Visualization and Analysis of HPC Simulation Data with VisIt

ATPESC 2025

Data Analysis and Visualization Track

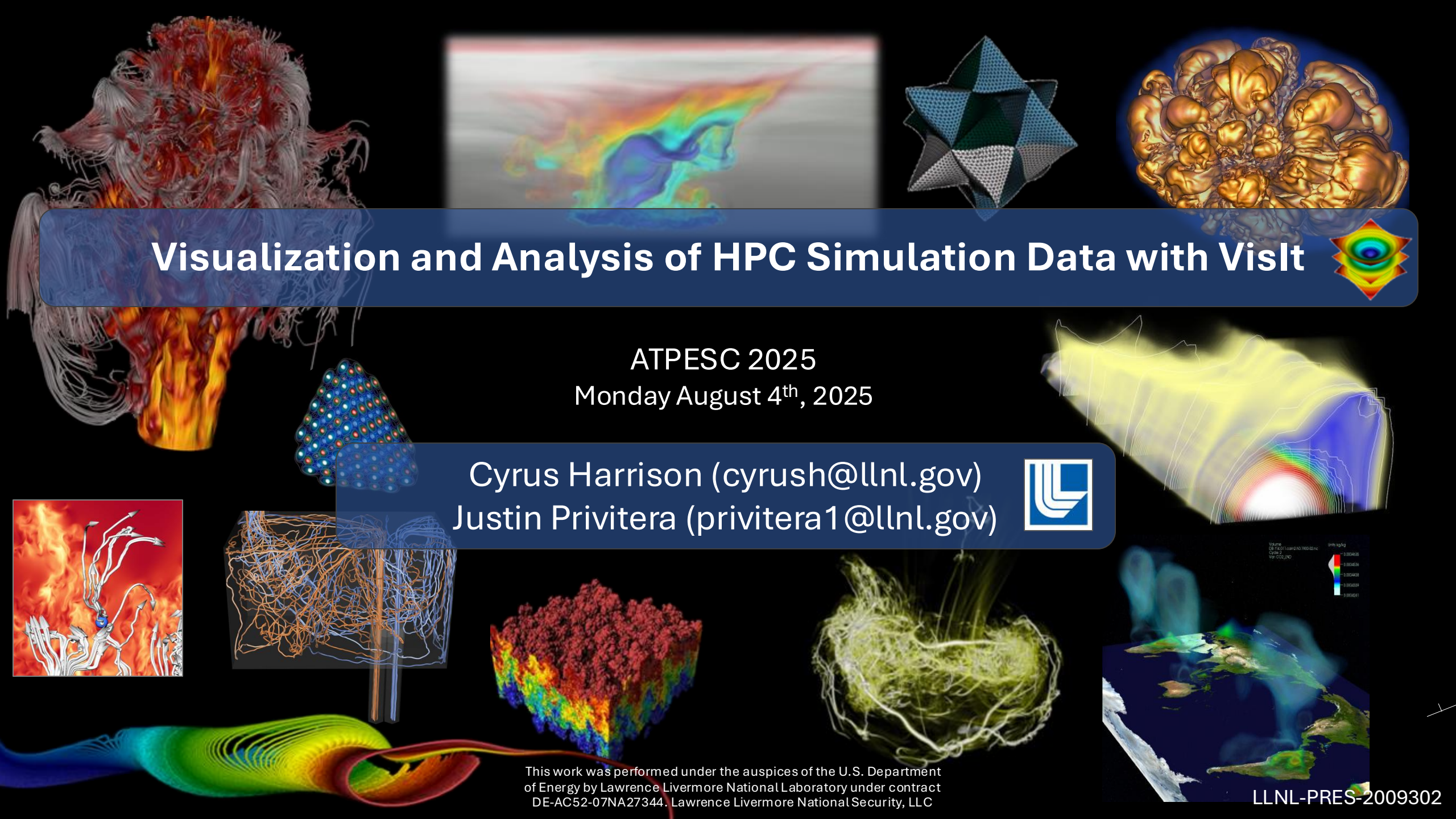
2025/08/04

Cyrus Harrison

Justin Privitera

LLNL

Prepared by LLNL under Contract DE-AC52-07NA27344.



Visualization and Analysis of HPC Simulation Data with VisIt

ATPESC 2025

Monday August 4th, 2025

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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

LLNL-PRES-2009302

Acknowledgements

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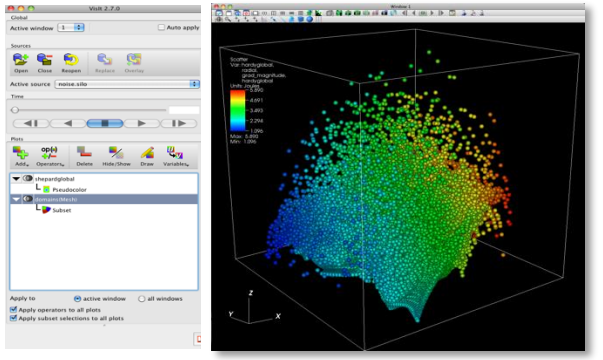
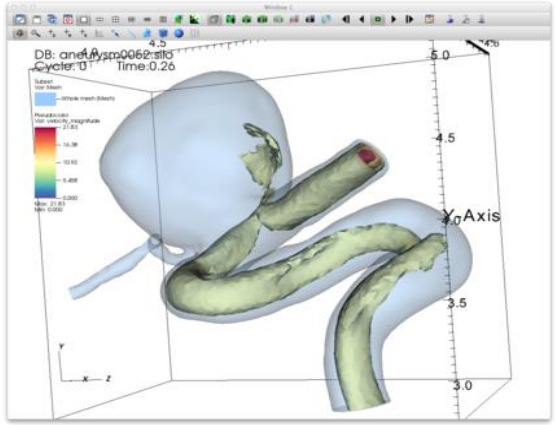
This research was supported by the Exascale Computing Project (17-SC-20-SC), a joint project of the U.S. Department of Energy's Office of Science and National Nuclear Security Administration, responsible for delivering a capable exascale ecosystem, including software, applications, and hardware technology,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

Tutorial Outline

- VisIt Project Introduction (20 min)
- Hands-on: (55 min)
  - Guided tour of VisIt (25 min)
  - Visualization of an Aneurysm (30 min) (Blood Flow) Simulation



Intro to VisIt



Simulation Exploration

Tutorial Resources

- **VisIt 3.4.2**
  - https://github.com/visit-dav/visit/releases
- **Tutorial Materials**
  - http://visitusers.org/index.php?title=VisIt_Tutorial
- **How to get in touch**
  - GitHub: https://github.com/visit-dav/visit
  - GitHub Discussions: https://github.com/visit-dav/visit/discussions

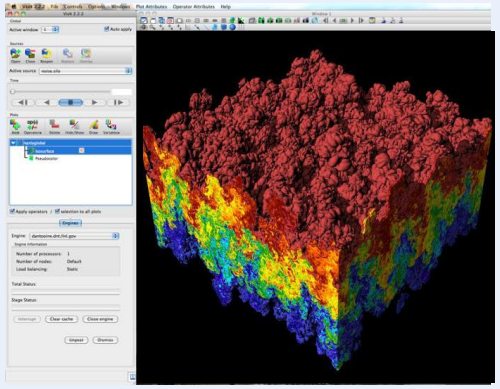
Tutorial Data Acknowledgements

- **Aneurysm Simulation Dataset**
  - Simulated using the LifeV finite element solver
  - **Available thanks to:**
    - Gilles Fourestey and Jean Favre
      Swiss National Supercomputing Centre (http://www.cscs.ch/)
- **Potential Flow Simulation Dataset**
  - Simple tutorial simulation built using MFEM (https://mfem.org/)
  - **Available thanks to:**
    - Aaron Fisher and Mark Miller, LLNL

VisIt Project Introduction

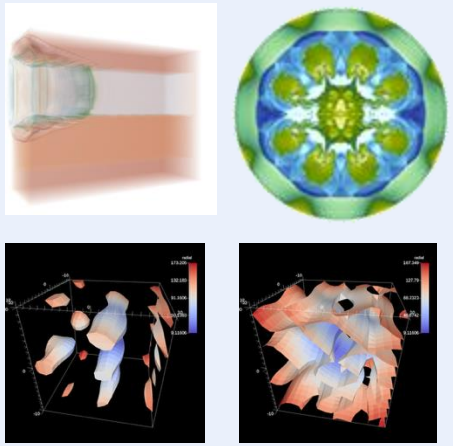
The VisIt team develops open-source Visualization, Analysis, and I/O tools

VisIt



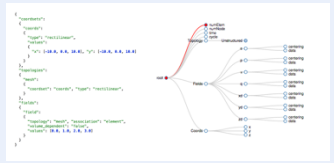
Turnkey HPC application for visualization and analysis of simulation data

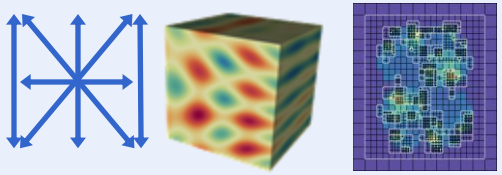
Ascent



Easy-to-use flyweight in situ visualization and analysis library for HPC simulations

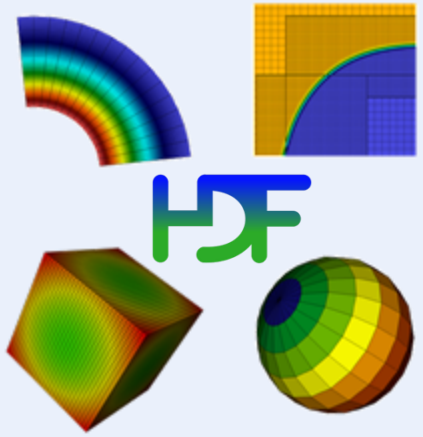
CONDUIT





In-memory data description, HPC I/O, and shared schemas for simulation data exchange

Silo



File-based, scientific data exchange library for checkpoint restart and visualization

vis·it

/ˈvizit/

verb

1. go to see and spend time with (someone) socially.
   "I came to visit my grandmother"
   synonyms: call on, call in on, pay a call on, pay a visit to, pay someone a call, pay someone a visit, go to see, come to see, look in on; More

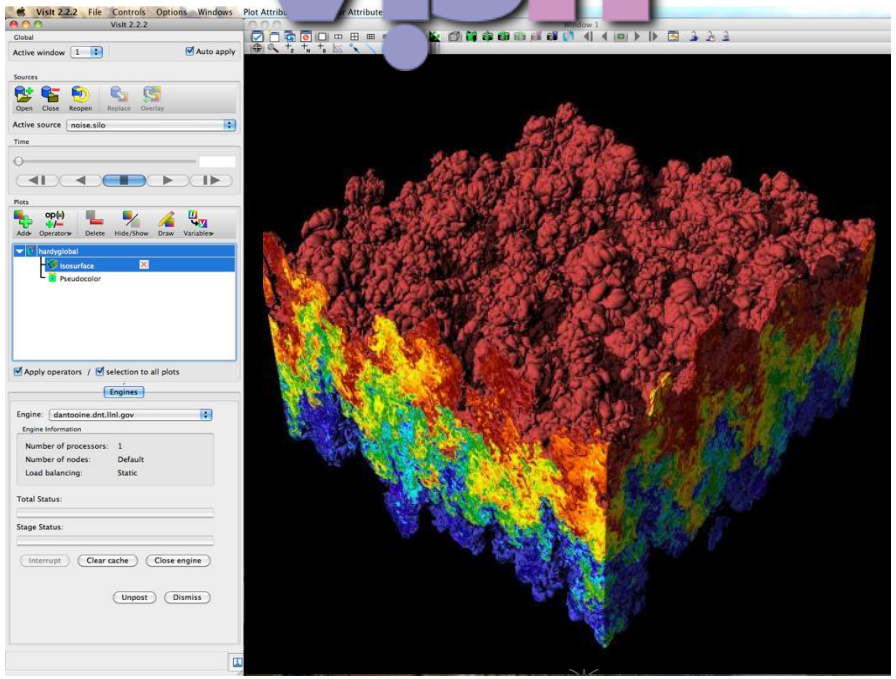
2. inflict (something harmful or unpleasant) on someone.
   "the mockery **visited upon** him by his schoolmates"
   synonyms: happen to, overtake, befall, come upon, fall upon, hit, strike
   "it is hard to imagine a greater psychological cruelty visited on a child"

noun

1. an act of going or coming to see a person or place socially, as a tourist, or for some other purpose.
   "a visit to the doctor"
   synonyms: social call, call
   "after reading the play she paid a visit to the poet"

