THREADS: THE WRONG ABSTRACTION AND THE WRONG SEMANTIC
Abstract

MPI+OpenMP is frequently proposed as the right evolutionary programming model for exascale. Unfortunately, the evolutionary introduction of OpenMP into existing MPI-only codes is fraught with difficulty. We will describe "The Right Way" to do MPI+OpenMP and ultimately conclude that MPI+MPI is a more effective alternative for legacy codes.
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HPC software design challenges

- To MPI or not to MPI...
- One-sided vs. two-sided?
- Does your MPI/PGAS need a +X?
- Static vs. dynamic execution model?
- What synchronization motifs maximize performance across scales?

Application programmers can afford to rewrite/redesign applications zero to one times every 20 years...
SHARED-MEMORY
Application motivations for shared-memory

Storage bottlenecks:
• Large, lookup (WORM) tables, e.g. Quantum Monte Carlo.
• Replicated data structures that scale with job size.
• Eliminate $O(ppn)$ halo buffers.

Communication bottlenecks:
• Load-store is (usually) faster than Send-Recv within a node.
• Complex data structures when dereferencing through indirection.
• Aggregation of small messages or I/O writes.
Threads versus processes...

Threads:

- Automatic variables (i.e. stack) all shared by default.
- Per-thread **privatization upon request** (OpenMP, C11, C++11,...).
- Dealing with NUMA requires OS interactions (e.g. page-faulting).
- All library calls must use mutual exclusion for shared state.

Processes:

- Automatic variables (i.e. stack) all private by default.
- Interprocess **sharing upon request** (Sys5, POSIX, MPI-3, XPMEM, ...).
- NUMA placement done by MPI, private data naturally local.
- Mutual exclusion required only for *explicitly* shared state.

PE = Processing Element = Thread or Process
MPI+THREADS
Design choices

Choose Threads:
• Data sharing: free everywhere.
• Race conditions: fork-join or mutex them all.
• Compute sharing: must parallelize extensively or Amdahl will get you.

Choose Processes:
• Data sharing: wherever necessary.
• Race conditions: only on shared data.
• Compute sharing: already done, up to MPI scalability.

Lack of libraries that exploit interprocess shared-memory is unfortunate, but compare ScaLAPACK to threaded LAPACK...
MPI-2 and Threads

MPI_Init_thread(., FUNNELED);
#omp parallel
{
  for (..) { Compute(..); }
  #omp master
  { MPI_Bar(..); }
}
MPI_Foo(.);

MPI_Init_thread(., SERIALIZE);
#omp parallel
{
  for (..) {
    Compute(..);
    #omp critical
    { MPI_Bar(..); }
  }
}
MPI_Foo(.);
MPI-2 and Threads

MPI_Init_thread(.., MULTIPLE);
#endif omp parallel
{
  Compute(..);
  MPI_Bar(..);
}
MPI_Foo(..);

This is the ONLY method that works reliably with more than one threading model!

int MPI_Bar(..)
{
  if (MULTIPLE) Lock(Mutex);
  rc = MPID_Bar(..);
  if (MULTIPLE) Unlock(Mutex);
  return rc;
}

int MPI_Bar(..)
{
  return MPID_Bar(..);
  /* ^ fine-grain locking inside of this call... */
}
Optimization work on threaded MPI


Software offloading for MPI_THREAD_MULTIPLE

• Application code is consistent with MPI_THREAD_MULTIPLE; implementation only requires MPI_THREAD_FUNNELED.

• Assumes agent thread can:
  • keep up with application
  • drive network

• Good for common use of NB p2p with bolt-on OpenMP.

• Side-effect: asynchronous progress

  MPI_Isend(ARGS)
  {
      /* insert uses atomics to be thread-safe without locking */
      insert(&queue,ARGS);
  }
  /* agent runs in a polling thread */
  agent_function()
  {
      ARGS = remove(&queue);
      PMPI_Send(ARGS);
  }
PRK
Programming model evaluation

Standard methods

- NAS Parallel Benchmarks
- Mini Applications (e.g. Mantevo, LULESH)
- HPC Challenge

There are numerous examples of these on record, covering a wide range of programming models, but is source available and curated?*

What is measured?

