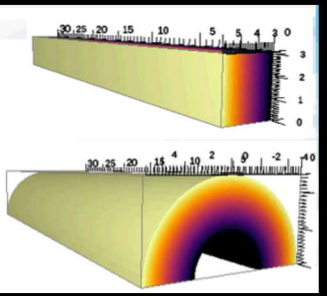
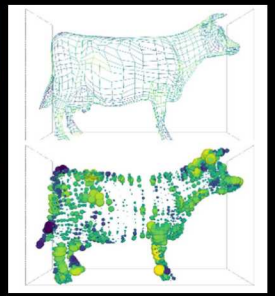
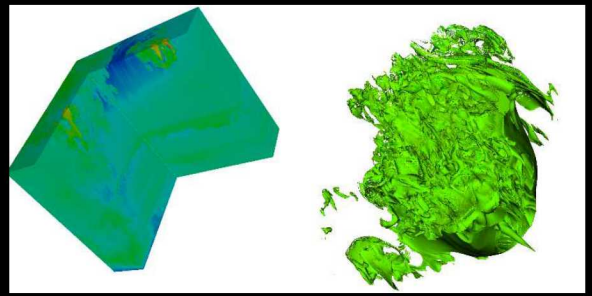
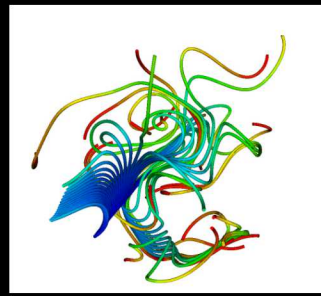
SAND2019-4261PE

VTK-m Update

DOECGF 2019

April 23 or 24, 2019

Kenneth Moreland Sandia National Laboratories

with lots of contributions from the VTK-m community

CCR Center for Computing Research

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Acknowledgements

- This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research, under Award Numbers 10-014707, 12-015215, and 14-017566.
- This research was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of two U.S. Department of Energy organizations (Office of Science and the National Nuclear Security Administration) responsible for the planning and preparation of a capable exascale ecosystem, including software, applications, hardware, advanced system engineering, and early testbed platforms, in support of the nation's exascale computing imperative.
- Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.
- **Thanks to many, many partners in labs, universities, and industry.**

Thanks to All Our Partners!

Sandia National Laboratories

Code Sprint, September 2015, LLNL

Code Sprint, April 2017, University of Oregon

Sandia National Laboratories

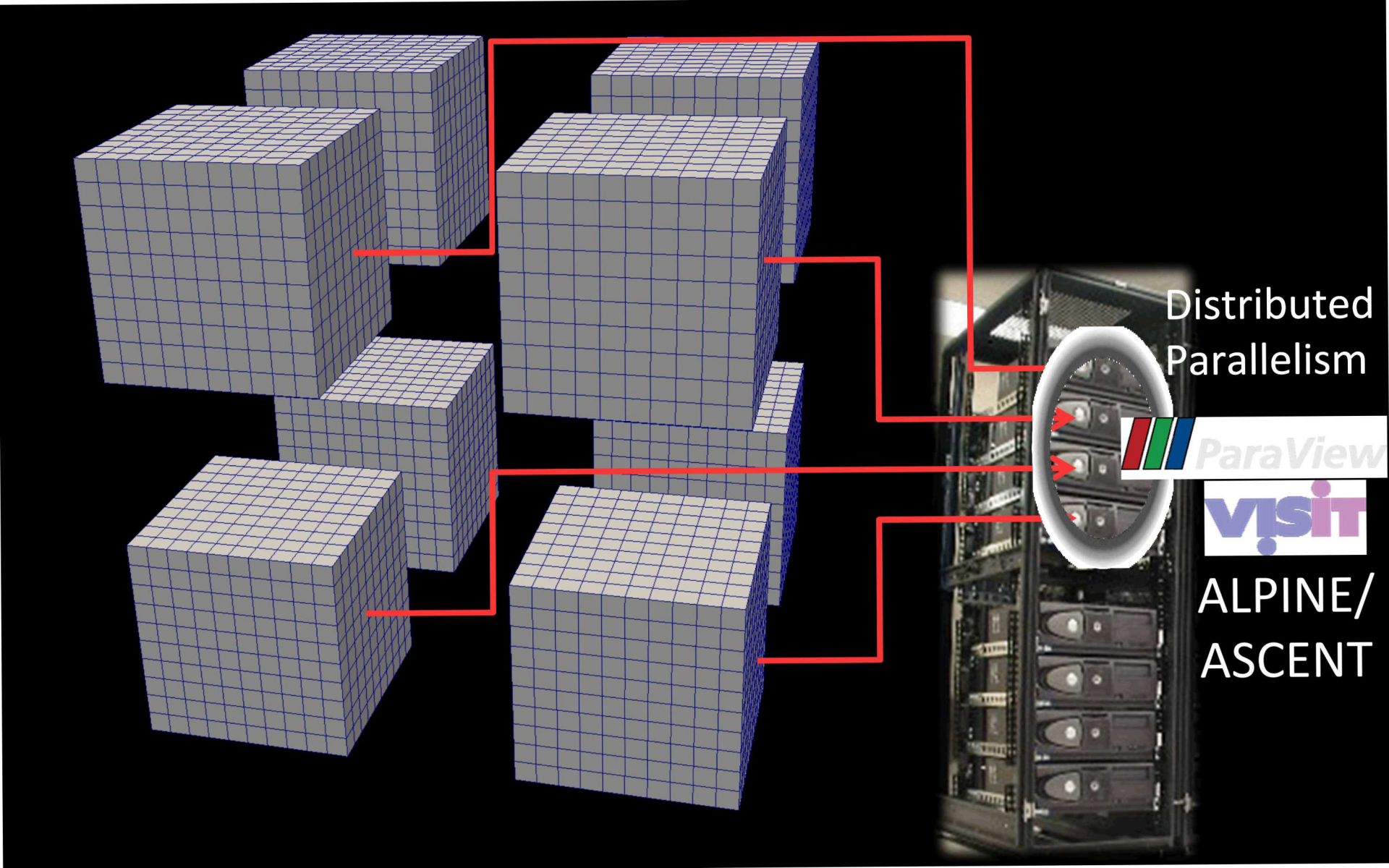
Why VTK-m?

