Implications of Numerical and Data Intensive Technology Trends on Scientific Visualization and Analysis

James Ahrens
Los Alamos National Laboratory
March 2015 - SIAM CSE
Technology Trends in Numerically and Data Intensive Computing

<table>
<thead>
<tr>
<th>Numerically intensive Trends</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hardware: Exascale challenges and solutions</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Data intensive Trends</th>
</tr>
</thead>
<tbody>
<tr>
<td>Software: Cloud challenges and solutions</td>
</tr>
</tbody>
</table>
Trends for HPC Scientific Visualization and Analysis

Relentless increase in data sizes
3 orders of magnitude every ten years

Adapting to changing infrastructure
Shared memory, clusters, threading, cloud

Advancing the fundamentals
Improved end-to-end workflow and cognitive understanding
How about the user experience?
Responding to the Trends: ParaView

- An open-source, scalable, multi-platform visualization application
- Support for distributed computation models to process large data sets
  - Billions of AMR cells, Scaling test over 1 Trillion cells
- Used by academic, government and commercial institutions worldwide
  - Downloaded ~100K times per year
  - Developed by Kitware, LANL, SNL...
- Originally designed to support a post processing workflow
  - Simulations save data to storage and scientist interactive visualizes results

http://paraview.org
Numerically Intensive Trends: Exascale Computing – The Vision

Achieve order $10^{18}$ operations per second and order $10^{18}$ bytes of storage

Address the next generation of scientific, engineering, and large-data problems

1,000X capabilities of today’s computers with a similar size and power footprint

Set the US on a new trajectory of progress – towards a broad spectrum of computing capabilities over the next decade

Productive system

- Usable by a wide variety of scientists and engineers
- “Easier” to develop software & management of the system

Based on marketable technology

- Not a “one off” system - Scalable, sustainable technology
- Deployed in early 2020s
### Potential Exascale System Architecture

With a cap of $200 M and 20 MW

<table>
<thead>
<tr>
<th>Feature</th>
<th>2013 Titan Computer</th>
<th>2023</th>
<th>Difference 2013 &amp; 2023</th>
</tr>
</thead>
<tbody>
<tr>
<td>System Peak</td>
<td>27 Pflops/s</td>
<td>1 Eflop/s</td>
<td>O(100)</td>
</tr>
<tr>
<td>Power</td>
<td>8.3 MW</td>
<td>20MW</td>
<td>2.5x</td>
</tr>
<tr>
<td>System Memory</td>
<td>0.7 PB</td>
<td>64 PB</td>
<td>O(100)</td>
</tr>
<tr>
<td>Node Performance</td>
<td>1.5 TF/s</td>
<td>15 TF/s</td>
<td>O(10)</td>
</tr>
<tr>
<td>Node Memory BW</td>
<td>0.2 TB/s</td>
<td>4 TB/s</td>
<td>O(10)</td>
</tr>
<tr>
<td>Interconnect BW</td>
<td>0.008 TB/s</td>
<td>0.4TB/s</td>
<td>O(100)</td>
</tr>
<tr>
<td>Number of Nodes</td>
<td>18688</td>
<td>100000</td>
<td>O(10)</td>
</tr>
<tr>
<td>Total concurrency</td>
<td>50M</td>
<td>O(billion)</td>
<td>O(100)</td>
</tr>
</tbody>
</table>

Power is very costly: 1 MW = ~ Million dollars

Without intervention on track to 200MW for Exascale
Data Access Delay

Diagram and Table from "Taming the Power Hungry Data Center", Fusion I/O.
Implication: The traditional post-processing approach is becoming unworkable at extreme scale

- Temporal simulation snapshots are saved at longer intervals
  - Full checkpoints are costly - less temporal data available for analysis

- Rate of improvement of rotating storage is not keeping pace with compute
  - Power, cost and reliability are becoming significant issues
Implication: Transition to an in situ focused approach

- In situ saves **reduced-sized data products** during simulation run
  - Benefits:
    - Save disk space
    - Save time in post-processing analysis
    - Produce higher fidelity results

