MPI3 Hybrid

Proposal Description

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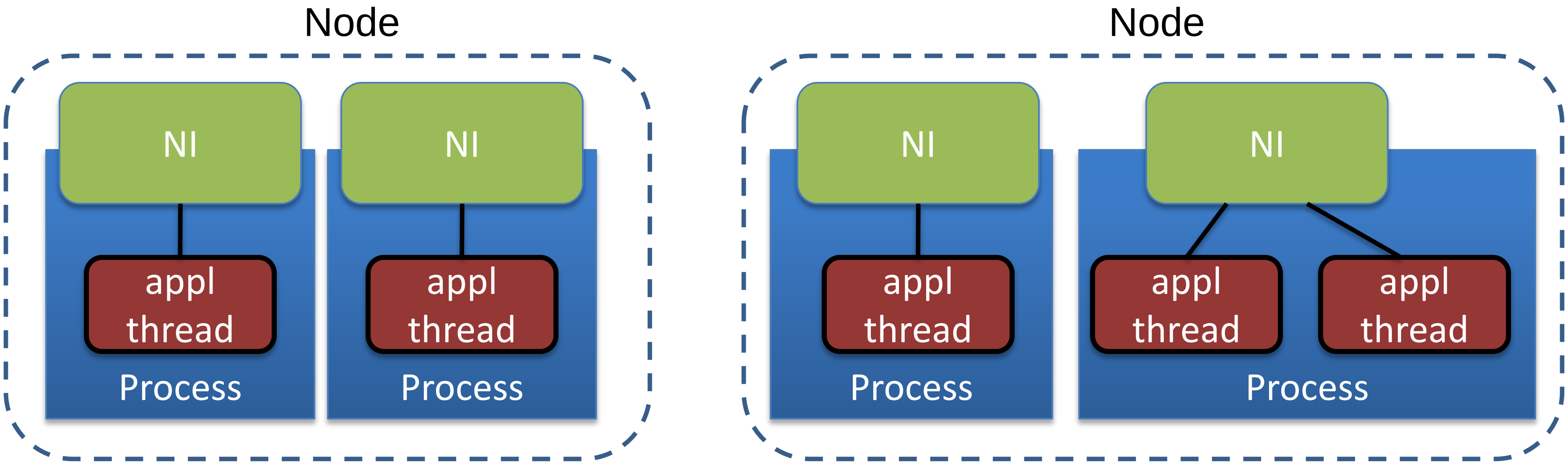
Goals

- Allowing more than one “MPI process” per node, without requiring multiple address spaces
- Having a clean binding to OpenMP and other thread-based parallel programming models
- Having a clean binding to UPC, CAF and similar PGAS languages

