DEEP Projects

ParaStation MPI

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ParTec Modular Supercomputing

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Outline

- ParaStation overview
- Modular MPI Jobs
  - Network Bridging
  - Workflows
  - MSA awareness
- CUDA awareness
- Persistent MPI Windows

ParaStation History

- 1995: ParaStation research project (→ University of Karlsruhe)
- 1999: ParTec was founded as a spin-off
- 2005: Open source (→ ParaStation Consortium)
- since 2004: Cooperation with JSC
  - various precursor clusters
  - DEEP-System (MSA Prototype)
  - JURECA (Cluster/Booster)
  - JUWELS (Cluster/Booster)
  - JURECA DC
- since 2010: DEEP Projects
  - Cluster/Booster → Modularity
- since 2017: ParaStation Modulo

ParaStation Modulo

- ParaStation ClusterTools
  - Tools for provisioning and management
- ParaStation HealthChecker & TicketSuite
  - Automated error detection & error handling
  - Ensuring integrity of the computing environment
  - Keeping track of issues
  - Powerful analysis tools
- ParaStation MPI & Process Management
  - Runtime environment specifically tuned to the largest distributed memory supercomputers

ParaStation Process Manager

- Scalable network of MPI process management daemons running on the computational nodes:
  - Process startup and control, I/O forwarding, …
  - Precise resource monitoring
  - Proper cleanup after jobs
- PSSLURM and PSMOM:
  - Plugins to the ParaStation Management daemons
  - For tight integration with Slurm & Torque
  - Reduce number of daemons

ParaStation MPI Library

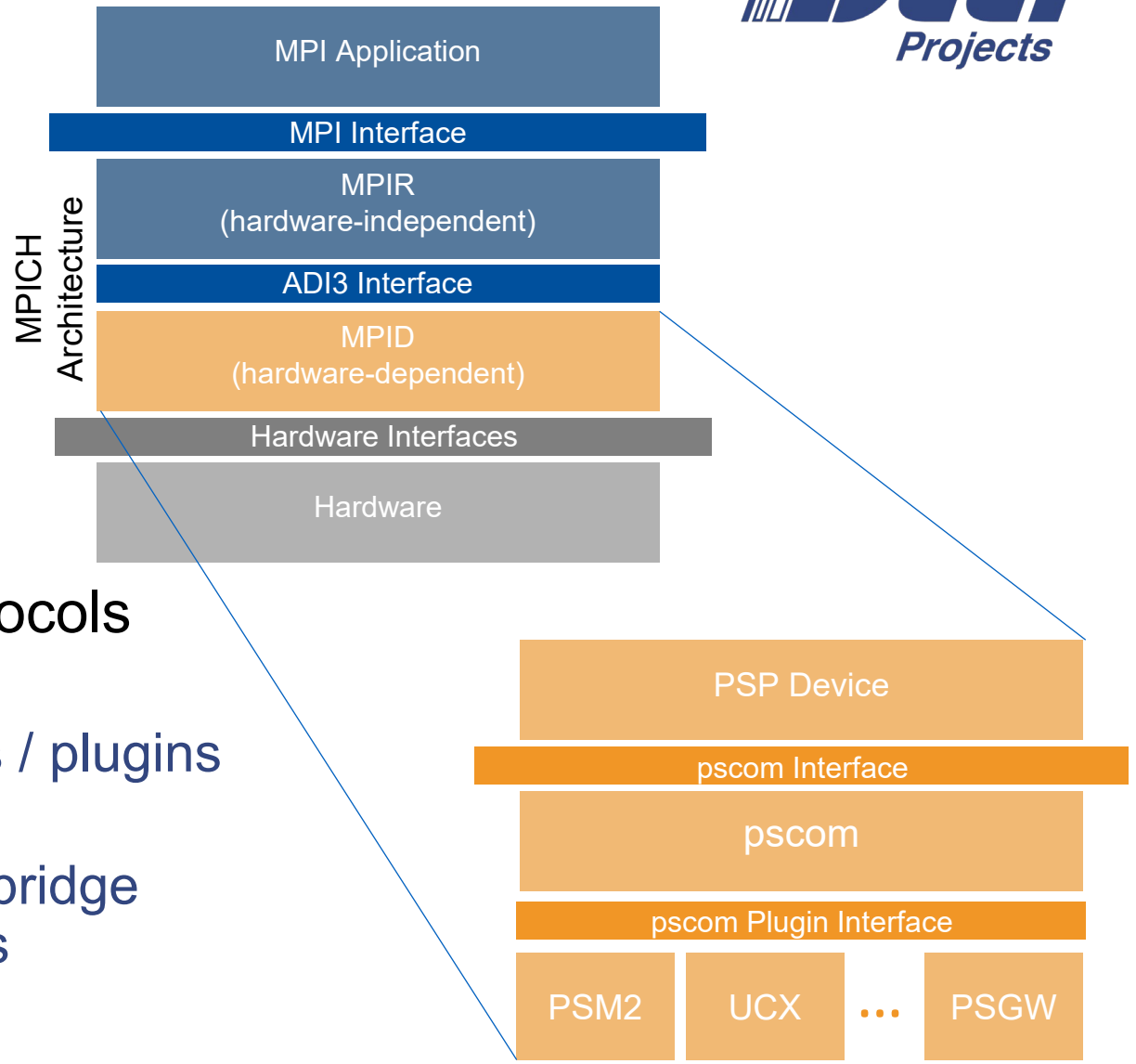
- Based on MPICH 3.3.2 (merge with 3.4.1 coming soon)
  - Maintains MPICH ABI compatibility
  - Supports all MPICH tools (tracing, debugging, …)
- MPI libraries for several compilers (especially for GCC and Intel)
- Supports a wide range of interconnect technologies, even in parallel:
  - InfiniBand on JURECA Cluster and JUWELS
  - Omni-Path on JURECA Booster
  - Extoll on DEEP projects research systems
  - BXI planned to be integrated in RED-SEA

