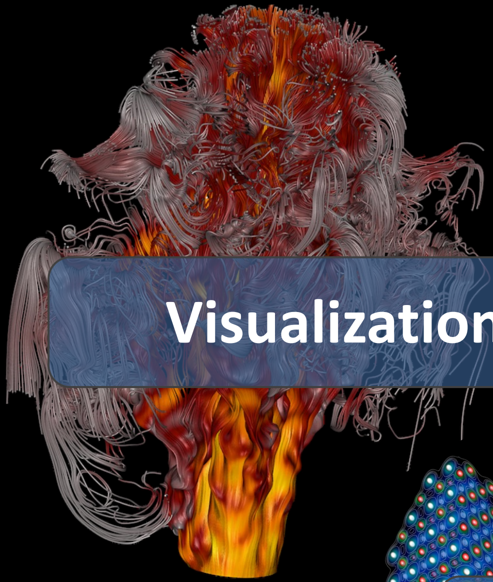
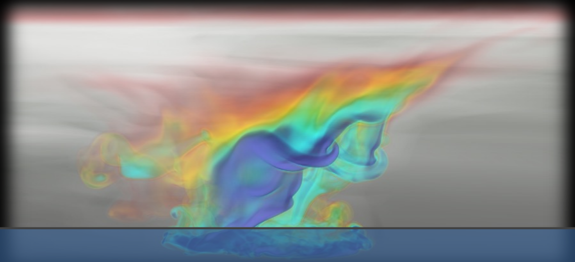
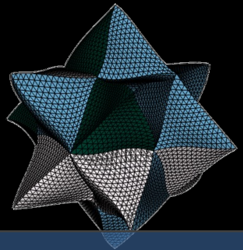
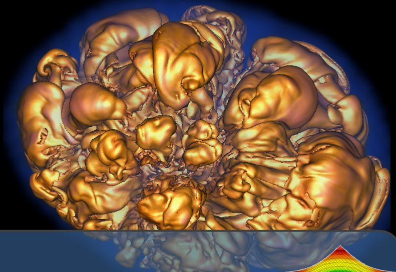
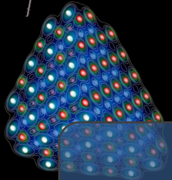
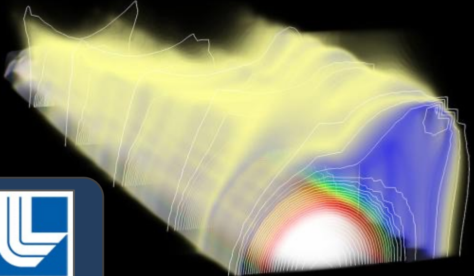





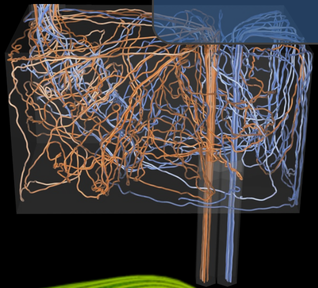
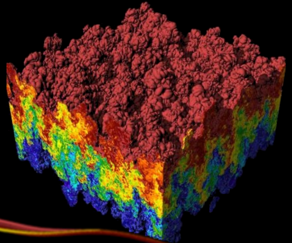
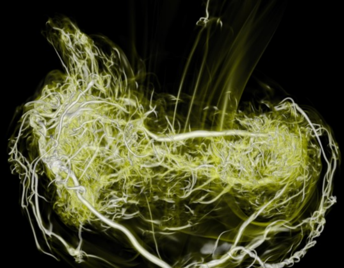
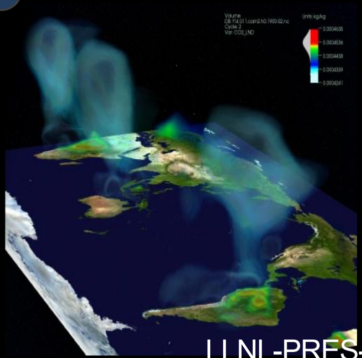
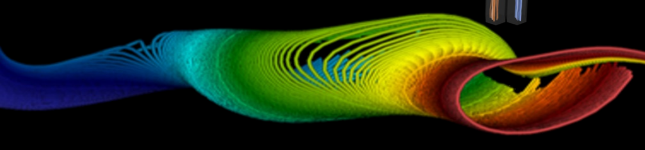
Visualization and Analysis of HPC Simulation Data with VisIt

ATPESC 2024

Monday August 5th, 2024

Cyrus Harrison (cyrush@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

LLNL-PRES-867585

Acknowledgements

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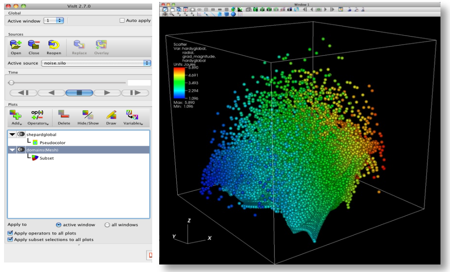
Lawrence Livermore National Security, LLC

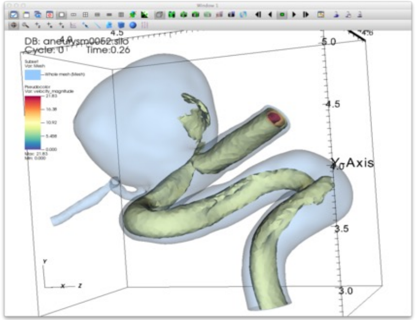
This research was supported by the Exascale Computing Project (17-SC-20-SC), a joint project of the U.S. Department of Energy's Office of Science and National Nuclear Security Administration, responsible for delivering a capable exascale ecosystem, including software, applications, and hardware technology,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

Outline

- VisIt Project Introduction (30 min)
- Hands-on: (60 min)
  — Guided tour of VisIt (30 min)
  — *[Lunch!]*
  — Visualization of an Aneurysm (30 min) (Blood Flow) Simulation



Intro to VisIt



Simulation Exploration

Tutorial Resources

- **VisIt 3.4.1**
  - 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 (http://www.lifev.org/) 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/)

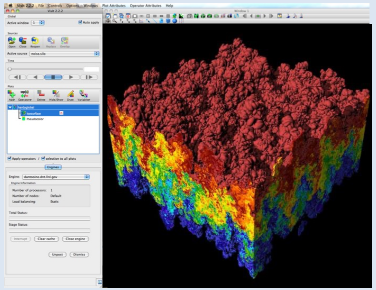
Available thanks to:

- Aaron Fisher and Mark Miller, LLNL

VisIt Project Introduction

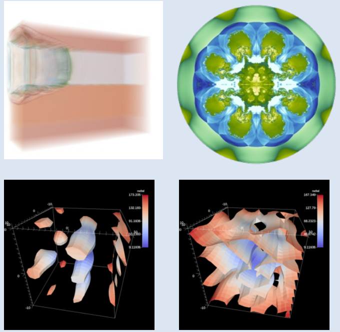
The VisIt team develops open-source Visualization, Analysis, and I/O tools.

