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Improving the Performance of Charm++ Applications on GPU Systems

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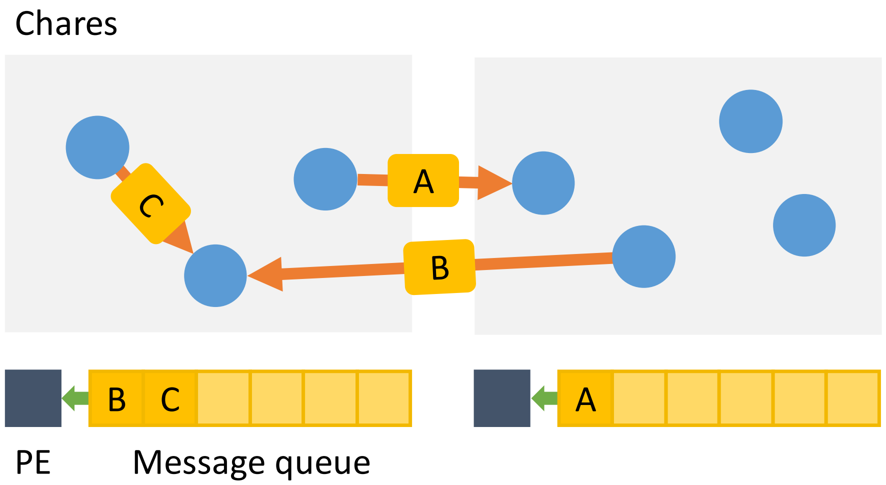
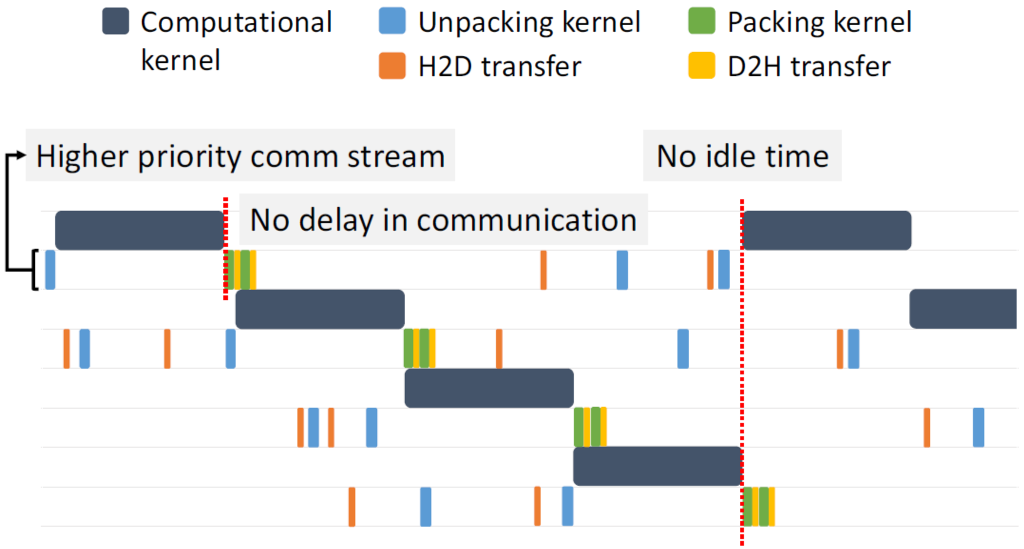
Charm++ on GPU Systems



- Chares can offload computational kernels to the GPU (e.g., CUDA)
- Need to maximize asynchrony to prevent chares from not yielding to other chares
  - CUDA streams
  - Charm++ Hybrid API (HAPI) for asynchronous completion notification