- Productivity (?), elegance (?)
- Implementation quality (runtime or application)
- Asynchrony/overlap
- Semantics:
  - Automatic load-balancing (AMR)
  - Atomics (GUPS)
  - Two-sided vs. one-sided, collectives

* PRK curation is TBD.
Goals of the Parallel Research Kernels

1. Universality: Cover broad range of performance critical application patterns.


3. Portability: Should be implementable in any sufficiently general programming model.

4. Extensibility: Parameterized to run at any scale. Other knobs to adjust problem or algorithm included.


6. Hardware benchmark: No! Use HPCChallenge, Xyz500, etc. for this.
Outline of PRK Suite

- **Dense matrix transpose**
- Synchronization: global
- **Synchronization: point to point**
- Scaled vector addition
- Atomic reference counting
- Vector reduction
- Sparse matrix-vector multiplication
- Random access update
- **Stencil computation**
- Dense matrix-matrix multiplication
- Branch
- Particle-in-cell

\[ A_{i,j} = A_{i-1,j} + A_{i,j-1} - A_{i-1,j-1} \]
PRK implementations

- Serial
- OpenMP
- MPI1 – MPI two-sided
  - FG-MPI – MPI1 using Fine Grain MPI from UBC
  - AMPI – MPI1 using Adaptive MPI from
- MPIOMP – MPI two-sided with local OpenMP
- MPISHM – MPI two-sided with MPI-3 shared-memory
- MPIRMA – MPI one-sided communication (multiple flavors)
- SHMEM
- UPC
- Fortran 2008 (serial, OpenMP, coarrays, intrinsics)
- Python (simple and Numpy)
- Grappa (C++)
- Charm++ (C++)

OpenMP, Serial and MPI support most of the PRKs. *Synch_p2p, Stencil* and *Transpose* are primary targets for distributed-memory evaluation.

In progress:
- Legion (Stanford)
- HPX (LSU & IU)
- OCR (Rice/Intel)
- Chapel (Cray)
Experimental apparatus

See paper for details.
Transpose, strong scaled (49152x49152*)

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MPI+X based models win (X=OpenMP/MPI3)

Aggregate performance MB/s

* Charm++: (47104x47104)
Stencil, strong scaled (49152x49152*)

Normalized performance (Mflops/#nodes)/Mflops_single_node_MPI1
Synch_p2p, strong scaled (49152x49152*)

Aggregate performance MFlops
Conclusions

• Private data is the right default, both for applications and for system software.

• Good OpenMP looks like MPI:
  • Fork threads once.
  • Very little data sharing.

• MPI+OpenMP usually entails bad OpenMP, especially when threaded libraries are involved.

• Good MPI+OpenMP is MPI+MPI.

I don't always compute in parallel but when I do, I prefer MPI.
MPI-3 RMA
### MPI-3 window constructor options

<table>
<thead>
<tr>
<th>Window ctor</th>
<th>Buffer</th>
<th>Restrictions</th>
<th>T/S*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alloc_mem, Win_create</td>
<td>input</td>
<td>static, coll.</td>
<td>B</td>
</tr>
<tr>
<td>Win_allocate</td>
<td>output</td>
<td>static, coll.</td>
<td>A</td>
</tr>
<tr>
<td>Win_allocate_shared</td>
<td>output</td>
<td>ld/st domain</td>
<td>A+</td>
</tr>
<tr>
<td>Alloc_mem, Win_{create_dynamic,attach}</td>
<td>input</td>
<td>-</td>
<td>?</td>
</tr>
</tbody>
</table>

- Win_create cannot use symmetric memory, likely will not allocate shm or registered buffers without info keys.
- Dynamic windows require not-yet-standard info keys to cache RDMA metadata, in addition to the restrictions of Win_create.
- Win_allocate_shared hopefully deprecated (into Win_allocate) in MPI-4.
MPI RMA memory allocation

• All RMA operations act on windows, which are handles to opaque objects that describe memory on which RMA can act.

