Optimizing Out-of-Core Nearest Neighbor Problems on Multi-GPU Systems Using NVLink

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Out-of-core GPU Computations

- **Definition:** ***Out-of-core*** computations refer to a class of problems in which either input data is too large to fit in the GPU's device memory or input data is partially available (e.g., *streaming* data)

- Out-of-core problems *are* **observed across a wide variety of application domains**:
  - Deep Learning: Training/Inference over large models
  - Big Data Analytics (e.g., Spark): Regression, Recommendation Systems, Clustering, Graph Analytics, ...
  - HPC: Seismic, Computational Chemistry, CFD, ...
  - Databases: Relational or NoSQL Databases, Spark
  - Streaming Data Analytics: Time-series processing for IoT workloads

Problem Under Consideration

- ***Problem Statement*:** How do we avoid performance degradation when end-to-end GPU performance and scalability is bound by memory allocation and data transfer costs?
- ***Solution:*** Only IBM's POWER Systems with the POWER8 processor and CPU-GPU NVIDIA NVLink improves performance and scalability of an out-of-core GPU-accelerated workload

What is NVLink 1.0?

- **CPU-GPU high-bandwidth Interface** with 19.2 GB/s peak uni-directional bandwidth per link
  - **IBM S822LC for HPC** (aka *Minsky*) has 2 NVLink links per CPU-GPU connection with 38.4 GB/s peak uni-directional bandwidth

Results with IBM POWER Systems 822LC (Minsky)

- **For a GPU-accelerated workload, without any code change, we observe on average 2.5X performance improvement when using CPU-GPU NVLINK over PCI-e based systems**
  - Results observed across various implementations

- ***At least 3X in allocation time is saved*** due to the POWER8 CPU and its memory subsystem

- With code optimizations for NUMA CPU data affinity, **we achieve scalability up to 4 GPUs for out-of-core workloads** when scaling on IBM's Power System

Coupling the POWER8 CPU, its memory subsystem and industry-unique CPU-GPU NVLink, IBM Power Systems drastically improves performance and reduces the impact of I/O costs on scalability as the number of GPUs is increased.

Motivating Workload: Cognitive Database Queries

- Cognitive relational database uses an ***unsupervised*** neural network model (Word Embedding) to capture relationships in the database tokens and uses the model to answer novel SQL semantic queries. Currently implemented in Spark.
- The word embedding model represents each token in the database by a vector
- At runtime, the SQL engine executes each semantic query via evaluating similarities between vectors corresponding to the relational tokens
  - Vector similarity is computed using nearest neighbor algorithms
- Database tables can have millions of tokens
  - Models can be very large (multi-GB)
  - Efficient out-of-core nearest neighbor implementations critical for fast query execution

Bordawekar and Shmueli: arXiv:1603.07185, March 2016 and DEEM 2017

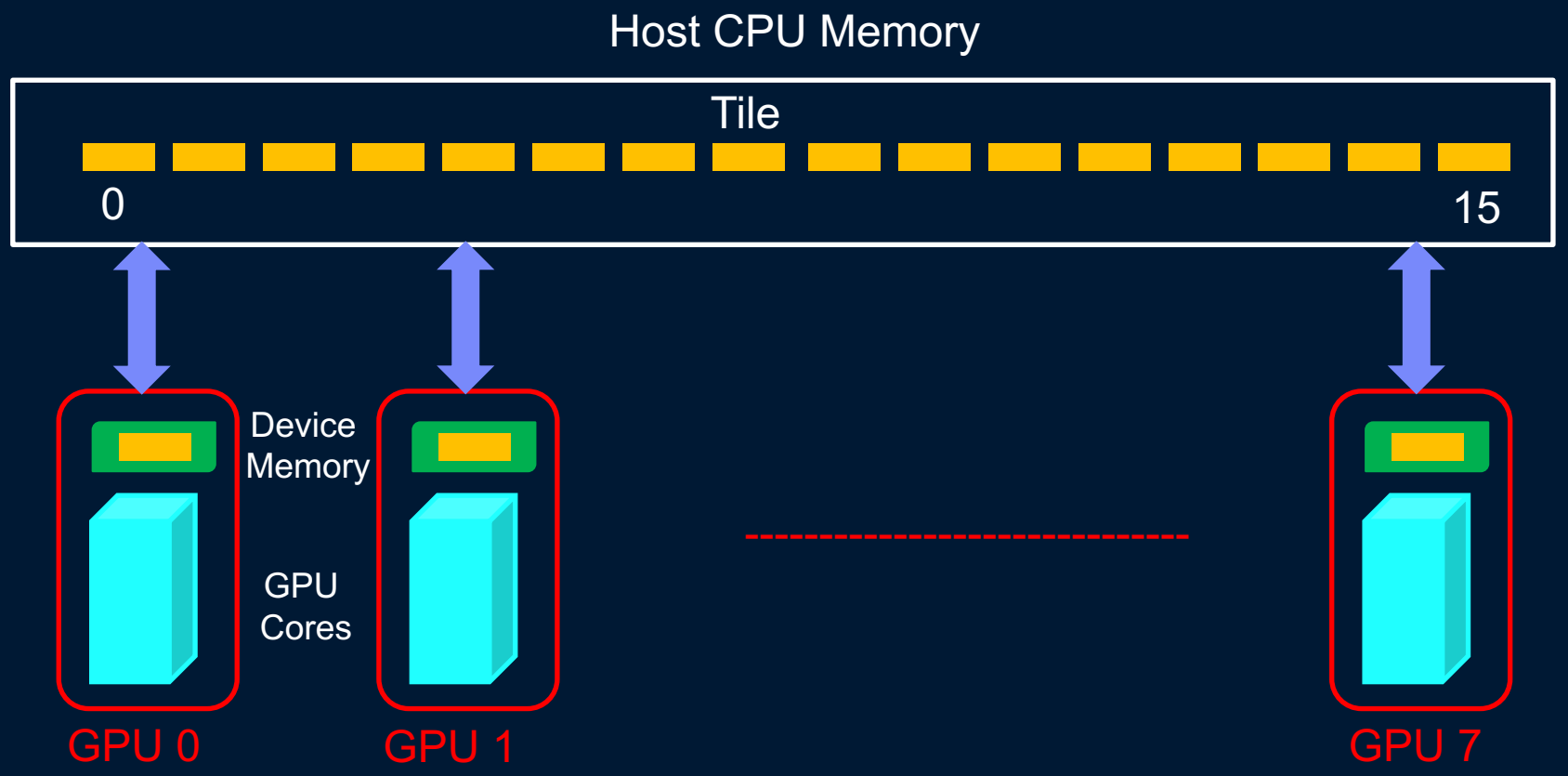
Nearest Neighbor Computations over Vectors

