# Achieving Computation-Communication Overlap with Overdecomposition on GPU Systems

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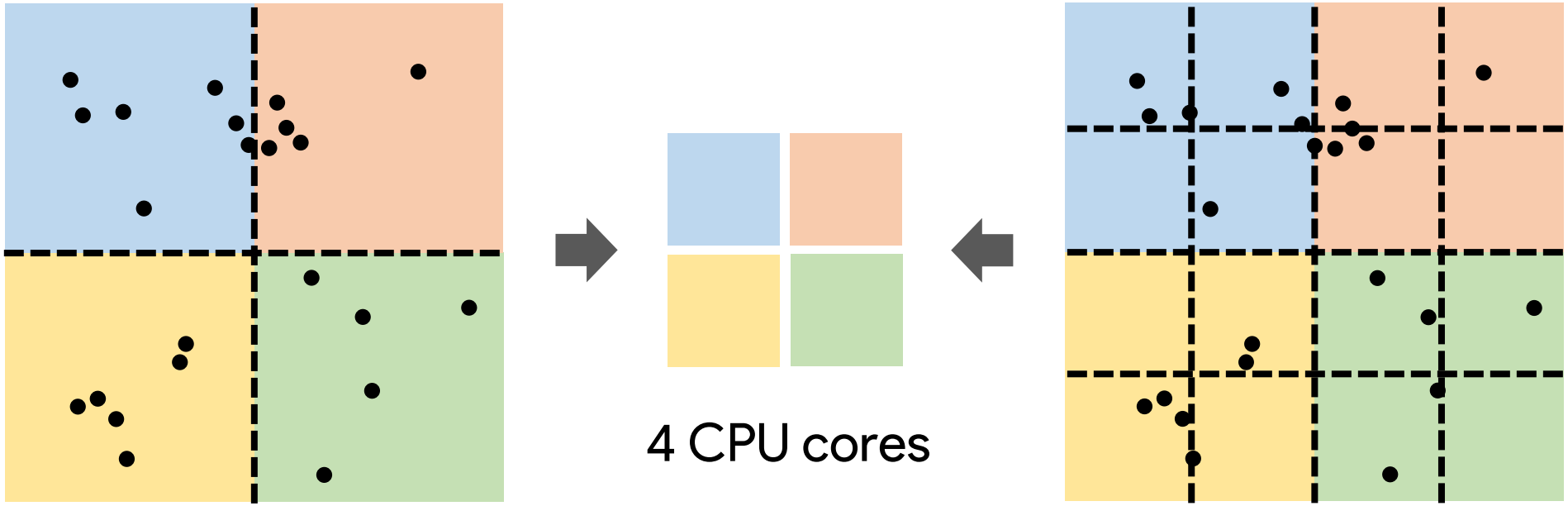
# Overview

- Increasing gap between single-node computational power and inter-node communication performance on modern supercomputers
- Can be tackled from at least 2 directions
  1. Improve communication performance itself with software optimizations and better utilization of hardware support (e.g. GPUDirect, SHARP, hardware tag-matching)
  2. Reduce impact of communication on overall performance (e.g. computation-communication overlap)
- Focus on computation-communication overlap

