VTK-m

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ECP Data Management, Data Analytics, and Visualization Overview

Kenneth Moreland
Sandia National Laboratories

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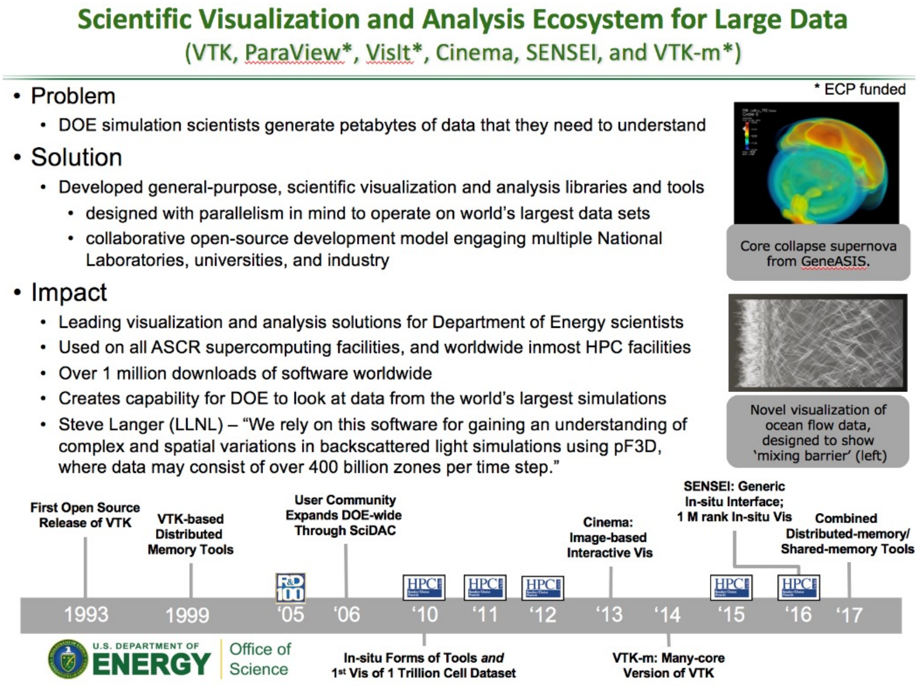
Why VTK-m?

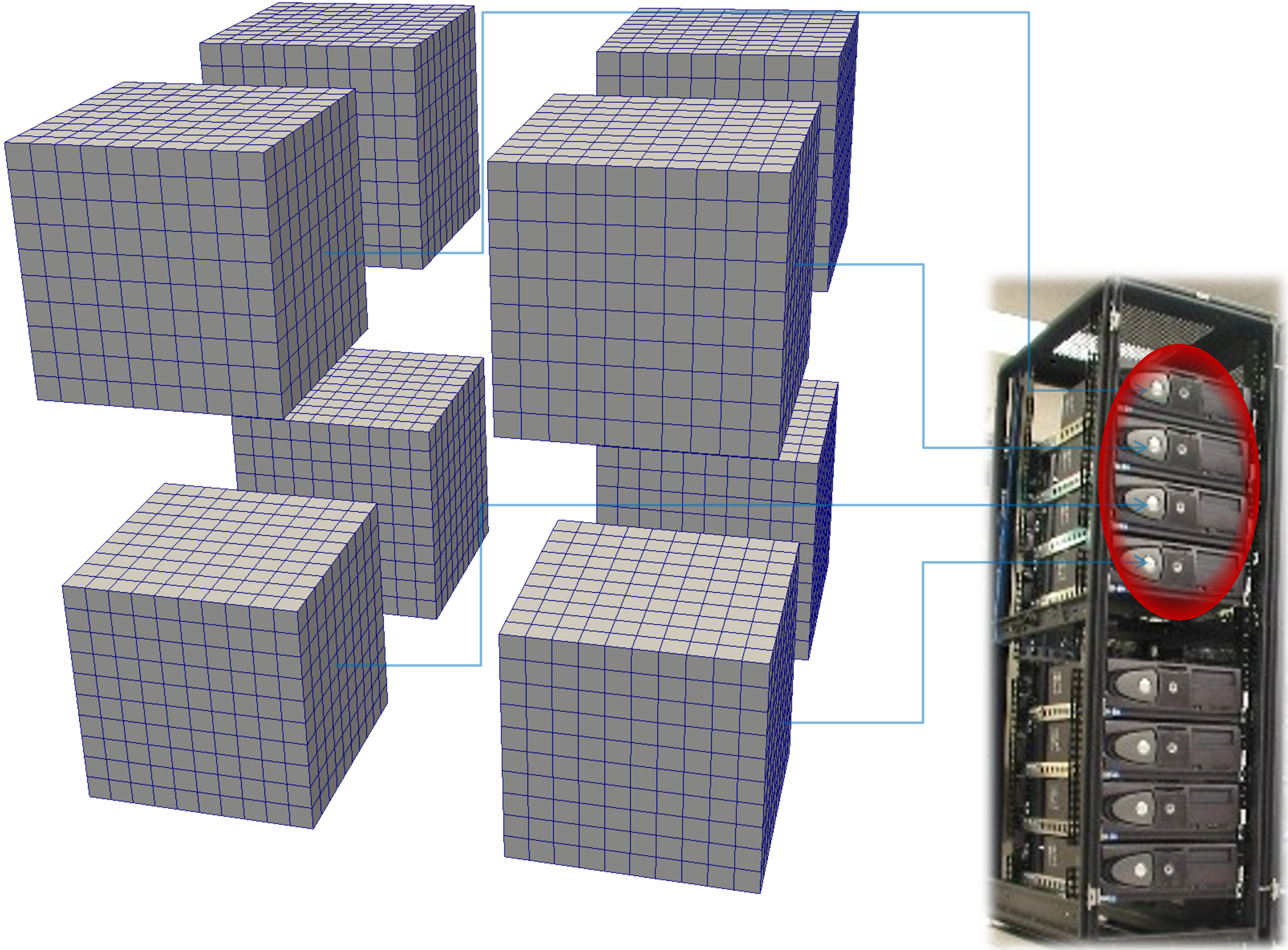
Visualization and Analysis for HPC: Current Status

- Developed popular, open source tools (ParaView, VisIt) based on the Visualization ToolKit library (VTK)
  – Widespread usage in DOE and >1 million downloads worldwide
  – Hundreds of person years of effort
- Two major problems for exascale:
  1) Many-core architectures (as current VTK-based investments are primarily only MPI parallelism)
  2) I/O limitations will require in situ processing



ASCR highlight slide for VTK-based tools.

ECP/VTK-m project focused on problem #1.
ECP ALPINE is focused on problem #2.
Our approaches are complementary and coordinated.