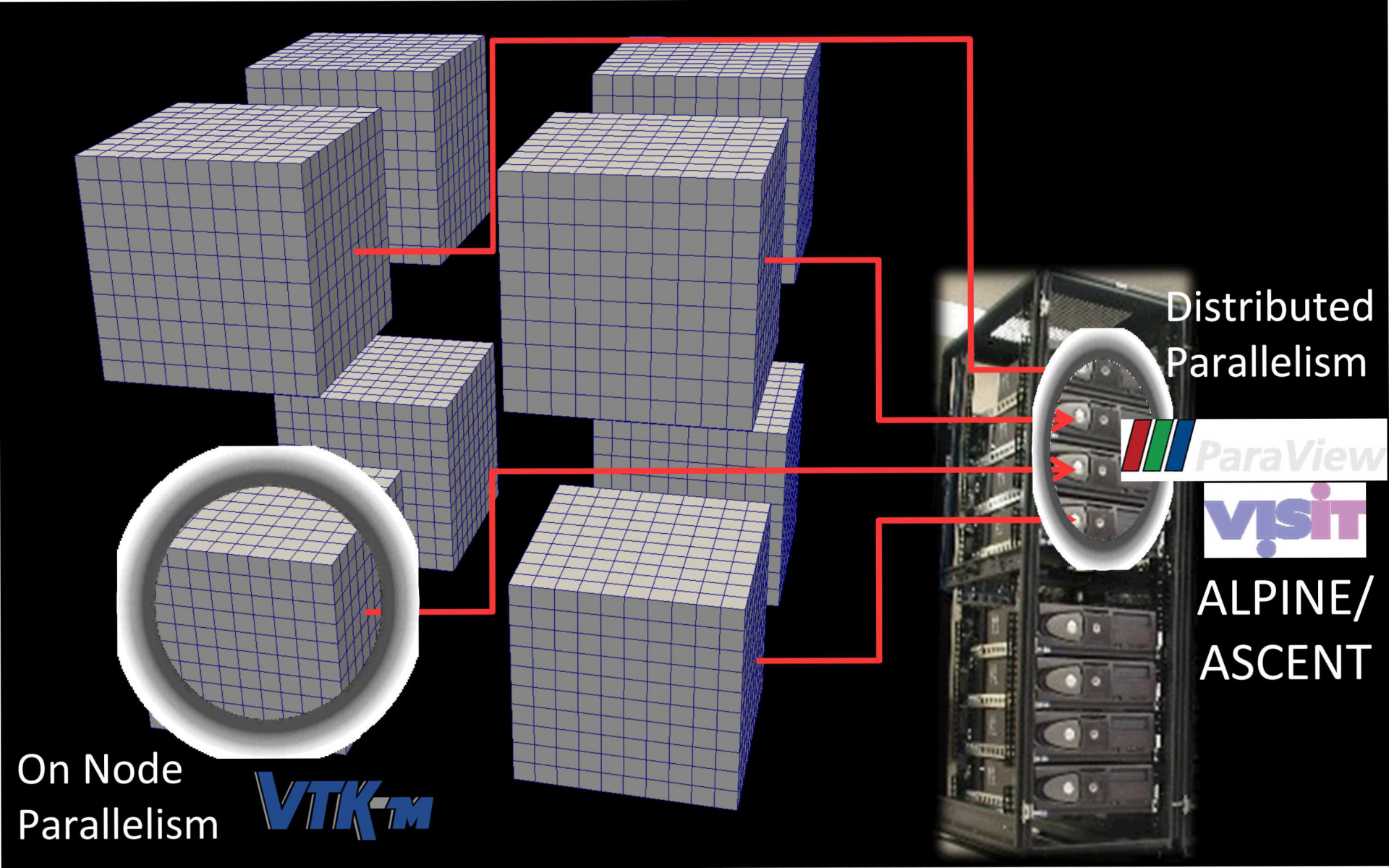
My new computer's got the clocks, it rocks
But it was obsolete before I opened the box

– “Weird” Al Yankovic, *It’s All About the Pentiums*, circa 1999

Moore’s Law is dead.