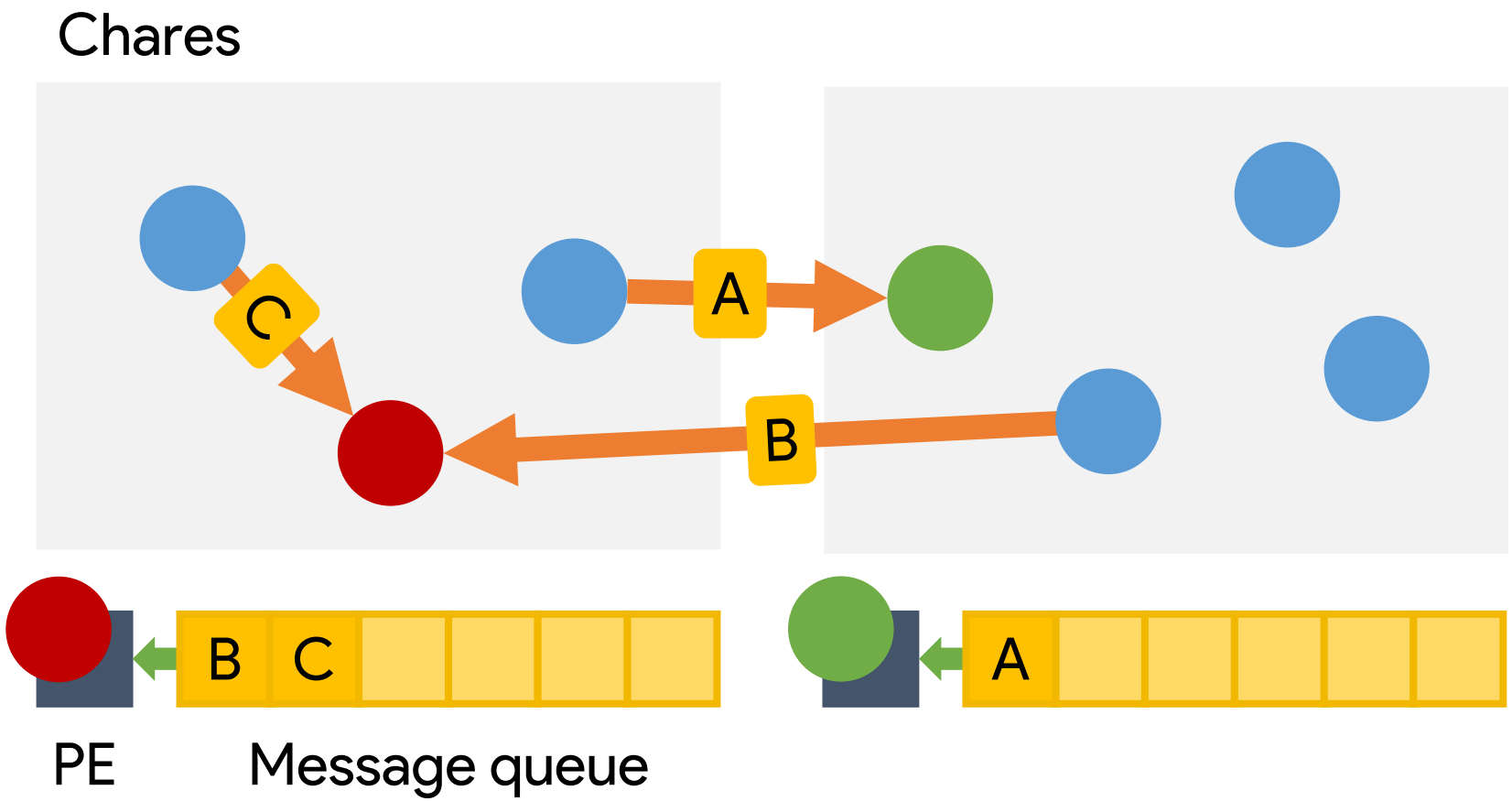
# Overdecomposition



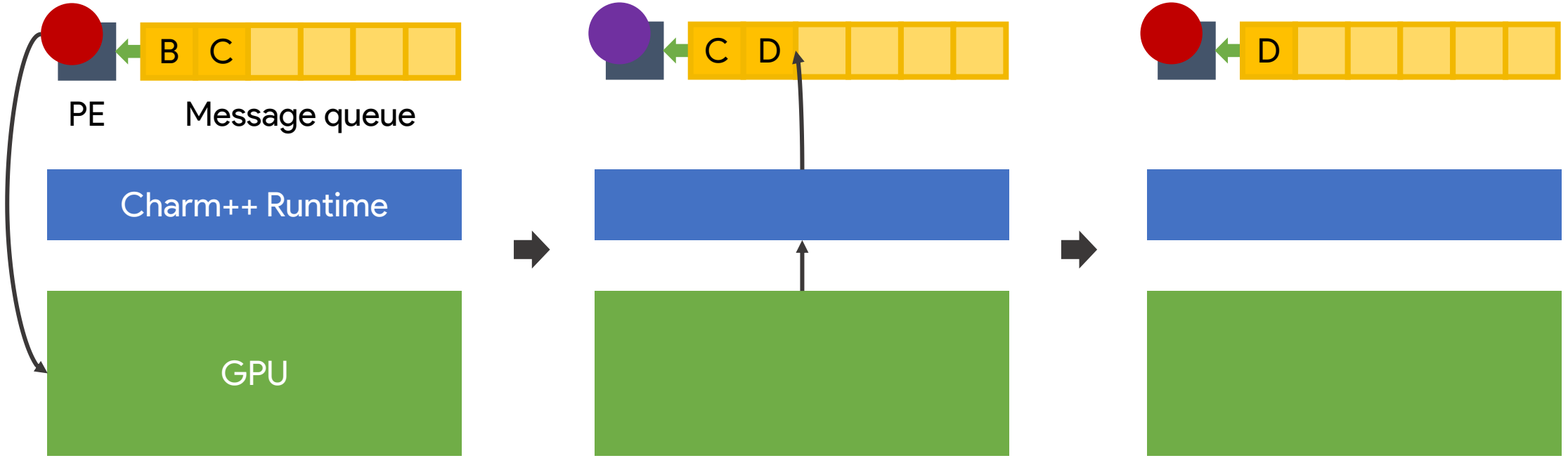

Per-process decomposition
(MPI)

Overdecomposition
(Charm++)

# Asynchronous Message-Driven Execution



# GPU Execution in Charm++




1. Asynchronously offload work to GPU

2-1. Scheduler progresses communication and executes next chare
2-2. GPU work completes, runtime enqueues new message

3. Work that depends on the completed GPU work can continue (e.g. another entry method of the original chare)

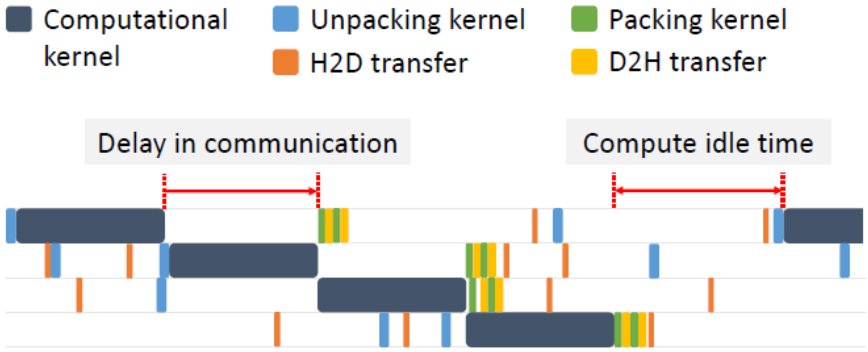
# Achieving Computation-Communication Overlap

1. **Support asynchronous progress in the runtime**
   - Avoid synchronization CUDA APIs (e.g. cudaStreamSynchronize)
     - Charm++ scheduler blocked from performing other chares' work
     - Cannot make forward progress on communication (without comm. threads)
   - Directly using CUDA async APIs to determine completion is infeasible
     - Scheduler-driven execution in Charm++
     - CUDA-generated thread disassociated from the Charm++ runtime
   - `hapiAddCallback(cudaStream_t stream, CkCallback* callback)`
     - Allows user to schedule a Charm++ callback to be invoked when GPU operations complete in the specified CUDA stream
     - Two compile-time configurable mechanisms based on CUDA Callback and CUDA Events (default)
   - https://charm.readthedocs.io/en/latest/charm++/manual.html#gpu-support

