PGAS in C++:

A Portable Abstraction for Distributed Data Structures

BENJAMIN BROCK

Cppcon
The C++ Conference
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About Me

- PhD candidate at Berkeley
- Advised by **Kathy Yelick** and **Aydın Buluç**
- Work on **large-scale parallel systems**
- Use a lot of LBL, ORNL **supercomputers**

This Talk

Background: how do we **write a program** for a **supercomputer**?

Introduce **PGAS Model**, RDMA

Building **Remote Pointer** Types

Building **Distributed Data Structures**

Extending to **GPUs**

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- A **distributed implementation** of the **STL**

- A full **evaluation** of **parallel computing models**

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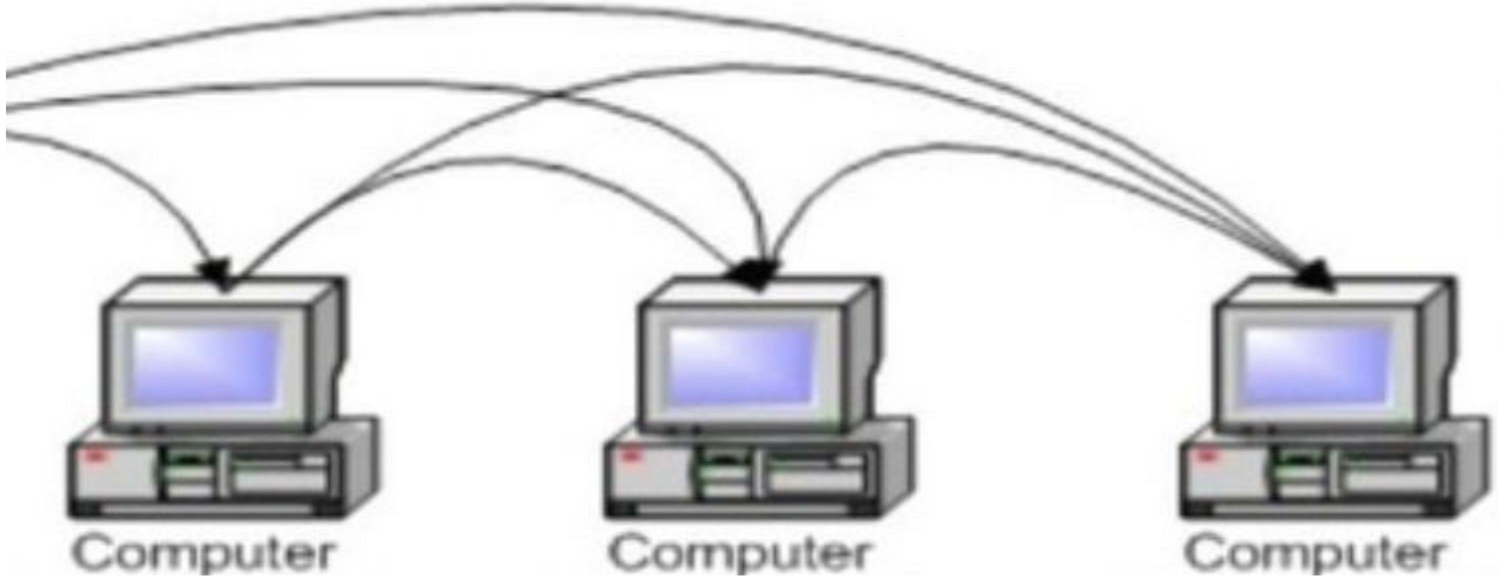
Background: How to supercompute?

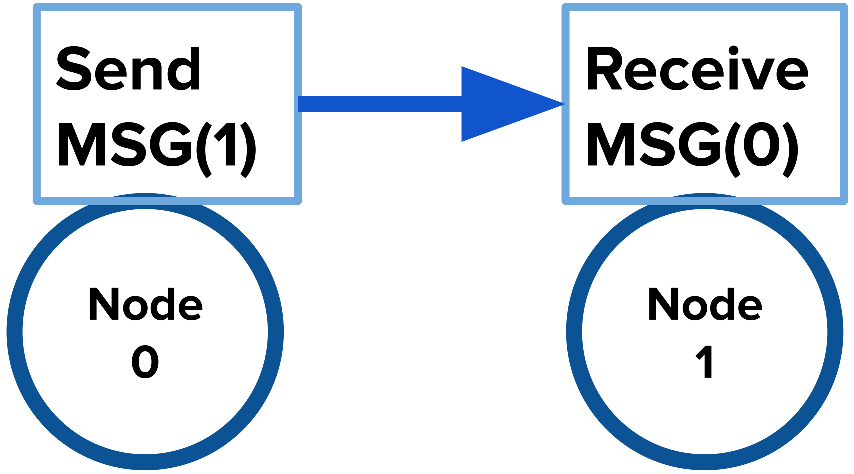
What is a Cluster?

- A collection of **nodes**, connected by a **network**.



How do I program one?

- **Message Passing** - processes issue matching **send** and **receive** calls



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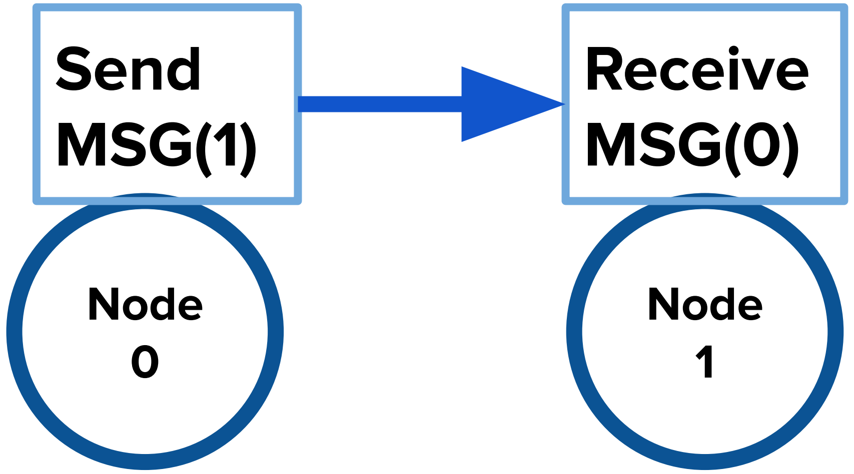

Process 0

```
// Calculate data
auto values =
   algorithm(1.0f, 3, data);

// Send data to proc. 1
MPI_Send(values.data(),
         values.size(),
         MPI_FLOAT, 1,
         0, MPI_COMM_WORLD);

// Data is now sent.
```

Process 1

```
// Allocate space for data
std::vector<float>
recv_values(num_values);

// Receive data from proc. 0
MPI_Recv(recv_values.data(),
         num_values,
         MPI_FLOAT, 0,
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// Data is now in
// `recv_values`
```

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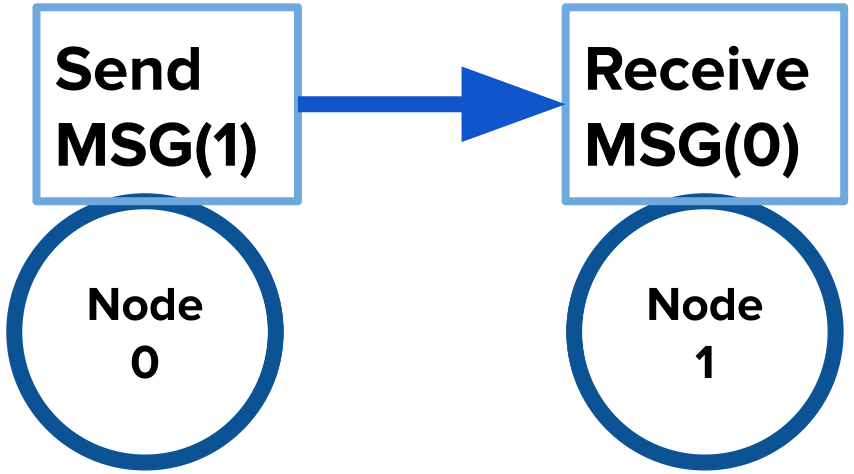

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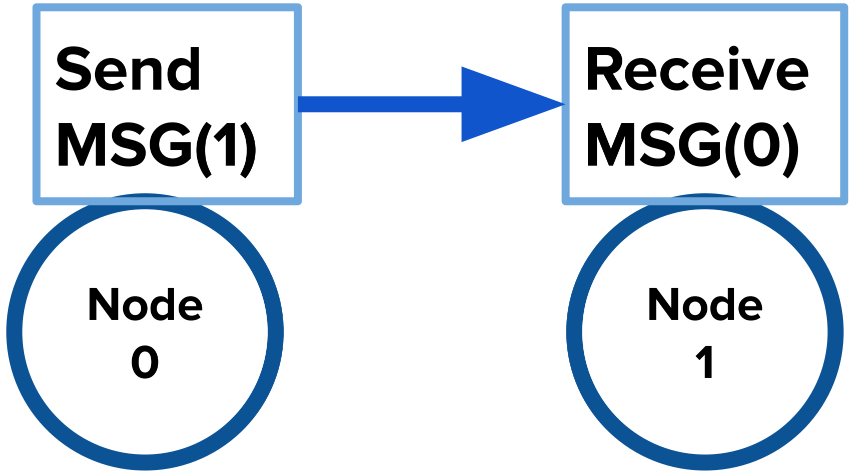

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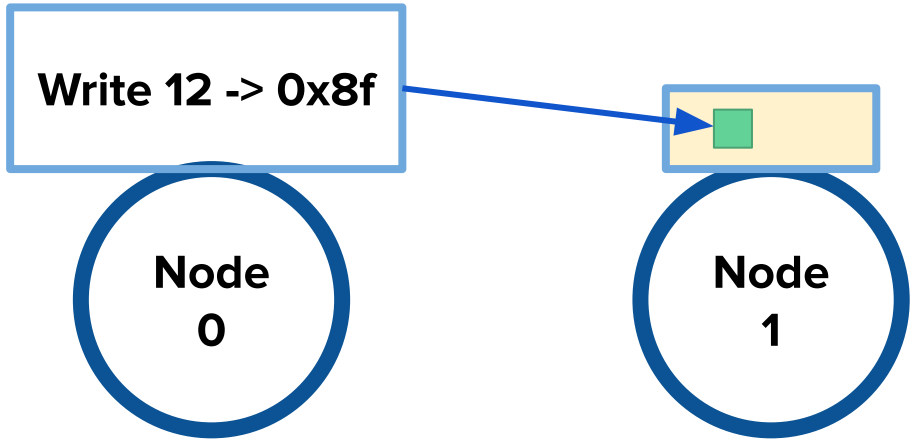
P0 and P1 must both participate in message.

How do I program one?

- **Message Passing** - processes issue matching **send** and **receive** calls

- **RDMA** - directly read/write to **remote memory**



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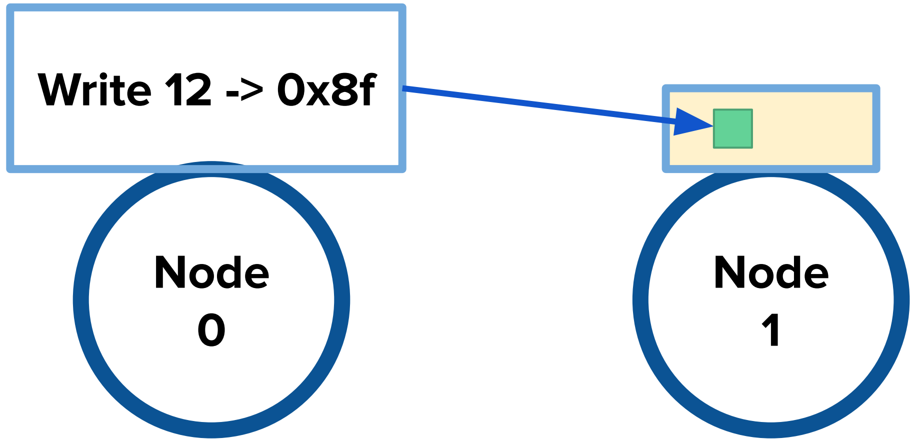

Process 0

```
auto remote_ptr = ...;
// Calculate data
auto values = algorithm(1.0f, 3, data);

// Send data to proc. 1
BCL::memcpy(remote_ptr, values.data(),
            values.size()*sizeof(float));

BCL::flush();

// Data is copied.
```

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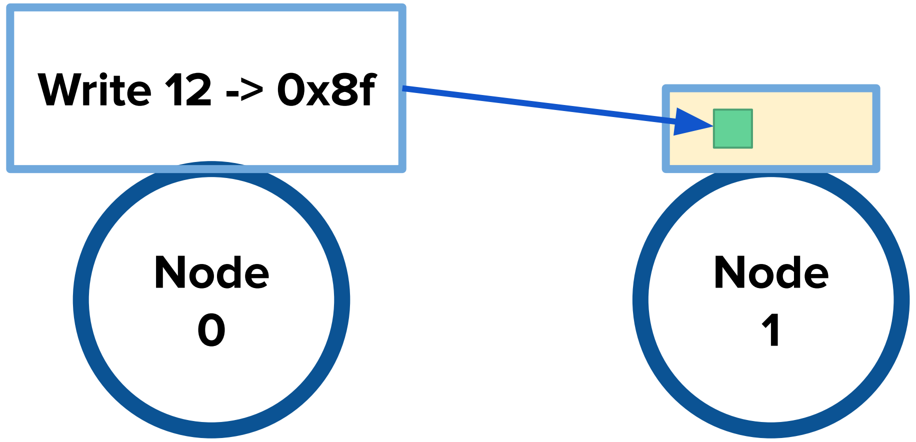
- **Message Passing** - processes issue matching **send** and **receive** calls

- **RDMA** - directly read/write to



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BCL::flush();