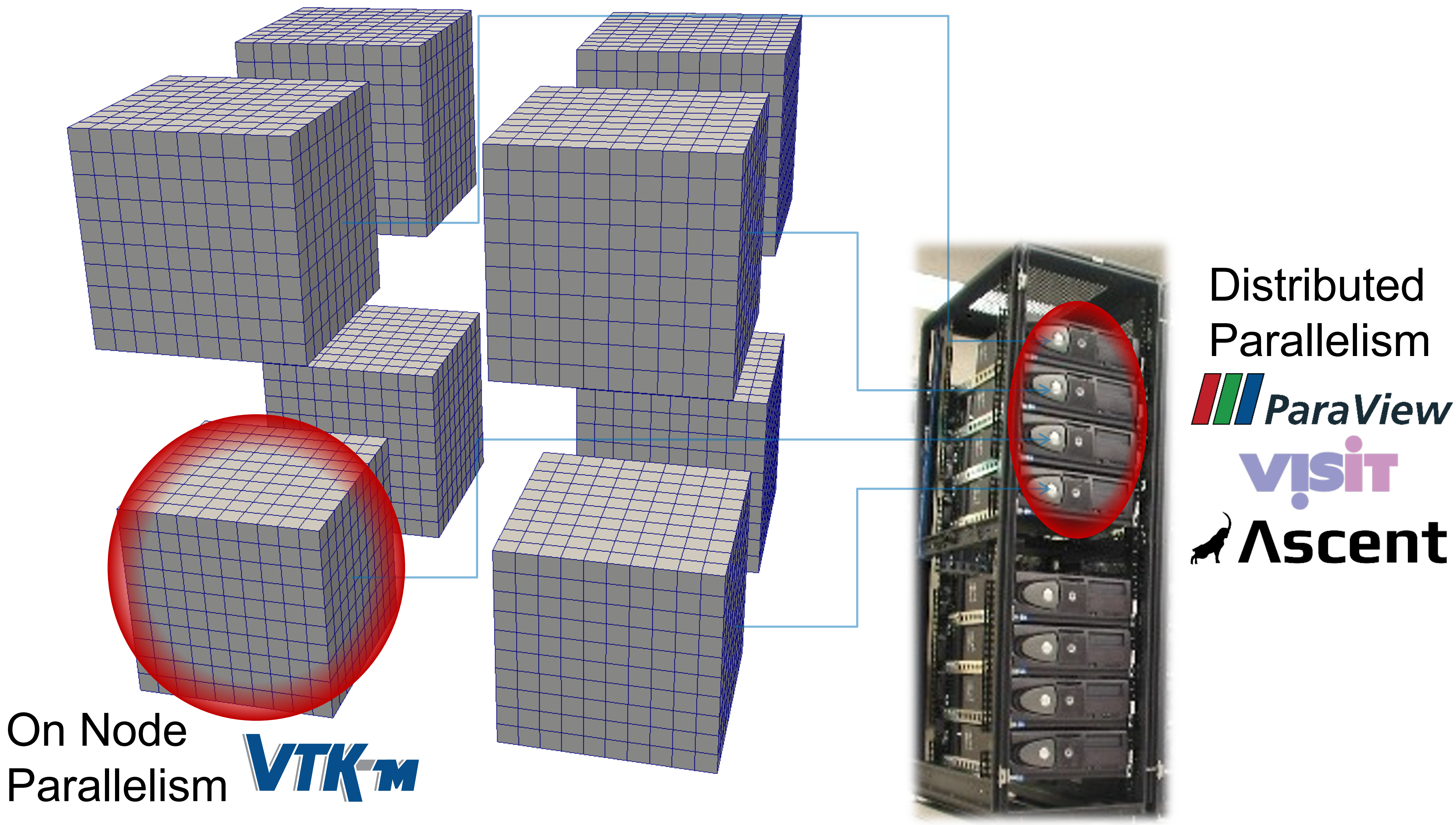


Distributed Parallelism

ParaView

VisIt

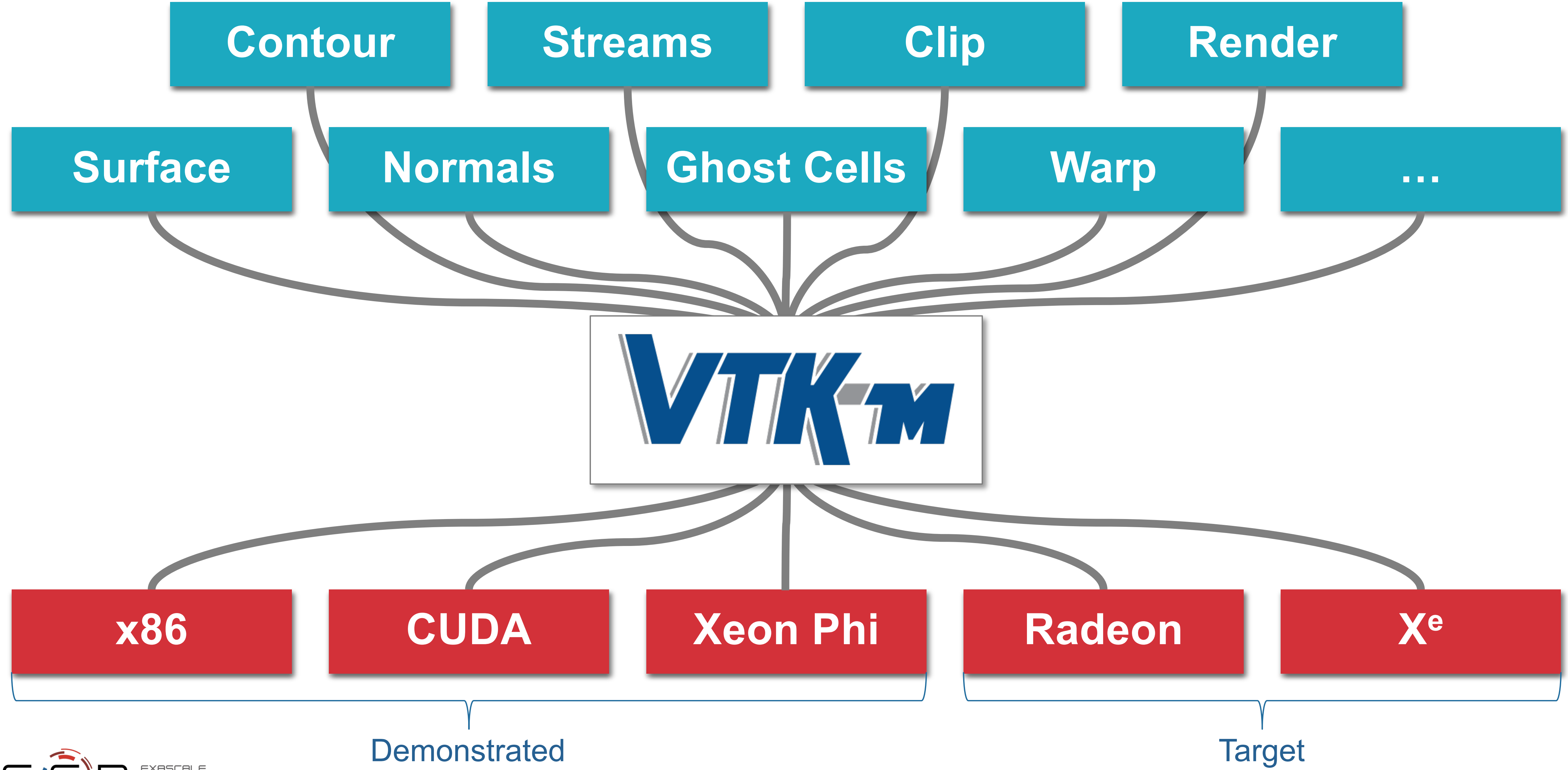
Ascent


Distributed
Parallelism
ParaView
VisIt
Ascent
On Node
Parallelism
VTK-m

VTK-m: the ’m’ is for many-core

- 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.

