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Enterprise

Optimizing the Cray Graph Engine for Performant Analytics on Cluster, SuperDome Flex, Shasta Systems and Cloud Deployment

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Cray User Group, May 3-5, 2021

Outline

- **Background**
  - Cray Graph Engine (CGE)
- **Enabling execution on multiple platforms**
  - Performant execution across architectures
- **Recent Optimizations**
  - Database build
  - Query Engine
- **Deployment Options**
  - Native and cloud deployments
- **Benchmarks**
  - Dictionary build
  - Query execution
- **Summary**

Background : The Cray Graph Engine

- CGE is a scalable parallel graph analytics framework
  - An in-memory semantic graph database
    - Basic graph pattern search
    - Graph-theoretic (whole graph) algorithms
  - A W3C Standards inspired triplestore
    - Uses RDF Data model
    - Uses SPARQL as query language
- Scales-out and scales-up, i.e. built for “vertical scaling” based on parallel and distributed computing principles
  - Most market competitors are scale-out databases.
  - Scale-up => faster with more compute resources
- Fast turn-around on queries, brings interactivity to graph-based discovery
  - Scaling and performance enables interactive analysis of very large datasets (1 – 100s of TBs)

2012: YarcData is formed to build Big Data solutions

2014: Urika-GD – an appliance for graph analytics using the XMT architecture

2016: Urika-GX – graph engine code ported to work on Aries interconnect and x86 architecture.

2017: Urika-XC – graph engine code scales on supercomputers.

2018: Demonstrated scaling and showed CGE as the best performing database on a trillion triples.

2020 : Ongoing work on porting Graph engine ported for HPE hardware architectures such as ProLiant, SuperDomeFlex, InfiniBand, Shasta and HPE Container Platform.

Enabling CGE on Multiple Architectures

- **CGE for XC based on Cray Coarray-C++**
  - Coarray-C++ built on Cray PGAS which leverages XPMEM/DMAPP and Aries interconnect
- **Changes required for multi-platform support:**
  - Developed simplified PGAS library to remove dependence on Cray hardware and software stack
    - Based upon POSIX shared memory and one-sided MPI communication
    - Implements only functionality required by CGE, such as:
      - Creation of symmetric virtual address space across images and symmetric memory allocations/frees
      - Blocking and non-blocking puts/gets
      - Barriers
      - Collectives
      - Direct memory access amongst images on same physical node
  - Modified Coarray-C++ to leverage simplified PGAS library
- **Advantages of using POSIX shared memory and MPI**
  - Portability
  - Performance across architectures

CGE PGAS Library

- **POSIX shared memory used for symmetric heap**
  - All images use shared memory to allocate symmetric heap
    - Used for all allocations in CGE, including memory for other allocators CGE maintains
  - Enables images on same node to directly read/write to each other's memory without XPMEM

- **MPI used for PMI, synchronization and RMA**
  - MPI window feature used to enable RMA access to symmetric heap
  - CGE put/get functions translated into memcpy if on same node or MPI_Put/MPI_Get if to remote node
    - If non-blocking put/get, CGE will track outstanding RMA until next atomic_image_fence()
  - atomic_image_fence() implemented using MPI_Win_flush_local for necessary ranks
  - sync_all() implemented as an atomic_image_fence() and MPI_Barrier()

- **Using MPI enables containerization with Singularity**
  - Container, cloud, Infiniband clusters, SuperDome Flex, and Shasta Cray EX supercomputers
  - Without significant loss in performance across architectures

CGE Coarray-C++ Template File

- **Only implemented features used by CGE**
  - Removed features such as cofuture and coatomic
- **Replaced calls to Cray PGAS library with new versions to CGE PGAS**
  - New API mimics Cray PGAS which simplified replacement
- **New functionality:**
  - coexchange(): templated utility function provided that performs all-to-all communication of single data elements in a group-aggregated manner
  - Separate image fence functions for puts/gets:
    - atomic_image_put_fence()
    - atomic_image_get_fence()
  - coexchange and separate put/get fences required corresponding support be added to CGE PGAS library

