MPICH for Exascale: Supporting MPI-4 and ECP

EXASCALE COMPUTING PROJECT

Approved for public release

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National Nuclear Security Administration

U.S. DEPARTMENT OF ENERGY | Office of Science

Agenda

- Intro
- MPICH Updates
  - GPU
  - Collective
  - MPI-4
- Partner Updates
  - Intel MPI (Nusrat Islam)
  - MVAPICH (Dr. Dhabaleswar Panda)
- Q&A

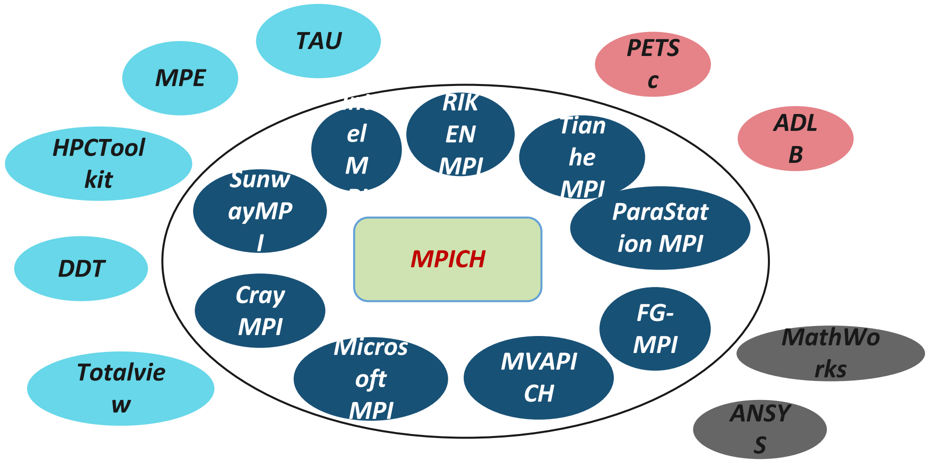
Exascale MPI (MPICH)

- Funded by DOE for 29 years
- Has been a key influencer in the adoption of MPI
  - First/most comprehensive implementation of every MPI standard
  - Allows supercomputing centers to not compromise on what features they demand from vendors
- DOE R&D100 award in 2005
- MPICH and its derivatives are the world's most widely used MPI implementations
  - Supports all versions of MPI including the recent MPI-3.1

- MPICH Adoption in US Exascale Machines
  - Aurora, ANL, USA (MPICH)
  - Frontier, ORNL, USA (Cray MPI)
  - El Capitan, LLNL, USA (Cray MPI)

MPICH is not just a software

It's an Ecosystem

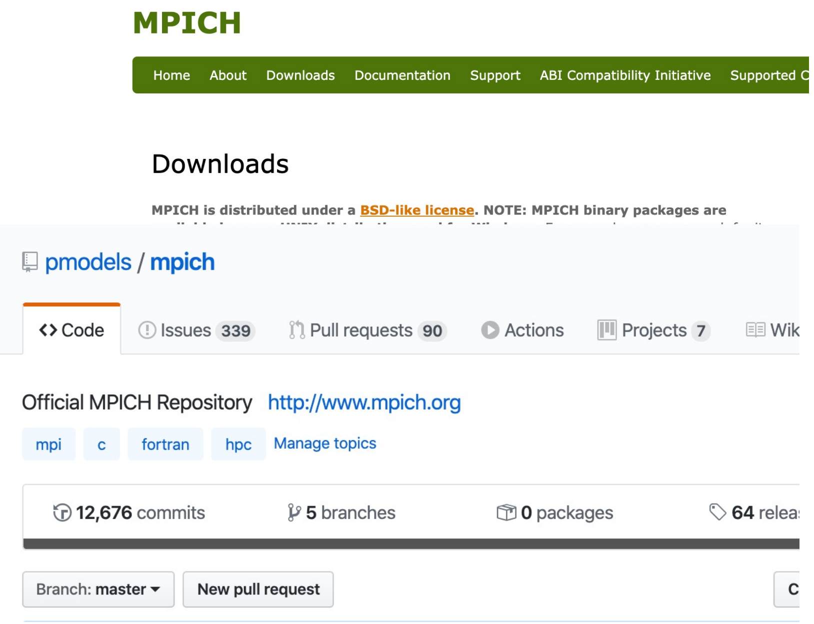


MPICH ABI Compatibility Initiative

- Binary compatibility for MPI implementations
  - Started in 2013
  - Explicit goal of maintaining ABI compatibility between multiple MPICH derivatives
  - Collaborators:
    - MPICH (since v3.1, 2013)
    - Intel MPI Library (since v5.0, 2014)
    - Cray MPT (starting v7.0, 2014)
    - MVAPICH2 (starting v2.0, 2017)
    - Parastation MPI (starting v5.1.7-1, 2017)
    - RIKEN MPI (starting v1.0, 2016)
- Open initiative: other MPI implementations are welcome to join
- http://www.mpich.org/abi