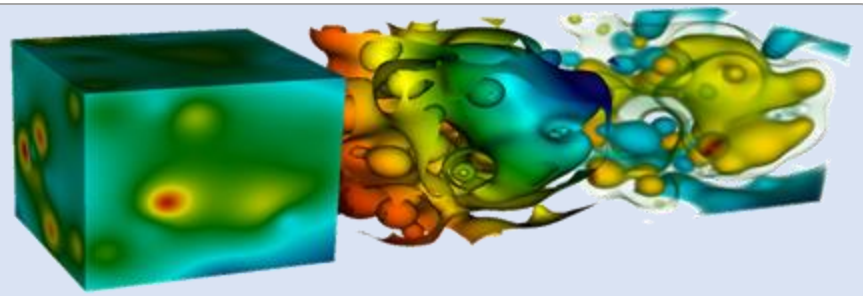
VisIt is an open source, turnkey application for data analysis and visualization of mesh-based data

- Production end-user tool supporting scientific and engineering applications.
- Provides an infrastructure for parallel post-processing that scales from desktops to massive HPC clusters.
- Source released under a BSD style license.

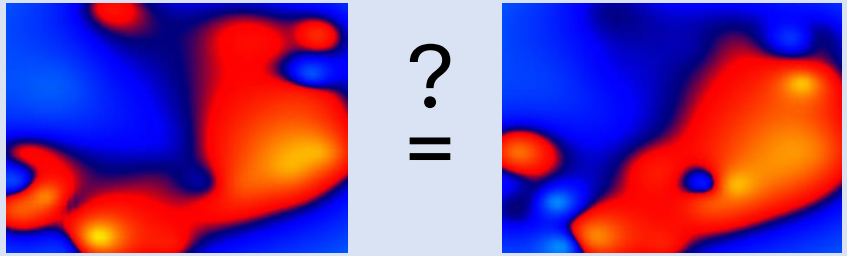


Pseudocolor plot of Density
(27 billion element dataset)

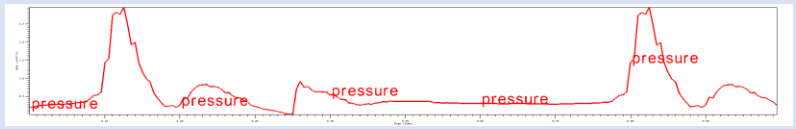
VisIt supports a wide range of use cases



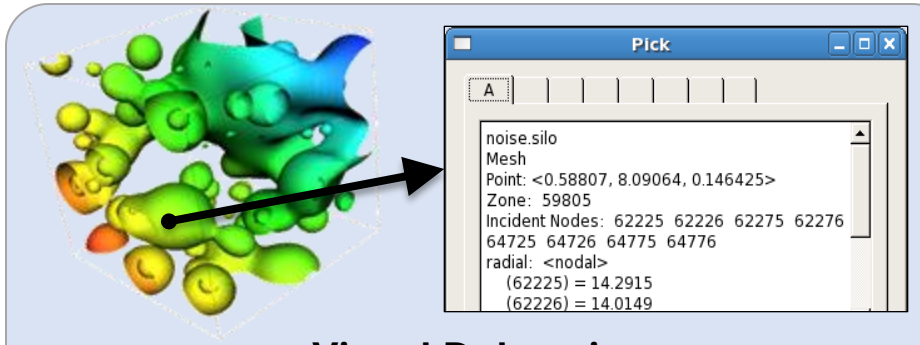
Data Exploration



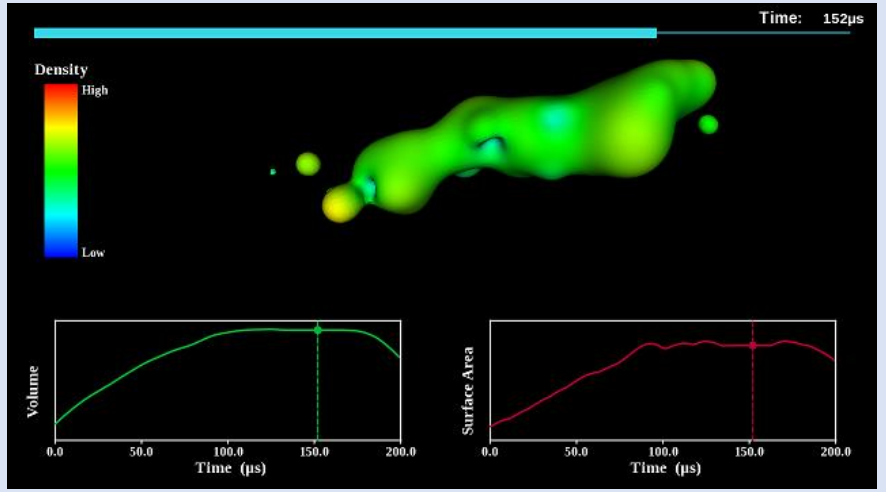
Comparative Analysis



Quantitative Analysis

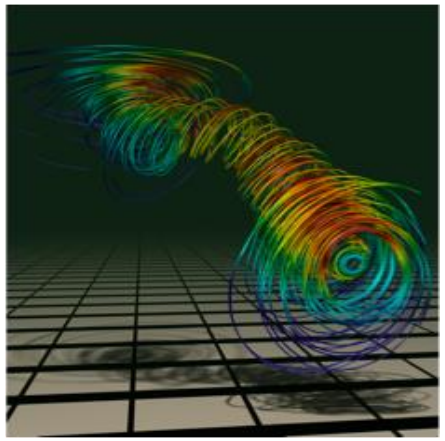


Visual Debugging

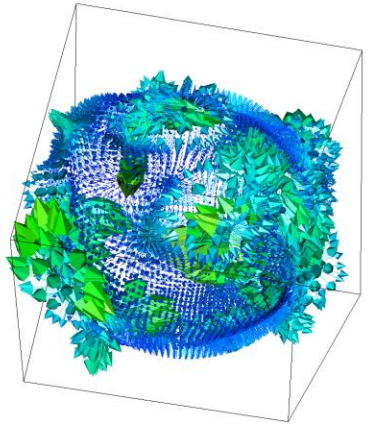


Presentation Graphics

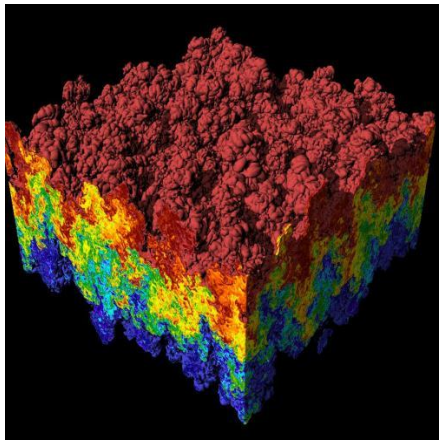
VisIt provides a wide range of plotting features for simulation data across many scientific domains



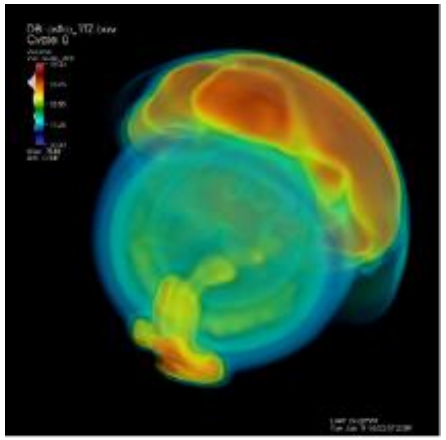
Streamlines / Pathlines



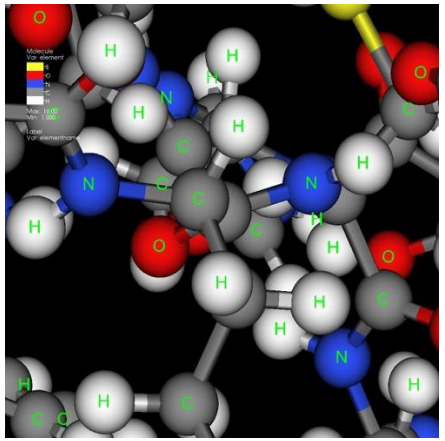
Vector / Tensor Glyphs



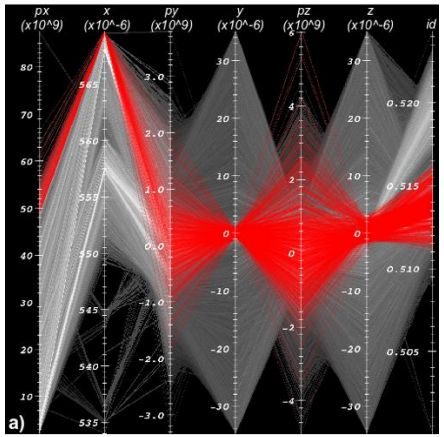
Pseudocolor Rendering



Volume Rendering



Molecular Visualization



Parallel Coordinates

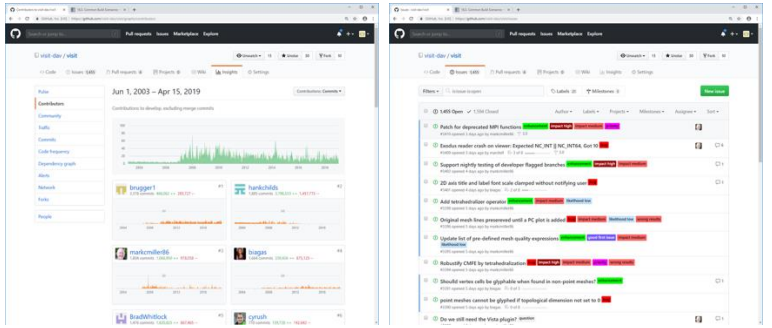
VisIt is a vibrant project with many participants

- The VisIt project started in 2000 to support LLNL's large-scale ASC physics codes.
- The project grew beyond LLNL and ASC with development from DOE SciDAC and other efforts.
- VisIt is now supported by multiple organizations:
  - LLNL, LBNL, ORNL, Univ of Oregon, Univ of Utah, Intelligent Light, …
- Over 100 person years of effort, 1.5+ million lines of code.

