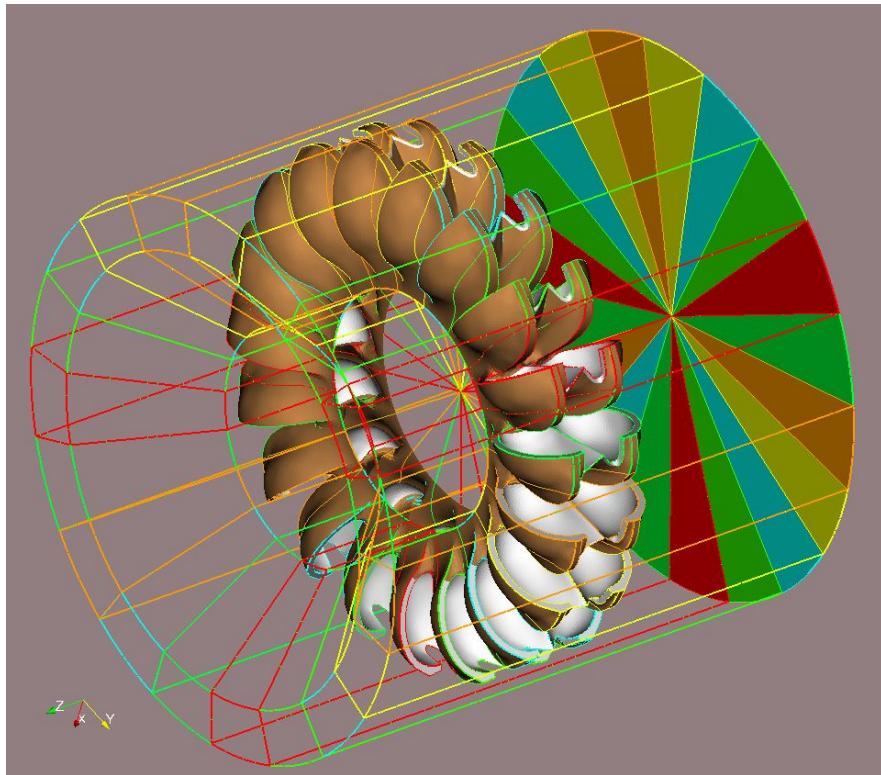


Source: Sandia National Lab



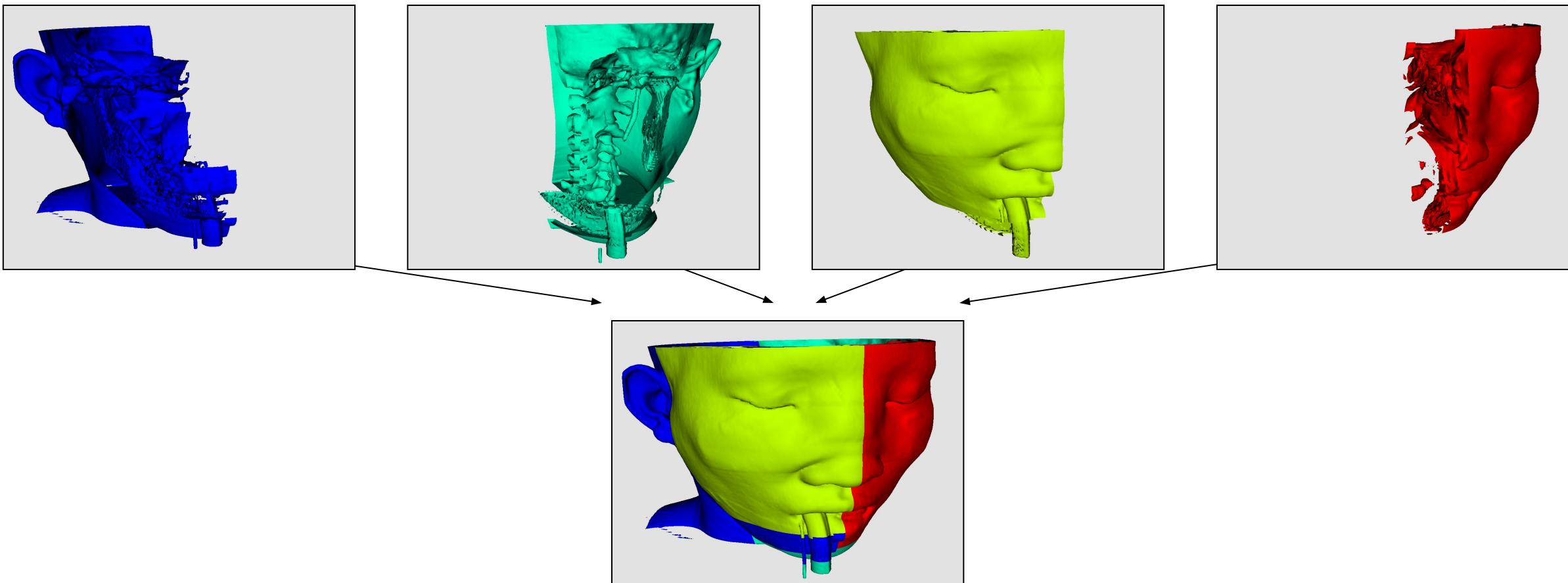
Fast Large Data Interaction

CFD simulation of 20-30 million cells
with load balancing

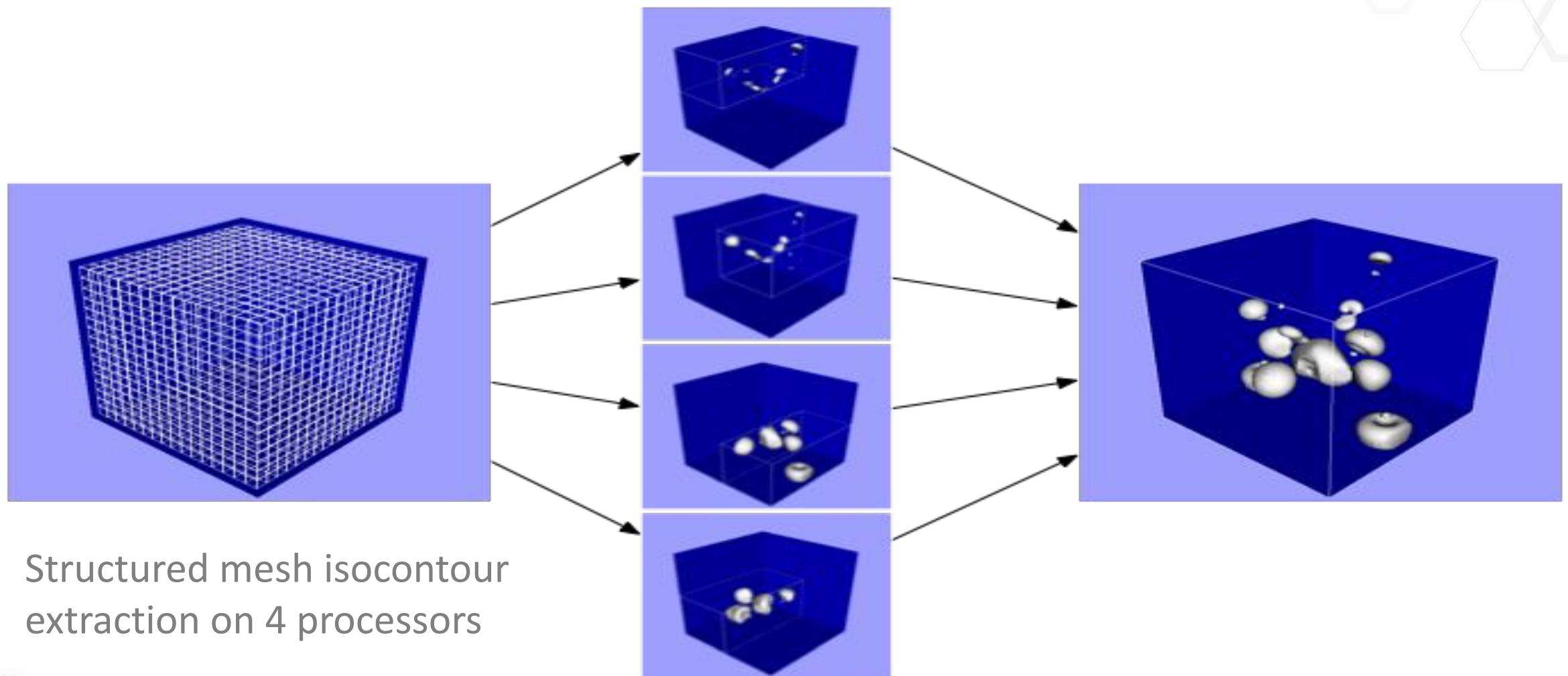


Source: Swiss National
Supercomputing center

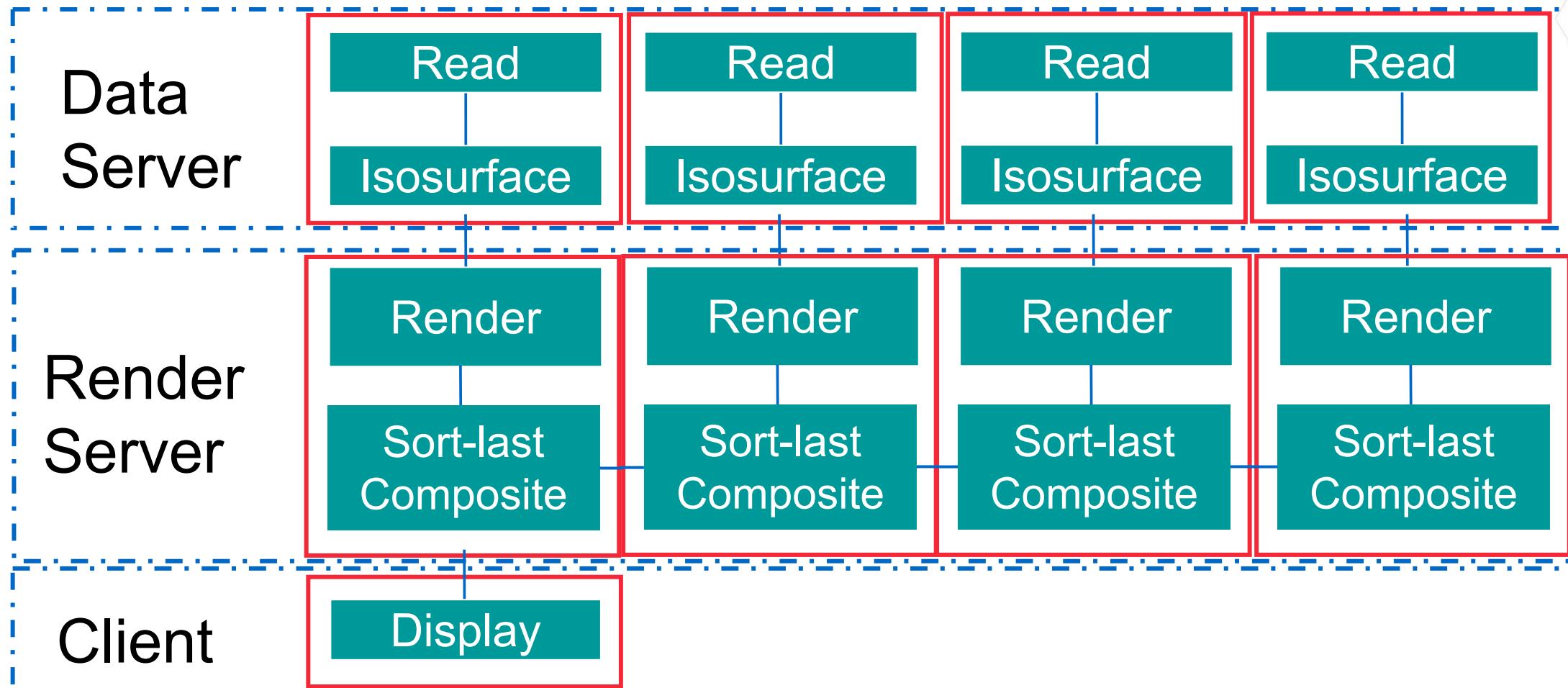
Parallel Rendering



Distributed Processing

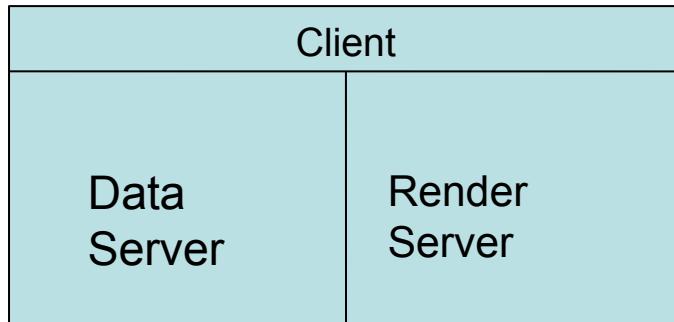


Data Parallel Pipelines

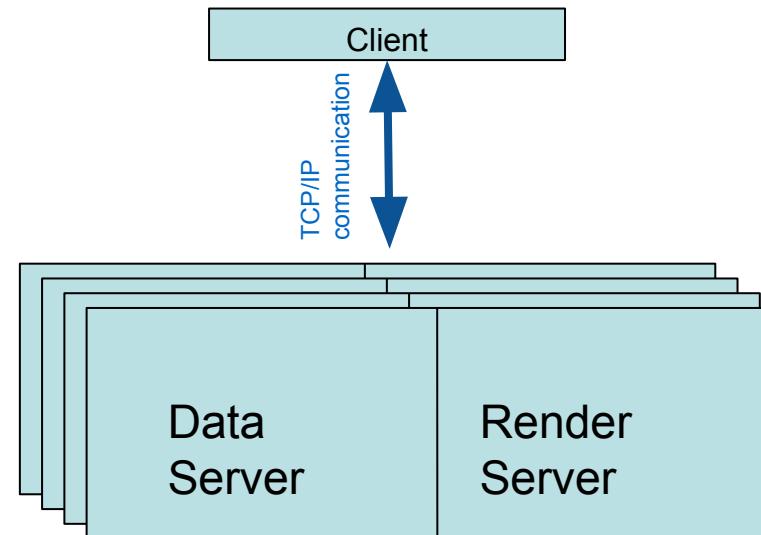


Deployment Topologies

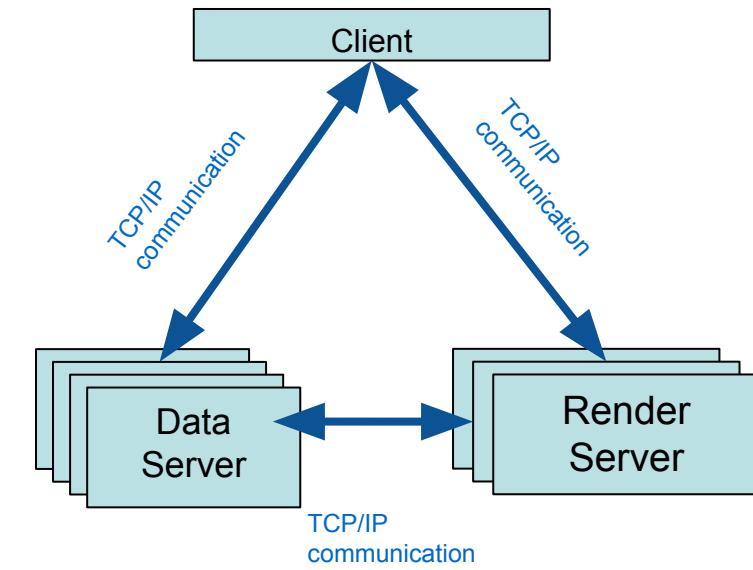
Builtin Server



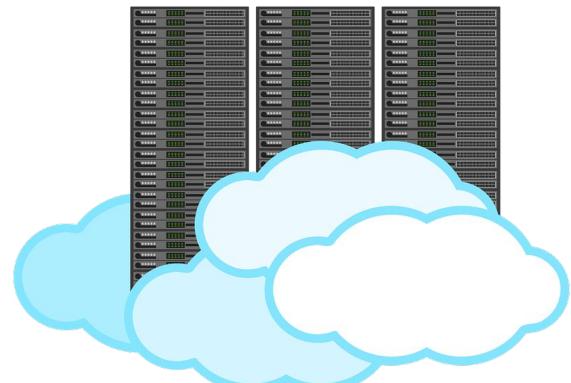
Client-Server