MPICH Distribution Model

- Source Code Distribution
  - MPICH Website, Github
- Binary Distribution through OS Distros and Package Managers
  - Redhat, CentOS, Debian, Ubuntu, Homebrew (Mac)
- Distribution through HPC Package Managers
  - Spack, OpenHPC
- Distribution through Vendor Derivatives



MPICH Releases

- MPICH typically follows an 18-month cycle for major releases (3.x), barring some significant releases
  - Minor bug fix releases for the current stable release happen every few months
  - Preview releases for the next major release happen every few months
- Current stable release is in the 3.4.x series
  - mpich-3.4.1 was released last week
- Upcoming major release is in the 4.0 series
  - mpich-4.0a1 is released

MPICH-3.4 Series

POC: Ken Raffenetti
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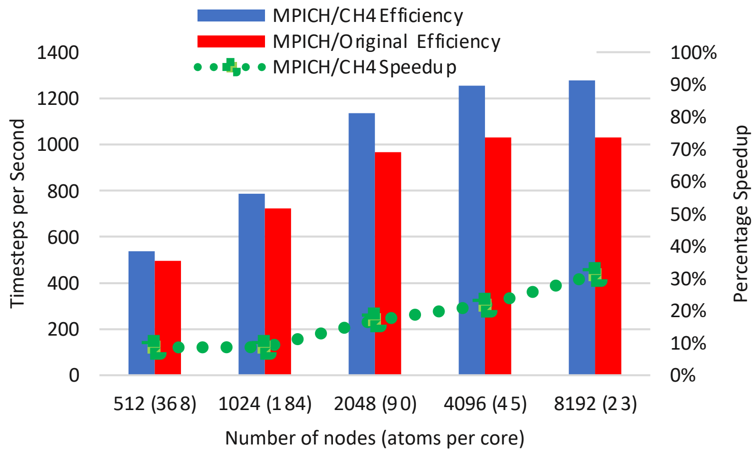
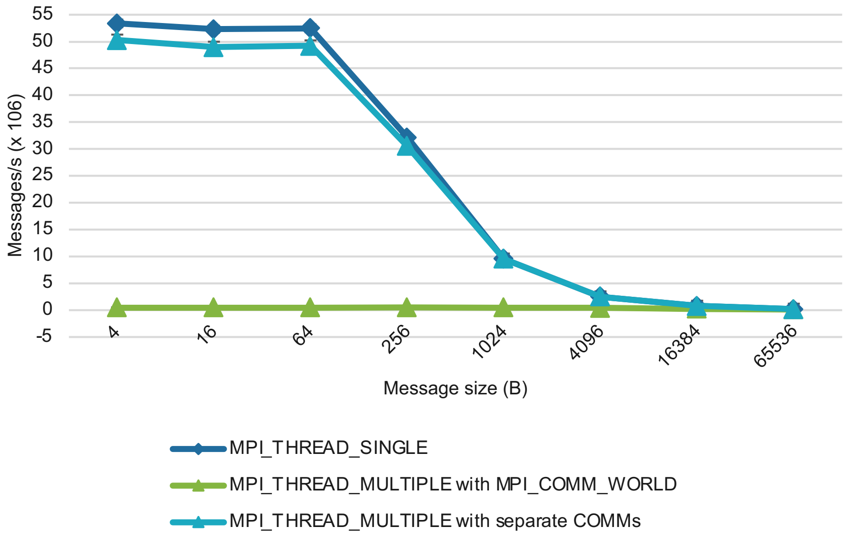
- **CH4 device being the default**
  - Replacement for CH3 as default option, CH3 still maintained till all of our partners have moved to CH4
  - Co-design effort
    - Weekly telecons with partners to discuss design and development issues
  - Three primary objectives:
    - Low-instruction count communication
      - Ability to support high-level network APIs (OFI, UCX)
      - E.g., tag-matching in hardware, direct PUT/GET communication
    - Support for very high thread concurrency
      - Improvements to message rates in highly threaded environments (MPI_THREAD_MULTIPLE)
      - Support for multiple network endpoints (THREAD_MULTIPLE or not)
    - Support for GPU