VisIt is hosted and developed using GitHub

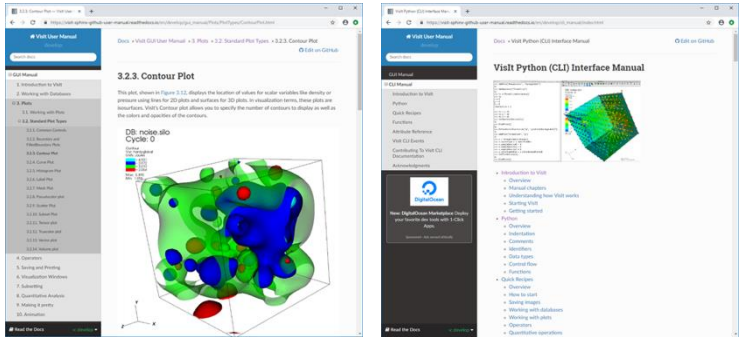
- Main Website
  - https://visit-dav.github.io/visit-website
- Our Source Code, Issue tracking, and Discussions are in the `visit-dav` GitHub organization
  - https://github.com/visit-dav/
- Our Docs are hosted on Read the Docs
  - https://visit-sphinx-github-user-manual.readthedocs.io/en/develop/

GitHub



VisIt source repo and issue tracking on GitHub

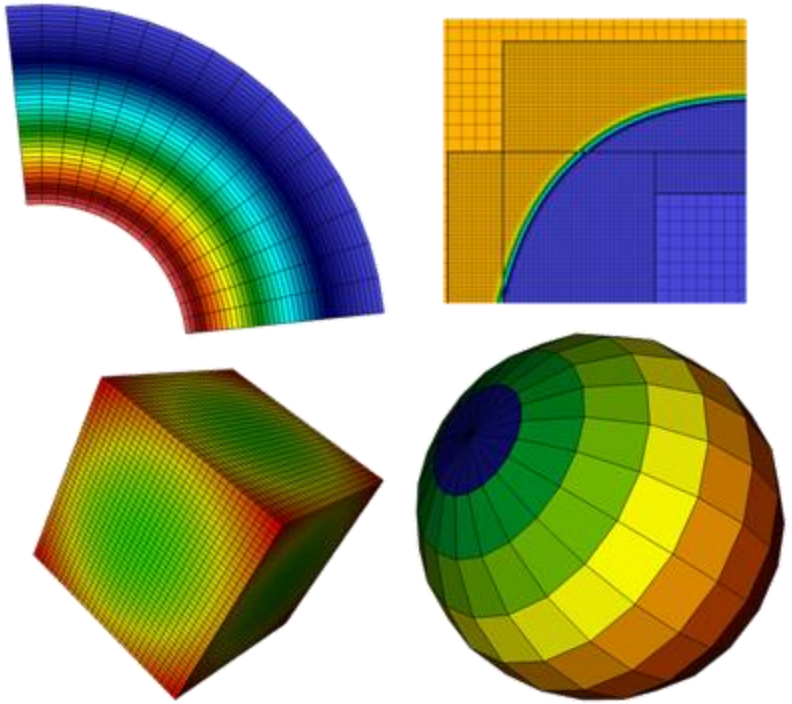
Read the Docs



VisIt manuals on Read the Docs

VisIt provides a flexible data model, suitable for many application domains

- **Mesh Types**
  - Point, Curve, 2D/3D Rectilinear, Curvilinear, Unstructured
  - Domain Decomposed, AMR
  - Time Varying
  - Primarily linear element support, limited quadratic element support
- **Field Types**
  - Scalar, Vector, Tensor, Material Volume Fractions, Species



The VisIt team releases binaries for several platforms and a script that automates the build process

“How do I obtain VisIt?”

- Use an existing build:
  - For your Laptop or Workstation:
    - Binaries for Windows, OSX, and Linux (RHEL, Ubuntu, and many other flavors): (https://github.com/visit-dav/visit/releases/)
  - Several HPC centers have VisIt installed
- Build VisIt yourself:
  - “build_visit” is a script that automates the process of building VisIt and its third-party dependencies. (also at: https://github.com/visit-dav/visit/releases/)
  - Fledgling support for building via spack (https://github.com/spack/spack)

VisIt supports more than 110 file formats

“How do get my data into VisIt?”

- The *PlainText* database reader can read simple text files (CSV, etc)
  - http://visitusers.org/index.php?title=Using_the_PlainText_reader
- Write to a commonly used format:
  - *VTK, Silo, Xdmf, PVTK, Conduit Blueprint (JSON/YAML, or HDF5 files)*
- We are investing heavily in Conduit Blueprint Support
  - http://llnl-conduit.readthedocs.io/en/latest/blueprint_mesh.html
- Consult the Getting Data Into VisIt Manual.

We continuously evolve our software development processes and resources

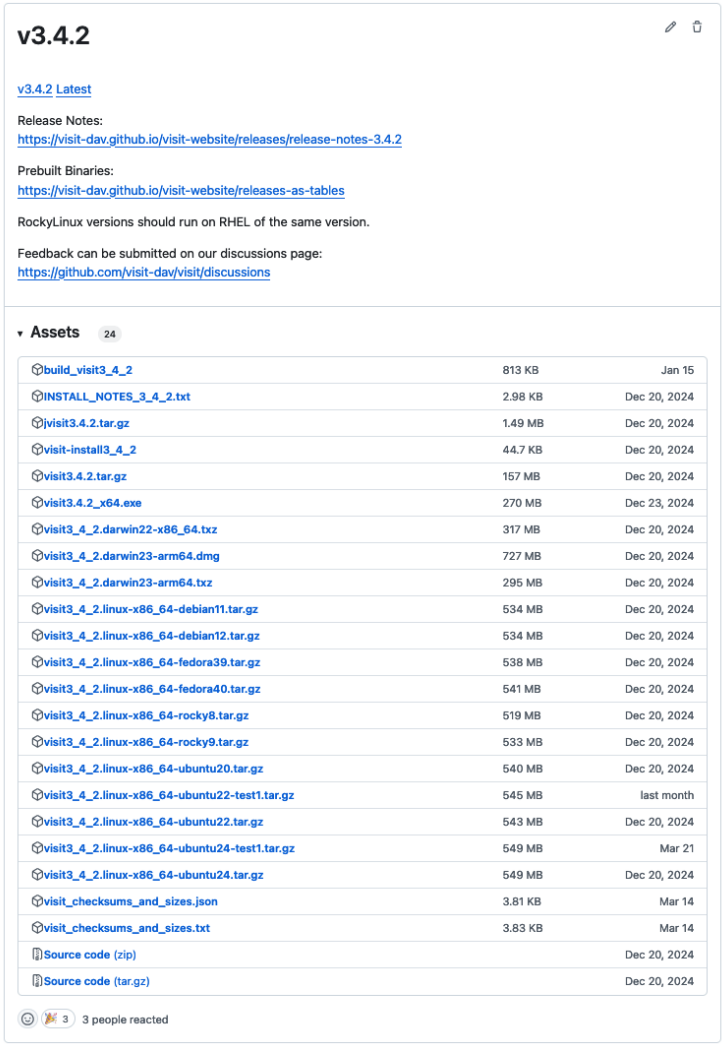
Overview of continuous technology refresh (CTR) on VisIt

	1999 (LLNL Internal)	2008 (NERSC)	2019 (GitHub)	Notes
Revision control	ClearCase (LLNL/Yellow)	Subversion (NERSC)	Git (GitHub)	Binary content, git-lfs, svn->git full history, custom scripts
Issue Tracking	ClearQuest (LLNL/Yellow)	Redmine (ORNL)	Issues (GitHub)	Tied to code
Testing+Dashboard	B-Div Irix (LLNL/Yellow)	LLNL-CZ + (NERSC)	LLNL-CZ + (GitHub)	3k image+2k txt, fix/rebase tests, exact vs. fuzzy match
CI Testing	N/A		Cicle-CI → Azure	Presently ensuring only compile of core
User contact	Majordomo (LLNL)	GNU Mailman (ORNL) 4-2Viz (LLNL)	Discussions (GitHub) 4-2Viz, Teams (LLNL)	Discoverable, attachments/size, notification controls Privacy, where users are hanging out
Documentation	FrameMaker	OpenOffice	Sphinx (ReadTheDocs)	Mergeable, committed & versioned w/code (docs like code)
Website	N/A	Drupal (LLNL, WSC web)	Jekyll + GH Pages	Developers can edit directly, GitHub Pages
Configuration	AutoTools	CMake		Native windows dev
Operating System • Windows • OSX/macOS • Linux	• XP Vista 7 8 9 10 11 • OSX-10.? 10.2 10.4 10.5/6 10.8 10.10 10.12 10.14 11 12 13 • RedHat +ubuntu +(fedora, debian, centos)			• Visual Studio, sys-call changes, manually trigger tests • Security changes getting harder to manage • No means to test variants fully
Core 3rd Party Libs • Qt • VTK • GL	• Qt3 Qt4 Qt5 Qt6 • VTK-5.0 VTK-5.8 VTK-6 VTK-8 VTK-9 • GL Drivers + Mesa (OpenGL, GL rendering changes)			**Qt+VTK+GL is a complex interdependency** • Integration w/GL tricky, no automated testing for GUI • API changes, baselines change • hw GL when possible, driver compat, baselines change
Language Standards • C++ • Python	• C w/classes templates OK C++ 11 allowed C++ 14Required • Python 2 Python 2or 3			• Very conservative in adopting new language features • A lot of users still using Python 2 workflows

We released VisIt 3.4.2 in December 2024

VisIt 3.4.2

- 45 bug fixes, 22 enhancements, 20 other changes
- Improvements for Blueprint, MFEM, Mili, MOAB, and Silo
- Improvements for Scalable Rendering and Ghost Zone Communication
- Investments during 3.4.1 release process were captured to make 3.4.2 release much faster
- Build hardening for Sierra, El Cap, and Crossroads, eliminating need for Qt5, using Qt6 everywhere
- Expanded use of Docker builds to support releases for a wide set of Linux platforms, inc. RHEL
  https://visit-dav.github.io/visit-website/releases/release-notes-3.4.2/



v3.4.2

v3.4.2 Latest

Release Notes:
https://visit-dav.github.io/visit-website/releases/release-notes-3.4.2

Prebuilt Binaries:
https://visit-dav.github.io/visit-website/releases-as-tables

RockyLinux versions should run on RHEL of the same version.