– Gordon Moore, circa 2005


Distributed
Parallelism
ParaView
VISIT
ALPINE/
ASCENT

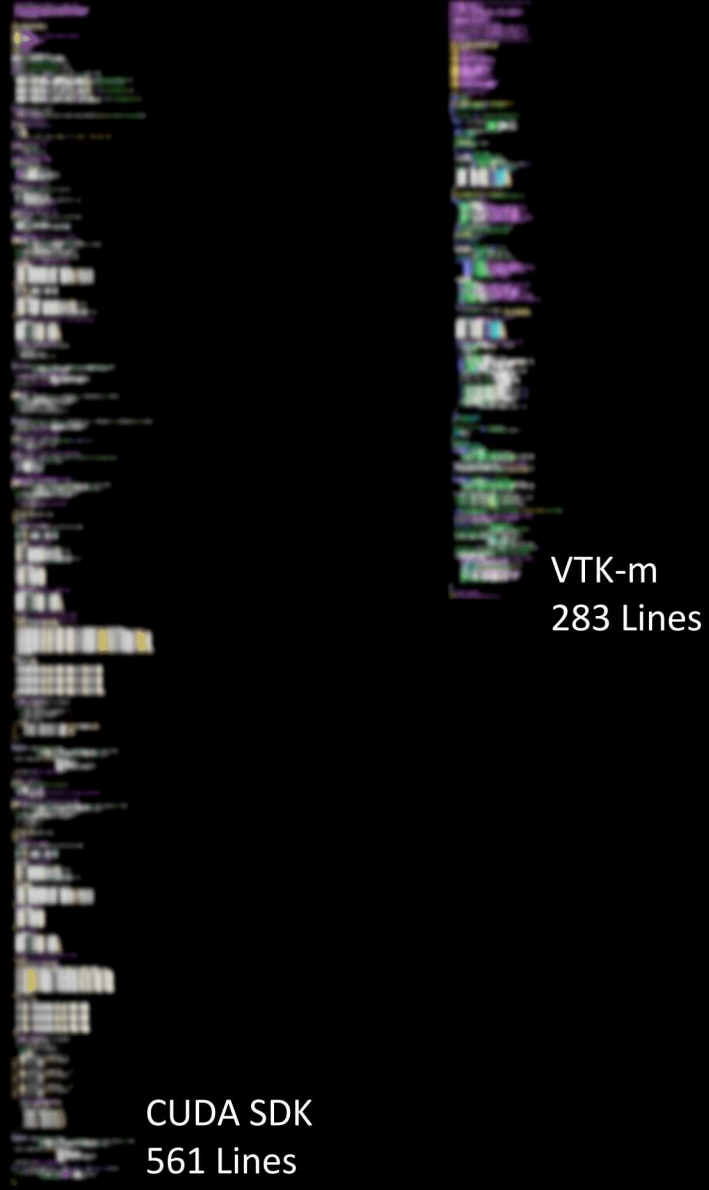

Distributed
Parallelism
ParaView
VISIT
ALPINE/
ASCENT
On Node
Parallelism
VTK-m

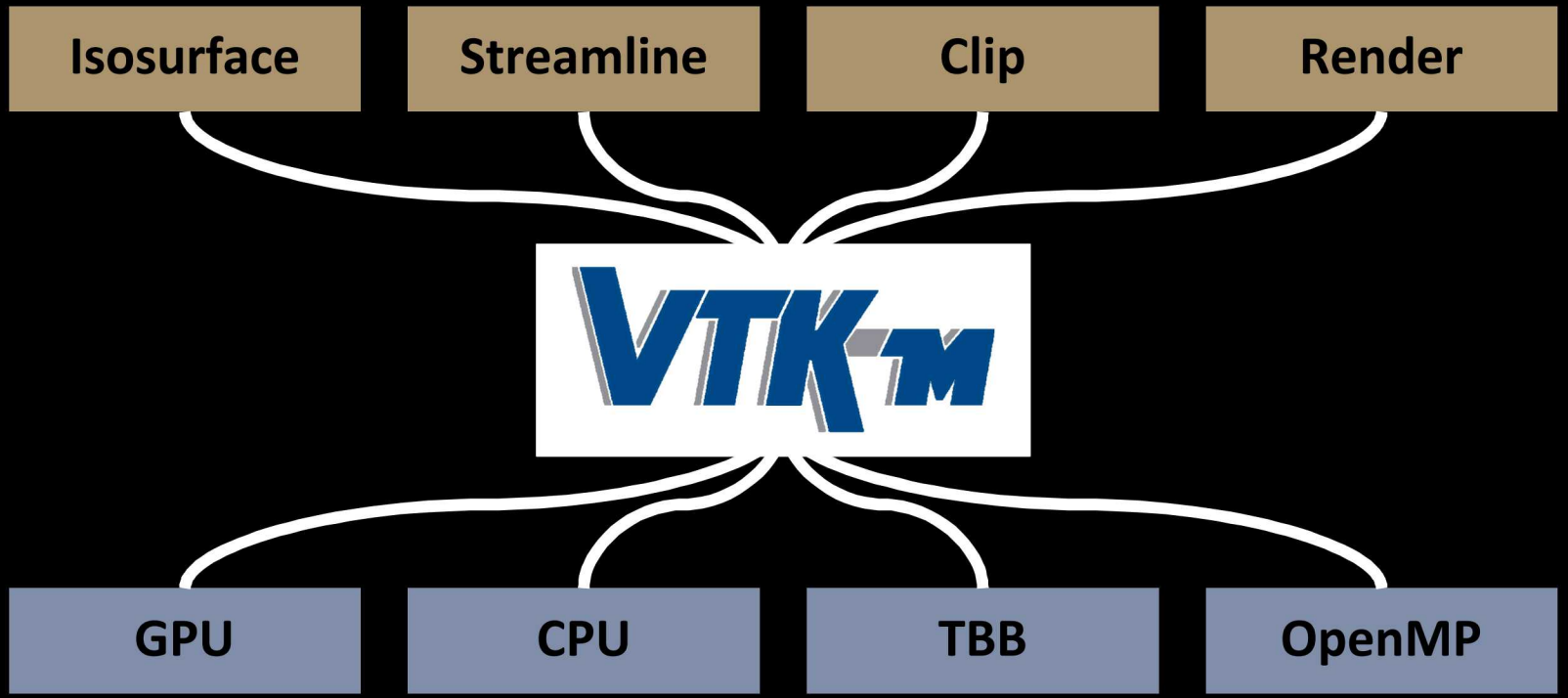
VTK-m: the ’m’ is for many-core

Sandia National Laboratories

- VTK:
  - popular, open source, supported by a community
  - … but primarily single core only.
- VTK-m:
  - name chosen to evoke the positive attributes of VTK
  - … but will support multi-core and many-core.

- VTK-m is the only DOE effort for many-core visualization.
  - Previously there were 3 predecessor projects, but the PI’s of those projects decided to join forces in 2014 to make VTK-m.


VTK-m
283 Lines
CUDA SDK
561 Lines


Isosurface
Streamline
Clip
Render
VTK-m
GPU
CPU
TBB
OpenMP

Simulations

In Situ Vis Library
(Integration with Sim)

GUI / Parallel Management

Base Vis Library
(Algorithm Implementation)

Libsim

Ascent

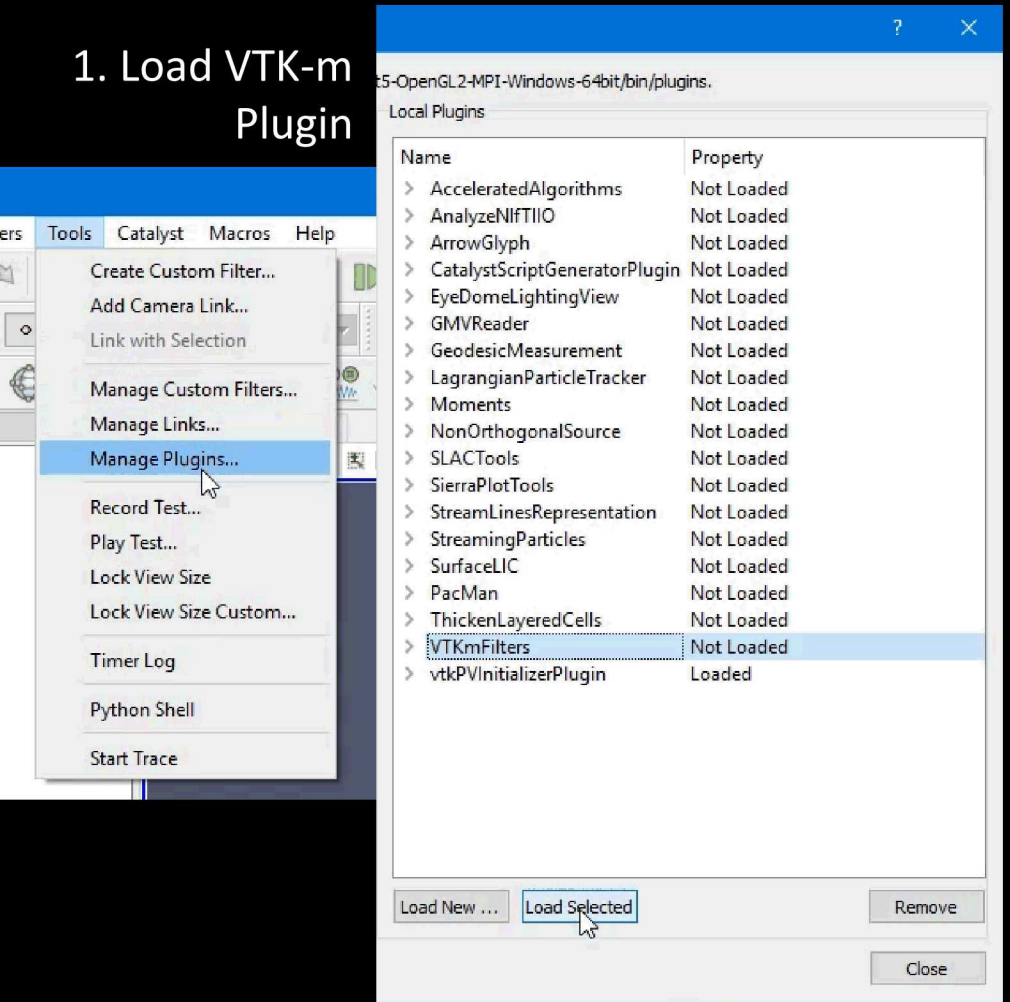
ADIOS

VTK-m

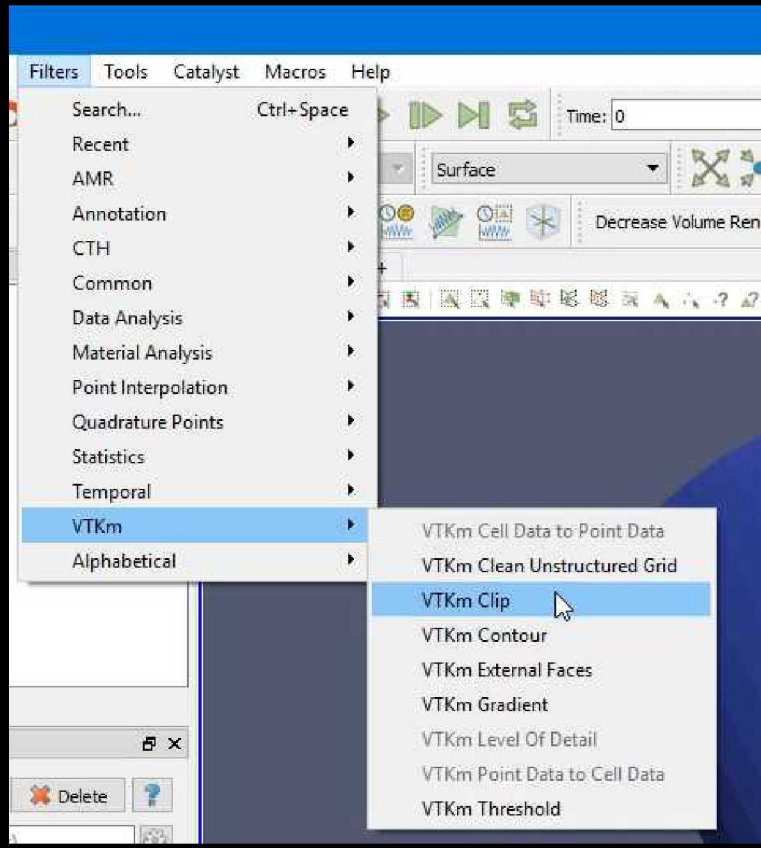
Multithreaded Algorithms
Processor Portability