- Nearest Neighbor (NN) calculations involve two stages: distance-based similarity calculations and finding a pair with minimum distances
- Vector similarity computed using the cosine distance between the vectors as a metric
  - Similarity varies from 1 (closest) to -1 (farthest)
- Can be implemented as a dot-product between two normalized vectors
  - Generalized as matrix multiplication for computing distances between two sets of vectors
- For very large datasets, e.g., in cognitive databases, the NN calculations will require multiplying the entire out-of-core matrix
- To reduce the costs, approximate NN algorithms are needed

Approximate Nearest Neighbor (ANN) Algorithms

- Use approximate NN algorithm to identify candidates and then use expensive matrix multiplication algorithm on the smaller dataset to compute exact results
- Requirements for the approximate Nearest Neighbor algorithms
  - Good accuracy, smaller memory footprint, easy to partition and parallelize on GPUs
- Two alternatives:
  - **Locality Sensitive Hashing** (LSH) using signed random projections (SRP-LSH)
    - Project each input vector onto k random planes. Use the resulting k element signature to approximate cosine distance between vectors [Charikar, 2002]
    - Map the signature to a hash bucket to cluster similar vectors
  - **Spherical K-Means** [Dhillon and Modha, 2001 and Hornik, 2012]
    - Cluster the vectors into a pre-determined number of classes using cosine distance as the clustering metric
    - Vectors in a cluster are very close (higher cosine distance) to the centroid vector

Multi-GPU Out-of-core Implementation



Computational *Strip-mining:* Each GPU fetches input data in smaller chunks (*tiles*) based on available device memory

Given available memory of 1 tile per GPU:
16 accesses for 1 GPU, 8 each for 2 GPUs,…, 2 each for 8 GPUs

Multi-GPU Out-of-core Implementations: SRP-LSH

- Input: An out-of-core feature matrix with *n* vectors of dimension *d*
- Output: *n*-element array representing hash positions for each vector
- Three stages:
  1. Project each vector of dimension d onto k random planes of dimension d, to compute a k element projection
  2. Convert the k-element projection to a k-element binary signature
  3. Hash the k-element signature
- Out-of-core Algorithm
  - Partition the input feature matrix into *k* tiles of *s* samples (last tile can have different size)
  - For each tile:
    1. Project all vectors in the tile by multiplying it by the in-core random planes matrix [k,d]. Use in-core CUBLAS Sgemm function
    2. Convert each of the *s* results to *s* k-element signatures
    3. Map each signature to a hash location value (steps 2 and 3 implemented by a single kernel)
- Overall algorithm embarrassingly-parallel, each tile can be executed independently
- Similar approach used for the naïve matrix multiplication scenario
  - Normalize vectors in each feature tile and do the multiplication with input vectors

Multi-GPU Out-of-core Implementations: Spherical K-Means

- Input: An out-of-core feature matrix with *n* vectors of dimension *d*, number of clusters C, iteration count "I"
- Output: Map of size *n* storing target cluster index
- Three stages: Initial clustering, finding new clusters, update total weights
- **Focus on the most expensive component: finding new clusters**
- Out-of-core Algorithm
  - Partition the input feature matrix into *k* tiles of *s* samples (last tile can have different size)
  - For each tile:
    1. Normalize each vector in the tile
    2. Compute cosine distances of each vector with *C* cluster centroid vectors using CUBLAS Sgemm
    3. For each vector, compute the largest distance among the *C* computed distance. Return the offset as the index of the next cluster
- Overall algorithm embarrassingly-parallel and each tile can be executed independently
  - Stage 2 implemented using in-core CUBLAS Sgemm
  - Stages 1 and 3 implemented as separate kernels

