## Visualization & Data Analysis

<table>
<thead>
<tr>
<th>Time</th>
<th>Title of presentation</th>
<th>Lecturer</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:30 am</td>
<td><strong>Data Analysis and Visualization Introduction</strong></td>
<td>Joe Insley ANL/NIU, Silvio Rizzi ANL, Victor Mateevitsi, ANL</td>
</tr>
<tr>
<td>9:15 am</td>
<td><strong>Scalable Molecular Visualization and Analysis Tools in VMD</strong></td>
<td>Alex Bryer UD</td>
</tr>
<tr>
<td>10:00 am</td>
<td>Break</td>
<td></td>
</tr>
<tr>
<td>10:30 am</td>
<td><strong>Large Scale Visualization with ParaView</strong></td>
<td>Dan Lipsa Kitware</td>
</tr>
<tr>
<td>12:00 pm</td>
<td><strong>Visualization and Analysis of HPC Simulation Data with VisIt</strong></td>
<td>Cyrus Harrison LLNL</td>
</tr>
<tr>
<td>12:30 pm</td>
<td>Lunch</td>
<td></td>
</tr>
<tr>
<td>1:30 pm</td>
<td><strong>Visualization and Analysis of HPC Simulation Data with VisIt (Cont.)</strong></td>
<td>Cyrus Harrison LLNL</td>
</tr>
<tr>
<td>2:30 pm</td>
<td><strong>Vapor</strong></td>
<td>Scott Pearse NCAR</td>
</tr>
<tr>
<td>3:30 pm</td>
<td>Break</td>
<td></td>
</tr>
</tbody>
</table>
| 4:00 pm    | **Exploring Visualization with Jupyter Notebooks**         | • David Koop NIU  
• Cyrus Harrison LLNL |
| 5:30 pm    | **Hands-on**                                               | All                                            |
| 6:30 pm    | **Dinner**                                                 |                                                |
| 7:30 pm    | **After-dinner talk: Growing up at Argonne National Lab**  | Jack Dongarra UT                              |
Here’s the plan...

— Examples of visualizations
— Visualization tools and formats
— Data representations
— Visualization for debugging
— Advanced Rendering
— In Situ Visualization and Analysis
Physics: Stellar Radiation

Data courtesy of: Lars Bildsten and Yan-Fei Jiang, University of California at Santa Barbara
ARTERIAL BLOOD FLOW

Data courtesy of: Amanda Randles, Duke University
Computational Fluid Dynamics

Data courtesy of Rao Kotamarthi, Ramesh Balakrishnan, Aleks Obabko, Argonne National Laboratory
Engineering Technologies: Combustion

Data courtesy of: Saumil Patel, Muhsin Ameen, Sicong Wu, Argonne National Laboratory; Tanmoy Chatterjee, GE Global Research
Materials Science / Molecular

Data courtesy of: Jeff Greeley, Nichols Romero, Argonne National Laboratory

Data courtesy of: Paul Kent, Oak Ridge National Laboratory, Anouar Benali, Argonne National Laboratory

Data courtesy of: Subramanian Sankaranarayanan, Argonne National Laboratory
Visualization Tools and Data Formats
All Sorts of Tools

Visualization Applications
- VisIt
- ParaView
- EnSight

Domain Specific
- VMD, PyMol, Ovito, Vapor

APIs
- VTK: visualization
- ITK: segmentation & registration

Analysis Environments
- Matlab
- Parallel R

Utilities
- GnuPlot
- ImageMagick

Available on Cooley
ParaView & VisIt vs. vtk

ParaView & VisIt
- General purpose visualization applications
- GUI-based
- Client / Server model to support remote visualization
- Scriptable / Extendable
- Built on top of vtk (largely)
- In situ capabilities

vtk
- Programming environment / API
- Additional capabilities, finer control
- Smaller memory footprint
- Requires more expertise (build custom applications)
## Data File Formats (ParaView & VisIt)