ParaStation MPI Library

- Proven to scale up to 3,500 nodes and 140,000 procs per job
- HPL runs with ParaStation MPI:
  - JURECA & Booster: No. 29 (Top500 Nov 2017)
  - JUWELS: No. 23 (Top500 Jun 2018)
  - JUWELS Booster: No. 7 (Top500 Nov 2020)

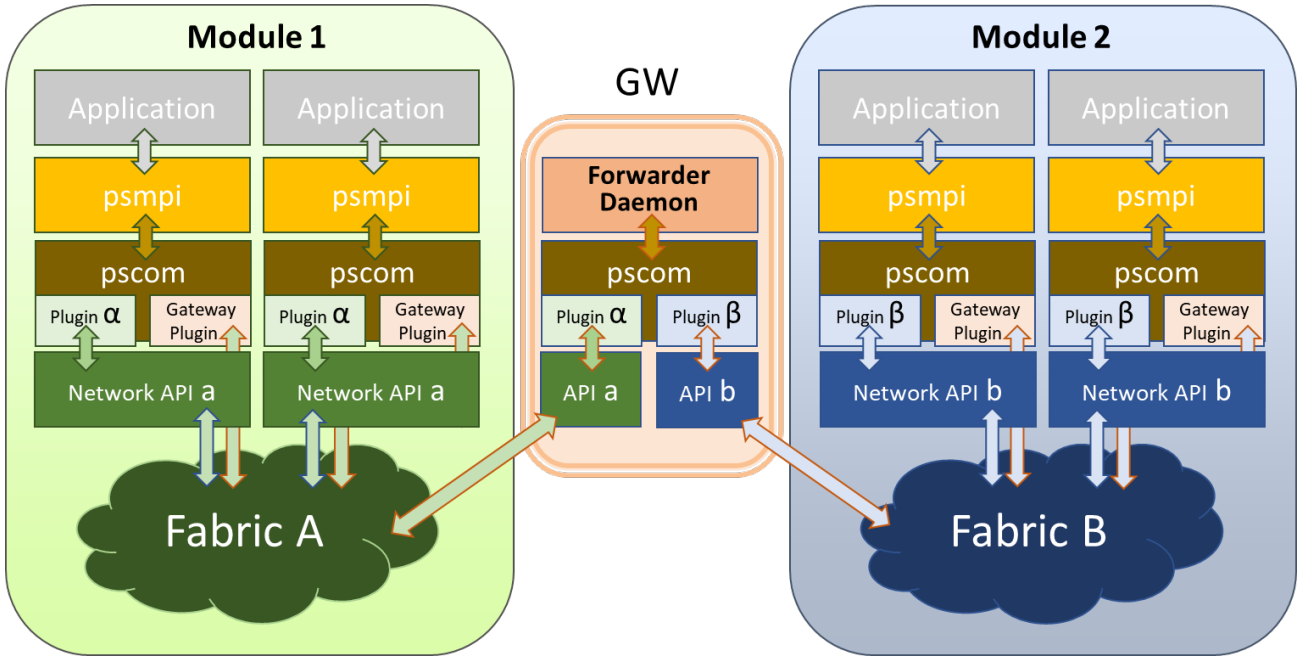
Software Architecture

- Upper (HW-independent) layers are derived from MPICH
- MPICH layers beneath ADI3 are replaced by:
  - ParaStation PSP Device, plus
  - pscom low-level communication library
- Support for various transports and protocols via pscom plugins
  - Applications may use multiple transports / plugins at the same time
  - Gateway capability via PSGW plugin to bridge transparently between different networks



Network Bridging

- Two processes communicate through a gateway if they are not directly connected by a high-speed network (e.g., IB, OPA, Extoll…)
- High-speed connections between processes and gateway daemons
- Static routing to choose a common gateway
- Virtual connection between both processes through the gateway, transparent for the application
- Virtual connections are multiplexed through gateway connections