Feedback can be submitted on our discussions page:
https://github.com/visit-dav/visit/discussions

Assets 24

build_visit3_4_2	813 KB	Jan 15
INSTALL_NOTES_3_4_2.txt	2.98 KB	Dec 20, 2024
jvisit3.4.2.tar.gz	1.49 MB	Dec 20, 2024
visit-install3_4_2	44.7 KB	Dec 20, 2024
visit3.4.2.tar.gz	157 MB	Dec 20, 2024
visit3.4.2_x64.exe	270 MB	Dec 23, 2024
visit3_4_2.darwin22-x86_64.txz	317 MB	Dec 20, 2024
visit3_4_2.darwin23-arm64.dmg	727 MB	Dec 20, 2024
visit3_4_2.darwin23-arm64.txz	295 MB	Dec 20, 2024
visit3_4_2.linux-x86_64-debian11.tar.gz	534 MB	Dec 20, 2024
visit3_4_2.linux-x86_64-debian12.tar.gz	534 MB	Dec 20, 2024
visit3_4_2.linux-x86_64-fedora39.tar.gz	538 MB	Dec 20, 2024
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visit3_4_2.linux-x86_64-rocky8.tar.gz	519 MB	Dec 20, 2024
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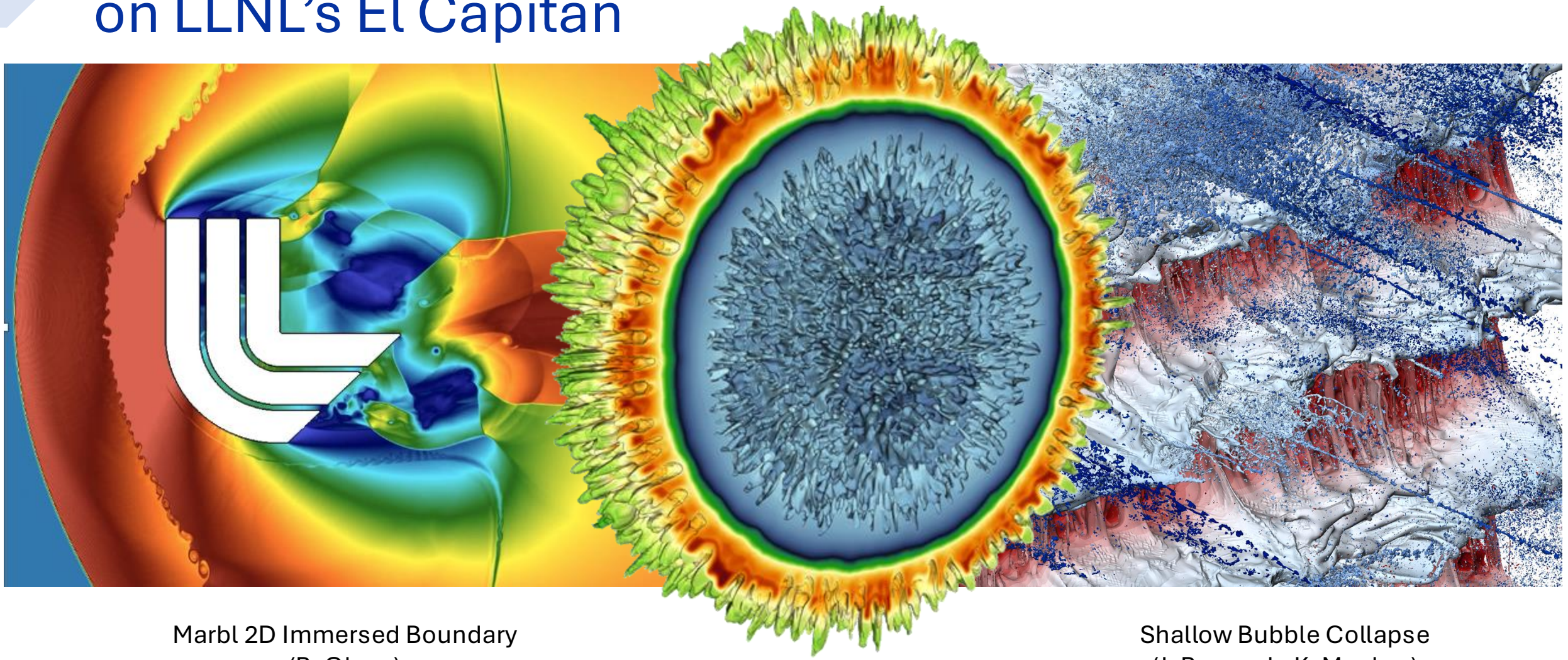
visit3_4_2.linux-x86_64-ubuntu20.tar.gz	540 MB	Dec 20, 2024
visit3_4_2.linux-x86_64-ubuntu22-test1.tar.gz	545 MB	last month
visit3_4_2.linux-x86_64-ubuntu22.tar.gz	543 MB	Dec 20, 2024
visit3_4_2.linux-x86_64-ubuntu24-test1.tar.gz	549 MB	Mar 21
visit3_4_2.linux-x86_64-ubuntu24.tar.gz	549 MB	Dec 20, 2024
visit_checksums_and_sizes.json	3.81 KB	Mar 14
visit_checksums_and_sizes.txt	3.83 KB	Mar 14
Source code (zip)		Dec 20, 2024
Source code (tar.gz)		Dec 20, 2024

3 people reacted

Release process improvements for 3.4.1 made the 3.4.2 release process much smoother

- We overhauled our build scripts to streamline builds
- Supporting 3 ASC ATS Systems (LLNL Sierra, LANL XR, and LLNL El Cap) is a still a challenge and key priority
- Several HPC X11 environments lack development packages to support Qt6, we now build `xkbcommon` and `xcb` ourselves
- Docker Builds are amazing for creating binary releases for a wide range of Linux distributions
- We are now supporting RHEL via Rocky Linux

VisIt 3.4.2 is a key tool for users running simulations on LLNL's El Capitan



Marbl 2D Immersed Boundary
(B. Olson)

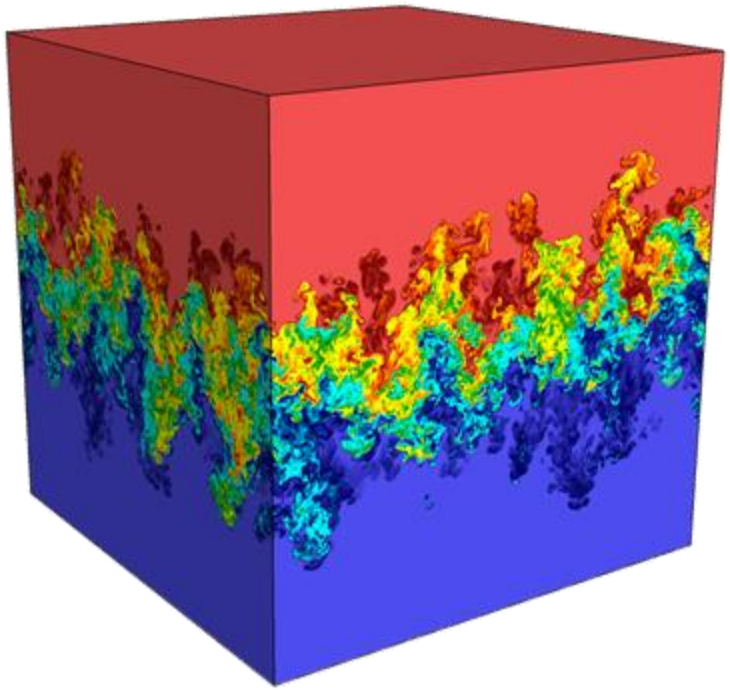
Marbl NIF N210808 Shot
(T. Stitt and R. Rieben)

Shallow Bubble Collapse
(J. Burmark, K. Mackay)

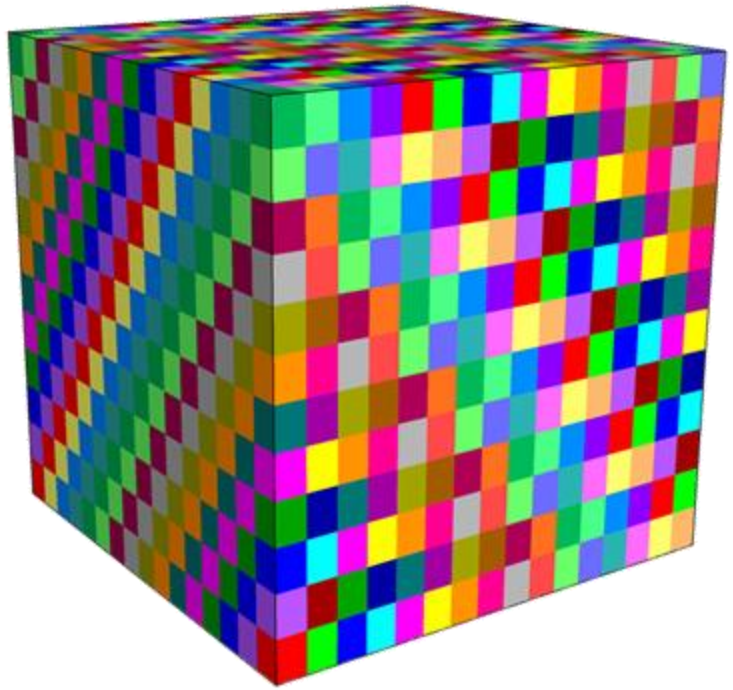
We will release VisIt 3.5.0 this fall

- Update to VTK 9.5 and leverage its new library GL strategy
- Add ANARI Rendering support
- Other TPL Updates (MFEM, Conduit)
- Revamped CMake infrastructure with BTL and Modern Targets
- Python CLI Improvements
- Bug fixes and removal of deprecated code
- Finish work on global mesh expressions
- And last but not least:
  - *New Splash Screens since we have released images from El Cap Simulations!*
- Beyond 3.5.0: We are going to explore ML Inference in DB Plugins

VisIt uses MPI for distributed-memory parallelism on HPC clusters

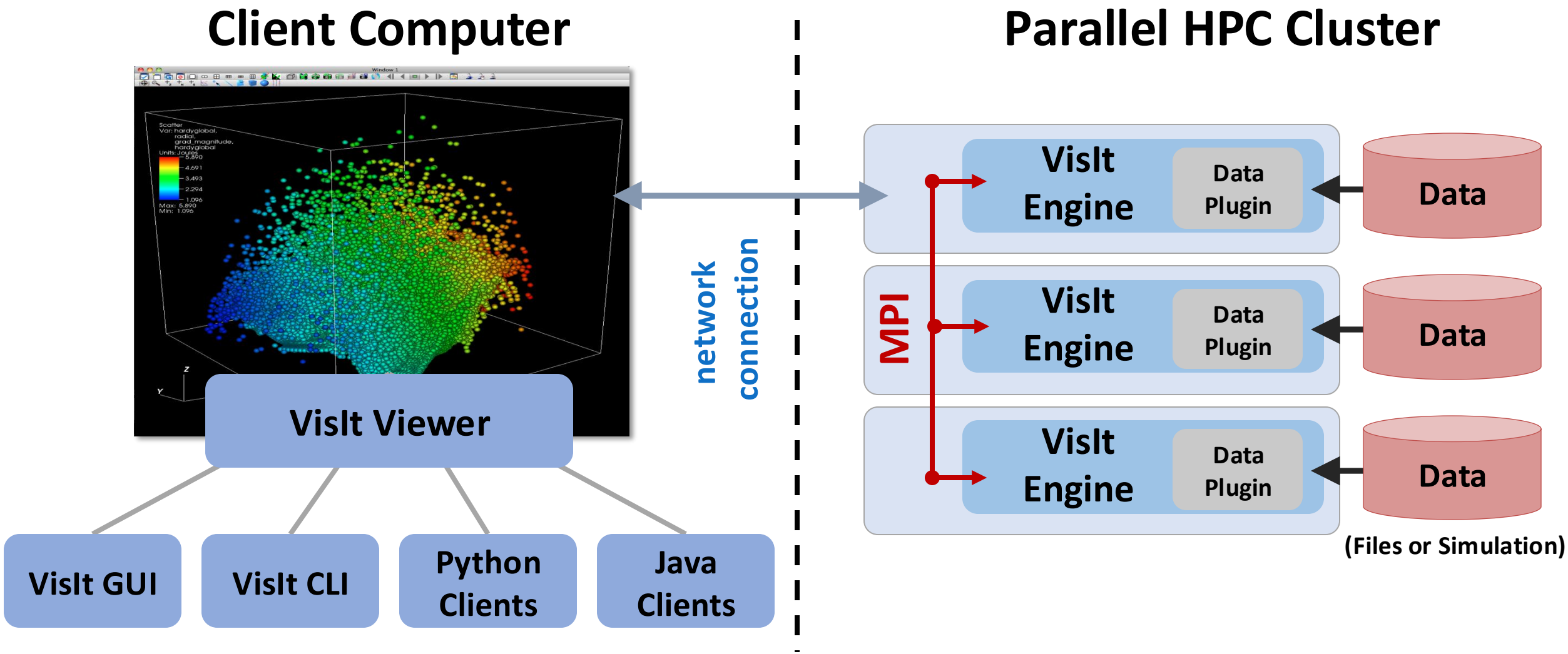


Full Dataset
(27 billion total elements)

