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Hey! You Got Your DWA in My HPC

Experiences Integrating Netezza and Cray XT3

Cray Hybrid Solutions Summit

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Why HPC and DWA

Increasing desire to use HPC for informatics

- Process massive amounts of data
  - Current approaches cull data before processing
  - HPC could identify global relationships in data
  - Time-series analysis to identify patterns (requires large time windows)
- Some problems have strong compute requirements
  - Eigensolves, LSA, LMSA (lots of matrix multiplies)
  - Graph algorithms
- National security interest

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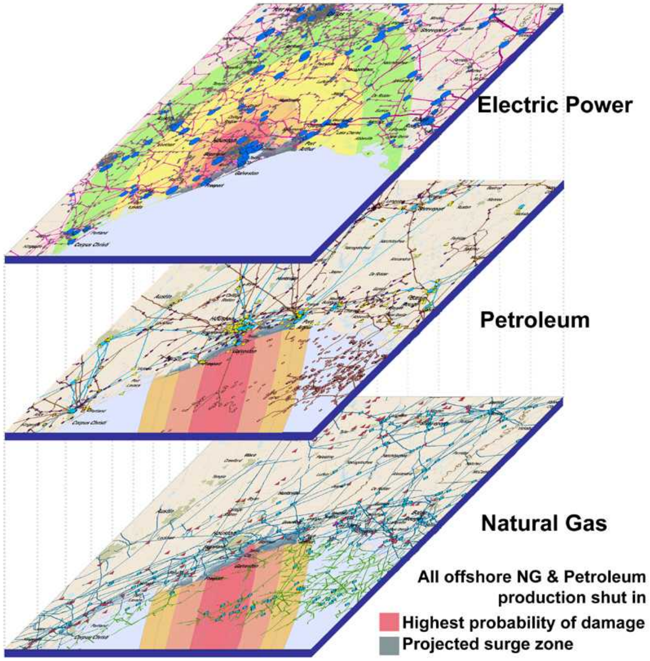
Increasing desire to use DWA in HPC-app workflow

- Post-processing sim data (e.g., economic modeling)
- I/O system metadata (fast indexing, searching)
- Feature selection/detection for “data triage” in DWA

Motivating Example: NISAC/N-ABLE

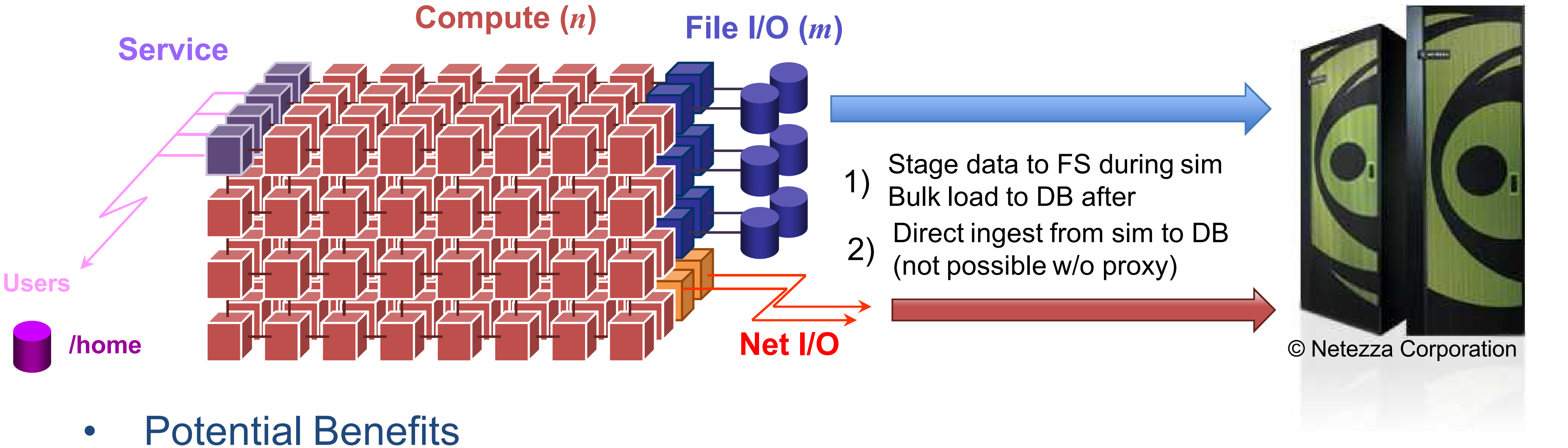
- Model economic impact of disruptions in infrastructure
  - Changes in U.S. Border Security technologies
  - Terrorist acts on commodity futures markets
  - Transportation disruptions on regional agriculture and food supply chains
  - Optimized military supply chains
  - Electric power and rail transportation disruptions on chemical supply chains