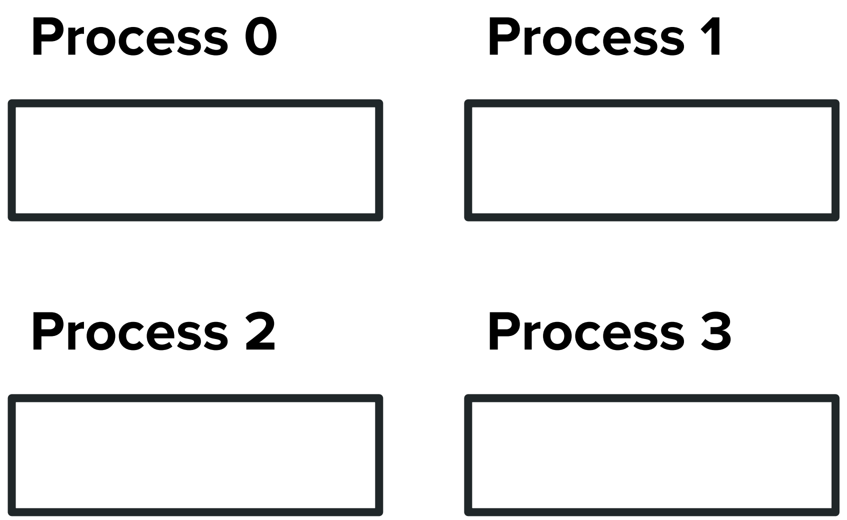
// Data is copied.
```

P1 does not participate in remote write.

PGAS Model

- **Partitioned** - **each process** has its own **shared segment**

- **Global address space** - each proc's **shared segment** can be **referenced** by **other processes**



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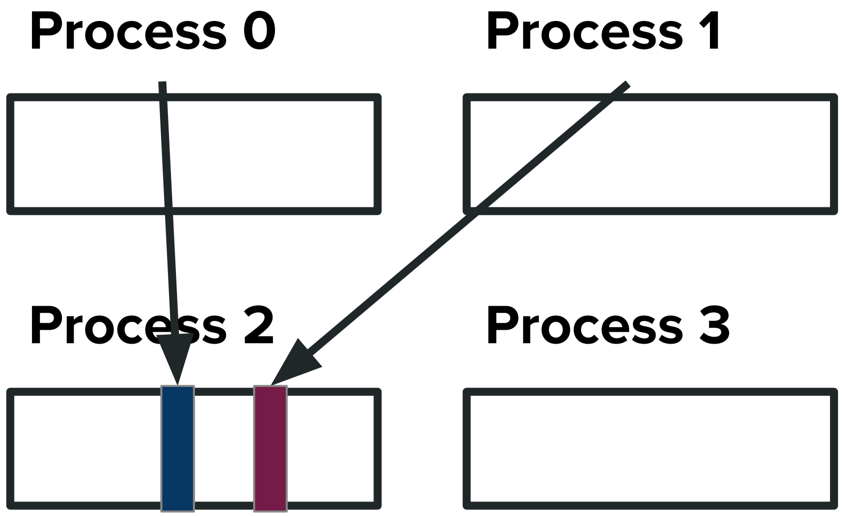

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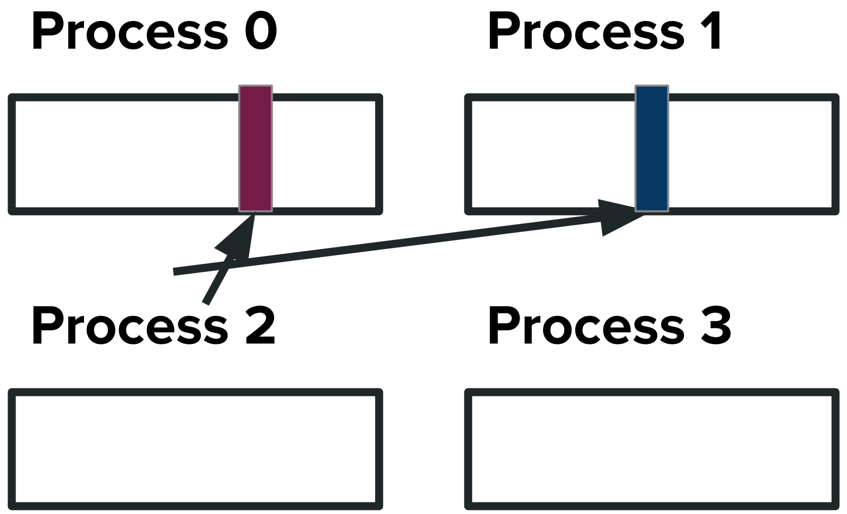
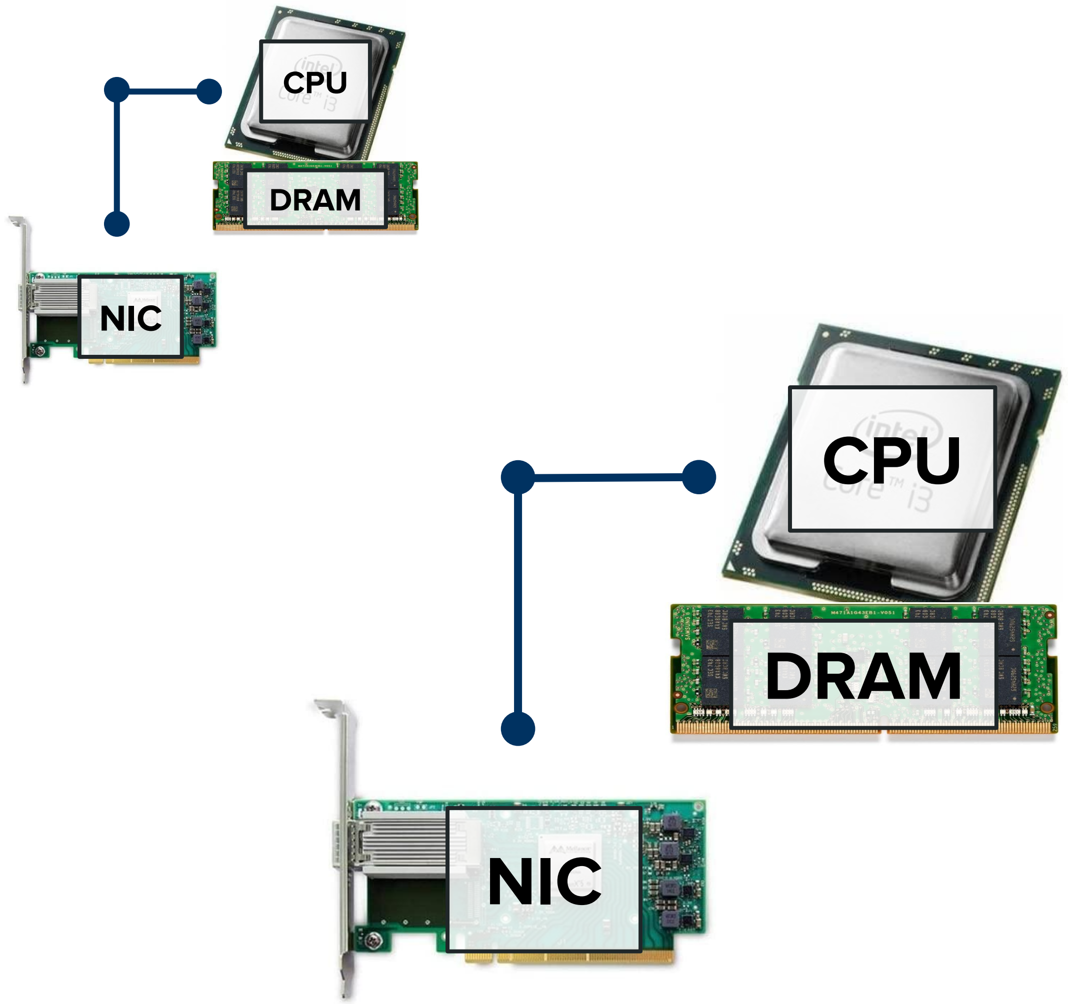


Advantages of PGAS

- **Asynchronous** - RDMA operations **executed by NIC**
- Allows **irregular**, one-sided access
- Maps well to **data structure** ops



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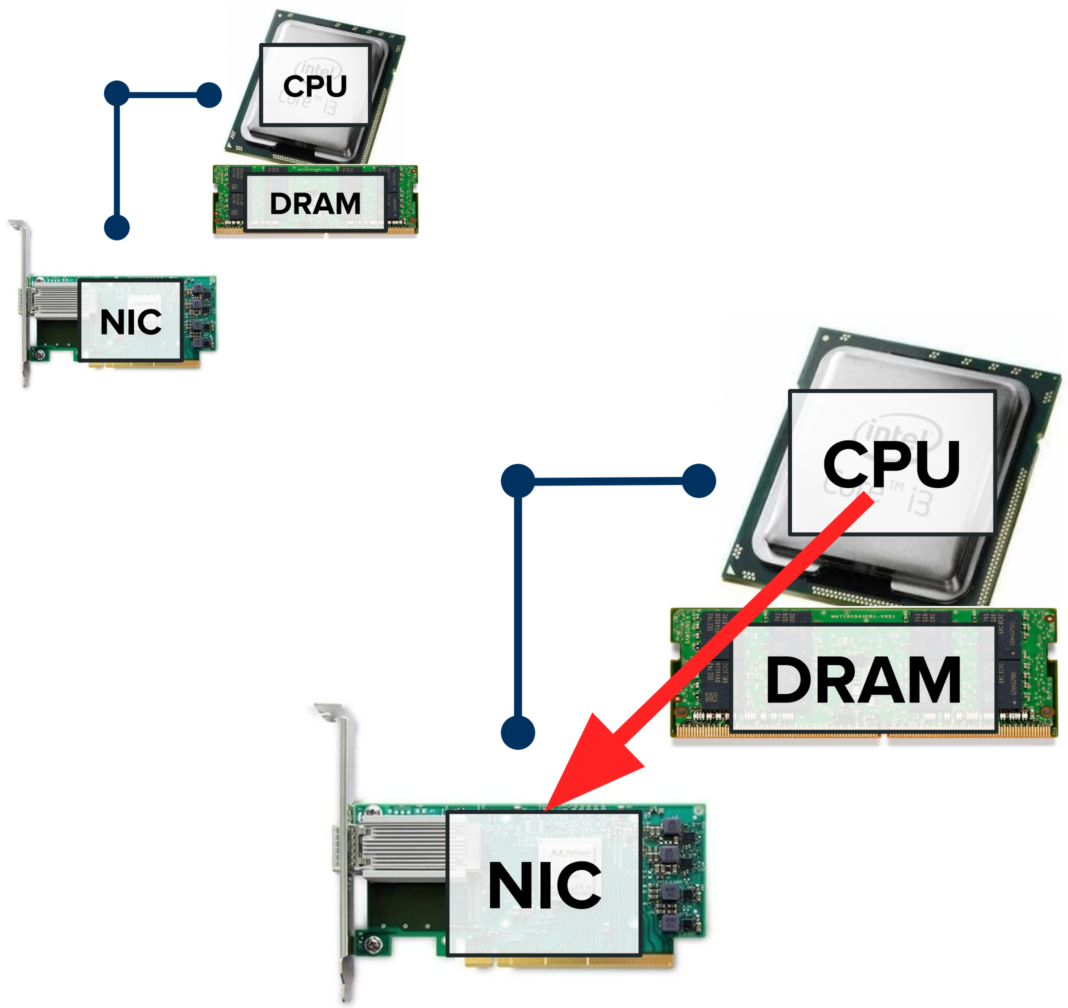

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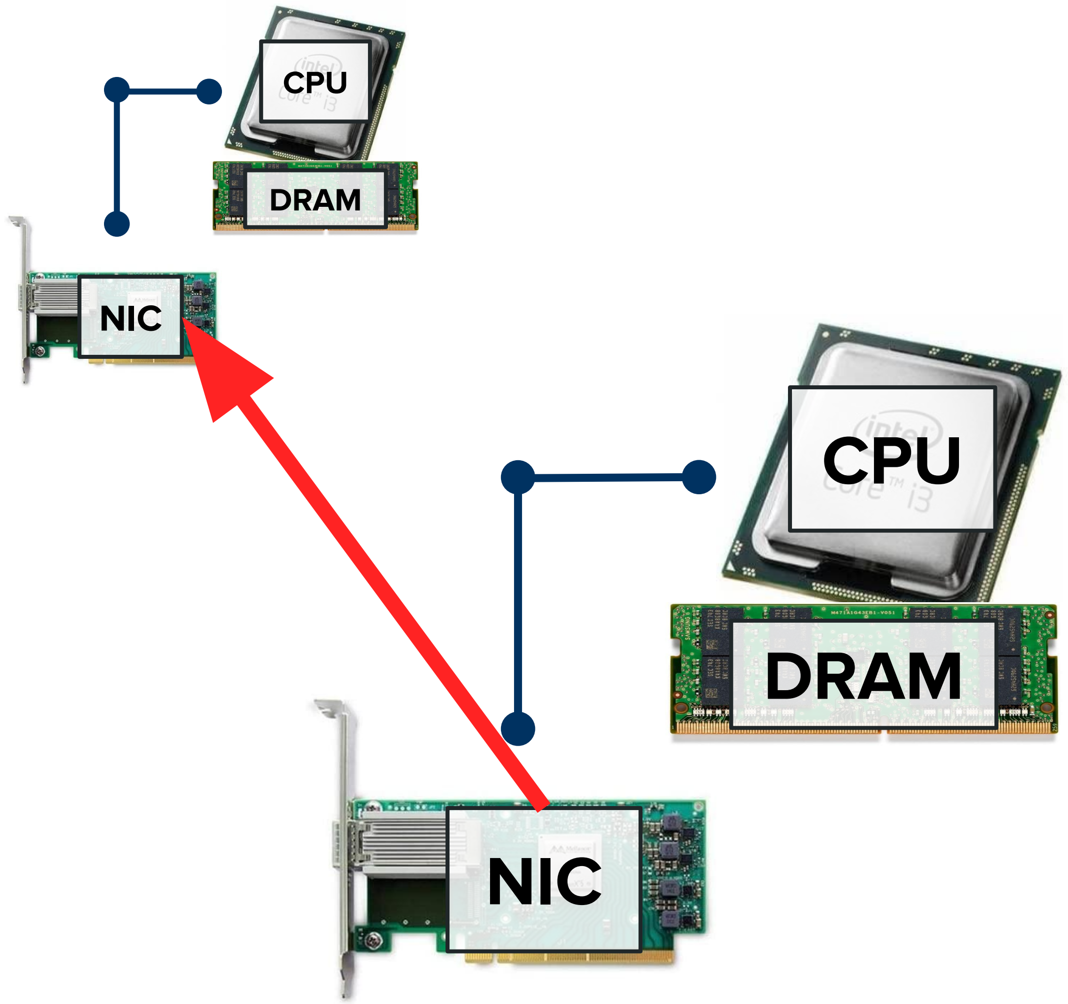

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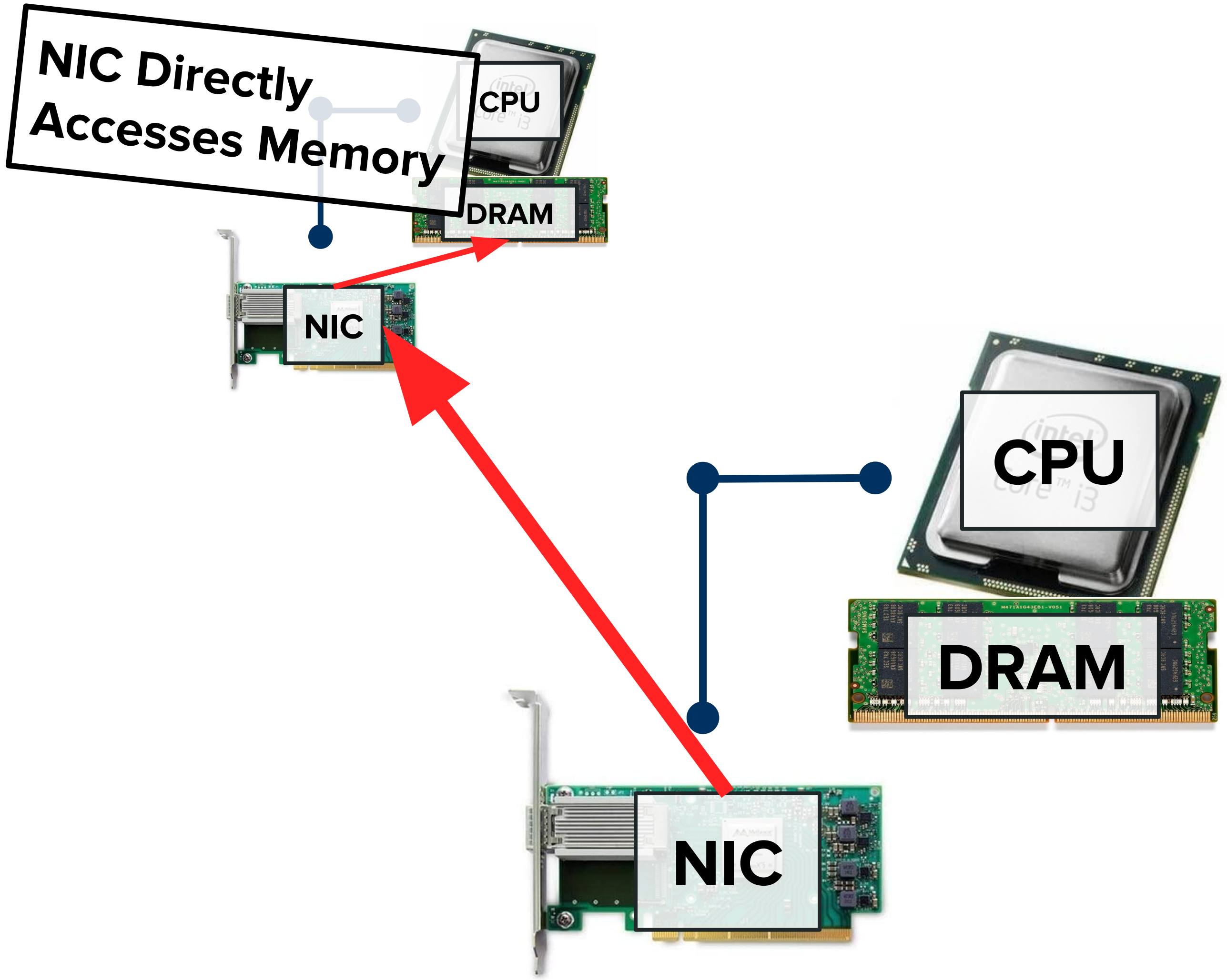

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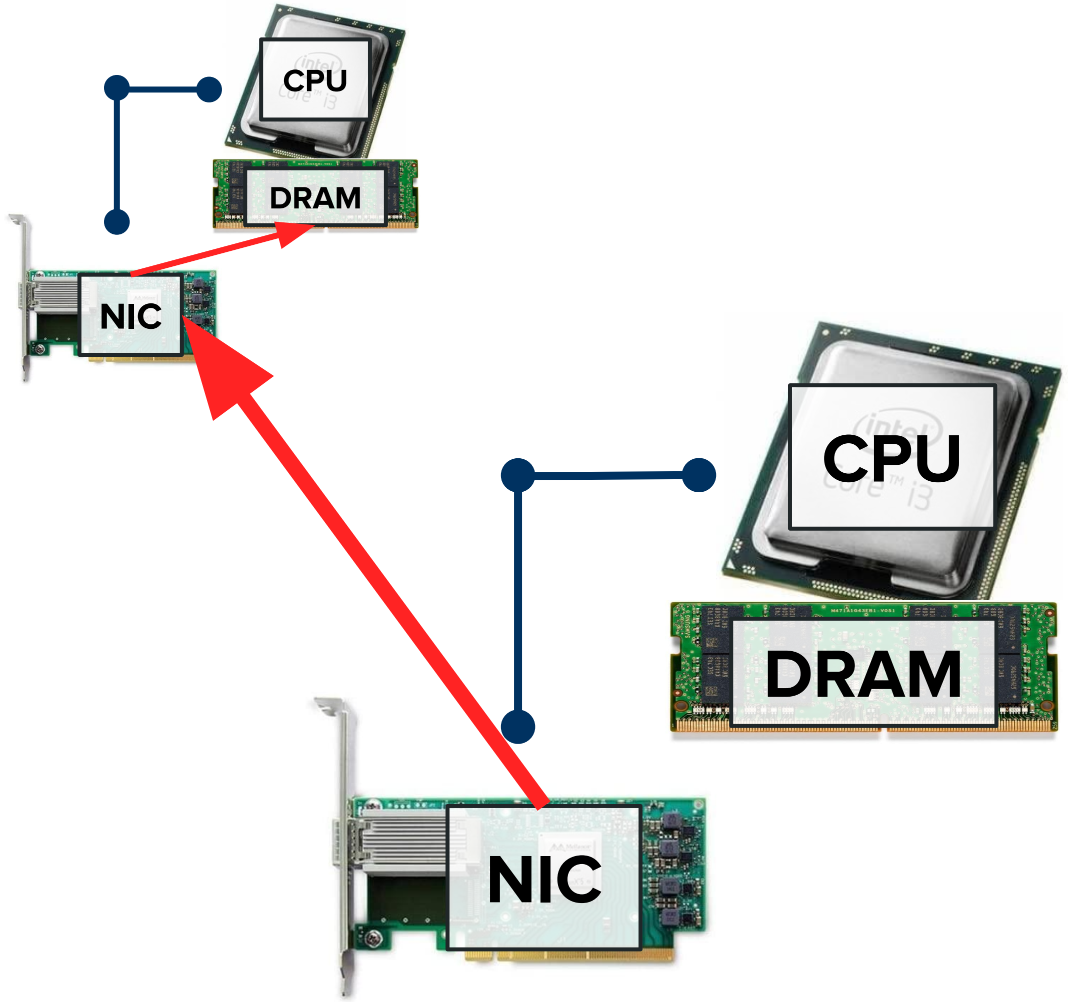

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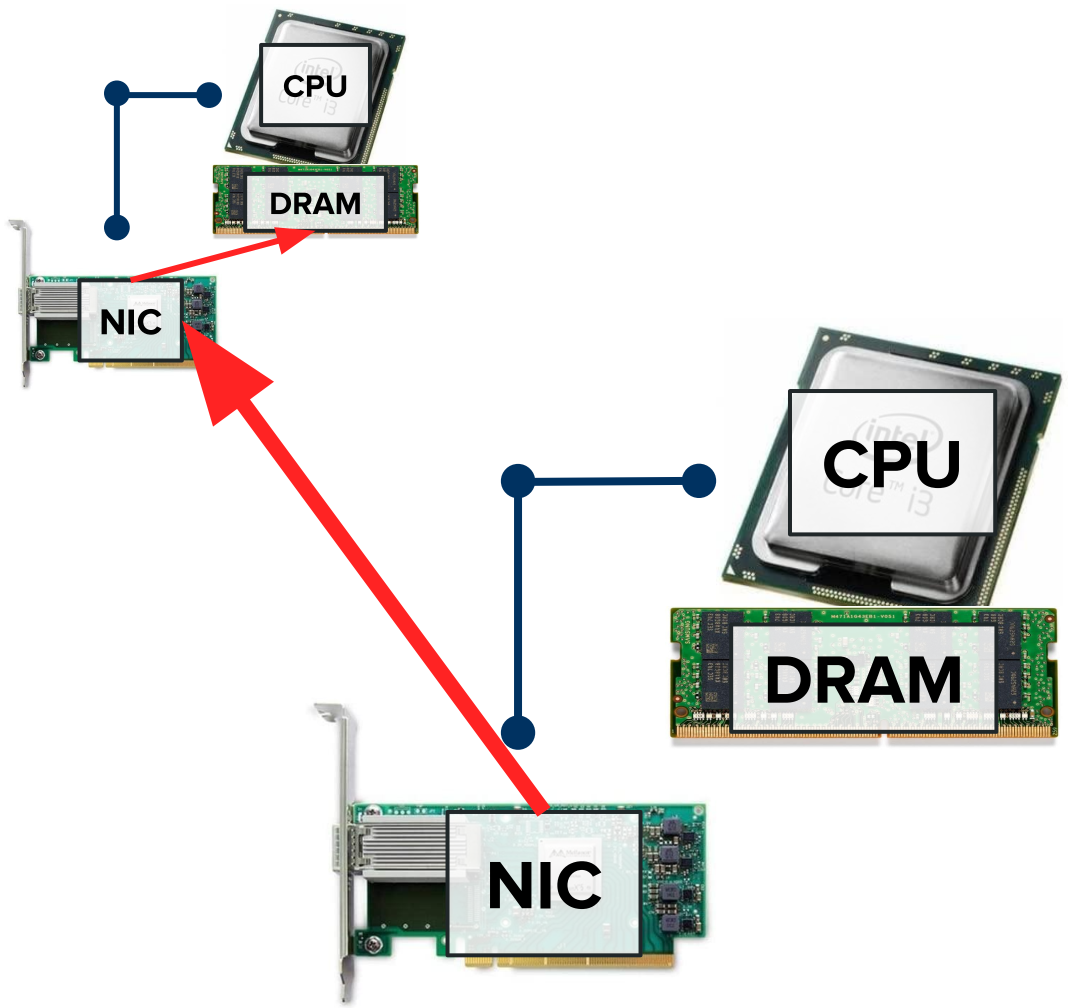

Background: Parallel Programs

Parallel Programs

- **Multiple processes** are executing a program
- Each process has its own **memory space**
- Two methods of communication: **shared memory** and **message passing**

A SPMD Program

```
#include <bcl/bcl.hpp>
#include <fmt/core.h>

int main(int argc, char** argv) {
  BCL::init();

  fmt::print(“Hello from rank {}\n”,
             BCL::rank());

  BCL::finalize();
  return 0;
}
```

A SPMD Program

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#include <bcl/bcl.hpp>
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int main(int argc, char**
  BCL::init();

  fmt::print("Hello from
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  BCL::finalize();
  return 0;
}
```

Output: `mpirun -n 4 ./test`

```
$ mpirun -n 4 ./test
Hello from rank 0
Hello from rank 1
Hello from rank 2
Hello from rank 3
```

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}
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Output: `mpirun -n 4 ./test`

```
$ mpirun -n 4 ./test
Hello from rank 0
Hello from rank 1
Hello from rank 2
Hello from rank 3
```

Each process runs the same program.

A SPMD Program

```
#include <bcl/bcl.hpp>
#include <fmt/core.h>

int main(int argc, char** argv) {
  BCL::init();

  if (BCL::rank() == 2) {
    fmt::print("Rank 2 says hi!\n");
  }

  BCL::finalize();
  return 0;
}
```

A SPMD Program

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int main(int argc, char** a
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```
$ mpirun -n 4 ./test
Rank 2 says hi!
```

Only one process runs portion in if statement.

Remote Pointers

Remote Pointers

- Remote pointers are **smart pointer classes** that **may reference remote memory**

1) We can use a remote pointer to do an **RDMA get / put**
2) Can also perform **atomic operations** (e.g. fetch-and-add, compare-and-swap)
3) If pointing to **shared memory in the current process**, can convert to regular (local) pointer

Building a Remote Pointer Type

```
template <typename T>
struct GlobalPtr {

  ...

private:
  size_t rank_;
  size_t offset_;
};
```

Remote Pointer Types

```
template <typename T>
struct GlobalPtr {

  ...

private:
  size_t rank_;
  size_t offset_;
};
```

```
void memcpy(void* dest,
            GlobalPtr<void> src,
            size_t n) {
  // Issue remote get operation to
  // copy `n` bytes from `src` to `dest`
  backend::remote_get(dest, src, n, ...);
}
```

Remote Pointer Types

- Can build **memcpy** to support **reading/writing** from/to remote memory

- Can write fetch_and_op, compare_and_swap, etc. **atomic ops**

- Can **dereference** remote pointer

Remote Pointer Types

```
template <typename T>
struct GlobalPtr {

  ...

  GlobalRef<T> operator*() {
    return GlobalRef<T>(*this);
  }

private:
  size_t rank_;
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Remote Pointer Types

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struct GlobalPtr {

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private:
  size_t rank_;
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```

Not possible to return a regular T&, since memory may be remote.

Remote Pointer Types

```
template <typename T>
struct GlobalPtr {

  ...

  GlobalRef<T> operator
    return GlobalRef<T>
  }

private:
  size_t rank_;
  size_t offset_;
};
```

```
template <typename T>
struct GlobalRef {
  T& operator=(const T& value) {
    memcpy(ptr_, &value, sizeof(T));
    return value;
  }

  operator T() const {
    T value;
    memcpy(&value, ptr_, sizeof(T));
    return *static_cast<T*>(value);
  }

private:
  GlobalPtr<T> ptr_;
};
```

Remote Pointer Types

- Allow referencing memory on **another process**
- Can support **memcpy**, **atomics**, pointer arithmetic, etc.
- Can support **dereferencing**, but must have **custom reference type** (cannot use **T&** across nodes)
- Limited to **trivially copyable** types