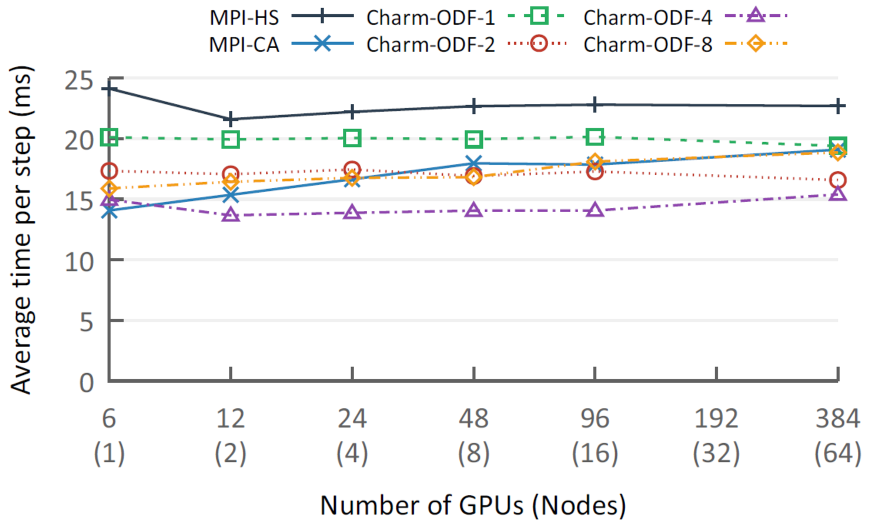
Computation-Communication Overlap

Automatic Computation-Communication Overlap

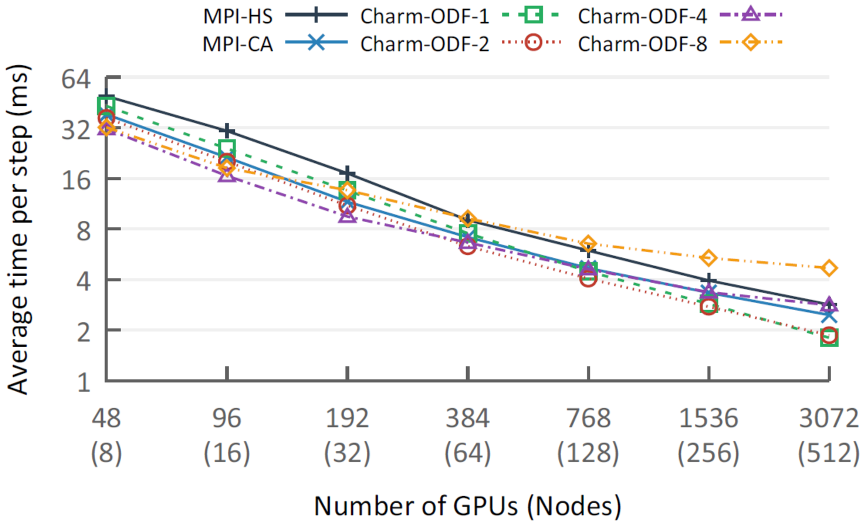


- Minimize synchronization for overlap
- Prioritize communication using CUDA stream priorities or coordination with CUDA events
- More details can be found in this ESPM2'20 paper

Automatic Computation-Communication Overlap



(a) Weak scaling on Summit.

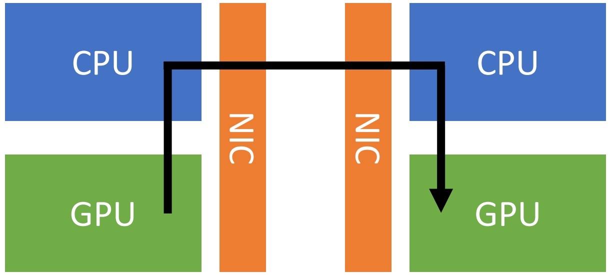


(c) Strong scaling on Summit.