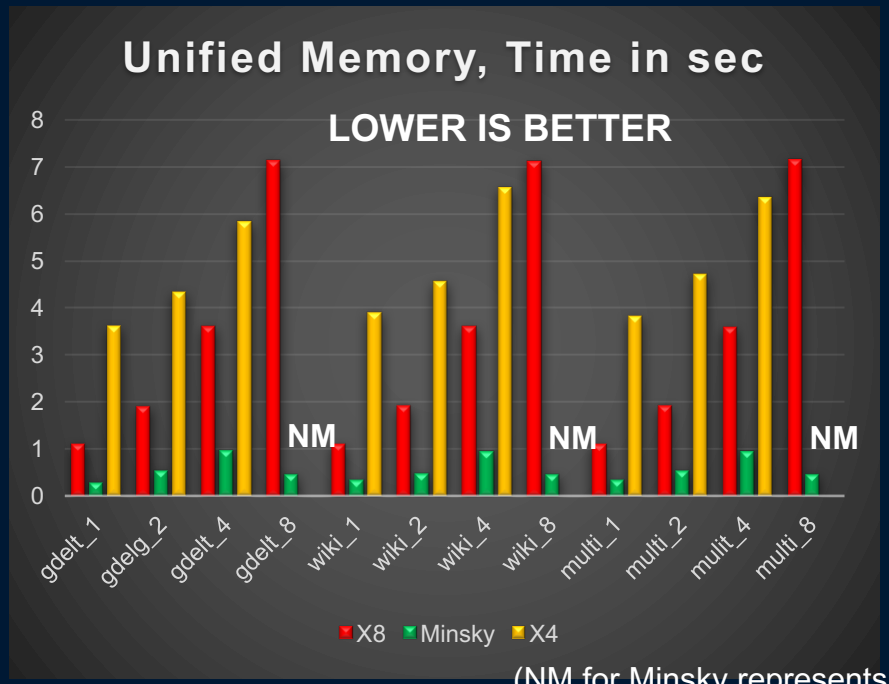
Experimental Evaluation: System Infrastructure

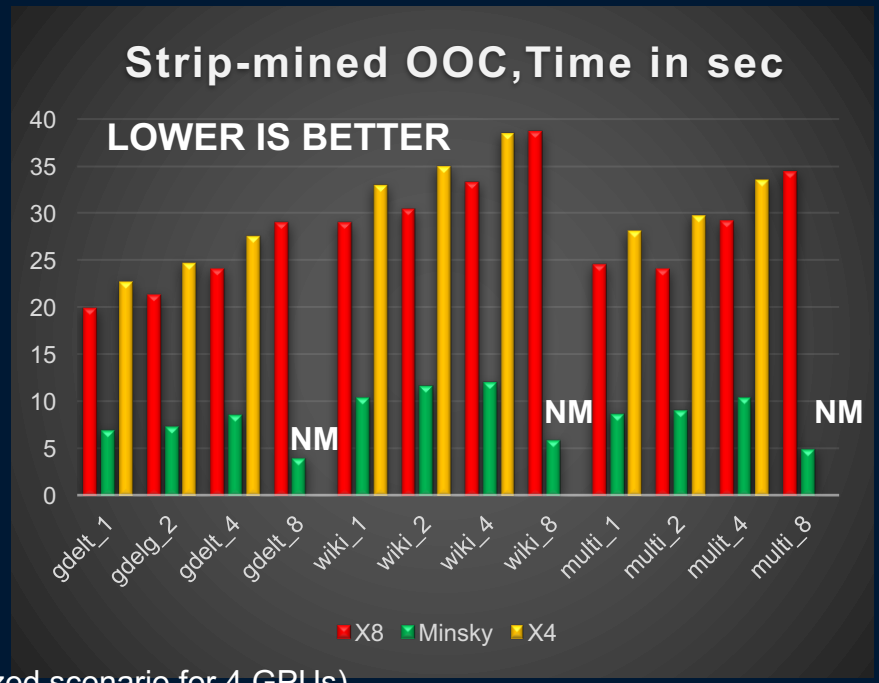
- 3 different multi-GPU Linux systems:
  - All using Pascal GPUs, each with 16 GB of device memory
  - Two x86 based: Both Dual Socket Xeons, X8 with 8 GPUs, X4 with 4 GPUs
  - Power8 based: IBM Minsky S822LC with Dual Socket Power 8s and 4 GPUs
- CPU-GPU Connectivity
  - Both x86 systems used PCIe Gen 3 x16 interconnect
  - IBM Minsky used NVLink 1.0 (2 links per CPU-GPU connection)
- All systems supporting CUDA 8.0
- Test data:
  - Three vector models built from datasets used in cognitive workloads
    - **GDELT:** vectors from an global events database with 10520822 vectors of dimension 300 (12 GB)
    - **WIKI**: vectors from Wikipedia with 5137305 vectors of dimension 1000 (20 GB)
    - **MULTI**: vectors from a multi-lingual dataset with 13120143 vectors of dimension 300 (15 GB)

Experimental Evaluation Methodology

- Each algorithm implemented using 2 approaches:
  - Unified Memory using CUDA 6+ Unified Memory primitives
    - ***cudaMallocManaged()*** used to allocate data structures shared across CPU and GPUs
  - Strip-mined Out-of-core implementation using explicit memory allocation & copy routines
    - ***cudaMallocHost()*** used to allocate host memory
- Each algorithm tested using three datasets, on the three machines: X8, X4, and Minsky
  - On each machine, number of GPUs varied from 1 to 4 or 8
  - On Minsky, we also evaluated NUMA-optimized code that ran 2 concurrent tasks assigned to two different sockets
- For each run, we measured
  - Allocation time: time for allocating memory regions
  - Execution time: compute time and memory allocation and copy time (for strip-mined case)
  - Total time = allocation time + execution time