The CH4 in MPICH is developed in close collaboration with vendor partners including Including AMD, Cray, Intel, Mellanox and NVIDIA

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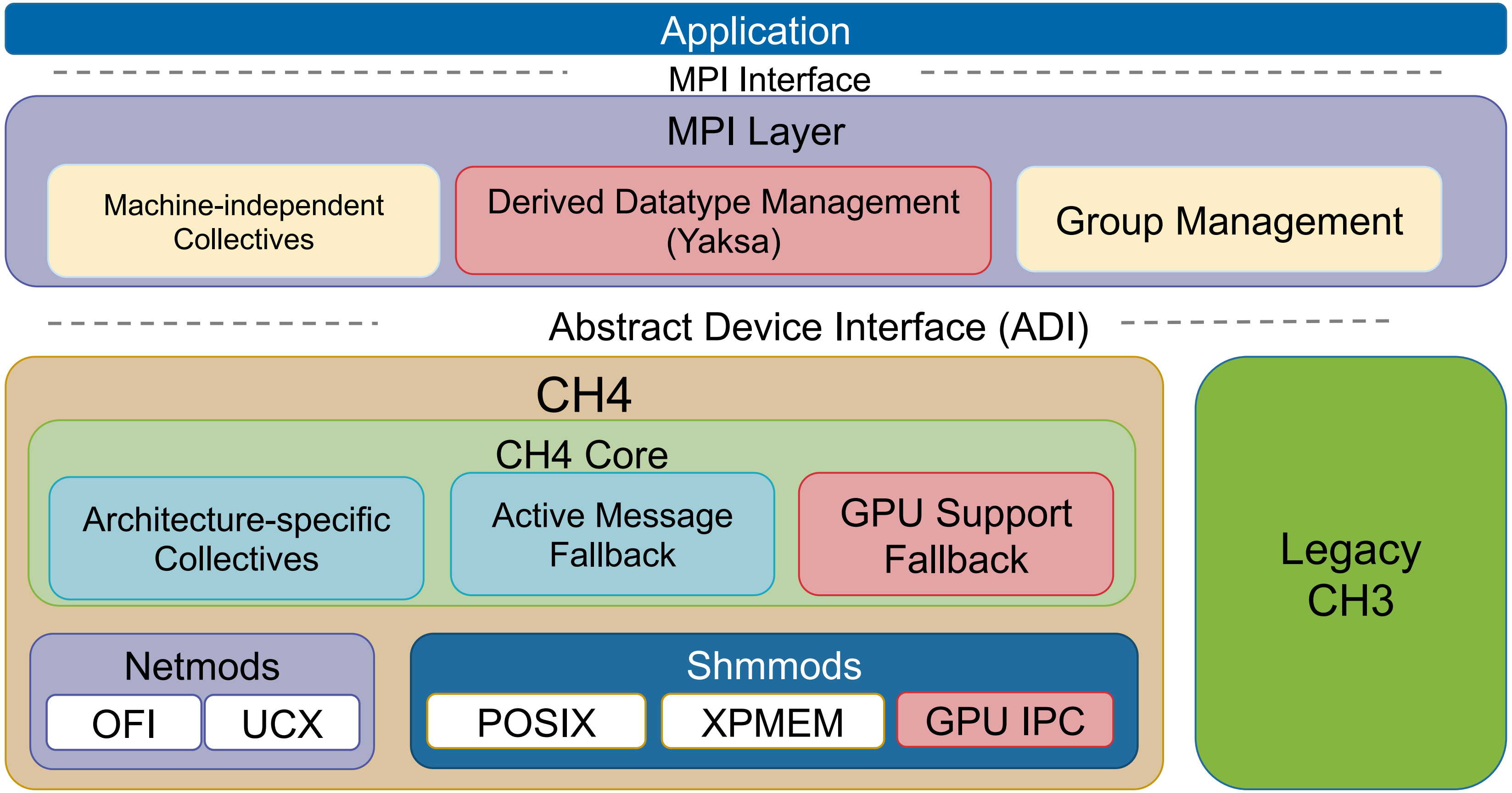
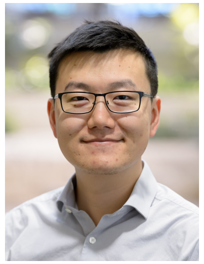
MPICH with CH4 Device Overview