- **Automatic visualization and analysis** during the simulation run
  - Prioritized by scientist's importance metrics

- Identify specific analysis questions

- Help manage cognitive and storage resource budget
Implication: Significant in situ data reduction

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Reduction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Data parallelism</td>
<td>Handle large datasets</td>
</tr>
<tr>
<td></td>
<td>Make reduction possible</td>
</tr>
<tr>
<td>Multi-resolution</td>
<td>Make focused exploration possible</td>
</tr>
<tr>
<td>Visualization and analysis operators (Isosurface)</td>
<td>A dimension reduction</td>
</tr>
<tr>
<td>Statistical sampling</td>
<td>1-2 orders of magnitude</td>
</tr>
<tr>
<td>Compression</td>
<td>1 order of magnitude</td>
</tr>
<tr>
<td>Feature extraction</td>
<td>2 orders of magnitude</td>
</tr>
</tbody>
</table>
Sampling

Random sampling provides a data representation that is unbiased for statistical estimators, e.g., mean and others.

Since the sampling algorithm is in situ: accuracy metric (simulation data, sampled representation)

Plotting

Red is 0.19% sample data, black is original simulation data

Feature Extraction: Halo Finding

The red, green, and blue curves are 0.19%, 1.6%, and 12.5% samples. The black curve is the original data. Calculate the halo mass function for different sample sizes of $256^3$ particles.
Example: Visual Downsampling

Cosmology visualization in ParaView
In Situ Compression with Quantified Accuracy

- *In situ* compression of simulation data
- Use JPEG 2000 to compress data
- Quantify the maximum/L-infinity norm data quality for scientific analysis

- Measure the maximum point error
- Guarantee accuracy to x decimal places
- Accuracy Metric (Simulation data – Compressed representation)

- User can trade read I/O time vs. data accuracy in a quantifiable manner
Isovalues on Compressed Simulation Data with Bounding Error - (32 bits, 3200x2400x42, 1.4 GB)

- 0.25 bits, 10.8 MB
- 0.5 bits, 21.6 MB
- 1.0 bits, 43.3 MB
- 2.0 bits, 86.5 MB
Implication: Automated Algorithms
Adaptive focus based on selected scientific metrics

- Create adaptive analysis-based grid
  - Histogram at each grid element
    - Across all axes (spatial, value, multivariate)
- Use for spatial, temporal selection
  - Cameras, storage, feature identification
Sampling Using Analysis Driven Refinement (ADR)

- Recursive metric-based refinement
- Multidimensional

Sampling in Time

Sampling in Space
Data Intensive Trends: Cloud Computing

The NIST Definition

- A model for enabling ubiquitous, convenient, on-demand network access to:
  - a shared pool of configurable computing parallel resources (e.g., networks, servers, storage, applications, and services)
  - rapidly provisioned and released with minimal interaction

The NIST Definition of Cloud Computing

Essential Characteristics

- On-demand self-service
- Resource pooling / Multi-tenancy (multiple jobs)
  - Virtualization
- Rapid elasticity
  - Scale rapidly commensurate with demand
- Measured service / Cost model
  - Resource usage is automatically monitored, controlled, and reported, providing transparency
The NIST Definition of Cloud Computing