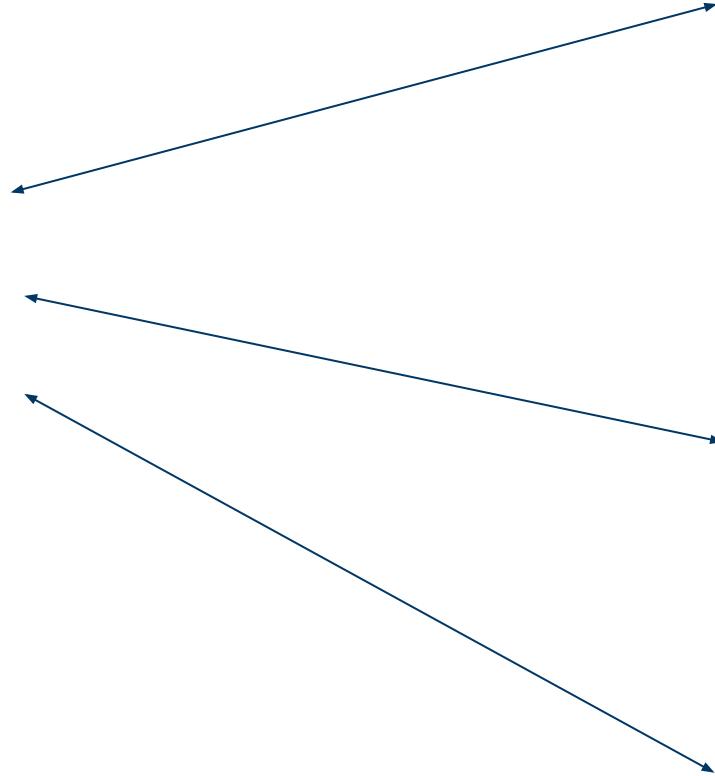
Client - Render Server - Data Server



Running ParaView

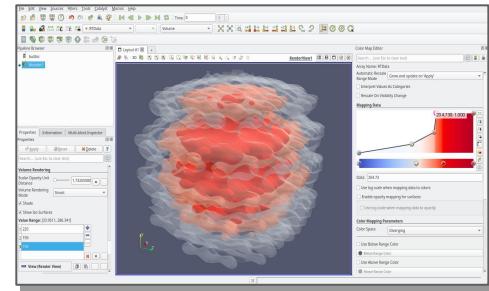


ParaView Server



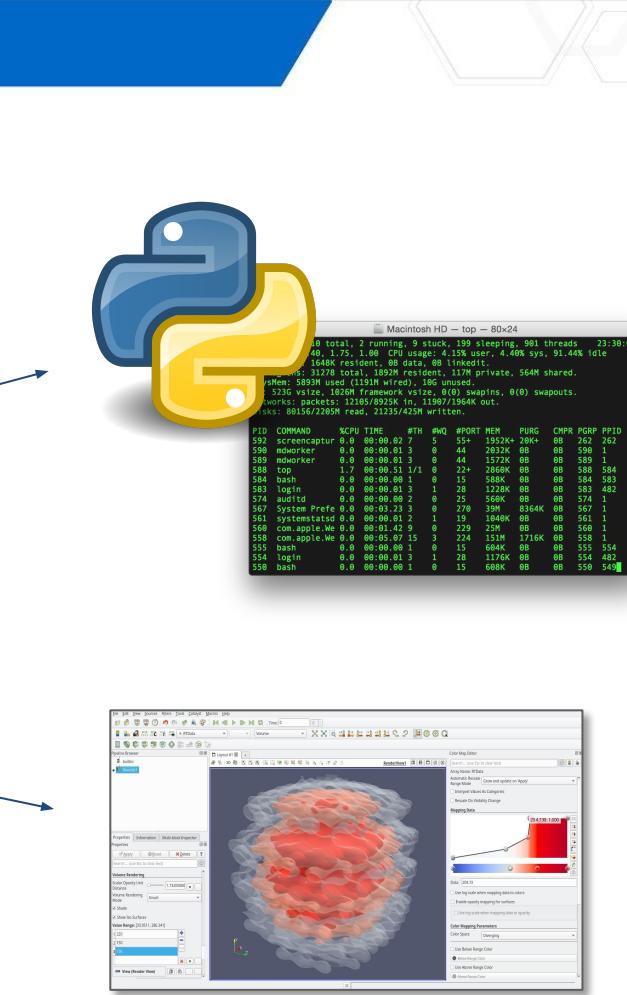
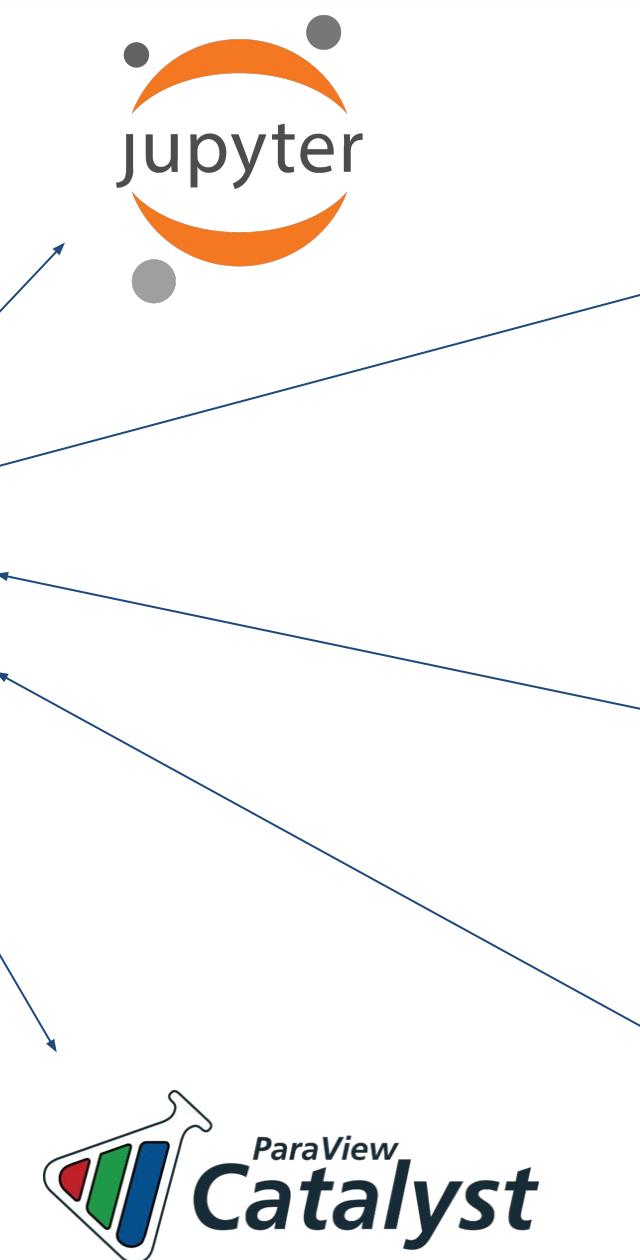
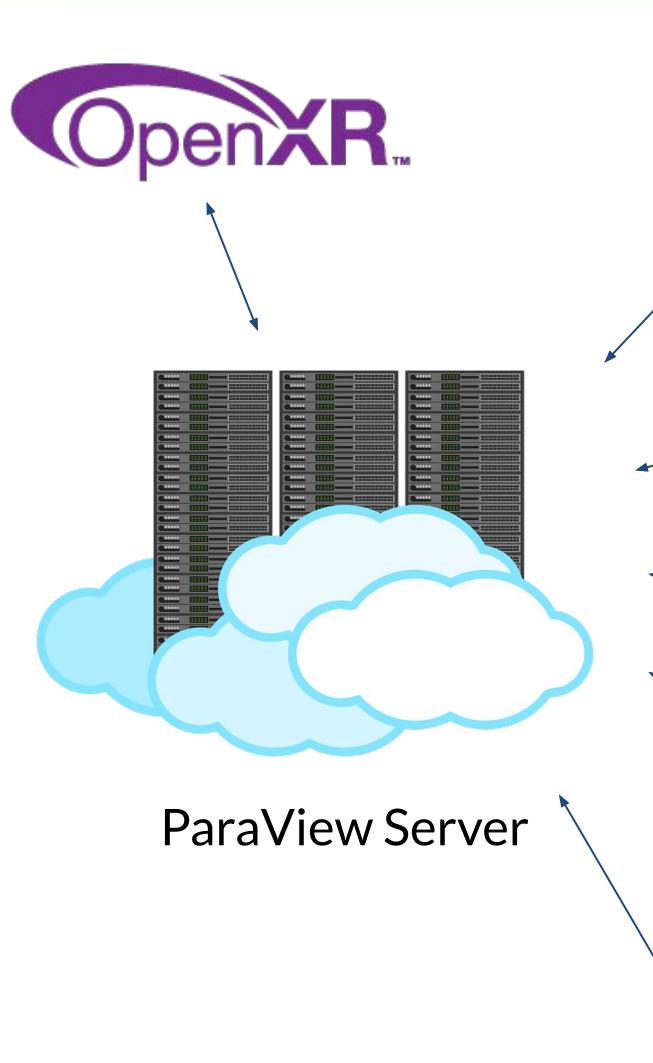
```
Macintosh HD - top - 80x24
PID COMMAND %CPU TIME #TH #MQ PORT MEM PURG CMR PGRP PPID
532 screencaptur 0.0 00:00:00 0 0 55+ 1952K 20K+ 0B 262 262
536 mencoder 0.0 00:00:00 0 0 40+ 1952K 20K+ 0B 262 262
589 mdworker 0.0 00:00:01 3 0 44+ 1572K 0B 0B 589 1
588 top 1.0 00:00:51 1/1 0 22+ 2868K 0B 0B 588 584
583 ssh 0.0 00:00:00 0 0 13+ 1572K 0B 0B 583 482
583 login 0.0 00:00:51 3 1 28+ 1228K 0B 0B 583 482