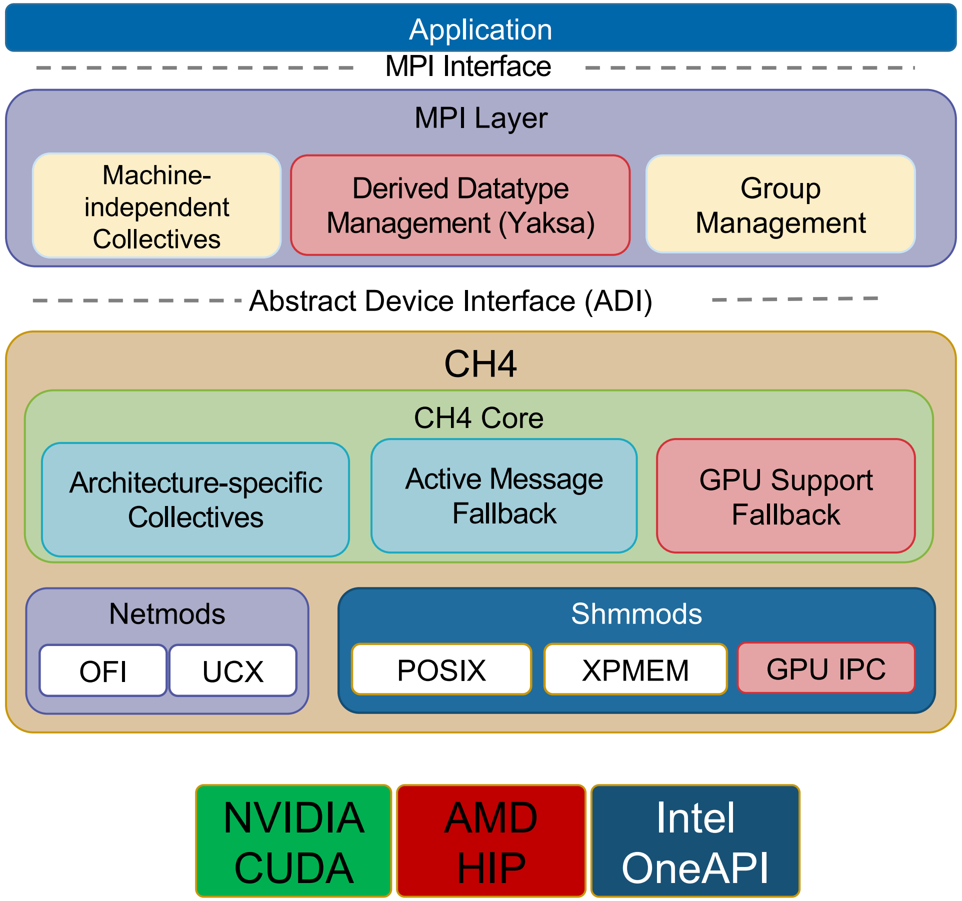


Supporting GPU in MPI Communication (1/3)



POC: Yanfei Guo
<yguo@anl.gov>

- **Native GPU Data Movement**
  - Multiple forms of “native” data movement
  - GPU Direct RDMA is generally achieved through Libfabrics or UCX (we work with these libraries to enable it)
  - GPU Direct IPC is integrated into MPICH
- **GPU Fallback Path**
  - GPU Direct RDMA may not be available due to system setup (e.g. library, kernel driver, etc.)
  - GPU Direct IPC might not be possible for some system configurations
  - GPU Direct (both forms) might not work for noncontiguous data
  - Datatype and Active Message Support



The GPU support in MPICH is developed in close collaboration with vendor partners including Including AMD, Cray, Intel, Mellanox and NVIDIA

