Near real-time processing of scientific data

WoNDP: 3rd workshop on near-data processing
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Outline

• Motivation
• Our contributions
• Examples
• SIRIUS: Next generation Multi-tier storage and I/O system
• Closing thoughts

Disclaimer: I do NOT pay much attention to hardware....
Where do we spend our time in science

• Goals
  • Accelerate this process
  • Make the process **predictable**
  • Make the process **adaptable**
  • Make the process **scalable** as the complexity increases
  • Make the software **easy-to-use**

• Observation
  • Most of the time is spent in managing, moving, storing, retrieving, and turning the science data into **knowledge**
Vision: Enable Rapid Collaborative Decision Making

• Vision: Enable distributed, collaborative, real-time decisions
  • Workflows including both experiments and simulations
  • Reduce cost, improve utilization of expensive experimental devices

• Metrics of Success:
  • Reduction of time to make a “good” decision, across the entire scientific process
  • Adoption of technology by “important users”
How to Enable Rapid Decision Making

• Effective data management
  • Easily express data accesses: high-level data model instead of offsets into files
  • Transparent accesses to remote data
  • Convenient querying operations

• Effective workflow management
  • Tight integration of workflow components to reduce latency
  • Make the best uses of known resources

• Reduce the time to solution
  • Streaming data accesses, avoid waiting for all data before analysis could start
  • Only access the necessary data records (selective data accesses)
  • Keep the data in memory as much as possible
Example: Fusion Experiments

• Complex DOE experiments, such as a fusion reactor, contain numerous diagnostics that need **Near-Real-Time analysis for feedback to the experiment**
  • For guiding the experiment
  • For faster and better understanding of the data

• Current techniques to write, read, transfer, and analyze “files” require a long time to produce an answer
  • Long delay due to slow disks involved to store and retrieve files
  • Slow start up of many workflow execution engines
Big Data in Fusion Science: ITER example

- **Volume**: Initially 90 TB per day, 18 PB per year, maturing to 2.2 PB per day, 440 PB per year
- **Value**: All data are taken from expensive instruments for valuable reasons.
- **Velocity**: Peak 50 GB/s, with near real-time analysis needs
- **Variety**: ~100 different types of instruments and sensors, numbering in the thousands, producing interdependent data in various formats
- **Veracity**: The quality of the data can vary greatly depending upon the instruments and sensors.

The pre-ITER superconducting fusion experiments outside of US will also produce increasingly bigger data (KSTAR, EAST, Wendelstein 7-X, and JT60-SU later).
Validation Laboratories

• **Goal**
  • Create a framework which can allow scientists to fuse experimental and computational data to aid in the validation process, transitioning this from an Art to a Science

• **Research Challenges**
  • Encapsulate sufficient semantic information in a workflow language to allow global optimizations to be performed
  • Scheduling across heterogeneous resources (memory, cores, systems, networks)
  • Fusion of data in an automated workflow
  • Ensemble comparison using comparative analytics
  • Extract relationships of experimental and simulation data

• **Metrics of Success**
  • Increasing the number of users who manually validate their data to automated workflows, decreasing their time in “baby-sitting”
  • Accuracy of data mining for discovery of correlations to aid validation
Synthetic Diagnostics

• Enables direct comparison of simulation results to experiment

• Example of beam emission spectroscopy (BES) using XGC1 simulation data
Example ITER workflow: Anomaly detection, analysis, and feedback

Hot spots detected & analyzed!!

Remote scientist

Image processing, anomaly detection, and near-real-time prediction at remote compute center

ICEE WAN data transfer

~600MB/s

( Resource management) offload compute depending on availability

Move the plasma gap 2cm inward

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Our Approach

• Create an I/O abstraction layer for
  • Writing data quickly on exa, peta, tera, giga scale resources transparently
  • Streaming data on these resources, and across the world

• Place different parts of a workflow at different locations
  • Move work to data whenever possible

• Research new techniques for quickly indexing data to reduce the amount of information moved in the experimental workflow
  • Prioritize data

• Create new techniques to identify important features, which turn the workflow into a data-driven streaming workflow
**ADIOS**

- An I/O abstraction framework
- Provides portable, fast, scalable, easy-to-use, metadata rich output
- Choose the I/O method at runtime
- Abstracts the API from the method
- Need to provide solutions for “90% of the applications”

- Astrophysics
- Climate
- Combustion
- CFD
- Environmental Science
- Fusion
- Geoscience
- Materials Science
- Medical:
- Pathology
- Neutron Science
- Nuclear Science
- Quantum
- Turbulence
- Relativity
- Seismology
- Sub-surface modeling
- Weather

http://www.nccs.gov/user-support/center-projects/adios/
The ADIOS-BP Stream/File format

- All data chunks are from a single producer
  - MPI process, Single diagnostic
- Ability to create a separate metadata file when “sub-files” are generated
- Allows variables to be individually compressed
- Has a schema to introspect the information
- Has workflows embedded into the data streams
- Format is for “data-in-motion” and “data-at-rest”