Current Design

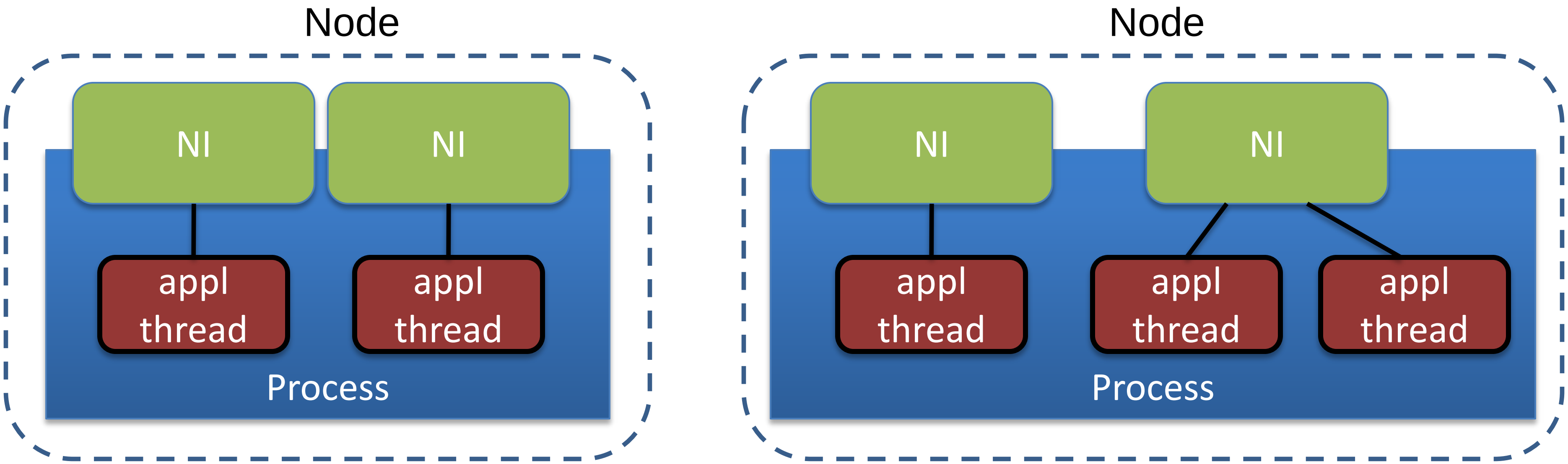


- Single-threaded

- Multi-threaded
  - Requires reentrant MPI library (hard) or mutual exclusion

Network Interfaces (NI): physical or virtual, disjoint interfaces

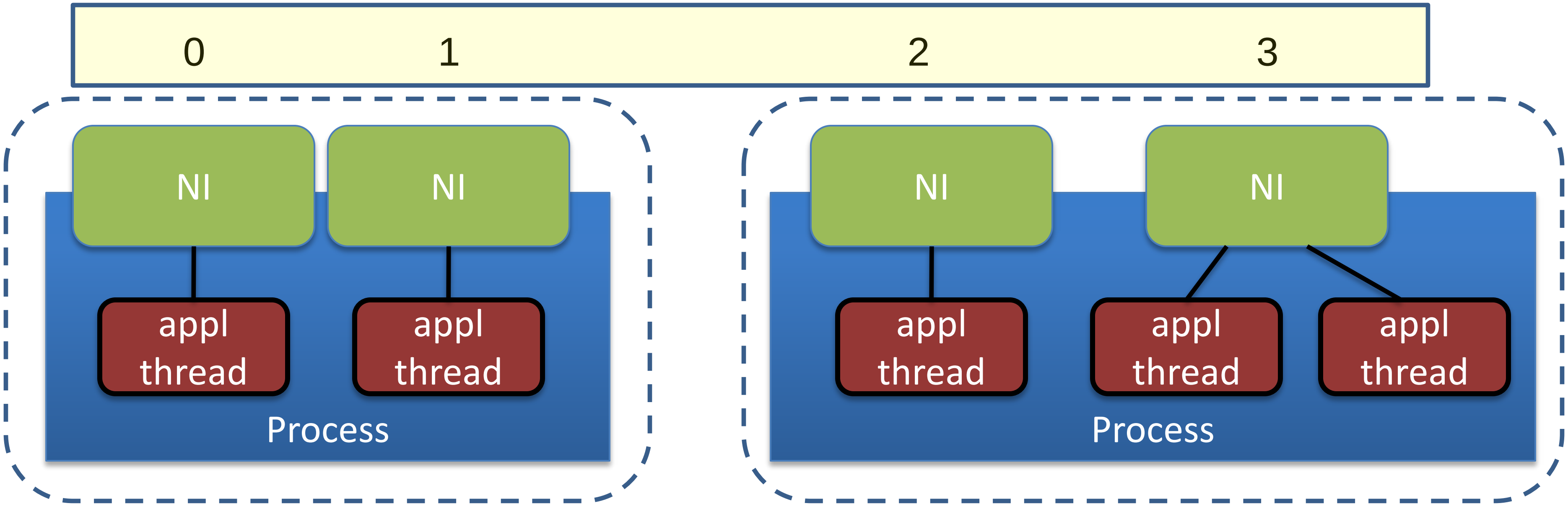
Proposed Design



- Single-threaded
  - Each NI (or virtual NI) is accessed by only one thread
- Multi-threaded
  - Some NIs are accessed by multiple threads

Same as before, except multiple NIs are mapped in same address space

MPI_COMM_EWORLD



- Each *MPI Endpoint* has unique rank in MPI_COMM_EWORLD
  - rank in derived communicators computed using MPI rules
- MPI code executed by thread(s) *attached* to endpoint
  - Including collectives
  - thread is attached to at most one endpoint

Binding Time

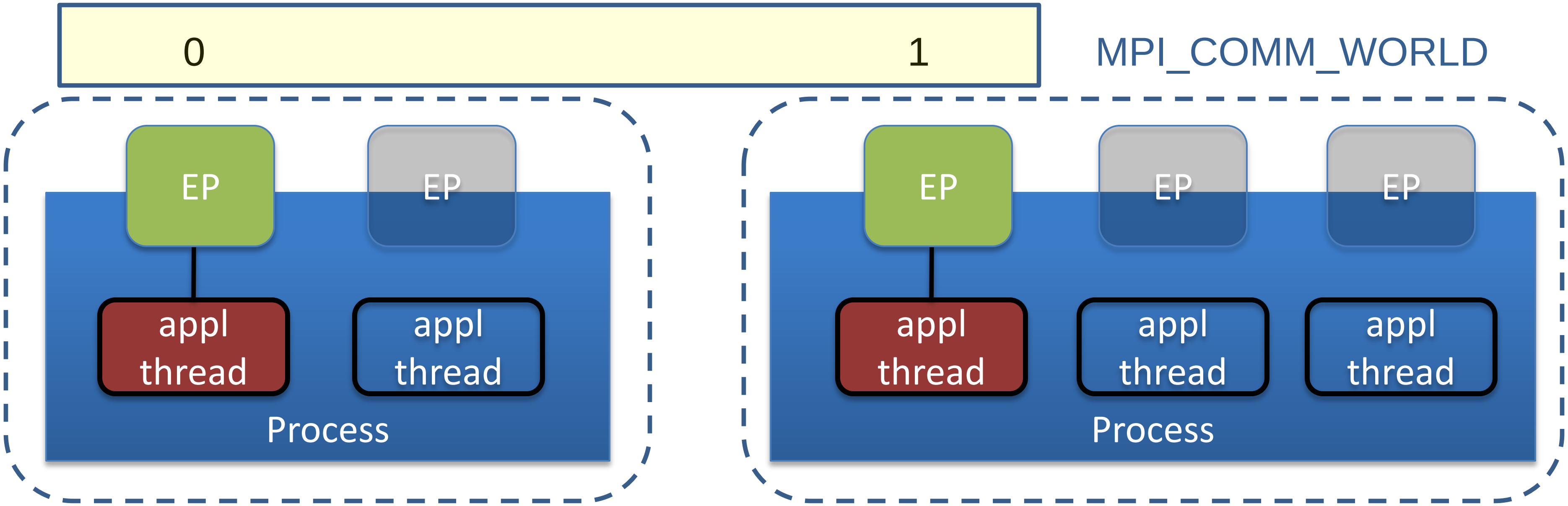
- Binding of MPI Endpoints to processes
  - done at MPI initialization time, or before
- Attachment of threads to MPI endpoints
  - done during execution; can change but expected to rarely change
  - threads can be created after endpoints