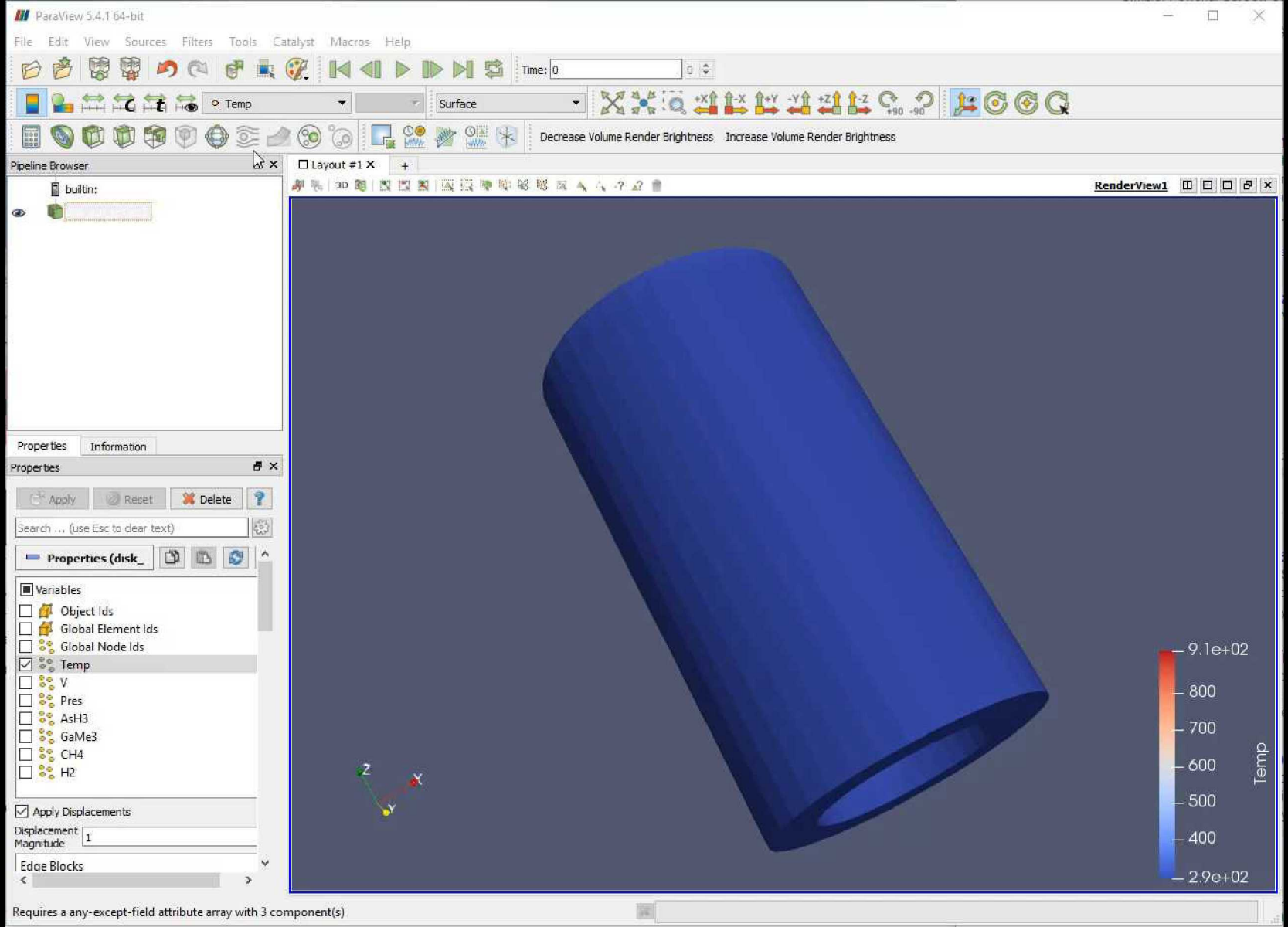
Using VTK-m in ParaView

1. Load VTK-m Plugin



2. Use a VTK-m filter like any other

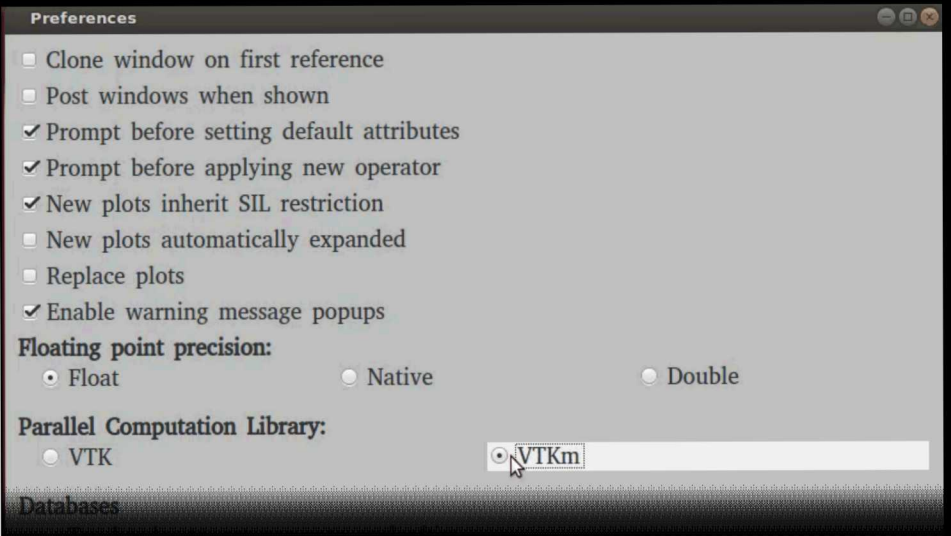



ParaView 5.4.1 64-bit
File Edit View Sources Filters Tools Catalyst Macros Help
Time: 0
Temp
Surface
Decrease Volume Render Brightness
Increase Volume Render Brightness
Pipeline Browser
builtin:
Properties
Information
Properties
Apply
Reset
Delete
Search ... (use Esc to clear text)
Properties (disk_
Variables
Object Ids
Global Element Ids
Global Node Ids
Temp
V
Pres
AsH3
GaMe3
CH4
H2
Apply Displacements
Displacement Magnitude
1
Edge Blocks
Layout #1
RenderView1
9.1e+02
800
700
600
500
400
2.9e+02
Temp
Requires a any-except-field attribute array with 3 component(s)

