The MPI+MPI programming model and why we need shared-memory MPI libraries

Jeff Hammond

Extreme Scalability Group & Parallel Computing Lab
Intel Corporation (Portland, OR)

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Hanlon’s Razor.
Abstract (for posterity)

The MPI-3 standard provides a portable interface to interprocess shared-memory through the RMA functionality. This allows applications to leverage shared-memory programming within a strictly MPI paradigm, which mitigates some of the challenges of MPI+X programming using threads associated with shared-by-default behavior and race conditions, NUMA and Amdahl’s law. I will describe the MPI shared-memory capability and how it might be targeted by existing multithreaded libraries.
MPI-3
What is **MPI**?

(A) A bulky, bulk-synchronous model.
(B) The programing model of Send-Recv.
(C) An explicit, CSP-like, private-address-space programming model.
(D) An industry-standard runtime API encapsulating 1-, 2- and $N$-sided blocking and nonblocking communication and a whole bunch of utility functions for library development.
(E) The assembling language of parallel computing!!
MPI_Init(..);
MPI_Comm_size(..); MPI_Comm_rank(..);
MPI_Barrier(..); MPI_Bcast(..);
MPI_Reduce(..); MPI_Allreduce(..);
MPI_Gather(..); MPI_Allgather(..);
MPI_Scatter(..); MPI_Alltoall(..);
MPI_Reduce_scatter(..); MPI_Reduce_scatter_block(..);
MPI_Send(..); MPI_Recv(..); /* [b,nb] x [r,s,b] */
...
MPI_Finalize();
MPI_Ibarrier(..); MPI_Ibcast(..);
MPI_Ireduce(..); MPI_Iallreduce(..);
MPI_Igather(..); MPI_Iallgather(..);
MPI_Iscatter(..); MPI_Ialltoall(..);
MPI_Ireduce_scatter(..);
MPI_Ireduce_scatter_block(..);

Go forth a write bulk-asynchronous code!
MPI_Comm_create_group(..);
MPI_Icomm_dup(..);
...
MPI_Dist_graph_create_adjacent(..);
MPI_Neighborhood_allgather(..);
MPI_Neighborhood_allgatherv(..);
MPI_Neighborhood_alltoall(..);

Virtual topologies corresponding to algorithmic topology; additional semantic information enables MPI to optimize.
Win_create(..); Win_allocate(..);
Win_allocate_shared(..); Win_shared_query(..);
Win_create_dynamic(..); Win_attach(..);
Win_detach(..);
Put(..); Get(..); Accumulate(..);
Fetch_and_op(..); Compare_and_swap(..);
Win_lock(..); Win_lock_all(..);
Win_flush(_local)(_all)(..); Win_sync(..);
...

MPI-3 is a superset of ARMCI and OpenSHMEM...

http://wiki.mpich.org/armci-mpi/
https://github.com/jeffhammond/oshmpi/
What is MPI_Win_allocate_shared(..)?

Historically, SysV shared memory used, but painfully.

POSIX shared memory good, but Windows, BSD/Mach...

In HPC, we have XPMEM (Cray and SGI). And BGQ...

MPI processes can be threads, in which case, all is shared.

The purpose of MPI is to standardize best practice!

Shared-memory is a “best practice.”
Limitations:

- Only defined for cache-coherent systems (WIN\_MODEL=UNIFIED).
- Allocated collectively.
- Memory allocated contiguously by default.

Features:

- It’s SHARED MEMORY: what don’t you love?
- Works together with RMA ops (e.g. atomics).
- Noncontiguous allocation upon request (hint).
MPI+X
The future is MPI+X (supposedly)

- MPI+OpenMP is too often fork-join.
- Pthreads scare people; can’t be used from Fortran (easily).
- Intel® has Cilk® and TBB.
- OpenCL is not a good model for application programmers and has no magic for portable performance (since such magic does not exist).
- CUDA® is an X for only one type of hardware (ignoring Ocelot).