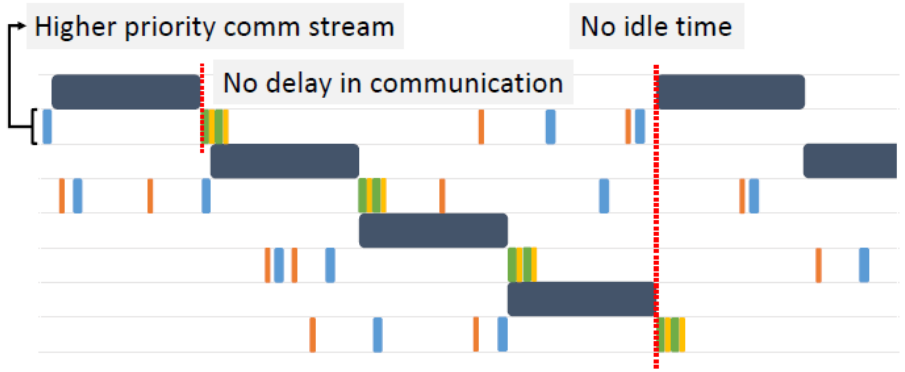
# Achieving Computation-Communication Overlap

2. **Prioritize communication-related GPU operations in the application**
   - Single CUDA stream per chare: delays in communication-related operations (host-device data transfers, packing/unpacking kernels) due to computational kernels offloaded from other chares to the same GPU
   - Need separate streams for compute and communication (with higher priority for communication)
   - More complex design may be necessary, as for MiniMD (described in paper)

# Achieving Computation-Communication Overlap




(a) Single CUDA stream per chare. Communication is delayed by a computational kernel enqueued from another chare, causing idle time between iterations.




(b) Separate compute/communication CUDA streams per chare, with the communication stream given higher priority. Iterations continue without idle times in between.

Fig. 3. Execution timelines of Jacobi2D with four chares mapped to a single GPU.

# Evaluation Platforms

- OLCF Summit
  - 6 NVIDIA Tesla V100s per node
- LLNL Lassen
  - 4 NVIDIA Tesla V100s per node
- PAMILRTS, SMP version of Charm++
- 1 process with 1 PE/core per GPU
  - e.g. 6 PEs and 6 GPUs per compute node on Summit

# Benchmarks

- Iterative proxy apps
- **Jacobi3D**
  - Jacobi iteration performed on 3D grid, overdecomposed into chares
  - Near-neighbor exchange of halo data (up to 6 neighbors)
- **MiniMD**
  - Proxy app for LAMMPS molecular dynamics code
  - Converted MPI-Kokkos to Charm++-Kokkos
  - CUDA-aware MPI converted to explicit host-device transfers and host messages
  - Kokkos responsible for computational kernels and intra-process data movement
  - Neighbor exchange of atoms, Lennard-Jones force calculation