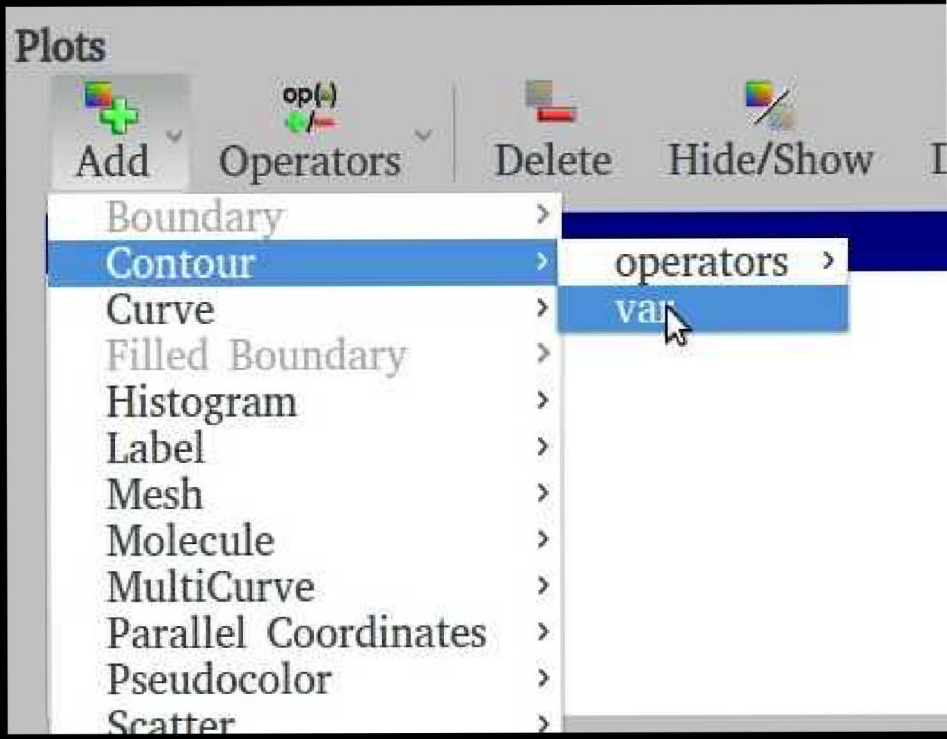
Using VTK-m in VisIt

Sandia National Laboratories

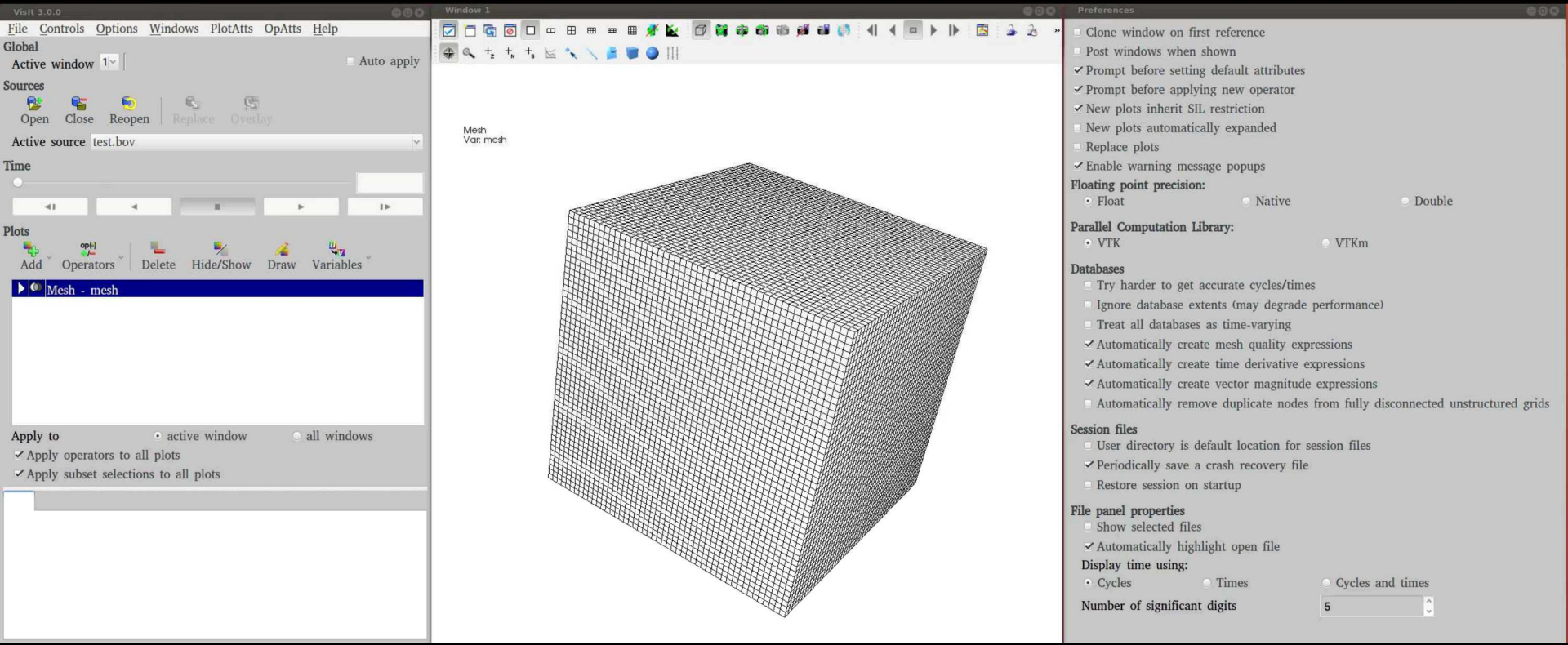
1. Turn on VTK-m in Preferences



2. Use VTK-m-enabled plots as normal



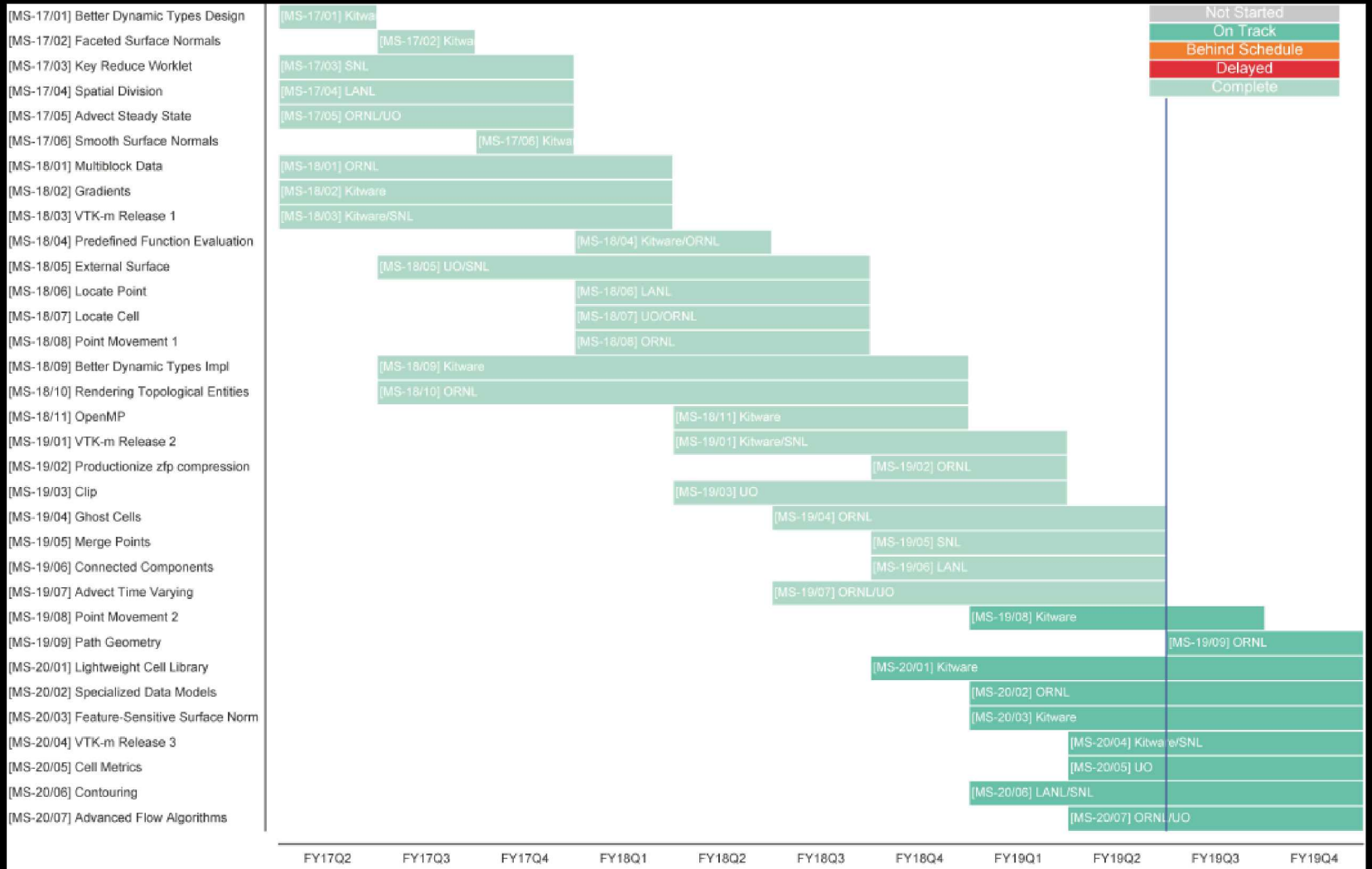
Slide Credit: David Pugmire



Slide Credit: David Pugmire

What is Going on Now?

ECP/VTK-m Schedule



Extracting External Mesh Surfaces in VTK-m

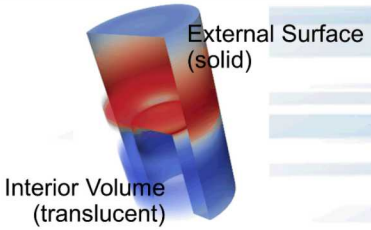
ECP WBS	2.3.4.13 ECP/VTK-m
PI	Kenneth Moreland, SNL
Members	ORNL, LANL, UO, Kitware

Scope and objectives

- ECP/VTK-m enables scientific visualization on the emerging processors required extreme scale computers
- Major focus on core functionality of HPC sci-vis software
- FY18 focus on field computation, computational geometry, and framework development/maintenance

Cool image

When rendering solid objects, it is only necessary to external surface of the object as the interior of the volume is hidden.



Impact

- External surfaces are used in most executions of ECP scientific visualization tools like ParaView and VisIt
  - Used by the rendering system to draw surfaces of solid volumes
- The accelerated external surface extraction will be integrated into the core behavior of vis tools

Project accomplishment

- The extraction of external surfaces are now supported by VTK-m
- Specialized “fast path” methods are provided for structured data sets
- VTK-m multicore code outperforms serial VTK external faces performance.

Deliverables FY18Q3 [MS-18/05-08] External Surface / Locate / Point Movement, WBS 2.3.4.13, Milestone STDA05-15
VTK-m source code repository available at: https://gitlab.kitware.com/vtk/vtk-m

Point Movement Operations in VTK-m

ECP WBS	2.3.4.13 ECP/VTK-m
PI	Kenneth Moreland, SNL
Members	ORNL, LANL, UO, Kitware

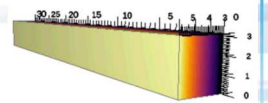
Scope and objectives

- ECP/VTK-m enables scientific visualization on the emerging processors required extreme scale computers
- Major focus on core functionality of HPC sci-vis software
- FY18 focus on field computation, computational geometry, and framework development/maintenance

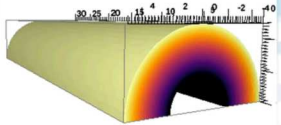
Cool image

Simulations represent data in different coordinates systems. Transformations allow visualizations to be done in the desired coordinate system

Cylindrical Coordinates



Cartesian Coordinates



Impact

- Transformations of point coordinates are commonly used in scientific visualization tools like ParaView and VisIt