Experimental Results: Scalability of MM Nearest Neighbor

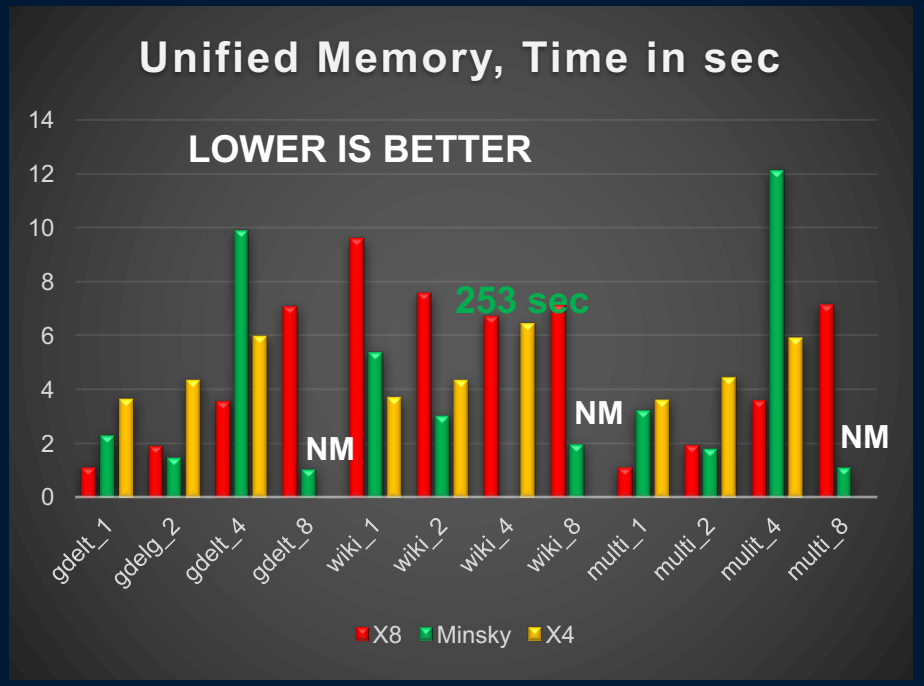


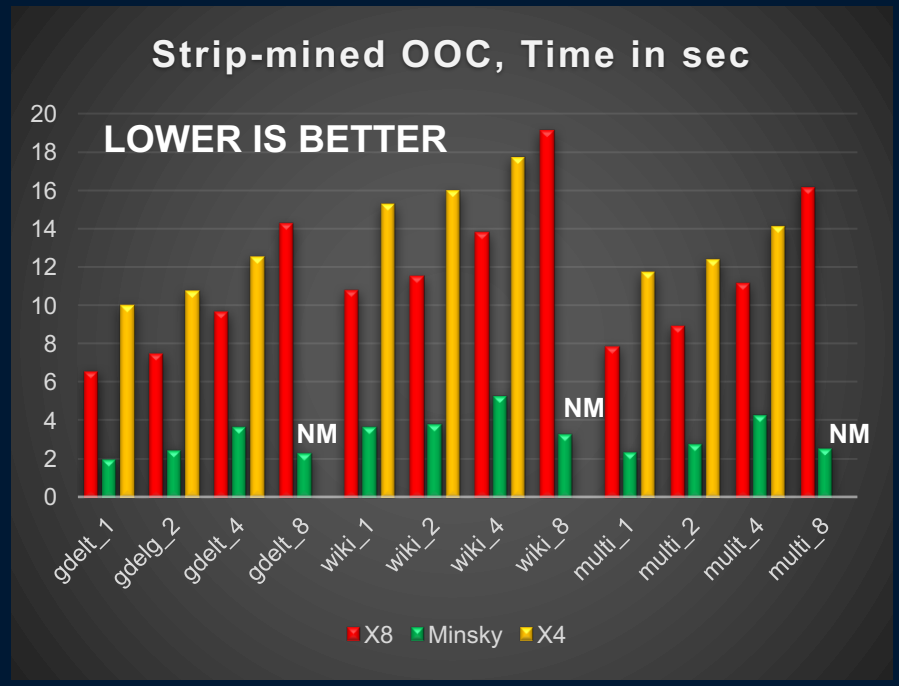


(NM for Minsky represents NUMA optimized scenario for 4 GPUs)

- GPU computation kernels executed concurrently by multiple GPUs
- End-to-end performance affected by I/O costs
- Performance does not scale as the number of GPUs is increased
- Unified Memory performs significantly better than the strip-mined approach
- In all cases, NVLink improves performance by at least 3X
- **With NUMA optimizations, 4 GPU performance scales on IBM Minsky**

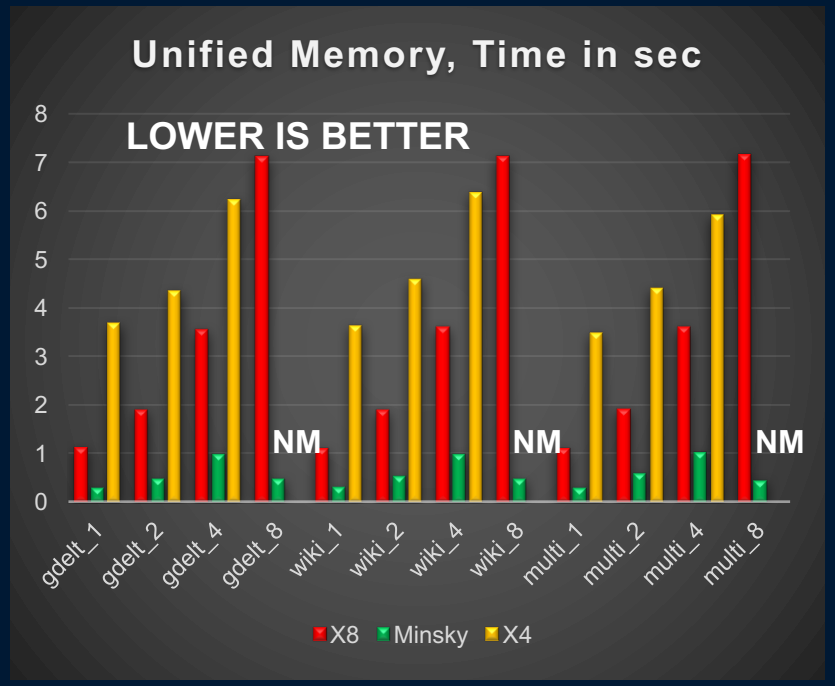
Experimental Results: Scalability of SRP-LSH Nearest Neighbor