574 auditd 0.0 00:00:00 2 0 6+ 568K 0B 0B 574 1
567 com.apple.Prefer 0.0 00:00:00 0 0 270+ 3104K 0B 0B 567 1
561 systemstatd 0.0 00:00:01 2 0 19+ 1848K 0B 0B 561 1
568 com.apple.Web 0.0 00:01:42 9 0 229+ 25M 0B 0B 568 1
553 com.apple.Web 0.0 00:00:00 15 0 224+ 2174K 0B 0B 553 1
355 bash 0.0 00:00:00 0 0 14+ 604K 0B 0B 355 554
554 login 0.0 00:00:01 3 1 28+ 1176K 0B 0B 554 482
559 bash 0.0 00:00:00 1 0 15+ 608K 0B 0B 559 549
```

Batch mode
(ParaView Python)



ParaView Client

/// **ParaView**
Web



Batch mode (ParaView Python)

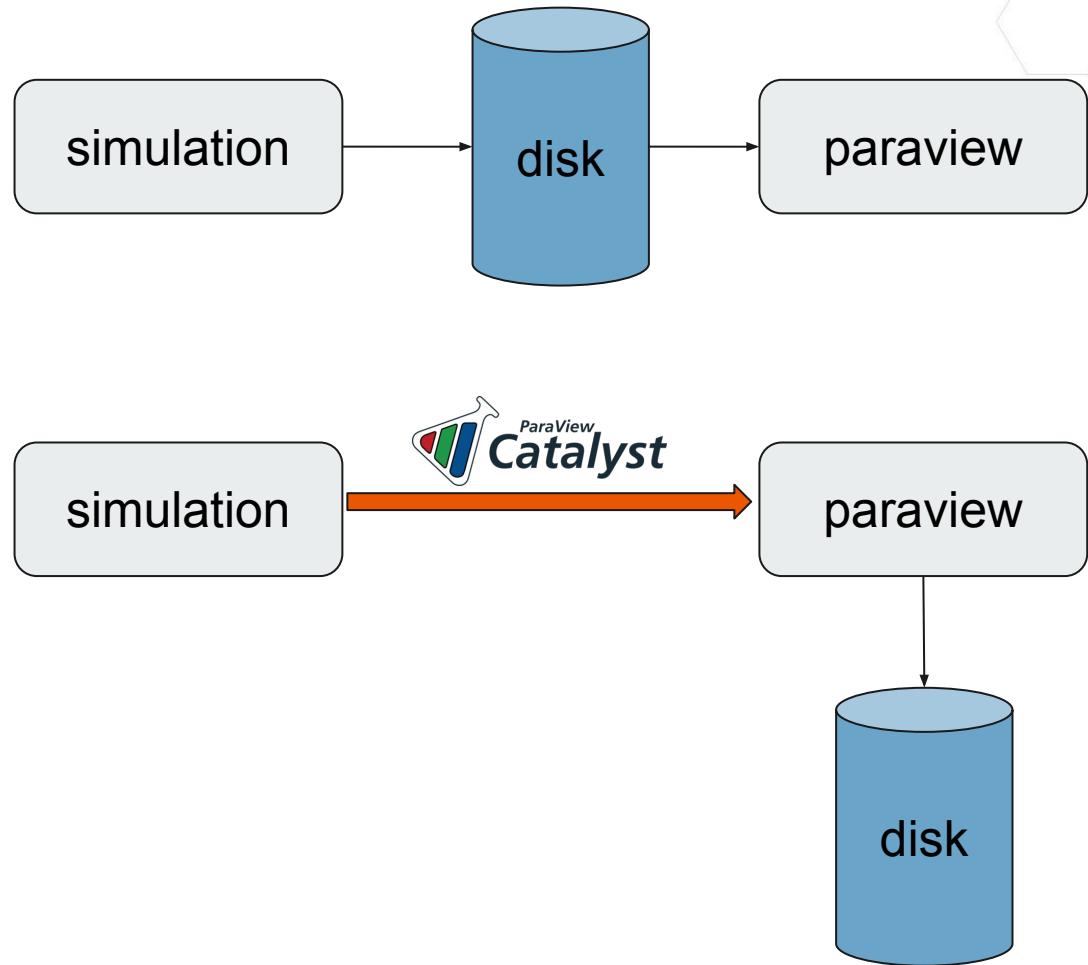




In-Situ Analysis

What is ParaView Catalyst?