  - Used for general transformations (e.g., translate, rotation, scale), as well as coordinate system transforms (e.g., cartesian, cylindrical, spherical)
- The accelerated point movement will be integrated into the core behavior of vis tools

Project accomplishment

- Implementations of two forms of point coordinate transformation
  - General affine transformations (any combinations of translate, rotate, and scale)
  - Coordinate system transformations (translations between Cartesian, cylindrical, and spherical representations)

Deliverables FY18Q3 [MS-18/05-08] External Surface / Locate / Point Movement, WBS 2.3.4.13, Milestone STDA05-15
VTK-m source code repository available at: https://gitlab.kitware.com/vtk/vtk-m

Cell and Point Locators in VTK-m

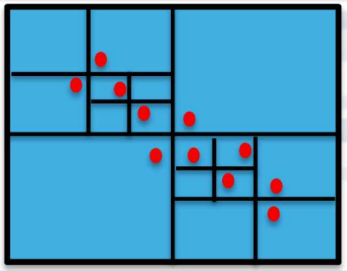
ECP WBS	2.3.4.13 ECP/VTK-m
PI	Kenneth Moreland, SNL
Members	ORNL, LANL, UO, Kitware

Scope and objectives

- ECP/VTK-m enables scientific visualization on the emerging processors required by extreme scale computers
- Major focus is core functionality of HPC sci-vis software
- FY18 focus on field computation, computational geometry, and framework development/maintenance

Cool image

Locators enable for quick spatial searching.
The time complexity for searching when using locators becomes logarithmic.



Impact

- Visualization algorithms in VTK-m that depend on cell or point location can now receive significant acceleration.
  - For example, particle advection depends on repeatedly evaluating a velocity field, which requires point location. This operation can now be done quickly for unstructured meshes.

Project accomplishment

- Implementation of VTK-m of point locators and cell locators
- Effort to make a consistent interface across all locators
- Work merged to VTK-m master
- API documented

Deliverables FY18Q3 [MS-18/06-07] Locate Point / Locate Cell, WBS 2.3.4.13, Milestone STDA05-24,25
VTK-m source code repository available at: https://gitlab.kitware.com/vtk/vtk-m

Rendering Topological Entities

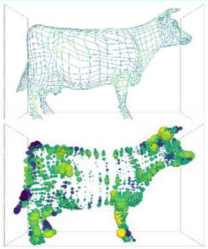
ECP WBS	2.3.4.13 ECP/VTK-m
PI	Kenneth Moreland, SNL
Members	ORNL, LANL, UO, Kitware

Scope and objectives

- ECP/VTK-m enables scientific visualization on the emerging processors required extreme scale computers
- Major focus on core functionality of HPC sci-vis software
- FY18 focus on field computation, computational geometry, and framework development/maintenance

Cool image

Examples of rendering a surface mesh based on edges (top) and points (bottom).