Modular MPI Jobs

- Example for a job on 2 modules of the DEEP-EST prototype:
  - Use of srun with colon notation

```
srun … : …
```

  - Modules: Cluster (CN) + Extreme Scale Booster (ESB)

```
--partition dp-cn … : … --partition dp-esb
```

  - 8 Nodes / 64 Procs on Cluster and 16 Nodes / 256 Procs on Booster

```
-N8 -n64 … : … -N16 -n256
```

  - Use of 1 gateway node in between

```
srun --gw_num=1 …
```

```
srun --gw_num=1 --partition dp-cn -N8 –n64 ./hello_mpi_world :
--partition dp-esb –N16 –n256 ./hello_mpi_world
```

Workflows

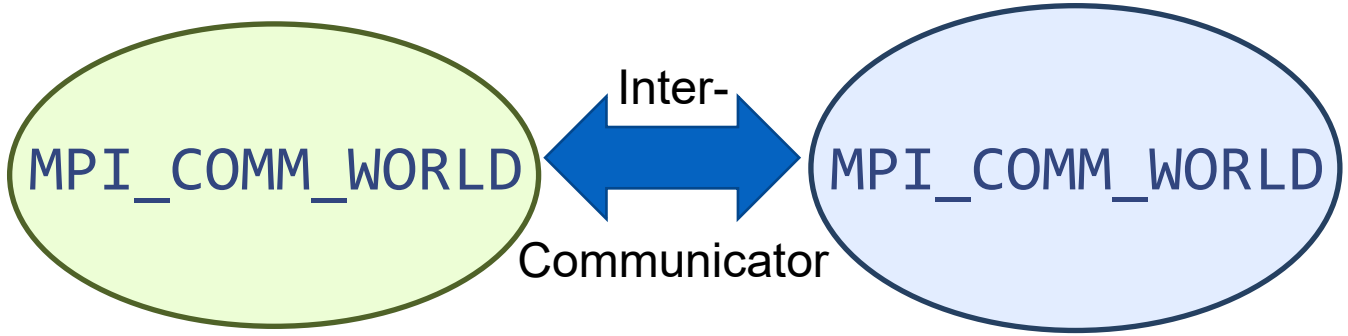
- An MPI job started with colon notation via srun will run in a *single* `MPI_COMM_WORLD`.
- Workflows may demand for multiple `MPI_COMM_WOLRDs` that may connect (and later disconnect) with each other during runtime.
- Simple job script example for such a case:

```
#!/bin/bash
#SBATCH --gw_num=1
#SBATCH --nodes=8 --partition=dp-cn
#SBATCH hetjob
#SBATCH --nodes=16 --partition=dp-esb

srun –n64  --het-group 0 ./mpi_hello_accept &
srun –n256 --het-group 1 ./mpi_hello_connect &

wait
```