Essential Characteristics

- Levels of cloud service
  - Infrastructure
  - Application

- Private cloud is an option...
<table>
<thead>
<tr>
<th>Axis</th>
<th>Sub-axis</th>
<th>Numerically Intensive</th>
<th>Data Intensive</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hardware</td>
<td>Nodes and Interconnect</td>
<td>High performance and power</td>
<td>Lower performance and power</td>
</tr>
<tr>
<td></td>
<td>Storage</td>
<td>Separate, independent</td>
<td>Integrated</td>
</tr>
<tr>
<td></td>
<td>SW</td>
<td>Synchronization</td>
<td>Tightly coupled</td>
</tr>
<tr>
<td></td>
<td>Reliability</td>
<td>Checkpoint restart</td>
<td>Replication</td>
</tr>
<tr>
<td>Workload</td>
<td>Number of Users</td>
<td>Single per node</td>
<td>Multiple per node</td>
</tr>
<tr>
<td></td>
<td>Data</td>
<td>Dynamic, heterogeneous (unstructured grid)</td>
<td>Static, homogeneous (text, images)</td>
</tr>
<tr>
<td></td>
<td>Algorithms</td>
<td>Global</td>
<td>Distributed</td>
</tr>
<tr>
<td></td>
<td>User Interface</td>
<td>Complex Application</td>
<td>Simple Web</td>
</tr>
<tr>
<td></td>
<td>Data Model</td>
<td>Files</td>
<td>Database</td>
</tr>
<tr>
<td></td>
<td>Workflow</td>
<td>Scheduling</td>
<td>Batch</td>
</tr>
<tr>
<td></td>
<td>Analysis</td>
<td>Offline post-processing</td>
<td>Online</td>
</tr>
</tbody>
</table>
Implications of Cloud Computing on HPC Visualization and Analysis

Multi-billion dollar market
- Leverage, collaborate and support

Virtual machine (VM) encapsulates a simulation with defined inputs/outputs

- Cloud infrastructure services require VM
  - Provenance - full lineage of data/process/environment
  - Resilience – follows from provenance
  - Data compression – VM and input deck instead of data
  - To do: Reduced VM size and VM composition
Implications of Cloud Computing on HPC Visualization and Analysis

Data-oriented applications
As an approach to massive data

- Beyond Map-Reduce
  - Environments – Spark
  - Scalable databases – Impala, MongoDB
  - Data analytics products

User/task-centric applications

- Cloud enables mobile/web
- Focus on usability and simplicity
Inspiration: Image Database Approach Cinema

Challenge
In situ is a batch process
Concern that exploratory aspect of analysis will be lost

Idea
Store many images that sample the visualization parameter space
In less than the space needed for a single scientific data dump
Ex: Cameras, operations, parameters

Create an image database from in situ analysis
Post-processing exploration of image database

<table>
<thead>
<tr>
<th></th>
<th>Mega</th>
<th>Giga</th>
<th>Tera</th>
<th>Peta</th>
<th>Exa</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$10^{6}$</td>
<td>$10^{9}$</td>
<td>$10^{12}$</td>
<td>$10^{15}$</td>
<td>$10^{18}$</td>
</tr>
<tr>
<td>Image</td>
<td>speed</td>
<td>Storage &amp;</td>
<td>Operations</td>
<td>Operations</td>
<td>Operations</td>
</tr>
<tr>
<td></td>
<td></td>
<td>network</td>
<td>speed</td>
<td>speed</td>
<td>speed</td>
</tr>
<tr>
<td>speed</td>
<td></td>
<td>speed</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Cinema Workflow

1. Simulation Code Run with In Situ Script
2. Image Database
3. Use Case 1 - Traditional Interactive Visualization
4. Use Case 2 - Image Database Exploration

Setup/Data Reduction In Situ Script
Setup / Data Reduction Phase

Setup / Data Reduction

In Situ Script

1

Simulation Code
Run with In Situ Script

- Interactively create or reuse a visualization pipeline
- Contains all operations
- Specifies information needed to generate images for the database
Setup / Data Reduction Phase

Upload visualization pipeline state

- Pipeline
  - Earth core
    - Color by
      - Option: 0.25 61
  - Simulation data
    - Simulation parameters
      - Simulation timesteps: ...
      - Output frequency: ...
  - CellDataToPointData
    - Contour
      - Parameters
        - Contour by
          - Option: Temperature, Salinity
        - Contour values
          - Option: 0.0, 0.5, 1.0, 1.5, 2.0
      - Color by
        - Option: Temperature, Salinity

Set camera and operator parameters to visualize
Example Script
For each (Time Step)
For each (Operator)
For each (Value)
For each (Camera Position)
Generate Image
Use Case 1 – Traditional interactive exploration

In all videos in this presentation:
Processing, combining and showing images from the image database
No raw scientific data is read, no geometry is created during viewing
Use Case 1 – Traditional interactive exploration