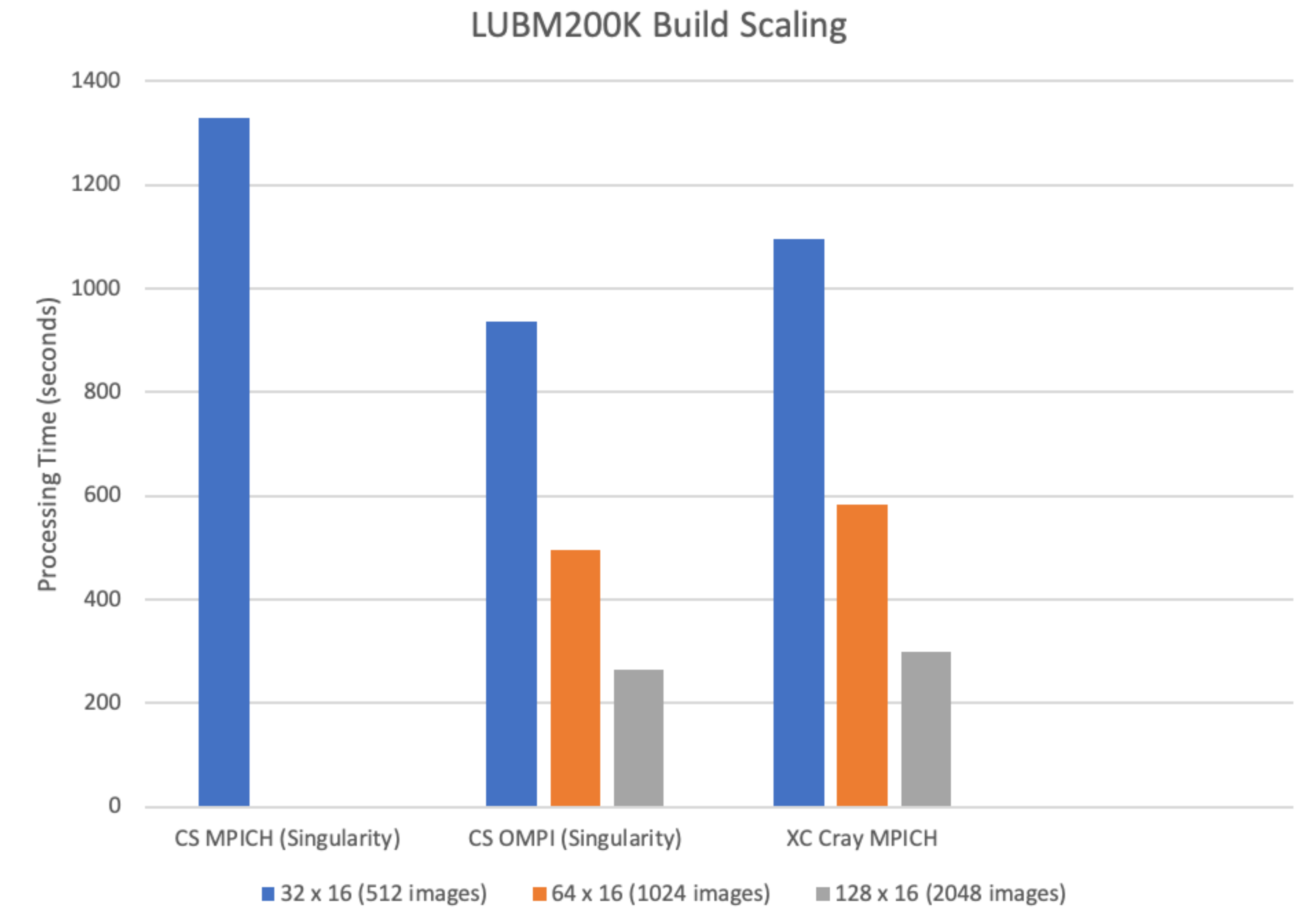
Recent Optimizations

- **Dictionary updated to support block-fetching of strings**
  - Given an array of IDs dictionary uses group-aggregated block fetching of strings
  - Used by query results writing, FILTER, Inferencing, etc.
- **Inferencer updated to use dictionary block fetching of strings**
  - Strings used to verify quads being inferred
  - Reduced inferencing time of LUBM100K on 512 images from 1796.6 seconds to 158.8 seconds
- **Scan/Join operators**
  - Optimized for shared memory machines to avoid data marshalling
  - Modified group-aggregated messaging so images hold data for consecutive images
    - Previously aggregated data from group based on one partner image per group – O(num_groups) messages
    - Reduces number of groups an image communicates with -- O(num_groups / group_size) messages
  - Reduced message sizes by returning bit-flag for 1/0 statuses rather than full words