Never confuse portability with portable performance!
Using MPI+OpenMP effectively

- Private data should behave like MPI but with load-store for comm.
- Shared data leads to cache reuse but also false sharing.
- NUMA is going to eat you alive. BG is a rare exception.
- OpenMP offers little to no solution for NUMA.
- If you do everything else right, Amdahl is going to get you.

Intranode Amdahl and NUMA are giving OpenMP a bad name; fully rewritten hybrid codes that exploit affinity behave very different from MPI codes evolved into MPI+OpenMP codes.
Fork-Join vs. Parallel-Serialize

Jeff Hammond

MPI+MPI
Fork-Join vs. Parallel-Serialize

```c
#pragma omp parallel
{
    /* thread-safe */
#pragma omp single
    /* thread-unsafe */
#pragma omp parallel for
    /* threaded loops */
#pragma omp sections
    /* threaded work */
}
 /* thread-unsafe */
```

```c
#pragma omp parallel for
{
    /* threaded loops */
}
 /* thread-unsafe */
```

```c
#pragma omp parallel for
{
    /* threaded loops */
}
 /* thread-unsafe work */
```
This is a toy DAXPY-like test I wrote for an ALCF tutorial...

```
> for n in 1e6 1e7 1e8 1e9 ; do ./numa.x $n ; done
n = 1000000   a: 0.009927  b: 0.009947
n = 10000000  a: 0.018938  b: 0.011763
n = 100000000 a: 0.123872  b: 0.072453
n = 1000000000 a: 0.915020  b: 0.811122
```

The first-order effect requires a multi-socket system.

For more complicated data access patterns, you may see this even with parallel initialization.
MPI⊗X
Threads are independent, long-lived tasks in a shared address space.

Threads all access MPI like they own it.

MPI_THREAD_MULTIPLE is non-trivial overhead.

Be sure you have a communicator per thread with collectives...

If your low-level network stack is not thread-safe...

God help you if you want to mix more than one threading model!¹

¹ See https://www.ieeetcsc.org/activities/blog/challenges_for_interoperability_of_runtime_systems_in_scientific_applications
Best of all worlds?

MPI-1 between nodes; MPI-Shm within the node...

- Private by default; shared by request. Safe.
- Memory affinity to each core; NUMA issues should be rare.
- No fork-join - end-to-end parallel execution, just a question of replicated or distributed (GA-like).
- No need to reimplement any collectives.
- Easily supports both task- and data-parallelism.
- Hierarchy via MPI communicators.
- One runtime to rule them all. No interop BS.
- MPI_THREAD_SINGLE sufficient.
Why not MPI+MPI?

- MPI shm allocation collective.
- MPI shm allocator not `malloc`.
- No cure for data races.
- Data races not cured.
- cured. races not Data
- All the intranode libraries use threads!!!
BLIS should be the first MPI-Shm library:

- BLIS thread communicator maps perfectly to MPI communicator.
- Need to put BLIS communicator outside of API calls, but that’s the only major change I can see.
- Tyler’s implementation with OpenMP is trivially mapped to MPI calls.
- API refactoring for this is incredibly useful in threading models for task-parallelism and batching.
Elemental should be the second MPI-Shm library:

■ Does OpenMP really meet the needs of Elemental within a node?
■ Lots of people don’t want to think about hybrid, just MPI-only.
■ Elemental with MPI-Shm within node could compete with threaded libraries and might beat them because of well-known fork-join issues in LAPACK.
■ DistMatrix object hides all of the allocation issues internally, as it’s already collective.
■ We have an MPI-3 RMA AXPY implementation as a related proof-of-concept.
MPI is dead. Long live MPI!
Acknowledgements

Tyler Smith and Jed Brown, for explaining and discussing thread communicators at length.

Jack Poulson, for Elemental discussions over the years.

NUMA and Amdahl’s Law, for holding OpenMP back and keeping MPI-only competitive in spite of the ridiculous cost of Send-Recv within a shared-memory domain.