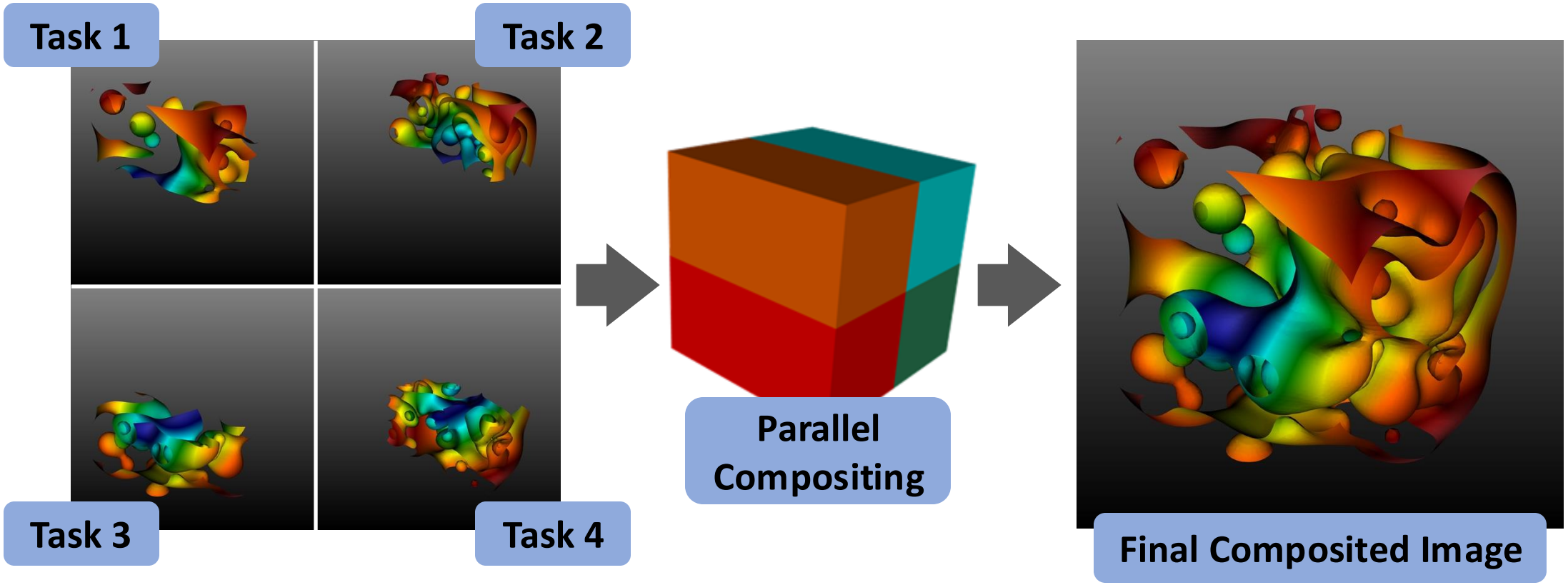


3072 sub-grids
(each 192x129x256 cells)

VisIt employs a parallelized client-server architecture



VisIt automatically switches to a scalable rendering mode when plotting large data sets on HPC clusters



In addition to scalable surface rendering, VisIt also provides scalable volume rendering

DOE's visualization community is collaborating to create open source tools for Exascale simulations

Addressing node-level parallelism

- Viskores (formerly VTK-m) is an effort to provide a toolkit of visualization algorithms that leverage emerging node-level HPC architectures from NVIDIA, AMD, Intel.

VISKORES

https://github.com/Viskores/

Addressing I/O gaps with in-situ

- Projects providing in-situ infrastructure and capabilities

CONDUIT

https://github.com/llnl/conduit

Ascent

https://github.com/Alpine-DAV/ascent

ParaView Catalyst

https://kitware.github.io/paraview-catalyst/

The VisIt team is investing in Conduit and Ascent to create next generation in situ infrastructure

Intuitive APIs for in-memory data description and exchange

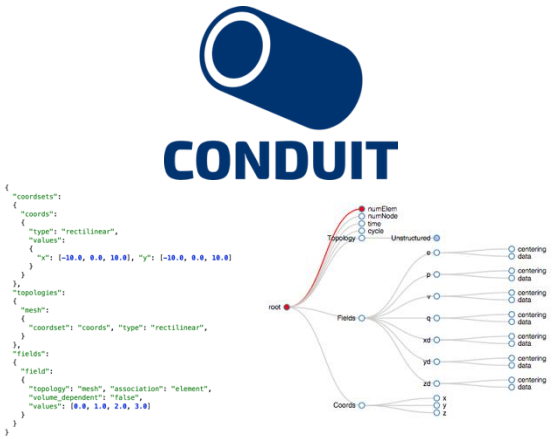
https://github.com/llnl/conduit

Flyweight in-situ visualization and analysis for HPC simulations

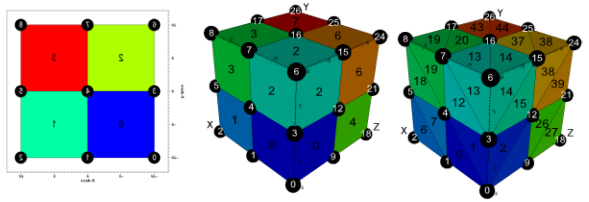
https://github.com/Alpine-DAV/ascent

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

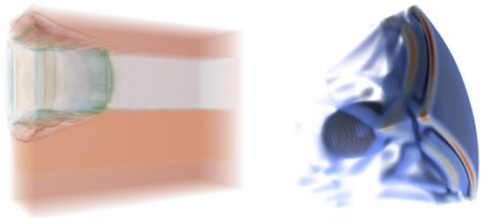
http://software.llnl.gov/conduit
http://github.com/llnl/conduit

Website and GitHub Repo

Ascent 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 fewer dependencies than current tools (ex: no OpenGL)

Ascent



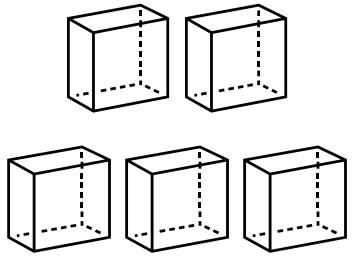
Visualizations created using Ascent

HDF python™ CINEMA

Extracts supported by Ascent

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

Website and GitHub Repo



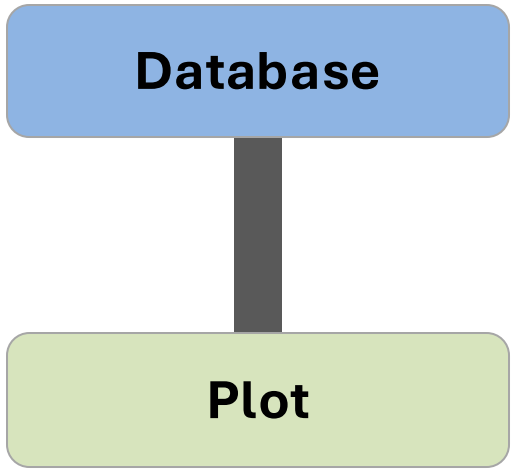
VisIt's Visualization Building Blocks

VisIt's interface is built around five core abstractions

- **Databases:** Read data
- **Plots:** Render data
- **Operators:** Manipulate data
- **Expressions:** Generate derived quantities
- **Queries:** Summarize data

Examples of VisIt Pipelines

- **Databases**: Read data
- **Plots:** Render data
- **Operators:** Manipulate data
- **Expressions:** Generate derived quantities
- **Queries:** Summarize data

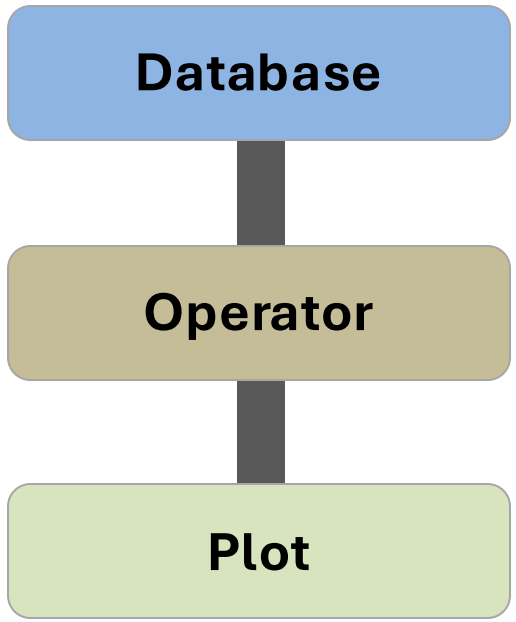


Open a database, which reads from a file
(Example: Open file1.hdf5)

Make a plot of a field in the database
(Example: Pseudocolor plot of *density*)

Examples of VisIt Pipelines

- **Databases**: Read data
- **Plots:** Render data
- **Operators:** Manipulate data
- **Expressions:** Generate derived quantities
- **Queries:** Summarize data



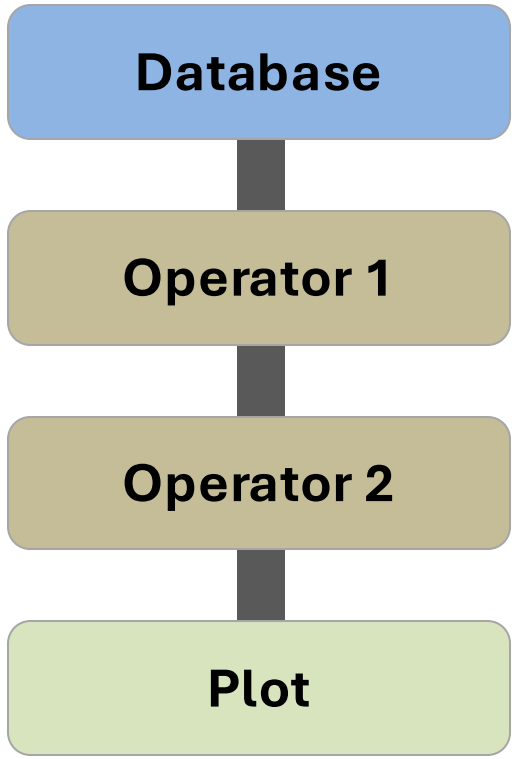
Open a database, which reads from a file
(Example: Open file1.hdf5)

Apply an operator to transform the data
(Example: Slice operator)

Make a plot of the result
(Example: Pseudocolor plot of *density*)

Examples of VisIt Pipelines

- **Databases**: Read data
- **Plots:** Render data
- **Operators:** Manipulate data
- **Expressions:** Generate derived quantities
- **Queries:** Summarize data



Open a database, which reads from a file (Example: Open file1.hdf5)