# Performance Results – Jacobi3D

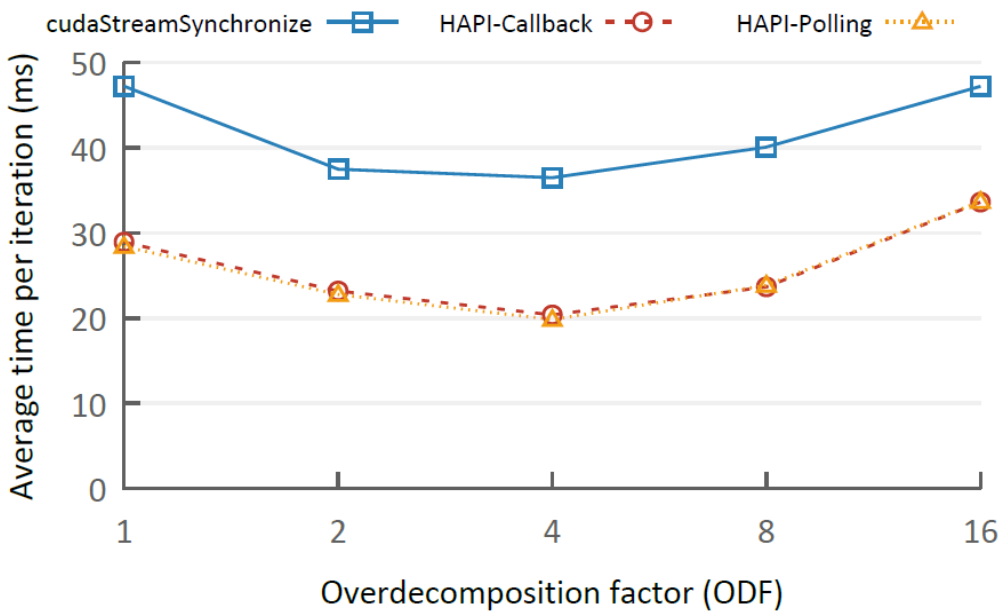
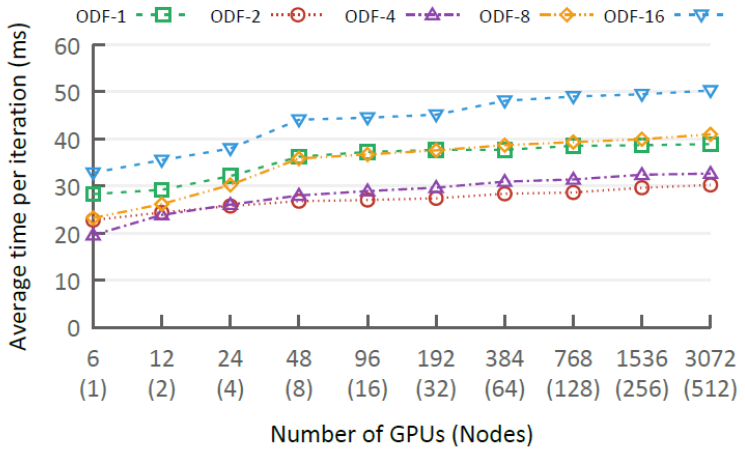
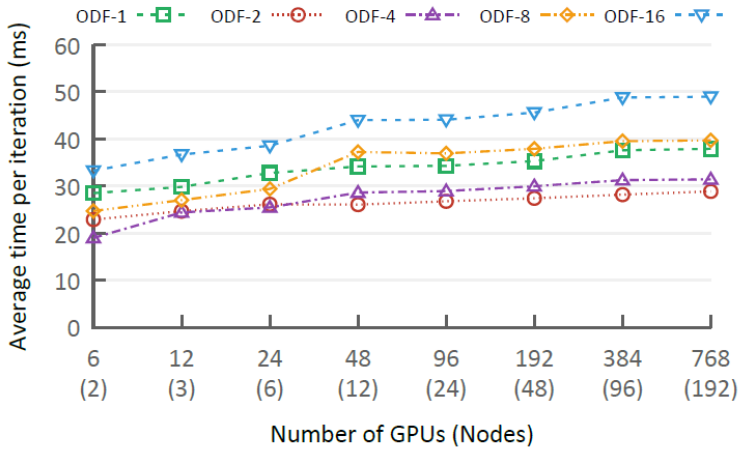



Fig. 5. Performance of Jacobi3D with varying overdecomposition factors on a single node of OLCF Summit.