Impact

- A mesh contains multiple distinctive features, all of which can affect the solution achieved by a solver
- Renderings of different topological features are important to understand mesh structures and data in the mesh

Project accomplishment

- Implemented multiple “mappers” that represent topologies in different ways
  - MapperCylinder: Represent edges as 3D tubes that can be sized based on physical properties
  - MapperPoint: Represent points as 3D spheres that can be sized based on physical properties
  - MapperQuad: Optimize render for surfaces of quads

Deliverables FY18Q4 [MS-18/09-10] Dynamic Types / Rendering Topologies, WBS 2.3.4.13, Milestone STDA05-16
VTK-m source code repository available at: https://gitlab.kitware.com/vtk/vtk-m

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OpenMP Thread Management in VTK-m

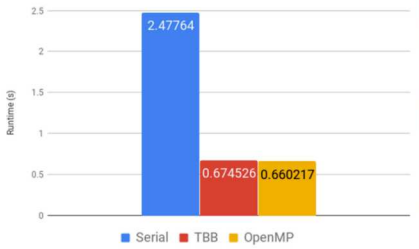
ECP WBS	2.3.4.13 ECP/VTK-m
PI	Kenneth Moreland, SNL
Members	ORNL, LANL, UO, Kitware

Scope and objectives

- ECP/VTK-m enables scientific visualization on the emerging processors required extreme scale computers
- Major focus on core functionality of HPC sci-vis software
- FY18 focus on field computation, computational geometry, and framework development/maintenance

Performance

The OpenMP backend performs similarly to the TBB backend. Benchmark shown is the Marching Cubes algorithm on a 512x512x512 volume on a quad core workstation.



Impact

- Many software products used and developed in ECP use OpenMP
- VTK-m's previous thread manager, TBB, could interact with OpenMP in poor ways
- VTK-m with OpenMP insures that VTK-m's threads will not interfere with other integrated software

Project accomplishment

- A "device adapter" using OpenMP was added to VTK-m
  - TBB device adapter still exists
  - Users can choose between the two
- Performance comparisons show that the OpenMP implementation is as efficient as our TBB implementation

Deliverables FY18Q4 [MS-18/09-10] Dynamic Types / Rendering Topologies, WBS 2.3.4.13, Milestone STDA05-16
VTK-m source code repository available at: https://gitlab.kitware.com/vtk/vtk-m

Dynamic Types in VTK-m

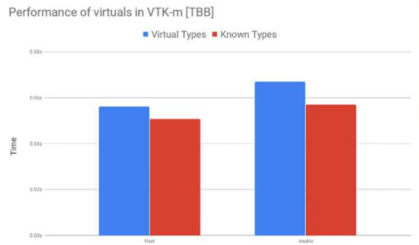
ECP WBS	2.3.4.13 ECP/VTK-m
PI	Kenneth Moreland, SNL
Members	ORNL, LANL, UO, Kitware

Scope and objectives

- ECP/VTK-m enables scientific visualization on the emerging processors required extreme scale computers
- Major focus on core functionality of HPC sci-vis software
- FY18 focus on field computation, computational geometry, and framework development/maintenance

Performance

Comparison of Black-Scholes with and without the overhead of virtual calls



Impact

- VTK-m is designed to adapt to other app data structures
- Often specific types of these structures are not known until run time.
- VTK-m's new dynamic data types hide the physical structure behind a virtual method interface.

Project accomplishment

- ArrayHandleVirtual was added to VTK as primary virtual method interface which works seamlessly across TBB, OpenMP, and CUDA.
- Support was added for filters to have full de-virtualization of specific type and layout combinations

Deliverables FY18Q4 [MS-18/09-10] Dynamic Types / Rendering Topologies, WBS 2.3.4.13, Milestone STDA05-16
VTK-m source code repository available at: https://gitlab.kitware.com/vtk/vtk-m

ZFP Compression Available in VTK-m

ECP WBS	2.3.4.13 ECP/VTK-m
PI	Kenneth Moreland, SNL
Members	ORNL, LANL, UO, Kitware

Scope and objectives

- ECP/VTK-m enables scientific visualization on the emerging processors required extreme scale computers
- Major focus on core functionality of HPC sci-vis software
- FY19 focus on computational geometry, flow visualization, and framework development/maintenance

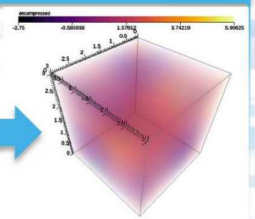
Ease of Integration

Enabling ZFP in rendering can be implemented in as little as 4 lines of code.

```
template<typename M, typename C, typename V3>
void RenderZFP(vtkm::cont::DataSet &compressedDS,
               vtkm::Float64 rate)
{
  vtkm::filter::ZFPDecompressor3D decompressor;
  decompressor.SetActiveField("compressed");
  decompressor.SetRate(rate);
  auto decompress = decompressor.Execute(compressedDS);

  vtkm::cont::ColorTable colorTable("inferno");
  colorTable.AddPointAlpha(0.0, .01f);
  colorTable.AddPointAlpha(1.0, .01f);

  vtkm::rendering::testing::Render<M, C, V3>(
    decompress, "decompressed", colorTable, "reg3D.pnm");
}
```



Impact

- ZFP provides fast, tunable compression
  - A critical technology for ECP (WBS 2.3.4.11)
- Benefits of implementing ZFP in VTK-m:
  - Device portability
  - Easier integration in visualization and other software

Project accomplishment

- Implement ZFP using VTK-m parallel primitives model
- Implement VTK-m compression filters
- Implement VTK-m compression worklets

Deliverables FY19Q1 [MS-19/01-03] ZFP / Release / Clip, WBS 2.3.4.13, Milestone STDA05-17
VTK-m source code repository available at: https://gitlab.kitware.com/vtk/vtk-m

Fast, Highly Parallel Mesh Clipping

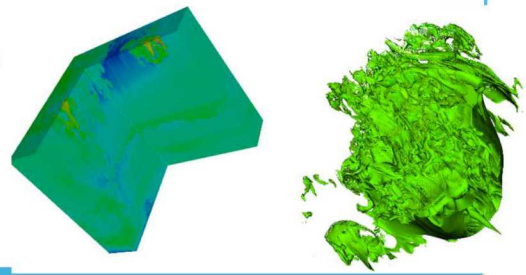
ECP WBS	2.3.4.13 ECP/VTK-m
PI	Kenneth Moreland, SNL
Members	ORNL, LANL, UO, Kitware

Scope and objectives

- ECP/VTK-m enables scientific visualization on the emerging processors required extreme scale computers
- Major focus on core functionality of HPC sci-vis software
- FY19 focus on computational geometry, flow visualization, and framework development/maintenance

Cool image

Two uses of clipping, applied to a buoyancy data set. Left: clipping away using two planes. Right: clipping away regions outside a scalar range.