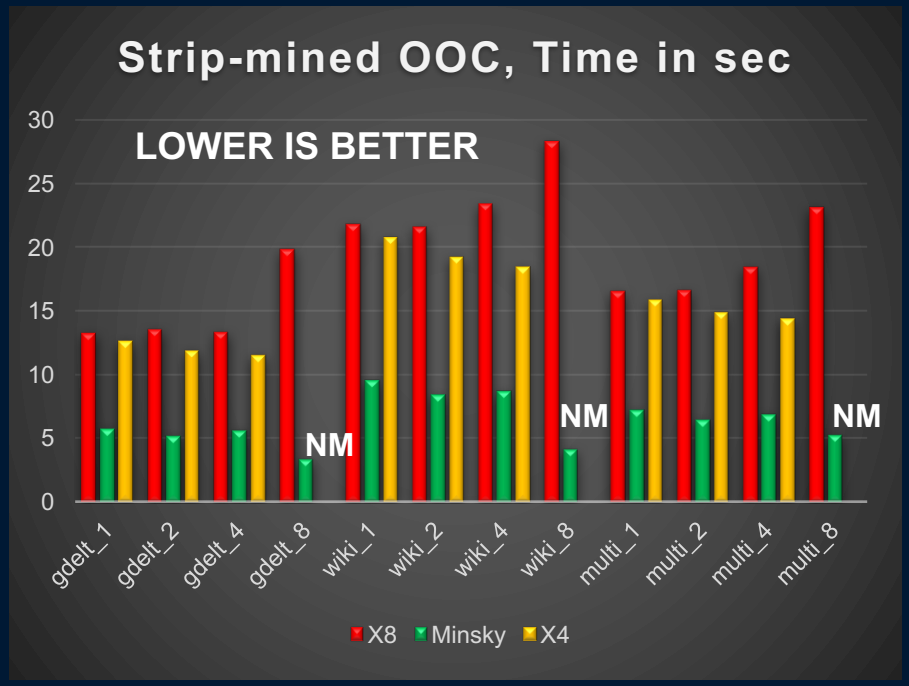




(NM for Minsky represents NUMA optimized scenario for 4 GPUs)

