Porting the Urika-GD Graph Analytic Database to the XC30/40 Platform

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Kristyn Maschhoff
James Maltby
Robert Vesse
Outline of Talk

● Introduction to Urika-GD
● Porting the Query Engine
● Performance - Urika-GD vs. XC40
● Porting the User Interface
● Bioinformatics Use Case
● Conclusion
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Urka-GD Graph Discovery Appliance

**Urka-GD**

**Standalone Semantic Database Appliance**
- Integrated semantic database software, server, and storage
- Designed and Optimized for graph analytics
- Standards Based (W3C/Linux + RDF/SPARQL)

**Unique Hardware Platform**
- Threadstorm Multithreaded Processors
- Cray SeaStar2 interconnect
- Uniform Shared Memory programming model

**Enterprise Software**
- SPARQL 1.1 graph query engine
- Browser-based Database front end

**Cray SPARQL Extensions**
- Built-in Graph Functions (BGFs)

Purpose Built for Graph Data Discovery
Motivation

- Cray provides two strong product offerings in Analytics with Urika-GD and Urika-XA
  - Extensive interest in Analytics on HPC
- Extending the Graph Analytics capabilities developed for the Urika-GD to the XC30/40 line
  - Cray Graph Engine (CGE)
  - Enables mixed workloads
    - Traditional HPC (simulation)
    - Graph Discovery (Urika-GD)
  - Creation of complex analytics workflows
    - Multi-step and mixed analytic workflows
    - Spark + CGE
  - Shared high performance network and storage
Porting the Query Engine - Early Investigations

● Data in an RDF database is unstructured
  ● Communication of information across the dataset can be highly irregular, may approach all-to-all for tightly connected graphs
  ● Maintaining optimal network performance for short remote references, both PUTs and GETs is essential
  ● Urika-GD does this very well
    ● ~100 Mrefs/s per node for single word loads and stores
    ● But all references are remote!

● Mapping to XC architecture
  ● Global address space for one-sided communication
  ● Leverage the low-level DMAPP library communication layer
    ● Non-blocking implicit GETs and PUTs (~50 Mrefs/s per node, single word)
  ● Utilize synchronization features and atomic operations available with Aries
Selection of Coarray C++ Programming Model

● **A more standard HPC programming methodology**
  ● Alternative was to develop an in-house programming environment to emulate shared memory model of XMT on XC to provide a single code base for both platforms

● **C++ template library that runs on top of Cray's Partitioned Global Address Space (PGAS) library**
  ● Provides the performance advantages of the low-level DMAPP communication
  ● Provides easy access to Aries synchronization features and atomic operations
  ● Urika-GD codebase is currently C++
Coarray C++ Programming Model (continued)

- Coarray provides an easy model for taking advantage of locality when available
  - Internal intermediate data structures
- Flexibility to add application specific functionality by customizing Coarray C++ template files
- Carrying forward the Basic Graph Function (BGFs) extensions
  - Custom graph algorithms written in Coarray C++
  - Coarray C++ can also be used with Cray MPI to incorporate third party graph libraries
    - Parallel Boost Graph Library
    - Knowledge Discovery Toolkit (using Combinatorial BLAS)
Extending Coarray C++ template files

- Started with the coarray_cpp.h template file provided with the Cray compiler
- Examples of customizations added for CGE
  - mget member function to simplify syntax for multi-word gets
  - New member functions to allow vanilla loads and stores for coatomics
    - Allow these to be more lightweight in regions where we know these are not being updated or where there are no conflicts (initialization loop)
  - Threading specific member functions
    - e.g. get_switch() member function that issues a non-blocking GET followed by a thread context switch
Performance on Standard Benchmarks

- **LUBM - Lehigh University BenchMark**
  - Concentrates primarily on the Basic Graph Pattern (BGP)
  - Communication intensive – tests parallel efficiency
  - LUBM25K is a moderate-sized benchmark (3 billion quads)
  - LUBM100K – 4x larger