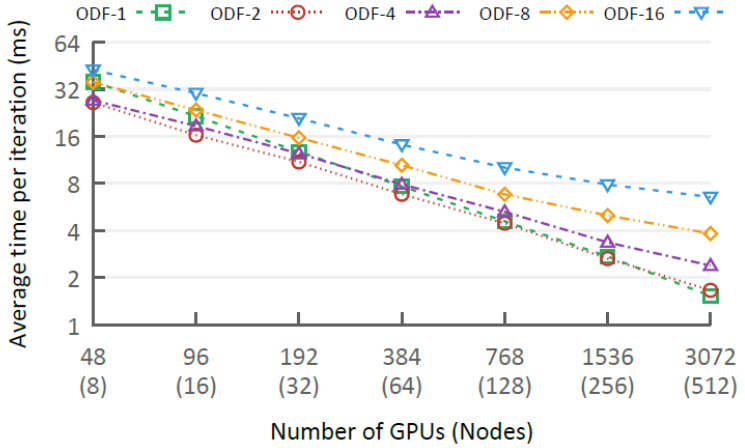
# Performance Results – Jacobi3D



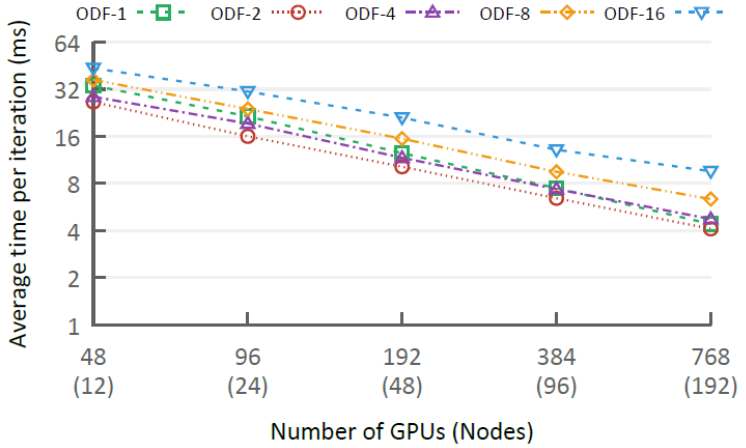

(a) Weak scaling on Summit.




(b) Weak scaling on Lassen.



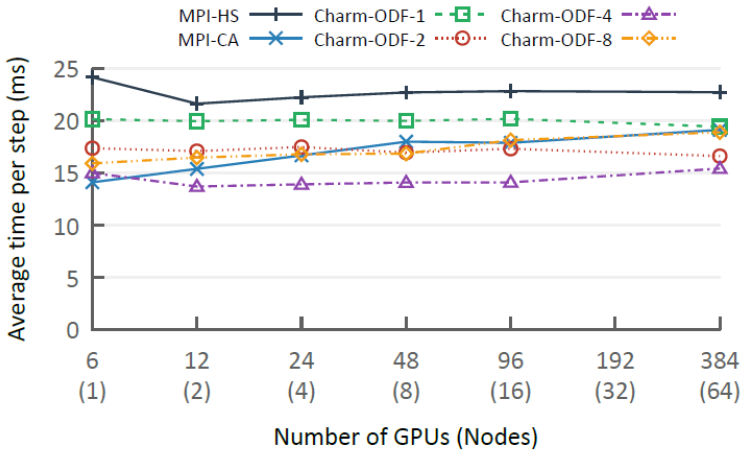

(c) Strong scaling on Summit.



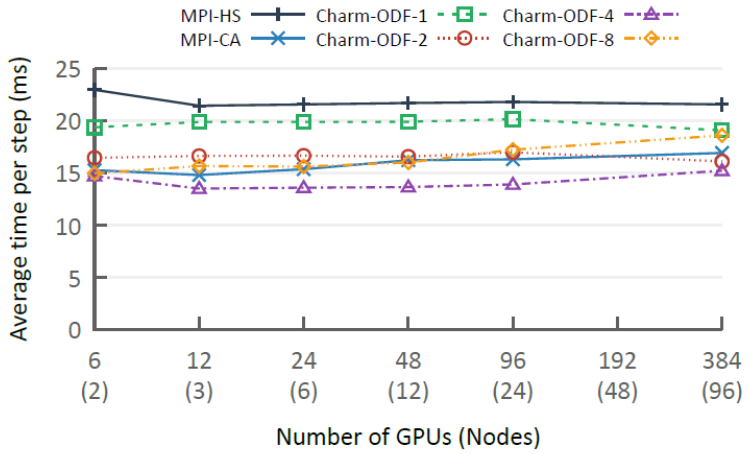

(d) Strong scaling on Lassen.

Fig. 6. Weak & strong scaling performance of Jacobi3D.