- Compute and data challenges
  - Models economy to the level of the individual firm
  - Model transactions from 10s of millions of companies
  - Simulation data ingested into DB for analysis
  - DB ingest is bottleneck (10x time to simulate data)
  - Time to solution is critical… want answers in hours


Electric Power
Petroleum
Natural Gas
All offshore NG & Petroleum production shut in
🟥 Highest probability of damage
▨ Projected surge zone

NISAC identifies potential consequences of disruptions to infrastructures and analyzes cascading impacts due to interdependencies

Integration Challenges for N-ABLE



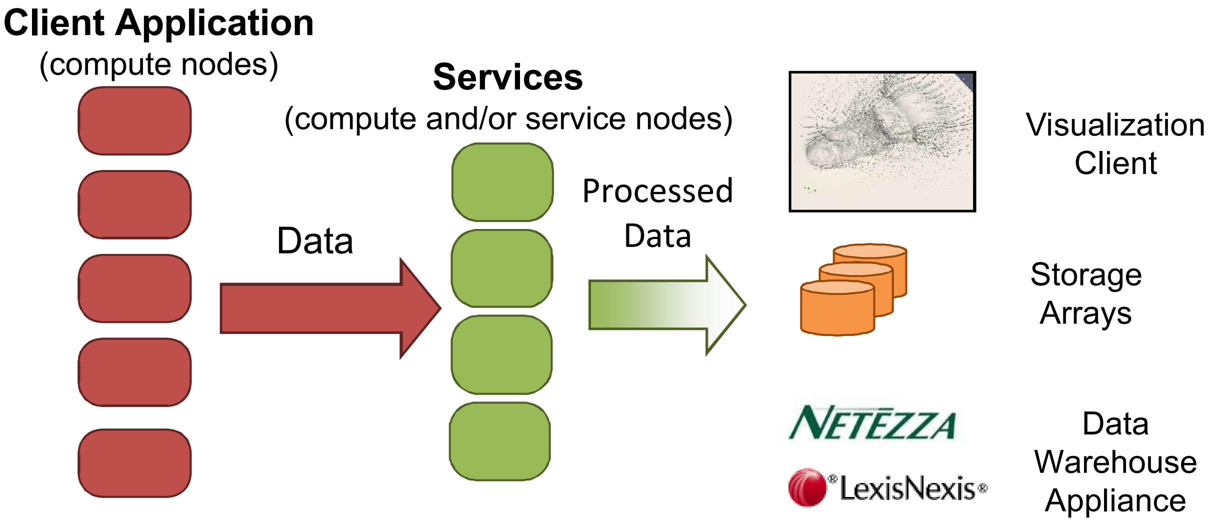
1) Stage data to FS during sim
Bulk load to DB after

2) Direct ingest from sim to DB
(not possible w/o proxy)

- Potential Benefits
  - Cray XT provides memory and compute resources for large-scale simulations
  - Netezza provides fast queries for post-analysis of data
- Software and Hardware Incompatibility
  - Specialized internal network APIs (Portals) for Cray
    - No support for standard DB interfaces (e.g., ODBC)
  - Fast network internally (2 GB/s/link), slow externally (1 Gb/s)
    - Networked integration of systems leads to I/O bottleneck

Scalable I/O Services

A Software Solution to Remote Access



Client Application
(compute nodes)

Data

Services
(compute and/or service nodes)