<table>
<thead>
<tr>
<th>VTK</th>
<th>PLOT2D</th>
<th>Meta Image</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parallel (partitioned)</td>
<td>PLOT3D</td>
<td>Facet</td>
</tr>
<tr>
<td>VTK</td>
<td>SpyPlot CTH</td>
<td>PNG</td>
</tr>
<tr>
<td>VTK MultiBlock</td>
<td>HDF5 raw image</td>
<td>SAF</td>
</tr>
<tr>
<td></td>
<td>data</td>
<td>LS-Dyna</td>
</tr>
<tr>
<td></td>
<td>DEM</td>
<td>Nek5000</td>
</tr>
<tr>
<td>Legacy VTK</td>
<td>VRML</td>
<td>OVERFLOW</td>
</tr>
<tr>
<td>Parallel (partitioned)</td>
<td>PLY</td>
<td>paraDIS</td>
</tr>
<tr>
<td>legacy VTK</td>
<td>Polygonal Protein</td>
<td>PATRAN</td>
</tr>
<tr>
<td>EnSight files</td>
<td>Data Bank</td>
<td>PFLOTRAN</td>
</tr>
<tr>
<td>EnSight Master</td>
<td>X Mol Molecule</td>
<td>Pixie</td>
</tr>
<tr>
<td>Server</td>
<td>Stereo Lithography</td>
<td>PuReMD</td>
</tr>
<tr>
<td>Exodus</td>
<td>Gaussian Cube</td>
<td>S3D</td>
</tr>
<tr>
<td>BYU</td>
<td>Raw (binary)</td>
<td>SAS</td>
</tr>
<tr>
<td>XDMF</td>
<td>AVS</td>
<td>Tetrad</td>
</tr>
<tr>
<td></td>
<td></td>
<td>UNIC</td>
</tr>
<tr>
<td></td>
<td></td>
<td>VASP</td>
</tr>
<tr>
<td></td>
<td></td>
<td>ZeusMP</td>
</tr>
<tr>
<td></td>
<td></td>
<td>ANALYZE</td>
</tr>
<tr>
<td></td>
<td></td>
<td>BOV</td>
</tr>
<tr>
<td></td>
<td></td>
<td>GMV</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Tecplot</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Vis5D</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Xmdv</td>
</tr>
<tr>
<td></td>
<td></td>
<td>XSF</td>
</tr>
</tbody>
</table>
Data Representations
Data Representations: Cutting Planes

Slice a plane through the data
– Can apply additional visualization methods to resulting plane
VisIt & ParaView & vtk good at this
VMD has similar capabilities for some data formats
Data Representations: Volume Rendering
Data Representations: Contours (Isosurfaces)

A Line (2D) or Surface (3D), representing a constant value

**VisIt & ParaView:**
- good at this

**vtk:**
- same, but again requires more effort
Data Representations: Glyphs

2D or 3D geometric object to represent point data
Location dictated by coordinate
  – 3D location on mesh
  – 2D position in table/graph
Attributes of graphical entity dictated by attributes of data
  – color, size, orientation
Data Representations: Streamlines

From vector field on a mesh (needs connectivity)
– Show the direction an element will travel in at any point in time.
VisIt & ParaView & vtk good at this
Data Representations: Pathlines

From vector field on a mesh (needs connectivity)
– Trace the path an element will travel over time.
VisIt & ParaView & vtk good at this
Data Representations: Pathlines

From vector field on a mesh (needs connectivity)
– Trace the path an element will travel over time.
VisIt & ParaView & vtk good at this
Molecular Dynamics Visualization

VMD:
- Lots of domain-specific representations
- Many different file formats
- Animation
- Scriptable

VisIt & ParaView:
- Limited support for these types of representations, but improving

VTK:
- Anything’s possible if you try hard enough
Visualization for Debugging
Visualization for Debugging
Visualization for Debugging
Visualization as Diagnostics: Color by Thread ID
Advanced Rendering
Intel® oneAPI Rendering Toolkit ("Render Kit"/"Render Framework")
Open Source Software for Advanced Rendering and Visualization

Stellar Radiation
Lars Bildsten (UC Santa Barbara),
Vis: Joe Insley (ANL), Greg Johnson (Intel)

51 M particle “Last Journey” HACC,
Katrin Heitmann (ANL) and Tom Uram (ANL),
Vis: Aaron Knoll (Intel)

Harvey Proxy Simulation
Amanda Randles (Duke University)
Vis: Silvio Rizzi (ANL), David DeMarle (Intel)

Kurth def/ simulation;
Jifu Tan and Michael Hood, (NIU),
Vis: Joe Insley, Silvio Rizzi,
Michael Papka and Janet Knowles, (ANL)

Slide courtesy of Intel Visualization Team
The Science

Internal Combustion Engine Simulation

TCC Engine Apparatus

Fluid Dynamics Simulation
Goal

Provide context to tell the story/explain the science
Integrate production tools into the existing visualization pipeline
Tools used:
- ParaView
- Maya
- Substance Painter
- V-Ray
- Custom scripts and HPC Resources
- ffmpeg
- Premiere/After Effects
THE VISUALIZATION PIPELINE