Starts two *separate* `MPI_COMM_WORLDs`

Establishing Communication

- According to the MPI standard, the following functions can be used to establish connections between two separate `MPI_COMM_WORLD`s:
  - `MPI_Open_port()`
  - `MPI_Comm_accept()`
  - `MPI_Comm_connect()`
  - `MPI_Comm_disconnect()`

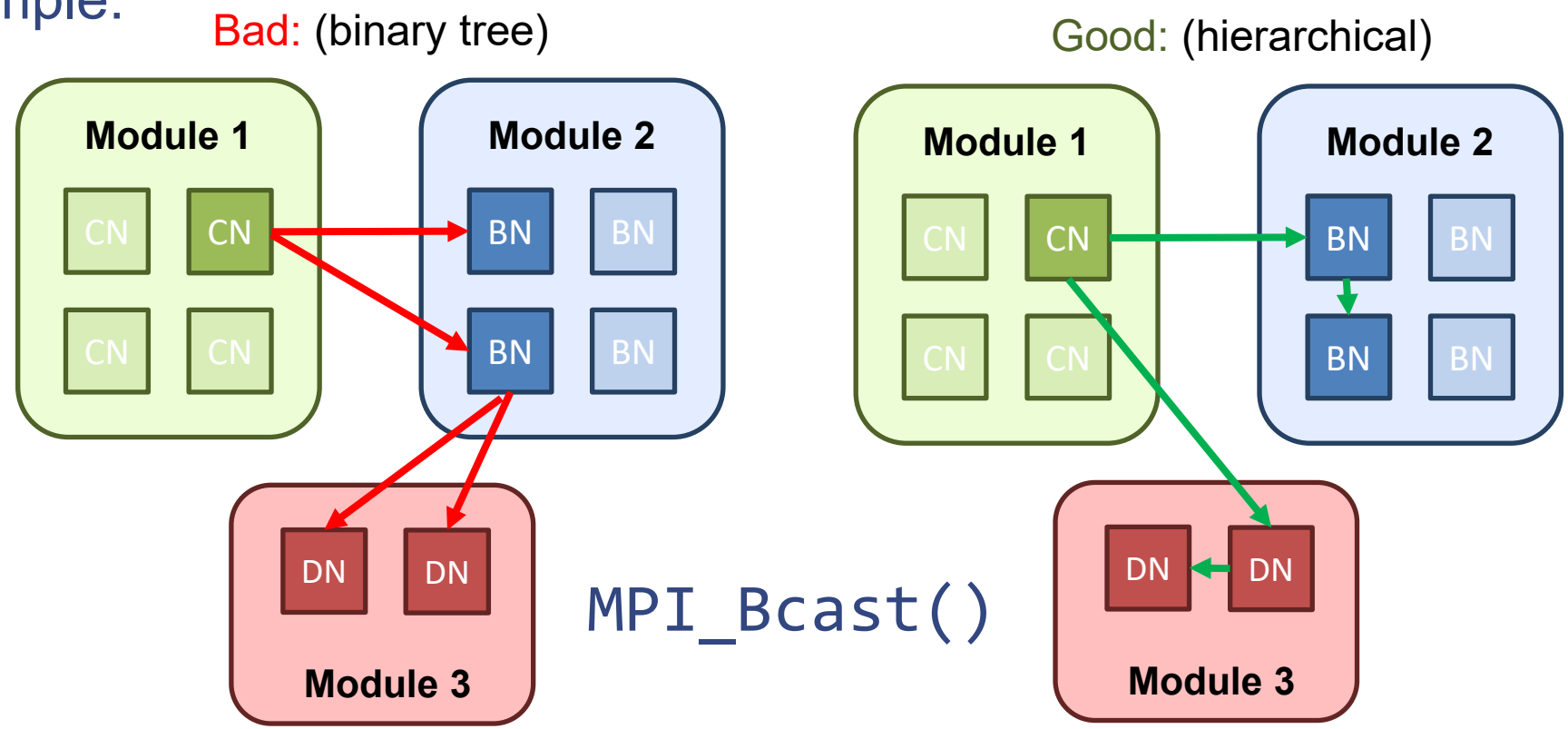


- ParaStation MPI supports all these functions – even for connections across module boundaries.
- …`MPI_Comm_spawn()` is supported, but currently not quite well for the inter-module case.

→ Is there a demand for this on application side?

MSA Awareness

- Modularity-aware MPI Collectives:
  - Optimized patterns for collectives that take the modularity into account
  - Assumption: Inter-module communication is the bottleneck
  - Example:



Hierarchical Collectives

- General rules used here to optimize collectives:
  1. First do all module-internal gathering and/or reduction operations — if required.
  2. Then perform the inter-module operation with only one process per module.
  3. Finally, distribute the data within each module in a strictly module-local manner.

- Multi-level hierarchy awareness:

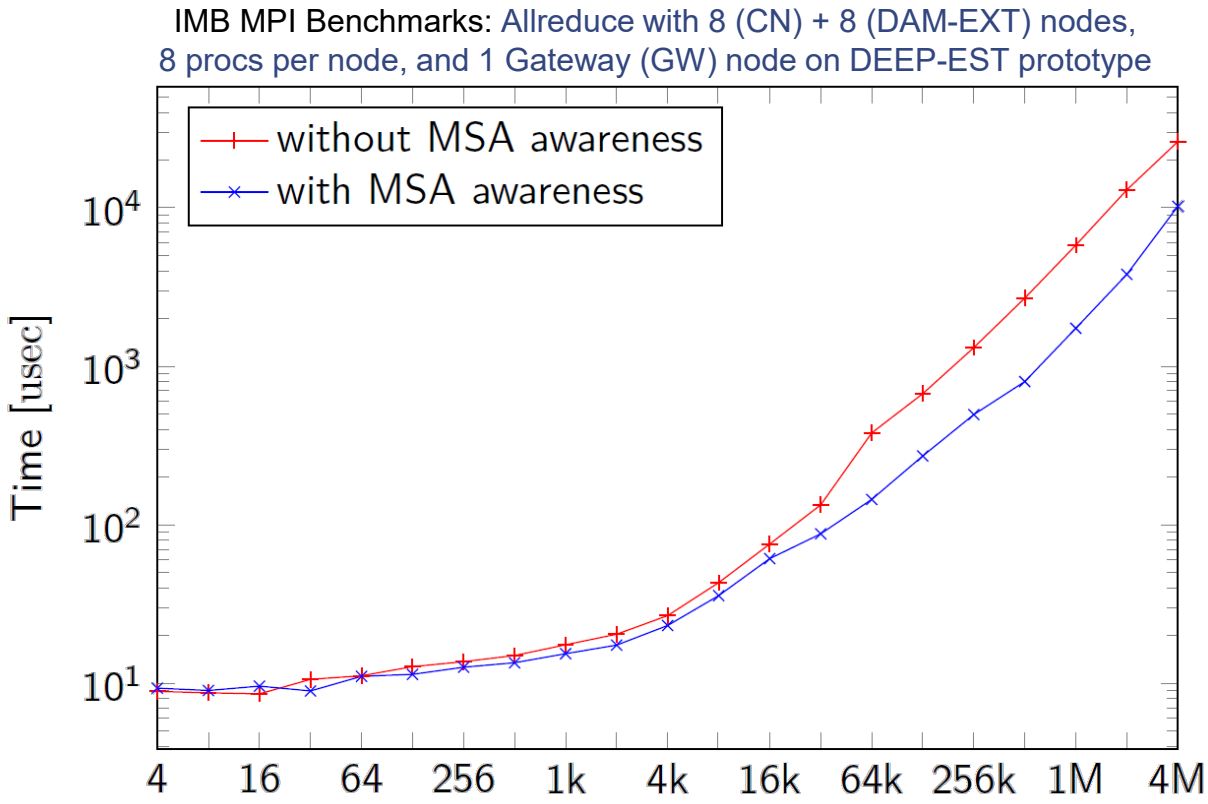
  → Apply this set of rules *recursively:* First on module level, then on node level…