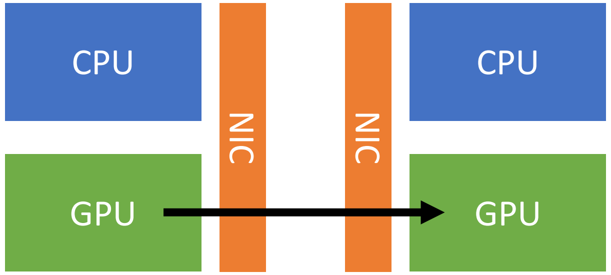
- **MiniMD**: proxy app for molecular dynamics
  - Charm++ (decomposition, communication) and **Kokkos** (GPU kernels, host-device transfers)
  - Beats CUDA-aware MPI even without GPU-aware communication due to overlap
  - Limitation: overlap with overdecomposition does not improve performance at end of strong scaling
  - https://github.com/minitu/miniMD/tree/charm/kokkos

GPU-aware Communication

GPU-Aware Communication



[Host-staged]



[Direct]

- **Productivity**: users can provide GPU buffers directly to the communication APIs
- **Performance**: direct transfers between GPUs (bypass host memory)
- Underlying technology: CUDA IPC, GPUDirect
- E.g., CUDA-aware MPI

GPU-Aware Communication in Charm++

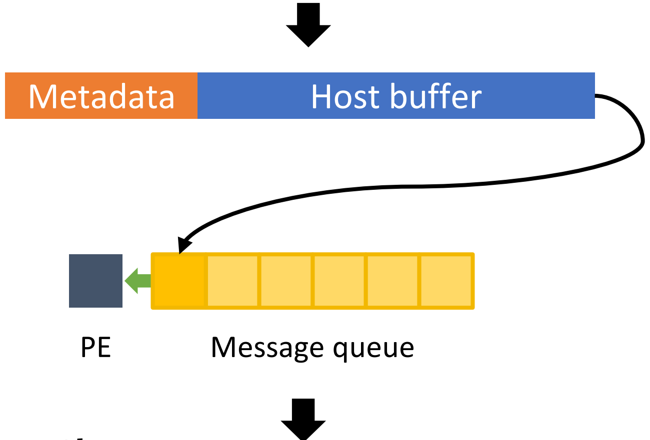
- Also, Adaptive MPI and Charm4py
- How can we support all of our parallel programming models?
- How do we retain message-driven execution?
- Our approach: build on GPU support in **UCX**
    - *Caveat*: UCX tagged API caters to MPI send/recv semantics

Unified Communication X

Messaging API in Charm++

Sender Chare

```
void Sender::foo() {
  // Send host buffer to a peer chare
  chare_proxy[peer].bar(1024, my_buf);
}
```



Receiver Chare

```
void Receiver::bar(int count, double* buf) {
  // Scheduler calls this method after picking
  // up message from its message queue
  for (i = 0; i < count; i++) {
    f(buf[i]);
  }
}
```

- Sender's data is packed together with metadata (e.g., information about target chare & method)
- Message asynchronously sent to receiver
- Sits in receiver's message queue until it is picked up by scheduler

GPU Messaging API

Sender Chare

```
void Sender::foo() {
  // Send GPU buffer to a peer chare
  chare_proxy[peer].bar(1024, CkDeviceBuffer(my_buf));
}
```

① Send host-side message ② Send GPU buffer

Host-side message arrival

Receiver Chare

```
// Post entry method: First called by the runtime
// Before receiving incoming GPU buffer
void Receiver::bar(int& count, double*& buf) {
  // Specify destination GPU buffer
  buf = recv_buf;
}
```

③ Post receive for GPU buffer

GPU buffer arrival

```
// Regular entry method: Called by the runtime
// once the GPU buffer has arrived
void Receiver::bar(int count, double* buf) {
  // Has access to received GPU buffer
  some_kernel<<<...>>>(count, buf);
}
```

- Documentation
- Builds on **Zero Copy API** to preserve message-driven execution
- Still need metadata on host memory
- **`CkDeviceBuffer`**
  - Contains information about GPU src/dst buffers
  - Sent to receiver together with other metadata
- Receiver posts separate receives for GPU data once host-side message arrives

Channel API

Sender Chare

```
void Sender::foo() {
  // Send GPU buffer to a peer chare
  channel.send(data, size, &future);
  CkWaitFuture(future);
}
```