Ensemble of chunks = file
• Use compute and deep-memory hierarchies to optimize overall workflow for power vs. performance tradeoffs
• Abstract complex/deep memory hierarchy access
• Placement of analysis and visualization tasks in a complex system
• Impact of network data movement compared to memory movement
DataSpaces – Rutgers

Coupled Scientific Workflow Applications

Programming Abstraction
- Coordination & Data Sharing
- Scalable Messaging
- Mapping & Scheduling

Distributed In-memory Object Store
- DART Communication Layer (Cray Gemini, Cray Portals, Infiniband, IBM DCMF, TCP/IP)

The DataSpaces Abstraction

- Virtual shared-space programming abstraction
  - Simple API for coordination, interaction and messaging
  - Distributed, associative, in-memory object store
  - Online data indexing, flexible querying

- Adaptive cross-layer runtime management
  - Hybrid in-situ/in-transit execution
  - Efficient, high-throughput/low-latency asynchronous

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Data Movement methods

- **ICEE**
- Using EVPath package (GATech)
- Support uniform network interface for TCP/IP and RDMA
- Easy to build an overlay network

- **Dataspaces (with sockets)**
  - Developed by Rutgers
  - Support TCP/IP and RDMA
  - Select only areas of interest and send (e.g., blobs)
  - Reduce payload on average by about 5X
Features

- ADIOS provides an overlay network to share data and give feedbacks
- Stream data processing – supports stream-based IO to process pulse data
- In transit processing – provides remote memory-to-memory mapping between data source (data generator) and client (data consumer)
- Indexing and querying with FastBit technology
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ICEE, Enabling International Collaborations

Example: KSTAR ECEI Sample Workflow (Electron cyclotron emission)

- **Objective**: To enable remote scientists to study ECE-Image movies of blobby turbulence and instabilities between experimental shots in near real-time.

- **Input**: Raw ECEi voltage data (~550MB/s, over 300 seconds in the future) + Metadata (experimental setting)

- **Requirement**: Data transfer, processing, and feedback within <15min (inter-shot time)

- **Implementation**: distributed data processing with ADIOS ICEE method
Index-and-Query Reduces Execution Time

- Remote file copy VS. index-and-query
  - Measured between LBL and ORNL to simulate KSTAR-LBL-ORNL connection
  - Indexed by FastBit. Observed a linear performance (i.e., indexing cost increased by data size) ➔ Expensive indexing cost
  - However, once we have index built, index-and-query can be a better choice over remote file copy
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Compute-Data Gap

- Data storage and management will be limiting factor for exascale and beyond
- New research into utilizing computation to fill in data gap
- Scientific data can be modelled and refactored
  - Exploit structure to optimize data storage and processing
  - Split data into blocks with varying precision
  - Remember how data was originally created to regenerate on demand
## Next Generation DOE Computing

<table>
<thead>
<tr>
<th>System attributes</th>
<th>NERSC Now</th>
<th>OLCF Now</th>
<th>ALCF Now</th>
<th>NERSC Upgrade</th>
<th>OLCF Upgrade</th>
<th>ALCF Upgrades</th>
</tr>
</thead>
<tbody>
<tr>
<td>Name Planned Installation</td>
<td>Edison</td>
<td>TITAN</td>
<td>MIRA</td>
<td>Cori 2016</td>
<td>Summit 2017-2018</td>
<td>Theta 2016</td>
</tr>
<tr>
<td>System peak (PF)</td>
<td>2.6</td>
<td>27</td>
<td>10</td>
<td>&gt; 30</td>
<td>150</td>
<td>&gt;8.5</td>
</tr>
<tr>
<td>Peak Power (MW)</td>
<td>2</td>
<td>9</td>
<td>4.8</td>
<td>&lt; 3.7</td>
<td>10</td>
<td>1.7</td>
</tr>
<tr>
<td>Total system memory</td>
<td>357 TB</td>
<td>710 TB</td>
<td>768 TB</td>
<td>~1 PB DDR4 + High Bandwidth Memory (HBM) + 1.5PB persistent memory</td>
<td>&gt;1.74 PB DDR4 + 2.8 PB persistent memory</td>
<td>&gt;480 TB DDR4 + High Bandwidth Memory (HBM)</td>
</tr>
<tr>
<td>Node performance (TF)</td>
<td>0.460</td>
<td>1.452</td>
<td>0.204</td>
<td>&gt; 3</td>
<td>&gt; 40</td>
<td>&gt; 3</td>
</tr>
<tr>
<td>Node processors</td>
<td>Intel Ivy Bridge</td>
<td>AMD Opteron</td>
<td>Nvidia Kepler</td>
<td>64-bit PowerPC A2</td>
<td>Intel Knights Landing many core CPUs Intel Haswell CPU in data partition</td>
<td>Multiple IBM Power9 CPUs &amp; multiple Nvidia Voltas GPUs</td>
</tr>
<tr>
<td>System size (nodes)</td>
<td>5,600 nodes</td>
<td>18,888 nodes</td>
<td>49,152</td>
<td>9,300 nodes, 1,900 nodes in data partition</td>
<td>~3,500 nodes</td>
<td>&gt;2,500 nodes</td>
</tr>
<tr>
<td>System Interconnect</td>
<td>Aries</td>
<td>Gemini</td>
<td>5D Torus</td>
<td>Aries</td>
<td>Dual Rail EDR-IB</td>
<td>Aries</td>
</tr>
<tr>
<td>File System</td>
<td>7.6 PB 168 GB/s, Lustre®</td>
<td>32 PB 1 TB/s, Lustre®</td>
<td>26 PB 300 GB/s GPFS™</td>
<td>28 PB 744 GB/s Lustre®</td>
<td>120 PB 1 TB/s Lustre®</td>
<td>10PB, 210 GB/s Lustre initial</td>
</tr>
</tbody>
</table>
Abstractions across File System to DB