Processed
Data

Visualization
Client

Storage
Arrays

NETEZZA
LexisNexis

Data
Warehouse
Appliance

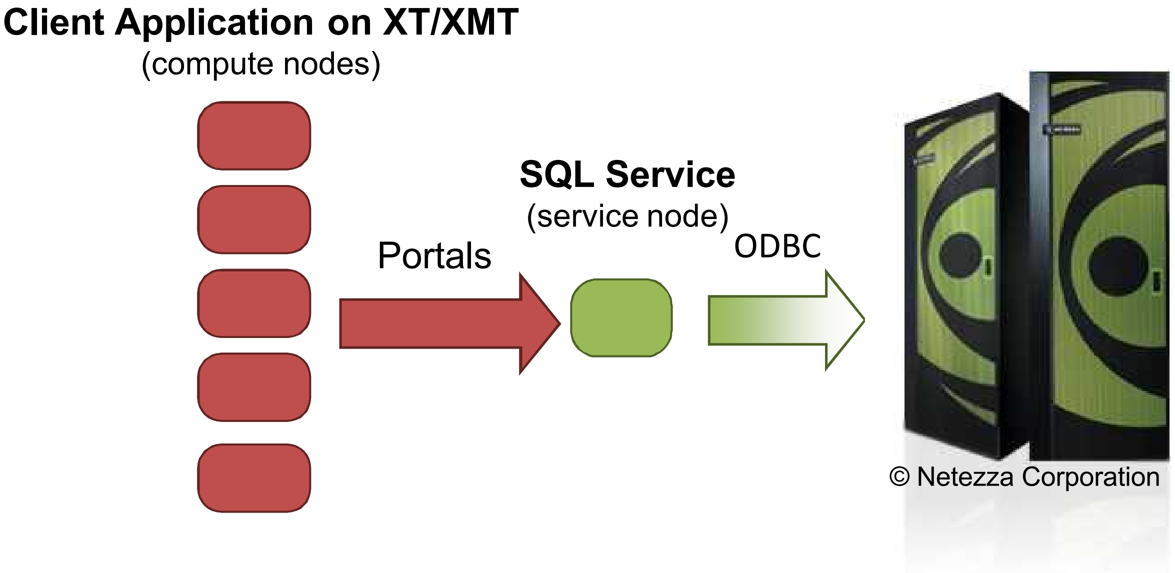
Network Scalable Service Interface (Nessie)

- Developed for the Lightweight File Systems Project
- Framework for HPC client/server development
- Designed for scalable data movement
- RPC-like API (client and server stubs)
- Implementations for Portals, InfiniBand, LUC (in development)

NEtwork-Scalable Service InterfacE

SQL Service

A Network Proxy Between Cray and Netezza



SQL Service Features

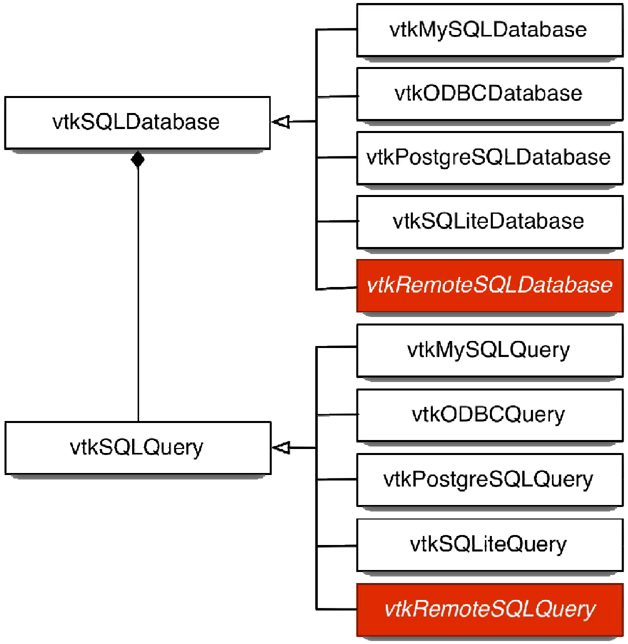
- Provides “bridge” between parallel apps and external DWA
- Runs on Red Storm/XMT network nodes
- Titan apps communicate with SQL service using Nessie (over Portals)
- Service accesses Netezza through standard interface (e.g., ODBC)