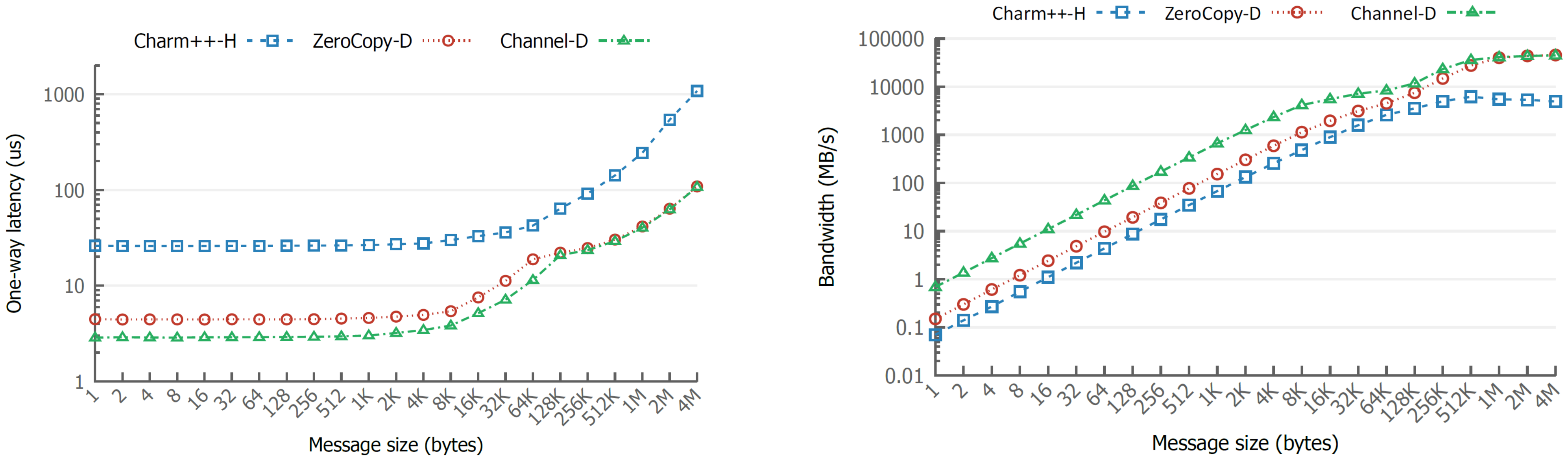
Receiver Chare

```
void Receiver::bar() {
  // Receive GPU buffer
  channel.recv(data, size, &future);
  CkWaitFuture(future);
}
```

* Can also use Charm++ callbacks instead of futures

- **Channels** can be created between a pair of chares (not constrained to GPU data)
- Exchange only data with explicit sends & receives (similar to MPI)
- Does not transfer control flow
- Reduces overhead from receive for GPU data being delayed
- Will be part of release 7.1
  - https://github.com/UIUC-PPL/charm/pull/3484

GPU-aware Communication Performance



Intra-node Latency and Bandwidth on OLCF Summit

- Substantial improvements in latency & bandwidth
- TODO: Combine computation-communication overlap & GPU-aware communication
- More details in AsHES’21 paper