VisIt



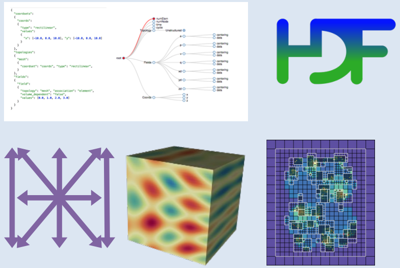
Turnkey HPC application for visualization and analysis of simulation data

Ascent



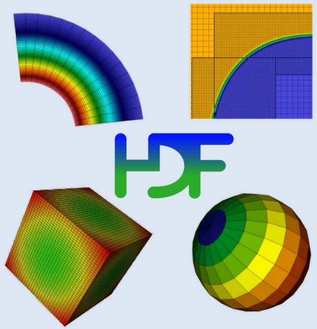
Easy-to-use flyweight in situ visualization and analysis library for HPC simulations

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

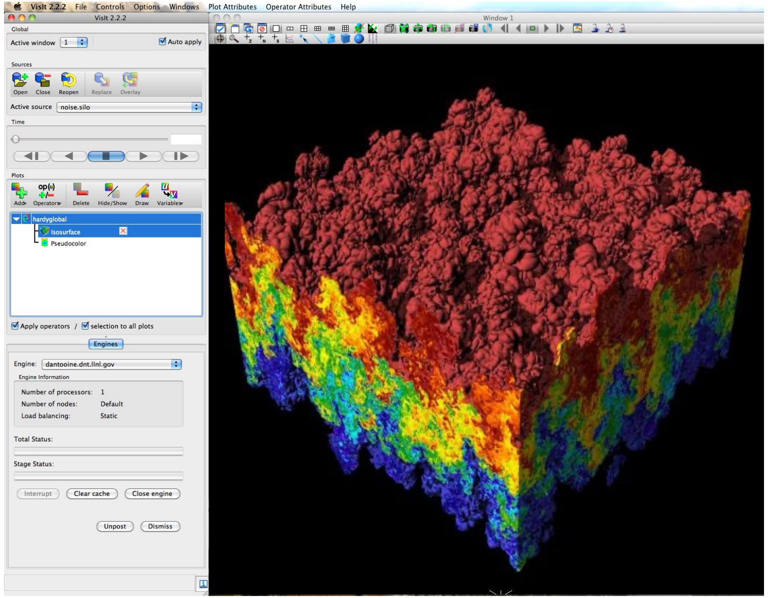
1. go to see and spend time with (someone) socially.
   "I came to visit my grandmother"
   synonyms: call on, call in on, pay a call on, pay a visit to, pay someone a call, pay someone a visit, go to see, come to see, look in on; More
2. inflict (something harmful or unpleasant) on someone.
   "the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

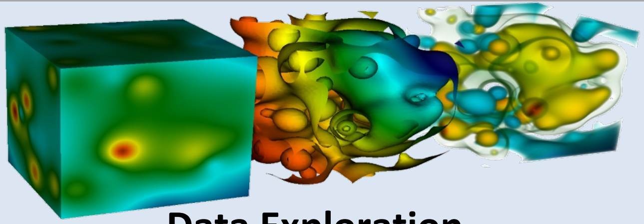
VisIt is an open source, turnkey application for data analysis and visualization of mesh-based data

- 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.

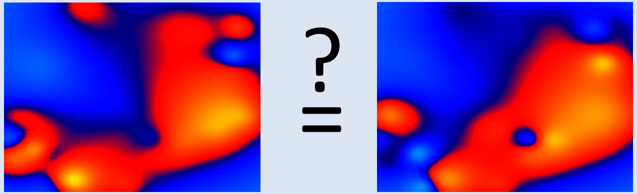


Pseudocolor plot of Density
(27 billion element dataset)

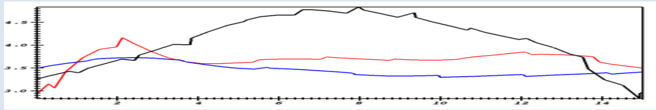
VisIt supports a wide range of use cases



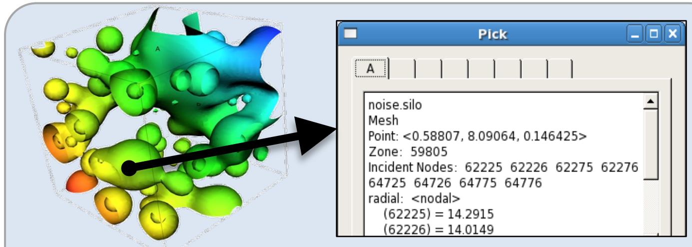
Data Exploration



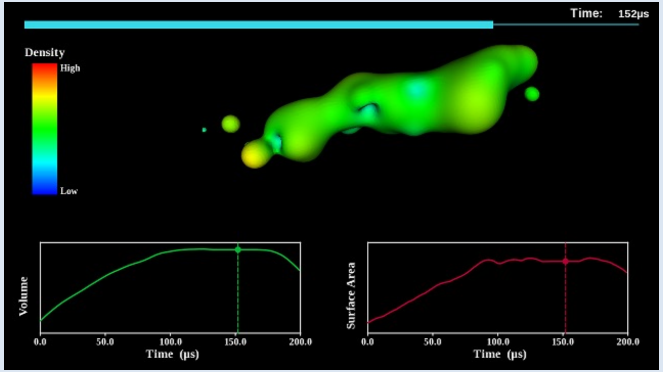
Comparative Analysis



Quantitative Analysis

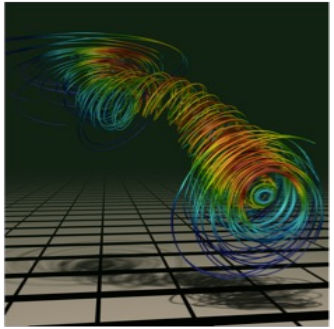


Visual Debugging

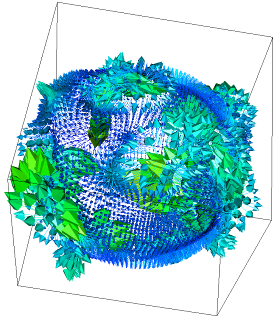


Presentation Graphics

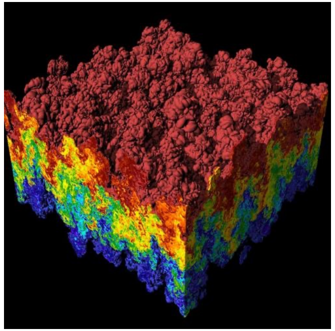
VisIt provides a wide range of plotting features for simulation data across many scientific domains