  - Uses separate fence for remote get to prevent blocking on put of status bits
  - LUBM100K Query 9 time on 32 nodes x 16 images per node reduced from 8.6 to 7.0 seconds

Deployment Options

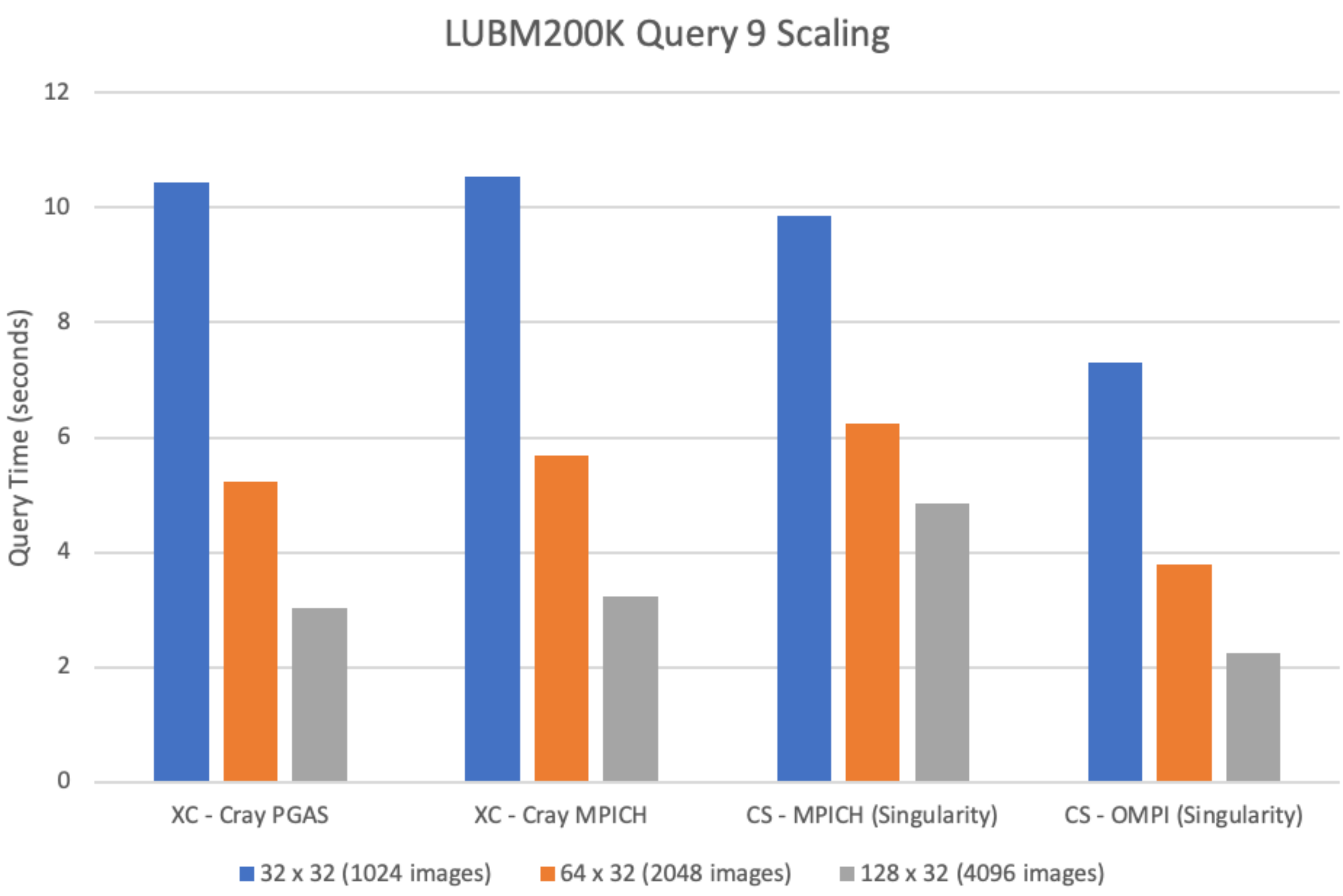
- **Build and execute natively using Cray MPICH**
  - Method used for executing on XC and EX
  - Enables optimal performance for given hardware using Cray MPI libraries
- **Containerization using Singularity**
  - Two models for MPI applications:
    - Bind – host MPI bind-mounted into container
    - Hybrid – MPI built into container and host MPI interacts with container MPI
  - CGE uses hybrid model for portability but requires container MPI to be configured for performance
    - Container includes: Mellanox OFED, UCX/OFI and MPI
  - Containers created for both OpenMPI and MPICH
    - OpenMPI 4.1 using UCX
      - Requires host OpenMPI install
    - MPICH 3.4 using OFI
      - Easy execution using slurm
      - Sometimes fails with OFI timeouts