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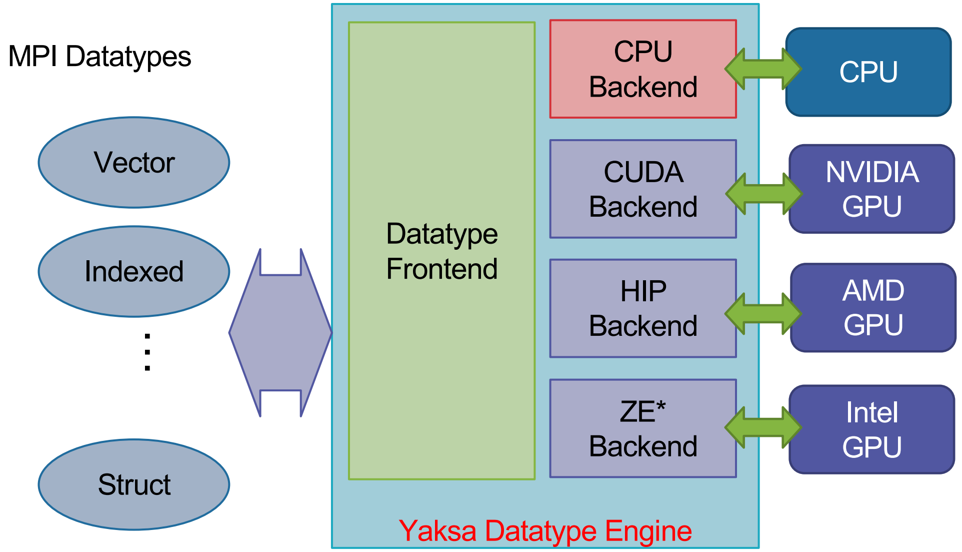
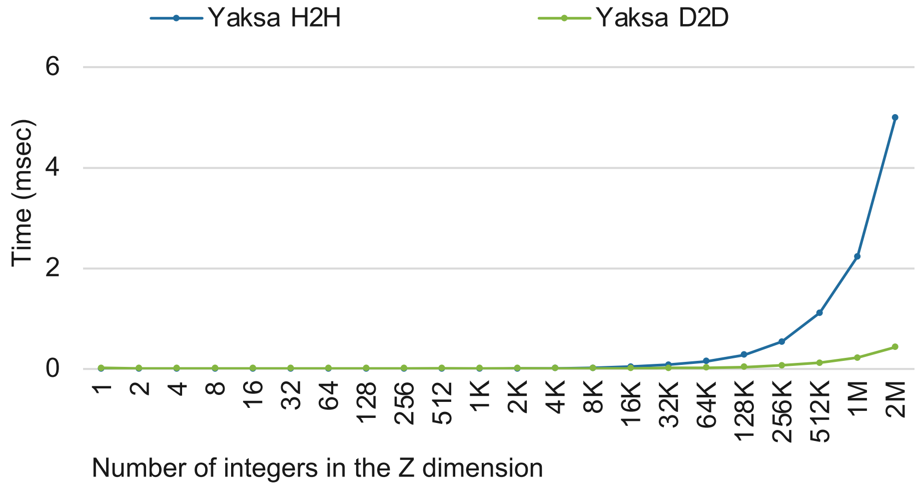
Supporting GPU in MPI Communication (2/3)

- **MPICH support for using complex noncontiguous buffers with GPU**
  - Buffer with complex datatype is not directly supported by the network library
  - Packing complex datatype from GPU into contiguous send buffer
  - Unpacking received data back into complex datatype on GPU
- **Yaksa: A high performance datatype engine**
  - Used for internal datatype representation in MPICH
  - Front-end provide interface for MPI datatypes
  - Multiple backend to leverage different hardware for datatype handle
  - Generated GPU kernels for packing/unpacking





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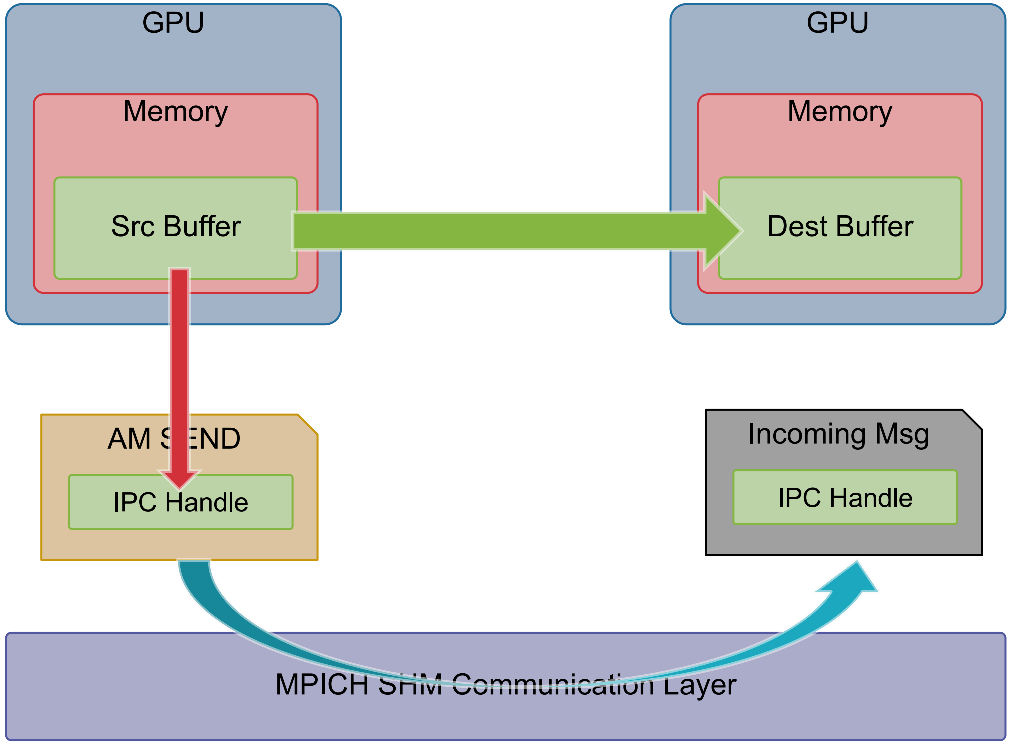
Supporting GPU in MPI Communication (3/3)