Endpoint Creation (1)

```
MPI_ENDPOINT_INIT(required, provided)
   IN required   desired level of thread support (integer)
   OUT provided  provided level of thread support (integer)
```

- `MPI_THREAD_FUNNELED`
  - each endpoint will have only one attached thread
- `MPI_THREAD_SERIALIZED`
  - multiple threads can attach to same endpoint, but cannot invoke MPI concurrently
- `MPI_THREAD_MULTIPLE`
  - multiple threads can attach to same endpoint and can invoke MPI concurrently
- Executed by one thread on each process; initializes MPI_COMM_WORLD

After MPI_ENDPOINT_INIT



- Attribute MPI_ENDPOINTS (on MPI_COMM_WORLD) indicates maximum number of endpoints at each process.
  - Can be different at each process (can depend on mpiexec arguments)

Endpoint Creation (2)

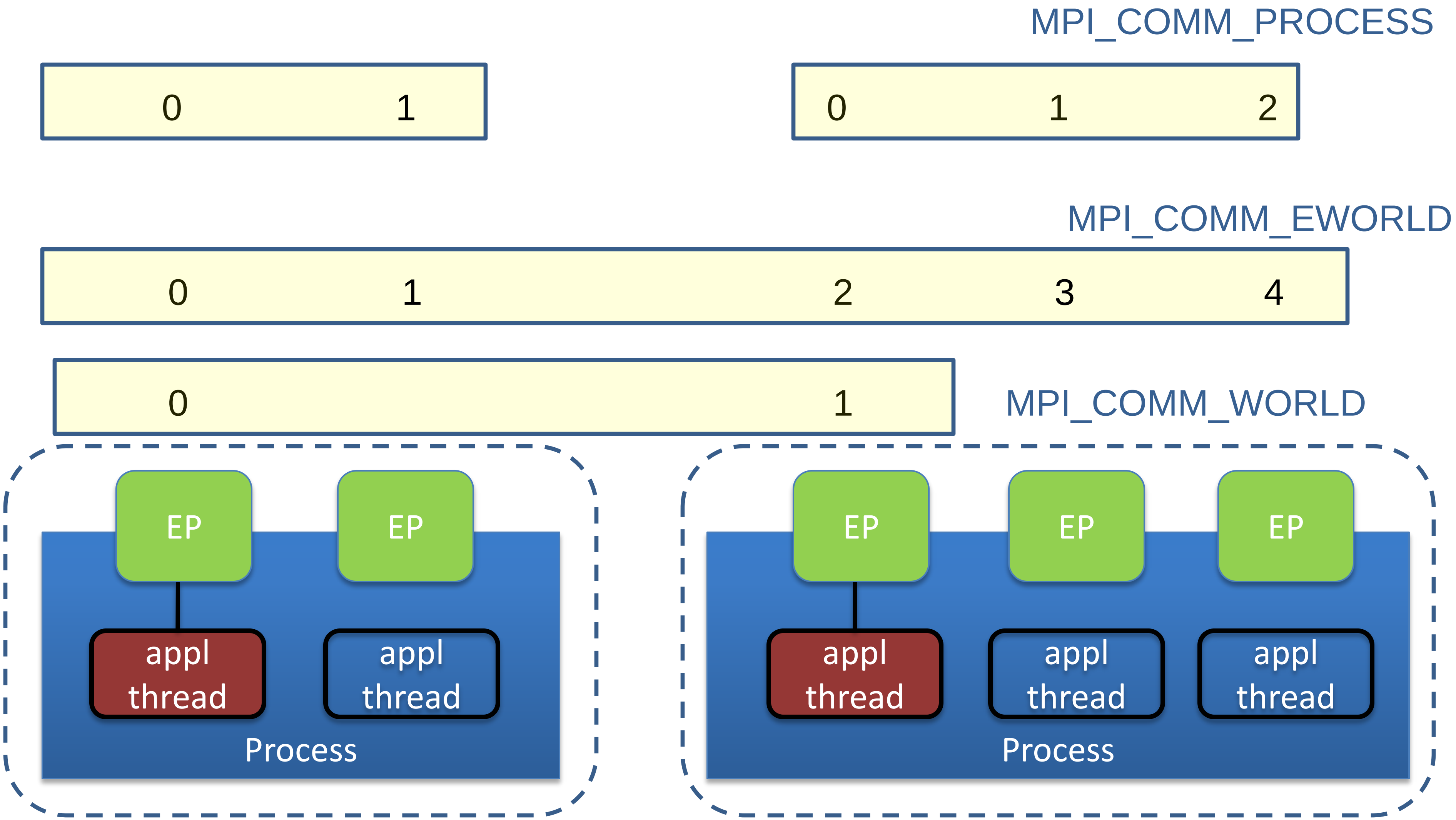
```
MPI_ENDPOINT_CREATE (num_endpoints,
  array_of_endpoints)
```

IN `num_endpoints` number of endpoints (integer)

OUT `array_of_endpoints` array of endpoint handles (array of handles)