CharminG: A GPU-resident Runtime System

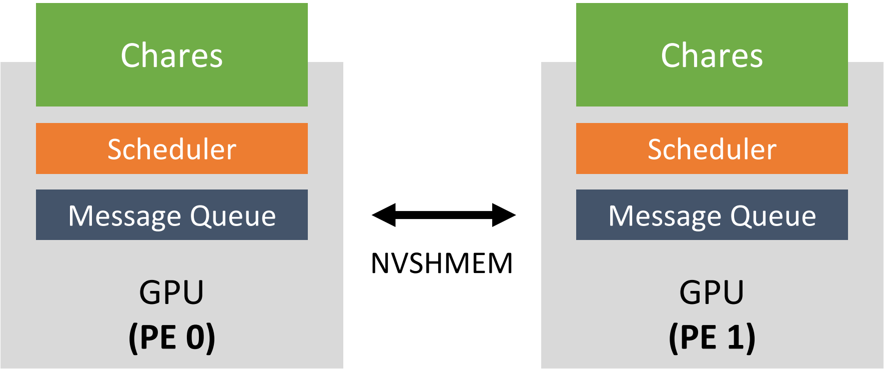
Motivation

- Computation is moving to GPU
- Program flow & communication are still driven by CPU
  - Overheads from interactions (e.g., synchronization) & data transfers between CPU and GPU
  - How do we utilize the upcoming direct GPU-NIC connections (e.g., OLCF Frontier) more efficiently?
- Can we improve performance by moving the entire execution to the GPU?
- Related work: Juggler [M. E. Belviranli, PPoPP '18]
  - Per-SM task scheduler
  - Task dependencies are resolved on the fly and entirely on the GPU
  - Limited to a single node
  - Not modularized, runtime system is embedded within the application

CharminG: Charm++ in GPUs

- Develop fully GPU-resident runtime system
- Using Charm++ principles
  - Overdecomposition
  - Asynchronous message-driven execution
  - Migratability
- Enable adaptive runtime features without interactions with host CPU
- Implemented working prototype

System Design



Chares

Scheduler

Message Queue

GPU
(PE 0)

NVSHMEM

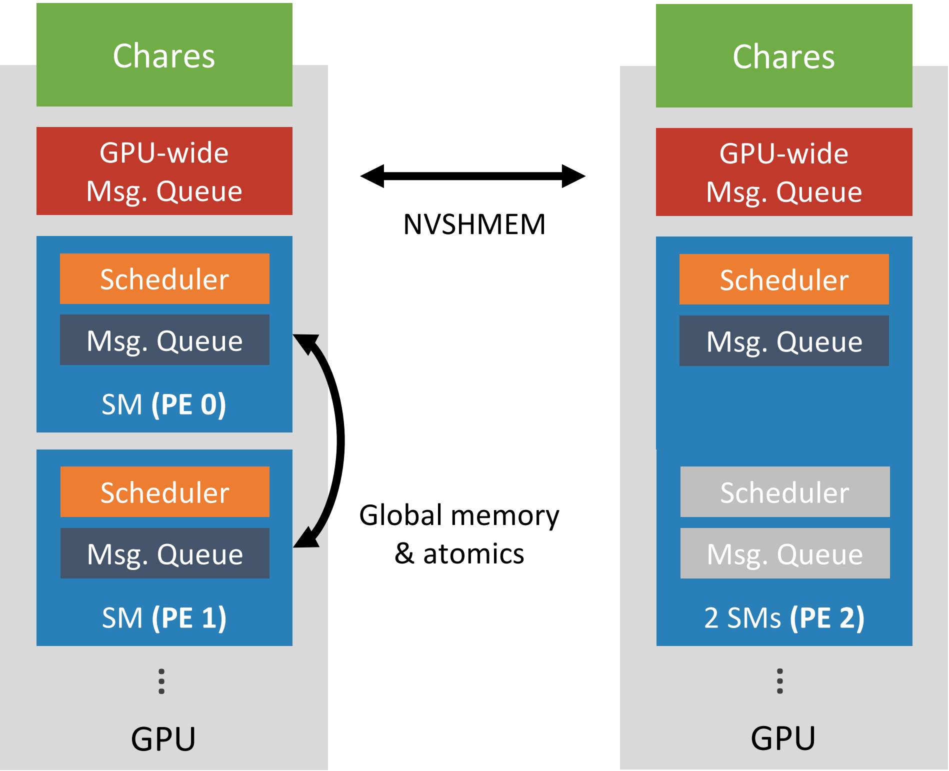
Chares

Scheduler

Message Queue

GPU
(PE 1)

[Current Prototype]