In all videos in this presentation:
Processing, combining and showing images from the image database
new scientific data is read, no geometry is created during viewing
Use Case 2 - Image database exploration

Query: theta = 90, phi = 45, time = 50

Sort by: contourIdx

Found 9 results.

contourIdx: [1 to 10 % 1]
phi: [0 to 345 % 15]
surfaceContour: [temperature, salinity]
theta: [30 to 150] % 30

time: [0 to 102] % 1

Traditional key-value pair queries
Keys: Camera (phi, theta), time, operator parameters
Use Case 2 – Image database exploration
Image-based approach reduces analysis exploration bias

- **Traditional post-processing approach**
  - Generate visualization and analysis result upon user request
  - User wait time is extremely variable
    - Rendering (seconds)
    - File system accesses (minutes)
  - Creates inherent bias in what is explored
    - For example: little significant interactive temporal analysis

- For an image-based approach
  - All "operations" take the same amount of time
    - Reduces bias of what get explored
Use Case 3 – Creation of new visualizations

- Use real time image compositing to build new pipelines
- Image representation: Color & depth buffer
- Multitude of combinations/visualizations possible
Use Case 3 – Creation of new visualizations

- Scientists can quickly create “arbitrary” pipelines to answer their analysis questions
Use Case 2 & 3 - Content based image search

- What image in the database contains the “best” view of a collection of visualization objects?
- Each image/pixel contains a list of the order/visibility of the objects for each view
- Pixel coverage is calculated for all views and objects
Use Case 2 & 3 – Content-based image search

- Light dust
- Dust
- Ground
- Deep ground
- Asteroid
- Pressure wave
- Slice X
- Slice Z
- Background

Compute pixel coverage: 17

Found 3072 results.

Query:
- time: 14
  phi: 180.0
  theta: 105.0
  Deep ground: 9.78%
  Asteroid: 2.91%
  Pressure wave: 1.55%
  Slice Z: 15.72%

Sort by:
- time: 13
  phi: 180.0
  theta: 105.0
  Deep ground: 9.74%
  Asteroid: 2.74%
  Pressure wave: 1.60%
  Slice Z: 15.83%

- time: 15
  phi: 180.0
  theta: 105.0
  Deep ground: 9.82%
  Asteroid: 3.06%
  Pressure wave: 1.49%
  Slice Z: 15.83%

+900 lines later

- time: 2
  phi: 270.0
  theta: 75.0
  Deep ground: 13.18%
  Asteroid: 0.12%

- time: 12
  phi: 270.0
  theta: 45.0
  Deep ground: 33.92%
  Asteroid: 0.11%
  Pressure wave: 0.10%
  Slice Z: 5.00%

- time: 3
  phi: 270.0
  theta: 75.0
  Deep ground: 13.18%
  Asteroid: 0.10%
  Pressure wave: 0.01%
- Databases
  - Plasma Code /Intel Ray tracer, MPAS/Cinema in-situ, HACC Cosmology data
- Code examples
  - Coupled MPAS/Cinema to create new databases

http://datascience.lanl.gov/Cinema.html
Weak Scaling of XRage Simulation and In Situ Analysis

In situ analysis of 10 contour objects and background Image size of 500x500

Summary: Scalable in situ performance to generate database
Disk usage reduction
Full XRage data files versus in situ

Summary: Orders of magnitude data saving with Cinema approach
Conclusions

- Next steps: http://datascience.lanl.gov

- In situ workflows are required for exascale
  - Benefits over traditional post-processing approach
  - Sampling is key

- Reduced simulation data approach
  - Error quantification is possible

- Image database approach
  - Offering unique interactive exploration options
    - Database search

Acknowledgements - This work was funded by Dr. Lucy Nowell, Program Manager for the Advanced Scientific Computing Research (ASCR) program office in the Department of Energy’s (DOE) Office of Science and Thuc Hoang, Program Manager, DOE NNSA.
Questions

Select a run from the Run menu in the header bar.

HACC Cosmo Cinema Volume Visualization