- Executed by one thread on each process; initializes MPI_COMM_EWORLD

After MPI_ENDPOINT_CREATE



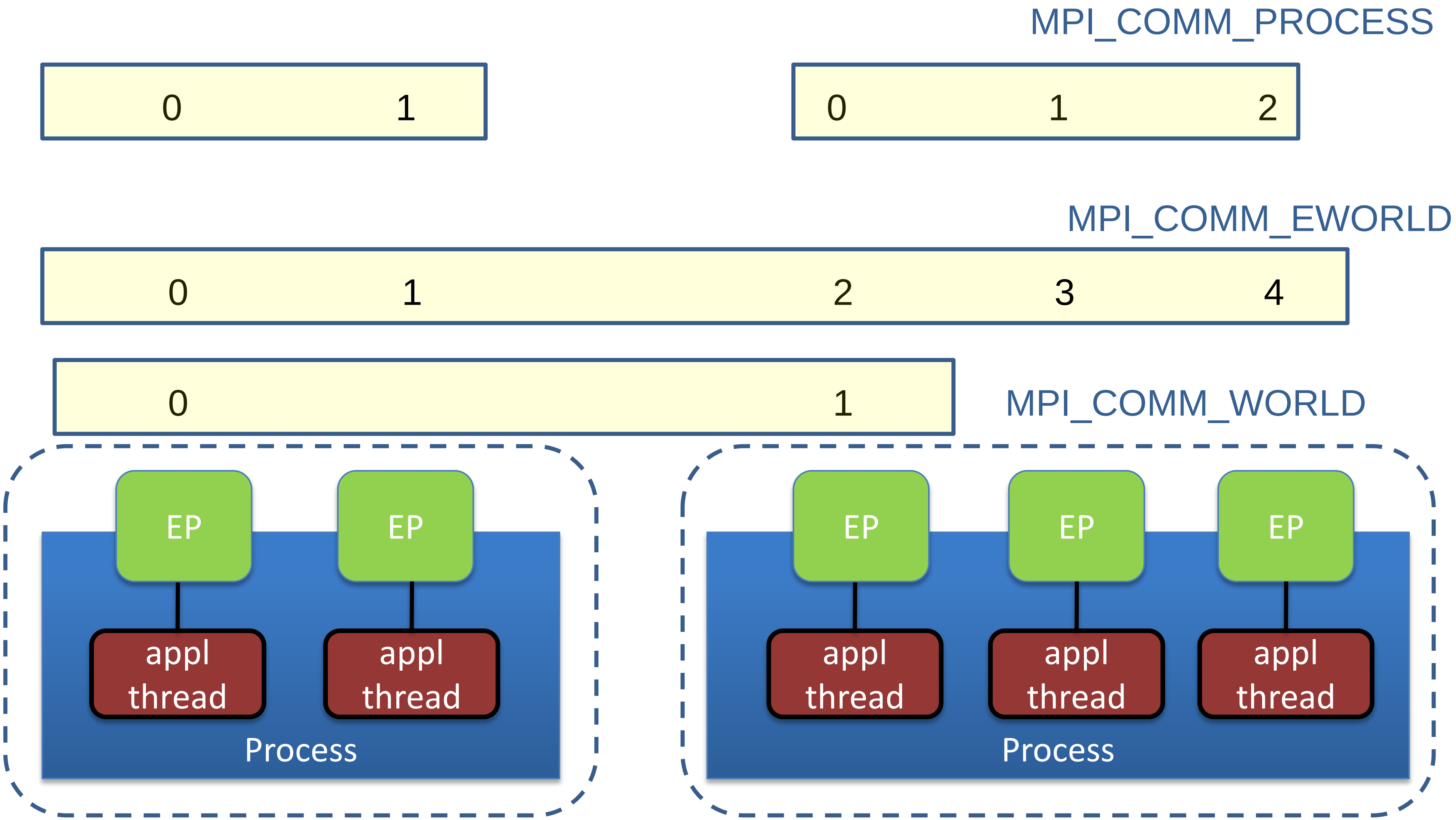
Thread Registration

```
MPI_THREAD_ATTACH (endpoint)
  IN endpoints endpoint handle (handle)

MPI_THREAD_DETACH (endpoint)
  IN endpoints endpoint handle (handle)
```

- Executed by each thread

After All Threads Attached



Remarks

- MPI calls invoked by thread pertain to endpoint the thread is attached to
  - E.g., sender rank is rank of endpoint
- MPI call may block if participation of endpoint is needed and no thread is attached to endpoint
  - E.g., collective or send to “orphan endpoint”
- Normally, endpoint will have attached thread after initialization

Missing Items

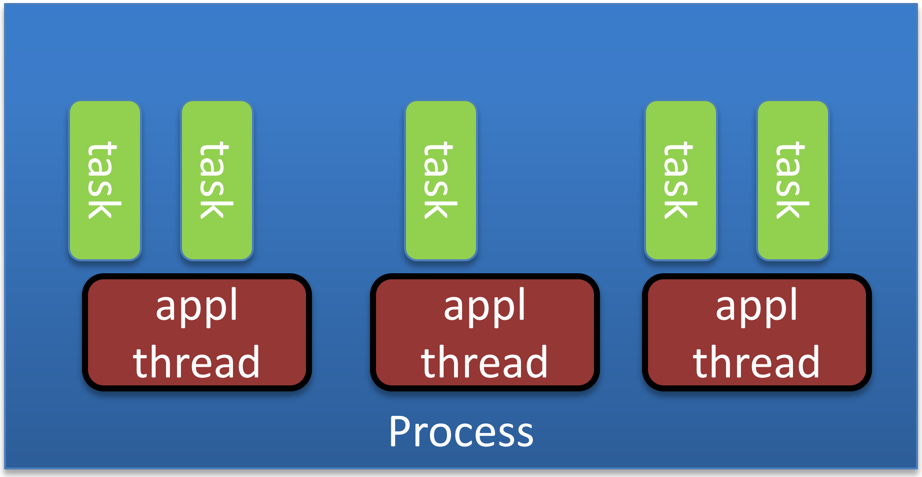
- MPI_FINALIZE()
- mpiexec
- Dynamic processes
- One-sided
- I/O
- Error codes
- …