Experimental Results: Spherical K-Means Clustering





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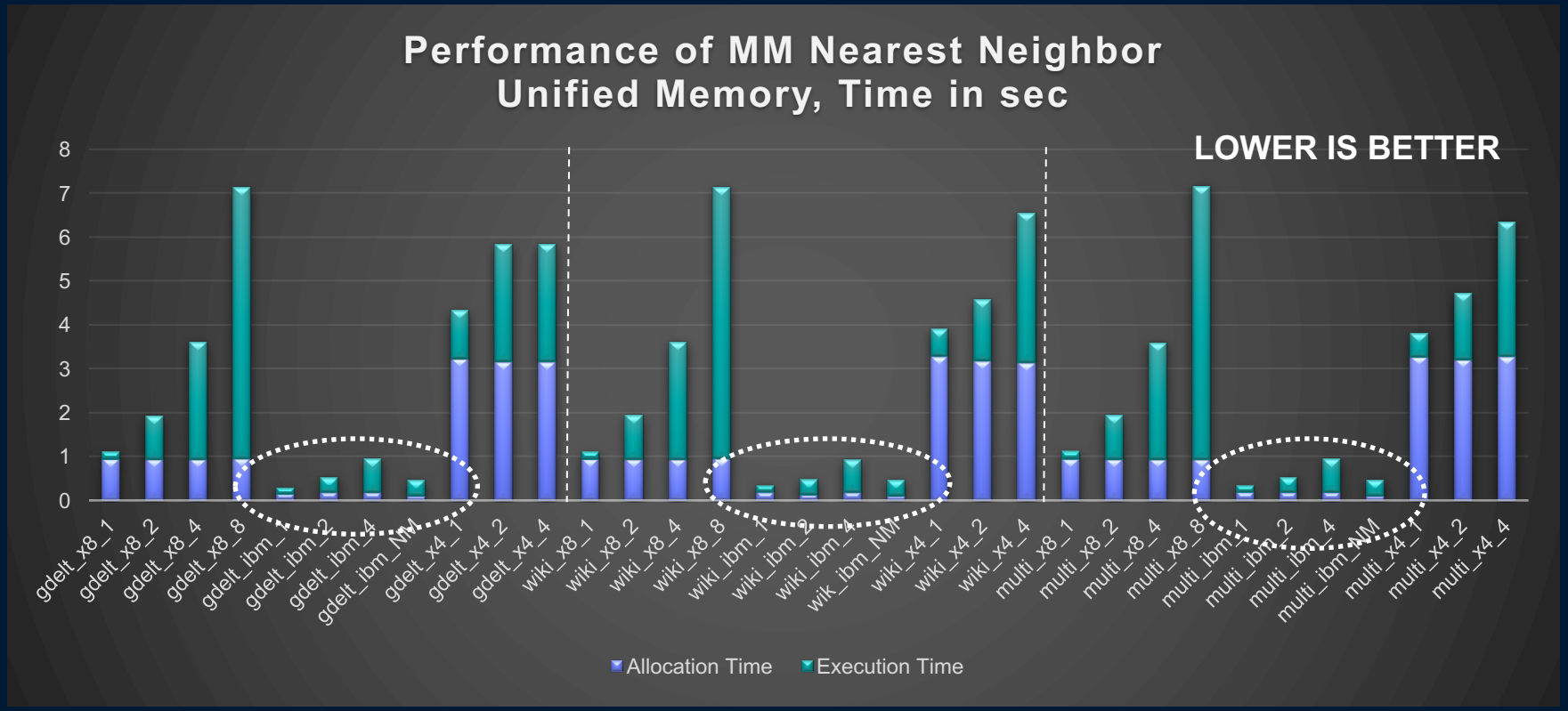
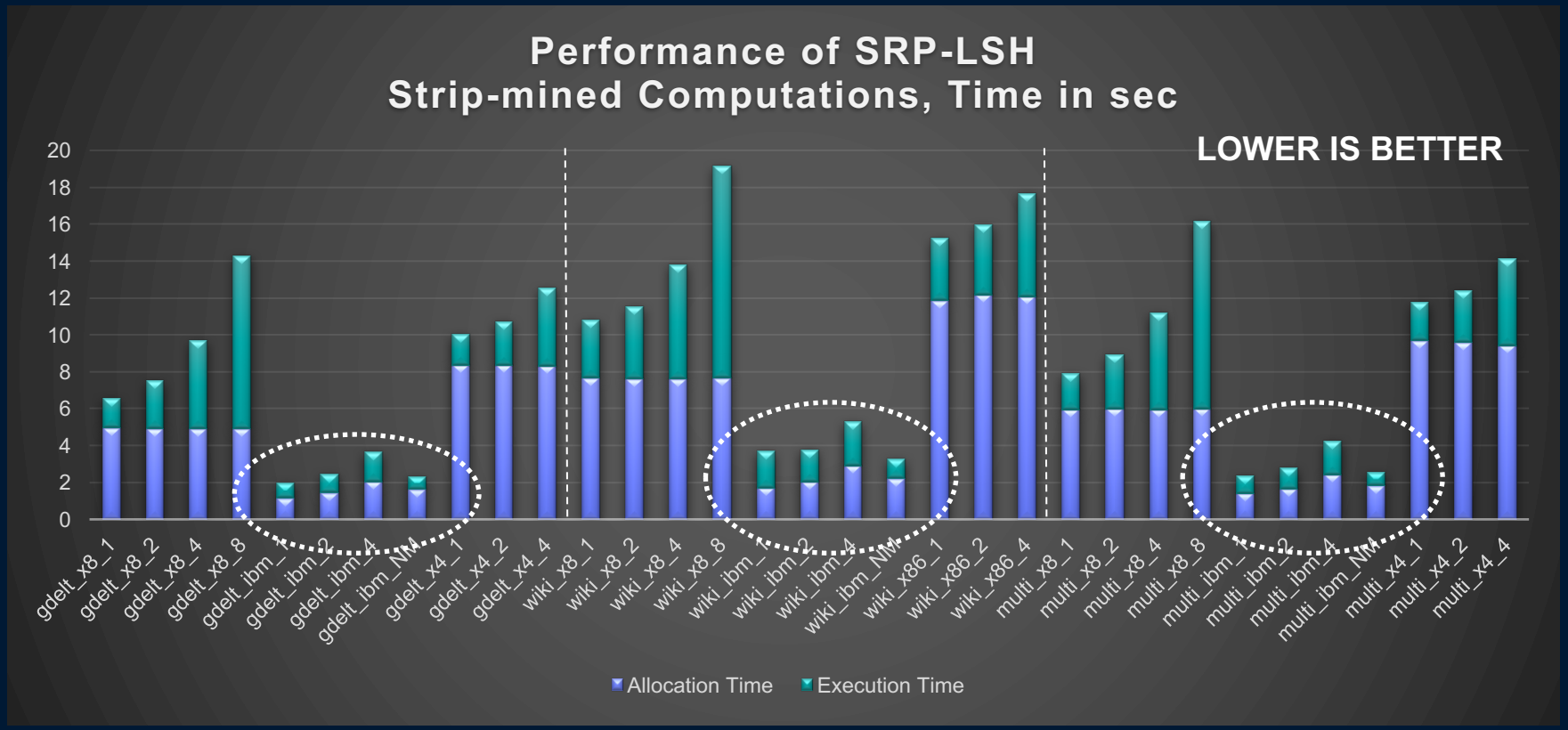
IBM Minsky Impact on Allocation and Execution Times



- In unified memory, overall performance is affected by allocation costs
- IBM Minsky's virtual memory manager (VMM) is able to improve allocations costs by up to 3X

IBM Minsky Impact on Allocation and Execution Times



For the strip-mined OOC scenario, both allocation and execution phase contribute to the overall performance. IBM Minsky is able improve both costs.

Experimental Results: Key Observations

- CUDA 6+ Unified Memory experiences
  - Very easy to use, simplifies programming tremendously
  - Does not scale as the number of GPUs is increased
  - Dependent on the Host OS memory management capabilities
- CUDA 6+ Unified Memory *always* performs better than the strip-mined OOC approach (using explicit I/O)
- In spite of GPU kernels executing concurrently, out-of-core applications do not scale across multiple GPUs
  - Performance affected by both memory allocation and copying costs
- Improving out-of-core performance requires support from both host CPU infrastructure and CPU-GPU networking fabric