Dictionary Build Step Scaling



- **Database build time excluding file I/O**
  - Parse, Sync, Sort, Update and Inference
- **Scales well by node count**
- **CGE using OMPI in Singularity is fastest**
- **CGE using MPICH fails to build using > 32 nodes**
  - OFI timeout errors

LUBM200K Query 9 Scaling



- **Strong scaling for all deployments except CS-MPICH**
  - 64 to 128 nodes had reduced scaling
- **Performance with Cray MPICH matches Cray PGAS**
- **CGE on CS using OMPI is fastest**
- **CGE on CS using MPICH required new coexchange**
  - OFI timeouts for small all-to-all puts/gets

Query Performance on EX, AWS and SDF

- **Benchmarked on AWS and Cray EX using LUBM100K (~18.2 billion quads)**
  - AWS parallel cluster with c5n.18xlarge nodes
  - Cray EX dual socket nodes with AMD 64-core EPYC processors
  - 32 nodes for both with either 16 or 32 images per node

Computing Platform	MPI	Query 9 time in seconds	
		512 images	1024 images
AWS efa cluster (singularity)	OpenMPI	11.60	8.40
Cray EX with Slingshot	Cray MPICH	6.17	4.24

- **SuperDome Flex (SDF) with LUBM25K (~4.6 billion quads)**

Computing Platform	MPI	Query 9 time in seconds	
		96 images	192 images
8 socket SDF (singularity)	MPICH	16.45	12.81

Summary

- **Described effort for enabling CGE to execute on multiple platforms**
  - Simplified PGAS and Coarray-C++ built on top of POSIX shared memory and one-sided MPI
  - Portability and performance using POSIX and MPI

- **Recent optimizations to CGE**
  - Dictionary build, inferencing and variable bindings

- **Demonstrated dictionary build and query performance and scaling**
  - CGE MPI based PGAS performance matches Cray PGAS
  - Containerized CGE performance on CS can match or exceed native XC performance

- **CGE now deployable either natively or in a Singularity container**
  - Native version for XC/EX enables leveraging Cray MPICH
  - Container enables easy deployment across platforms as well as in the cloud

THANK YOU

- **Questions?**