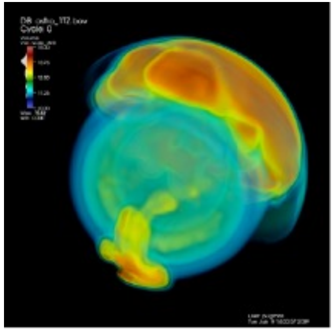
Streamlines / Pathlines



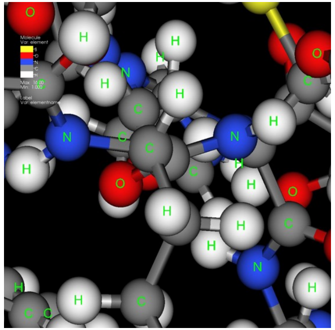
Vector / Tensor Glyphs



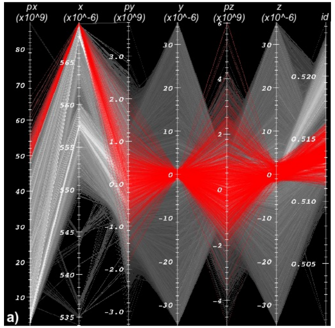
Pseudocolor Rendering



Volume Rendering



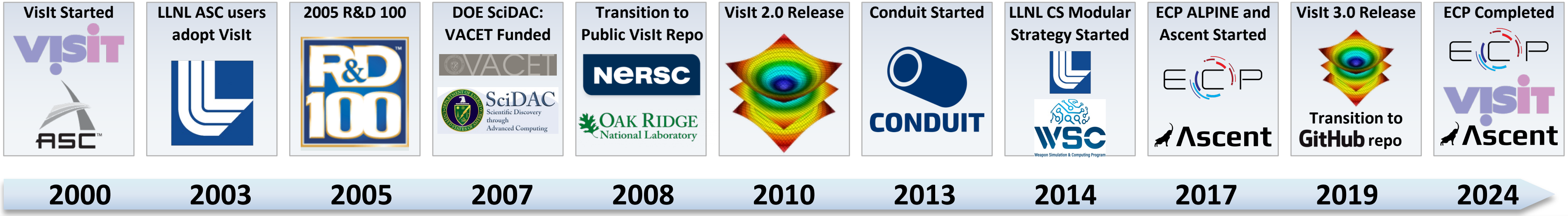
Molecular Visualization



Parallel Coordinates

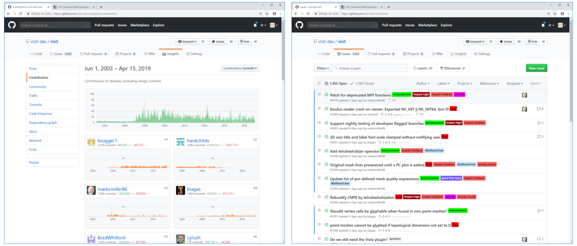
VisIt is a vibrant project with many participants

- 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.



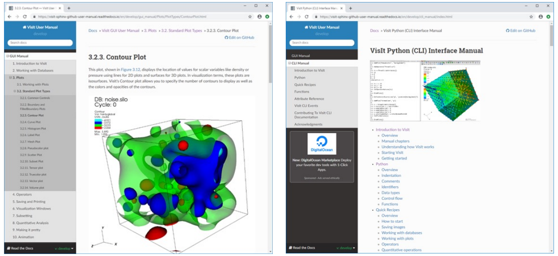
VisIt is hosted and developed using GitHub

- Our Source Code, Issue tracking, and Discussions are in the `visit-dav` GitHub organization:
  - https://github.com/visit-dav/



VisIt source repo and issue tracking on GitHub

- Our Docs are hosted on Read the Docs
  - https://visit-sphinx-github-user-manual.readthedocs.io/en/develop/

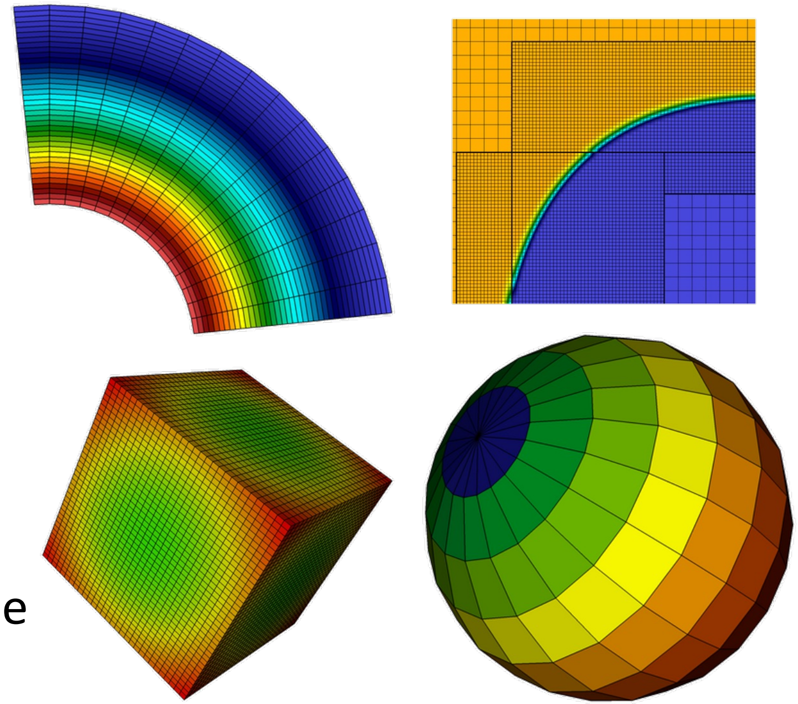


VisIt manuals on Read the Docs

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 I 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
- Experiment with the *visit_writer* utility.
- 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 • OSX-10.? 10.2 • RedHat +ubuntu	7 8 9 10 10.4 10.5/6 10.8 10.10 10.12 +(fedora, debian,	11 10.14 11 12 13 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 • VTK-5.0 VTK-5.8 • GL Drivers + Mesa	Qt4 Qt5 VTK-6 VTK-8 (OpenGL, GL rendering changes)	Qt6 VTK-9	**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 Required templates OK • Python 2	C++ 11 allowed	C++ 14 Python 2 or 3	• Very conservative in adopting new language features • A lot of users still using Python 2 workflows

We are actively developing VisIt's 3.4 release series

- VisIt 3.4.0
  - Initial Qt6, VTK-9, Ospray 3 support
  - Keyframing + Colorable Improvements, Hypertree Grid Export
  - 25+ enhancements, 19 bugfixes
  - https://visit-dav.github.io/visit-website/releases/release-notes-3.4.0/