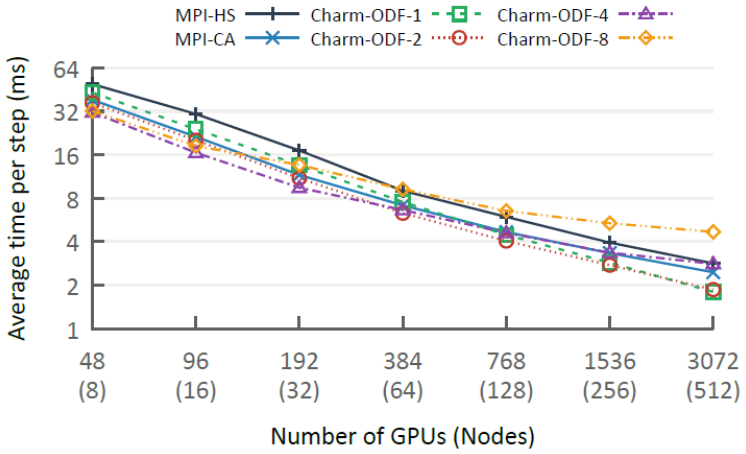
# Performance Results – MiniMD



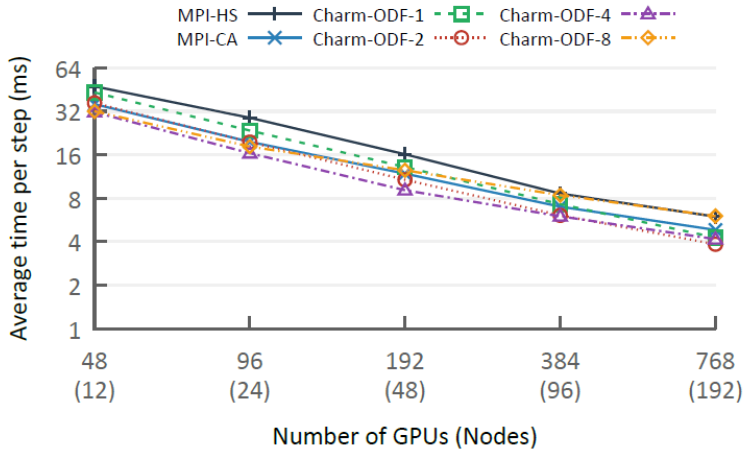

(a) Weak scaling on Summit.




(b) Weak scaling on Lassen.




(c) Strong scaling on Summit.




(d) Strong scaling on Lassen.

Fig. 7. Weak & strong scaling performance of MiniMD.