BCL Global Pointer Example

```
BCL::GlobalPtr<int> ptr = nullptr;

if (BCL::rank() == 0) {
  ptr = BCL::alloc<int>(BCL::nprocs());
}

ptr = BCL::broadcast(ptr, 0);

ptr[BCL::rank()] = BCL::rank();
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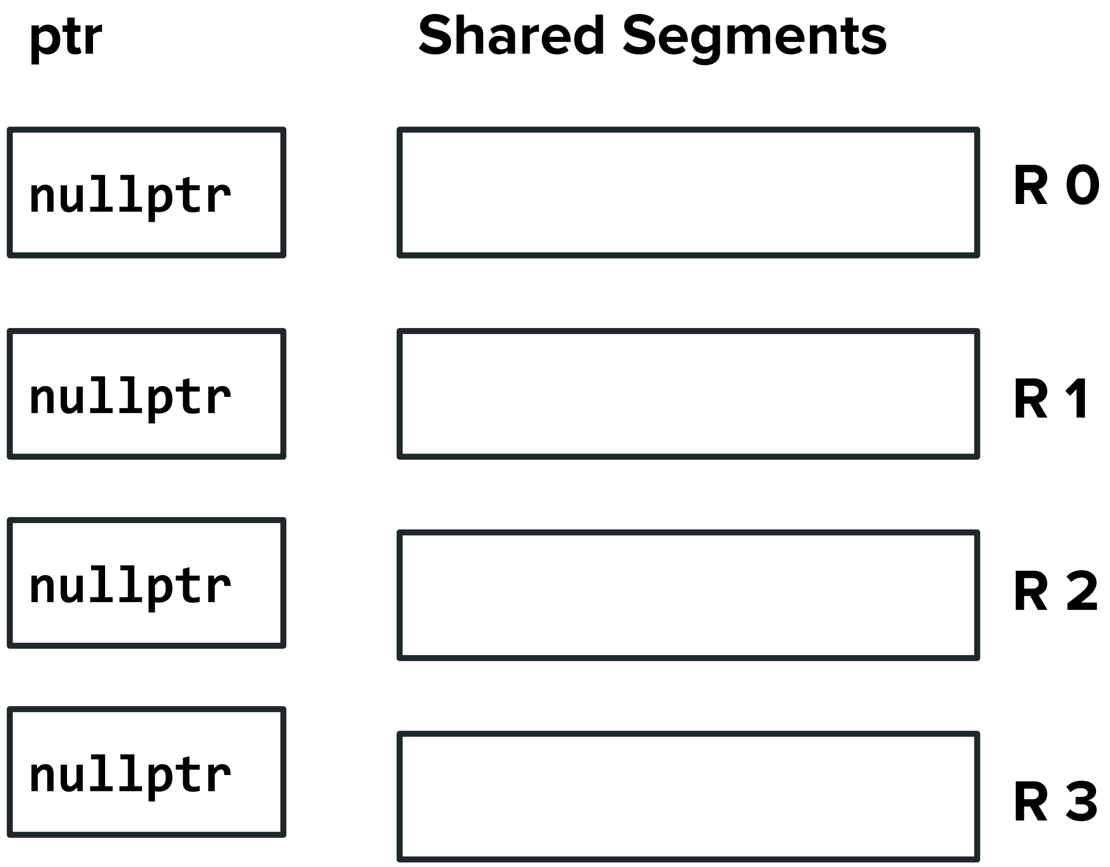

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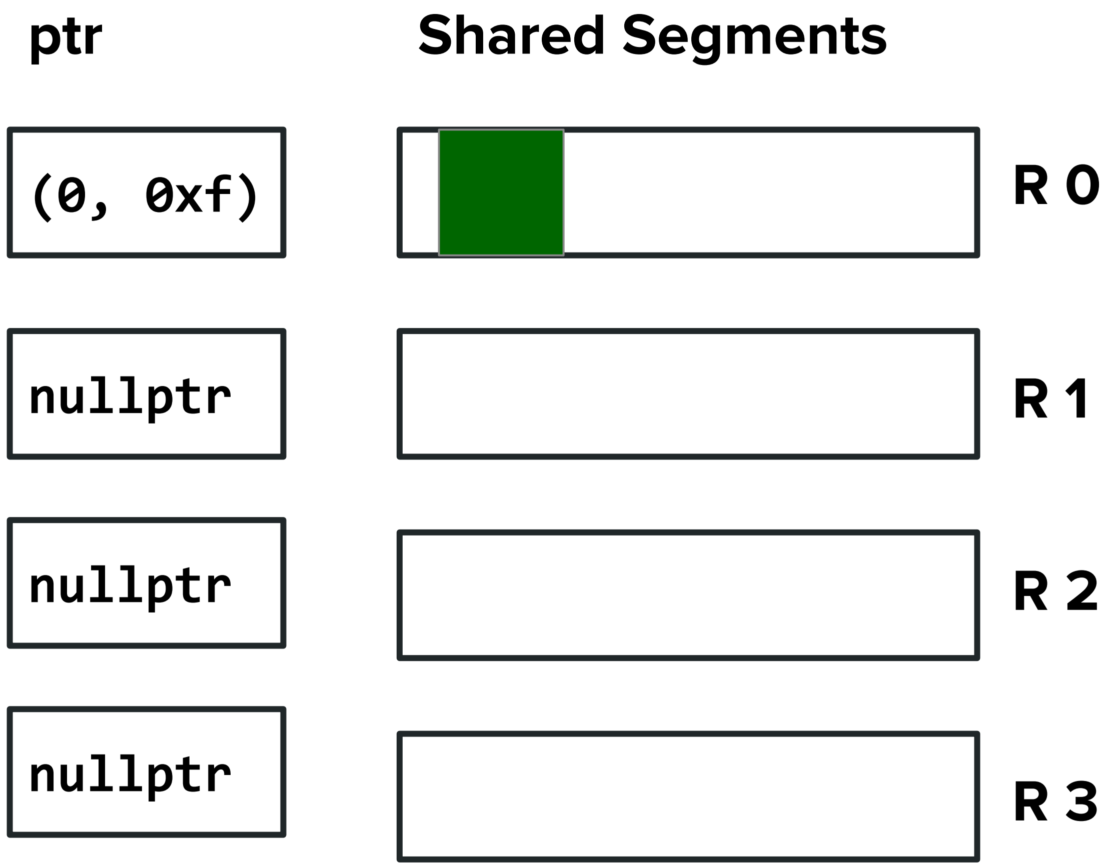

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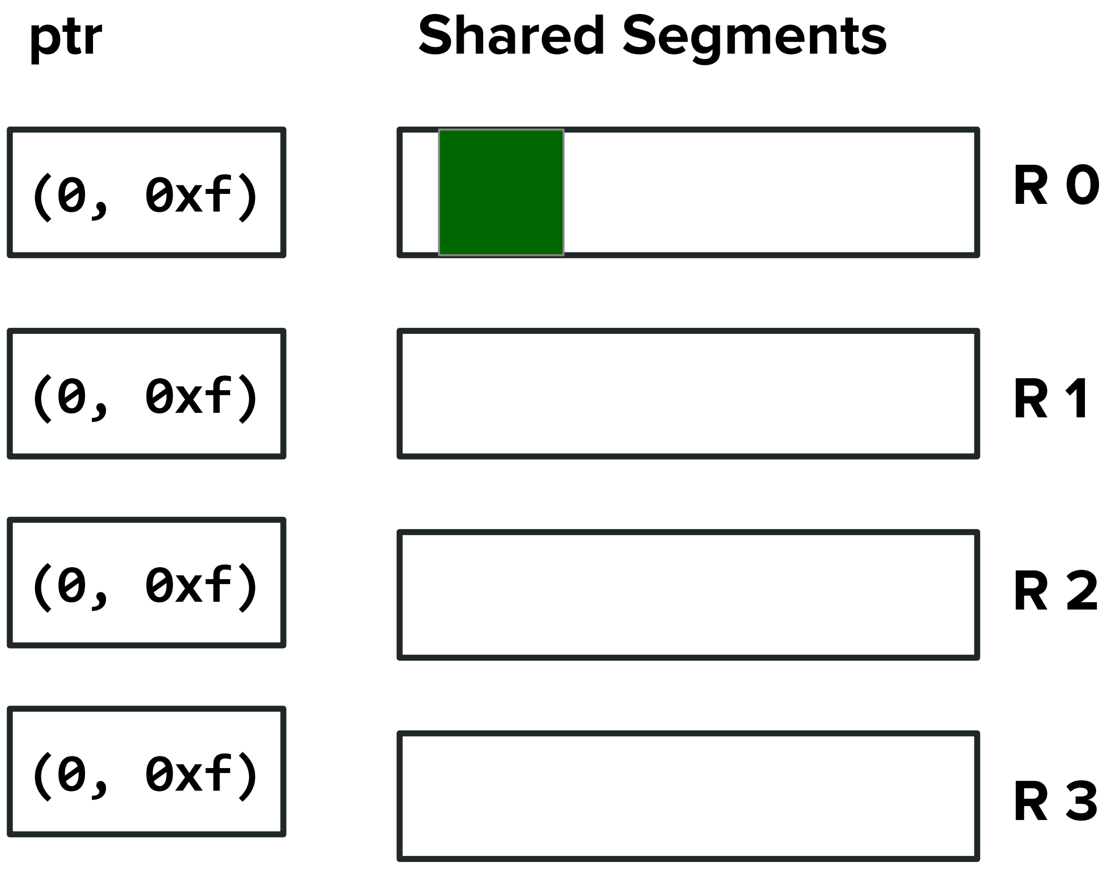

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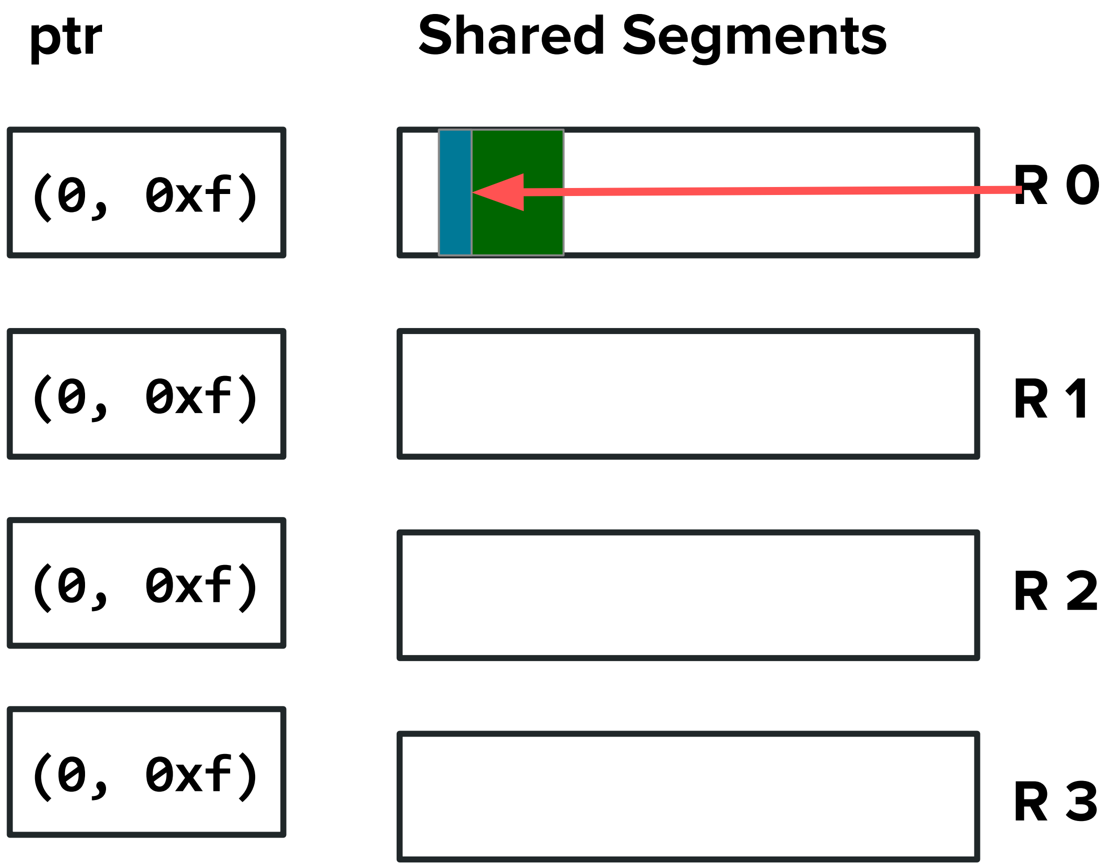

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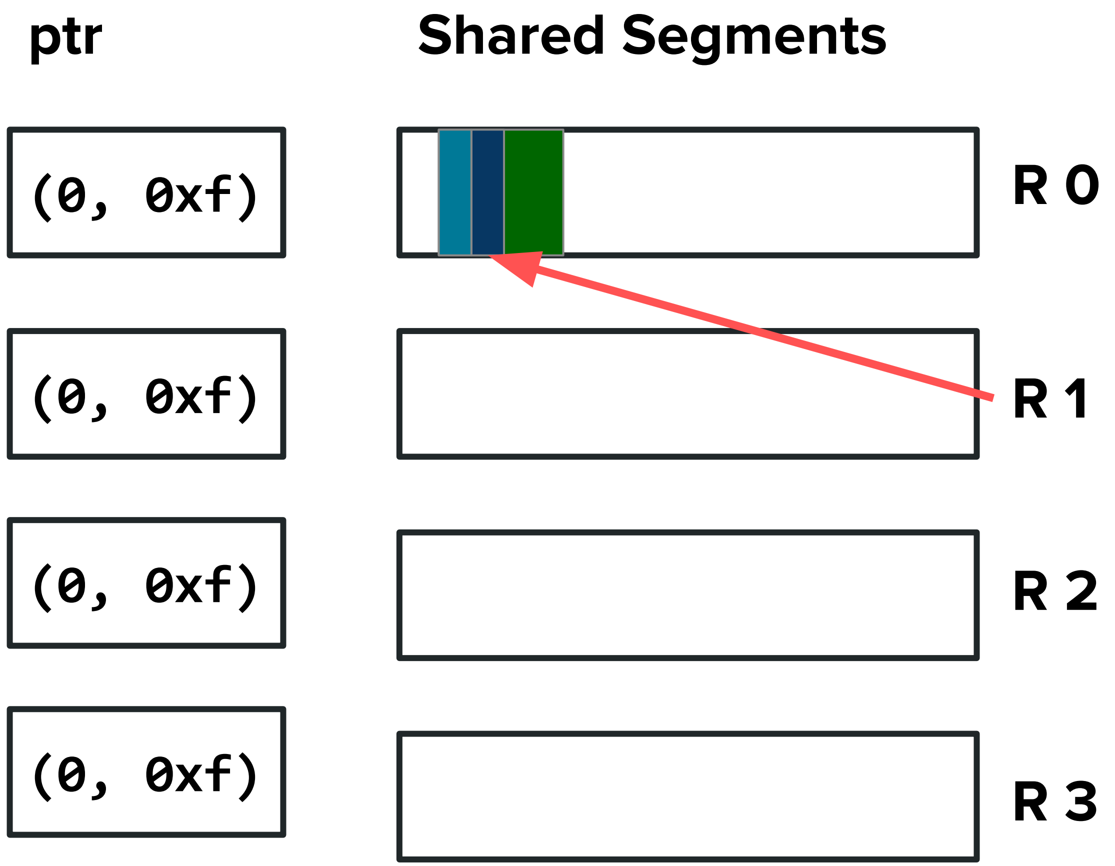

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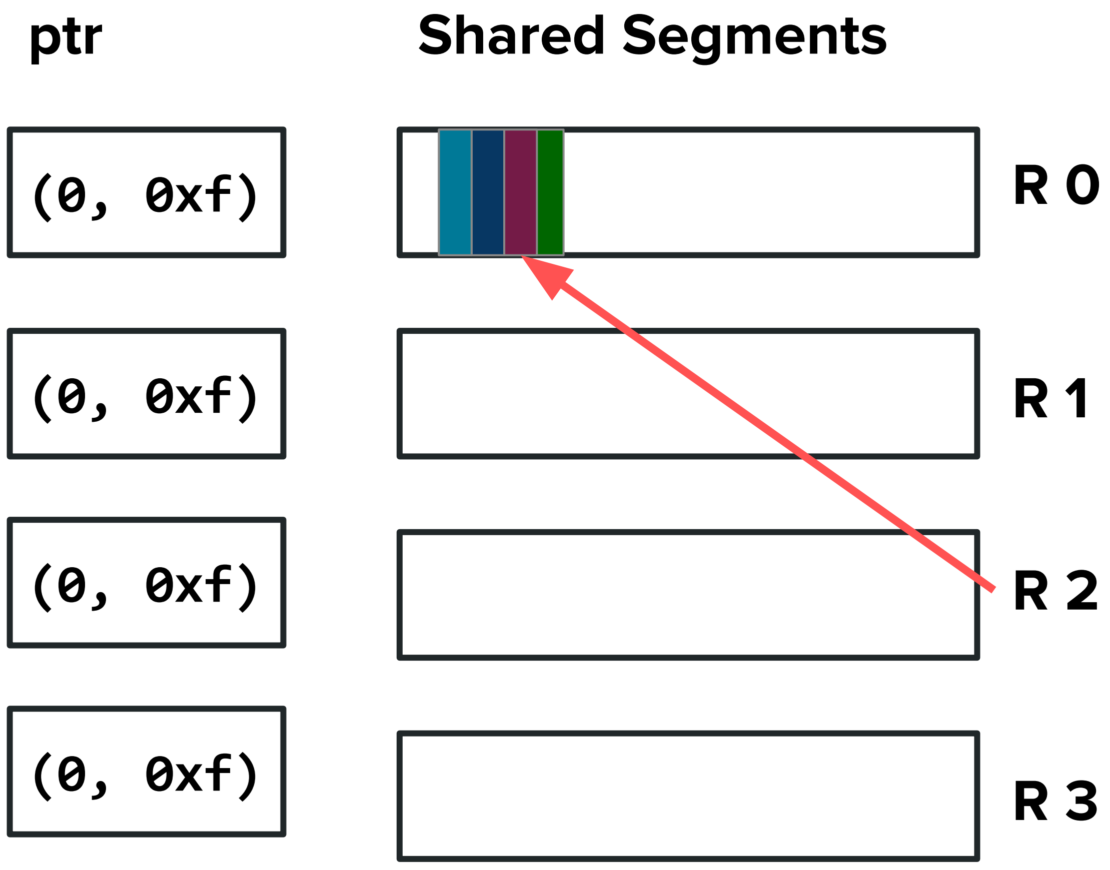

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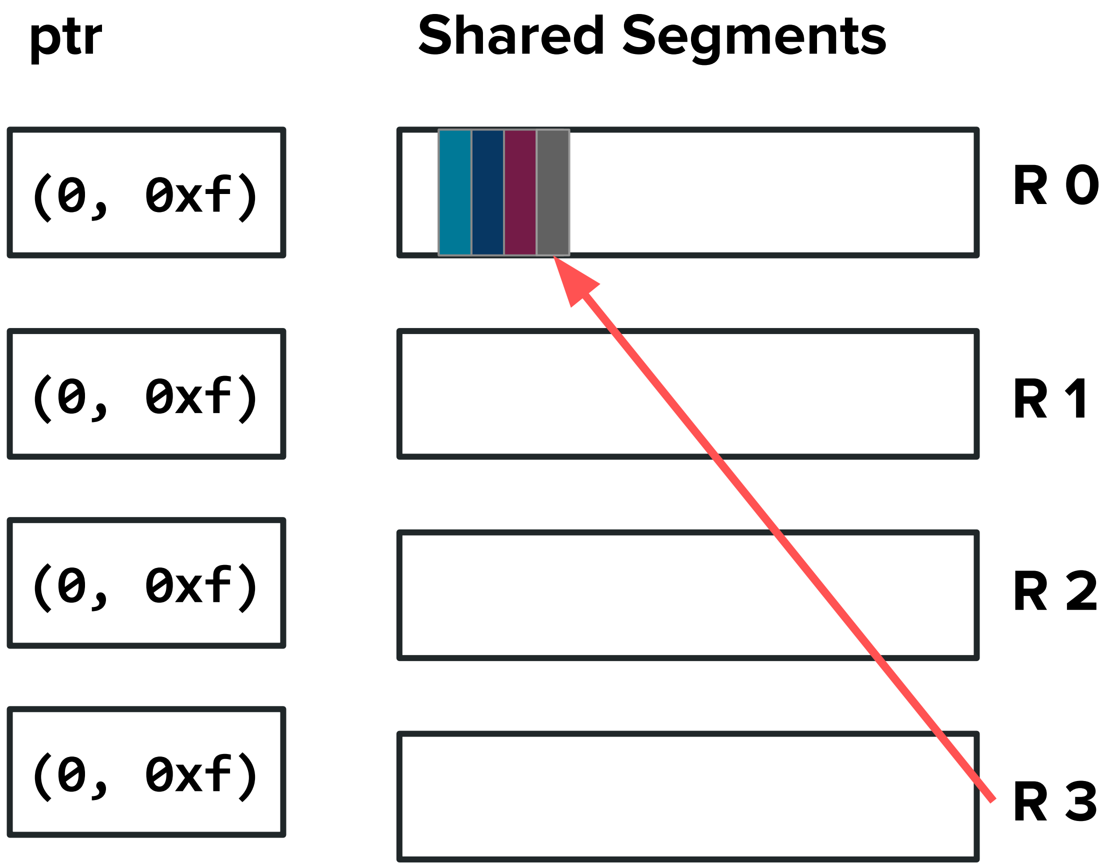

Data Structures

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- Data structures are **split into two types**:

1) **Remote** data structures
   - Data **located** on a **single process**
   - **Globally** accessible

2) **Distributed** Data structures
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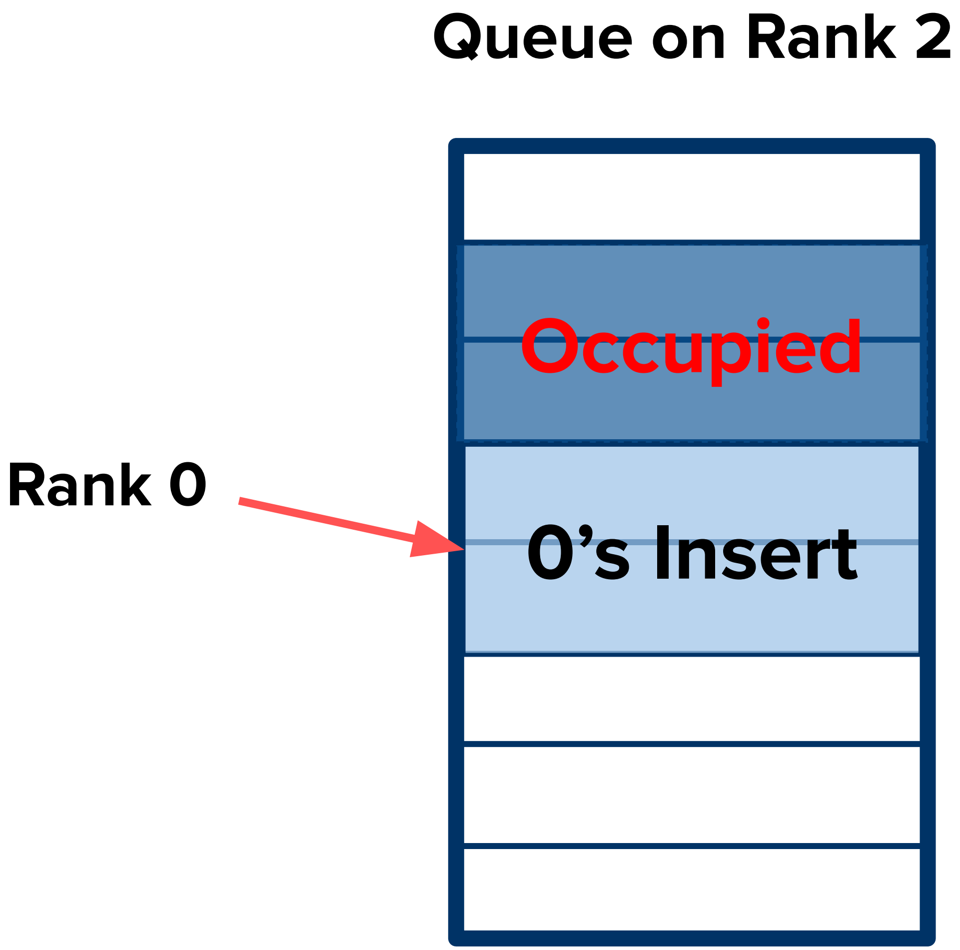

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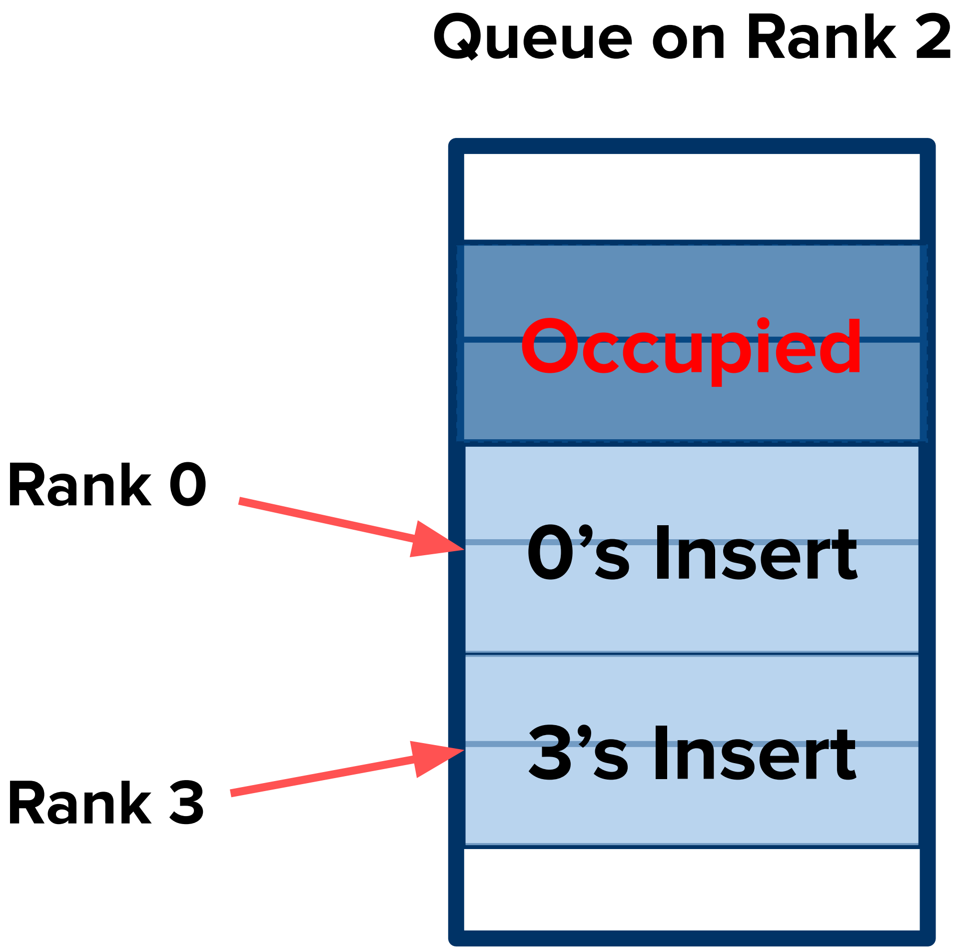

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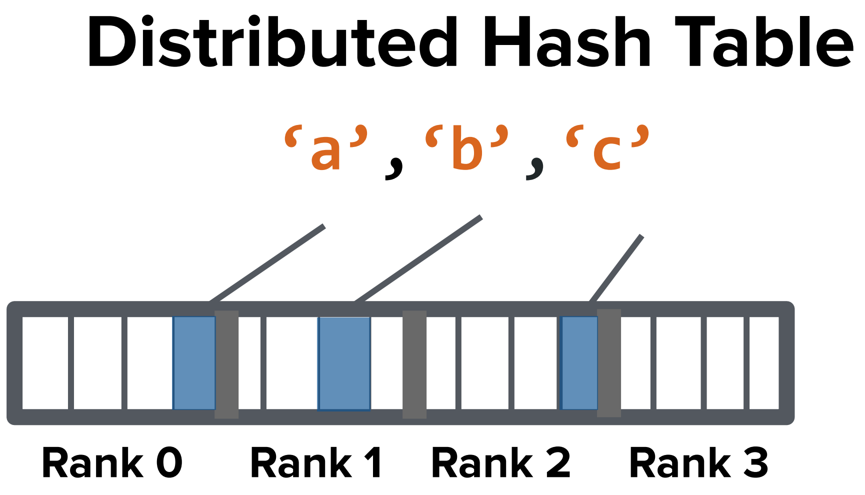

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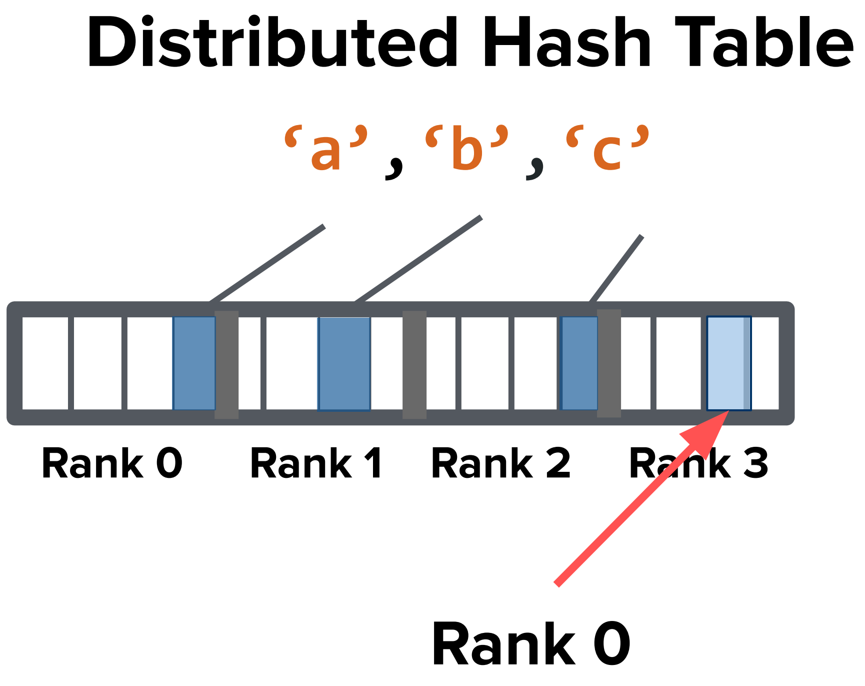

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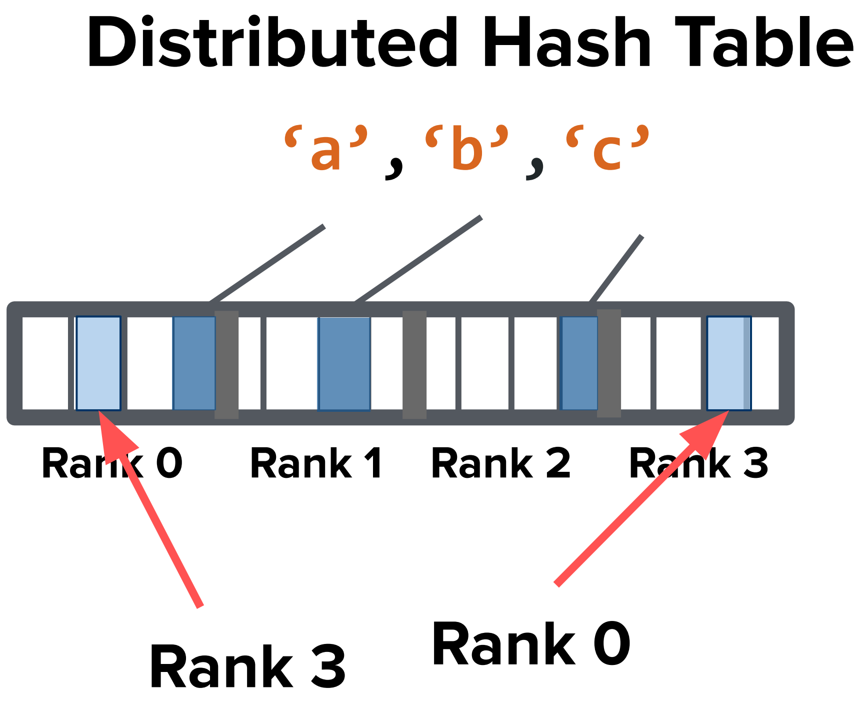

Data Structures

- **Constructors/destructors** that must be called **collectively**
- Each process has **global view** of data structure
- **Most methods** (e.g. insert, find) not collective

```
#include <bcl/bcl.hpp>

int main(int argc, char **argv) {
  BCL::init();

  BCL::HashMap<std::string, int> map(BCL::nprocs());

  if (BCL::rank() == 0) {
    for (int i = 0; i < BCL::nprocs(); i++) {
      map.insert({std::to_string(i), i});
    }
  }
  ...
}
```

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  if (BCL::rank() == 0) {
    for (int i = 0; i < BCL::nprocs(); i++) {
      map.insert({std::to_string(i), i});
    }
  }
  ...
}
```

Each process invokes constructor collectively

Data Structures

- **Constructors/destructors** that must be called **collectively**
- Each process has **global view** of data structure
- **Most methods** (e.g. insert, find) not collective

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}
```

Rank 0 inserts

Iteration - Global and Local

- “**Global Iteration**” supported over **distributed range** of elements

- “**Local iteration**” supported over **local range** of elements

```cpp
#include <bcl/bcl.hpp>

int main(int argc, char **argv) {
  BCL::init();

  BCL::HashMap<std::string, int> map = ...;

  if (BCL::rank() == 0) {
    for (auto iter = map.begin();
              iter != map.end(); ++iter) {
      auto&& [key, value] = *iter;
      fmt::print("{}: {}", key, value);
    }
  }
  ...
}
```

Iteration - Global and Local

- "**Global Iteration**" supported over **distributed range** of elements

- "**Local iteration**" supported over **local range** of elements in process' memory

```
#include <bcl/bcl.hpp>

int main(int argc, char **argv) {
  BCL::init();