Overview

Visualization Cluster

ParaView

Export geometry

Convert to VRMESH

v-ray

Transfer VRSCENE

Local Workstation

Transfer a few time steps

Materials

Modeling

Lighting

Export to VRSCENE

Colors
In Situ Visualization and Analysis
Five orders of magnitude between compute and I/O capacity on Titan Cray system at ORNL

Computation 125 PB/s
Node memory 4.5 PB/s
Interconnect 24 TB/s
Storage 1.4 TB/s

Image courtesy Ken Moreland
What are the problems?

• Not enough I/O capacity on current HPC systems, and the trend is getting worse.
• If there’s not enough I/O, you can’t write data to storage, so you can’t analyze it: lost science.
• Energy consumption: it costs a lot of power to write data to disk.
• Opportunity for doing better science (analysis) when have access to full spatiotemporal resolution data.
# In Situ Frameworks and Infrastructures at ALCF

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
<th>Contact person at ATPESC</th>
</tr>
</thead>
<tbody>
<tr>
<td>ALPINE</td>
<td>In Situ algorithms and infrastructure for the Exascale Computing Project</td>
<td>Silvio Rizzi, Cyrus Harrison</td>
</tr>
<tr>
<td>ASCENT</td>
<td>A flyweight in situ visualization and analysis runtime for multi-physics HPC simulations</td>
<td>Cyrus Harrison</td>
</tr>
<tr>
<td>SENSEI</td>
<td>Write once run anywhere. Multiple backends. MxN in transit communication patterns</td>
<td>Silvio Rizzi, Joe Insley</td>
</tr>
<tr>
<td>ParaView/Catalyst</td>
<td><em>In situ</em> use case library, with an adaptable application programming interface (API), that orchestrates the delicate alliance between simulation and analysis and/or visualization tasks</td>
<td>Dan Lipsa</td>
</tr>
<tr>
<td>Libsim</td>
<td>Originally developed to facilitate interactive connections from VisIt to running simulations</td>
<td>Cyrus Harrison</td>
</tr>
<tr>
<td>SmartSim</td>
<td>SmartSim is a software framework that facilitates the convergence of numerical simulations and AI workloads on heterogeneous architectures</td>
<td>Silvio Rizzi</td>
</tr>
</tbody>
</table>
Exascale Computing Project
Software Technology Data and Visualization

Apps

In situ Infrastructure

ALPINE

ASCENT

VisIt Libsim

ParaView Catalyst

In situ Algorithms

New Algorithms

Traditional Algorithms

Compression

ZFP

Output/Artifacts

Cinema

Traditional Output

ParaView

VisIt

Post Processing

Slide courtesy of the ECP ALPINE project
- Flyweight design, minimizes dependencies
- Data model based on Conduit from LLNL
- Vis and analysis algorithms implemented in VTK-m

///
// Run Ascent
///
Ascent ascent;
ascent.open();
ascent.publish(data);
ascent.execute(actions);
ascent.close();
SENSEI: Write once run everywhere

- “Write once, run everywhere” design
- Data model based on VTK from Kitware
- Supports a variety of backends, including ParaView/Catalyst, VisIt/LibSim, ADIOS, Python
- MxN in transit capabilities
The SmartSim open-source library enables scientists, engineers, and researchers to embrace a “data-in-motion” philosophy to accelerate the convergence of AI/data science techniques and HPC simulations.

SmartSim enables simulations to be used as engines within a system, producing data, consumed by other services enable new applications:
- Embed machine learning training and inference with existing in Fortran/C/C++ simulations
- Communicate data between C, C++, Fortran, and Python applications
- Analyze and visualize data streamed from HPC applications while they are running
- Launch, configure, and coordinate complex simulation, analysis, and visualization workflows

All of these can be done without touching the filesystem, i.e. data-in-motion

slide courtesy of the HPE SmartSim team
Infrastructures
VTK-m’s main thrust: a write-once-run-everywhere framework

- Contour
- Streams
- Clip
- Render
- Surface
- Normals
- Ghost Cells
- Warp
- ...
What is Cinema?