- **VisIt 3.4.1** -the one you want!
  - LANL Crossroads (XR) Install
  - Hardened Qt6, VTK-9 Support
  - Blueprint, MFEM LOR, X Ray Image Query Improvements
  - Python 3.9+ Support
  - 18 enhancements, (also) 19 bug fixes
  - https://visit-dav.github.io/visit-website/releases/release-notes-3.4.1/

v3.4.1 Latest

Release Notes:
https://visit-dav.github.io/visit-website/releases/release-notes-3.4.1

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

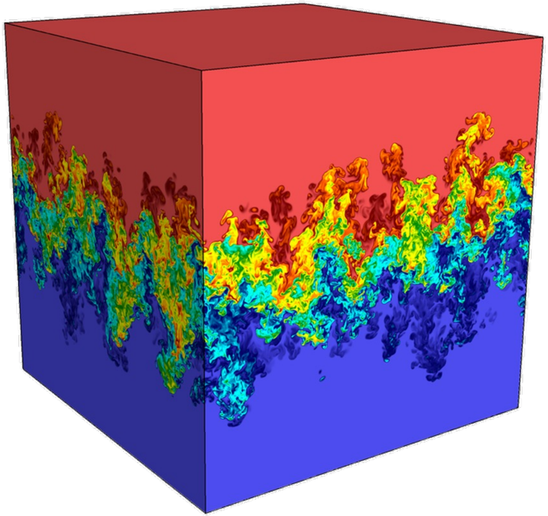
▾ Assets 18

build_visit3_4_1	804 KB	5 days ago
INSTALL_NOTES_3_4_1.txt	2.98 KB	5 days ago
jvisit3.4.1.tar.gz	1.49 MB	5 days ago
visit-install3_4_1	45.6 KB	5 days ago
visit3.4.1.tar.gz	175 MB	5 days ago
visit3.4.1_x64.exe	238 MB	5 days ago
visit3_4_1.linux-x86_64-debian10.tar.gz	481 MB	5 days ago
visit3_4_1.linux-x86_64-debian11.tar.gz	484 MB	5 days ago
visit3_4_1.linux-x86_64-debian12.tar.gz	483 MB	5 days ago
visit3_4_1.linux-x86_64-fedora31.tar.gz	469 MB	5 days ago
Source code (zip)		5 days ago
Source code (tar.gz)		5 days ago

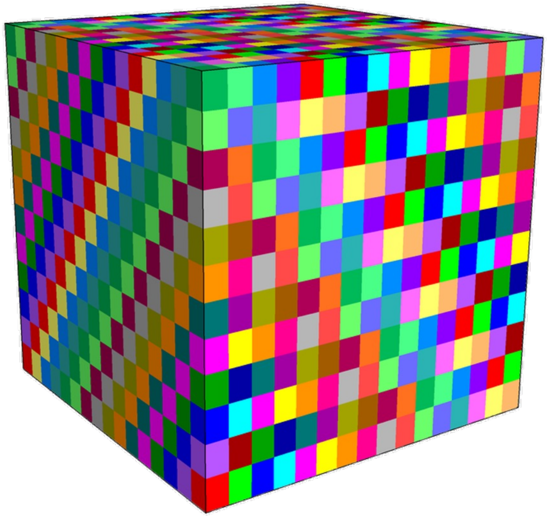
Show all 18 assets

1 · 1 person reacted

VisIt uses MPI for distributed-memory parallelism on HPC clusters

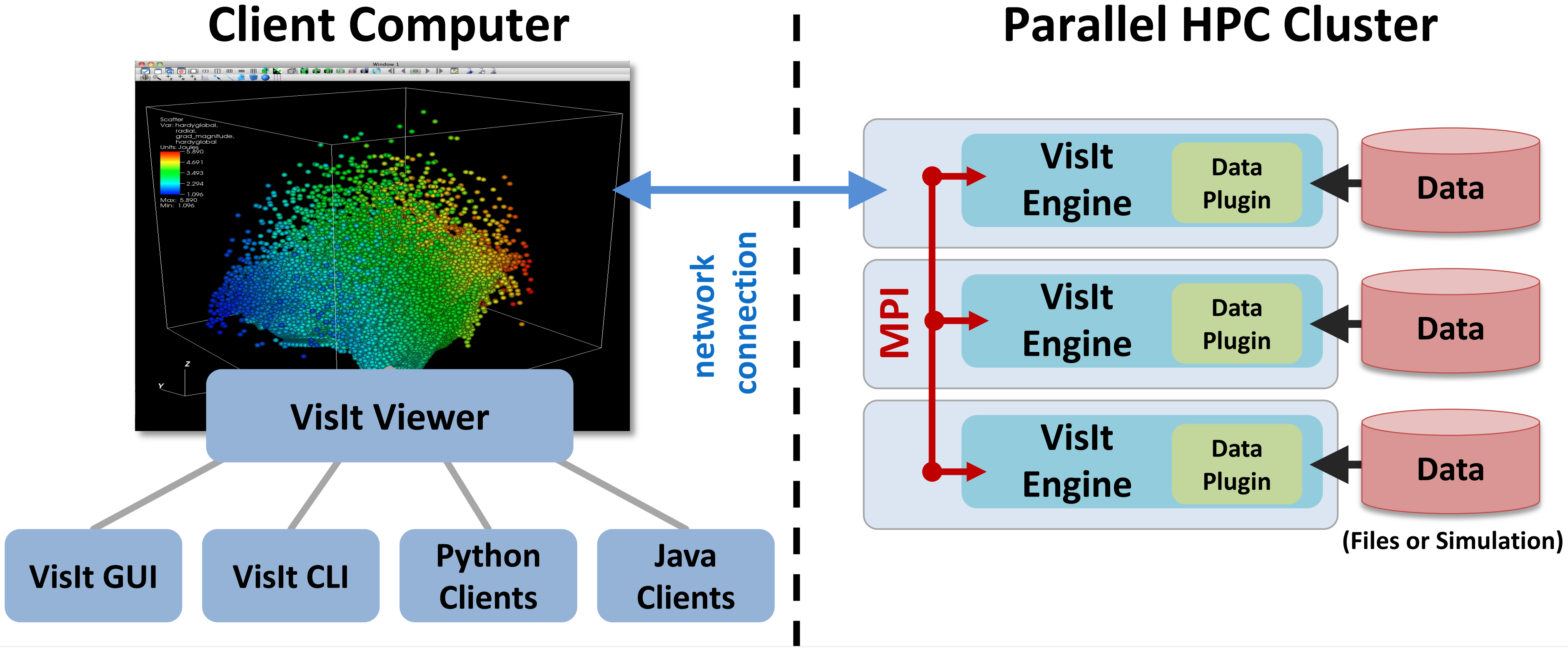


Full Dataset
(27 billion total elements)