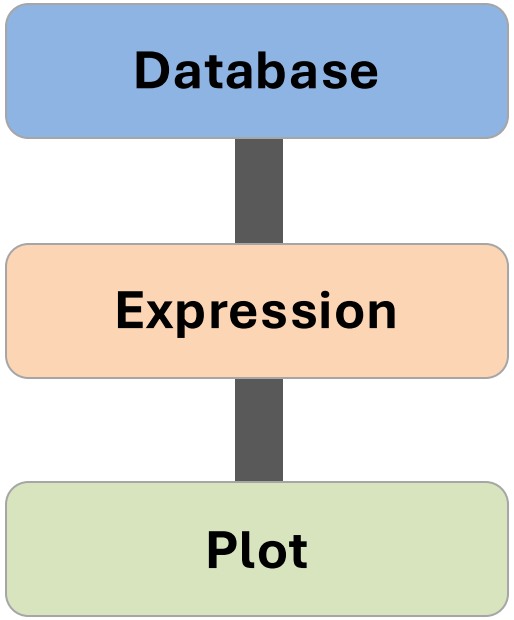
Apply an operator to transform the data (Example: Slice operator)

Apply a second operator to transform the data (Example: Elevate operator)

Make a plot of the result (Example: Pseudocolor plot of *density*)

Examples of VisIt Pipelines

- **Databases**: Read data
- **Plots:** Render data
- **Operators:** Manipulate data
- **Expressions:** Generate derived quantities
- **Queries:** Summarize data



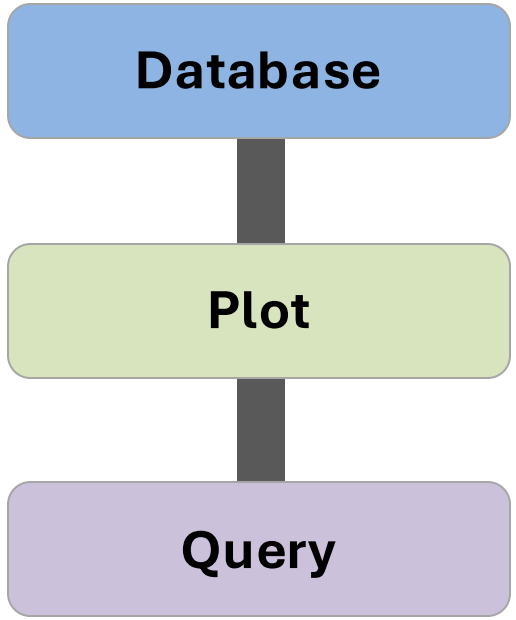
Open a database, which reads from a file
(Example: Open file1.hdf5)

Create derived quantity from existing fields
(Example: *speed* = *magnitude(velocity)*

Make a plot of the result
(Example: Pseudocolor plot of *speed*)

Examples of VisIt Pipelines

- **Databases**: Read data
- **Plots:** Render data
- **Operators:** Manipulate data
- **Expressions:** Generate derived quantities
- **Queries:** Summarize data



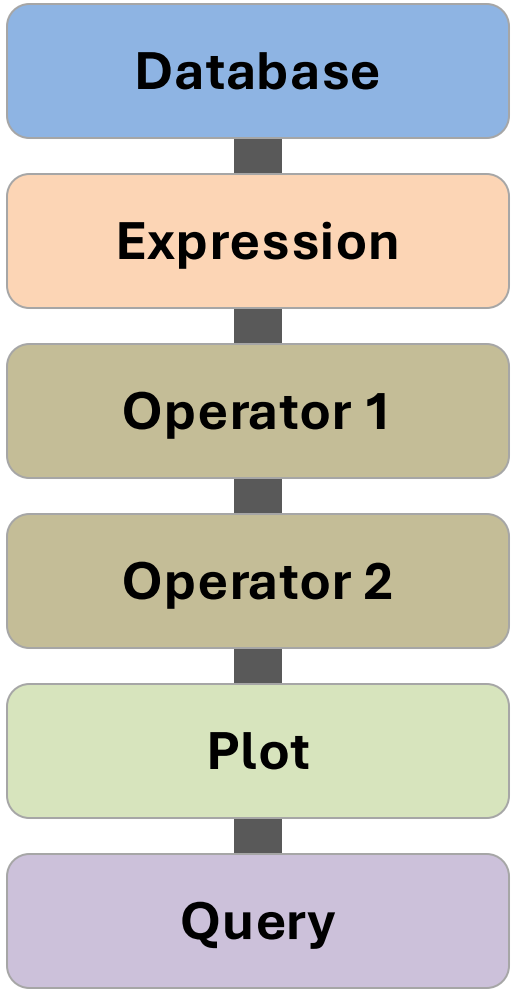
Open a database, which reads from a file
(Example: Open file1.hdf5)

Make a plot of a field in the database
(Example: Pseudocolor plot of *density*)

Extract quantitative information
(Example: integrate *density* to find *mass*)

Examples of VisIt Pipelines

- **Databases**: Read data
- **Plots:** Render data
- **Operators:** Manipulate data
- **Expressions:** Generate derived quantities
- **Queries:** Summarize data



Open a database, which reads from a file (Example: Open file1.hdf5)

Create derived quantity from existing fields (Example: *speed = magnitude(velocity)*

Apply an operator to transform the data (Example: Slice operator)

Apply a second operator to transform the data (Example: Elevate operator)

Plot a field (Example: Pseudocolor plot of *speed*)

Extract quantitative information (Example: Maximum speed over cross-section)

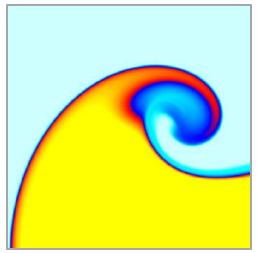
Contact info and Resources

Presenter Contact Info:

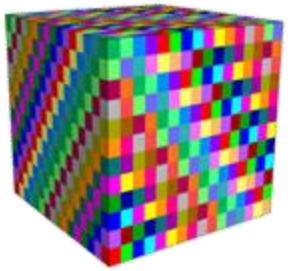
- Cyrus Harrison: cyrush@llnl.gov
- Justin Privitera: privitera1@llnl.gov

Resources:

- Main website: http://www.llnl.gov/visit
- Github: https://github.com/visit-dav/visit
- GitHub Discussions: https://github.com/visit-dav/visit/discussions
- Wiki: http://www.visitusers.org

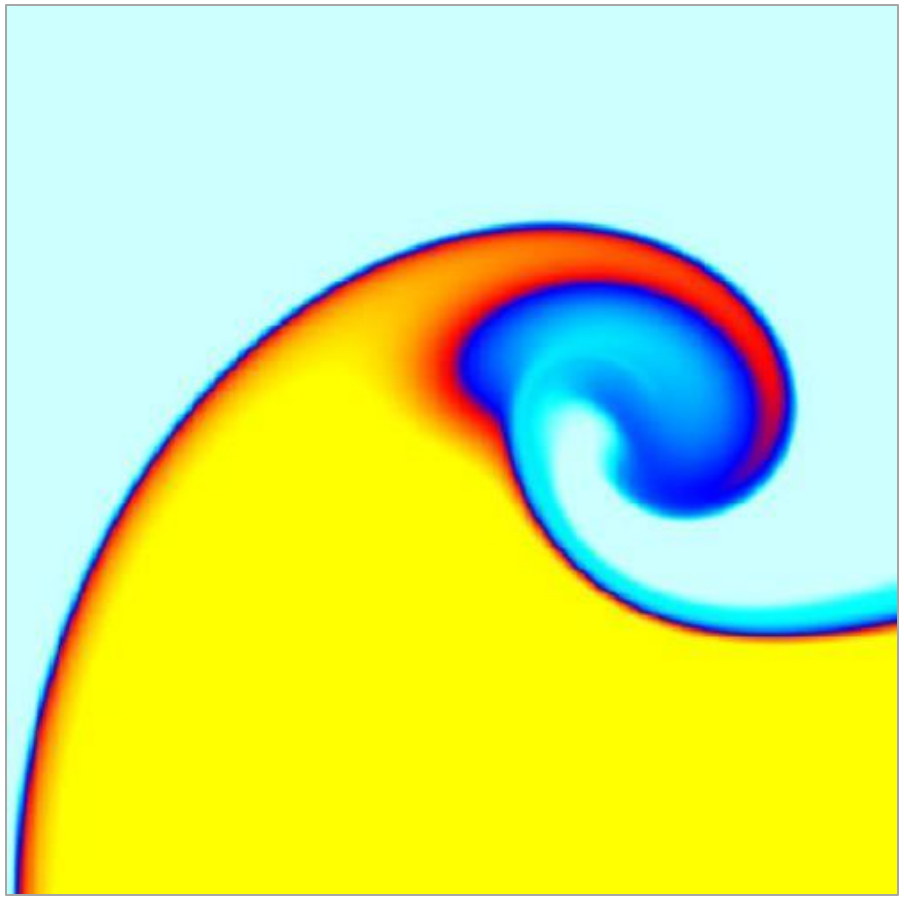


Visualization Techniques for Mesh-based Simulations



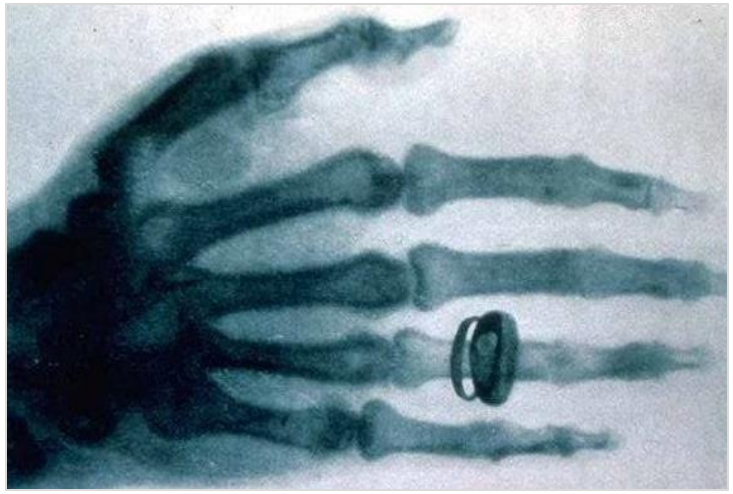
Pseudocolor rendering maps scalar fields to a range of colors

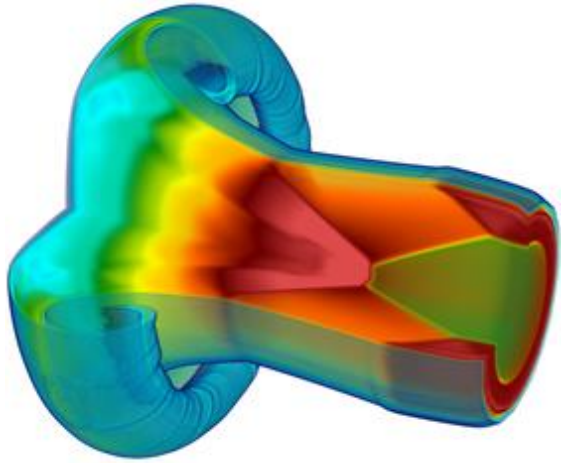
Pseudocolor rendering of Elevation

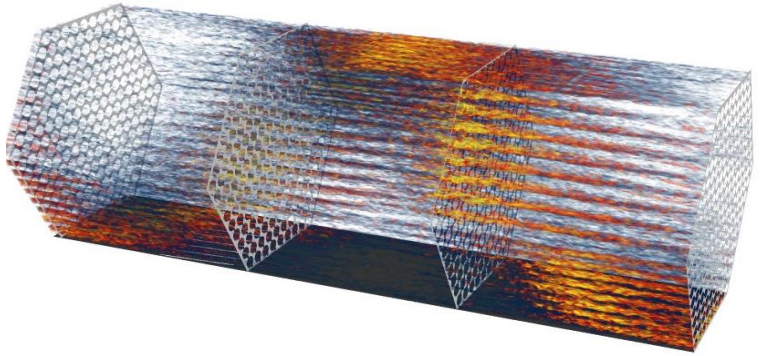


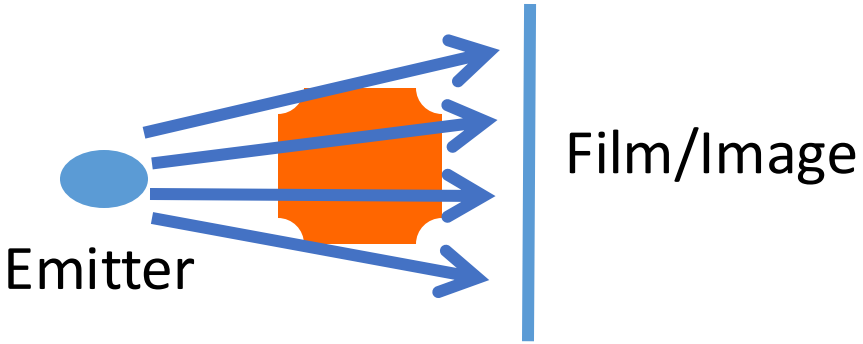
Pseudocolor rendering of Density

Volume Rendering cast rays though data and applies transfer functions to produce an image