Overall Strategy: A framework to write-once-run-everywhere

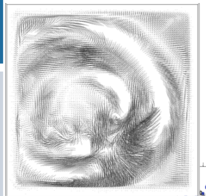
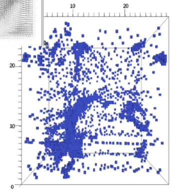
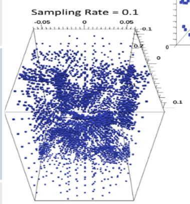


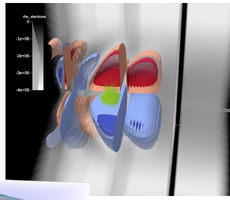
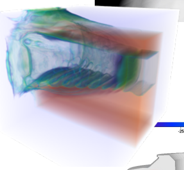
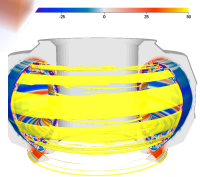
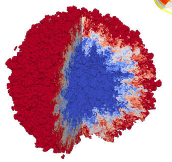
EXASCALE COMPUTING PROJECT

Recent Accomplishments

Capability Delivery

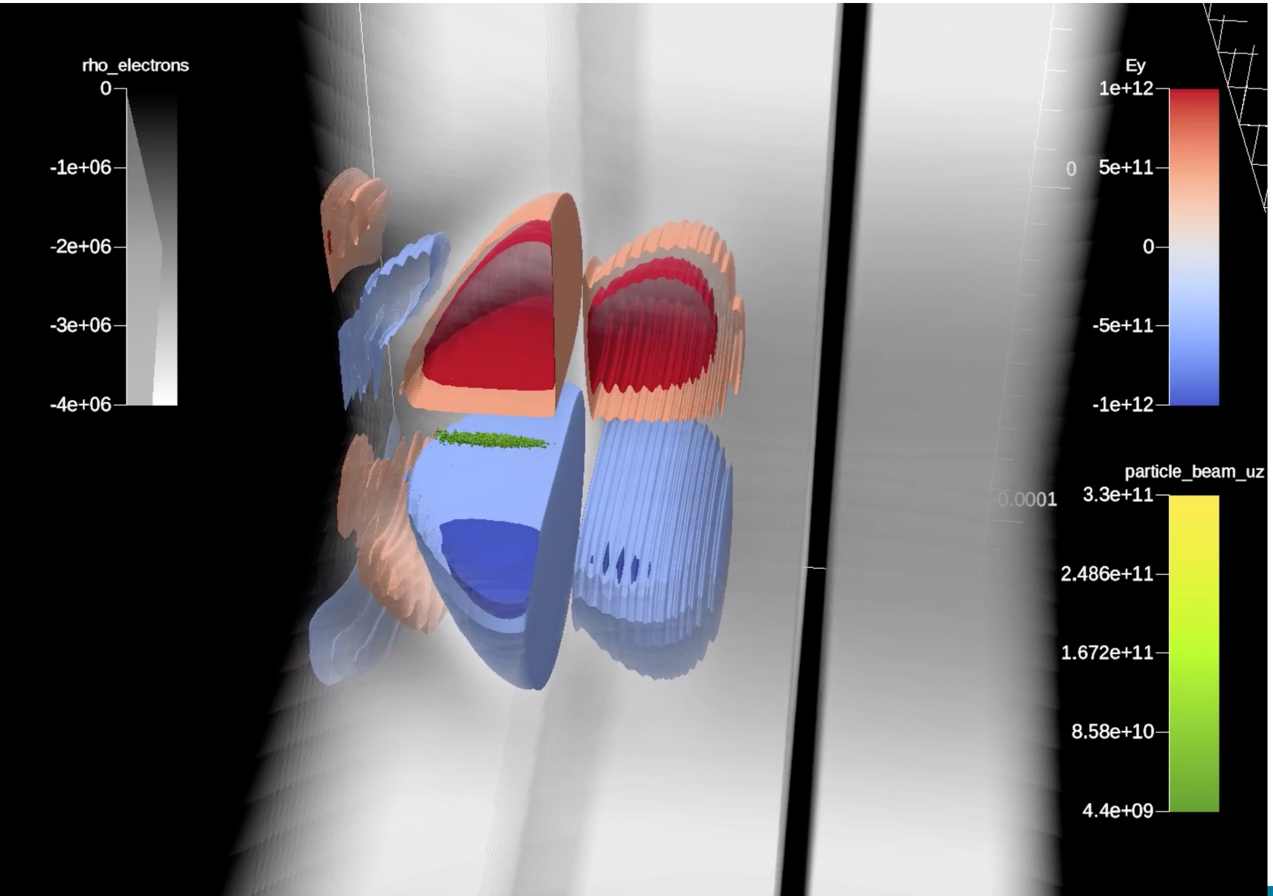
ECP App	ST Partner	Machine	Notes
EQSIM:SW4	Alpine	Summit (384 GPUs across 64 nodes for Lagrangian, 2000 nodes for traditional algs)	Scale increased in FY20
ExaSky:Nyx	Alpine	Summit (512 nodes with 1 MPI task per node and 1 GPU per MPI task)	Nyx on CPU with OpenMP
PeleC	Alpine	Summit (64 MPI processes)	VTK-m on CPU with OpenMP
WarpX	Alpine	Cori (1024 compute nodes, 65,536 cores with hyperthreading)	40X scaling improvement in FY20
WarpX	Alpine	Summit (27,000 GPUs)	Featured in ISAV keynote
MARBL	Alpine	Sierra (16,384 GPUs across 4096 nodes)	
WDMApp	ADIOS	Summit (100 nodes)	VTK-m incorporated in EFFIS
External	LLNL	Sierra (16,384 GPUs across 4096 nodes)	This image is of an idealized Inertial Confinement Fusion (ICF) simulation of a Rayleigh–Taylor instability with two fluids mixing in a spherical geometry.