- Usage: Set environment variables…
  - `PSP_MSA_AWARENESS=1`
  - `PSP_MSA_AWARE_COLLOPS=1`
  - `PSP_SMP_AWARE_COLLOPS=1`

As these features are not always beneficial and/or are still experimental, they are disabled by default!

Performance Improvement

- Improvement heavily depends on the setting, for example:
  - number of processes / gateway nodes involved
  - rank distribution in communicator
  - message sizes of the pattern
  - …and the pattern itself
- Currently supported patterns:
  - `MPI_Bcast / MPI_Ibcast`
  - `MPI_Reduce / MPI_Ireduce`
  - `MPI_Allreduce / MPI_Iallreduce`
  - `MPI_Scan / MPI_Iscan`
  - `MPI_Barrier`



API Extensions

- Besides this kind of transparent MSA awareness, there is also the possibility for the application to adapt to modularity explicitly.
- API additions by ParaStation MPI for retrieving topology information:
  - Querying the module ID via the `MPI_INFO_ENV` object:

```
MPI_Info_get (MPI_INFO_ENV , "msa_module_id", …, value, …);
```

  - Splitting communicators according to the topology by utilizing a newly added split type for `MPI_Comm_split_type()`:

```
MPI_Comm_split_type (oldcomm, MPIX_COMM_TYPE_MODULE, …,
                     &newcomm);
```

CUDA awareness

- In the first instance, CUDA awareness just means that an application is allowed to pass GPU-Device pointers to the MPI.
- Otherwise, if the memory is not managed by the CUDA runtime, an explicit staging is required by the application.

Back then, without CUDA awareness:

```
cudaMemcpy(temp_buffer_on host,                    // <- Staging
  buffer_in_device_memory, cudaDeviceToHost);

MPI_Send(temp_buffer_on_host, …);
```

Today, with CUDA awareness:

```
MPI_Send(buffer_in_device_memory, …);
```

CUDA and ParaStation MPI

- CUDA awareness supported by the following MPI APIs:
  - Point-to-point (e.g., `MPI_Send`, `MPI_Recv`, ...)
  - Collectives (e.g., `MPI_Allgather`, `MPI_Reduce`, ...)
  - One-sided (e.g., `MPI_Put`, `MPI_Get`, ...)
  - Atomics (e.g., `MPI_Fetch_and_op`, `MPI_Accumulate`, ...)
- CUDA awareness for all transports / pscom plugins via staging
- CUDA optimization / GPUDirect: UCX plugin (`pscom4ucp`)

CUDA and ParaStation MPI

- Ability to query CUDA awareness at compile time:

```
#if defined(MPIX_CUDA_AWARE_SUPPORT) && MPIX_CUDA_AWARE_SUPPORT
printf("The MPI library is CUDA-aware\n");
#endif
```

- …and also at runtime via API extensions:

```
if (MPIX_Query_cuda_support())
    printf("The CUDA awareness is activated\n");
```

```
MPI_Info_get(MPI_INFO_ENV, "cuda_aware", … , value, …);
```

Similar to Open MPI's CUDA extensions

- As CUDA awareness adds some cycles to latency, it is disabled by default!

