High Performance Computing for Data Intensive Science

John R. Johnson
Computational Sciences & Mathematics Division
Fundamental & Computational Sciences Directorate
john.johnson@pnl.gov
Data Intensive High Performance Computing

Traditional Computational Sciences

- Computations have spatial and temporal locality
- Problems fit into memory
- Methods require high precision arithmetic
- Data is static

Data Intensive Sciences

- Computations have no or little locality
- Problems do not fit into memory
- Variable precision or integer based arithmetic
- Data is dynamic

Problems where data is the dominating factor

- Speed
- Volume
- Complexity
- Uncertainty

Data Intensive Research Areas

- Discovering algorithms for real-time processing and analysis of raw data from high throughput scientific instruments
- Developing techniques to interactively analyze massive (PB) archives
- Quantifying uncertainty in data, models, and methods
- Designing methods for signature exploitation and discovery
- Developing new techniques for scientific data storage and management that actively enable analytics
- Understanding the structure, mechanics, and dynamics of complex real-world networks
- Modeling, simulation, and analysis of large-scale networks
- Developing scalable mathematical techniques for manipulating and transforming large complex networks
21\textsuperscript{st} Century Scientific Method

Theory suggests hypotheses that are verified through Experiment.

Theory is developed and explored through Computation.

Hypotheses are discovered in Data and drive Theory.

Data

Computation

Experiment

Computations inform the design of Experiments.
Cyber Analytics: Canonical Problem for Data Intensive Science

- Analysis needs to identify malicious activity in high-throughput streaming data
  - More than 10 billion transactions/day
  - Tens of millions of unique IP addresses observed each month
  - Adjacency matrix may contain over a quadrillion elements but is sparse, with billions of values
  - Tens of TBs → PBs of raw data
  - Patterns can span seconds, months

- Current data analysis tools operate on thousands to hundreds of thousands of records
PNNL Capabilities Leveraging HPC

New initiative for FY11 start
Data-intensive HPC architectures
Solving the problem of irregular data access

Multithreading in Hardware
- Assumes no locality
- Hides latency for applications that don’t have locality
- When memory references stall computation, switch to new computational thread

Preprocessing Data Before it gets to the CPU
- Assumes problems will be disk-bound
- Allows for online compression/decompression
- Can filter and reduce data as it is being requested

Combining approaches optimizes data extraction at the PB-EB level and latency tolerant computing at the TB-PB level

The Cray XMT can switch between threads of execution at the hardware level in a single cycle – each processor supports 128 concurrent threads

The Netezza TwinFin processes data between disk and CPU by compressing and filtering data using reconfigurable hardware (FPGAs).
Data Intensive Supercomputing Architecture

Enabling researchers and analysts from desktop to supercomputer

Netezza Twin Fin 12

Supermicro Server

LSI 7900

Cray XMT
128 Threads per node, 128 nodes, 1 TB memory

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Enabling Commercial Tools and Technology

Tableau Business Intelligence Software
Data-intensive computing
Analysis of massive aggregates

1. Anomalous spike in traffic from Switzerland

By leveraging supercomputers, analysts have the ability to aggregate across billions of records (terabytes of data) using commercial desktop tools to perform sophisticated analysis in minutes rather than days.

2. Analyzing traffic from Switzerland shows anomalous traffic is of one type – Reset Packets (over 7 million)

3. Further analysis shows evidence of port-scans just prior to Switzerland traffic

4.2 Billion Records – 4 weeks
Graph analytics
Deep analytics of attack signatures

- **Over a trillion nodes**
- **Over ½ PB simulated network traffic data**
- Multi-hop path analysis
- 48 minutes
- 8 rack Netezza Twin Fin
  - Linear scalability

Easy to detect direct connections between bad actors and protected systems by monitoring network header traffic.

Extremely difficult to detect whether attack moves through intermediate nodes, especially low and slow attacks that span many months and are embedded in petabytes of data.