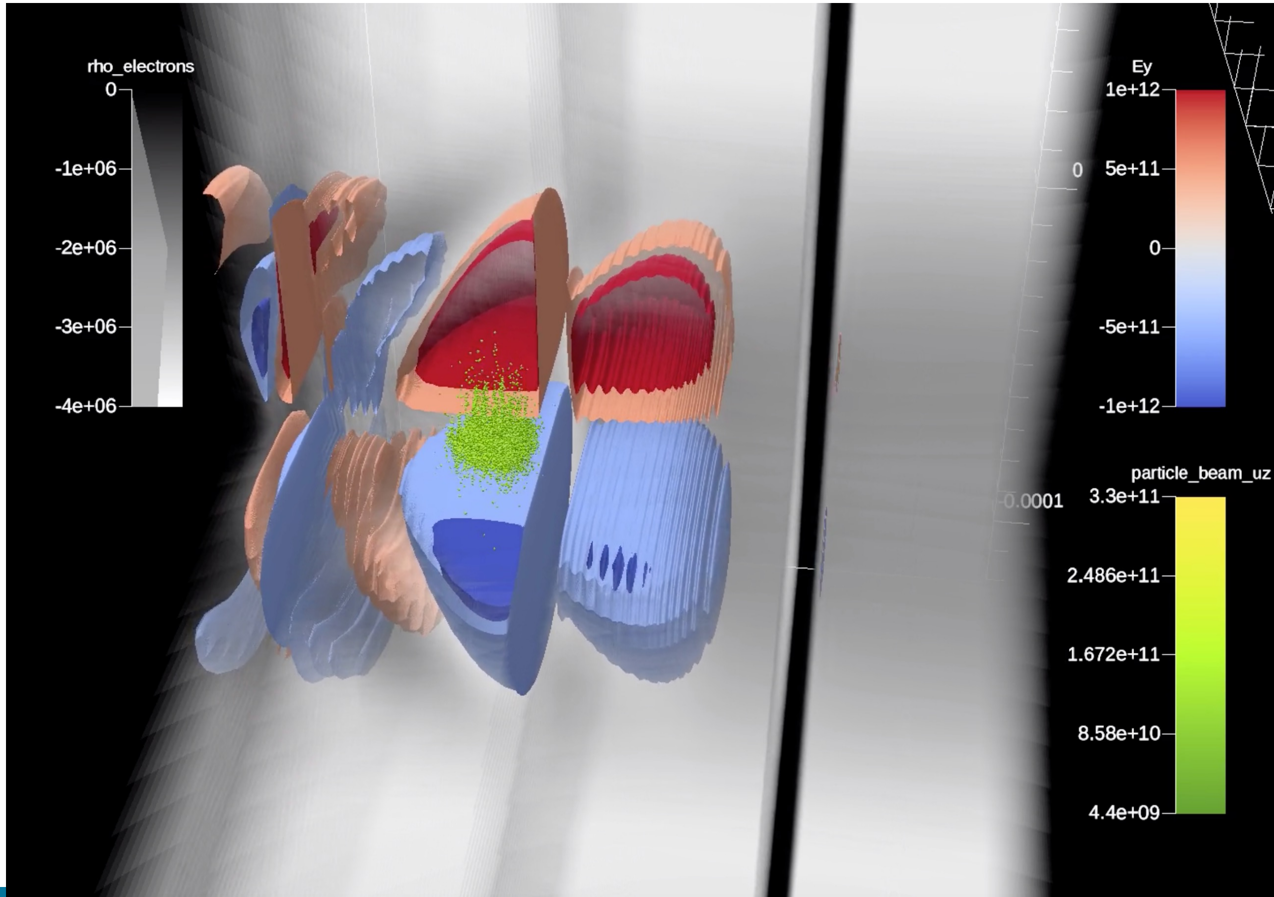




In Situ/In Transit Visualization with WarpX

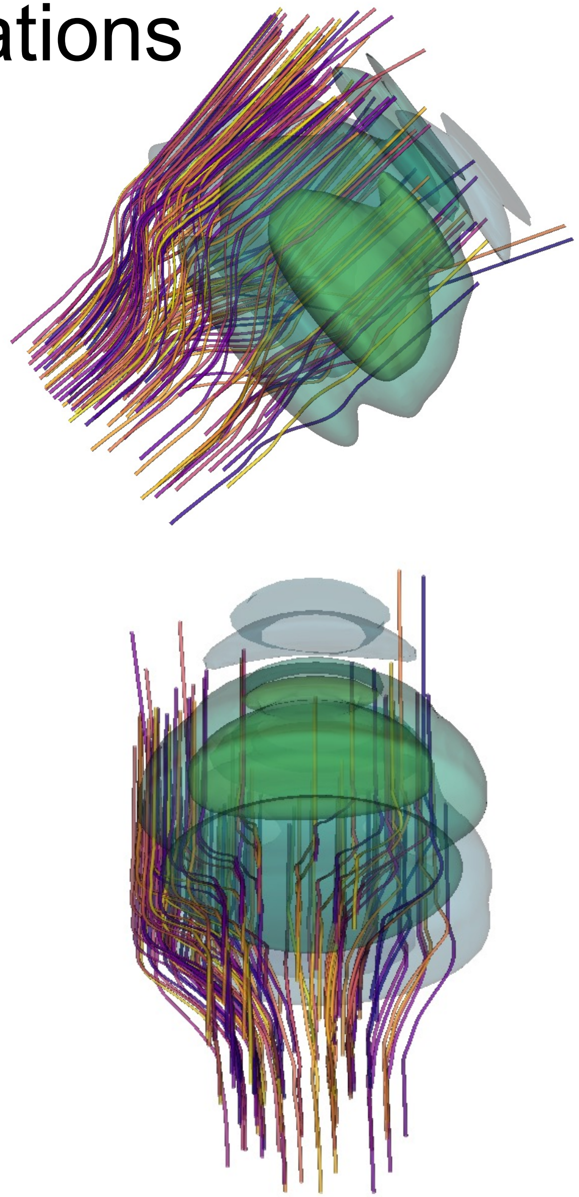
- VTK-m is providing in situ capabilities to WarpX (using Ascent)
- Simulation run on 600 GPUs on Summit
  - Modeling a 10-stage laser-wakefield accelerator
- Functionality featured in keynote for ISAV 2020: *Uses of In Situ/In Transit Methods in Large-Scale Modeling of Plasma-Based Particle Accelerators*





Flow Visualization in WarpX Laser Wakefield Simulations

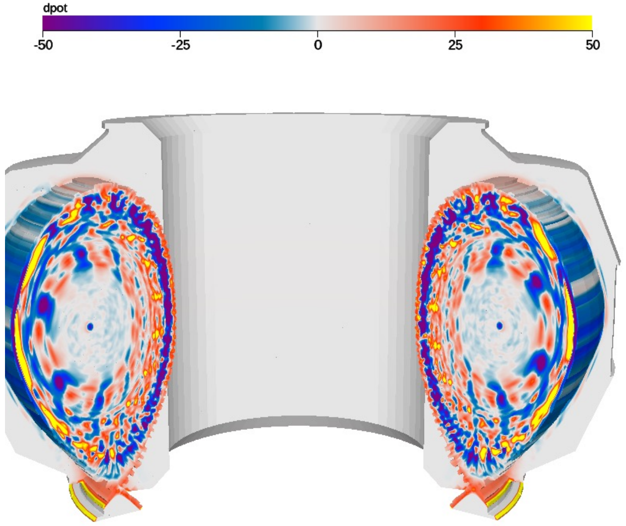
- Science Problem
  - The Exascale Modeling of Advanced Particle Accelerators (WarpX) project aims to answer outstanding questions in the physics of acceleration and transport of particle beams in chains of plasma channels. One of the core efforts in this project is the simulation of laser wakefields in plasma-based particle accelerators.
  - Modeling the flow of particles is critical to understanding the physics.
- Technical Solution
  - Unlike flow in typical fluids, the velocity of particles must be inferred from magnetic and electric fields by solving the Lorentz force equation.
  - The frame of reference of the simulation shifts to follow particle advancement, and the flow vectors must be translated to compensate.
  - VTK-m's flow visualization system was tailored to this application.
- Science Impact
  - The numerically accurate particle tracking provides numerous flow visualization techniques to better understand the flow in the simulated particle accelerators.