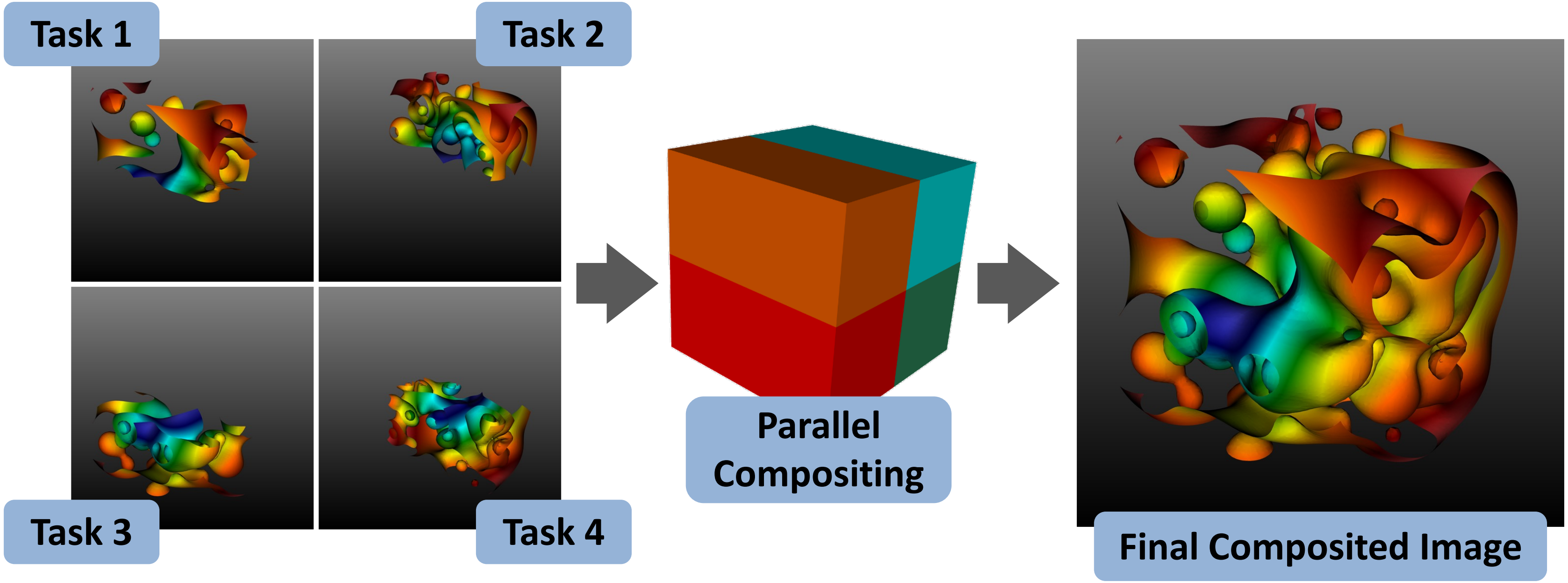


3072 sub-grids
(each 192x129x256 cells)

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 ready for Exascale simulations

Addressing node-level parallelism

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

VTK-m

http://m.vtk.org

Addressing I/O gaps with in-situ

- There are several efforts focused on in-situ infrastructure and algorithms

ALPINE (ParaView/VisIt) http://alpine.dsscale.org

ParaView Catalyst http://www.paraview.org/in-situ

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

SENSEI in situ http://www.sensei-insitu.org

VisIt LibSim https://visit.llnl.gov

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

CONDUIT

Intuitive APIs for in-memory data description and exchange

http://software.llnl.gov/conduit

Ascent

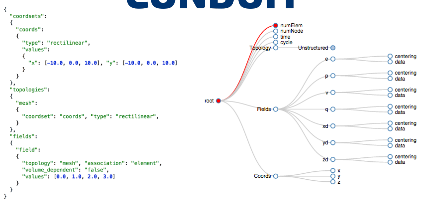
Flyweight in-situ visualization and analysis for HPC simulations

http://ascent-dav.org

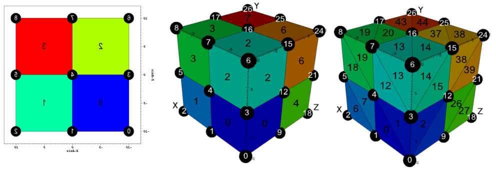
Conduit provides intuitive APIs for in-memory data description and exchange

- **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 (eg: *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)

CONDUIT



Hierarchical in-memory data description



Conventions for sharing in-memory mesh data

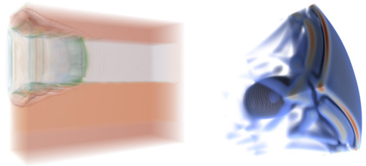
http://software.llnl.gov/conduit
http://github.com/llnl/conduit

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***
  - Supports 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

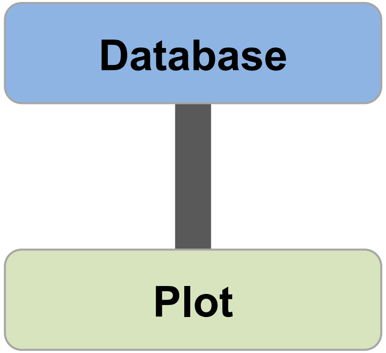
VisIt's Visualization Building Blocks

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

Database

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

Operator

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

Plot

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

Examples of VisIt Pipelines

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

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Examples of VisIt Pipelines

- **Databases**: Read data
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Database — Open a database, which reads from a file (Example: Open file1.hdf5)

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

Plot — 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
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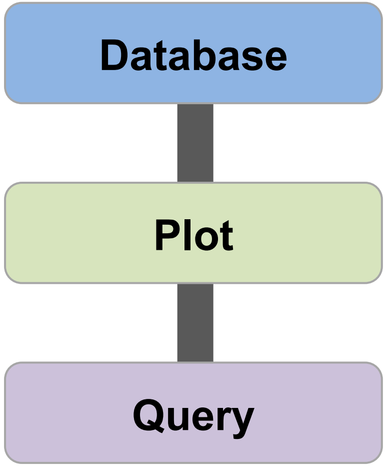


Open a database, which reads from a file
(Example: Open file1.hdf5)

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

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

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

Operator 1 — Apply an operator to transform the data
(Example: Slice operator)

Operator 2 — Apply a second operator to transform the data
(Example: Elevate operator)

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

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

Resources

Presenter Contact Info:

- Cyrus Harrison: cyrush@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

Aneurysm Simulation Exploration

https://visit-sphinx-github-user-manual.readthedocs.io/en/develop/tutorials/Aneurysm.html

Remote Usage Tips

https://visit-sphinx-github-user-manual.readthedocs.io/en/develop/tutorials/RemoteUsage.html

Python Scripting Basics

https://visit-sphinx-github-user-manual.readthedocs.io/en/develop/tutorials/Scripting.html

Connected Components

https://visit-sphinx-github-user-manual.readthedocs.io/en/develop/tutorials/CCL.html