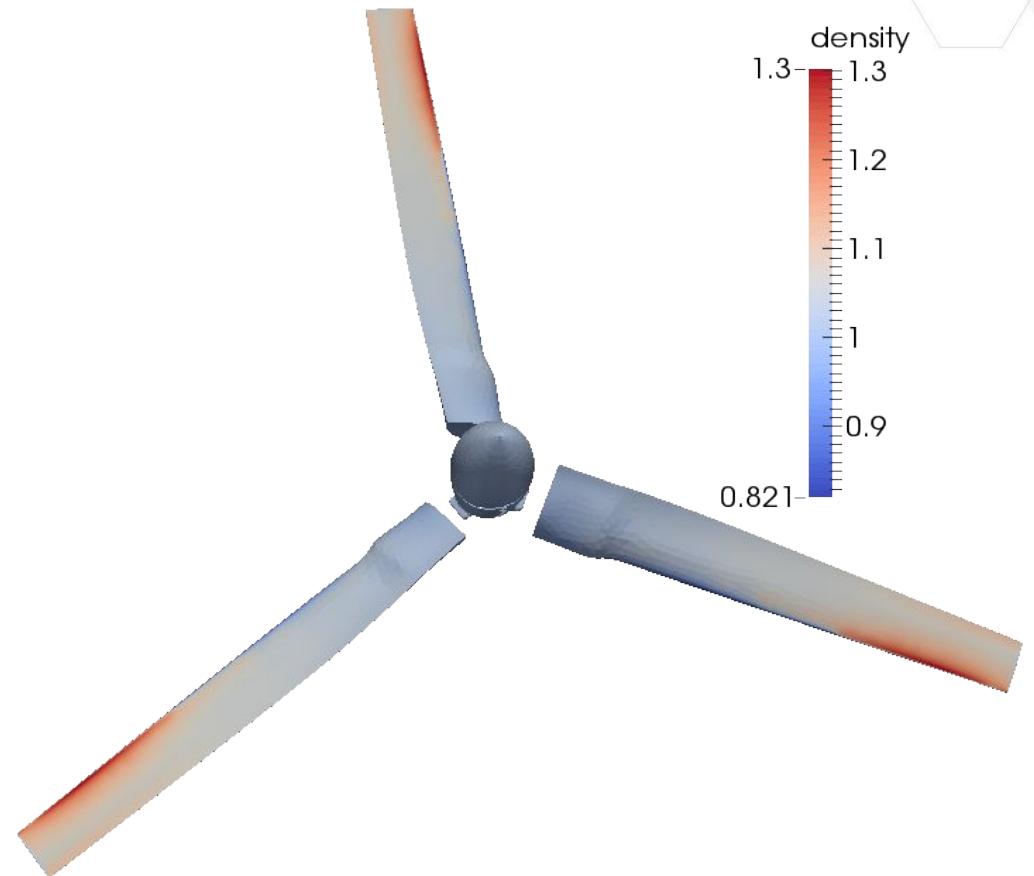
- ◆ An in-situ framework embedded with ParaView
 - in-situ analysis: uses ParaView analysis capabilities
 - live visualization: uses ParaView to connect to the simulation
 - easy configuration: uses ParaView to generate scripts
 - open source
- ◆ Challenges : explosion of scientific data
 - Storage
 - Bandwidth



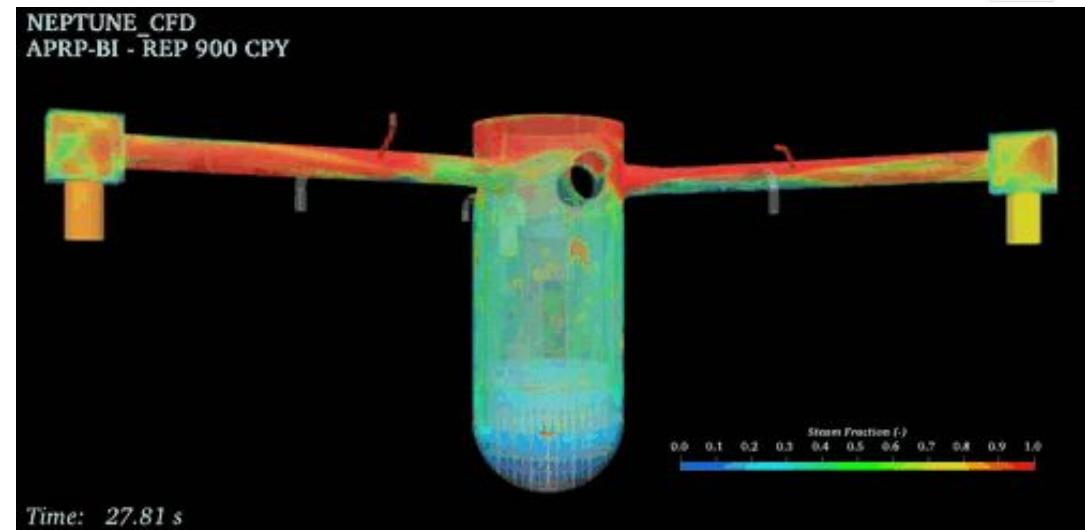
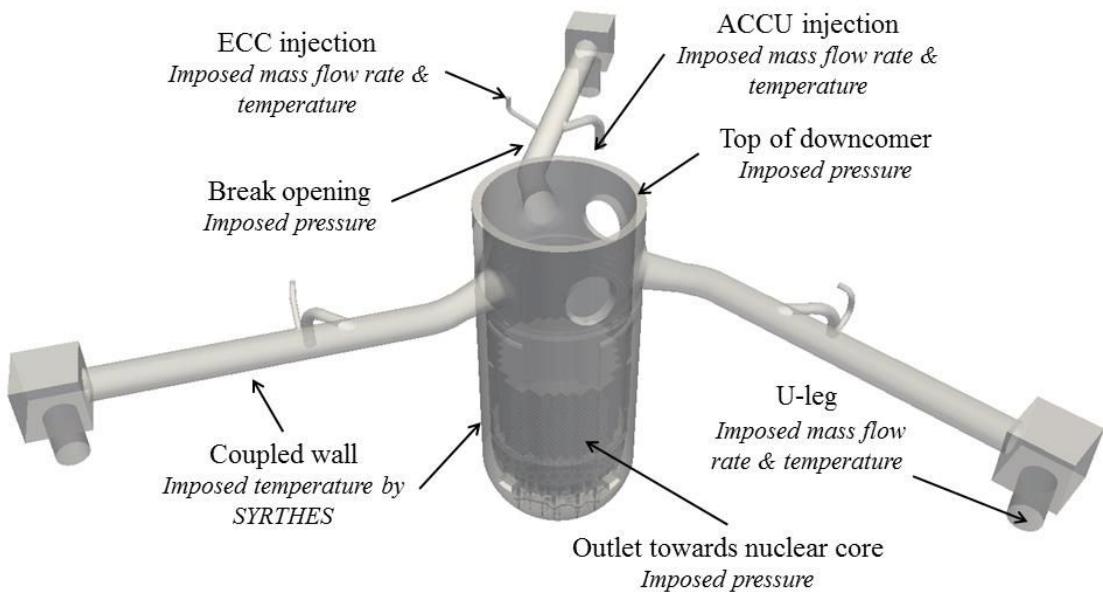
Saving Data Storage

Rotorcraft simulation output size for a single time step:

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



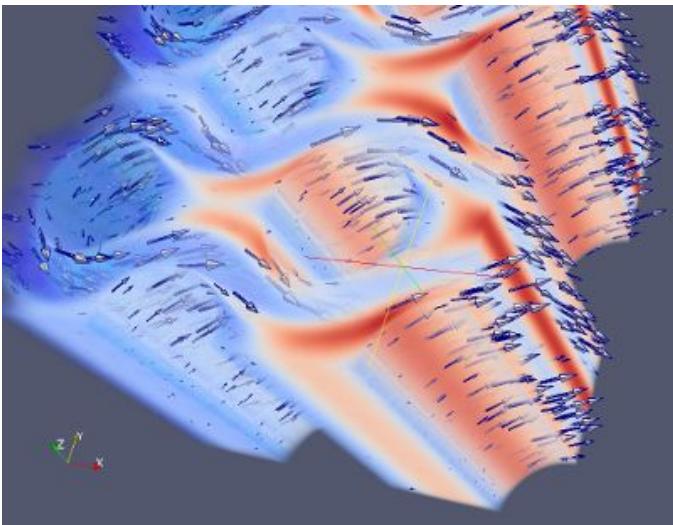
ParaView Catalyst in Code_Saturne Example



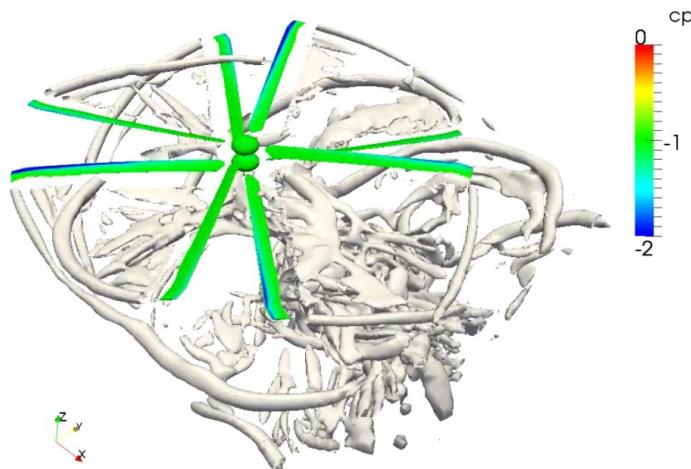
- Fluid mesh: about 6 500 000 cells
- Solid mesh: around 4 000 000 cells