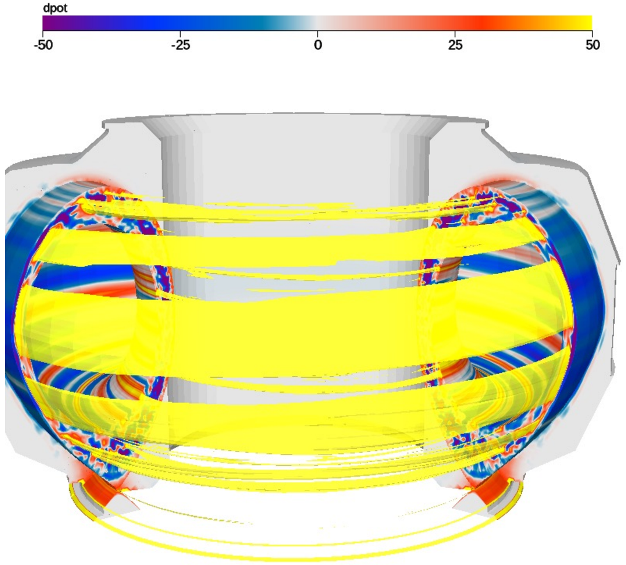
Streamlines depicting possible paths of particles in a laser wakefield.

In Situ Visualization in WDMApp Using VTK-m

- Science Problem
  - The Whole Device Model Application (WDMApp) project aims to develop a high-fidelity model of magnetically confined fusion plasmas, which is needed to plan experiments on ITER and optimize the design of future fusion facilities. One of the core efforts in this project is the development of a framework to couple two advanced and highly scalable gyrokinetic codes: XGC and GENE.
  - Large-scale simulations require real-time feedback on the current state.
- Technical Solution
  - Code coupling is facilitated by EFFIS, which orchestrates the codes and numerous analysis and visualization services. The ECP/VTK-m team incorporated an in situ visualization capability into EFFIS, which provides WDMApp with 3D renderings of the electrostatic potential within the plasma.
- Science Impact
  - These renderings provide near real-time insight to the running codes, as well as for post-run analysis. VTK-m is used for visualization and rendering. ADIOS is used for coupling with the running applications.



Rendering of electrostatic potential and streamer features in the plasma.



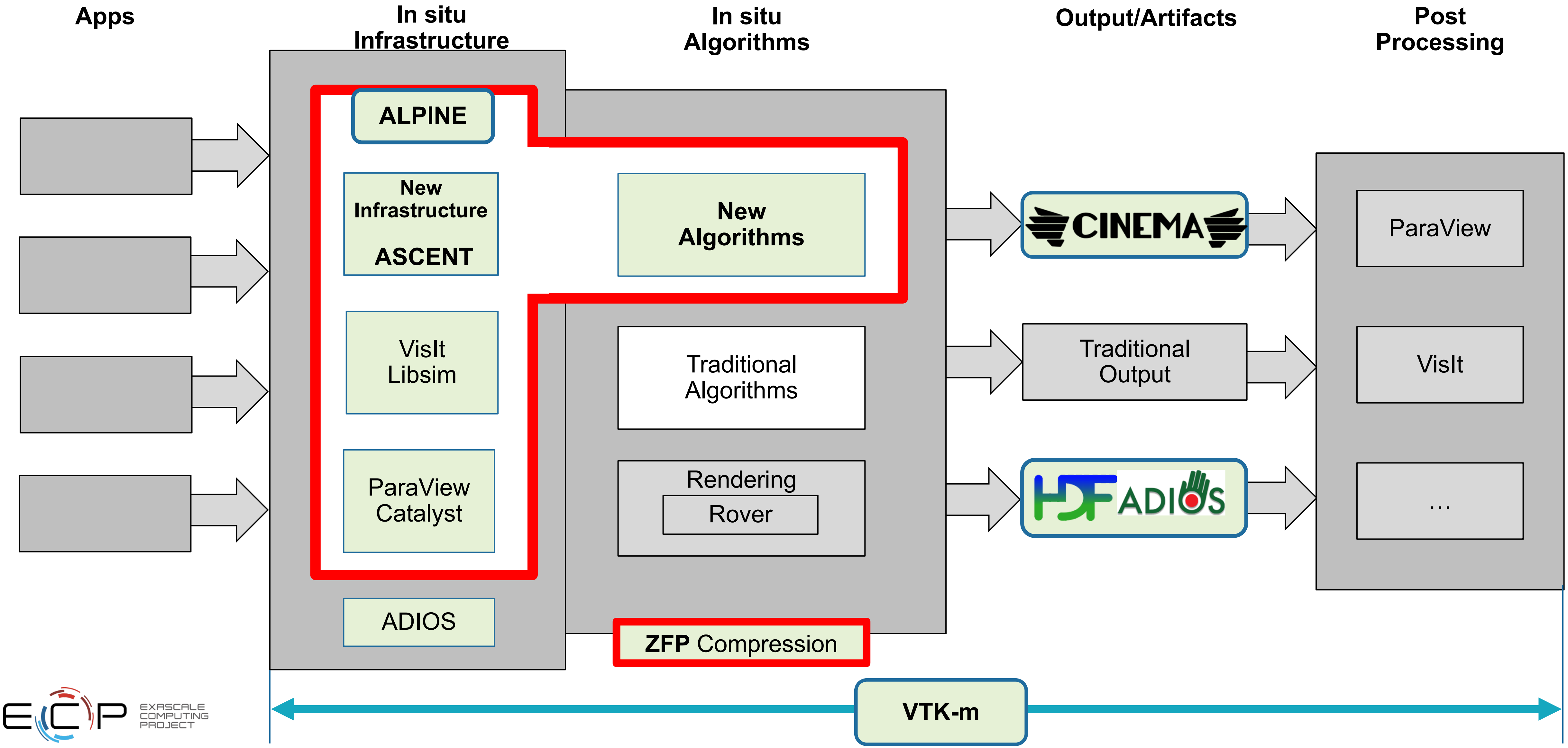
Cuts are made in the plasma to highlight the edge coupling region.

EXASCALE COMPUTING PROJECT
U.S. DEPARTMENT OF ENERGY
OAK RIDGE National Laboratory

How Do I Use VTK-m?