- **Supporting Multiple GPU Node**
  - Data movement between GPU devices
  - Utilizing high bandwidth inter-GPU links (e.g. NVLINK)
- **GPU-IPC Communication via Active Message**
  - Create IPC handles for GPU buffers
  - Send IPC handles to target process
  - Receiver initiate Read/Write using the IPC handle
- **Fallback Path in General SHM Active Message**
  - When IPC is not available for the GPU-pair



The GPU support in MPICH is developed in close collaboration with vendor partners including Including AMD, Cray, Intel, Mellanox and NVIDIA

New Collective Infrastructure

- Thanks to Intel for the significant work on this infrastructure
- Two major improvements:
  - C++ Template-like structure (still written in C)
    - Allows collective algorithms to be written in template form
    - Provides “generic” top-level instantiation using point-to-point operations
    - Allows device-level machine specific optimized implementations (e.g., using triggered operations for OFI or HCOLL for UCX)
  - Several new algorithms for a number of blocking and nonblocking collectives (performance tuning still ongoing)

Contributed by Intel (with some minor help from Argonne)

Collective Selection Framework

- Choose Optimal Collective Algorithms
  - Optimized algorithm for certain communicator size, message size
  - Optimized algorithm using HW collective support
  - Making decision on each collective call
- Generated Decision Tree
  - JSON file describing choosing algorithms with conditions
  - JSON file created by profiling tools
  - JSON parsed at MPI_Init time and applied to the library

Contributed by Intel (with some minor help from Argonne)