Courtesy of Nicolas MERIGOUX & Yvan FOURNIER, EDF R&D

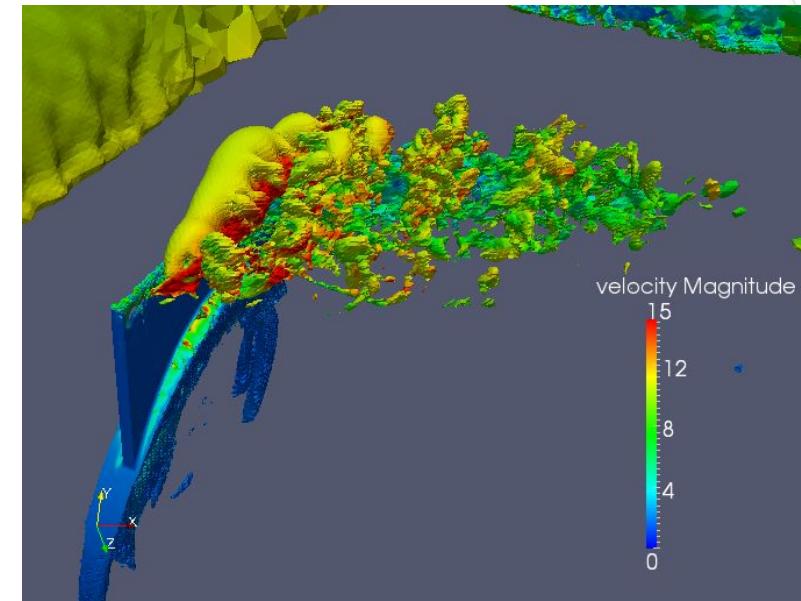
More Catalyst Examples



Code Saturne (EDF)

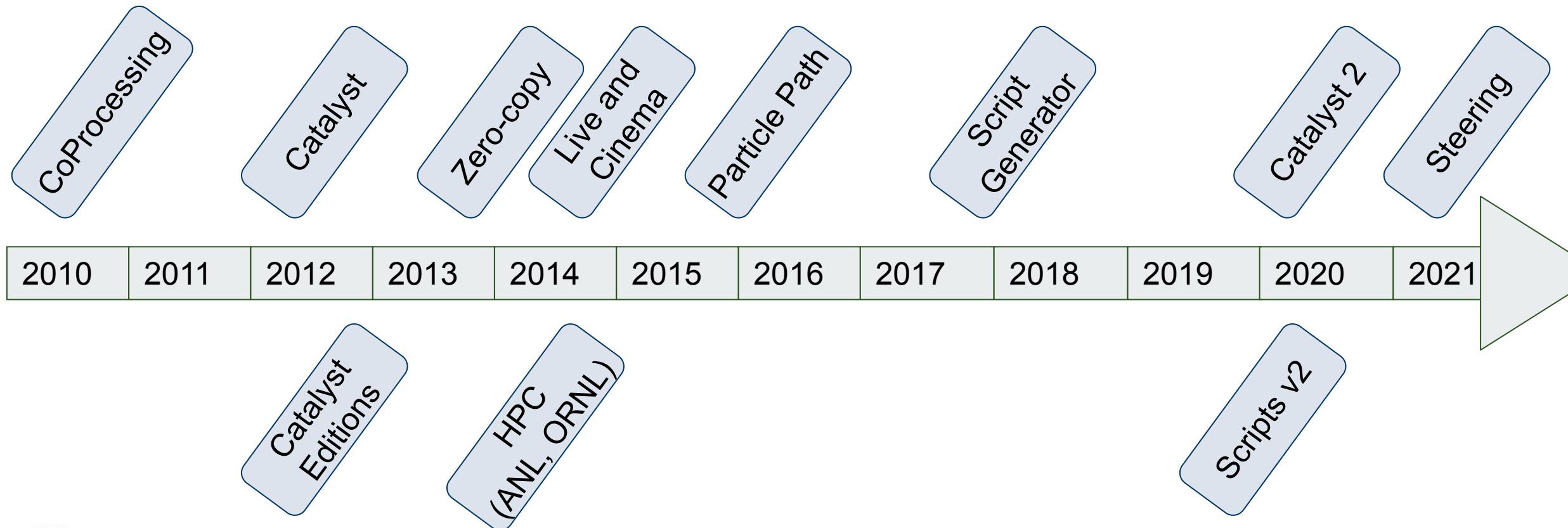


Helios
(Army Aeroflightdynamics
Directorate)



Phasta (UC-Boulder)

Catalyst History



Catalyst 2

Catalyst 2 : challenges

- ◆ Make it easy to develop
- ◆ Make it easy to build
- ◆ Make it easy to deploy
- ◆ Make it easy to maintain and upgrade

Catalyst 2 : easy development



- Avoid need to understand VTK data model
- Provide mechanism to expose data with zero-copy & meta-data to interpret it

→ Conduit !



Conduit



- ◆ JSON-inspired hierarchical description of parameters and in-code data
- ◆ Can be used to communicate control parameters or simulation data

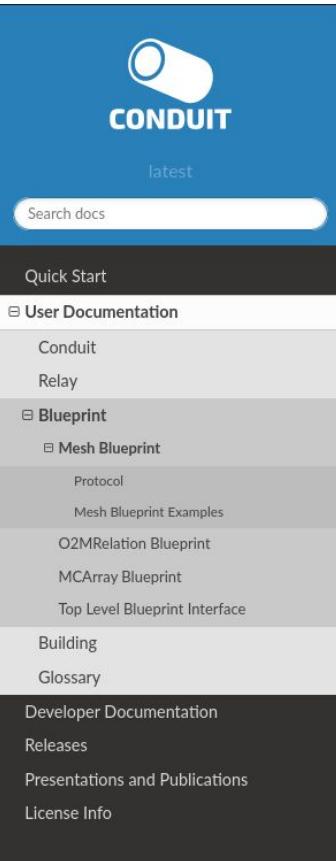
<https://llnl-conduit.readthedocs.io>

```
{  
  "catalyst":  
  {  
    "steerable":  
    {  
      "coordsets":  
      {  
        "coords":  
        {  
          "type": "explicit",  
          "values":  
          {  
            "x": 0.9,  
            "y": 0.9,  
            "z": 0.9  
          }  
        },  
        "topologies":  
        {  
          "mesh":  
          {  
            "type": "unstructured",  
            "coordset": "coords",  
            "elements":  
            {  
              "shape": "point",  
              "Connectivity":  
              (...)  
            }  
          }  
        }  
      }  
    }  
  }  
}
```

Mesh Blueprint

- ◆ Standard protocol to describe mesh :
 - Mesh Blueprint

<https://llnl-conduit.readthedocs.io/en/latest/blueprint.html>



An important nuance to the structure of a **polyhedral** shape topology is that the `elements/connectivity` path indexes into the `subelements` object to list the *many* faces associated with each one polyhedron. Similarly, the `subelements/connectivity` path indexes into the `coordset` path to list the *many* vertices associated with each one polyhedral face. There is no assumed ordering for constituent polyhedral faces relative to their source polyhedra.

The following diagram illustrates a simple **polyhedral** topology:

```
#          0
#          / \
#          / | \ <- e0
#          /   \
#          /_.-3-.\_\
#          1., | , .4
#          \-'2'-
#          \ | /
# e1 -> \ | /
#          \|/
#          5
#]

topologies:
topology:
  coordset: coords
  type: unstructured
  elements:
    shape: polyhedral
    connectivity: [0, 1, 2, 3, 4, 0, 5, 6, 7, 8]
    sizes: [5, 5]
    offsets: [0, 5]
  subelements:
    shape: polygonal
    connectivity: [1, 2, 4, 3, 1, 2, 0, 2, 4, 0, 4, 3, 0, 3, 1, 0, 1, 2, 5, 2, 4, 5, 4, 3,
    sizes: [4, 3, 3, 3, 3, 3, 3, 3]
    offsets: [0, 4, 7, 10, 13, 16, 19, 22, 25]
```

Catalyst 2 : simple API and stable API

<https://catalyst-in-situ.readthedocs.io>

```
enum catalyst_status catalyst_initialize(const conduit_node* params);  
enum catalyst_status catalyst_finalize(const conduit_node* params);  
  
enum catalyst_status catalyst_execute(const conduit_node* params);  
enum catalyst_status catalyst_results(conduit_node* params);  
  
enum catalyst_status catalyst_about(conduit_node* params);
```

Catalyst 2 API

- Inspired by “**MPICH ABI compatibility initiative**”
(<https://www.mpich.org/abi/>)

MPICH

High-Performance Portable MPI

Home About Downloads Documentation Support ABI Compatibility Initiative Supported Compilers

MPICH is a high performance and widely portable implementation of the **Message Passing Interface (MPI)** standard.

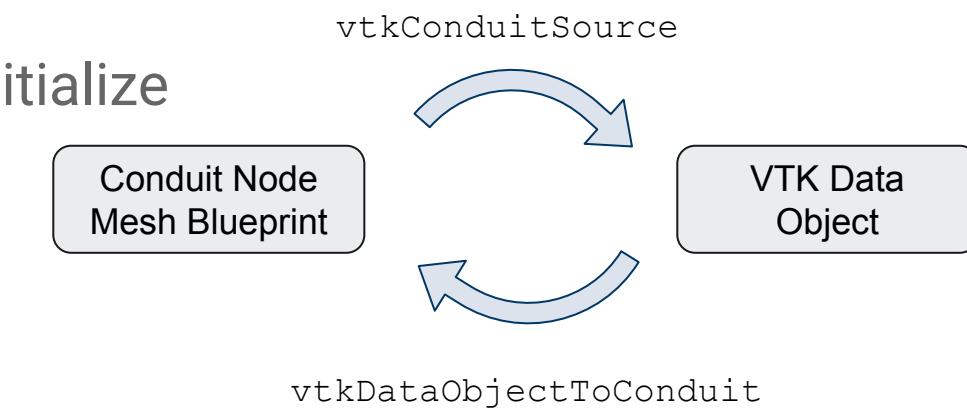
MPICH and its derivatives form the most widely used implementations of MPI in the world. They are used exclusively on nine of the top 10 supercomputers (June 2016 ranking), including the world's fastest supercomputer: Taihu Light.