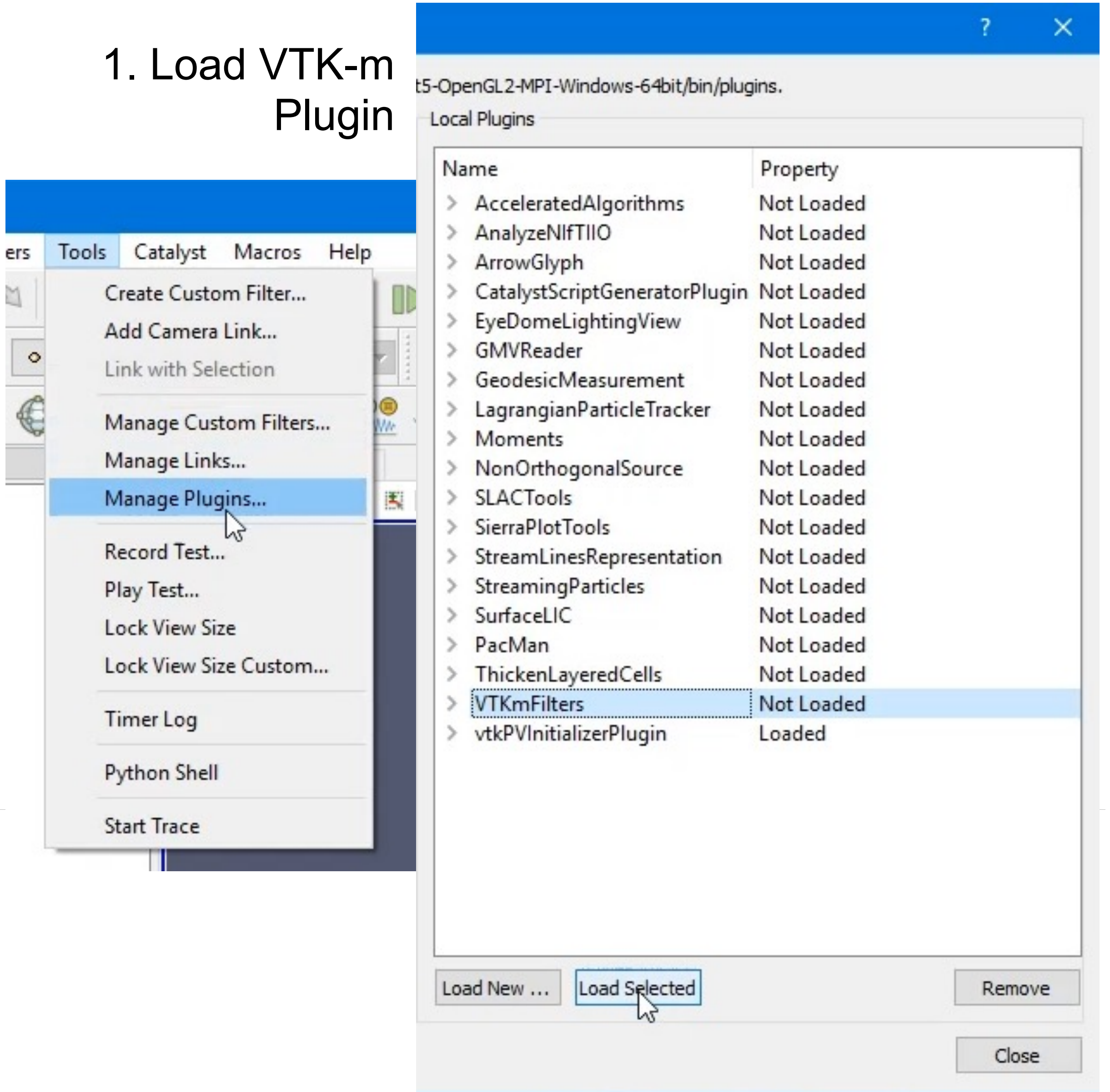
2.3.4.16 ALPINE/ZFP

2.3.4 ECP Data and Visualization products form an integrated workflow

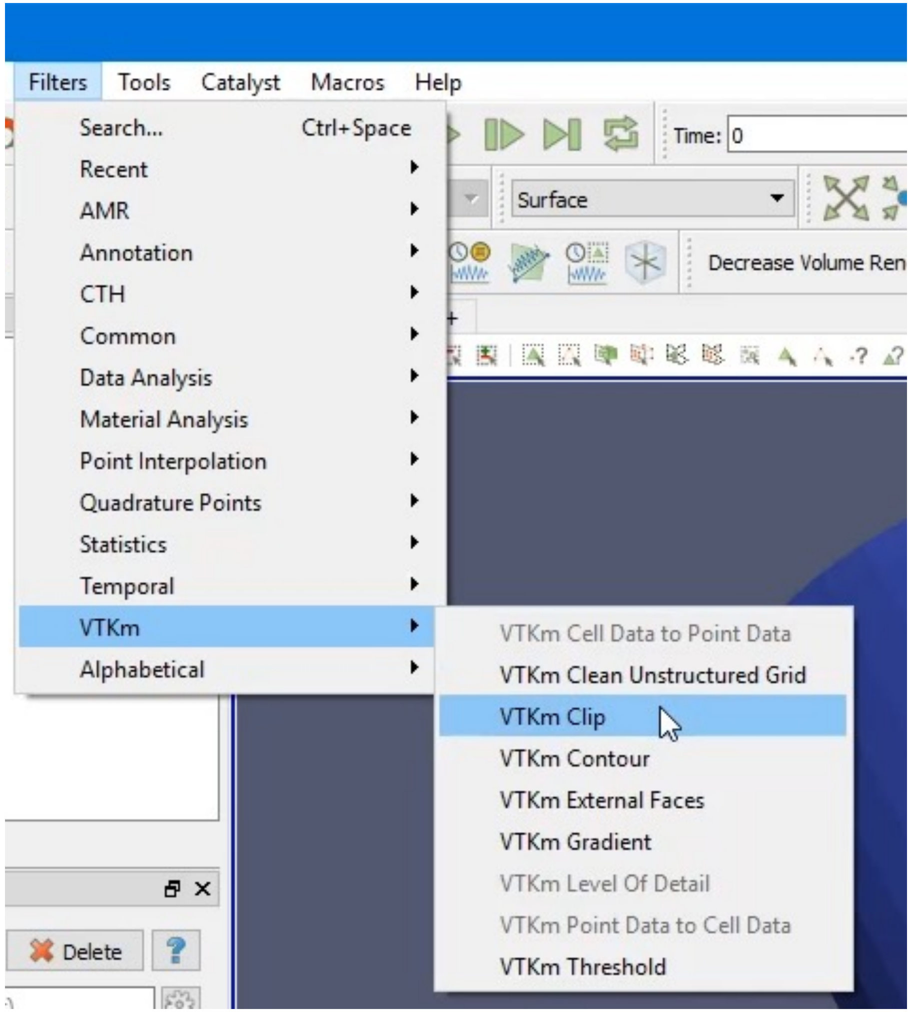


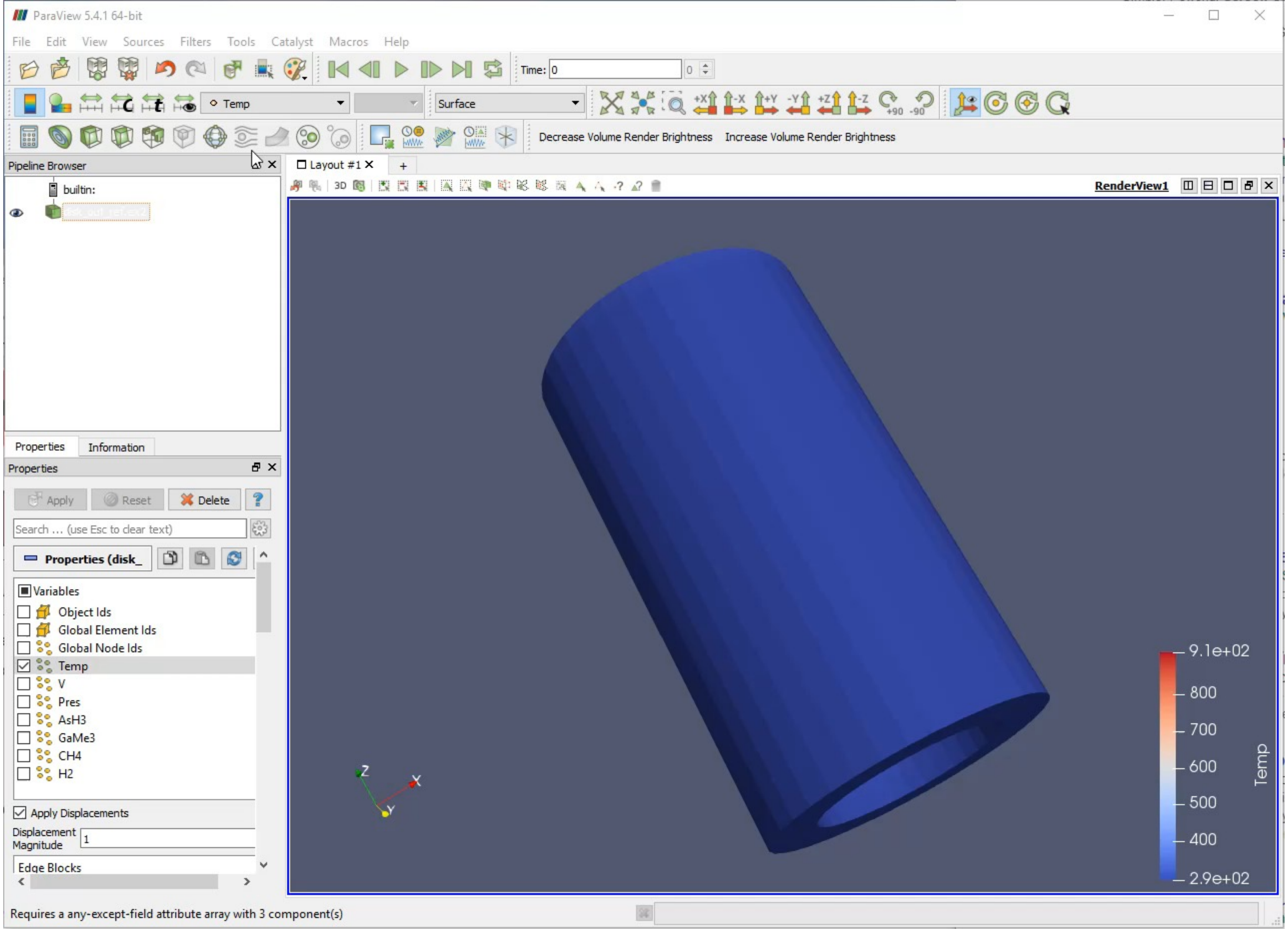
Using VTK-m in ParaView

1. Load VTK-m Plugin



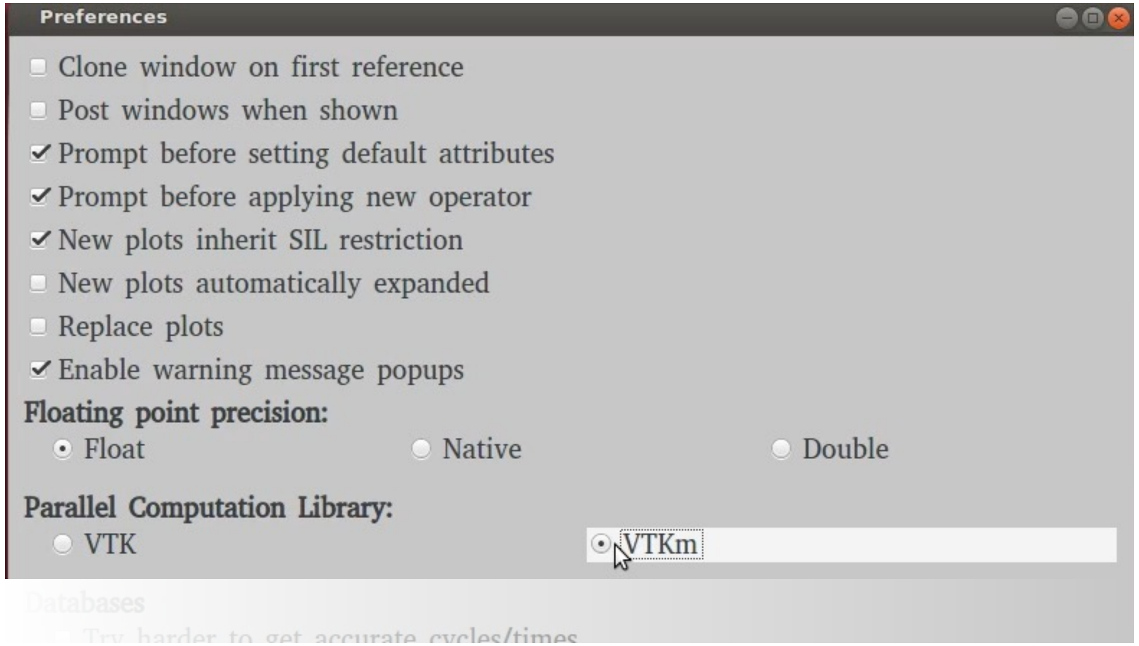
2. Use a VTK-m filter like any other



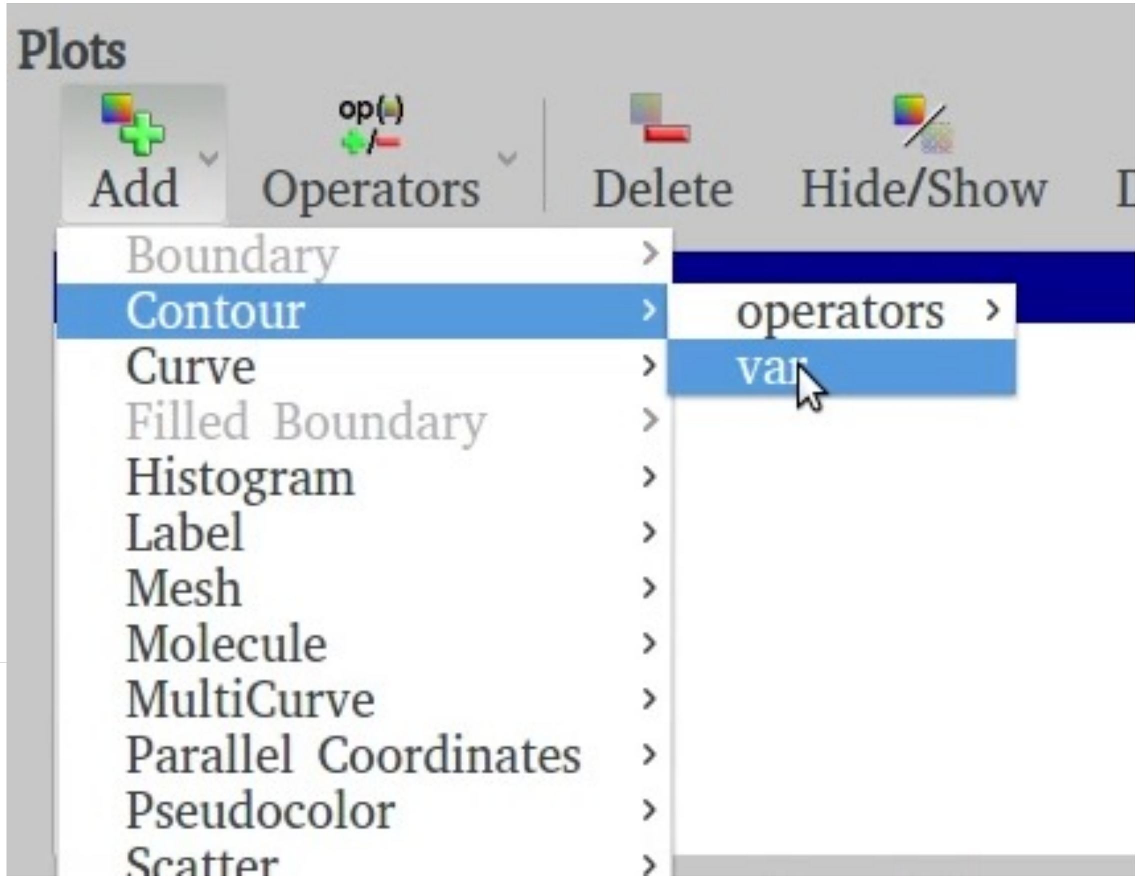

ParaView 5.4.1 64-bit
File
Edit
View
Sources
Filters
Tools
Catalyst
Macros
Help
Time: 0
Temp
Surface