Impact

- Clipping is a common visualization operation for extracting regions of interest.
- The algorithm intersects a mesh with spatial or field region to provide cutaways and isovolumes (the region of a volume between a minimum and maximum scalar value)

Project accomplishment

- Evolved the VTK-m clipping functionality to work natively on all cell types, rather than just tetrahedrons.
  - This work was carried out by adapting the routines from from the VisIt visualization tool to VTK-m.
- This minimizes the amount of memory needed to carry out the algorithm and also produces more accurate visualizations.

Deliverables FY19Q1 [MS-19/01-03] ZFP / Release / Clip, WBS 2.3.4.13, Milestone STDA05-17
VTK-m source code repository available at: https://gitlab.kitware.com/vtk/vtk-m

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Better Ghost Cell Support in VTK-m

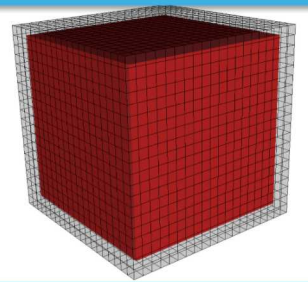
ECP WBS	2.3.4.13 ECP/VTK-m
PI	Kenneth Moreland, SNL
Members	ORNL, LANL, UO, Kitware

Scope and objectives

- ECP/VTK-m enables scientific visualization on the emerging processors required extreme scale computers
- Major focus on core functionality of HPC sci-vis software
- FY19 focus on computational geometry, flow visualization, and framework development/maintenance

Cool image

Grid with boundary layer cells marked as ghost cells. The ghost cells are rendered transparently and the other cells in red.



Impact

- Support for ghost cells allows for better representation of raw simulation data
- Support will allow for zero-copy data required for in situ visualization scenarios
- Support for both simulation embedded visualization as well as tools in the ALPINE project

Project accomplishment

- Ghost cells are critical for simulations to ensure boundary continuity
- Two VTK-m filters provided for working with ghost cells
  - Filter to mark boundary layers as ghost cells
  - Filter to remove ghost cells from dataset preserving structured topology when possible

Deliverables FY19Q2 [MS-19/04-07] Ghost / Merge / Connected / Advect Time, WBS 2.3.4.13, P6 Activity STDA05-18
VTK-m source code repository available at: https://gitlab.kitware.com/vtk/vtk-m

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Fast Point Merging in VTK-m

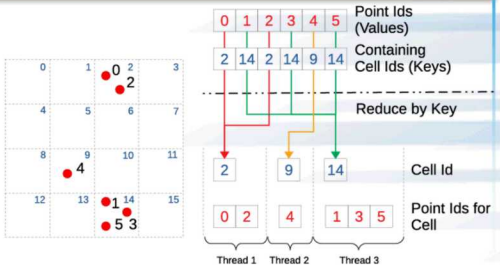
ECP WBS	2.3.4.13 ECP/VTK-m
PI	Kenneth Moreland, SNL
Members	ORNL, LANL, UO, Kitware

Scope and objectives

- ECP/VTK-m enables scientific visualization on the emerging processors required extreme scale computers
- Major focus on core functionality of HPC sci-vis software
- FY19 focus on computational geometry, flow visualization, and framework development/maintenance

Cool image

Our “virtual grid” approach quickly identifies nearby points much like a spatial search structure but without building the structure itself.



Impact

- Mesh structures can contain coincident points, and it may be necessary to merge these coincident points
- Efficiency is important for large points sets (naïve algorithm is $O(N^2)$)
- Point merging can: save space, make a mesh watertight, help identify malformed cells, simplify geometry

Project accomplishment

- Developed a “virtual grid” approach to point merging
  - Faster than an explicit search structure
  - Demonstrates scalable performance
- Adjustable tolerance for distance of “coincident”
  - Can manage floating point error at different scales

Deliverables FY19Q2 [MS-19/04-07] Ghost / Merge / Connected / Advect Time, WBS 2.3.4.13, P6 Activity STDA05-18
VTK-m source code repository available at: https://gitlab.kitware.com/vtk/vtk-m

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Identifying Connected Components in VTK-m

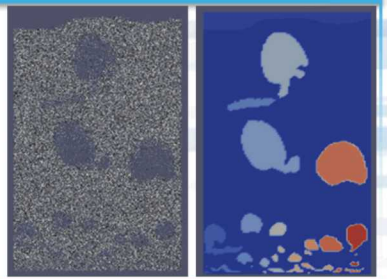
ECP WBS	2.3.4.13 ECP/VTK-m
PI	Kenneth Moreland, SNL
Members	ORNL, LANL, UO, Kitware

Scope and objectives

- ECP/VTK-m enables scientific visualization on the emerging processors required extreme scale computers
- Major focus on core functionality of HPC sci-vis software
- FY19 focus on computational geometry, flow visualization, and framework development/maintenance

Cool image

Bubble detection for MFIX particle data, identifying low particle density regions in the simulation.



Impact

- Identifying subsets with common property is a widely used data analysis technique.
- Simulations like ExSky and MFIX can use Connected Components to identify region of dense/sparse particle distributions.

Project accomplishment

- Implement ImageConnectivity filter for structured grid based on cell data.
- Implement CellSetConnectivity filter for unstructured grid based on cell to cell connectivity.

Deliverables FY19Q2 [MS-19/04-07] Ghost / Merge / Connected / Advect Time, WBS 2.3.4.13, P6 Activity STDA05-18
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Time Varying Particle Advection in VTK-m

ECP WBS	2.3.4.13 ECP/VTK-m
PI	Kenneth Moreland, SNL
Members	ORNL, LANL, UO, Kitware

Scope and objectives

- ECP/VTK-m enables scientific visualization on the emerging processors required extreme scale computers
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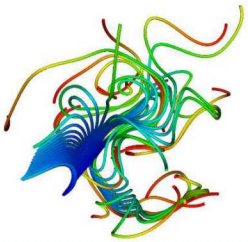
VTK-m Particle Advection

Particle advection is a foundational operation for many flow visualization algorithms
VTK-m's particle advection system supports diverse flow visualization algorithms, and does so efficiently in a performance portable, parallel manner



Impact

- Time-varying flow visualization algorithms are often needed by ECP Applications to understand their data
  - With this work, we will be able to deliver the most meaningful analysis to stakeholders, as opposed to our previous generation of code that supported only steady-state flow

Project accomplishment

- Enhanced the VTK-m particle advection system to support unsteady flow data
  - Extensive development task, requiring all previous components to add support for time information, as well as support for handling multiple time steps, and temporal interpolation

Deliverables FY19Q2 [MS-19/04-07] Ghost / Merge / Connected / Advect Time, WBS 2.3.4.13, P6 Activity STDA05-18
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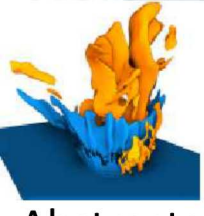
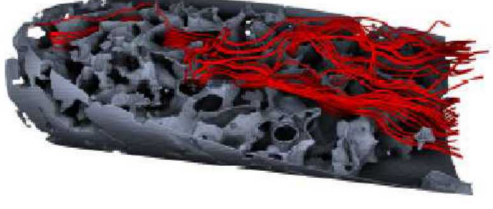
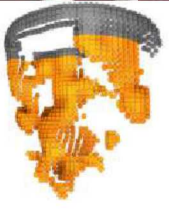
LDAV 2019

The 9th IEEE Symposium on Large Data Analysis and Visualization

in conjunction with IEEE VIS 2019,
Vancouver, BC, Canada, October 21, 2019







Abstracts Due: June 17
Papers Due: June 24