Download MPICH

Catalyst 2 implementations

- **Change implementation at run-time**
 - Environment variables
 - CATALYST_IMPLEMENTATION_PATHS
 - CATALYST_IMPLEMENTATION_NAME
 - Dedicated keys in conduit node of catalyst_initialize
 - catalyst_load/search_paths
 - catalyst_load/implementation
 - Legacy way: LD_LIBRARY_PATH



- **Several implementations**
 - catalyst-stub: no external dependencies, suitable for building
 - catalyst-paraview: uses ParaView and VTK to work on data
 - Debug, replay, etc.

Catalyst 2 Steering

Drive the simulation from ParaView via
Catalyst API and Live Visualization

```
enum catalyst_status  
catalyst_results(conduit_node* params);
```



Catalyst 2 : goals achieved!

◆ Easy to develop

- No need to understand VTK
- No data conversion

◆ Easy to deploy

- Several catalyst implementations deployment
- Not link to specific ParaView version

◆ Easy to build

- Few dependencies using catalyst-stub
- No CMake

◆ Easy to maintain

- Stable C API/ABI
- No need to rebuild simulation for new ParaView version

Catalyst : a VTK-based API

vs.

a Conduit-based API

Original API (ParaView before v5.9)

- Writing a data adaptor requires an intimate understanding of VTK. VTK Mesh types, Data types.
- Knowledge of how to efficiently transform simulation data structures to VTK is a must.
- Not for the faint-at-heart
- Not for a simulation code developer, without a hobby for Visualization software development

Catalyst : a VTK-based API

vs.

a Conduit-based API

Original API (ParaView before v5.9)

- Writing a data adaptor requires an intimate understanding of VTK. VTK Mesh types, Data types.
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- Not for a simulation code developer, without a hobby for Visualization software development

(with v5.9 and onwards)

- Writing an adaptor requires a discreet knowledge of Conduit, which I acquired in one afternoon.
- Catalyst is a lightweight API and a simulation can be linked against its stub implementation, without requiring a ParaView SDK
- A ParaView 5.9+ build provides a Catalyst API implementation, which is now referred to as *ParaView-Catalyst*
- [Catalyst in ParaView 5.9: Blog article](#)

ParaView Catalyst

- ParaView-Catalyst is an implementation of the Catalyst *in situ* API that uses ParaView for data processing and rendering.
- ParaView-Catalyst supports a subset of the [Mesh Blueprint](#). Simulations that can use the Mesh Blueprint to describe their data can directly use ParaView's Catalyst implementation for *in situ* analysis and visualization.
- [ParaView-Catalyst](#)
- [ParaView-Catalyst Blueprint](#)

ParaView Catalyst practical how-to

- Download (or build) ParaView:
 - <https://www.paraview.org/download> OR
 - Follow instructions at
<https://gitlab.kitware.com/paraview/paraview/-/blob/master/Documentation/dev/build.md>
- Download Catalyst and build Catalyst:
 - git clone https://gitlab.kitware.com/paraview/catalyst
 - mkdir build_catalyst
 - cd build_catalyst
 - cmake ../catalyst
 - make

ParaView Catalyst practical how-to

- Build SPH-EXA with Catalyst support:
 - git clone <https://github.com/unibas-dmi-hpc/SPH-EXA.git>
 - mkdir build_sphexa
 - cd build_sphexa
 - cmake -DINSITU=Catalyst
-Dcatalyst_DIR=../build_catalyst/lib/cmake/catalyst-2.0 .. /SPH-EXA
 - make sphexa
- Note: If you are using ParaView binaries from paraview.org, use an MPICH compatible MPI version (not OpenMPI)
- Launch SPH-EXA with Catalyst:
 - export CATALYST_IMPLEMENTATION_PATHS=/path/to/paraview/lib/catalyst/
 - export CATALYST_IMPLEMENTATION_NAME=paraview
 - sphexa (init options...) --catalyst my_catalyst_pipeline.py

ParaView Catalyst practical how-to

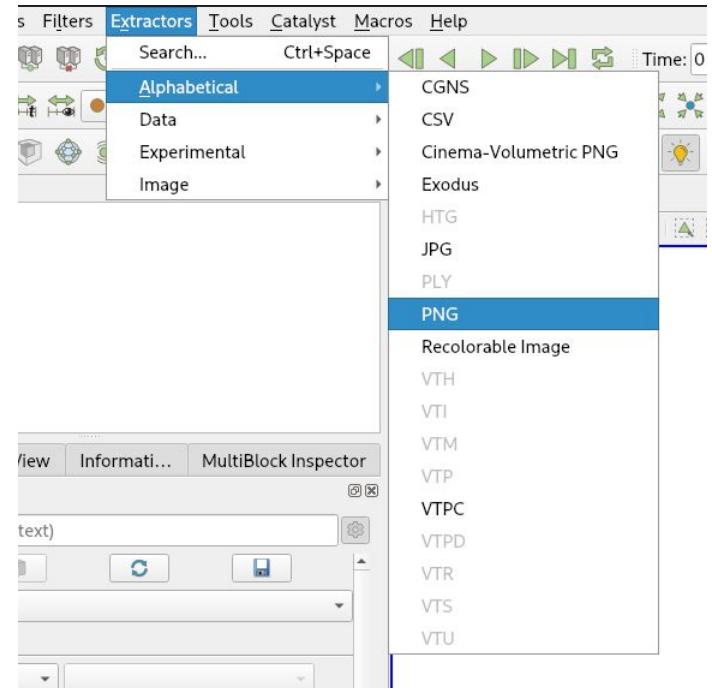
- Instrumented our simulation code? Yes!
- Compiled with ParaView Catalyst? Yes!
- How do we run and specify visualization tasks????

The ParaView Catalyst Python scripts

- Python scripts, are written by the ParaView application, given a representative template input file, and a set of visualization filters interactively tuned by the user in an *offline* fashion [not connected to a running solver]
- We create a visualization pipeline with the numerous visualization filters and rendering options available in ParaView, and we add “Extractors”
- ParaView provides hybrid parallelism out-of-the-box
 - MPI-enabled
 - TBB multi-threading
 - CUDA-enabled filters
- Some [or most of the] ParaView visualization code will be tightly integrated with the solver memory and execution space.

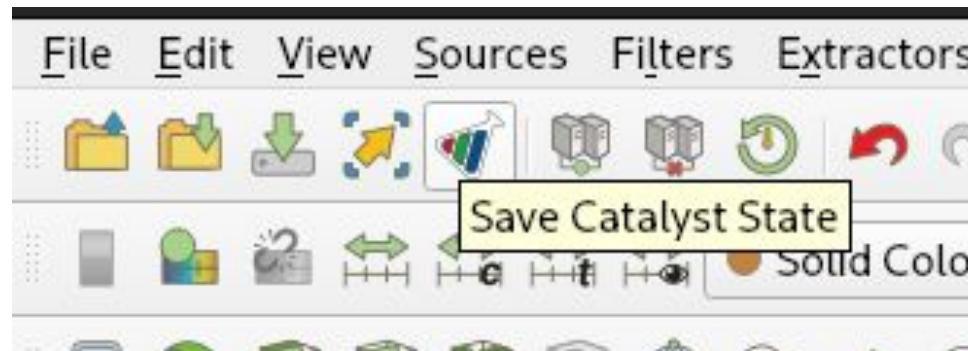
The ParaView Extractors

- Extractors are items in the visualization pipeline that can save data or images at a user-chosen temporal frequency.
 - Data Extractors
 - Image Extractors
- Using Extractors, no custom code per iteration is really necessary in the majority of cases. One can simply use Extractors to save out images from views or data extracts from filters and other data producers. (*more on that later*)



ParaView Catalyst Python scripts

- Can be generated from an interactive ParaView session, and later fine-tuned
- Are completely interchangeable between the batch-mode ParaView execution (reading data from disk), and the in-situ execution



Catalyst scripts (batch-mode

vs.

in-situ mode)

```
grid = OpenDataFile(registrationName='grid',  
filename=['/LULESH/datasets/data_000009.vtpd'])
```

```
renderView1 = GetRenderView()  
rep = Show()  
ColorBy(rep, ['POINTS', 'velocity'])  
Render()
```

execute in batch-mode with data read from disk

```
from paraview.simple import  
    SaveExtractsUsingCatalystOptions  
SaveExtractsUsingCatalystOptions(options)
```

```
grid = TrivialProducer(registrationName='grid')
```

```
renderView1 = GetRenderView()  
rep = Show()  
ColorBy(rep, ['POINTS', 'velocity'])
```

```
v = CreateExtractor('VTPD', grid)  
v.Trigger = 'TimeStep'  
v.Trigger.Frequency = 30  
v.Writer.FileName = 'data_{timestep:06d}.vtpd'
```

ParaView-Catalyst Blueprint

The Protocol is rather simple:

- Defines the options accepted by **catalyst_initialize()**; these include things like ParaView Python scripts to load, directories to save data
- Defines the protocol for **catalyst_execute()** and includes information about Catalyst channels i.e. ports on which data is made available to in situ processing as well as the actual data from the simulation
- Defines the protocol for **catalyst_finalize()**

ParaView-Catalyst Blueprint

Similar to the Conduit Mesh Blueprint.

node[“catalyst/scripts/script/filename”] =

node[“catalyst/state/cycle”] =

node[“catalyst/state/time”] =

node[“catalyst/channels/grid/type”] = “mesh”

node[“catalyst/channels/grid/data”] =

Example 1: Instrument an SPH simulation package with Ascent

- The smooth particle hydrodynamics (SPH) technique is a purely Lagrangian method. SPH discretizes a fluid in a series of interpolation points whose distribution follows the mass density of the fluid.
- [PASC](#), the Swiss Platform for Advanced Scientific Computing initiative, supports the SPH-EXA project developing an SPH library.
- [SPH-EXA](#) is a C++17 headers-only code with no external software dependencies. The parallelism is currently expressed via the following models: MPI, OpenMP, CUDA and HIP.