SQL Service Implementation

Client

- Compute-Node Client
  - Extensions of vtkSQL{Database,Query) classes
  - Marshal args (id, string) for remote func.

```
bool vtkRemoteSQLQuery::Execute()
{
    // handle to the RPC request
    nssi_request req;

    // XDR data structure for args and results (these get serialized)
    vtk_sql_query_execute_args args;
    vtk_sql_query_execute_res res;

    // Set the arguments for the remote Execute function.
    args.qid = this->GetRemoteQueryID();
    args.qstr = this->GetQuery();

    // Marshal and send the request to the SQL Service
    nssi_call_rpc(this->GetRemoteService(),
        VTK_SQL_QUERY_EXECUTE_OP, &args, NULL, 0, &res, &req);

    // Wait for async request to complete (no timeout used)
    nssi_wait(&req,NSSI_INFINITY);

    return res.status;
}
```



SQL Service Implementation

Server

- Server (on network node)
  - De-serialize request
  - Execute query on behalf

```
int vtk_sql_query_execute_stub(
        const nssi_remote_pid *caller,
        const vtk_sql_query_execute_args *args,
        const nssi_rma *data_addr,    // not used
        const nssi_rma *res_addr)
{
    // A data structure for the result
    vtk_sql_query_execute_res res;

    // Lookup the partner query object (stored in an STL map)
    query = query_map[args->qid];

    // Execute the query
    if (query) {
        query->SetQuery(args->qstr);
        status = query->Execute();

        res.status = status;
    }

    // Send the result of the Execute back to the client
    return nssi_send_result(VTK_SQL_QUERY_EXECUTE_OP, rc, &res, res_addr);
}
```