  BCL::HashMap<std::string, int> map = ...;

  if (BCL::rank() == 0) {
    for (auto iter = map.local_begin();
         iter != map.local_end(); ++iter) {
      auto&& [key, value] = *iter;
      fmt::print("{}: {}", key, value);
    }
  }
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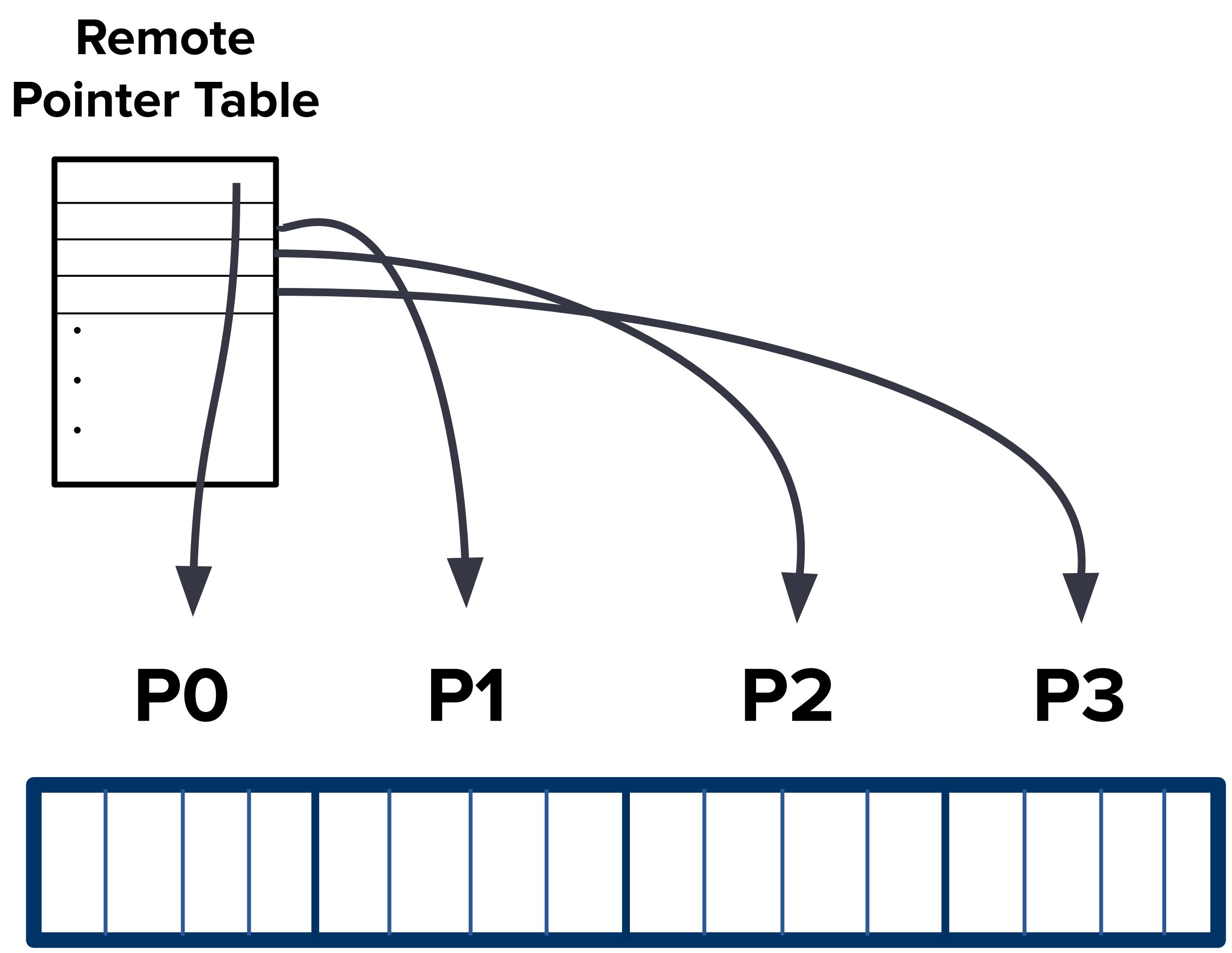
```

Distributed Hash Table

- Open addressing -- hash table buckets are split among procs
- To manipulate a bucket, **directly read/write using RDMA**.
- **Resizing** must be done collectively



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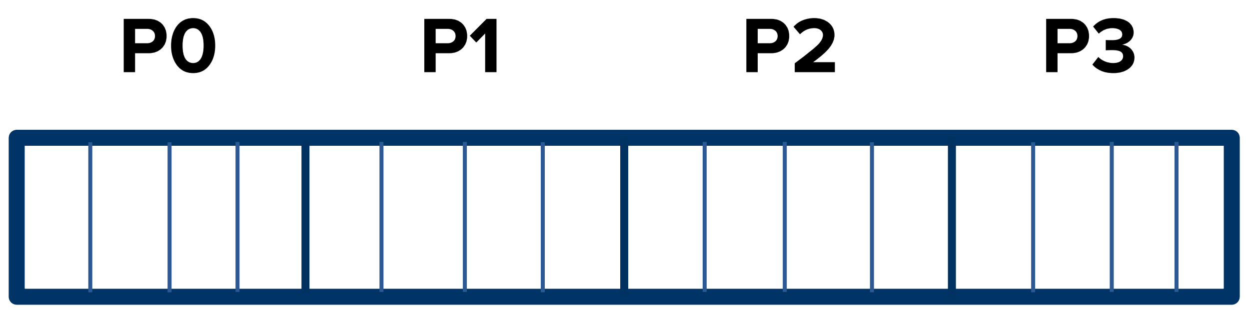

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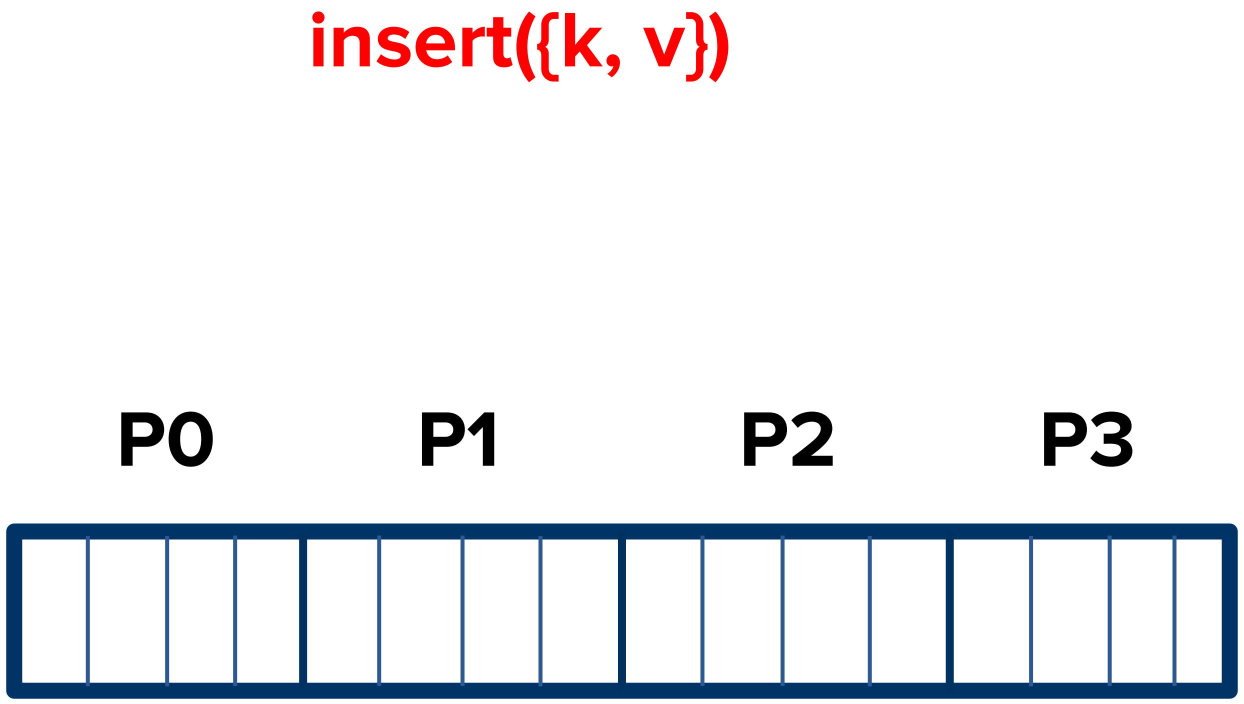

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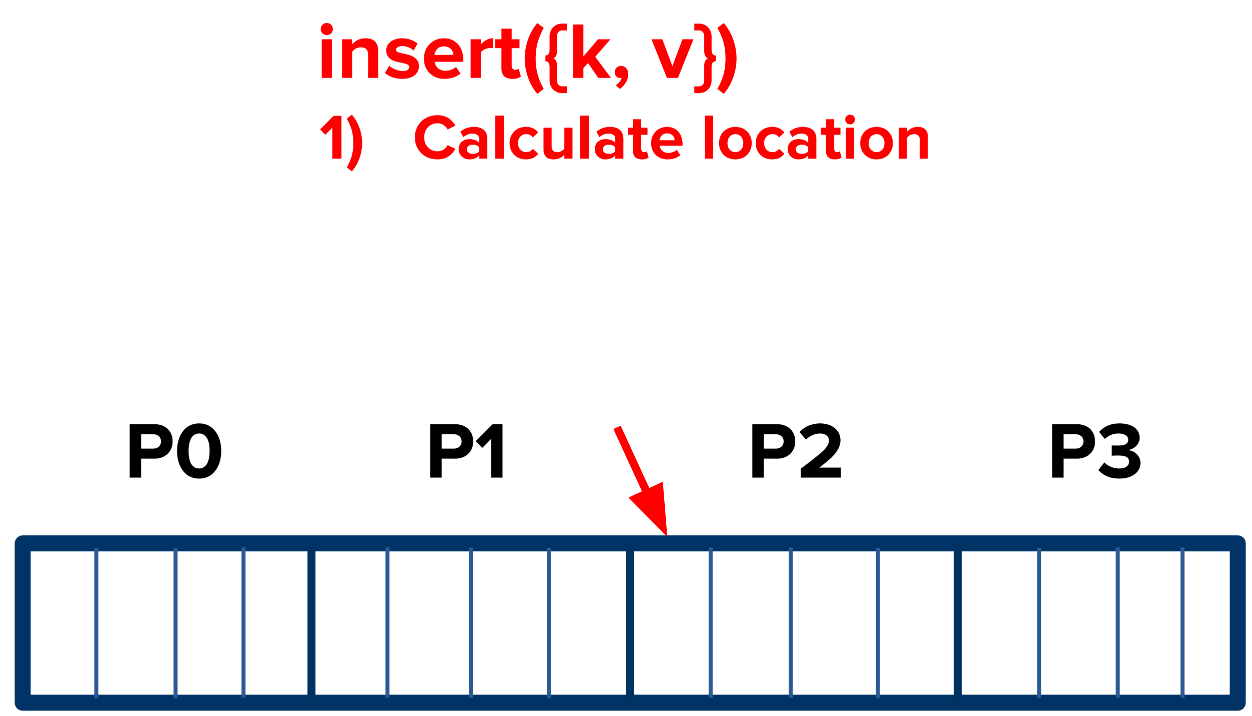

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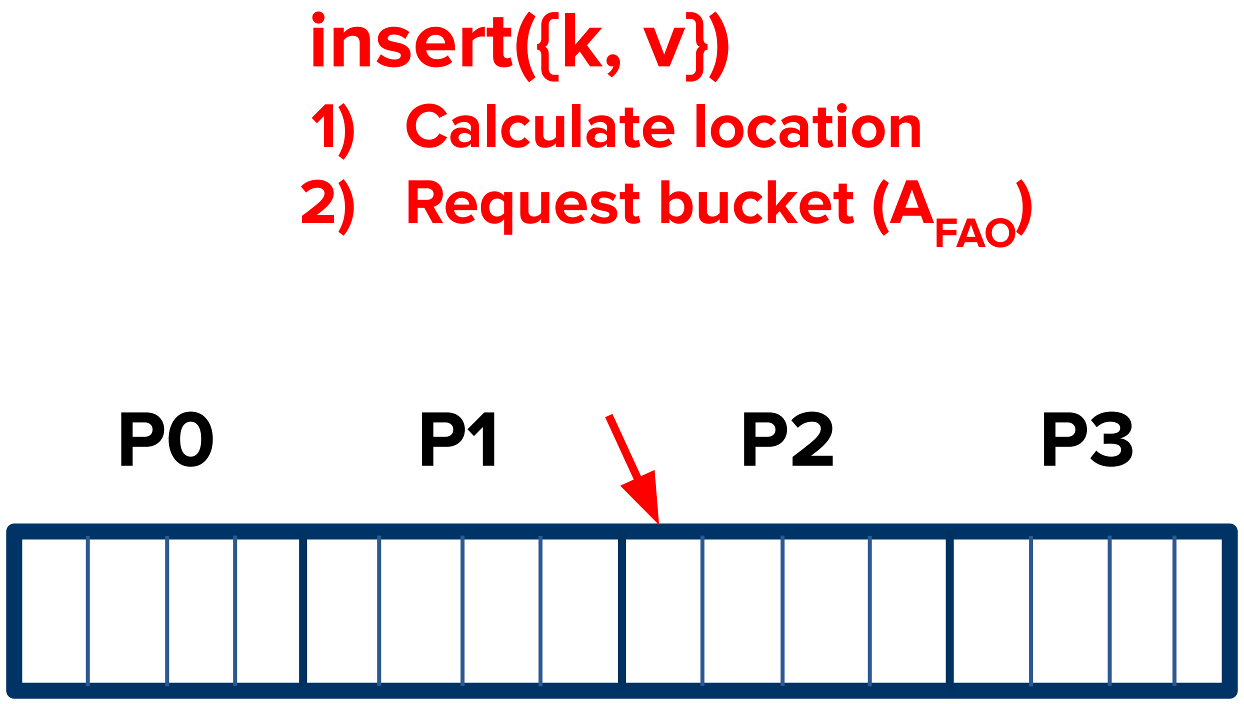

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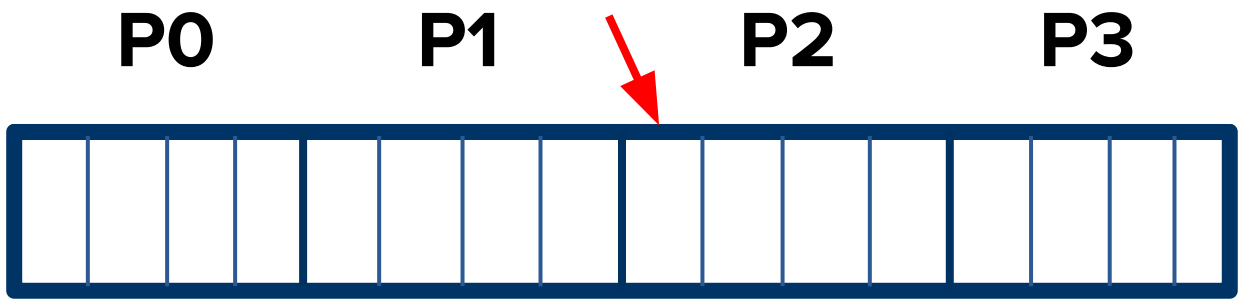

[1] ICPP'19, Brock, et. al

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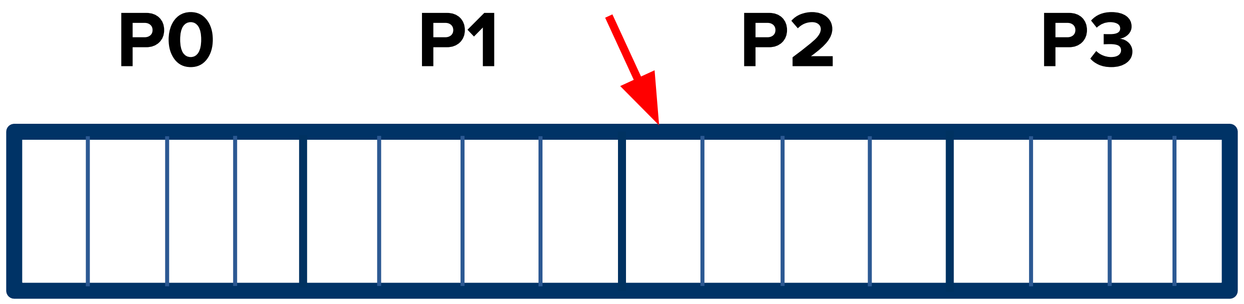

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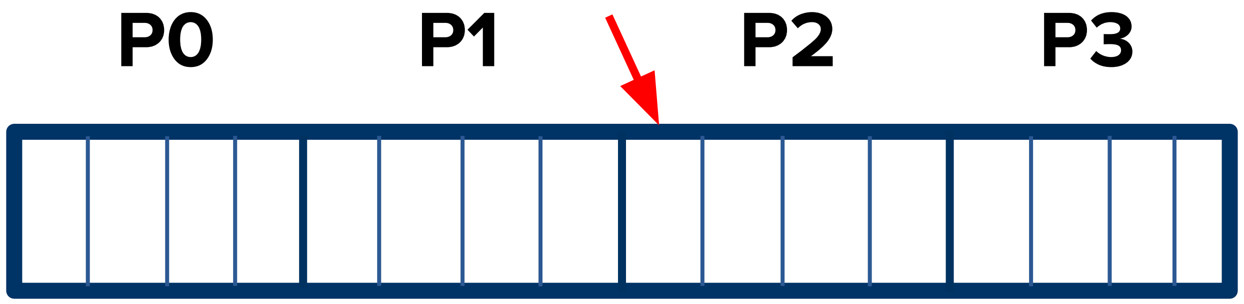

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Latency bound!
Can we do better?

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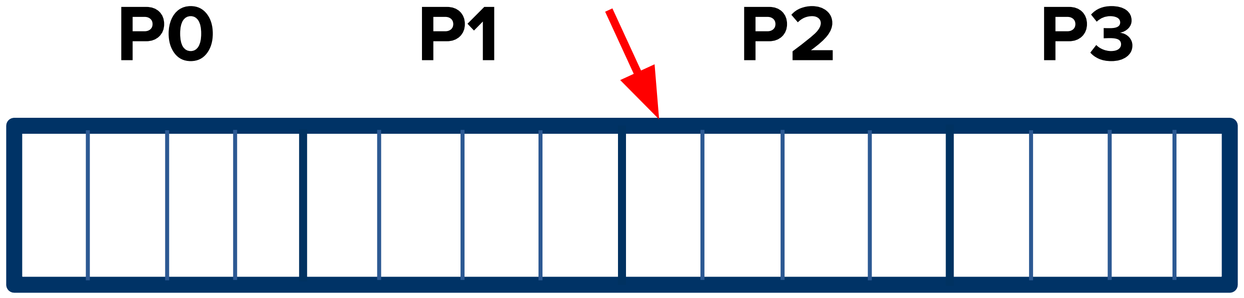

HashMapBuffer