Using Conduit, a particle set is trivially described [the coordinates]

```
particle_set = """  
coordsets:  
    coords:  
        type: "explicit"  
        values:  
            x: [0.0, 10.0, 20.0, 30.0]  
            y: [0.0, 10.0, 20.0, 30.0]  
            z: [0.0, 10.0, 20.0, 30.0]  
        """"
```

```
conduit::Node mesh;  
mesh["state/cycle"].set_external(&d.iteration);  
mesh["state/time"].set_external(&d.ttot);  
mesh["coordsets/coords/type"] = "explicit";  
mesh["coordsets/coords/values/x"].set_external(&d.x);  
mesh["coordsets/coords/values/y"].set_external(&d.y);  
mesh["coordsets/coords/values/z"].set_external(&d.z);  
// The heavy-data is available via shallow-copy links
```

Using Conduit, a particle set is trivially described [the topology]

```
particle_set = """  
topologies:  
    mesh:  
        type: "unstructured"  
elements:  
    shape: "point"  
    connectivity: [0, 1, 2, 3]  
    coordset: "coords"  
"""
```

```
mesh["topologies/mesh/type"].set("unstructured");  
mesh["topologies/mesh/elements/shape"].set("point");  
mesh["topologies/mesh/coordset"].set("coords");  
  
std::vector<int> conn(N); // N is # of particles  
std::iota(conn.begin(), conn.end(), 0);  
mesh["topologies/mesh/elements/connectivity"].set(conn);
```

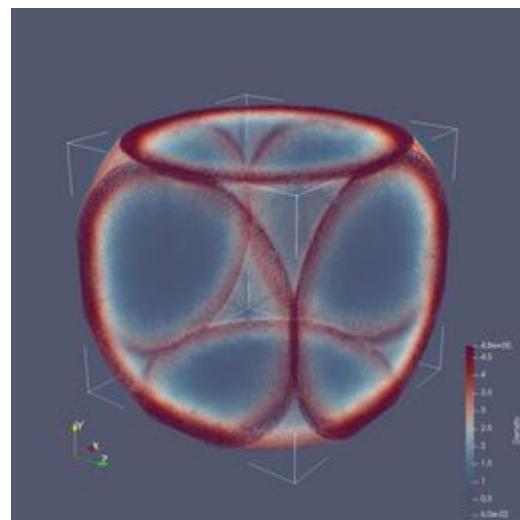
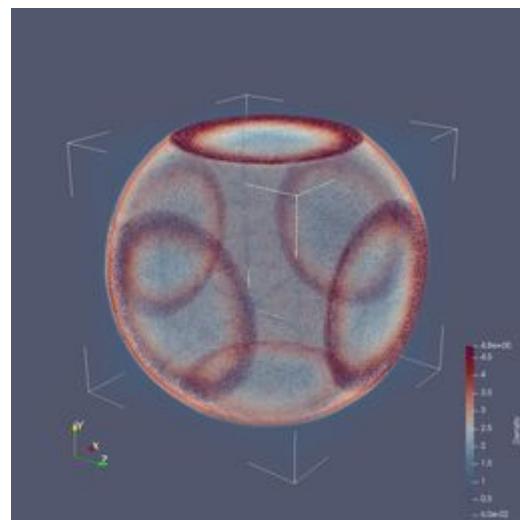
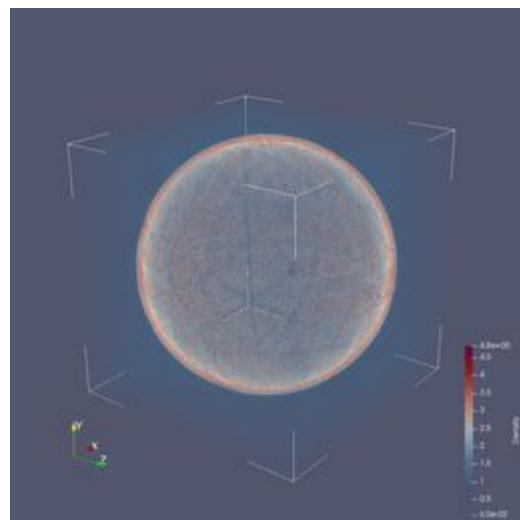
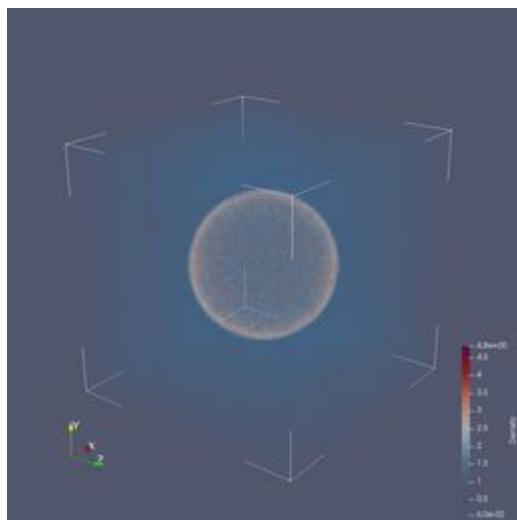
Using Conduit, a particle set is trivially described [the solution fields]

```
particle_set = """  
fields:  
  rho:  
    association: "vertex"  
    values: [-1, -2, -3, -4]  
    topology: "mesh"  
    volume_dependent: "false"  
    units: "g/cc"  
"""
```

```
auto fields = mesh["fields"];  
// Density scalar field  
fields["rho/association"].set("vertex");  
fields["rho/topology"].set("mesh");  
fields["rho/volume_dependent"].set("false");  
// Conduit supports shallow copy  
fields["rho/values"].set_external(&d.rho);
```

Instrument SPH-EXA with Catalyst

- Define a Conduit mesh definition



Use one of conduit's relay protocol to save data to disk?

c++: [extract node from SPH-EXA](#)

In Python

```
import conduit.relay as relay  
  
if relay.io.about()["protocols/hdf5"] == "enabled":  
  
    relay.io.save(mesh, "/dev/shm/foo.hdf5")
```

```
h5ls -r /dev/shm/foo.hdf5  
/  
    Group  
/coordsets  
    Group  
/coordsets/coords  
    Group  
/coordsets/coords/type Dataset {9}  
/coordsets/coords/values Group  
/coordsets/coords/values/x Dataset {4}  
  
...  
/fields  
    Group  
/fields/rho  
    Group  
/fields/rho/values Dataset {4}  
  
....  
/topologies  
    Group  
/topologies/mesh  
    Group  
/topologies/mesh/coordset Dataset {7}  
/topologies/mesh/elements Group  
/topologies/mesh/elements/connectivity Dataset {4}
```

Code instrumentation -

The Catalyst glue code for the SPH-EXA solver is 144 lines of code

Enabling in-situ visualization can be optionally compiled

before

```
int main(int argc, char** argv)
{
    MPI_Init_and_Code_Init();

    for (d.iteration = 0; d.iteration <= maxStep; d.iteration++)
    {
        Solve_For_Each_Timestep();

    }

    return exitSuccess();
}
```

Code instrumentation -

- The Catalyst glue code for the SPH-EXA solver is 144 lines of code
- The execution driver is instrumented with 4 lines of code
- Total: 148 lines of code

after

```
#include "CatalystAdaptor.h"

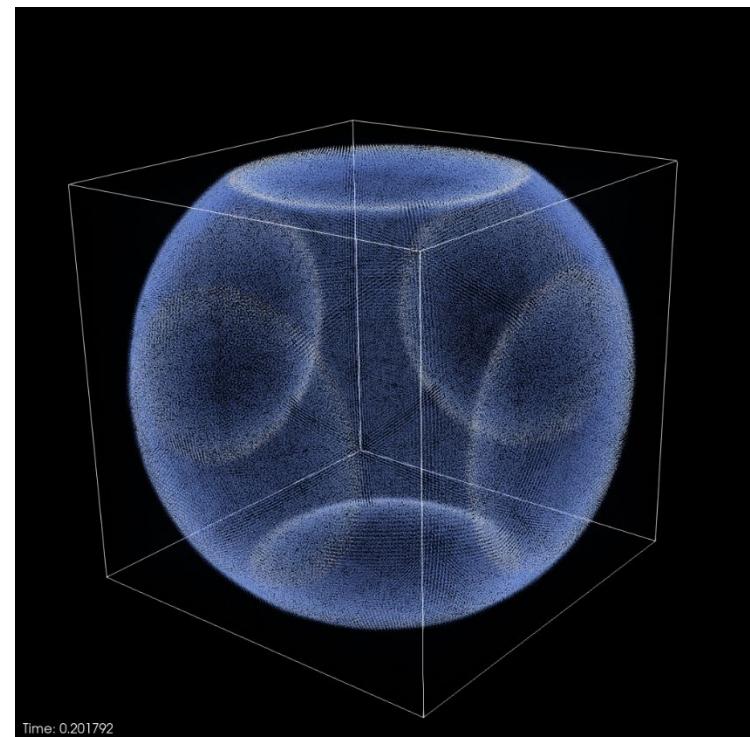
int main(int argc, char** argv)
{
    MPI_Init_and_Code_Init();
    CatalystAdaptor::Initialize(argc, argv);
    for (d.iteration = 0; d.iteration <= maxStep; d.iteration++)
    {
        Solve_For_Each_Timestep();
        CatalystAdaptor::Execute(d, domain.startIndex());
    }
    CatalystAdaptor::Finalize();
    return exitSuccess();
}
```

What about “Operations Control”?