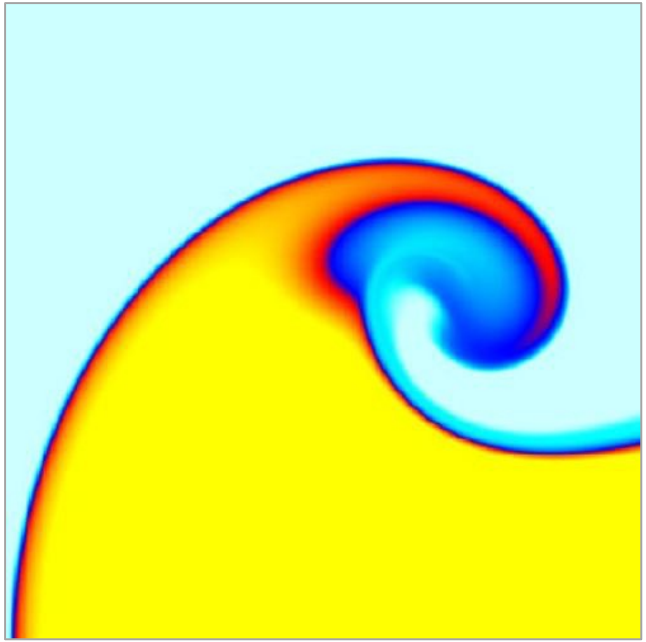
Additional Hands-on Materials

- **Potential Flow Simulation Exploration**
  - https://visit-sphinx-github-user-manual.readthedocs.io/en/develop/tutorials/PotentialFlow.html
- **Water Flow Simulation Exploration**
  - http://visitusers.org/index.php?title=Water_Flow_Tutorial
- **Volume Rendering**
  - http://visitusers.org/index.php?title-Visit-tutorial-Volume-Rendering
- **Movie Making**
  - https://visit-sphinx-github-user-manual.readthedocs.io/en/develop/tutorials/MakingMovies.html
- **Advanced Movie Making**
  - http://visitusers.org/index.php?title=Visit-tutorial-Advanced-movie-making

Visualization Techniques for Mesh-based Simulations

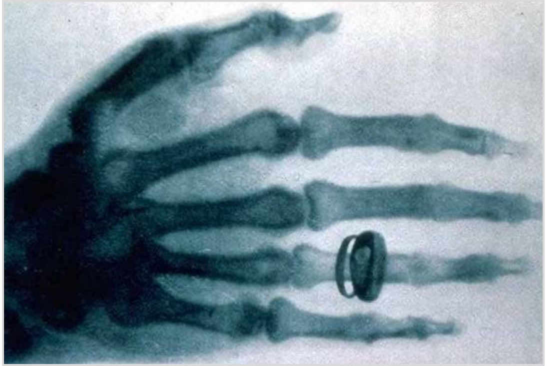
Pseudocolor rendering maps scalar fields to a range of colors