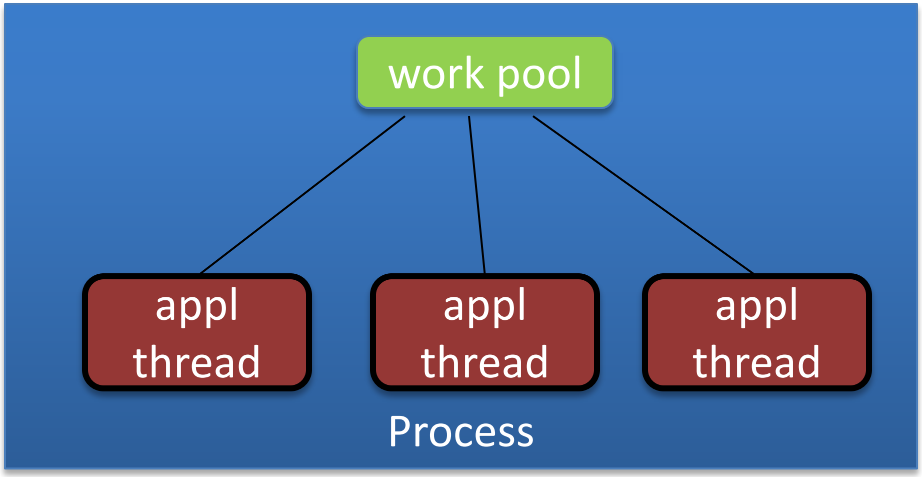
MPI + Shared Memory Language/Library

- Goals
  - Allow more than one MPI endpoint per shared memory program
  - Simple use (but not for naïve users!)
  - Simple implementation

Shared Memory Programming Models

- Number of threads can vary
- Tasks can be migrated from one thread to another
- Work can be shared dynamically





General Binding

- MPI calls can be executed anywhere in the shared memory program, with “natural semantics”
  - blocking MPI call blocks task/iterate
  - nonblocking call can be completed in any place in the program execution that causally follows the initial nonblocking call
  - registrations are per task, and are inherited when control forks

```
#pragma omp for
  for(i=0; i<N; i++)
    {
     MPI_Irecv(...,req[i]);
     }
MPI_Waitall(N,req,stat);
```

Issues

- Blocking MPI call blocks thread; this may block work sharing
- OpenMP/TBB/… scheduler does not know about MPI; communication performance may be affected
- OpenMP (TBB, etc.) runtime needs to migrate implicit MPI state (e.g., identity of associated MPI endpoint) when task migrates or forks
- Need MPI_THREAD_MULTIPLE
- Recommend to specify but not to require
  - Detailed specification missing in current document

Restricted Binding

- MPI endpoint is associated with thread
- User has to make sure that MPI calls execute on “right” thread

OpenMP Rules

- MPI_ENDPOINT_CREATE is invoked in the initial, sequential part of the program.
- Each endpoint is attached by one OpenMP thread
- Only OpenMP threads attached to an endpoint invoke MPI.
- Each handle should be used in MPI calls by the same thread through program execution.
  - Handle is `threadprivate`
  - Handle is `shared` and is not reused in different parallel regions unless they are consecutive, neither is nested inside another parallel region, both regions use the same number of threads, and *dyn-var = false*
  - An MPI handle should not be used within a work sharing construct.
  - An MPI handle should not be used within an explicit task.

Example (1)

```
... // omit declarations
MPI_Endpoint_Init(argc, argv, MPI_THREAD_SINGLE,
  &provided);
MPI_Comm_get_attr(MPI_COMM_WORLD, MPI_ENDPOINTS, &pnum,
  &flag);
#pragma omp parallel private(myid)
   {
  #pragma omp master
      {
/* find number of threads in current team */
      Nthreads = omp_get_num_threads();
      if (Nthreads != *pnum) abort();
/* create endpoints */
      MPI_Endpoint_create(Nthreads, *endpoints);
      }
```