- **Cinema** is part of an integrated workflow, providing a method of extracting, saving, analyzing or modifying and viewing complex data artifacts from large scale simulations.
  - If you’re having difficulty exploring the complex results from your simulation, Cinema can help.
- **The Cinema ‘Ecosystem’** is an integrated set of writers, viewers, and algorithms that allow scientists to export, analyze/modify and view Cinema databases.
  - This ecosystem is embodied in widely used tools (*ParaView, VisIt, Ascent*) and the database specification.
In Situ Computational Fluid Dynamics
NekRS

- CFD code
- Simulates turbulent incompressible or low Mach-number flows with heat transfer and species transport.
- Supports heterogeneous platforms
- Legacy code: Nek5000

As the resolution of the simulation increases, scientists turn to performing analysis in situ, doing their analysis while data is still resident in memory. Such capabilities enable study of turbulence statistics at these extremely high resolutions.
NekRS + Ascent

- Data is passed by reference (zero-copy)
  - CPU -> CPU or GPU -> GPU
- Ascent is disabled by default
  - Binary is bit by bit identical with non-instrumented code
- Full functionality of Ascent at your disposal
- Closely working with NekRS team, who are testing the instrumentation and providing feedback
Argonne Leadership Computing Facility

Polaris - 40 ranks

70.103.01 Driver Version: 470.103.01 CUDA Version: 11.4

<table>
<thead>
<tr>
<th>Pers. Ml</th>
<th>Bus-Id</th>
<th>Disp.A</th>
<th>Volatile Uncorr. ECC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wrf Pwr:Usage/Cap</td>
<td>Memory-Usage</td>
<td>GPU-Util</td>
<td>Compute M. MIG M.</td>
</tr>
</tbody>
</table>

- **100-SXM... On**: 00000000:07:00.0 Off
  - P0: 318W / 400W
  - 13934MiB / 40536MiB
  - 93% GPU-Util
  - Default
  - Disabled

- **100-SXM... On**: 00000000:46:00.0 Off
  - P0: 289W / 400W
  - 13928MiB / 40536MiB
  - 95% GPU-Util
  - Default
  - Disabled

- **100-SXM... On**: 00000000:85:00.0 Off
  - P0: 319W / 400W
  - 13952MiB / 40536MiB
  - 90% GPU-Util
  - Default
  - Disabled

- **100-SXM... On**: 00000000:07:00.0 Off
  - P0: 343W / 400W
  - 13952MiB / 40536MiB
  - 90% GPU-Util
  - Default
  - Disabled

### GPU Memory Usage

<table>
<thead>
<tr>
<th>ID</th>
<th>PID</th>
<th>Type</th>
<th>Process name</th>
<th>GPU Memory Usage</th>
</tr>
</thead>
<tbody>
<tr>
<td>V/A</td>
<td>12689</td>
<td>C</td>
<td>-ascent-polaris/bin/nekrs</td>
<td>13931MiB</td>
</tr>
<tr>
<td>V/A</td>
<td>12690</td>
<td>C</td>
<td>-ascent-polaris/bin/nekrs</td>
<td>13925MiB</td>
</tr>
<tr>
<td>V/A</td>
<td>12691</td>
<td>C</td>
<td>-ascent-polaris/bin/nekrs</td>
<td>13949MiB</td>
</tr>
<tr>
<td>V/A</td>
<td>12692</td>
<td>C</td>
<td>-ascent-polaris/bin/nekrs</td>
<td>13949MiB</td>
</tr>
</tbody>
</table>
Next steps…

Bi-directional steering
Visualization Help
support@alcf.anl.gov

Publication Images & Covers

Animations
- SC Visualization Showcase [Best Vis Finalist 2014-2020]
- APS Division of Fluid Dynamics Gallery of Fluid Motion
- SC Gordon Bell Submissions
- Press Releases

In Situ Vis and Analysis
Additional information

ALPINE: https://alpine.dsscale.org/
Ascent: https://github.com/Alpine-DAV/ascent
SENSEI: https://sensei-insitu.org/
SmartSim: https://developer.hpe.com/platform/smartsim/home/
ParaView/Catalyst: https://www.paraview.org/in-situ/
Libsim: https://www.visitusers.org/index.php?title=VisIt-tutorial-in-situ
VTK-m: https://m.vtk.org/
Cinema: https://cinemascience.github.io/
OSPRay: https://github.com/ospray/ospray
QUESTIONS?

Joe Insley
insley@anl.gov

Silvio Rizzi
srizzi@anl.gov

Janet Knowles
jknowles@anl.gov

Victor Mateevitsi
vmateevitsi@anl.gov