MPICH 4.0 Release Series

Implement MPI-4 Standard

and more …

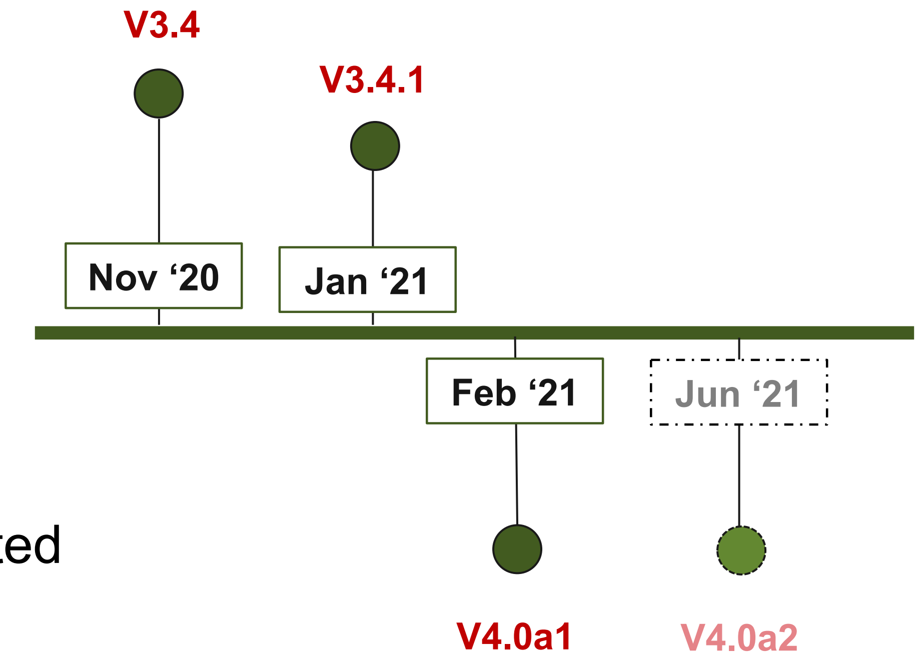
Focuses in MPICH 4.0 Release Series

POC: Hui Zhou
<zhouh@anl.gov>

- Full implementation of MPI 4 specification
  - MPI Sessions
  - Partitioned Communications
  - Persistent Collectives, Tool Events, Large Count, and more
  - https://www.mpi-forum.org/docs/
- Enhance GPU and threading support
  - Make the support more stable and user experience smoother
  - Push the production performance to our research projection
- Improve useability
  - Explore MPIX space for more natural/direct semantics

MPICH 4.0 Roadmap

- MPICH-4.0a1 released in February
  - Majority of the MPI 4 API implemented



- MPICH-4.0a2 will release in June
  - Synchronized to MPI Forum meeting with the expected official ratification of MPI 4 standard
  - Full implementation of MPI 4 API
  - More stable GPU/threading support

- Beta and GA release in early 2022

- Most bug fixes will be back ported to 3.4.x

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C Binding Generation

- \+ 3,000 lines of Python script
- \- 40,000 lines of C

```
MPI_Bcast_init:
    .desc: Creates a persistent request for broadcast
```

- API extracted from mpi-standard repo
- Generates –
  - Profiling interface
  - API documentation
  - Parameter validation
  - Handle object pointer conversion
- Fortran binding generation will be updated to Python and unified
  - F08 binding generation 80% done

MPI Session

```c
void library_foo_init(void)
{
    MPI_Session_init(info, errhan, &session);
    MPI_Group_from_session_pset(session, "mpi://world", &group);
    MPI_Comm_create_from_group(group, "foo (string tag)",
                               info, errhan, &comm);
    ...
}
```

- Libraries to keep MPI usage opaque to user
- Basic implementation internally initializes “world” in the first `MPI_Session_init/MPI_Init`
- Better implementation will delay the world initialization to first world-comm
- Fully *correct* implementation need to support first-class dynamic processes

Partitioned Communication

- In-between two-sided (pt2pt) and one-sided (RMA) communication
- Basic implementation done, plenty of optimization opportunity ahead!

```
if (rank == sender) {
  MPI_Psend_init(buf, parts, cnt, datatype,
                 recver, tag, comm, info, &req);
  MPI_Start(&req);
  ...
  MPI_Pready(i);
  ...
  MPI_Wait(&req, MPI_STATUS_IGNORE);
  MPI_Request_free(&req);
}
```

```
if (rank == recver) {
  MPI_Precv_init(buf, parts, cnt, datatype,
                 sender, tag, comm, info, &req);
  MPI_Start(&req);
  ...
  MPI_Parrived(req, i, &flag);
  ...
  MPI_Wait(&req, MPI_STATUS_IGNORE);
  MPI_Request_free(&req);
}
```

Large Count API

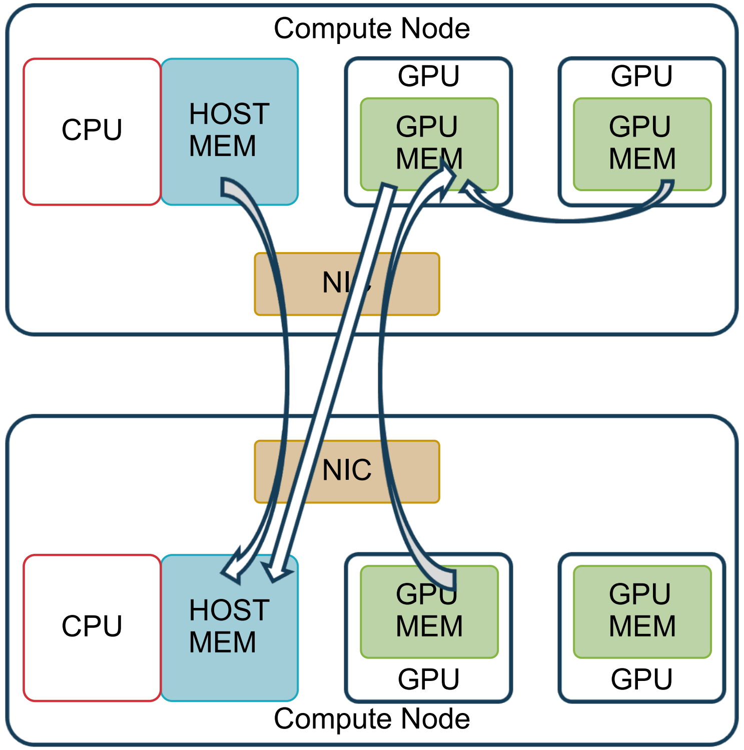
- A large count version for every API that has a ”count” or “displacement” argument (guess how many?)
- No more work-arounds!
- API use `MPI_Count`, internally we use `MPI_Aint` where-ever possible

```
MPI_Type_contiguous_c(10000000000, MPI_INT, &my_type);
```

```
MPI_Send_c(buf, 10000000000, MPI_INT, dest, tag, comm);
```