- Constructed from a **HashMap**

- Similar to a **range adaptor**, but relaxes when operations take place

- **Aggregates** fine-grained insertions into large transfers

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int main(int argc, char **argv) {
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  for (const auto&& value : data) {
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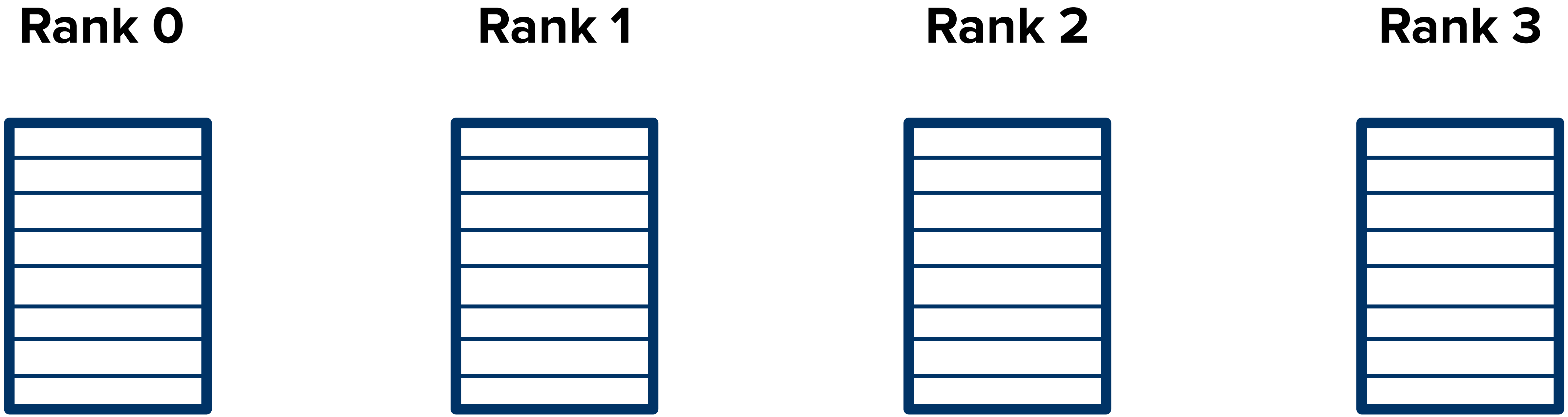
Bulk Transfers Using Queues

Queues allow **asynchronous all-to-all communication**



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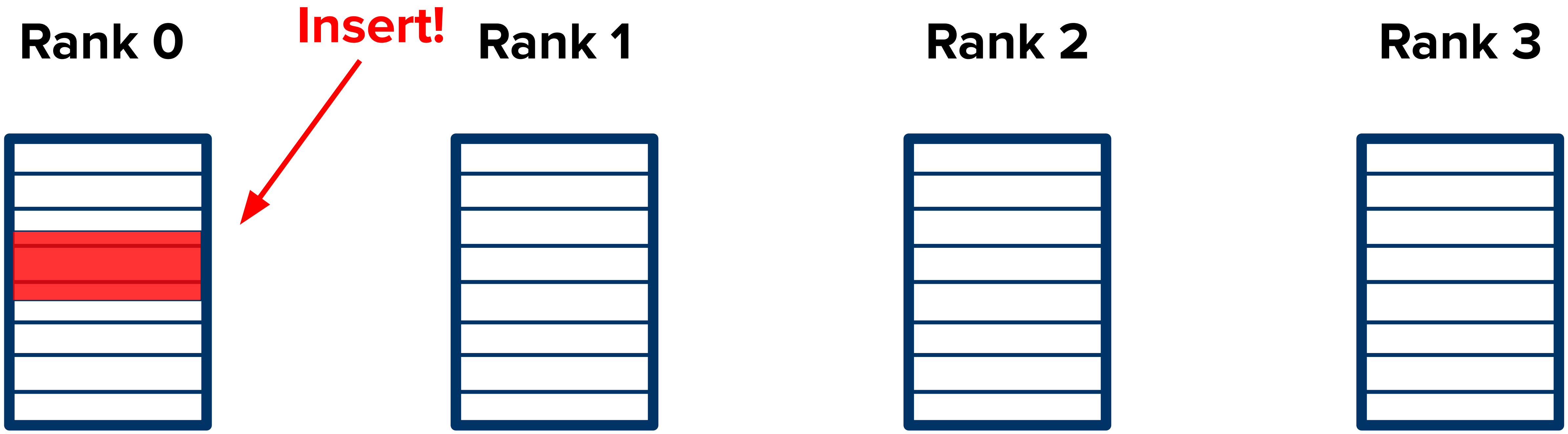

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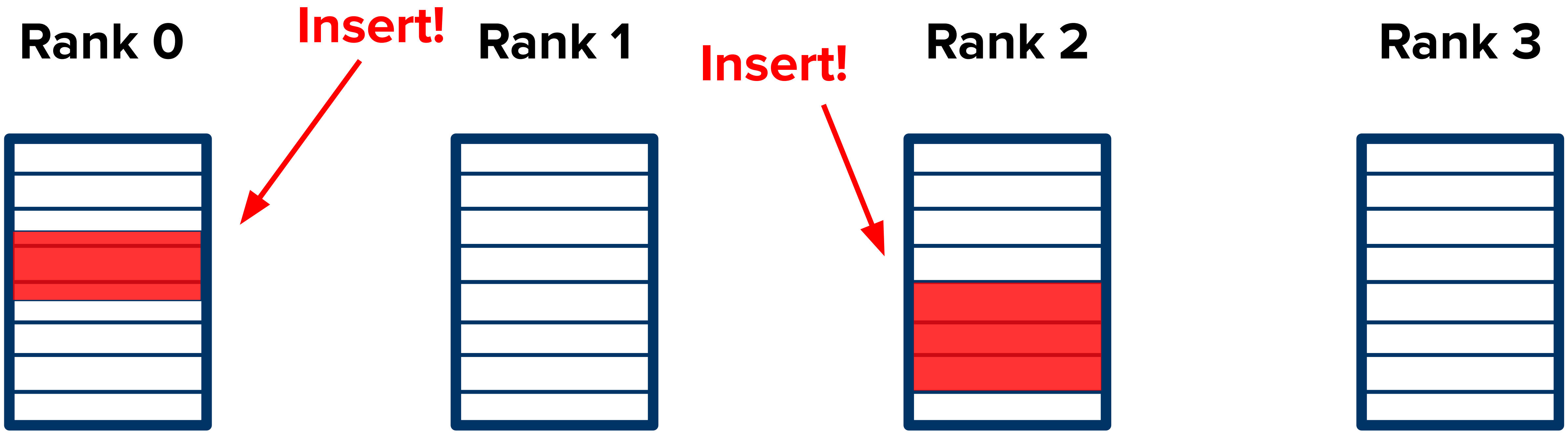

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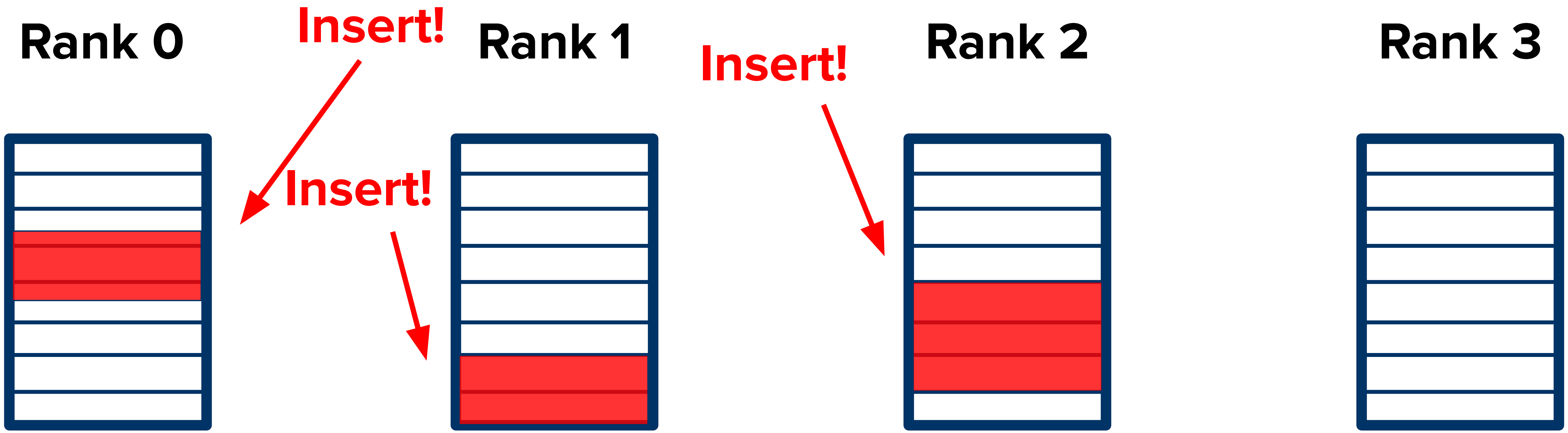
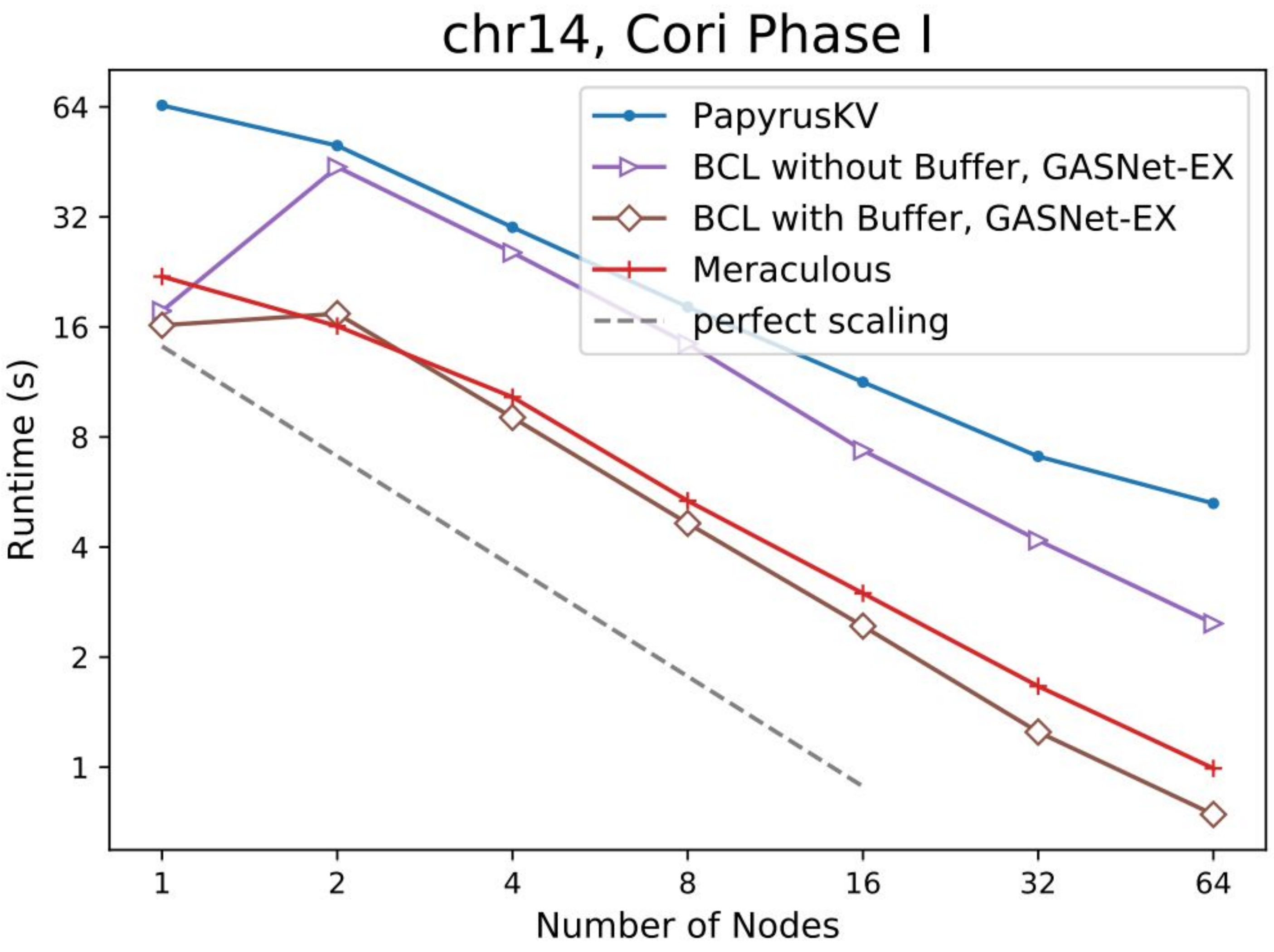


Genomics Benchmark



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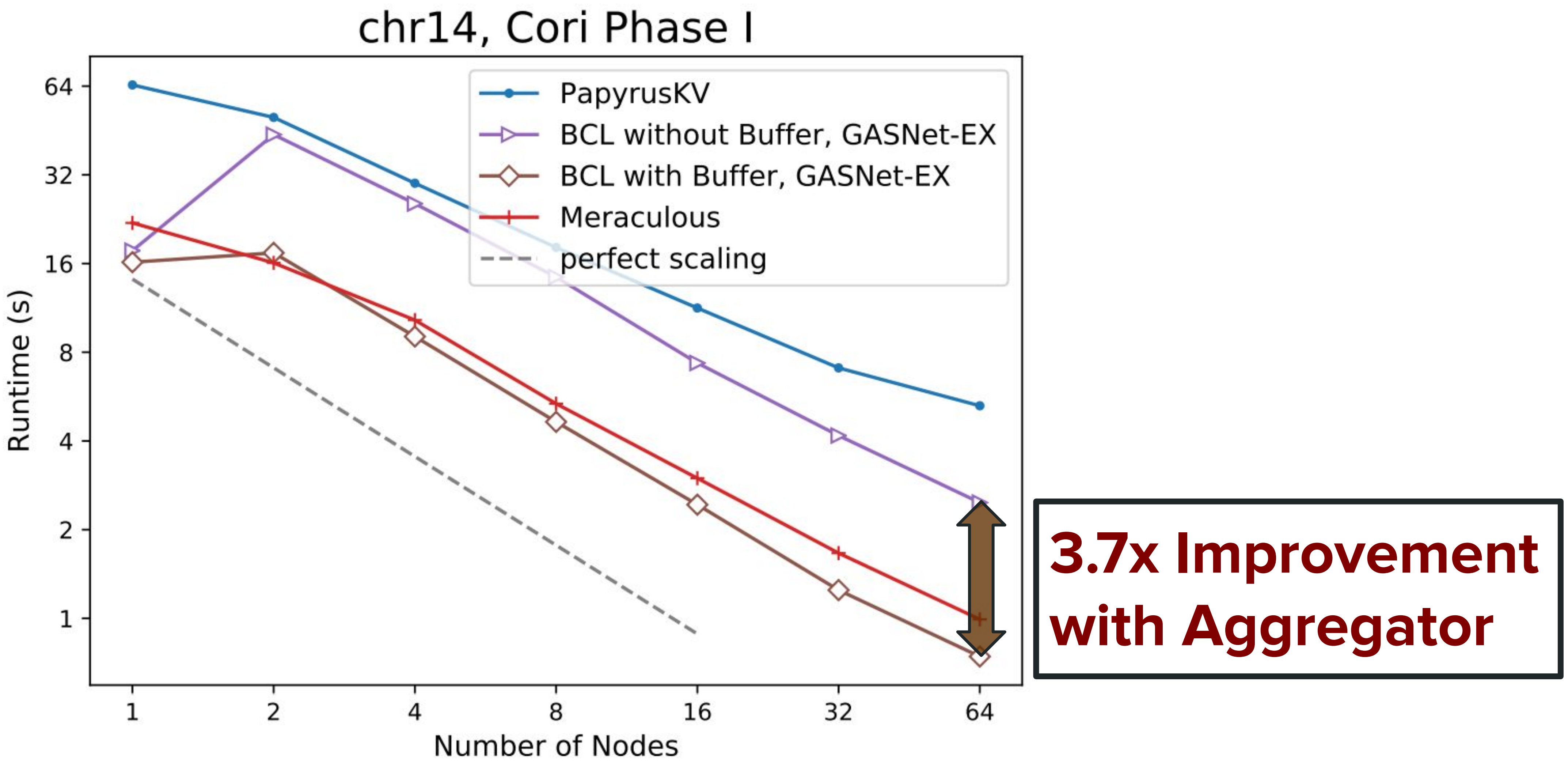

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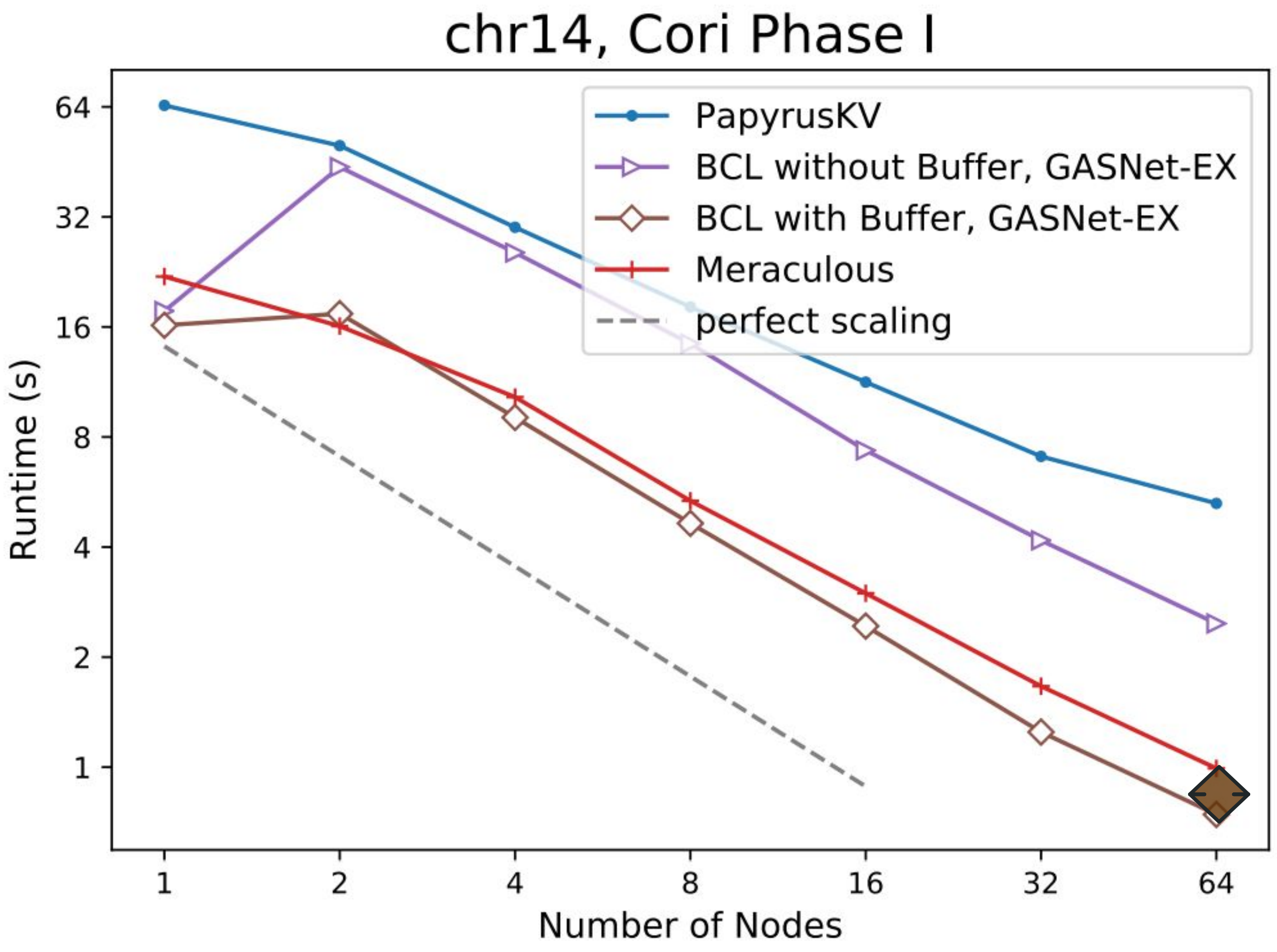
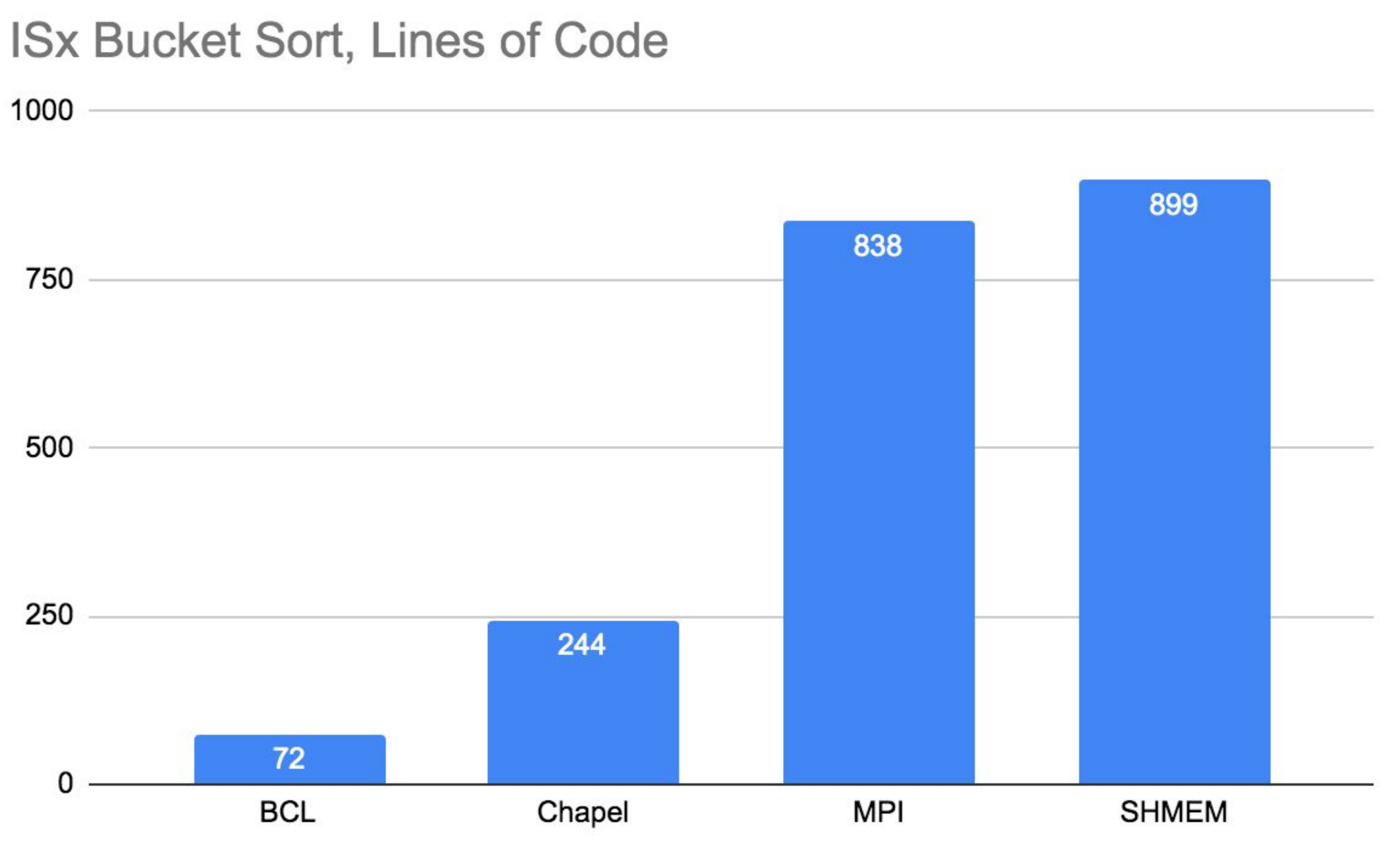
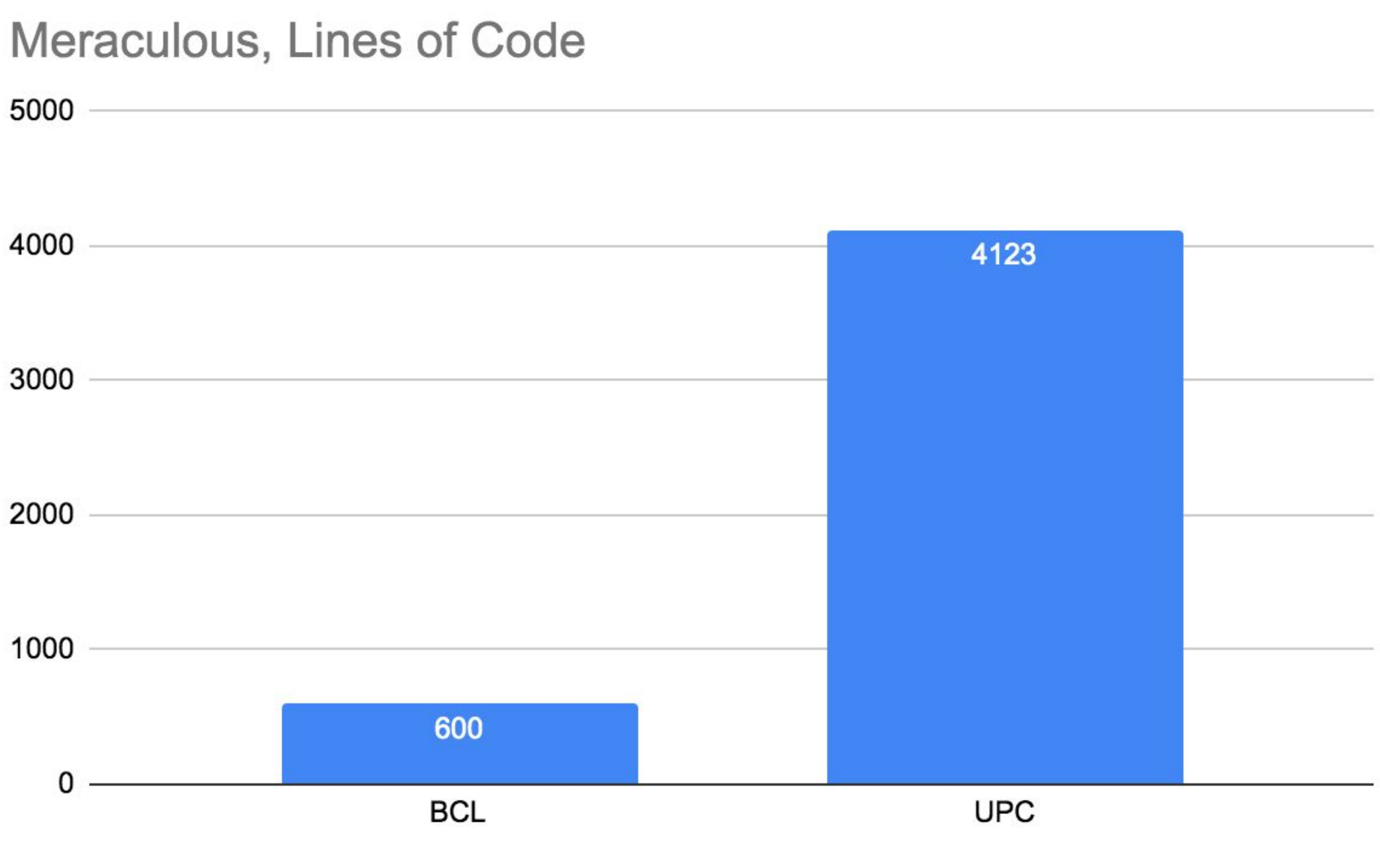


Match Perf. of Expert-Tuned Impl.

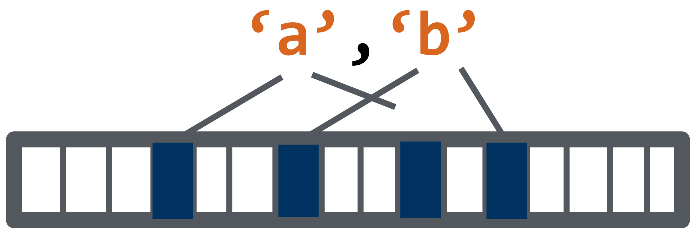
[1] ICPP’19, Brock, et. al

Comparison: Lines of Code

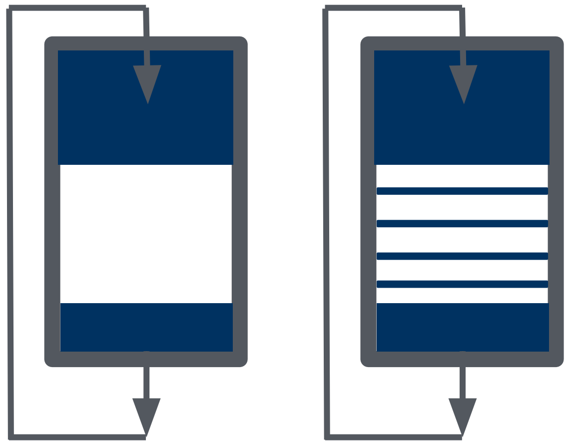




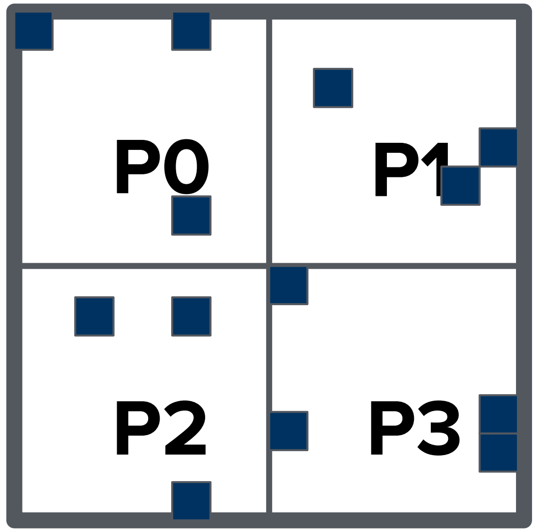
Some Data Structures We’ve Worked On



Bloom Filters