Decrease Volume Render Brightness
Increase Volume Render Brightness
Pipeline Browser
builtin:
Layout #1
RenderView1
3D
Properties
Information
Properties
Apply
Reset
Delete
Search ... (use Esc to clear 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
9.1e+02
800
700
600
500
400
2.9e+02
Temp
Z
X
Y
Requires a any-except-field attribute array with 3 component(s)

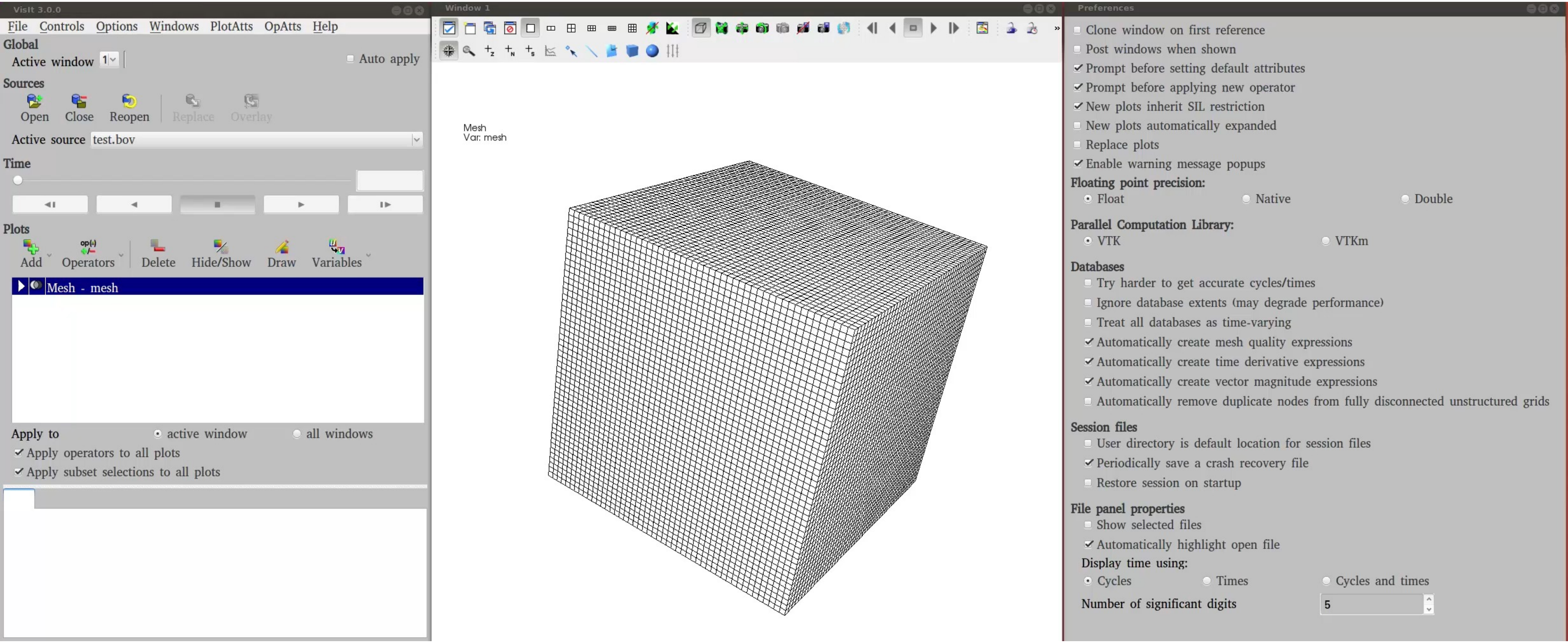
Using VTK-m in VisIt

1. Turn on VTK-m in Preferences



2. Use VTK-m-enabled plots as normal





Slide Credit: David Pugmire

Conclusion

- Let us know what further help you would like
  - Do you want a more focused, more in depth tutorial?
- Let us know how to prioritize our development
  - Is there something in particular you do a lot with ParaView, VisIt, Catalyst, Libsim, ASCENT, etc.?
  - Is there something that seems to be running slower in ParaView, VisIt, Catalyst, Libsim, ASCENT, etc.?
  - Is there functionality missing from ParaView, VisIt, Catalyst, Libsim, ASCENT, etc.?