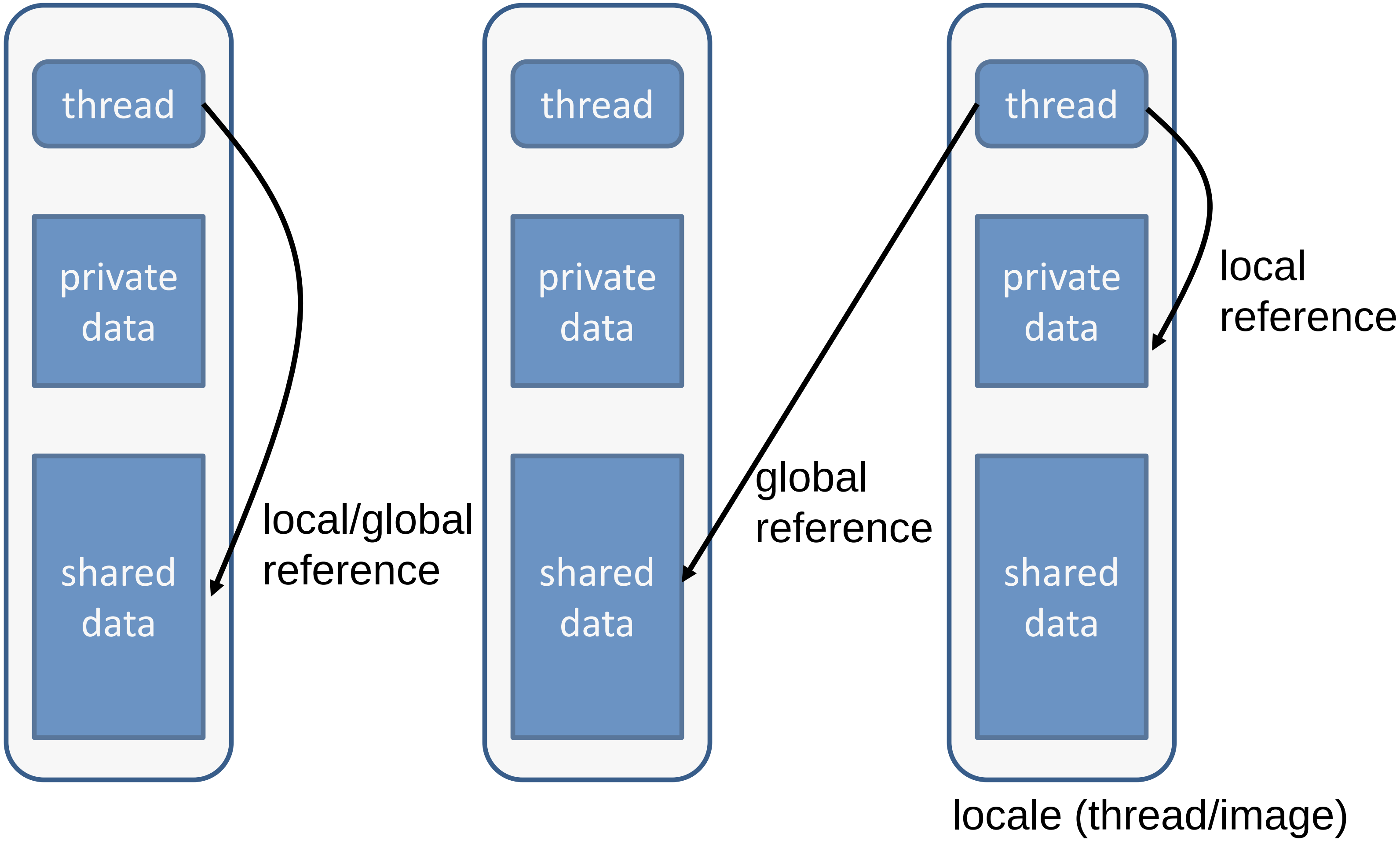
Example (2)

```
/* associate each thread with an endpoint */
  myid = omp_get_thread_num();
  MPI_Endpoint_register(myid, *endpoints);
/* MPI communication involving all threads */
  MPI_Comm_rank(MPI_COMM_EWORLD, &myrank);
  MPI_Comm_size(MPI_COMM_EWORLD, &size);
  MPI_Comm_rank(MPI_COMM_PROCESS, &mythreadid);
  if (myid != mythreadid) abort();
  if (myrank > 0) MPI_Isend(buff, count, MPI_INT,
      myrank-1, 3, MPI_COM_EWORLD, &req[mythreadid);
  if (myrank < size) MPI_Recv(buff1, count, MPI_INT,
      myrank+1, 3, MPI_COMM_EWORLD);
  MPI_Wait(&req[mythreadid], &status[mythreadid]); }
  ...
```