→ Set `PSP_CUDA=1` to enable it.

Persistent MPI Windows

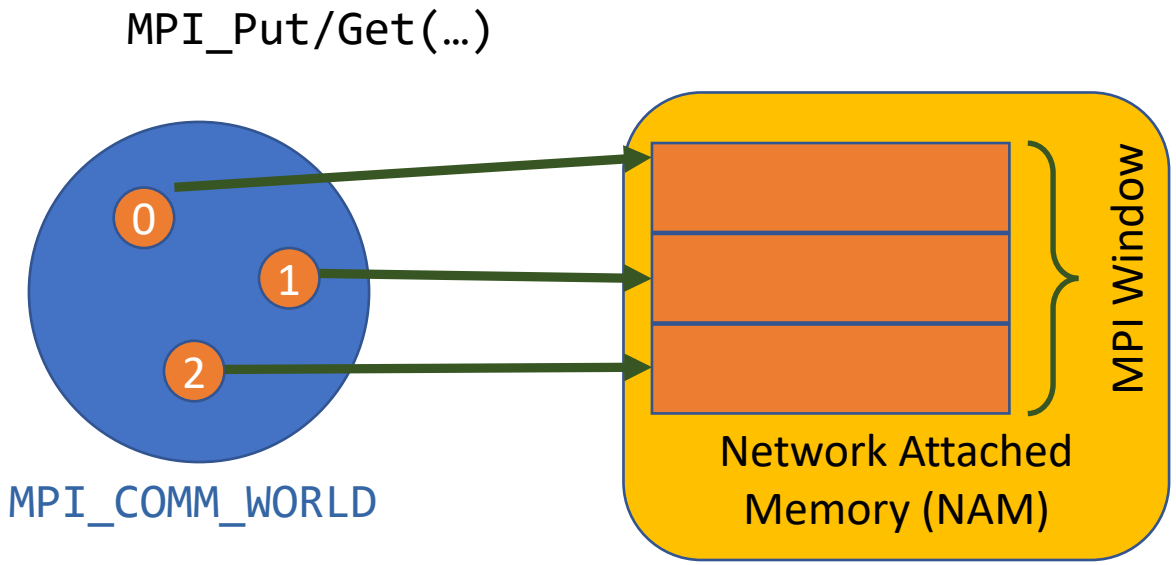
- Extension stemming from DEEP-EST: persistent MPI RMA windows
- Primarily developed for addressing so-called *Network Attached Memory*

  …but persistent RMA windows can also be built with *shared-memory* on common compute nodes as well!

- The idea of Network Attached Memory (NAM):
  - Network nodes without (significant) compute power, but equipped with a lot of fast and byte-addressable memory
  - Plus an interconnect technology that allows direct RDMA Put/Get operations onto this memory from remote compute nodes
- How to integrate this into the world of MPI and its RMA interface?