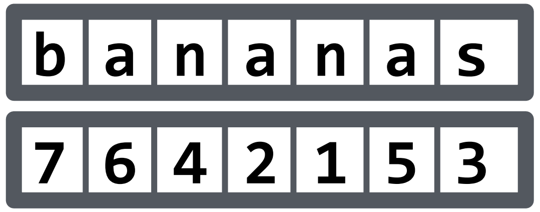


Queues

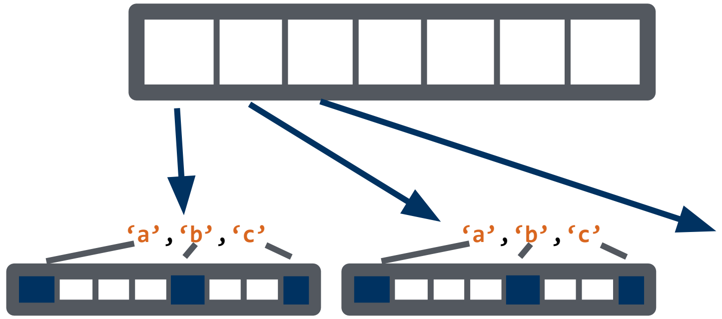


Dense and Sparse Matrices

. . .



Suffix Arrays



Hash Tables

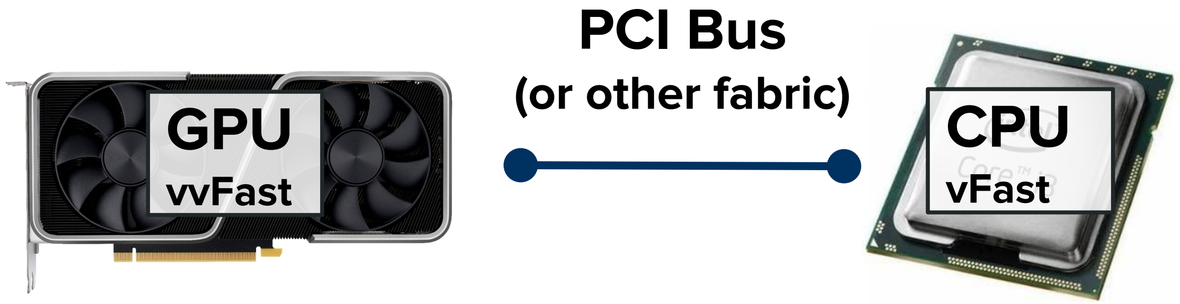
PGAS on GPUs

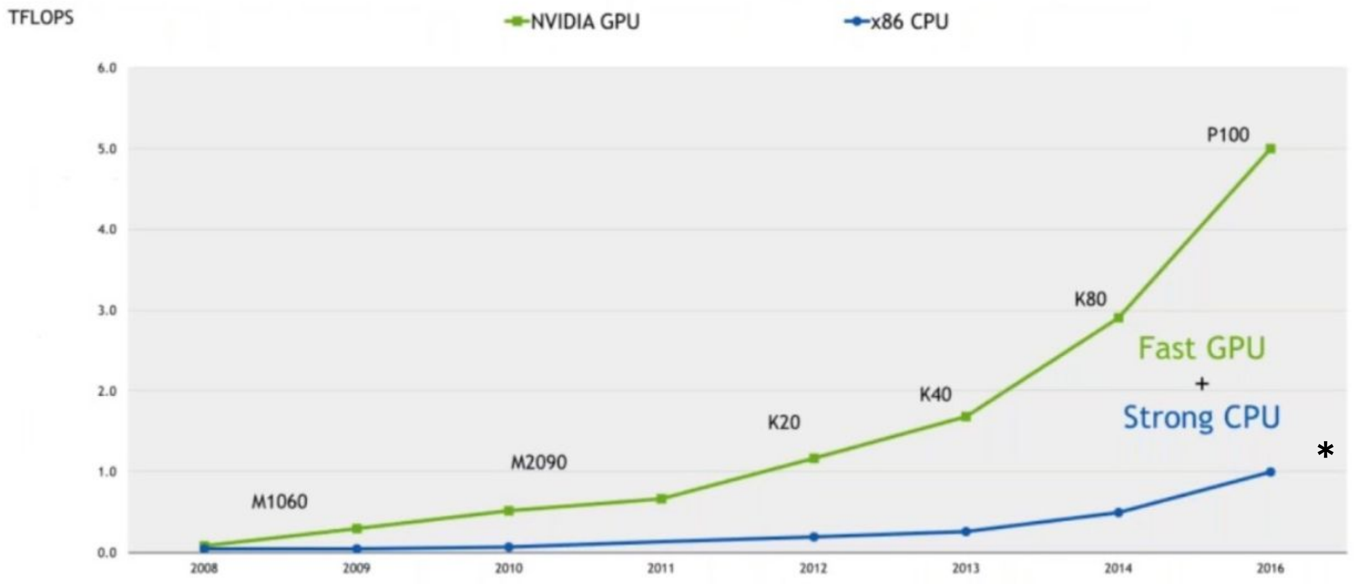
GPUs as a First-Class Computing Resource

- **GPUs** play an important role in modern large-scale computing systems

- **All three** DOE exascale systems **will use GPUs**

- **~10x** more compute, BW





* John Barco, Nvidia. https://youtu.be/wvk9zYbOmYc

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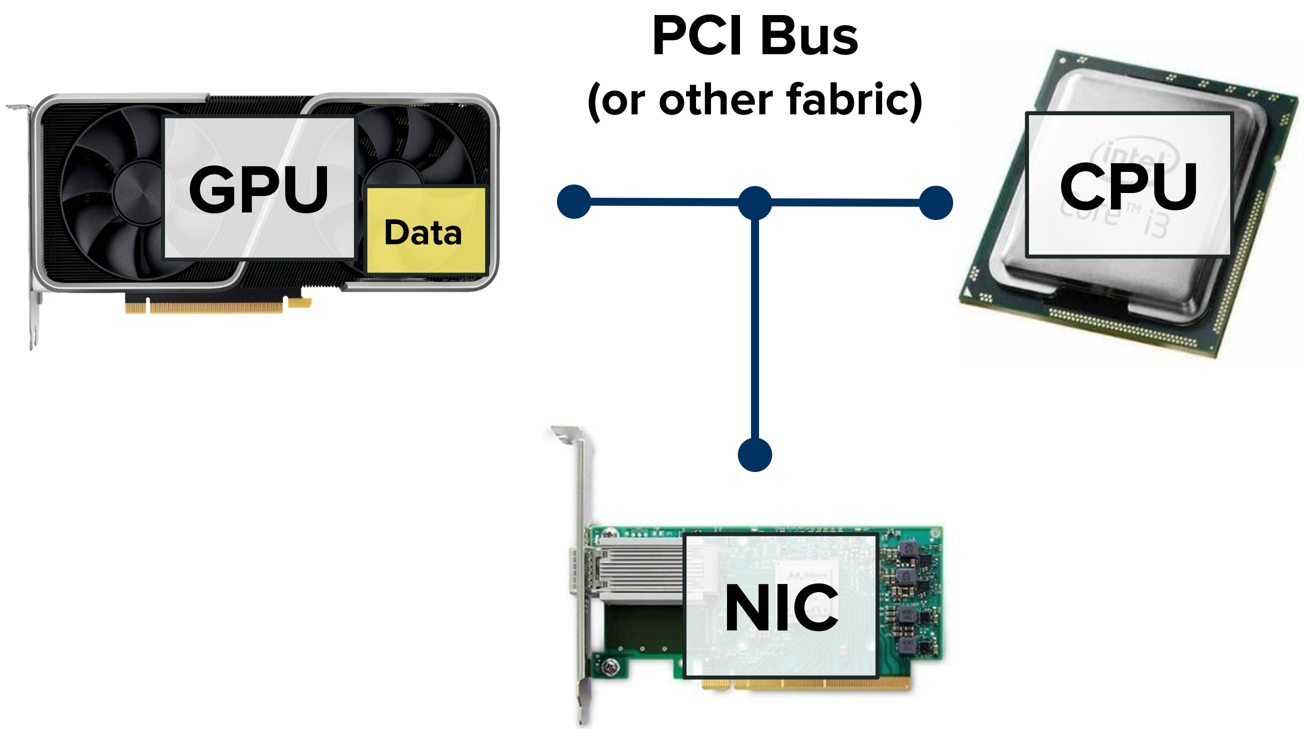
GPUs as a First-Class Computing Resource

- **Historically**, network comm. was CPU-centric

1) Direct GPU access to **Infiniband** allows **GPU-to-GPU** network transfers

2) **Fast in-node fabrics** like NVLink, Infinity Fabric allow very fast **intra-node transfers**



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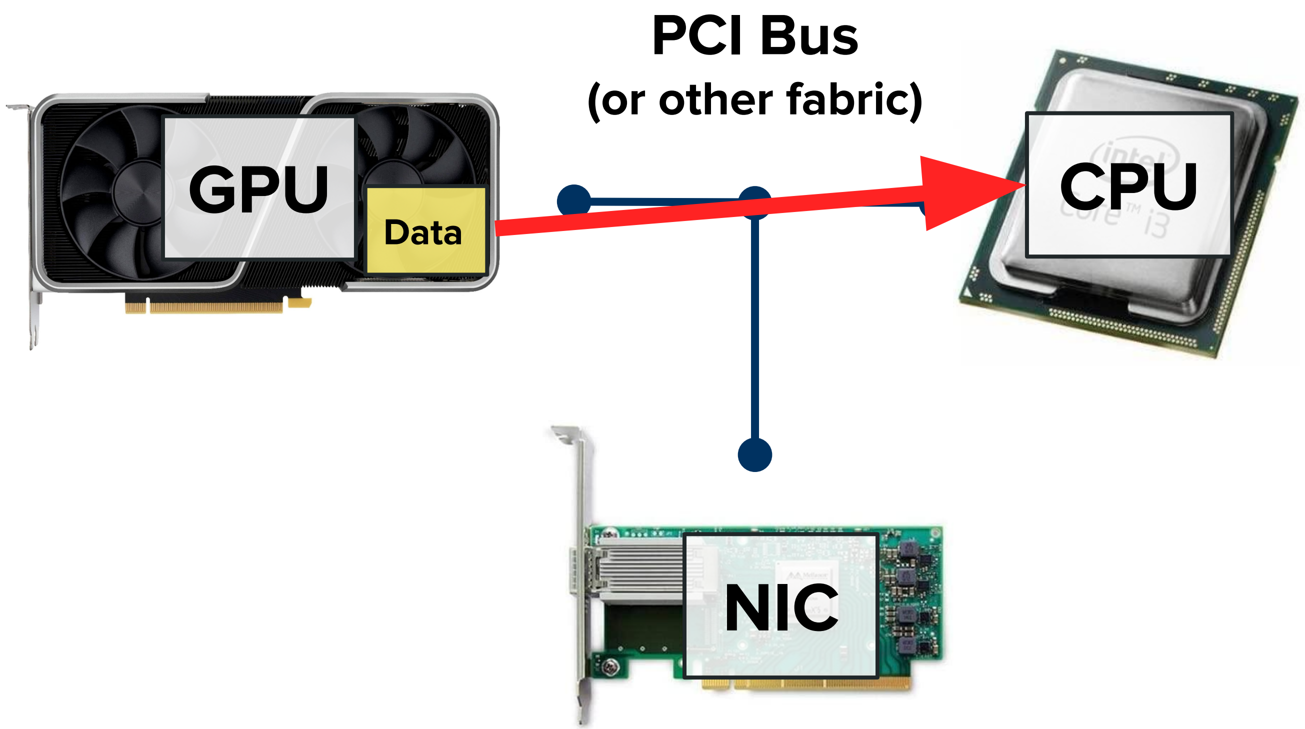

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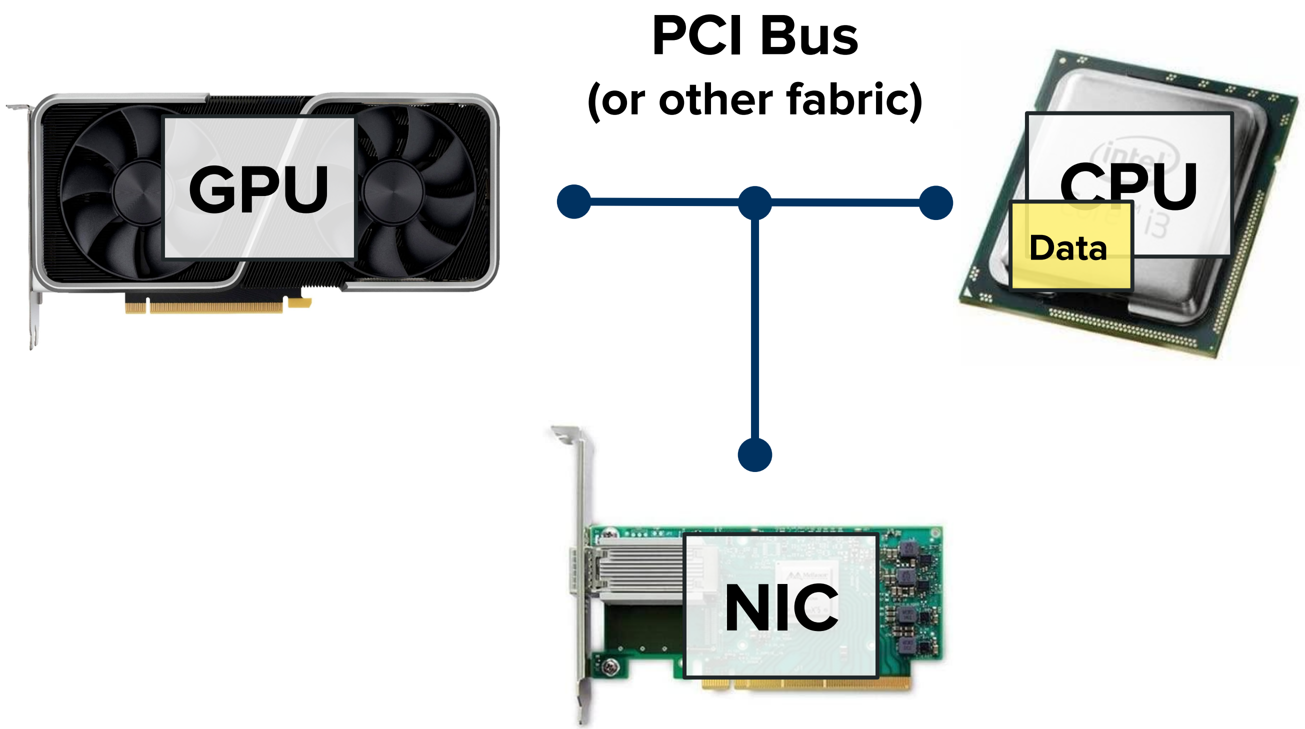

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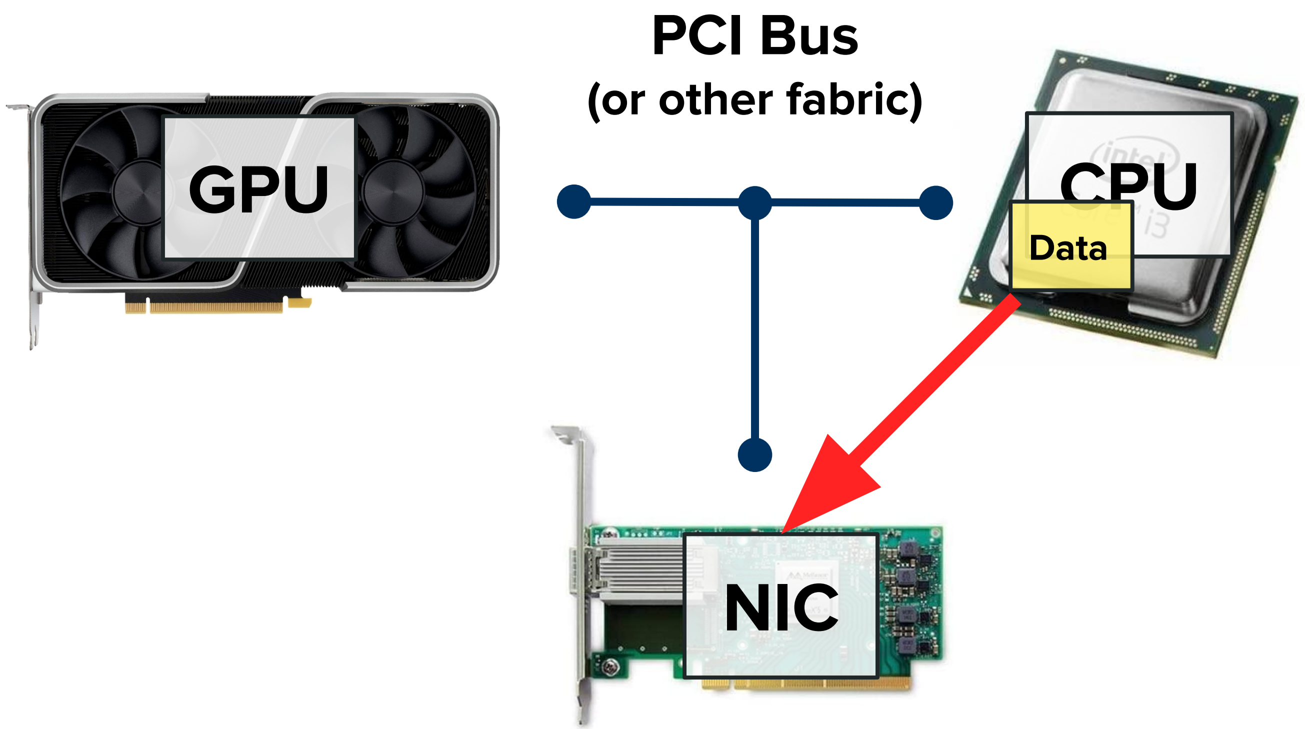

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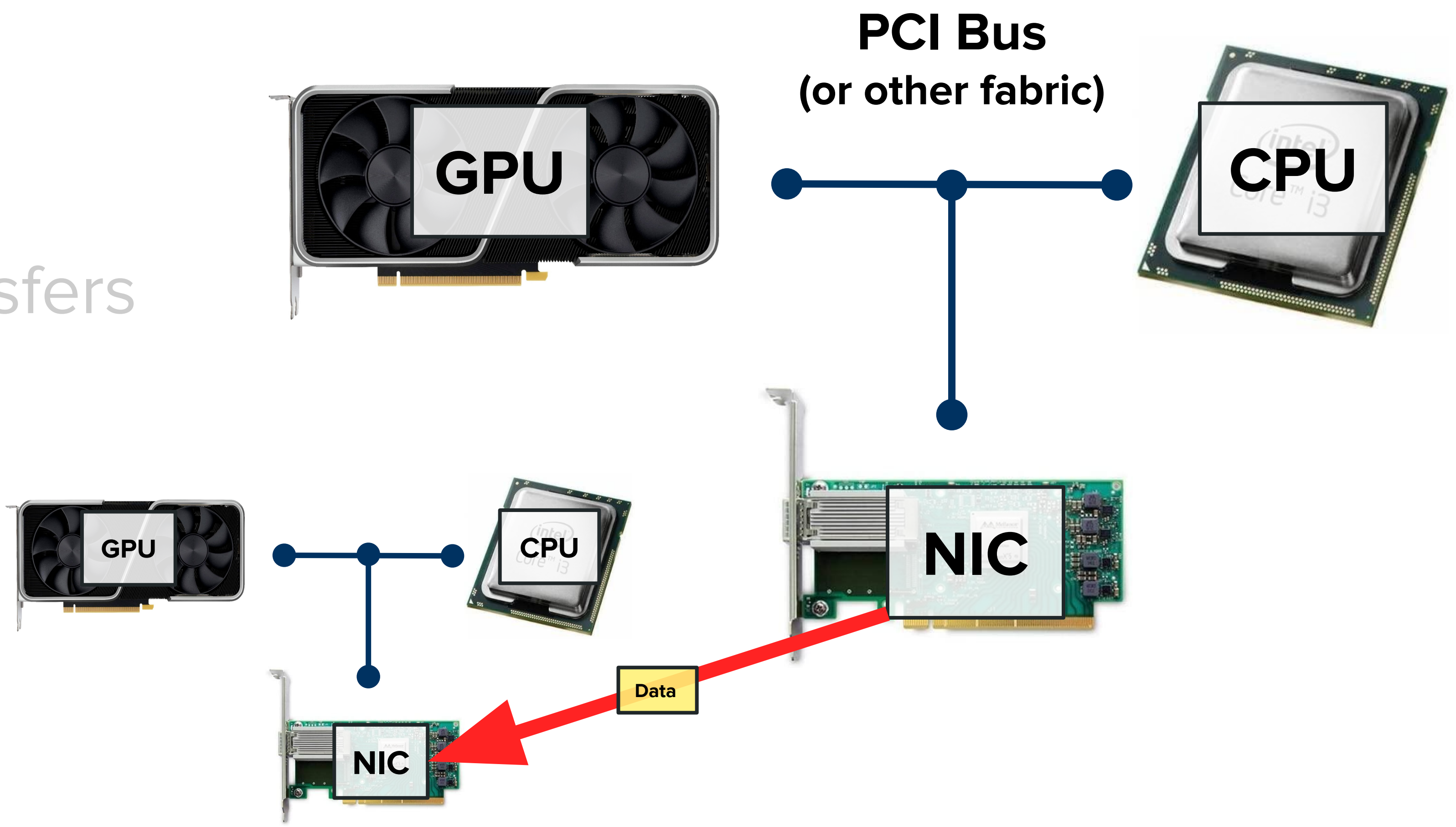

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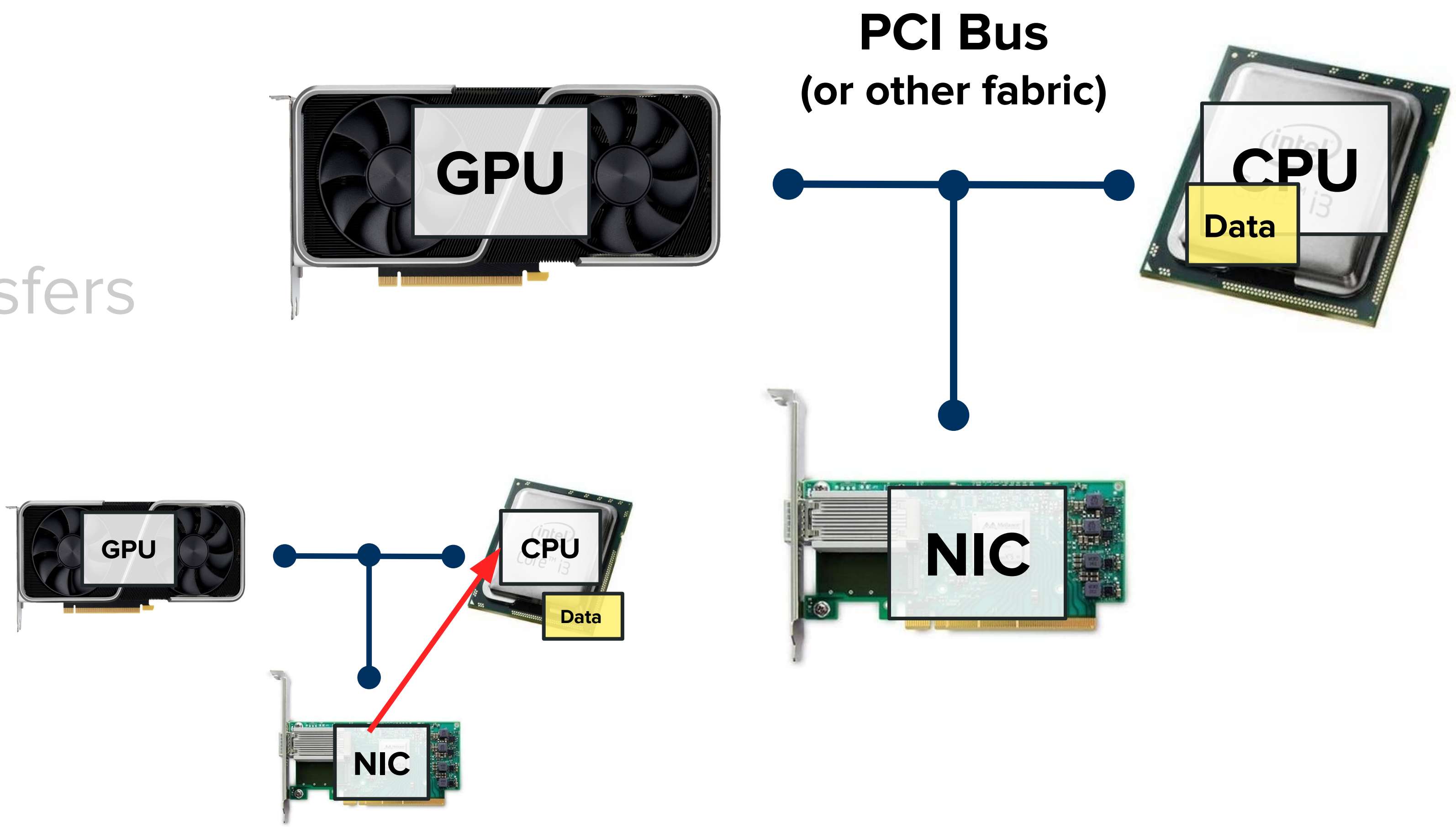

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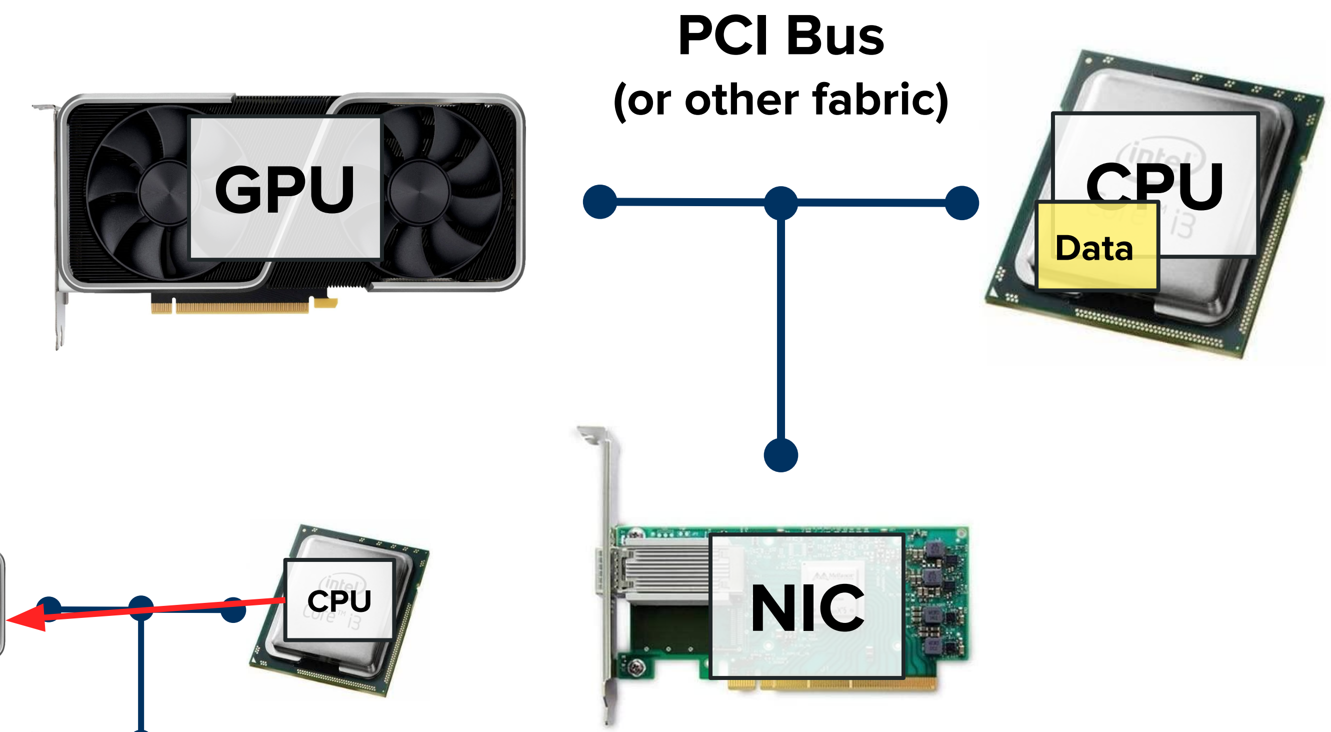

