Extreme Data Management Analysis and Visualization for Exascale Supercomputers

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Center for Extreme Data Management, Analysis, and Visualization

- 10 Faculty + scientists, developers, students, ...
- Primary partners: UU & PNNL
- Other partnerships: NSA, INL, LLNL, ANL, Battelle, ...
- Involvement in national Initiatives

$1.6B NSA data center (1.5 million-square-foot facility)
Massive Simulation and Sensing Devices Generate Great Challenges and Opportunities

- BlueGene/Q
- Satellite
- Earth Images
- Carbon Seq. (Subsurface)
- Hydrodynamic Inst.
- Retinal Connectome
- Molecular Dynamics
- Porous Materials
- Turbulent Combustion
- Cameras
- Titan
- Climate
- Photography
Lithium-Ion Battery
KAUST PowerWall: Fully Operational in a Few of Hours Steaming from Shaheen
We scaling of data movement infrastructure based on most advanced technology available

Live demonstration at SC14:
• ~4TB per time step (100s of PF 3D timesteps) steaming live from ANL visualization cluster Tukey
• Also steaming live from:
  • KAUST supercomputer Shaheen
  • Uintah simulation executed on CHPC clusters via Remus
  • LLNL server of climate data

Infrastructure that scales gracefully with available hardware resources
A Science Cyberinfrastructure Requires Efficient Big Data Management and Processing

• **Advanced data storage techniques:**
  - Data re-organization.
  - Compression.

• **Advanced algorithmic techniques:**
  - Streaming.
  - Progressive multi-resolution.
  - Out of core computations.

• **Scalability across a wide range of running conditions:**
  - From laptop, to office desktop, to cluster of PC, to BG/L.
  - Memory, to disk, to remote data access.
We Redesigned the Data Management and Visualization Pipeline with New Principles

- Basic core techniques:
  - Slicing, Volume rendering, Iso-surfaces
  - Topology
  - Statistics
- **Cache-oblivious** out-of-core processing optimizing access locality for any size of data blocks
- Pipelines of **progressive algorithms**
- **Coarse-to-fine** construction of multi-resolution models
- **Remote data streaming**
We Consider the Three Main Components Defining a Computing Infrastructure

Processing Network
(Data Access Path)

Data Layout
(Cache Oblivious)

Algorithm Design
(Progressive Processing)
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- Processing Network (Data Access Path)
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REMOTE DATA ACCESS AND ACQUISITION

MEDIUM AND LONG TERM STORAGE

VISUALIZATION

LOCAL FEEDBACK

FEEDBACK LINES

Algorithm Design

(Progressive Processing)
We Characterize Algorithmic Classes Based on Effect in a Processing Network

1. Standard data access (bricks, slices, row-major, …)
2. Linear Streaming
3. Guided Streaming
4. Progressive Streaming
5. Adaptive Progressive Streaming

Cache oblivious raw data access

- main memory
- local disk
- remote data

Data Layout (Cache Oblivious)
Order of Computation: Data vs Useful Information

Comparison of Convergence of Loop Orderings
Temporal Average - 3 month hourly data

Error of Output vs Quantity of Input

Iteration

linear rmse  lb rmse  rb rmse
Data Encoding: Incremental Data Decoding

Bit ordering (2D slice Miranda density field)

Ideal Upper Bound
Possible Encoding Schemes With Difference Performance Characteristics

Quality of Output vs. Quantity of Input

Quality of Output (PSNR) vs. Number of bits

by levels
by bit planes
static optimal
adaptive levels
adaptive levels (per bit plane)
greedy cut
dynamic optimal
Super Slow, High Quality Encoding/Decoding

Original Data → Stored Data → Reconstructed Data

Data Reduction → Data Reconstruction
ViSUS Remote climate Data Analysis and Visualization

- ViSUS data streams allow to merging multiple datasets in real time
- Time interpolation of and concurrent visualization of climate data ensembles defined on different time scales
- Server side and client side computation of statistical functions such as median, average, standard deviation, ……

Standard Deviation and Average of ten climate models
ViSUS Remote climate Data Analysis and Visualization

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High Performance Data Movements for Real-Time Monitoring of Large Scale Simulations

Scale simulation dumps to 130K cores with better performance than state of the art libraries while enabling real-time, remote visualization.