TBB et al

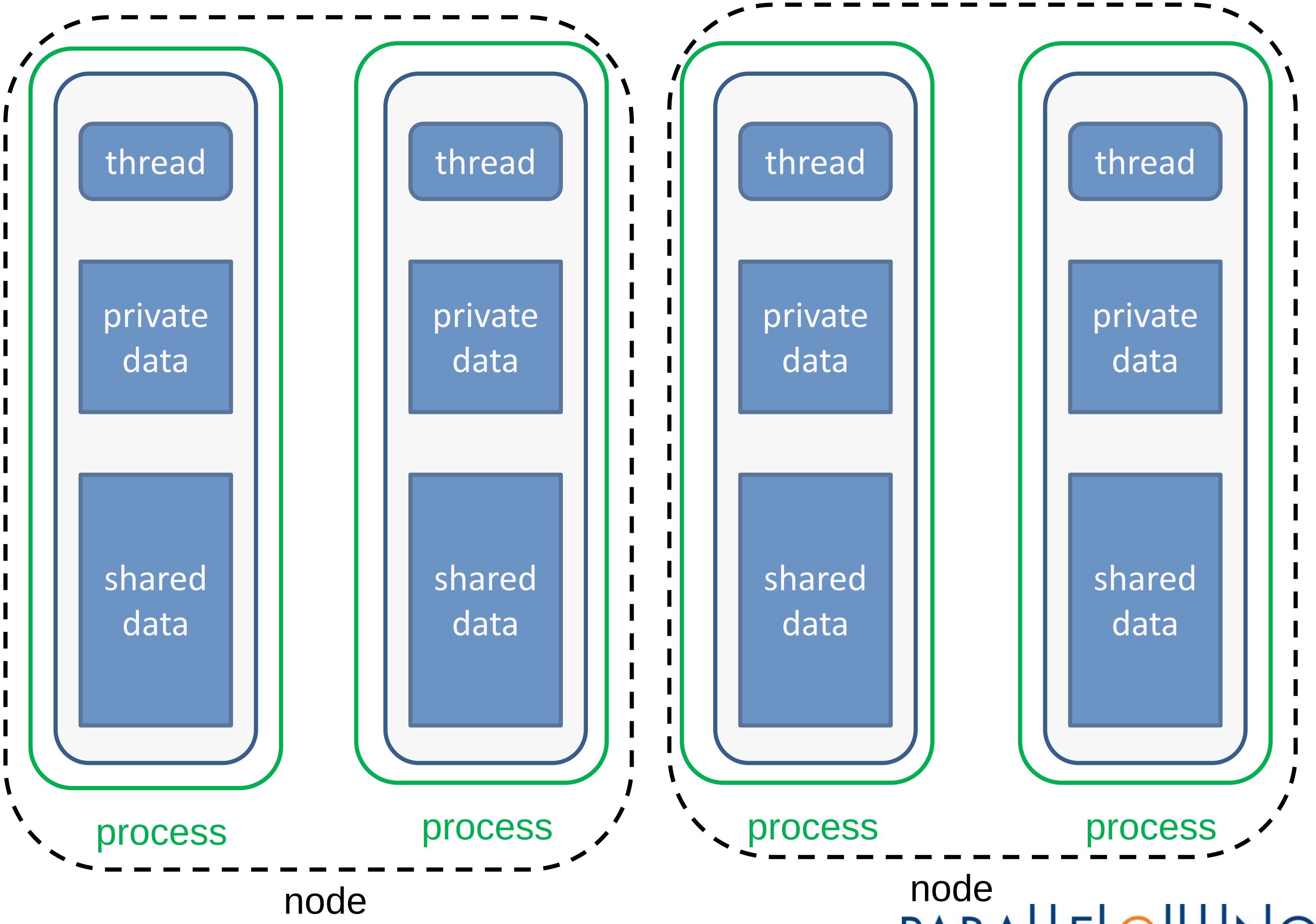
- Need TBB to provide a construct that binds a task to a specific thread.
  - Similar construct may be needed for GPU tasks and other similar messes

PGAS (UPC, Fortran 2008)

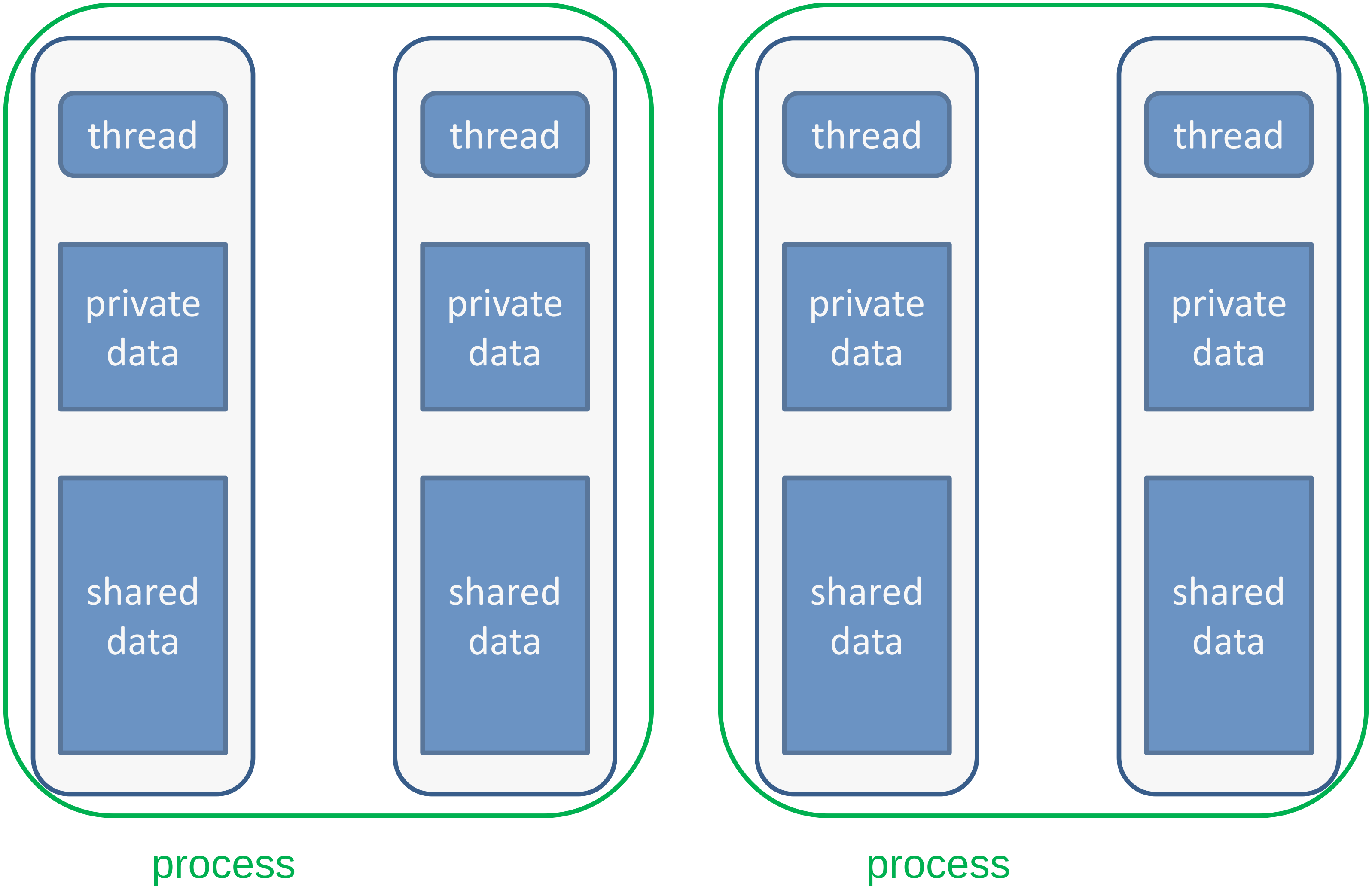


- One thread of control per locale (+ work sharing, in UPC)