• MPI-2 had one way to construct a window. MPI-3 added 2.5 new ways. All of them are formally collective (more on this later).

• Most PGAS models require a suballocator, compiler and/or OS hooks for memory management in general...

The purpose of multiple window constructors is to make the tradeoffs between flexibility and performance explicit. MPI is nothing if not explicit.
Synchronization epochs

MPI_Win w;
/* construct window */
MPI_Win_lock_all(MPI_MODE_NOCHECK,w); /* “PGAS mode” */
{
    ...
    MPI_Put(...,pe,w); /* all RMA communications are nonblocking */
    MPI_Win_flush_local(pe,w); /* local completion */
    MPI_Win_flush (pe,w); /* remote completion = global visibility */
    ...
}
MPI_Win_unlock_all(w);
MPI_Win_free(w);

This is the only synchronization motif PGAS programmers should ever use.
Direct local access

```c
int * ptr; MPI_Win w;
MPI_Win_{allocate_shared,shared_query}(&ptr,&w);
...
if (pe==0) {
    MPI_Put(...,pe=1,w); /* Write */
    MPI_Win_flush (pe=1,w); /* Release */
    MPI_Send(...,pe=1); /* Send */
} else if (pe==1) {
    MPI_Recv(...,pe=0); /* Recv */
    MPI_Win_sync(w); /* Acquire*/
    int tmp = *ptr; /* Read */

This approach to memory consistency is consistent with OpenMP “flush”...
```
Direct local access

```c
#include <stdatomic.h>

... if (pe==0) {
    *ptr = 0x86; /* Write */
    atomic_thread_fence(...release); /* Release */
    MPI_Send(...,pe=1); /* Send */
} else if (pe==1) {
    MPI_Recv(...,pe=0); /* Recv */
    atomic_thread_fence(...acquire); /* Acquire */
    int tmp = *ptr; /* Read */
}
```

- Shared-memory is equivalent to threads.
- Threads cannot be implemented as a library.
- MPI is a library.

→ Use language (C11 or C++11) features instead of MPI_WIN_SYNC*.
Direct local access

```
#include <stdatomic.h>
atomic_flag *flag; MPI_Win wf;
MPI_Win_{allocate_shared,shared_query}(&flag,&wf);
ATOMIC_FLAG_INIT(*flag);
...
if (pe==0) {
    atomic_store_explicit(ptr,0x86,release); /* Write + Release */
    atomic_store_explicit(flag,1,release); /* Send */
} else if (pe==1) {
    while (!atomic_load_explicit(flag,acquire)); /*Recv */
    int tmp = atomic_load_explicit(ptr,acquire); /* Acquire + Read */
}
```

Here MPI is just a portable wrapper around shared memory.
Topology

Cartesian communicators were just the beginning – distributed graph topology allows expression of any communication pattern to the runtime.

Neighborhood collectives express $O(pairs)$ of communication in a single call. Runtime can allocate persistent network resources because it knows the pattern in advance.

Boundary element exchange as $N \text{ isend-irecv} + \text{waitall}$ is perhaps the most common MPI pattern.
MPI-3 SHARED MEMORY
mpi-3 shared memory

/* numa optimization */
MPI_Info_set(sheap_info, "alloc_shared_noncontig", "true");

double * my_base_ptr;
MPI_Win_allocate_shared(per_proc_shm_size, sizeof(double), sheap_info,
    node_comm, &my_base_ptr, &shm_win); /* collective ☹ */

double** all_base_ptrs = malloc( node_comm_size * sizeof(double*) );
for (int rank=0; rank<node_comm_size ; rank++) {
    MPI_Aint size;
    int disp;
    MPI_Win_shared_query(shm_win, rank, &size, &disp, &all_base_ptrs[rank]);
}
Exascale Computing without Threads*

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