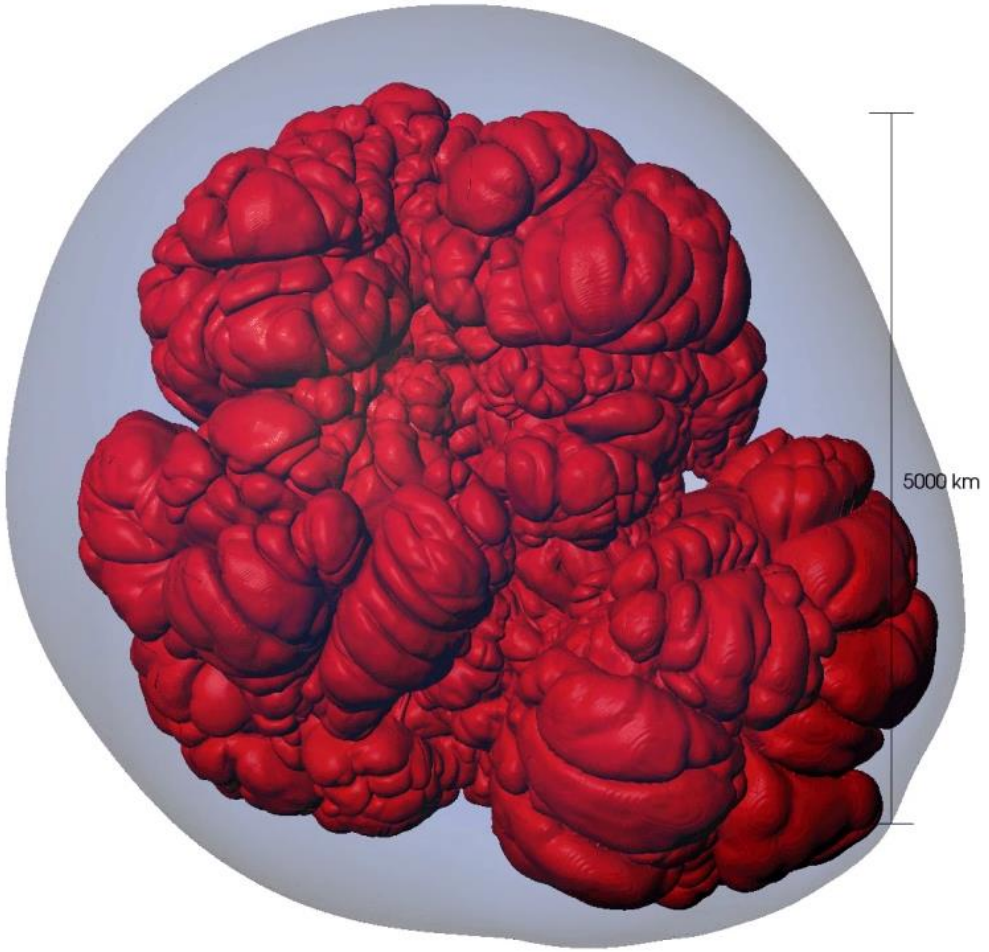








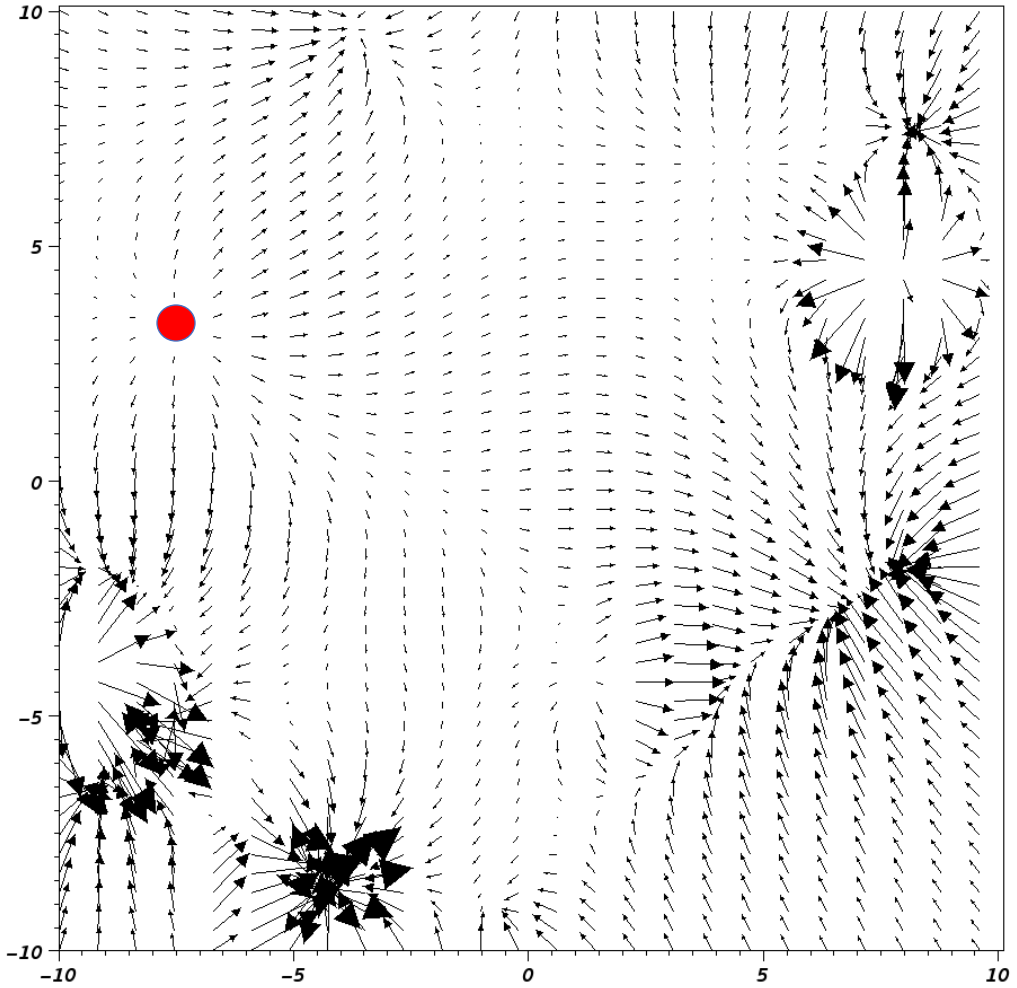
Isosurfacing (Contouring) extracts surfaces of that represent level sets of field values



Particle advection is the foundation of several flow visualization techniques

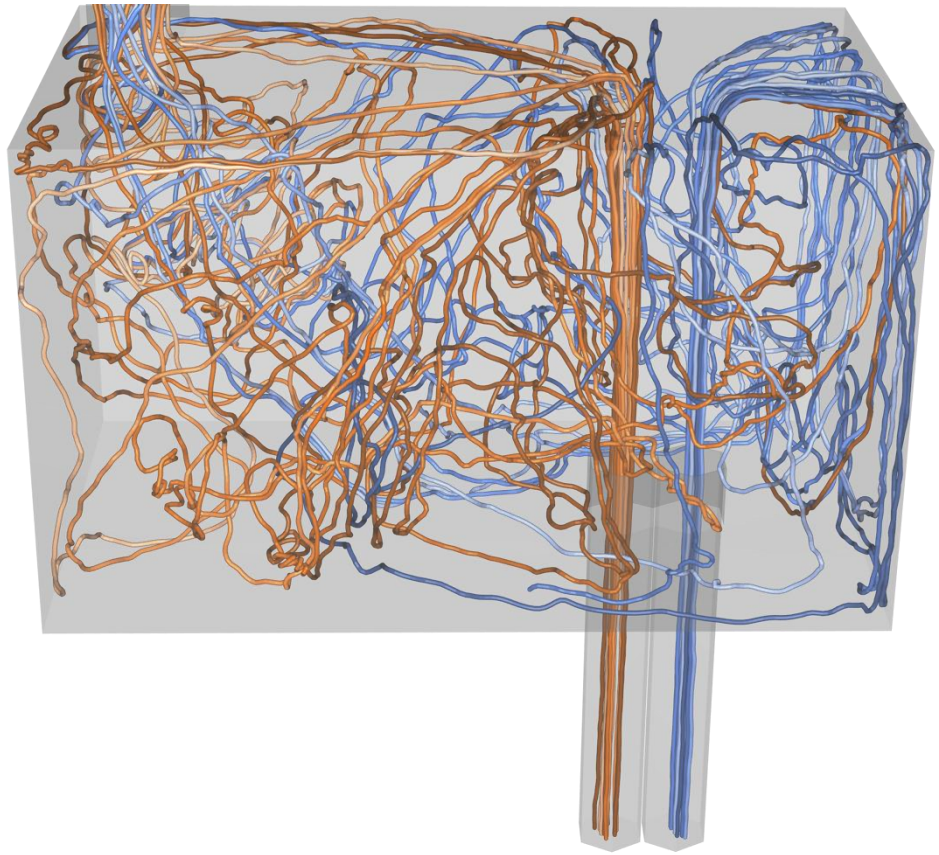
- S(t) = position of particle at time t
- $S(t_0) = p_0$
  - t_0: initial time
  - p_0: initial position
- S’(t) = v(t, S(t))
  - v(t, p): velocity at time t and position p
  - S’(t): derivative of the integral curve at time t

This is an ordinary differential equation.