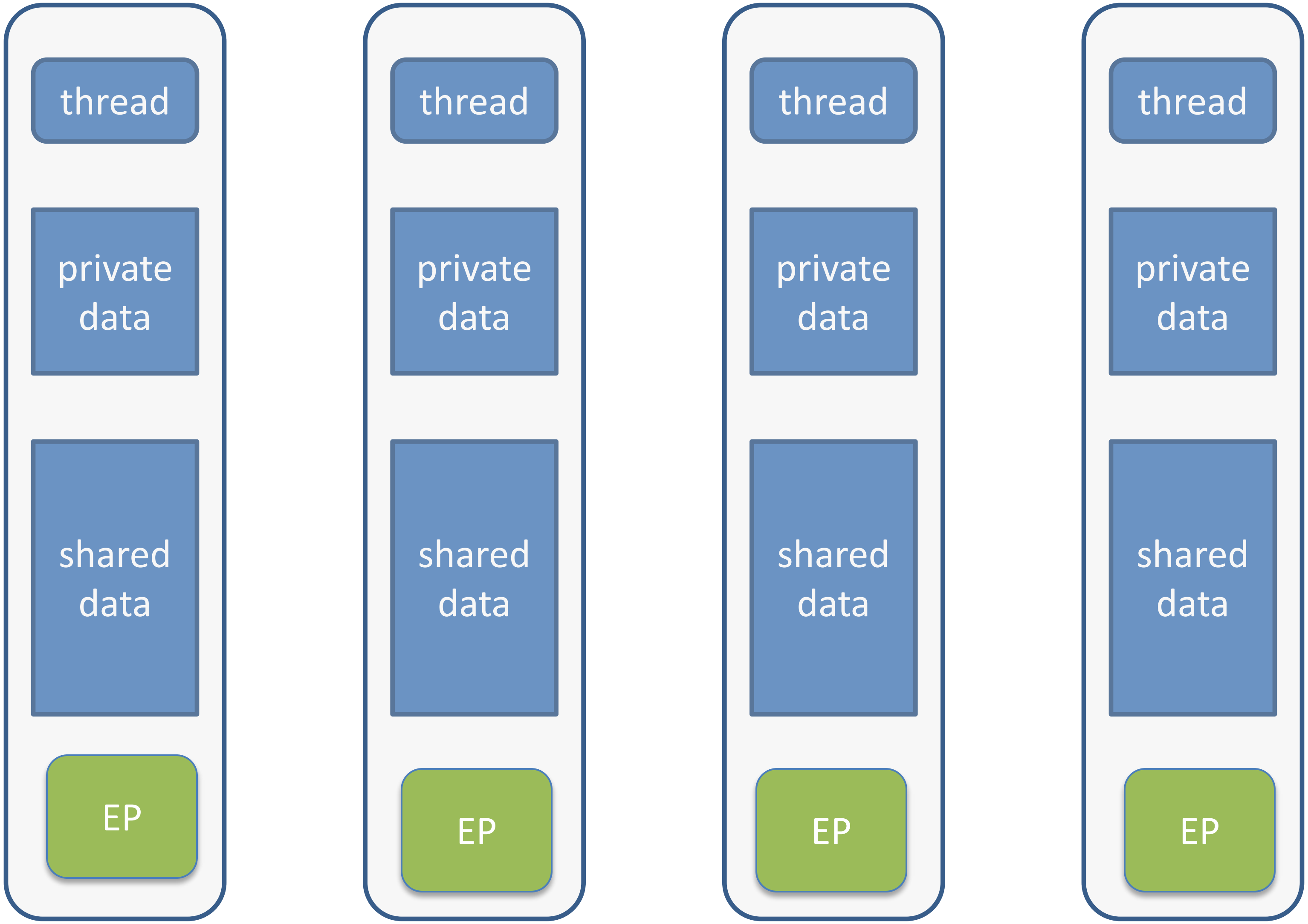
PGAS Implementations (1)



PGAS Implementations (2)



PGAS Invokes MPI



PGAS Invokes MPI (cont.)

- Each locale (thread/image) has MPI_COMM_EWORLD rank corresponding to its PGAS rank
- Each locale can invoke MPI (one endpoint per locale)
  - all arguments must be local
  - cannot be done within work sharing construct
- Model does not depend on chosen PGAS implementation
- Requires joint initialization of PGAS and of MPI
  - Both are initialized before user code starts running

MPI Invokes PGAS

Need “awareness” of PGAS language within MPI code

- Link and invoke UPC routine from (SPMD) C
  - Collective call over all MPI processes (endpoints) in communicator
- Create shared array from (SPMD) C
  - collective malloc; shared array descriptor
- Pass shared array as argument
- Query shared arrays

Problems mostly are on PGAS side; should we address them?