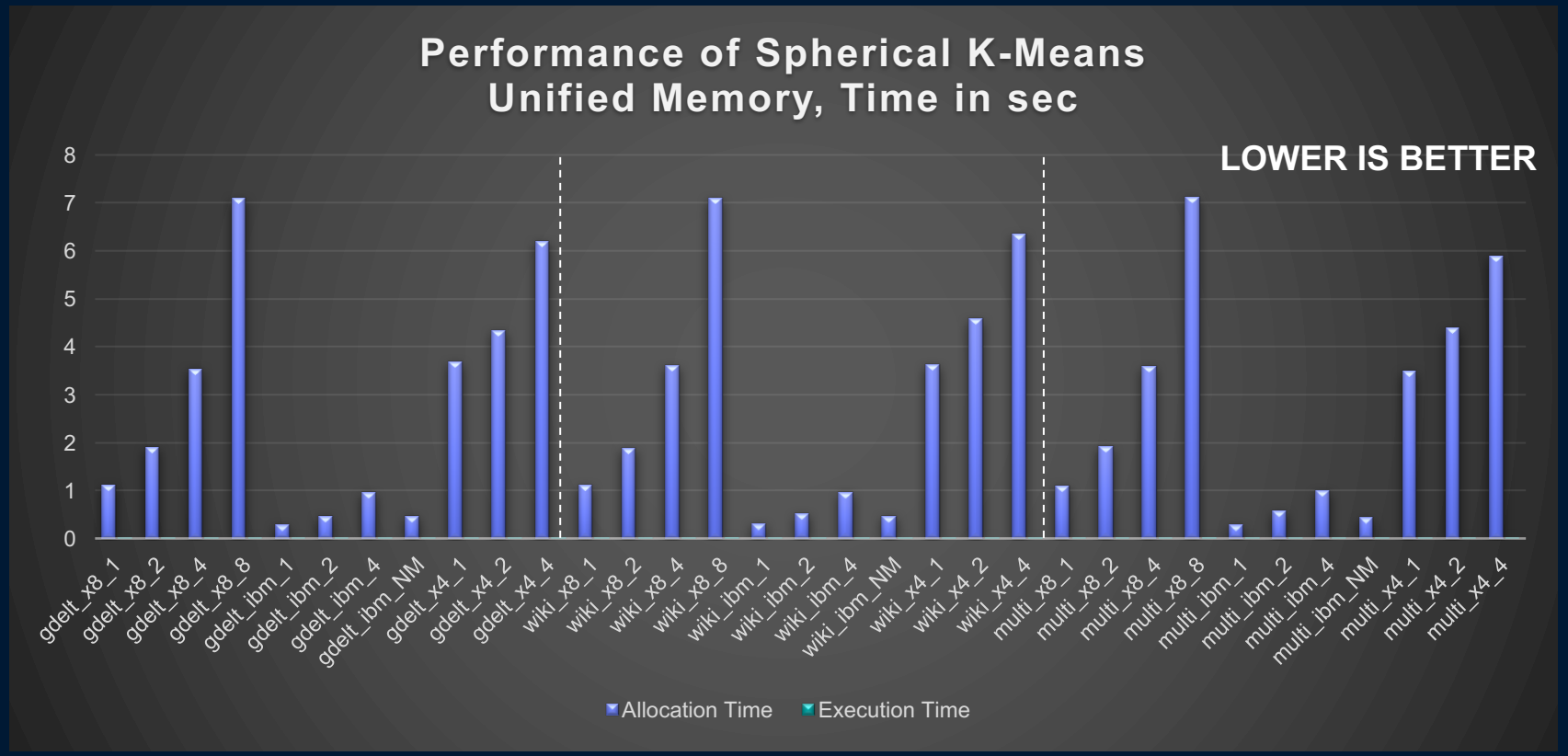
Summary

- Investigated performance of a key cognitive computation, Nearest Neighbor calculations, for out-of-core multi-GPU scenarios
- Evaluated three different implementations of Nearest Neighbor algorithms on both POWER and x86-based multi-GPU Pascal systems
- Analyzed performance of the algorithms using real datasets and identified key performance issues
- Demonstrated that IBM Minsky not only improves performance significantly (at least 2.5X) but achieves scalability for out-of-core multi-GPU scenarios

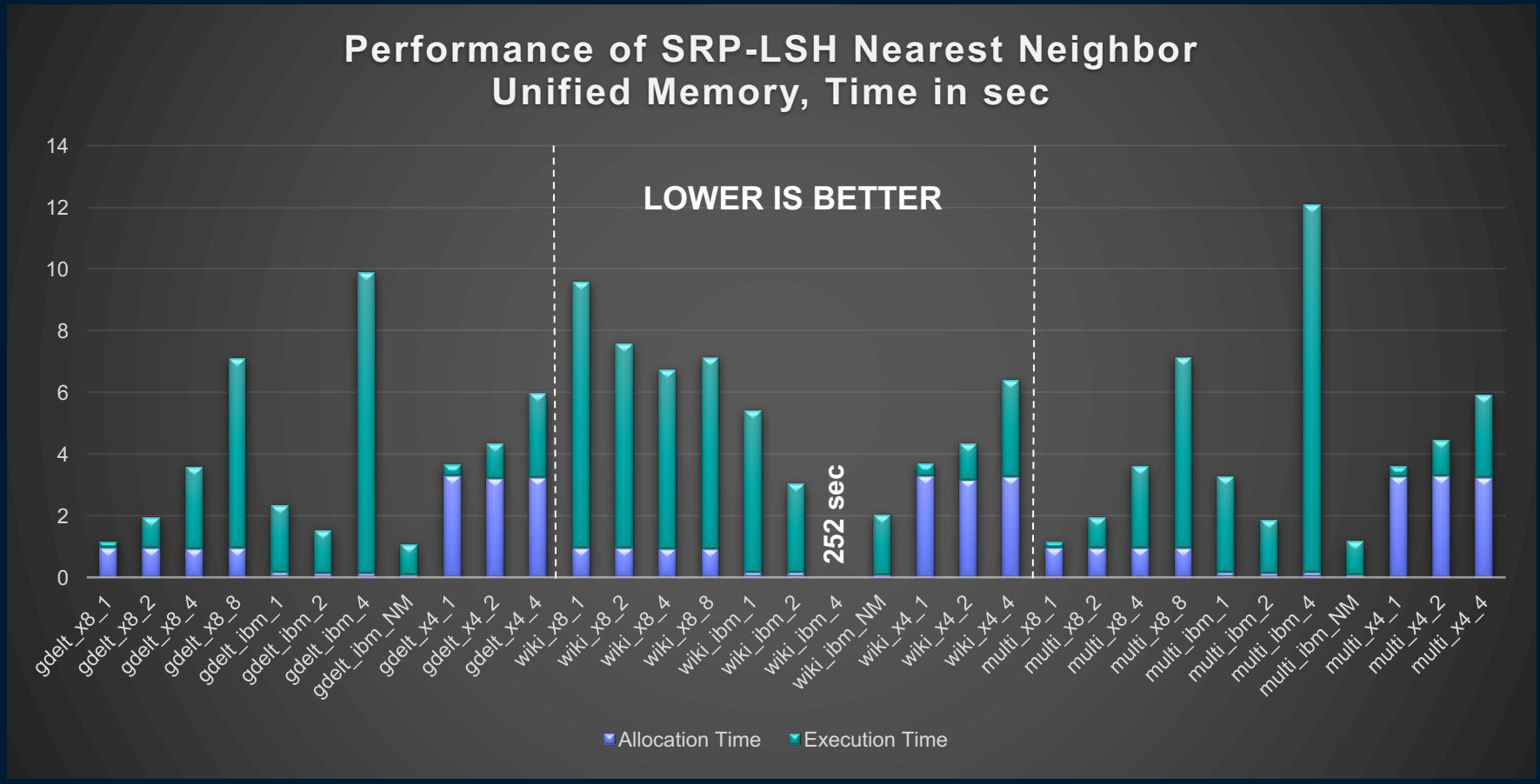
IBM Minsky is able to effectively use all three system components – CPU system stack, NVLink interconnect, and Pascal GPUs to deliver scalability and performance for out-of-core multi-GPU applications