Adaptive Control

- Choose different paths of execution based on queries/triggers
- The `catalyst_execute(ConduitNode)` script can be customized

```
def catalyst_execute(node):
    threshold = 1.4
    if reader.PointData[“Density”].GetRange()[1] > threshold:
        print(“density at timestep”, node.timestep)
        # Extract particles where Density > threshold
    else:
        # use ALL particles
```



What about “Operations Control”?

Human in the loop

ParaView has a very efficient client-server mode for post-hoc visualization

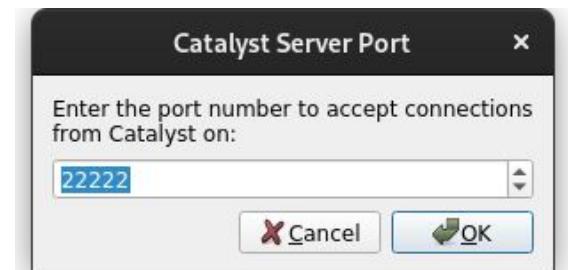
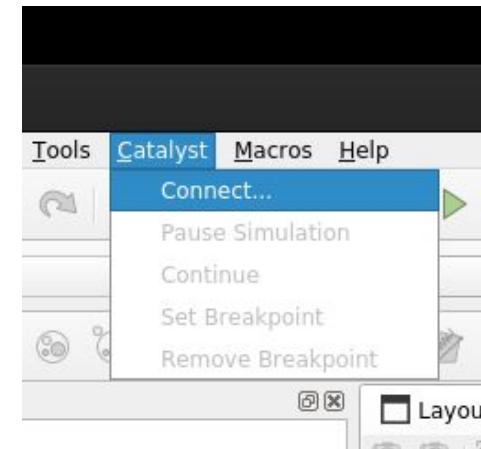
- Uses a powerful, remote server to do the heavy work:
 - Parallel I/O
 - Parallel filtering
 - Parallel Image Composition
- Has a very efficient, threshold-based, **Image Delivery** engine
- The results of the different visualization operations stay on the server (Mbytes, Gbytes, Tbytes (choose your flavour))
- Only the image gets sent over to the client (1024x1024 pixels, RGB).

ParaView-Catalyst Live Visualization

- Open ParaView and launch Catalyst via the menu “Connect...”
 - The ParaView desktop client sends a request for connection on that port
 - the code instrumentation listens to incoming calls with few additional lines of Python code:

```
from paraview import catalyst
options = catalyst.Options()
options.EnableCatalystLive = 1
```

Demonstration of Catalyst Live



Other examples: LULESH instrumented for ParaView Catalyst

[ASC Proxy Apps](#)

Instrumented with the [VTK-based](#) Catalyst

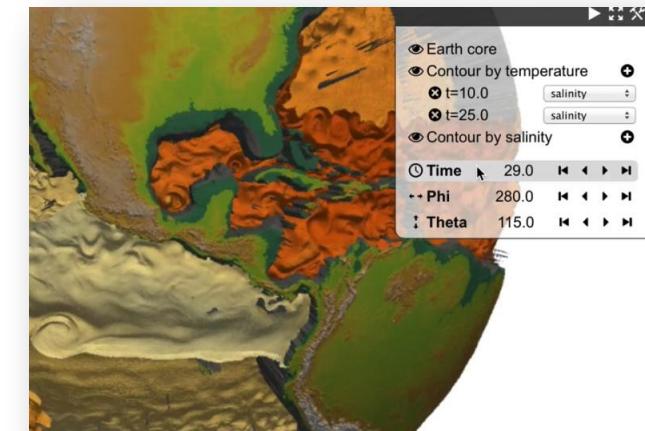
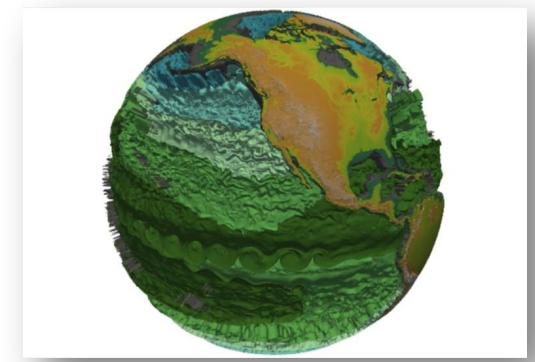
Instrumented with the [Conduit-based](#) Catalyst

Thanks to Utkarsh Ayachit (Kitware)



- Image output is orders magnitude less than an entire data set
- Use ParaView/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 desktop client or web-browser to view/analyze images later

<http://www.cinemascience.org>



Cinema and Catalyst



ParaView pipeline

vs.

Ascent pipeline

```
renderView1 = CreateView('RenderView')

selection=SelectPoints()
selection.QueryString="Density >= 1.4"

extractSelection = ExtractSelection()
thresholdDisplay = Show(extractSelection)
ColorBy(thresholdDisplay, ['POINTS', 'Density'])

pNG1 = CreateExtractor('PNG', renderView1)
pNG1.Trigger = 'TimeStep'
pNG1.Writer.FileName =
'threshold_{timestep:06d}{camera}.png'
pNG1.Trigger.Frequency = 100
```

```
"action": "add_pipelines",
"pipelines": {
    "pl1": {
        "f1": {
            "type": "threshold",
            [...]
        }
    }
}
"action": "add_scenes",
"scenes": {
    "s1": {
        "plots": {
            "p1": {
                "type": "pseudocolor",
                "pipeline": "pl1",
                [...]
            }
        }
    }
}
"renders": {
    "r1": {
        "image_prefix": "ThresholdImage.%05d",
```



CSCS

Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETHzürich

To close the loop: Use Ascent and ParaView Python scripts

Ascent can pass data to a ParaView script

- [Ascent Documentation](#)
- The instrumented simulation sends a tree structure (json like) that describes the simulation data using the Conduit Blueprint Mesh specification.
- A ParaView plugin constructs one of the following datasets: vtkImageData, vtkRectilinearGrid, vtkStructuredGrid or vtkUnstructuredGrid
- This data is converted to a VTK format using shallow copies for data arrays

Ascent, passing data to a ParaView script

- Ascent's “action” node is:

```
- action: "add_extracts"
extracts:
  e1:
    type: "python"
    params:
      file: "paraview-vis.py"
```

- The ParaView script describes a “standard” ParaView pipeline and can save images and any other derived data to disk

Catalyst Road Map

- **Meta data on meshes (ParaView 5.11)**
 - Defined in the mesh/state/my_meta_data conduit node
 - Becomes VTK Field Data
- **In-transit analysis with Catalyst (On-going work...)**
 - Based on ADIOS

Ascent Road Map

Conduit:

- Simplifying use of multi-domain Mesh Blueprint transforms
- Expanding support for ND-strides in Mesh Blueprint conventions
- Continuing to productize complex Mesh Blueprint transforms (e.g. AMR to Polyhedral)

Ascent:

- Migrating close dependences (Devil Ray, VTK-h) into Ascent source for future development
- Unifying Expressions features to support both JIT and non-JIT execution
- Adding pipeline support for re-partitioning and load balancing meshes
- Adding support to flatten mesh fields for use as tables in external analysis
- Adding new features to the Devil Ray filtering and rendering infrastructure
- Continuing to explore and productize interactive uses (Jupyter and other web technologies)

Thanks to Cyrus Harrison (LLNL) for this input.

Code milestones at <https://github.com/Alpine-DAV/ascent/milestones>

Summary

- Adopting the Conduit-based environments presented is rather simple, very intuitive. The bridges to ParaView or Ascent are hiding most complexity from code developers
- Both environments have proven tracks of high-scale deployments
- What's next:
 - evaluate performance, memory consumption,
 - visualization pipeline creation and tuning, and re-usability
- For the first time in several decades of developing data formats plugins (converters, adaptors, ..), we don't have to worry about this anymore, and each developer can concentrate on what they do best:
 - the simulation code itself, or
 - the visualization
- Already 10 years ago, while presenting libSim, people would tell me

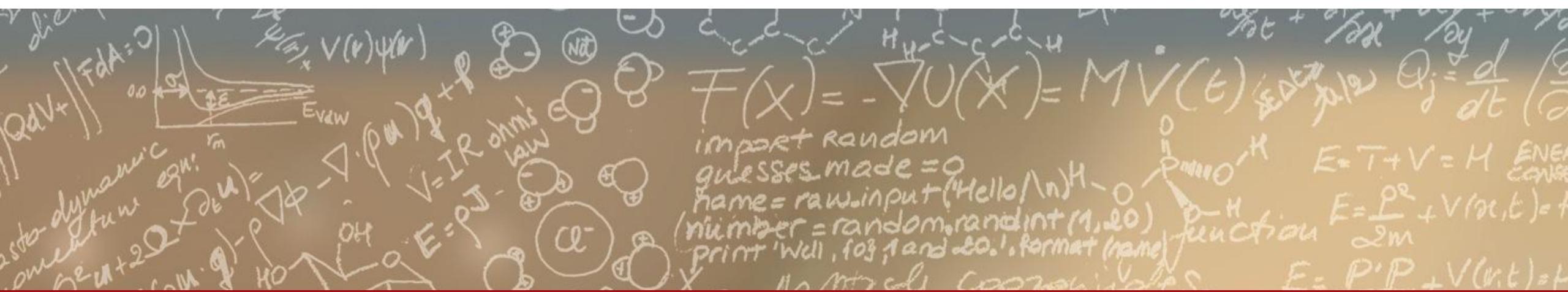
*“we're **very** tight on memory”*
- Adding an in-transit layer is the next venue to explore.

Resources

- <https://github.com/jfavre/InSitu-Vis-Tutorial2022>
- This ISC 2022 tutorial's [slides](#)
- https://dav.lbl.gov/events/SC21_SENSEI_Ascent_Tutorial/

Your feedback is encouraged. You should find a feedback link for this tutorial on the event platform.

Private emails are also encouraged: jfavre@cscs.ch, francois.mazen@kitware.com



Thank you for attending.