Enhanced GPU Support

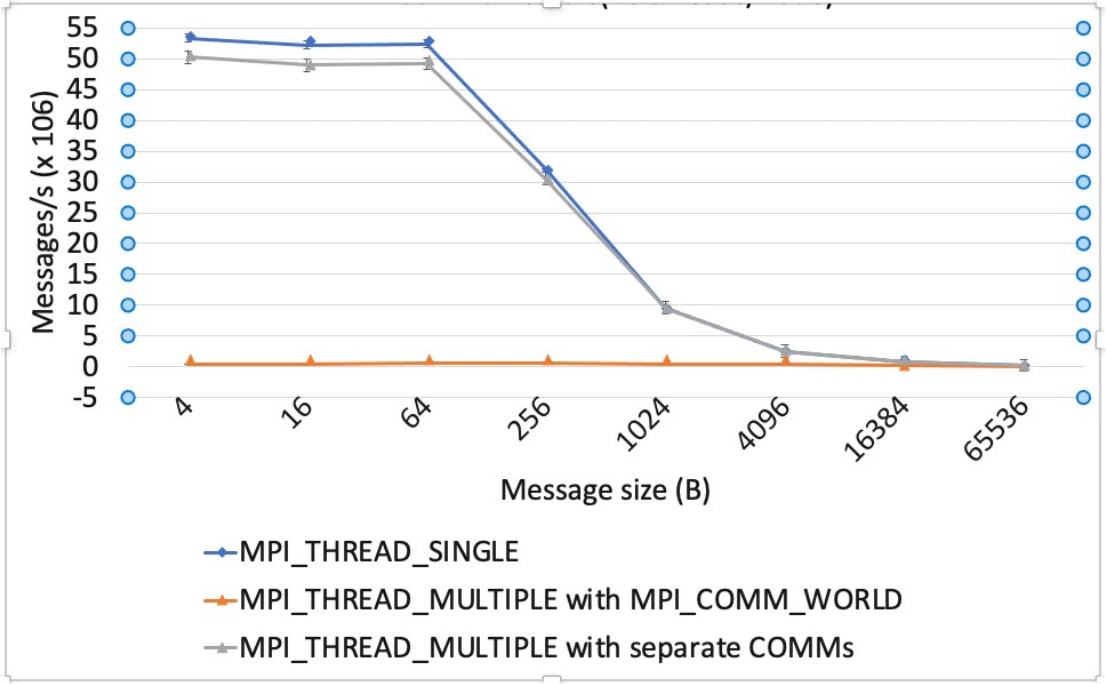
- MPICH is fully GPU-aware since 3.4.0
- But …
  - May experience degraded performance even for non-GPU app
    - GPU initialization cost, GPU pointer query cost, …
  - Cloudy with a chance of crash
    - GPU testing takes 8 hours!
  - Need GPU-aware API
- We are working on it …
  - `MPIR_CVAR_ENABLE_GPU=0` should recover full CPU-only performance
  - Fine-tuned usable GPU-testing and keeping it green
  - GPU direct IPC, GPU specific algorithm, …
- Explore `MPIX` extension



Better Threading Support

- Enable strong scaling with multiple VCI (virtual communication interface)
- Multi-VCI for Point-to-point implemented in 3.4.0
- Multi-VCI for RMA added in 4.0a1
- Multi-VCI for Active Messages coming

- Parallel semantics based on `communicator/rank/tag`
- Explore MPIX for direct threading semantics



Weekly MPICH Development Update

If you are excited with we are doing and like to get more technical –

https://bluejeans.com/266293319

Give us a whistle and we'll send you an invite.