Questions?

IBM Minsky Impact on Allocation and Execution Times



NVLink Impact on Allocation and Execution Times



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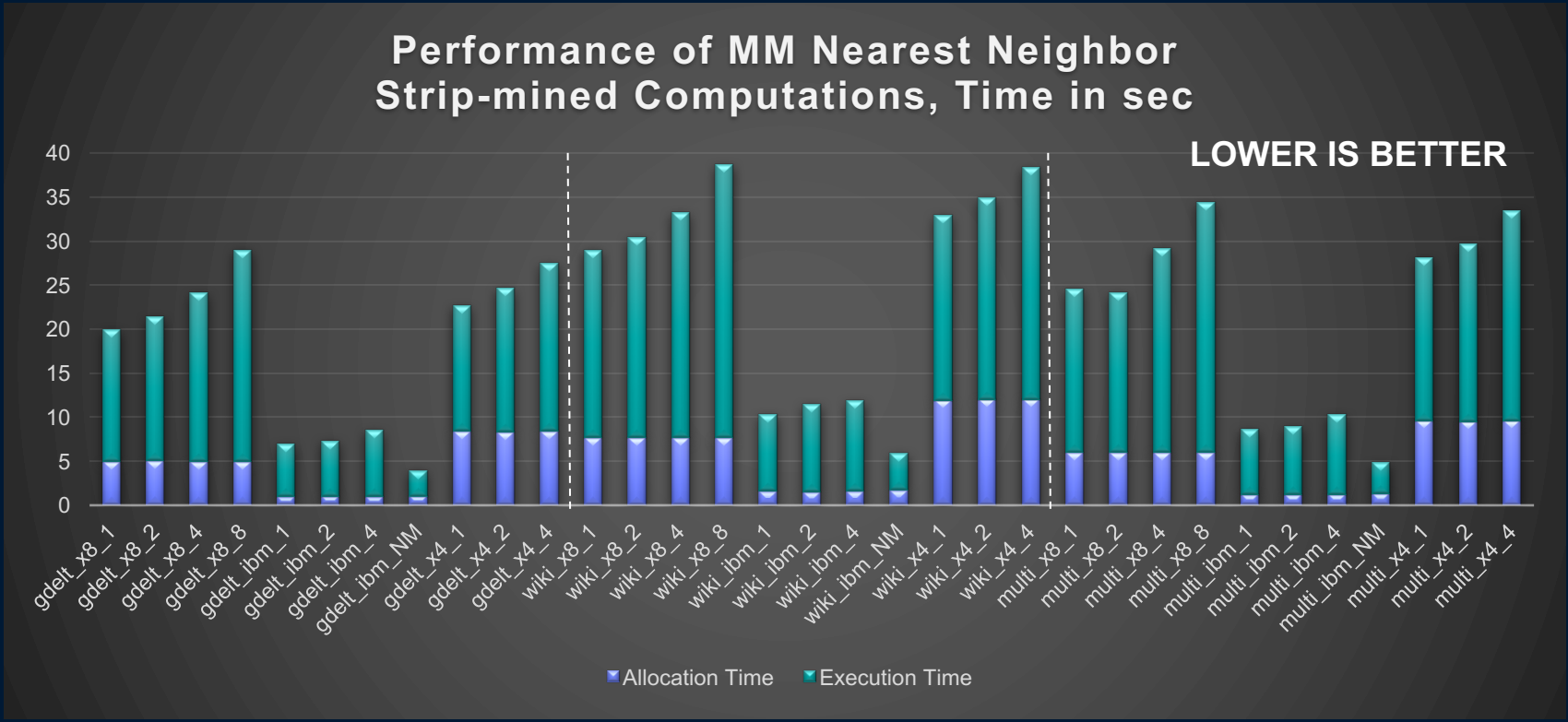

NVLink Impact on Allocation and Execution Times