- **SP2B - SParql Performance Benchmark**
  - More dependent on the other SPARQL operators such as FILTER, DISTINCT and ORDER BY
  - Less sensitive to communications and more sensitive to node compute power

- **Test setup**
  - Load database and run all queries
  - Time reported is time within query engine for each query
  - LUBM25K tested on 64 node systems
  - LUBM100K and SP2B500M tested on 256 nodes
LUBM25K, 64 nodes
LUBM100K, 256 nodes

LUBM 100K

Execution Time (seconds)

Query Number

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SP2B500M, 256 nodes

![Graph showing execution time for different query numbers with bars for different systems: SP2B 500M, Urika-GD 256 nodes, CGE on XC40 - 256 nodes.](image-url)
Conclusions from Benchmarking

● Customers transitioning from Urika-GD will in general see improved performance on XC
  ● Based on comparison of equal number of nodes
    ● Equal number of network injection ports
● Even on the most complex query (LUBM Q9), CGE on XC is able to match the performance of Urika-GD
  ● Additional optimizations to improve scaling are in development
● For simpler queries or queries which make use of compute intensive SPARQL operators, CGE on XC really shines
  ● Benefits from powerful compute nodes
● Potential to scale to much larger node counts on XC than is possible using Urika-GD hardware as the back-end
User Interface Model

- Database owner launches the database server
- Users interact via their preferred interface
  - Command Line
  - Web Browser
  - SPARQL Tools & APIs
- CLI may be used for scripted workflows
Institute for Systems Biology (ISB) cancer drug repurposing study

- Multiple compute-intensive steps
- Multiple compute platforms
- Extensive data motion

Now could all be performed in a single platform!
Conclusions

- The Urika-GD Graph Analytic Database has been successfully ported from the Threadstorm architecture to the XC30/40, with good preliminary performance.
- The Coarray C++ programming model provided a bridge from a shared memory architecture to distributed memory.
- An interactive user interface and data security were retained, despite the differences in platform.
- This exciting new capability will enable multi-step and mixed analytics workflows on a single platform.
- For more information on this capability, contact Jim Maltby, jmaltby@cray.com.
Thank You!

kristyn@cray.com
jmaltby@cray.com
rvesse@cray.com
Backup Slides
## PGAS Porting Recommendations

<table>
<thead>
<tr>
<th>Issue</th>
<th>Recommendation</th>
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<tbody>
<tr>
<td>Improve performance of remote PUTs and GETs</td>
<td>Disable SW Ordering by setting the environment variable setenv PGAS_NO_SW_ORDERING 1</td>
</tr>
<tr>
<td></td>
<td>Any ordering constraints must be handled explicitly by the user.</td>
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<tr>
<td>Increase concurrency for remote GETs</td>
<td>Issue multiple non-blocking operations before issuing an atomic_image_fence</td>
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<tr>
<td>Expose concurrency for remote GETs in deeply nested calls</td>
<td>Using lightweight threading layer to increase the number of non-blocking GETs issued</td>
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<tr>
<td>Reduce latency due to waiting on GET requests to complete</td>
<td>Overlap computation and communication</td>
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## PGAS Porting Recommendations (continued)

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<tr>
<td>Use of asymmetric coarrays incur additional overhead for remote address lookup.</td>
<td>When possible, use symmetric coarray allocations.</td>
</tr>
<tr>
<td>Improve performance of remote GETs.</td>
<td>Cache coptrs to remote memory.</td>
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<tr>
<td>DMAPP resource errors. Running out of resources for registering memory.</td>
<td>Explicitly register memory with PGAS. Currently using internal PGAS library registration function.</td>
</tr>
<tr>
<td>Memory fragmentation using tcmalloc. Prevents CGE from running lots of queries against a loaded database.</td>
<td>Preallocate memory to be managed by the application, using a custom buddy allocator.</td>
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