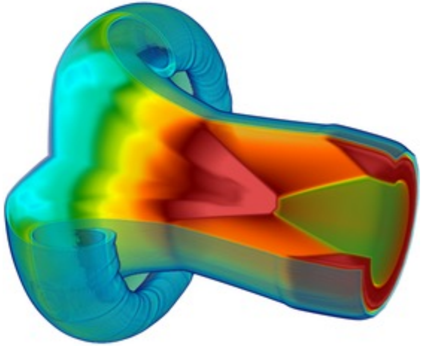
Pseudocolor rendering of Elevation

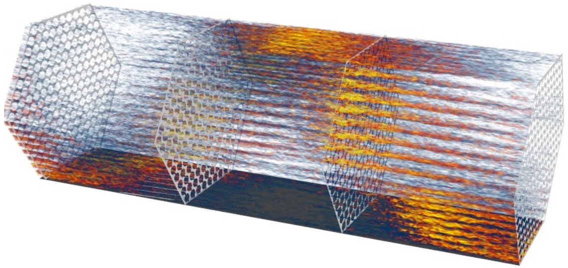


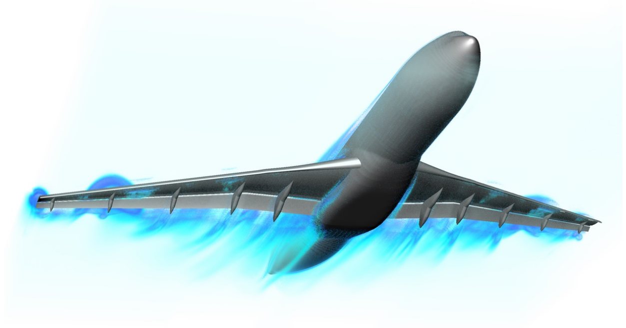
Pseudocolor rendering of Density

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

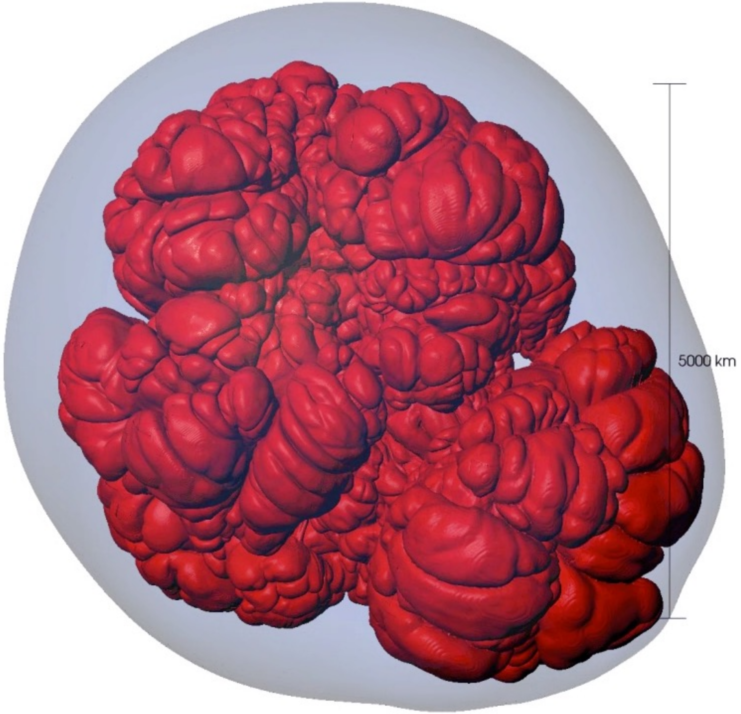






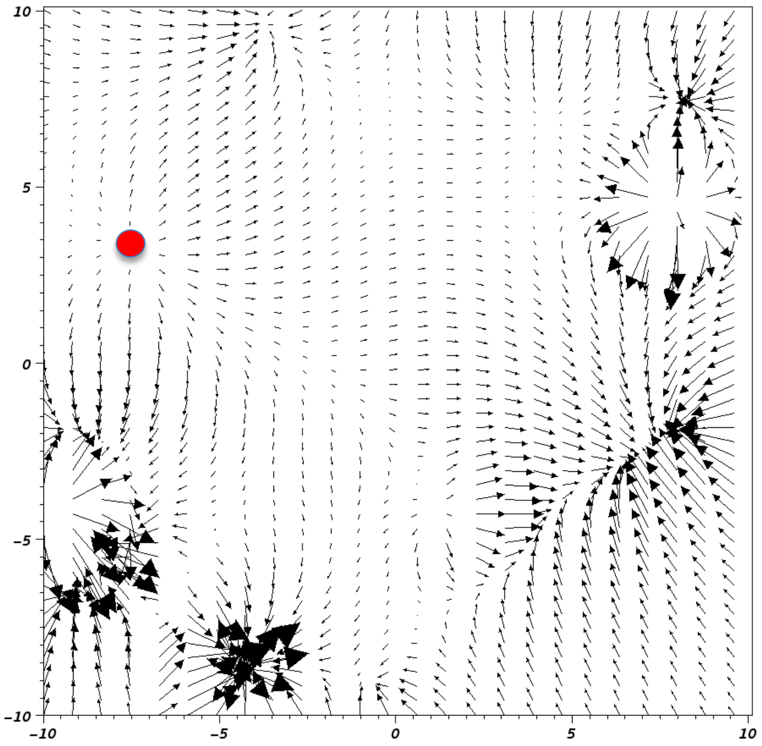


Isosurfacing (Contouring) extracts surfaces of that represent level sets of field values



Particle advection is the foundation of several flow visualization techniques

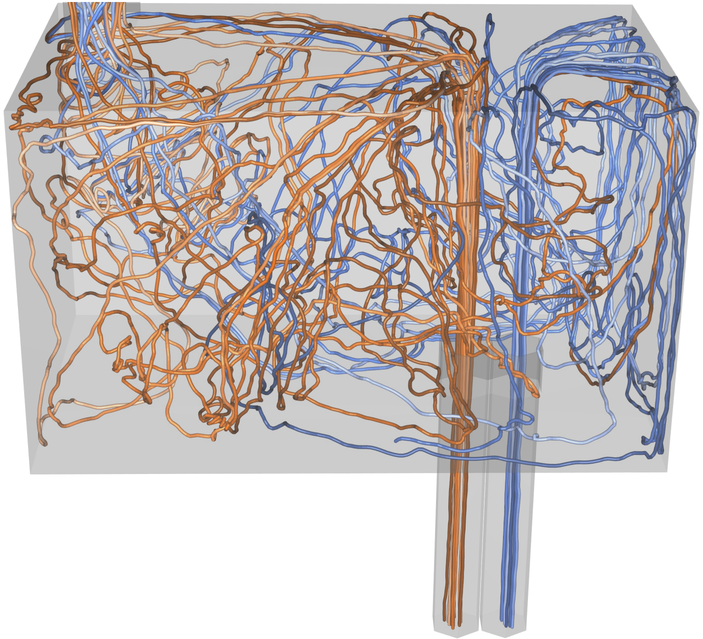
- $S(t)$ = position of particle at time t
- $S(t_0) = p_0$
  - t_0: initial time
  - p_0: initial position
- $S'(t) = v(t, S(t))$
  - $v(t, p)$: velocity at time t and position p
  - $S'(t)$: derivative of the integral curve at time t



This is an ordinary differential equation.

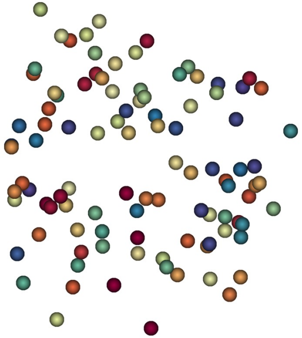
Streamline and Pathline computation are built on particle advection

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

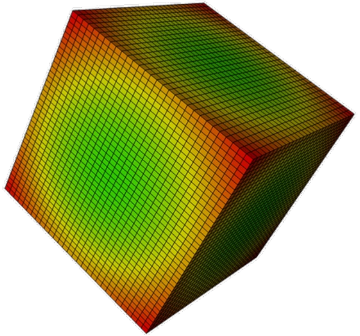


Meshes discretize continuous space

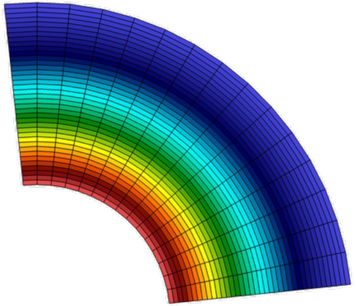
- **Simulations use a wide range of mesh types, defined in terms of:**
  - — A set of coordinates (“nodes” / “points” / “vertices”)
  - — A collection of “zones” / “cells” / “elements” on the coordinate set



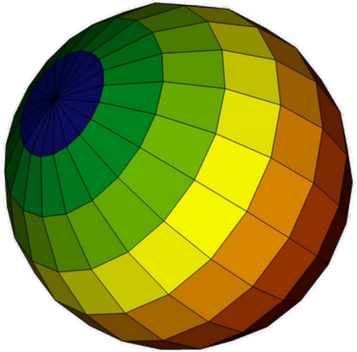
Points



Uniform



Curvilinear



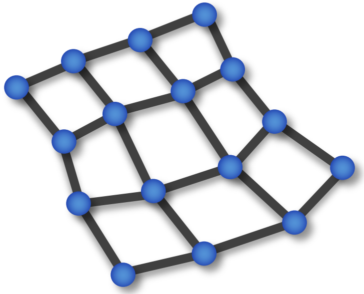
Unstructured

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

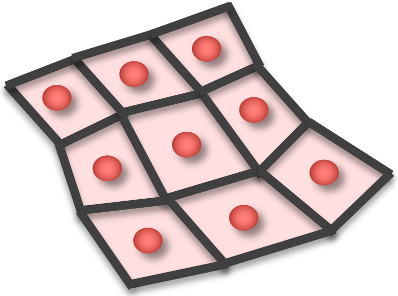
Mesh fields are variables associated with the mesh that hold simulation state

- 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

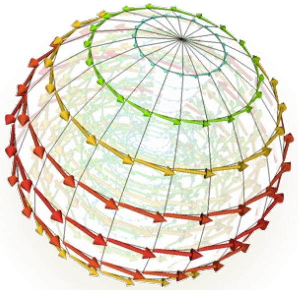
- Field values for each zone or node can be scalar, or multi-valued (vectors, tensors, etc.)