[SC12a] Efficient Data Restructuring and Aggregation for IO Acceleration in PIDX
High Performance Data Movements for Real-Time Monitoring of Large Scale Simulations

- 6 Terabytes per timestep
- 190 GB/sec
- 80% of max declared bandwidth
SC14 Demonstration of data streaming analytics and visualization

Live demonstration at SC14:
• Streaming live from KAUST Supercomputing Laboratory to New Orleans
• ~4TB per time step (100s of PF 3D timesteps generated on Intrepid) streaming live from ANL visualization cluster
• Live Uintah simulation run on CHPC (Utah) and visualized real-time at SC
Data restructuring mitigates inefficiency in access of memory.

Restructuring: Early blocking to optimize the layout for I/O.

Aggregate optimize disk access.

Large Size File I/O writes.
ROI writes for S3D data reduces both storage footprint and I/O time.

Full resolution data storage and I/O:
- 16 Seconds On 30,000 Cores Takes 16 GB

Region-of-Interest storage and I/O:
- 6 Seconds On 30,000 Cores Takes ~4 GB
Topology Has Been Successful for Analysis and Visualization of Massive Scientific Data

- Molecular Analysis (simulated)
- Materials Analysis (simulated)
- Turbulent Mixing Analysis (simulated)
- Materials Analysis (simulated)
- Molecular Analysis (simulated)
- Materials Analysis (imaged)
- Biomedical Analysis (imaged)
- Cosmology Analysis (simulated)
- Combustion Analysis (simulated)
Topology Provides a Well Defined Formalism for Communicating Shape

Morse Function:

Ascending Manifold:

Descending Manifold:

MS Complex:
Analysis of Extinction and Reignition Regions for Hydrogen Combustion
Scaling In-Situ Analytics to Full Titan with Computational Overhead < 1%
Strong Scaling – Full machine scale on Titan

HCCI rr_OH field - 1120x1120x1120
Strong Scaling with different core counts per node

- 1 core per node
- 2 cores per node
- 4 cores per node
- 8 cores per node
- 16 cores per node

Number of Nodes

Time (sec)
Strong Scaling – Full machine scale on Titan

Lifted Ethylene Jet - chi field - 1600 x 800 x 2025
Strong Scaling with different core counts per node

1 core per node
2 cores per node
4 cores per node
8 cores per node
16 cores per node

Number of Nodes

Time (sec)
Topology Provides a Well Defined Formalism for Communicating Shape

- B-separatrices
- M-separatrices
- Ridge/Valley lines
- Saddle Connectors
Exploration of High Dimensional Functions for Analysis of Complex Phenomena

Integrated presentation of statistics and topology
Topological Abstractions Improve Techniques for Visualizing and Exploring High Dim. Data

Reduce dimensionality and then extract structure

Gerber et al, 2010
Analysis of Combustion Simulations

Combustion Simulation of Jet CO/H2-Air Flames

Input: Composition of 10 chemical species

Output: Temperature
The Framework Allows Detailed Visualization and Analysis of High Dimensional Functions

10 dimensional data set describing the heat release wrt. to various chemical species in a combustion simulation
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The Framework Allows Detailed Visualization and Analysis of High Dimensional Functions

10 dimensional data set describing the heat release wrt. to various chemical species in a combustion simulation
Testbed for LOSSYY compressed data for restart dump

- Can you restart from a dump compressed LOSSY???
- Most of the data is being thrown away anyway…
- We spend a lot of data to encode bit that are known to be virtually random
- Lessons learned from UQ efforts say yes!!!
Integrated Data Management, Analysis, and Visualization Can be a Catalyst for a Virtuous Cycle of Collaborative Activities

• Tight cycle of:
  – basic research,
  – software deployment
  – user support
  – commercialization

• Coordination among many projects:
  – unified techniques for several applications

• University-Lab-Industry collaboration

• Focused technical approaches:
  – performance tools for fast data access
  – general purpose data exploration
  – error bounded quantitative analysis
  – feature extraction and tracking
  – ........

• Wide Spectrum of Interdisciplinary collaborations:
  – motivating the work
  – formal theoretical approaches
  – feedback to specific disciplines