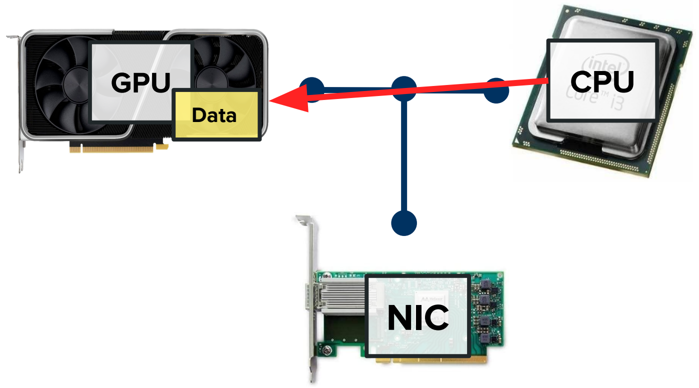

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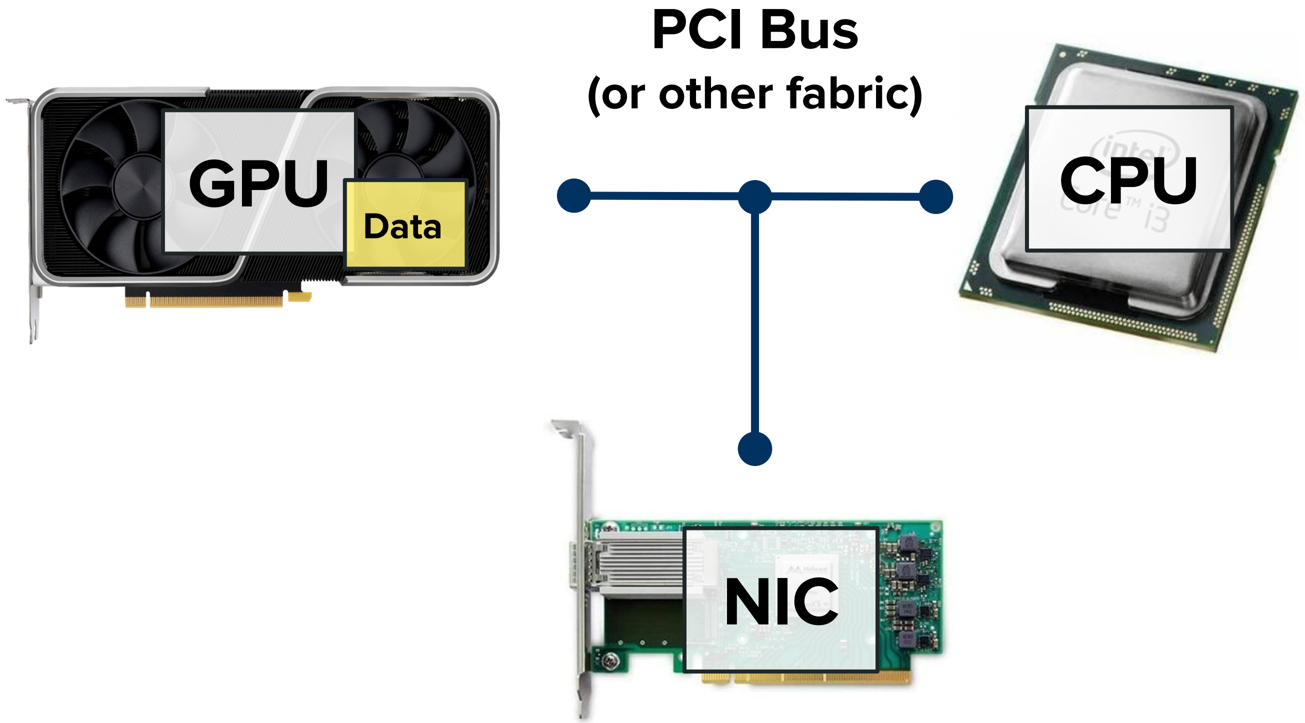

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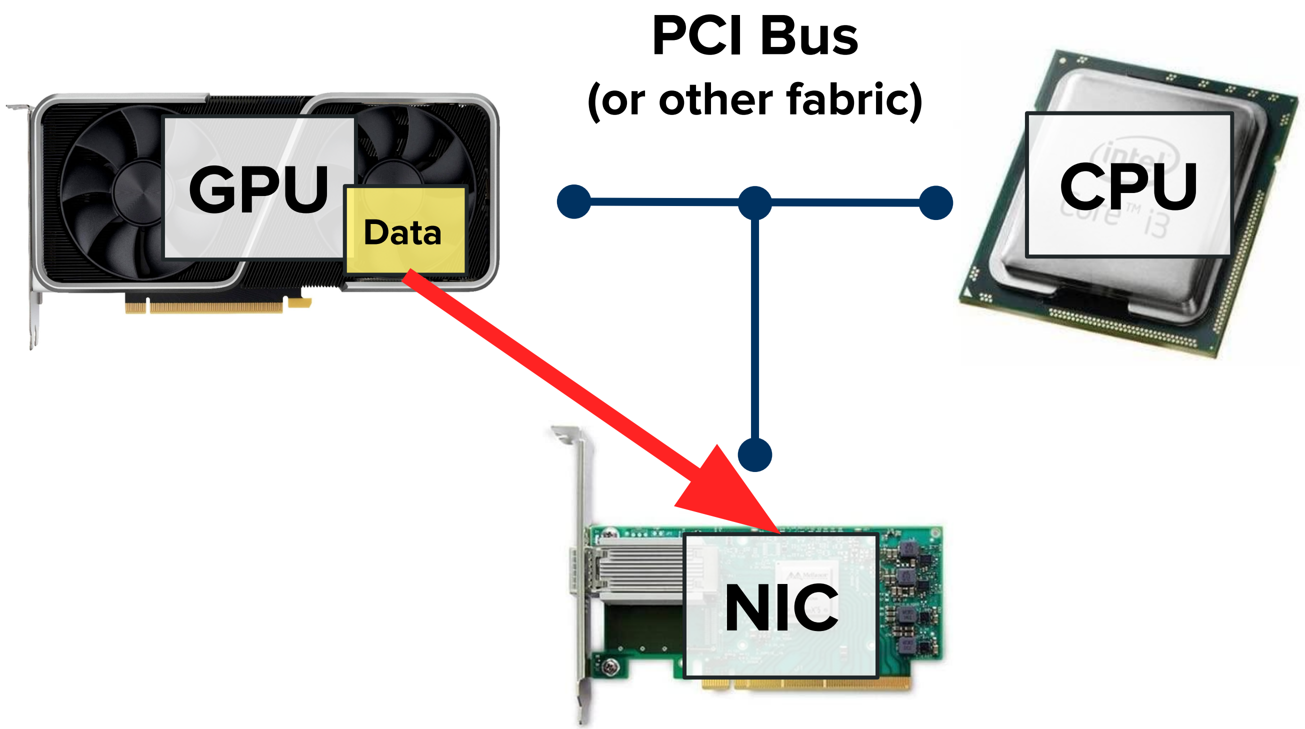

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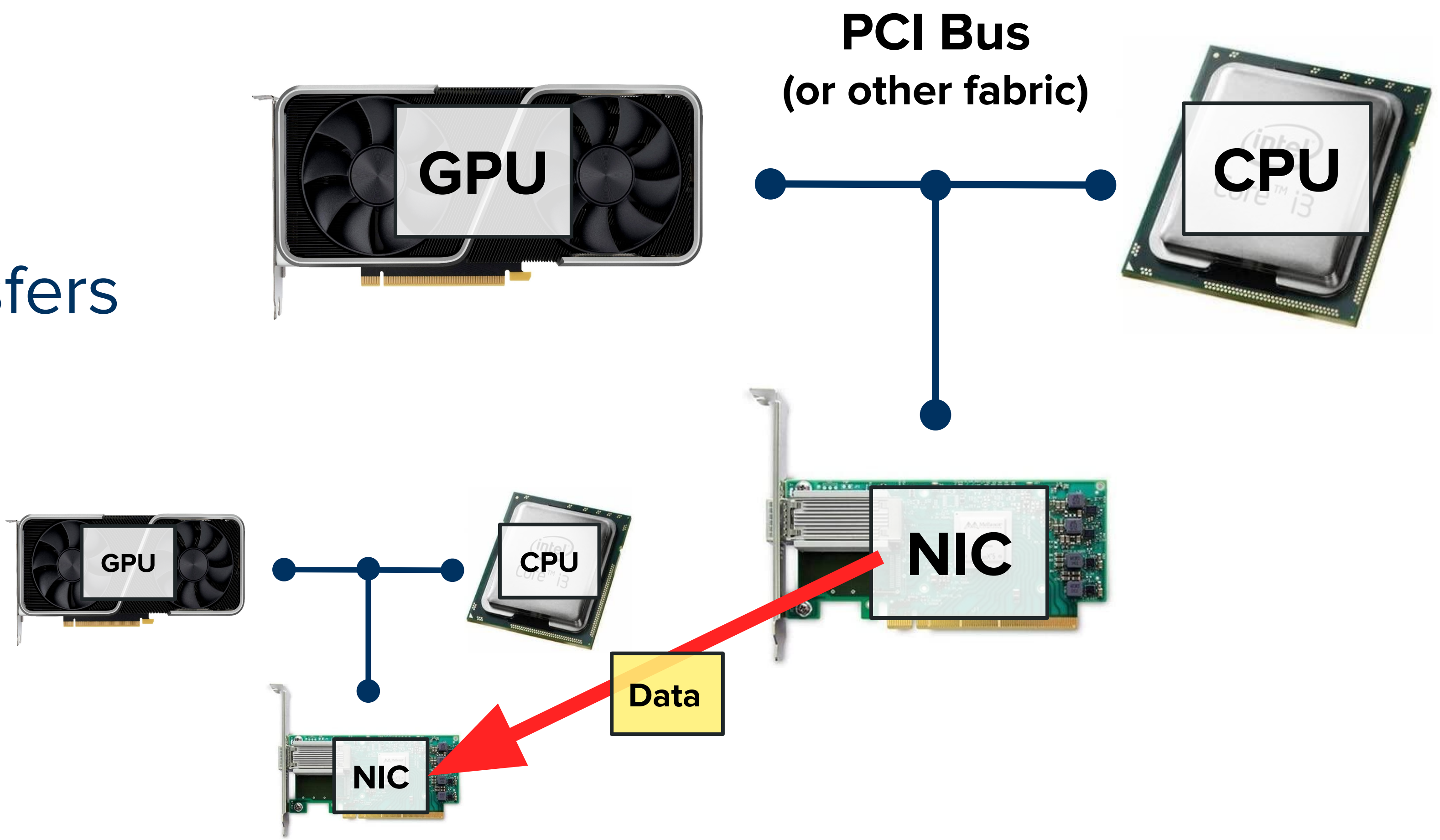

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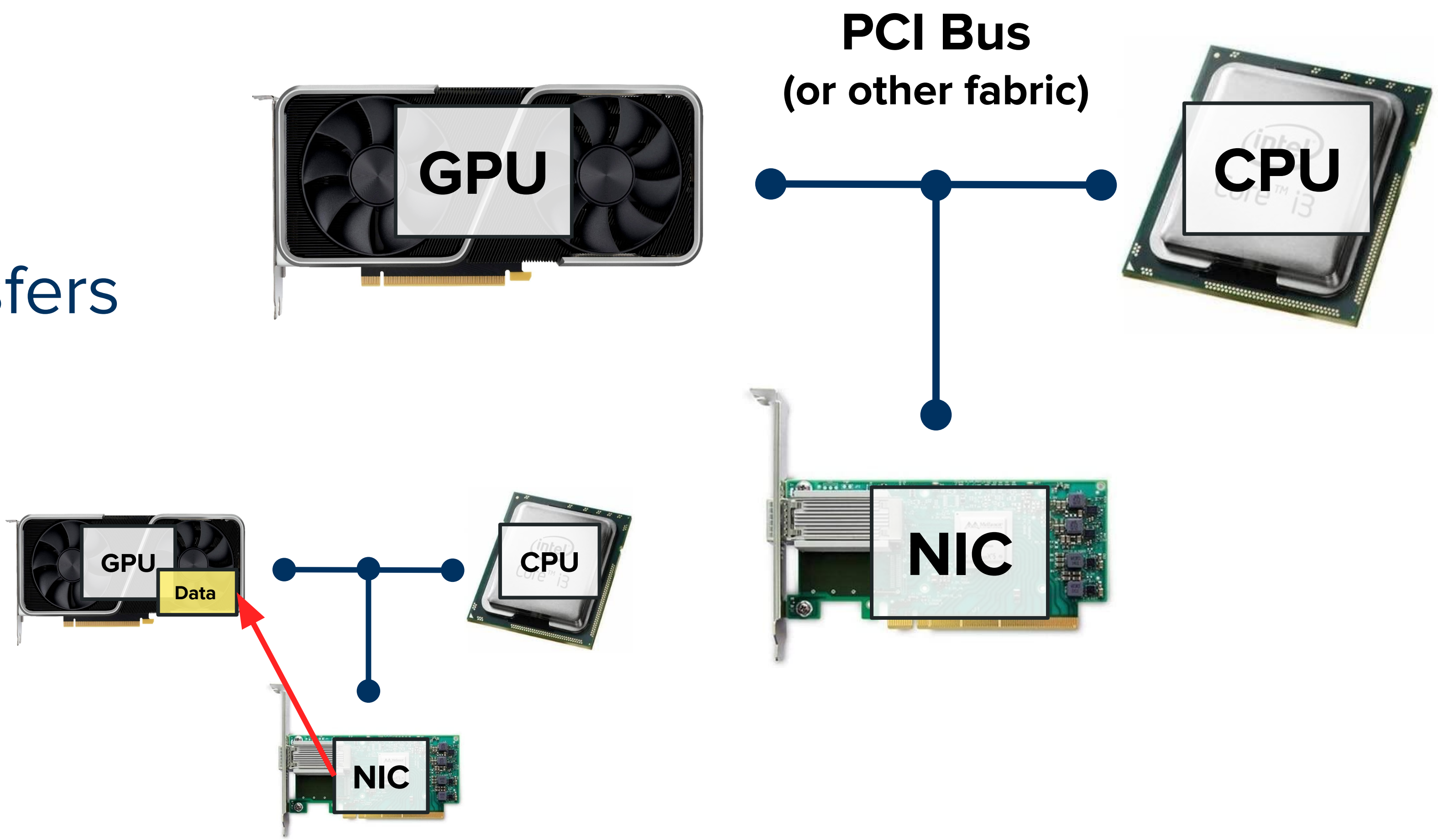

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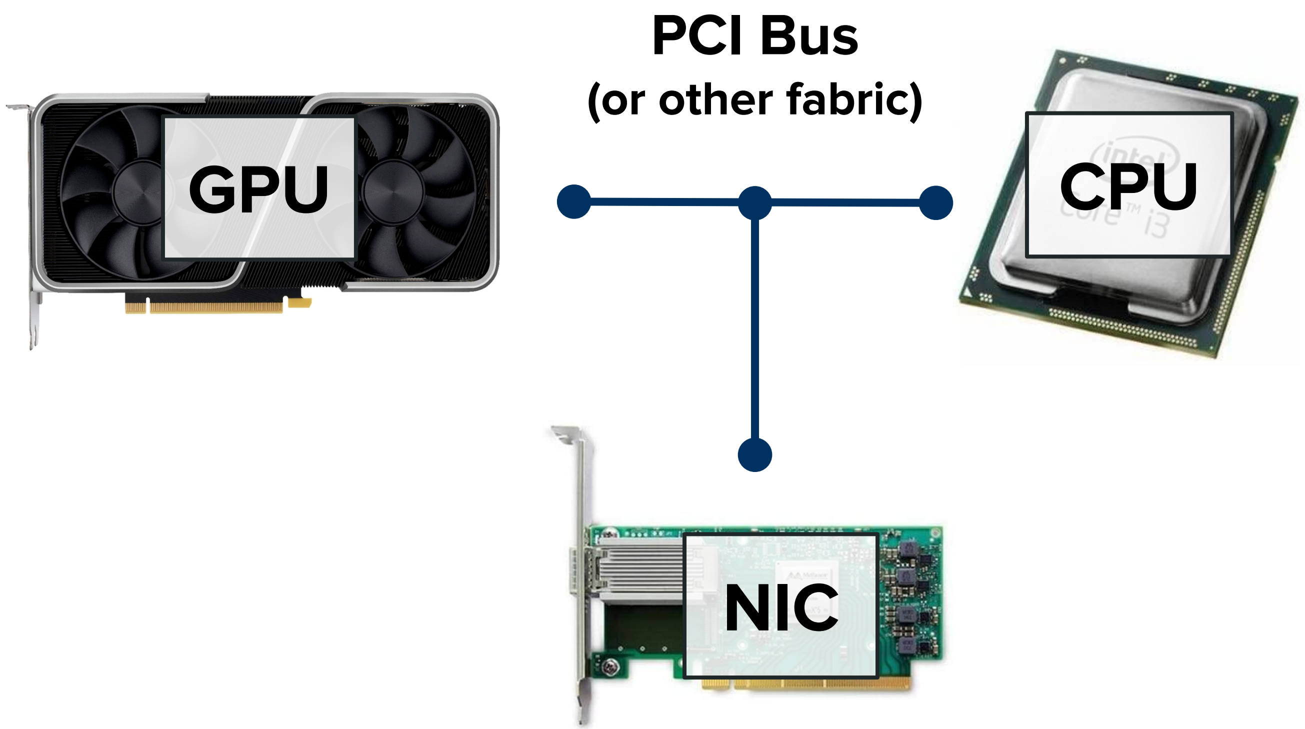

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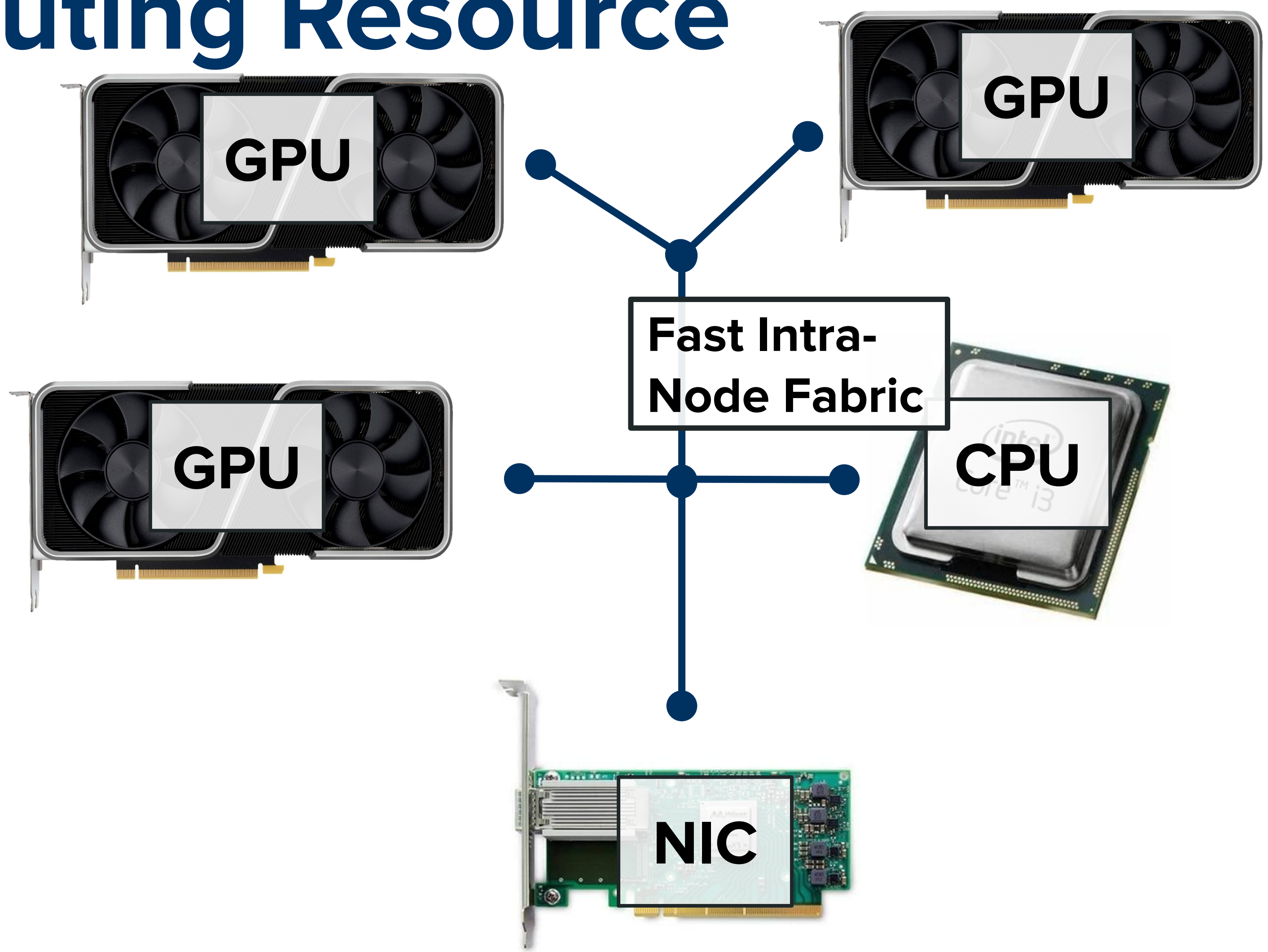

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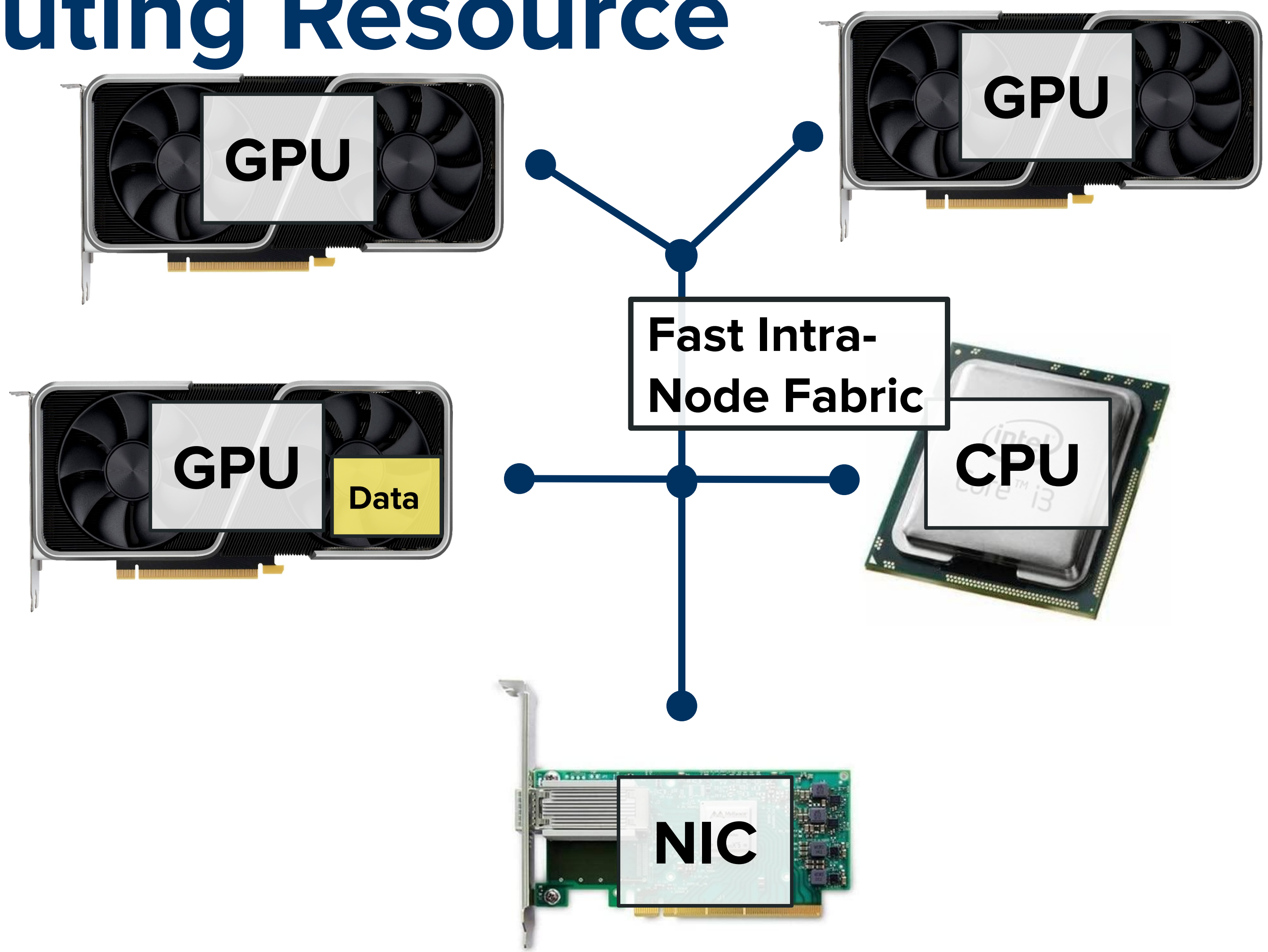

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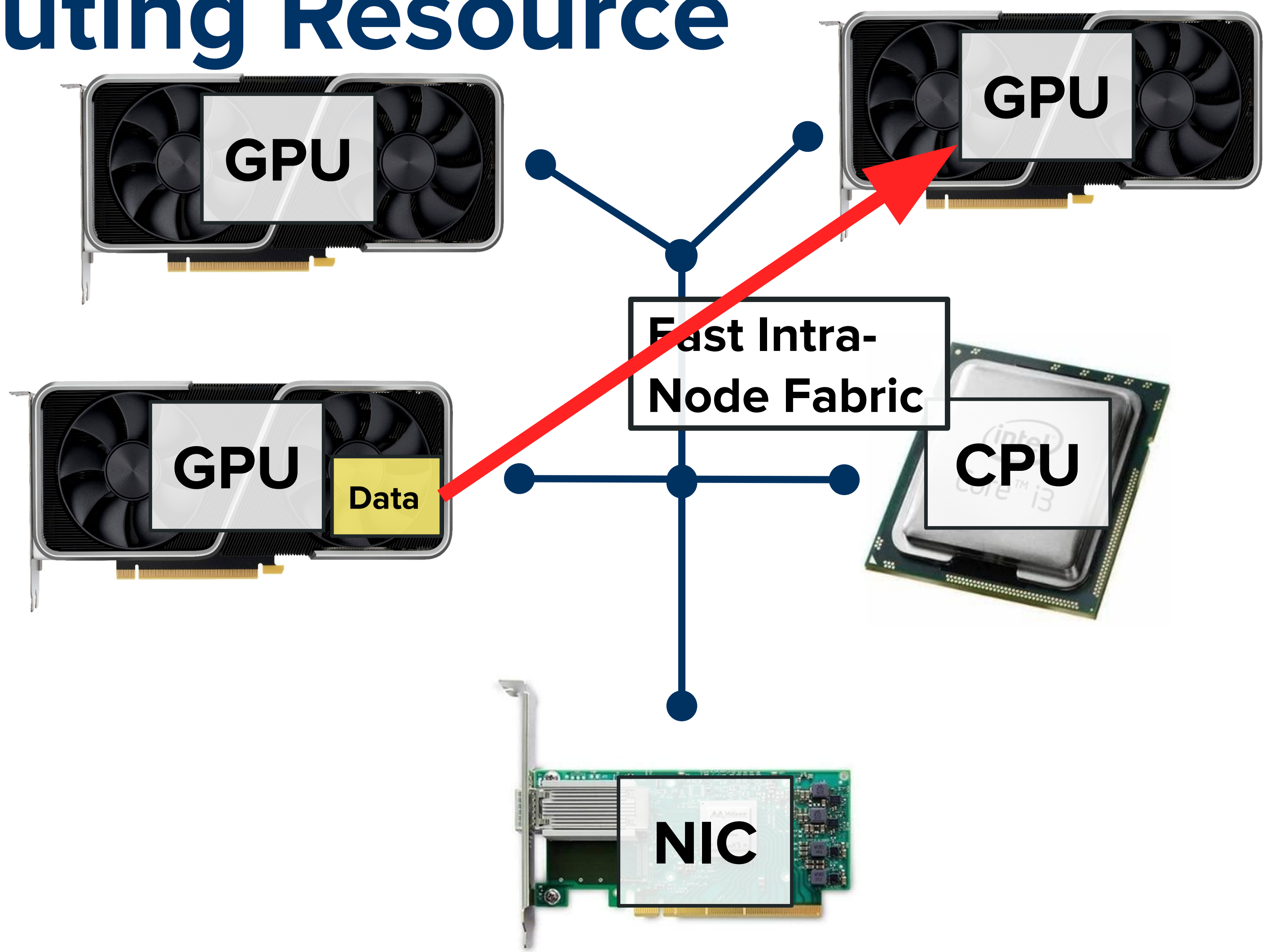

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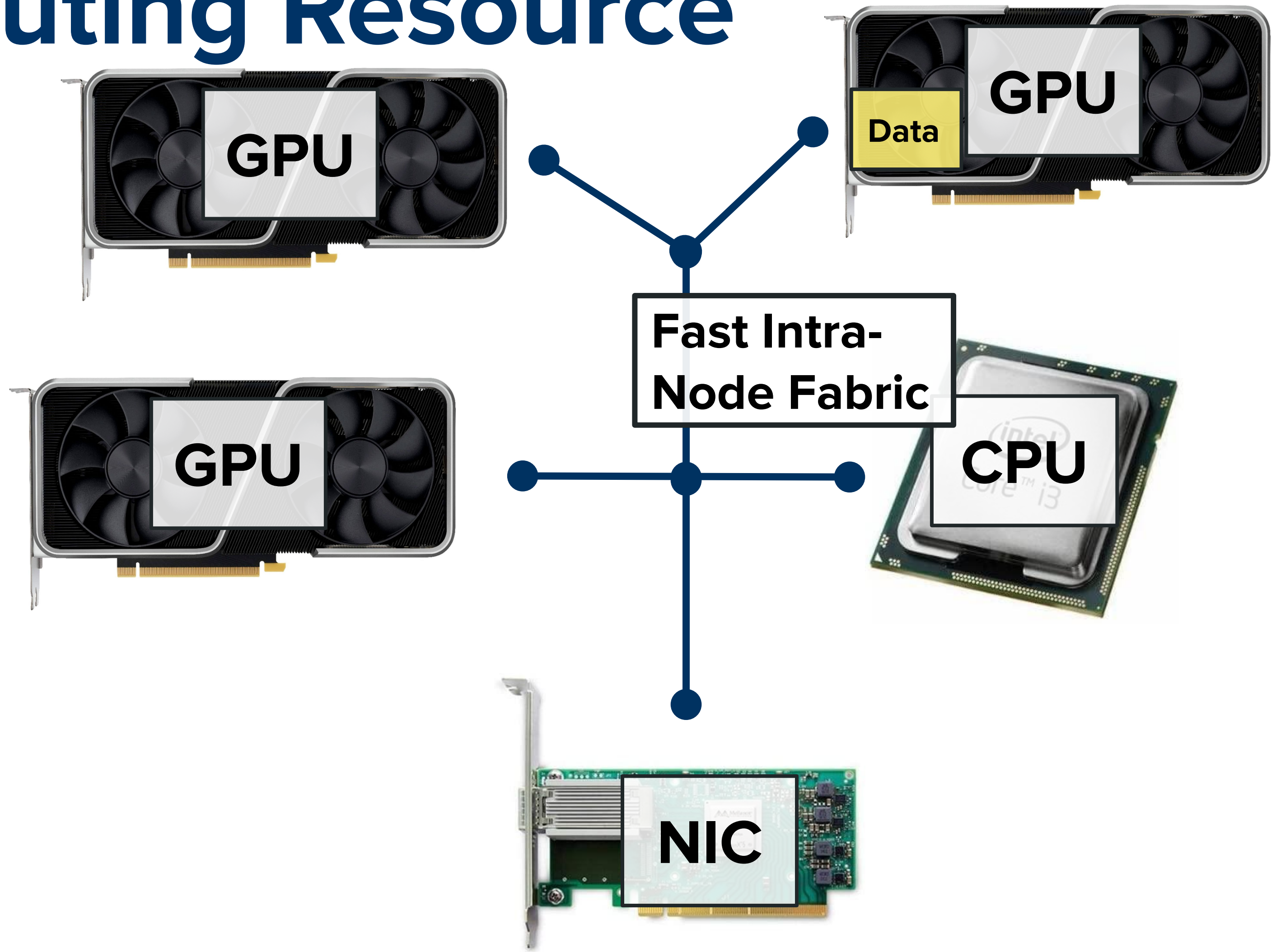
2) **Fast in-node fabrics** like NVLink, Infinity Fabric allow very fast **intra-node transfers**



GPU Communication Libraries

- **Communication libraries** offering increasing support for GPU-to-GPU transfers

- Currently **only PGAS-based libraries** offer **GPU-initiated** communication

- **NVSHMEM** will utilize both **GPUDirect RDMA** and **NVLink**

CUDA-Aware MPI

GASNet-EX
Memory Kinds

NVSHMEM

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Remote Pointer Types

CPU Remote Pointer