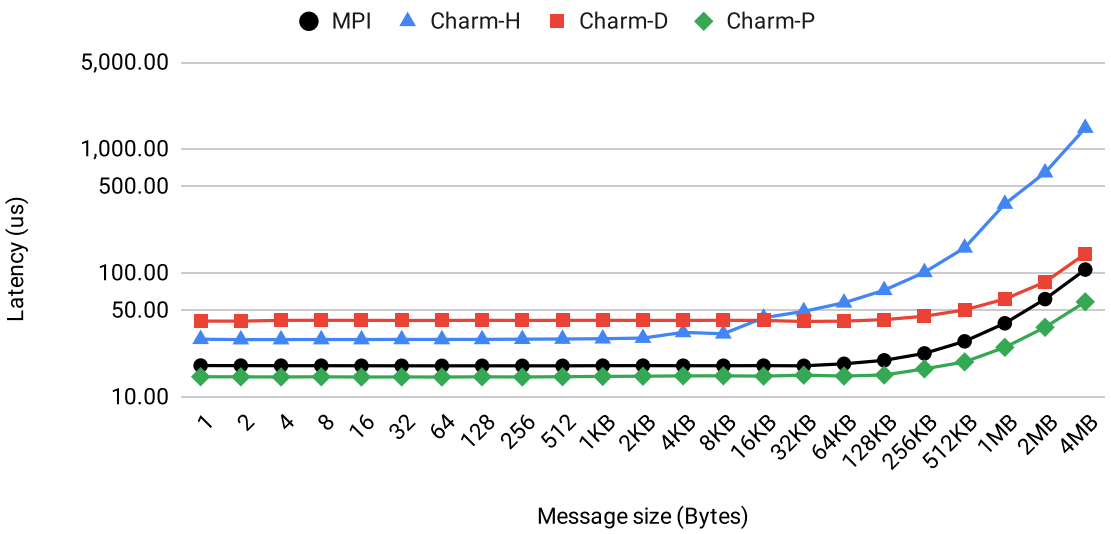
# Conclusion

- Up to **50%** and **47%** improvement in overall performance with Jacobi3D and MiniMD, respectively
- With careful design of the application to prioritize communication and support for asynchronous progress of GPU work in the runtime system, computation-communication overlap can significantly improve performance (esp. in weak scaling)
- Future work: improve communication performance with GPU messaging

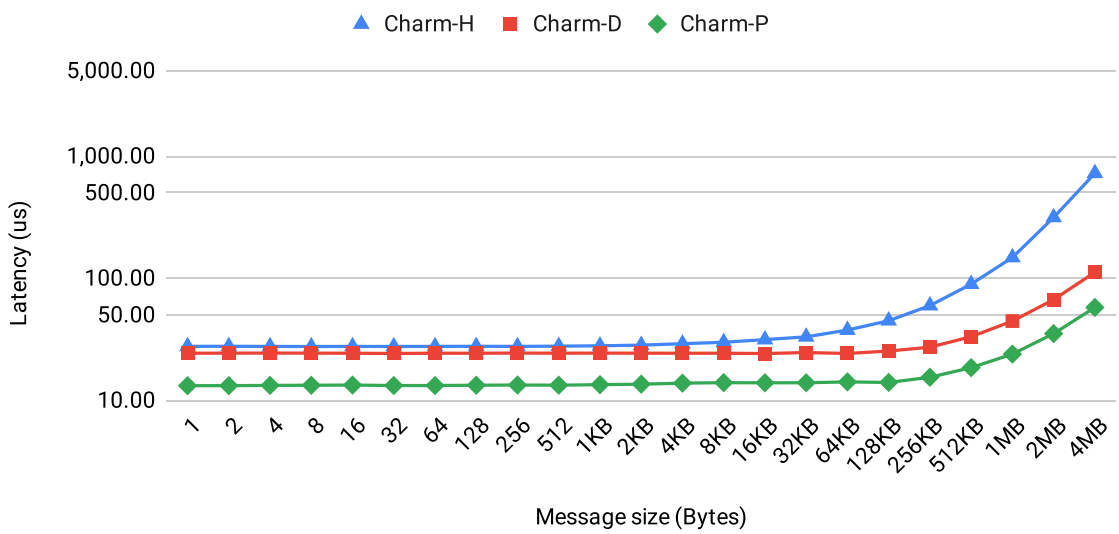
# GPU Messaging in Charm++ 6.11

- Direct data transfer between GPUs using GPUDirect & CUDA IPC, bypassing host memory
- Currently supports intra-node messages, support for inter-node coming soon
- Regular API
  - For point-to-point messages between chares
  - Currently undergoing performance optimizations
  - Included in 6.11-beta as experimental feature
  - Similar to Zerocopy Post Entry Method API, sender sends metadata & receiver performs a get
  - Documentation: https://charm.readthedocs.io/en/latest/charm++/manual.html#direct-gpu-messaging
- Persistent API
  - For persistent P2P messages between chares (reuse of GPU buffers)
  - Useful for iterative applications
  - Will also be part of 6.11 (merged for 2nd beta)

# GPU Messaging Performance




Inter-process




Intra-process

- Charm-H: Host-staged / Charm-D: Regular GPU messaging / Charm-P: Persistent GPU messaging
- OSU latency benchmark (CUDA-aware MPI and Charm++ versions) on OLCF Summit

Thank you! Questions?