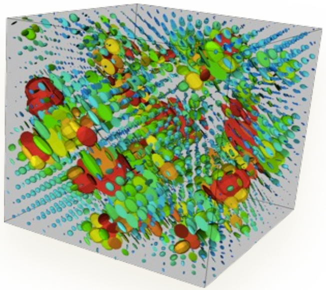
Nodal Association



Zonal Association



Vector Field

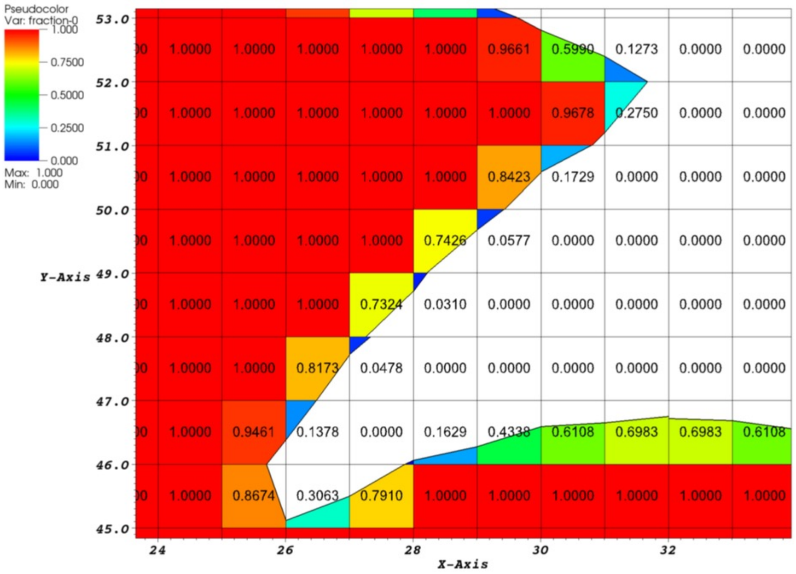


Tensor Field

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

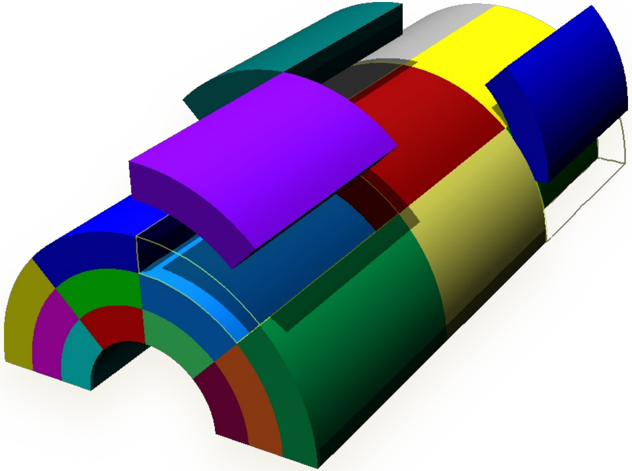
- Species describe sub-grid variable composition
  - Example: Material “Air” is made of species “N2” ,“O2”, “Ar”, “CO2”, etc.

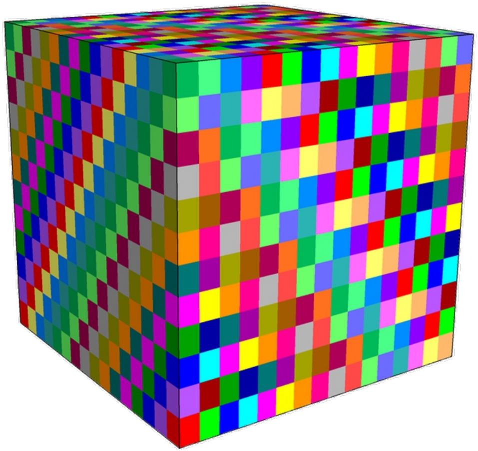
- Species are used for weighting, not to indicate sub-zonal interfaces.
  - They are typically used to capture fractions of “atomically mixed” values.

Domain decomposed meshes enable scalable parallel visualization and analysis algorithms

- Simulation meshes may be composed of smaller mesh "blocks" or "domains".

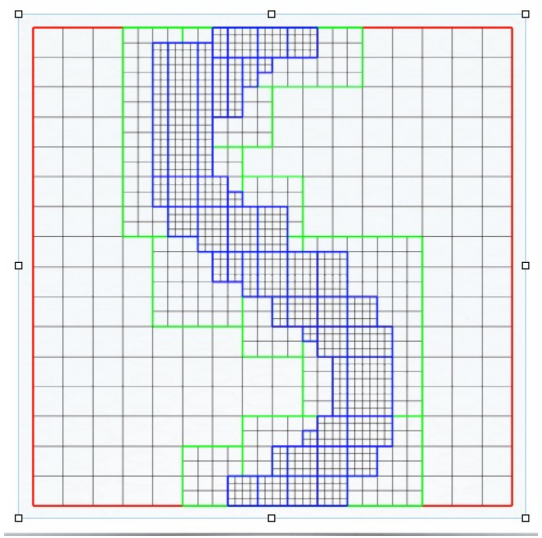
- Domains are partitioned across MPI tasks for processing.

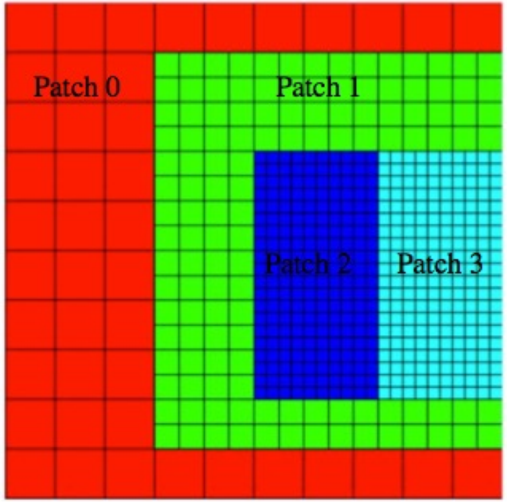


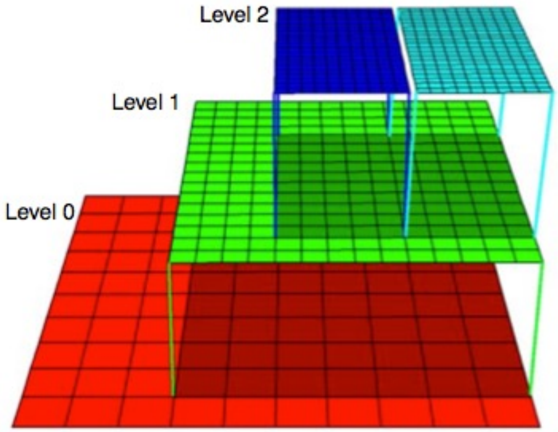


Adaptive Mesh Refinement (AMR) refines meshes into patches that capture details across length scales

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







Resources

Presenter Contact Info:

- Cyrus Harrison: cyrush@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

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Lawrence Livermore National Security, LLC

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Lawrence Livermore National Laboratory