```
BCL::GlobalPtr<int> ptr = nullptr;

if (BCL::rank() == 0) {
  ptr = BCL::alloc<int>(BCL::nprocs());
}

ptr = BCL::broadcast(ptr, 0);

ptr[BCL::rank()] = BCL::rank();
```

Remote Pointer Types

CPU Remote Pointer

```
BCL::Glob

if (BCL::
  ptr = B
}

ptr = BCL

ptr[BCL::
```

Remote GPU Pointer

```
BCL::cuda::ptr<int> ptr = nullptr;

if (BCL::rank() == 0) {
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```

Remote Pointer Types

CPU Remote

```
BCL::GlobalP

if (BCL::ran
  ptr = BCL:
}

ptr = BCL::b

ptr[BCL::ran
```

Remote GPU Pointer (Accessing on GPU)

```
__global__ void kernel(BCL::cuda::ptr<int> ptr) {
  size_t tid = ...;

  ptr[tid] = tid;
}

...

BCL::cuda::ptr<int> ptr = nullptr;

if (BCL::rank() == 0) {
  ptr = BCL::cuda::alloc<int>(BCL::nprocs());
}

ptr = BCL::broadcast(ptr, 0);

if (BCL::rank() == 1) {
  kernel<<<1, BCL::nprocs()>>>(ptr);
}
```

Remote Pointer Types for GPUs

CPU Remote Pointer

```
template <typename T>
struct GlobalPtr {

  ...

private:
  size_t rank_;
  size_t offset_;
};
```

Remote Pointer Types for GPUs

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struct GlobalPtr {

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};
```

```
void memcpy(void* dest,
            GlobalPtr<void> src,
            size_t n) {
  // Issue remote get operation to
  // copy `n` bytes from `src` to `dest`
  backend::remote_get(dest, src, n, ...);
}
```

Remote Pointer Types for GPUs

GPU Remote Pointer

```
template <typename T>
struct ptr {

  ...

private:
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GPU Remote Pointer

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struct ptr {

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};
```

```
__host__ __device__
void memcpy(void* dest,
            cuda::ptr<void> src,
            size_t n) {
  // Issue remote get operation to
  // copy `n` bytes from `src` to `dest`
#ifdef __CUDA_ARCH__
  nvshmem_getmem(dest,
                 src.rptr(), n,
                 src.rank());
#else
  ...
#endif
}
```

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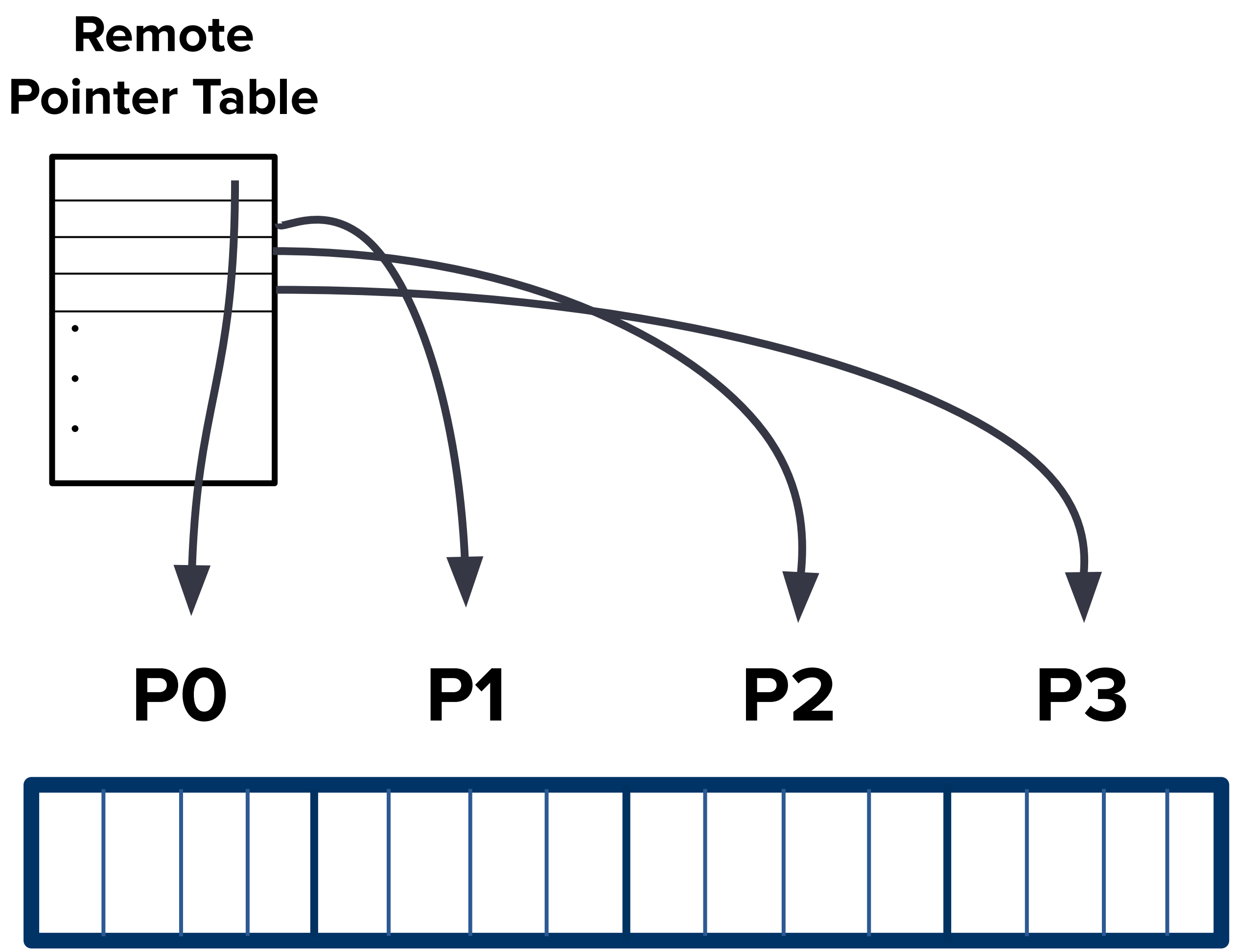
On CPU, necessary to stage data if transferring to host (CPU) memory.

Distributed Data Structures on GPUs

- Recall that **each process** needs a **table of pointers** to access data

- To implement **GPU-side methods**, need **GPU-accessible** table

- Is this enough to implement **GPU-side data structure methods**?



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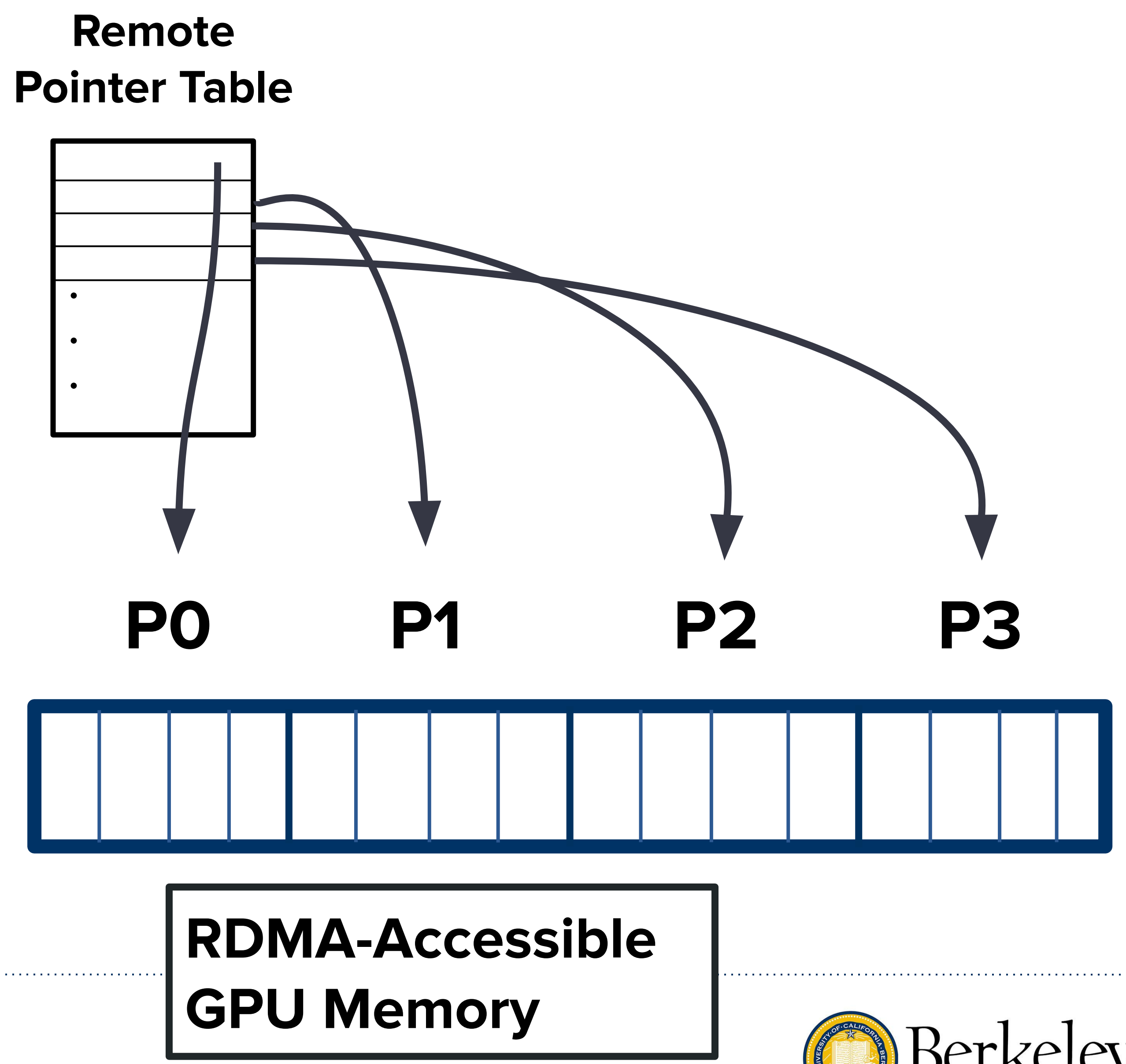

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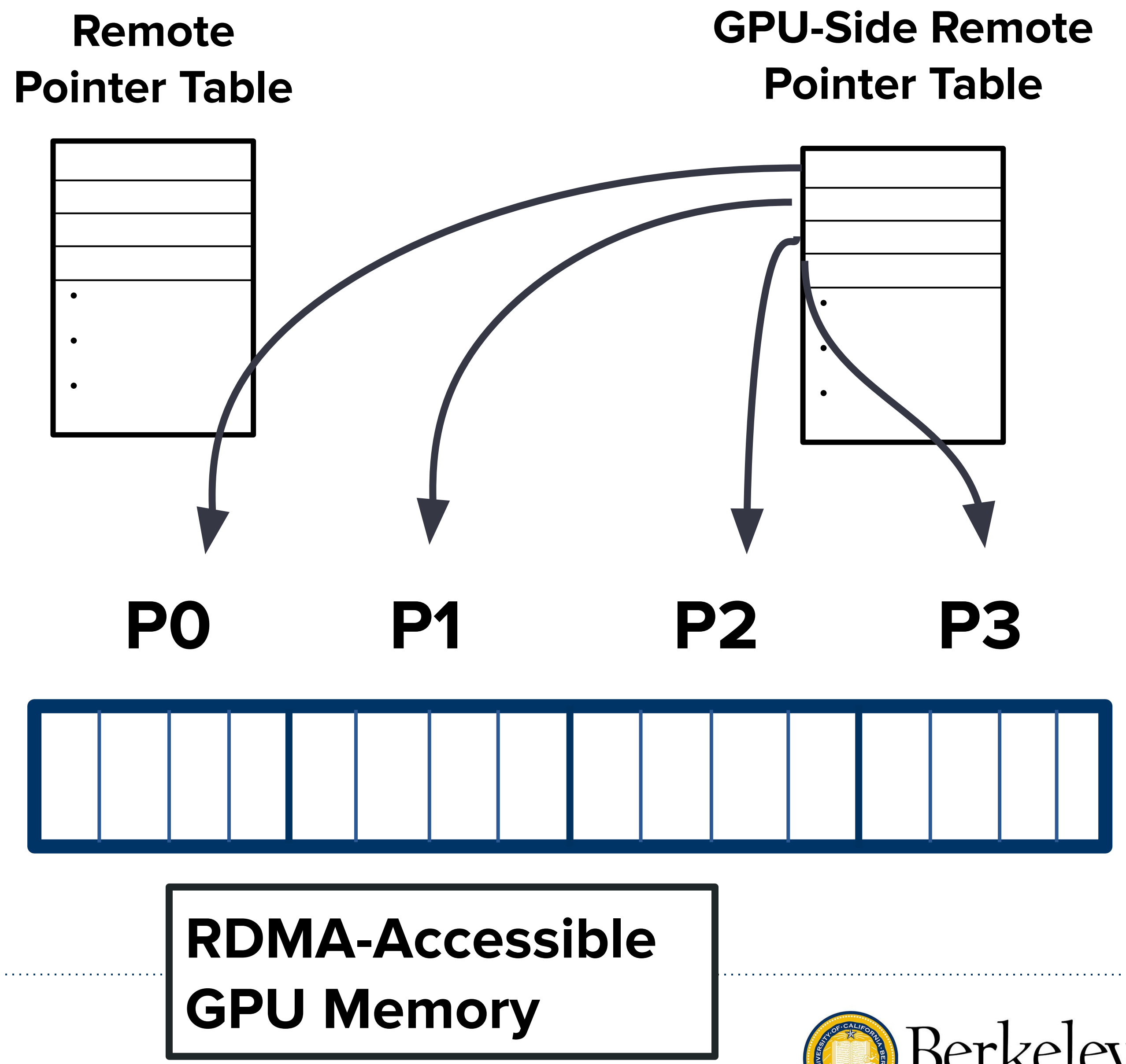

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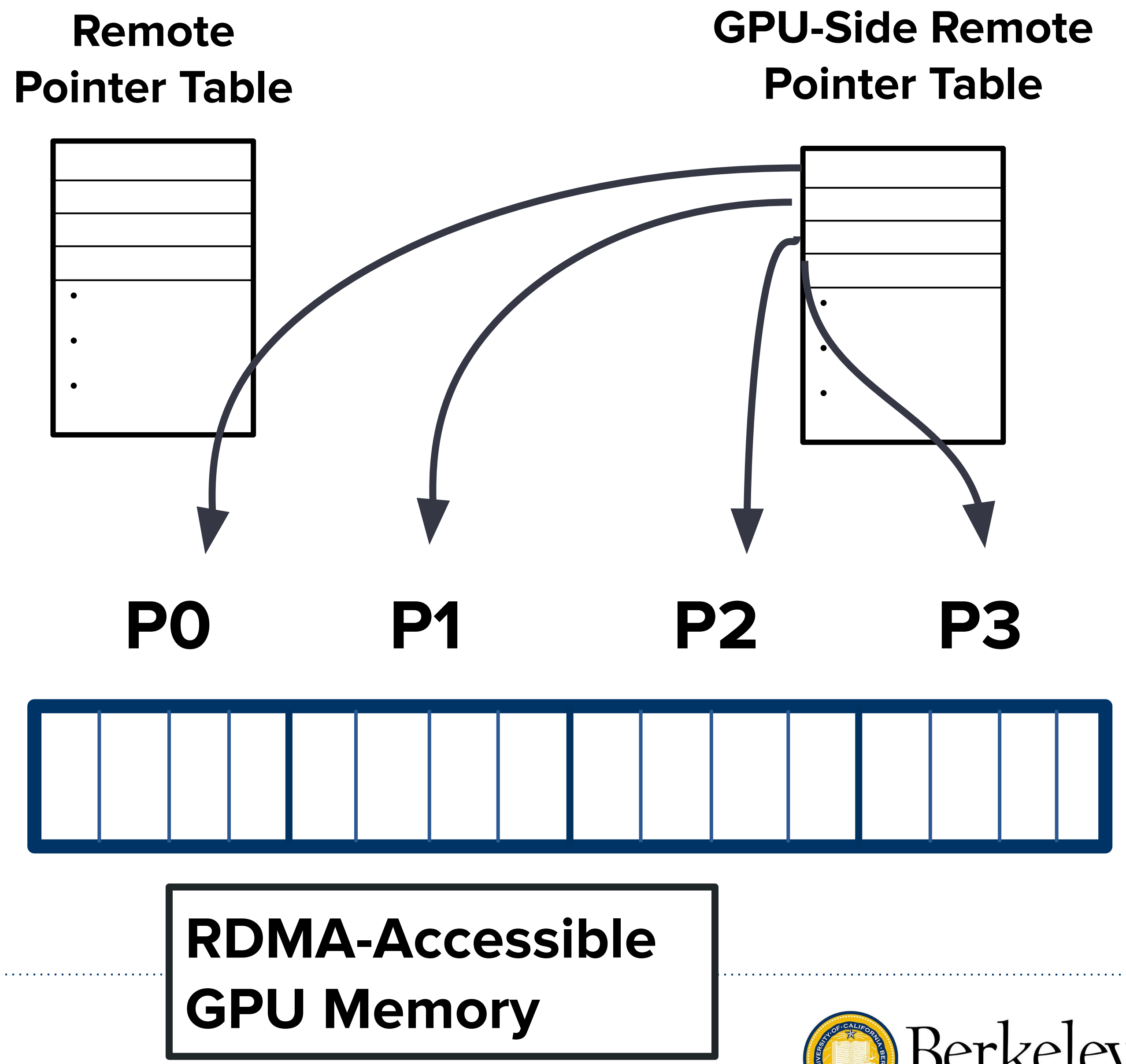


Passing Objects into CUDA Kernels

- Passing an **object by value** into a **CUDA kernel** results in a **copy**

- Object **likely destroyed** before kernel completes

- We need a **copy constructible** placeholder object

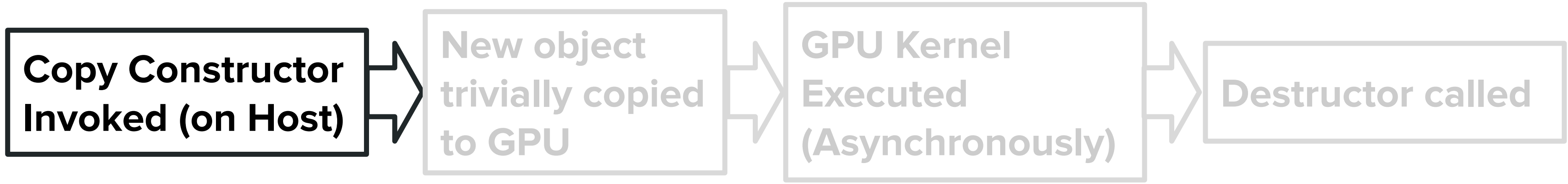
```
__global__
void kernel(BCL::cuda::HashMap <int, int> map) {
  size_t tid = ...;

  size_t value = tid*2
  map[tid] = value;
}

...

BCL::cuda::HashMap<int, int> map(100);

kernel<<<1, 100>>>(map);
```



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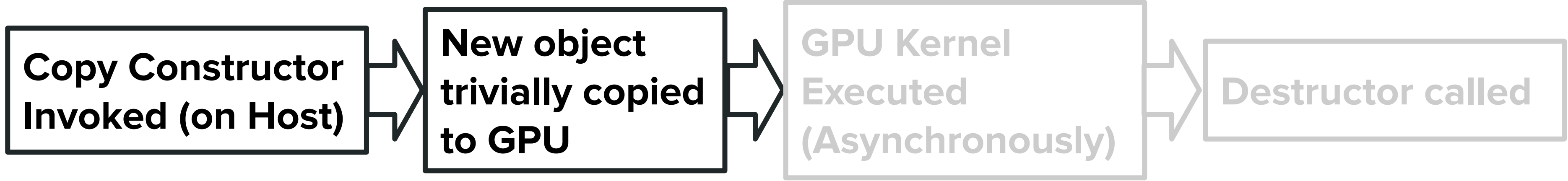

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Copy Constructor Invoked (on Host) → **New object trivially copied to GPU** → **GPU Kernel Executed (Asynchronously)** → Destructor called

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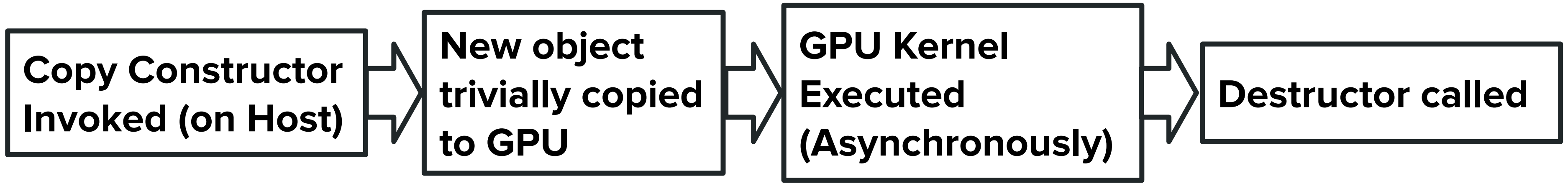

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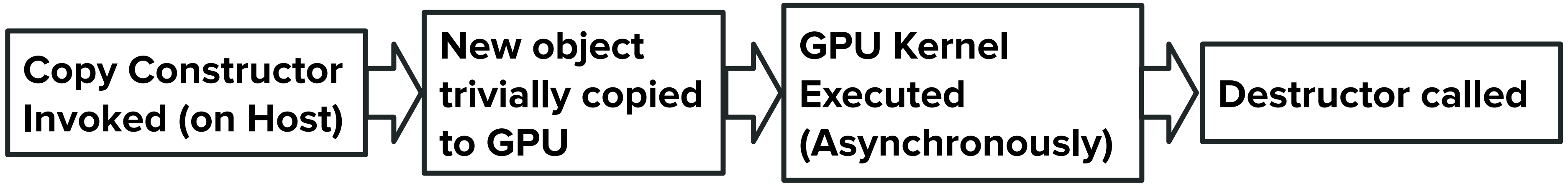

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Using GPU Views within Kernels

- First create a **`dmatrix_view`** view object

- `dmatrix_view` has **O(1)** copy constructor (does not copy data)

- View can be used to access data on GPU

```
__global__
void kernel(cuda::dmatrix_view<float> x_view) {
  size_t tid = ...;

  size_t i = tid / x.shape()[0];
  size_t j = tid % x.shape()[0];

  x_view[{i, j}] = tid;
}

...

cuda::DMatrix<float> a({8, 8});

kernel<<<1, 64>>>(cuda::dmatrix_view(a));
```

Wrap-Up

- **Remote pointer types** are a **useful abstraction** for implementing distributed data structures

- Extendable to **multi-GPU data structures** both intra-node and multi-node

- Having the correct **high-level distributed data structures** can unlock performance competitive with highly tuned implementations

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Pointers

Links

BCL, Our PGAS-Based C++ Distributed Data Structures Library

https://github.com/berkeley-container-library/bcl

My Website

https://cs.berkeley.edu/~brock

Interested in irregular data structures? Check out my other talk:

GraphBLAS: Building a C++ Matrix API for Graph Algorithms (CppCon'21)