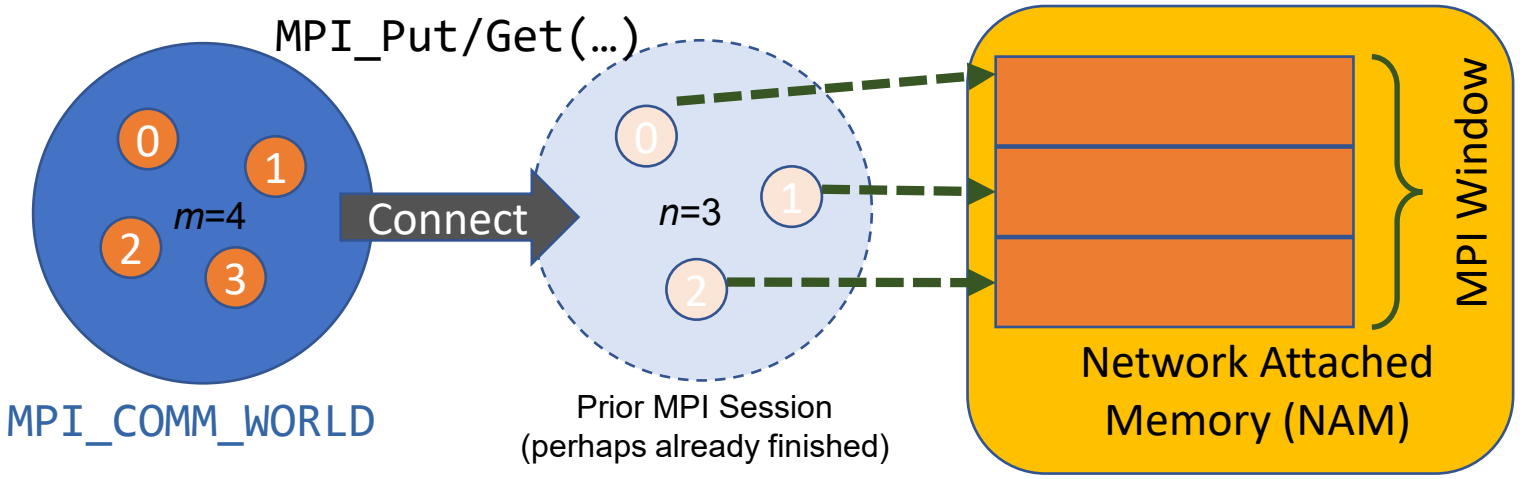
Persistent MPI Windows

- Idea followed in DEEP-EST:
  - Use `MPI_Win_allocate()` with special MPI Info key/value pairs to allocate
  - One NAM region is then associated with each MPI rank in the window
  - Use common `MPI_Put/Get()` operations for accessing these regions
  - Persistency: freeing the MPI window does *not* release the associated memory



Persistent MPI Windows

- Scenario for application workflows:
  - Prior MPI session has called `MPI_Win_allocate()` for NAM with n ranks
  - A new MPI session with m ranks now wants to attach to that window
  - New session calls `MPI_Comm_connect()`, returning an inter-comm and uses this inter-comm for creating an RMA window object by attaching
  - Window now has as many NAM regions as ranks n in former session, and NAM regions are addressable by remote ranks in the inter-comm



Summary and Outlook

- Which of these features are of interest for DEEP-SEA Applications?
  - Support for modular MPI jobs? (i.e., jobs across multiple MSA modules)
  - Transparent features to optimize communication on MSA systems?
  - API extensions to adapt applications explicitly to modularity?
  - Support for workflows (i.e., jobs with multiple `MPI_COMM_WORLD`s) via
    - *MPI_Comm_connect/accept()?*
    - *MPI_Comm_spawn()?*
    - *Persistent RMA windows?*
  - Awareness/interoperability for CUDA and/or other programming models?
- Any further demands, ideas, or special wishes towards MPI support?

Resources and Contact

- ParaStation MPI description on the DEEP Projects webpage:
  https://www.deep-projects.eu/software/programming-environment/parastation-mpi.html
- Documents on the BSCW: DEEP-SEA → Seminar → ParaStation MPI
  https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3597441
- ParaStation MPI as open-source on GitHub:
  https://github.com/ParaStation/psmpi
- For further questions and/or discussions just contact me directly:
  clauss@par-tec.com

DEEP-SEA

Software for Exascale Architectures