- RAM
- NVRAM
- Remote NVRAM
- Parallel Storage System
- Campaign Storage
- Tape (HPSS)

Evolution of Data to Information

Typical FS workload

Typical DB workload

Data Size (MB)

R/W Ratio

Time (days)

250 M Files on the Atlas File System

- > 1 GB: 1%
- 512 MB: 8%
- 16 MB: 6%
- 4 MB: 7%
- 1 MB: 3%
- < 1 MB: 75%
AUDITOR: New techniques for “Data Intensive Science”

AUDITOR: An additional “simulation” whose purpose is to monitor the fine scale simulation and initiate appropriate actions when anomalies are detected.

Examples
- Trigger a: checkpoint, roll-back, local change in a function, ...
- Not confined to stability issues because it will always reset
- Can allow data regeneration cheaply

Basic quantities in Information Theory
- Data stream $S$ and for $x \in S$ let $P_r(X=x) = p_x \in [0,1]$
- Shannon Information Content: $h(x) = - \log_2 p_x$
- Entropy $H(S) = - \sum p_x \log_2 p_x$
- Noisy/random data has HIGH ENTROPY
Current practices of today

• Want to write data every \(n\)th timestep
  • Because of the Storage and I/O requirements users are forced to writing less

• Common practice is to write data at every \(m\)th timestep, stride = \(M\)

• If the users reconstruct their data, \(u(t)\), at the \(n\)th timestep, they need to interpolate between the neighboring timesteps
  • \(\Phi_M(u)\) = interpolant on coarser grid (stride \(M\)), reduce storage my \(1/M\)

• Assume (\(C=\text{constant depending on the complexity of the data}\))
  • Original storage cost = 32*N bits (floats)
  • New storage cost = 32*N/M bits + \{ 23 – \log_2 (C M^2 Δt^2)\}N
  • Ratio = \((1/M – 1/16 \log_2 M) – 1/16 \log_2 Δt + \text{constant}\)
Compression with an interpolation auditor

• Linear interpolation (LA) is the auditor
• If we look at 10MB output, with a stride of 5
  • Total output = 50MB for 5 steps
  • 10 MB, if we output 1 step, 43MB “typical lossless compression”, 18MB, using linear auditing but lossless
• Investigating adaptive techniques

<table>
<thead>
<tr>
<th>Stride</th>
<th>1 step (MB)</th>
<th>lossless compression (MB)</th>
<th>Linear Audit (MB)</th>
<th>Total Data in 50 steps, typical compression</th>
<th>Total data in 50 steps in LA</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>10</td>
<td>43</td>
<td>18</td>
<td>430</td>
<td>180</td>
</tr>
<tr>
<td>10</td>
<td>10</td>
<td>85</td>
<td>25</td>
<td>850</td>
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<tr>
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<td>10</td>
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<td>40</td>
<td>1700</td>
<td>100</td>
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<tr>
<td>50</td>
<td>10</td>
<td>425</td>
<td>100</td>
<td>4250</td>
<td>100</td>
</tr>
</tbody>
</table>
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Lessons Learned

• Velocity
  • Critical to quickly build an index which can be done in a timely fashion

• Veracity
  • Understand the trade-offs for accuracy (of the query) vs. accuracy of the results vs. performance (time to solution).

• Volume
  • Reduce the volume of data being moved and processed over the WAN (size vs. accuracy)

• Variety
  • Enable multiple streams of data to be analyzed together

• Value
  • Provide the freedom for scientists to access and analyze their data interactively
Next steps

• **Zetascale** computing will usher a new age of computing

• Knowledge discovery in the validation process will become the overarching theme of scientific computing
  • Design of computation
  • Design of experiments

• Data Movement is the costly factor (you know this)

• Too many cores ....
  • Tradeoff between more cores and specialized accelerators

• Move from the “Big Data” age to the knowledge discover age
  • Move, process, only what’s necessary
Questions