Chares

GPU-wide
Msg. Queue

Scheduler

Msg. Queue

SM **(PE 0)**

Scheduler

Msg. Queue

SM **(PE 1)**

⋮

GPU

NVSHMEM

Global memory
& atomics

Chares

GPU-wide
Msg. Queue

Scheduler

Msg. Queue

Scheduler

Msg. Queue

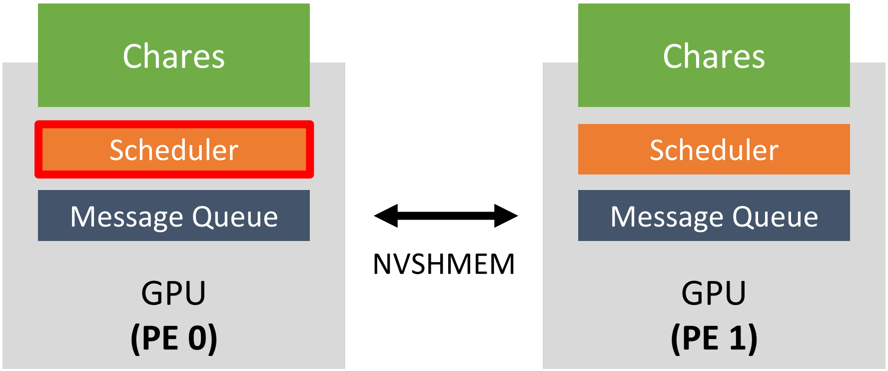
2 SMs **(PE 2)**

⋮

GPU

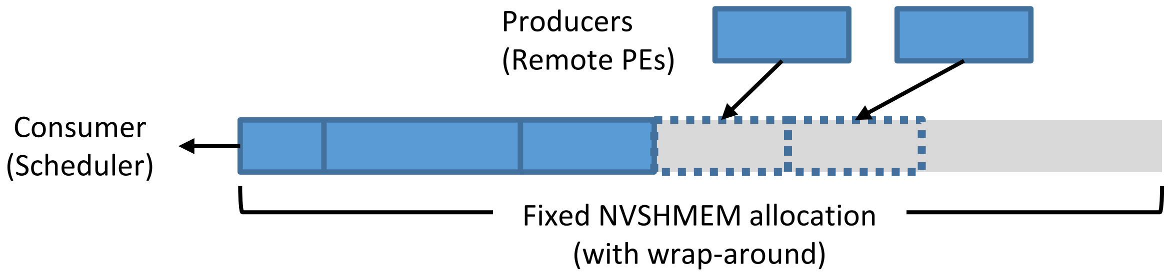
[Future]

Scheduler



- Persistent kernel, single thread per GPU
- PE 0 (thread 0 on GPU 0) executes user's main function
  - Creates chare objects and initiates program flow (invoke entry methods)
- All PEs keep receiving messages and executing entry methods until termination
  - New kernels launched using CUDA dynamic parallelism to perform user's data parallel tasks

Message Queue



[Multi-Producer Single-Consumer (MPSC) Ring Buffer]

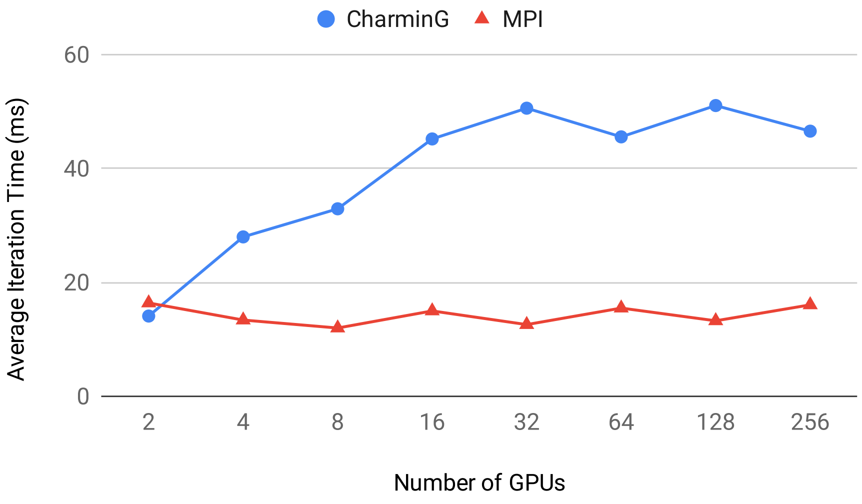
- Implemented as MPSC ring buffer with wrap-around to utilize fixed NVSHMEM allocation
  - Also working on SPSC-based implementation (O(N^2) memory usage in exchange for less remote atomic operations)
- Producers (remote PEs)
  - Try to acquire space in the consumer's message queue using **NVSHMEM atomics**
  - Once acquired, transfer message using **NVSHMEM one-sided put**
- Consumer (local PE, scheduler)
  - Consumes messages starting from the lowest address