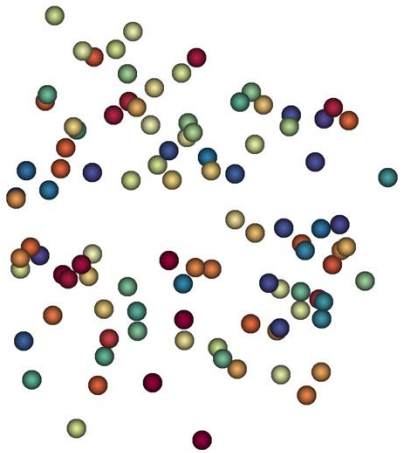
Streamline and Pathline computation are built on particle advection

- **Streamlines** – Instantaneous paths
- **Pathlines** – Time dependent paths

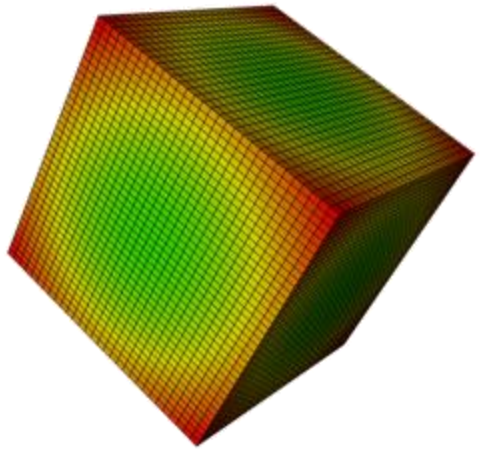


Meshes discretize continuous space

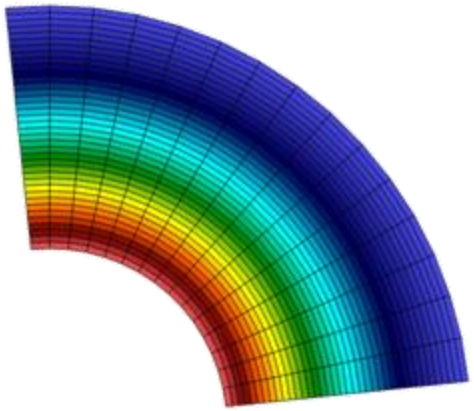
- **Simulations use a wide range of mesh types, defined in terms of:**
  - A set of coordinates (“nodes” / “points” / “vertices”)
  - A collection of “zones” / “cells” / “elements” on the coordinate set



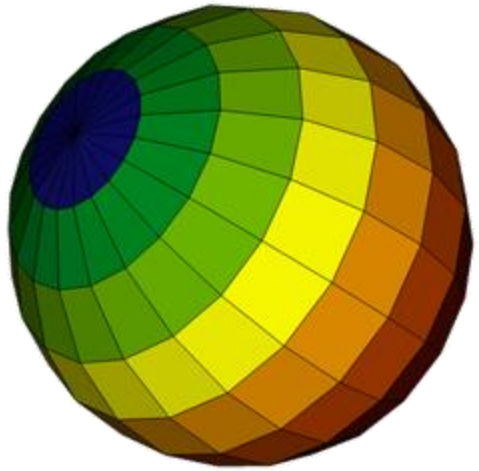
Points



Uniform



Curvilinear

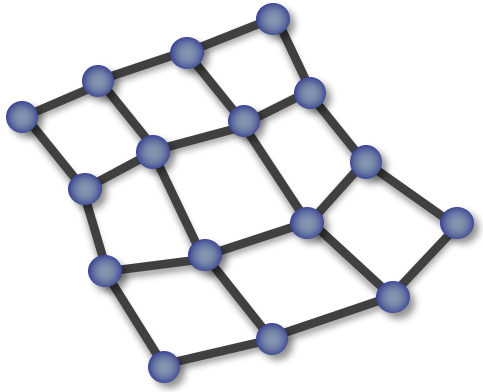


Unstructured

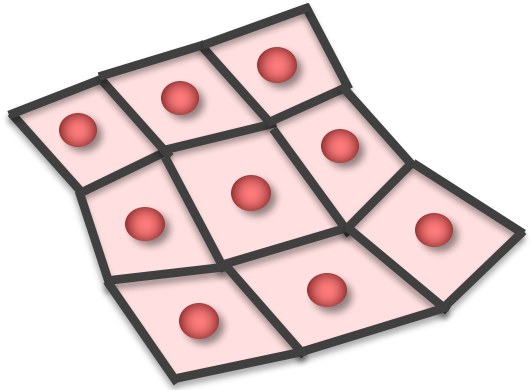
VisIt uses the “Zone” and “Node” nomenclature throughout its interface.

Mesh fields are variables associated with the mesh that hold simulation state

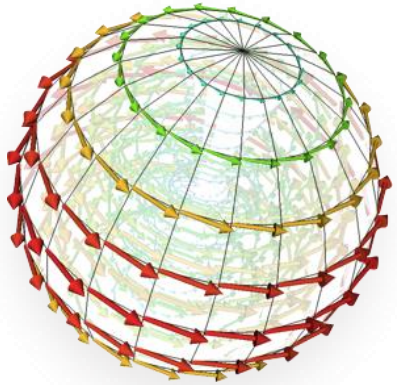
- Field values are associated with the zones or nodes of a mesh
  - Nodal: Linearly interpolated between the nodes of a zone
  - Zonal: Piecewise Constant across a zone
- Field values for each zone or node can be scalar, or multi-valued (vectors, tensors, etc.)



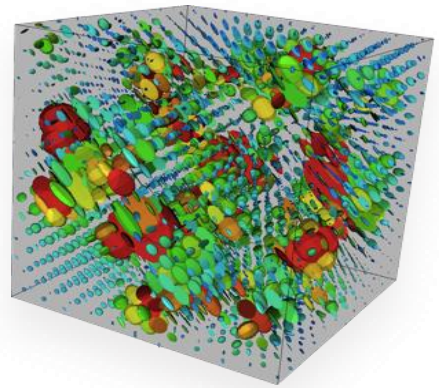
Nodal Association



Zonal Association



Vector Field

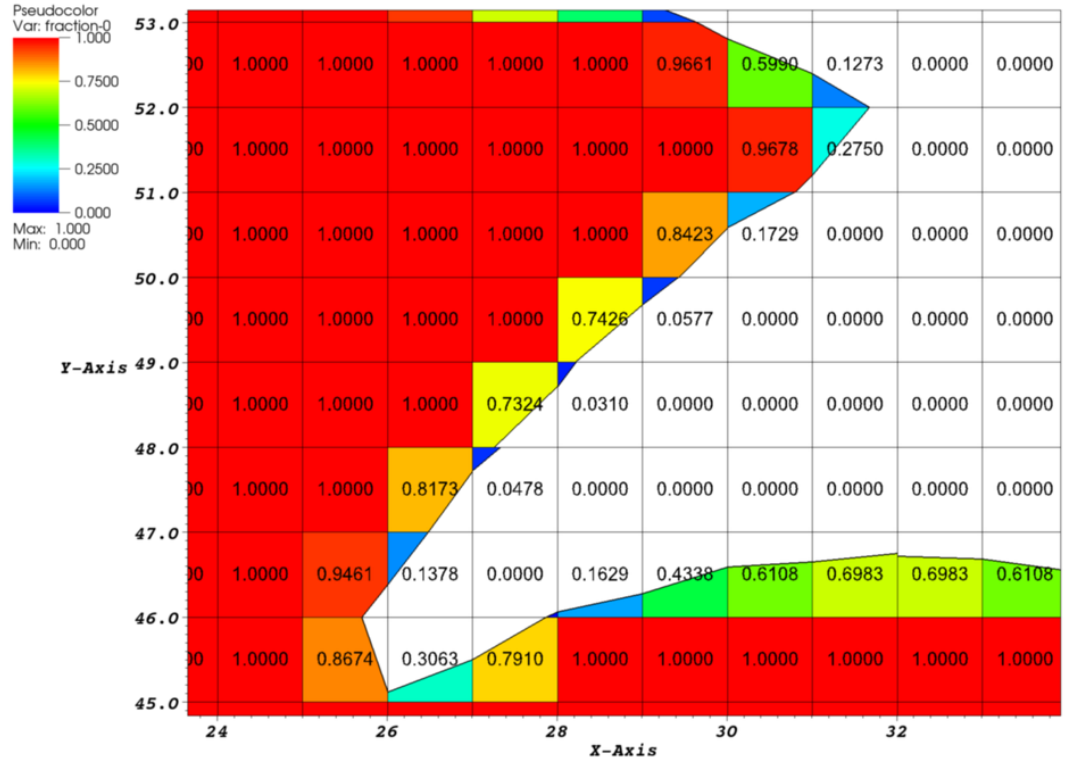


Tensor Field

Material volume fractions are used to capture sub-zonal interfaces

- Multi-material simulations use volume/area fractions to capture disjoint spatial regions at a sub-grid level.

- These fractions can be used as input to high-quality sub-grid material interface reconstruction algorithms.

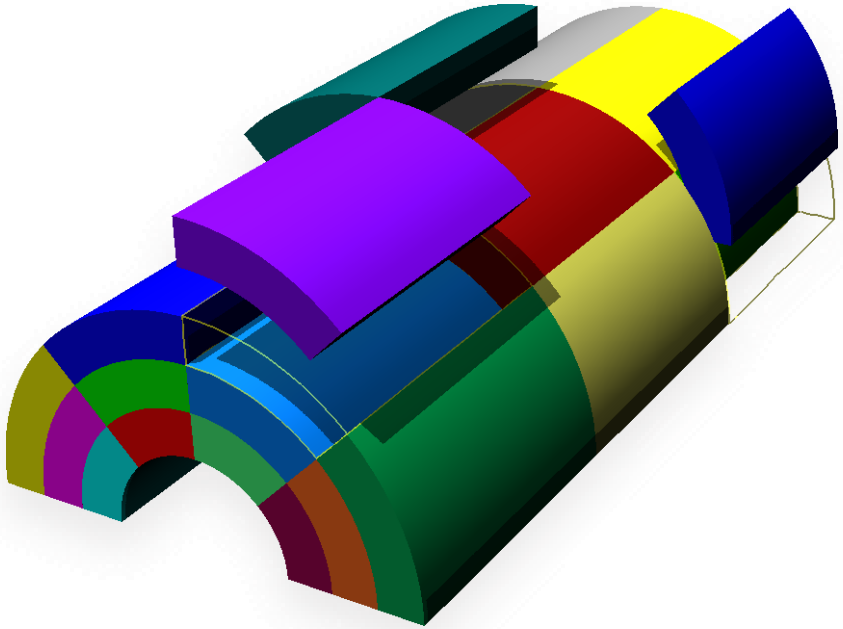


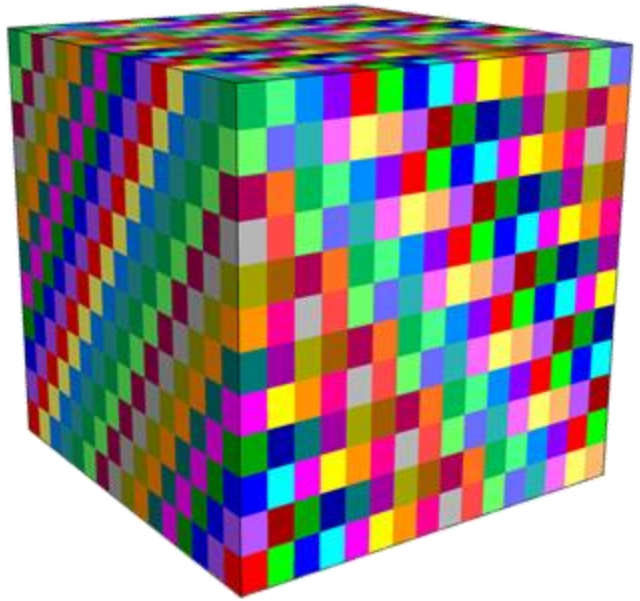
Species are used to capture sub-zonal weightings

- Species describe sub-grid variable composition
  - Example: Material “Air” is made of species “N2” ,“O2”, “Ar”, “CO2”, etc.
- Species are used for weighting, not to indicate sub-zonal interfaces.
  - They are typically used to capture fractions of “atomically mixed” values.

Domain decomposed meshes enable scalable parallel visualization and analysis algorithms

- Simulation meshes may be composed of smaller mesh “blocks” or “domains”.
- Domains are partitioned across MPI tasks for processing.





Adaptive Mesh Refinement (AMR) refines meshes into patches that capture details across length scales

- Mesh domains are associated with patches and levels
- Patches are nested to form a AMR hierarchy