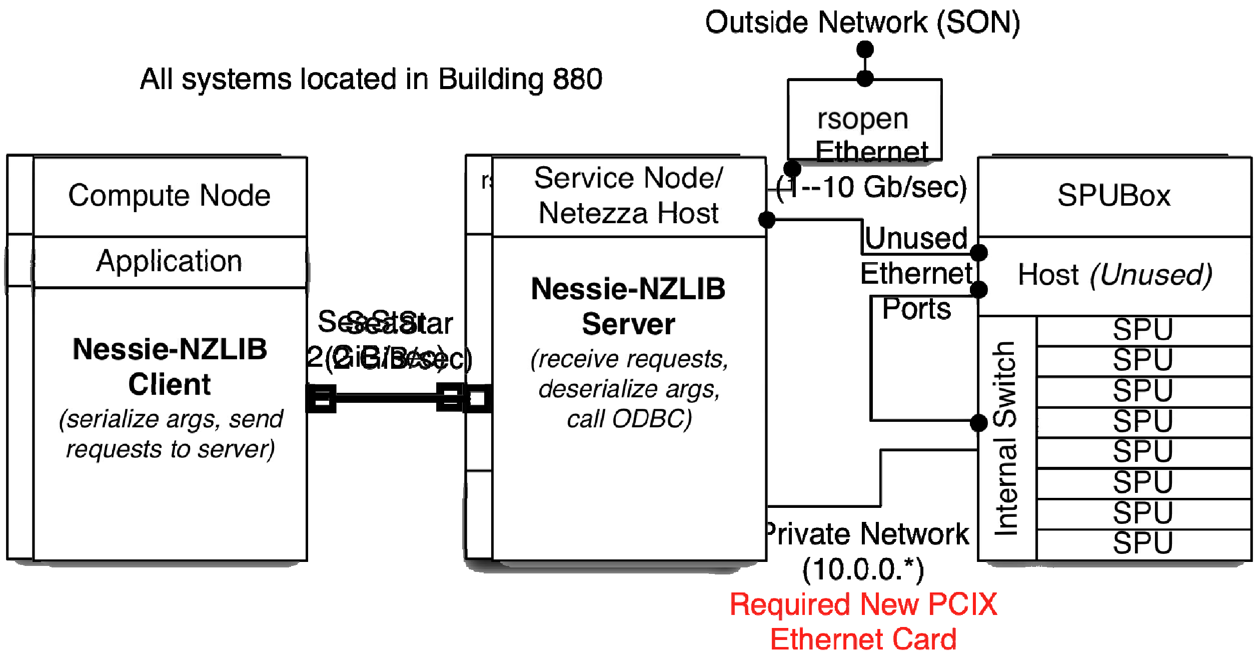
Parallel Statistics Demonstration

- Implemented Parallel Statistics Code as Demo
  - Pull one or more data sets from Netezza using SQL Service
  - Use MPI to distribute rows of query results evenly to compute nodes
  - Compute mean, variance, skewness, kurtosis, covariance, Cholesky decompositon
  - Insert results in a new table on remote Netezza using SQL Service
- Demonstration of functionality, not performance
  - Implemented minimal set of methods to demonstrate functionality
- Performance issues
  - Limitations of API (small requests)
  - ODBC implementation
  - Netezza limited to one head node (1 GigE/s max)

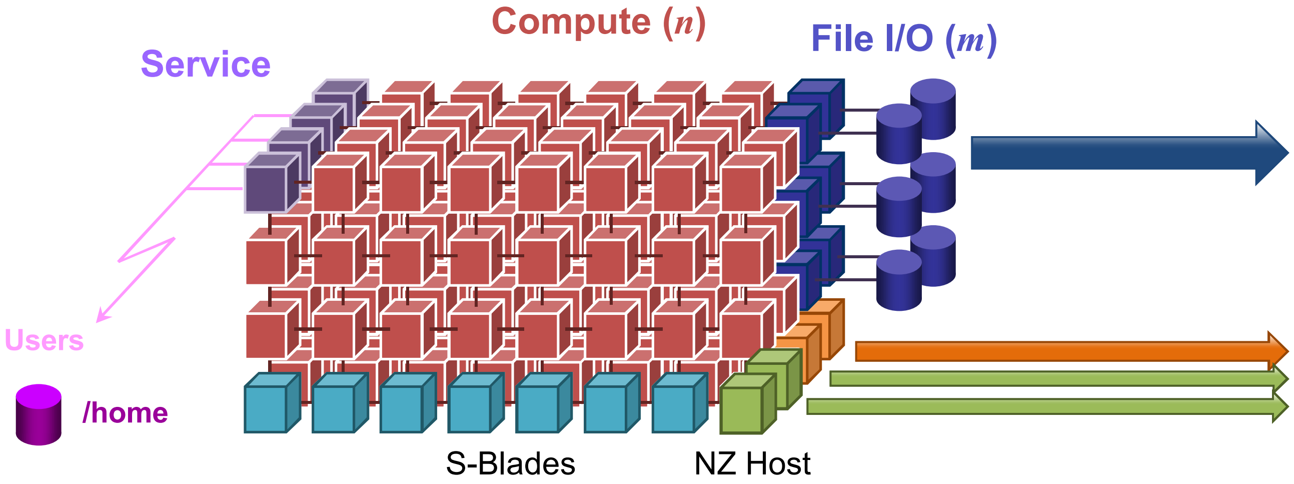
Tight Coupling of Cray and Netezza

Original Network Implementation

Move Host to Service Node



Hybrid Architecture Evolution



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Research Questions (yet to be answered)

- What ingest rates will keep up with scientific workloads?
- Where are bottlenecks? Between host and S-BLADE?
- What software/networking infrastructure will resolve the bottlenecks?

An evolving architecture to support rapid ingest for HPC workloads

1) Stage data to FS during sim, bulk load to DB after. (post-processing)
2) SQL Server sends ODBC requests to remote Netezza (slow network to host)
3) SQL Server becomes host (fast access to host, slow to S-BLADEs)
4) Multiple service-node hosts (parallel access to back-end S-BLADEs)
5) Really wacky! Hosts and S-BLADEs on fast network (fully integrated)