Jacobi2D Proxy App

```
__global__ void jacobi_kernel(double* temp, double* new_temp,
                              int block_width, int block_height) {
  int i = blockDim.x * blockIdx.x + threadIdx.x + 1;
  int j = blockDim.y * blockIdx.y + threadIdx.y + 1;
  if (i < block_height + 1 && j < block_width + 1) {
    new_temp[IDX(i,j)] = (temp[IDX(i,j)] + temp[IDX(i,j-1)]
      + temp[IDX(i,j+1)] + temp[IDX(i-1,j)] + temp[IDX(i+1,j)]) * 0.2;
  }
}

// Block is a chare object
struct Block : charming::chare {
  __device__ Block() {}
  __device__ void send_boundaries();
  __device__ void recv_ghost(void* arg);
  __device__ void update();
};
```

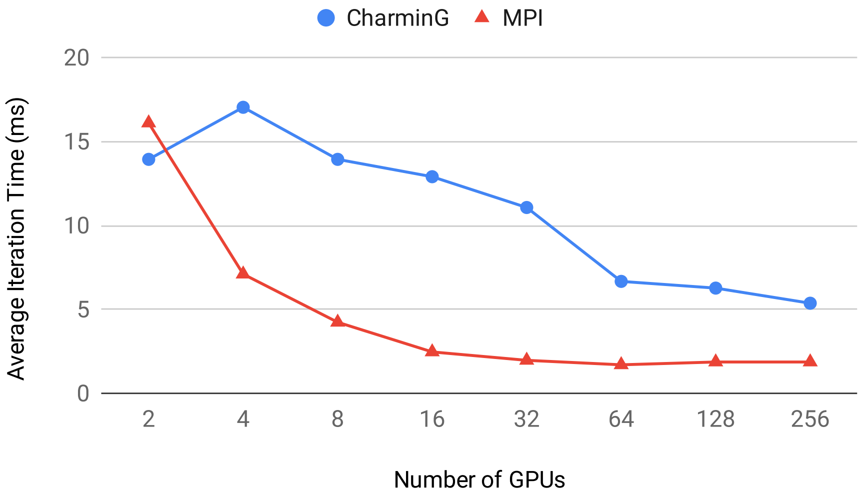
```
__device__ void Block::send_boundaries() {
  block_proxy->invoke(left_neighbor, 1, left_boundary, ghost_size);
  ...
}

__device__ void Block::recv_ghost(void* arg) {
  int dir = *(int*)arg;
  double* ghost = (double*)((int*)arg + 1);
  switch (dir) { ... } // Unpack if necessary
  if (++recv_count == neighbor_count) update();
}

__device__ void Block::update() {
  jacobi_kernel<<<grid_dim, block_dim>>>(...);
  cudaDeviceSynchronize();

  if (++iter == n_iters) charming::exit();
  else send_boundaries();
}
```

Jacobi2D Preliminary Performance



[Weak Scaling]

Base: 16K x 16K doubles



[Strong Scaling]

16K x 16K doubles

- Comparison against non-blocking CUDA-aware MPI based implementation
- Up to 64 nodes (256 NVIDIA V100 GPUs) on LLNL Lassen
- Much room for performance improvement

Current Status & Future Work

- Prototype working on NVIDIA GPUs
  - C++ templates to support user-defined chare types
  - NVSHMEM for device-initiated GPU communication
  - CUDA dynamic parallelism to launch new kernels
- Future work
  - Analyze and improve performance (communication, scheduler, launching of user kernels)
  - Explore computation-communication overlap with overdecomposition

Summary

- GPU features in Charm++
  - Asynchronous execution & completion notification using CUDA streams & HAPI
  - GPU-aware communication: GPU Messaging API, Channel API
- CharminG: GPU-resident runtime system

Thank You!