Advanced MPI: New Features of MPI-3

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Online materials: http://htor.inf.ethz.ch/teaching/mpi_tutorials/eurompi14/
Tutorial Outline

1. Introduction to Advanced MPI Usage
2. Nonblocking Collective Communication
3. One-Sided Communication
4. Topology Mapping and Neighborhood Collective Communication
5. Bonus Material (only if time)
   1. Hybrid Programming Primer
   2. Datatypes

- All materials (slides, code examples) at:
  http://htor.inf.ethz.ch/teaching/mpi_tutorials/eurompi14/
Used Techniques

- Benjamin Franklin "Tell me, I forget, show me, I remember, involve me, I understand."
  - **Tell**: I will explain the abstract concepts and interfaces/APIs to use them
  - **Show**: I will demonstrate one or two examples for using the concepts
  - **Involve**: You will transform a simple MPI code into different semantically equivalent optimized ones

- Please interrupt me with any question at any point!
Section I - Introduction
Introduction

- Programming model Overview
- Different systems: UMA, ccNUMA, nccNUMA, RDMA, DM
Introduction

- Different programming models: UMA, PGAS, DM

TBB, CILK, OpenMP, MPI-3 SM  UPC, CAF, MPI-2 OS  MPI-1, PVM

- The question is all about memory consistency
Programming Models

- Provide abstract machine models (contract)
  - Shared memory
  - PGAS
  - Distributed memory

- All models can be mapped to any architecture, more or less efficient (execution model)

- MPI is not a programming model
  - And has never been one!
MPI Governing Principles

- (Performance) Portability
  - Declarative vs. imperative
  - Abstraction

- Composability (Libraries)
  - Isolation (no interference)
  - Opaque object attributes

- Transparent Tool Support
  - PMPI, MPI-T
  - Inspect performance and correctness
Main MPI Concepts

- **Communication Concepts:**
  - Point-to-point Communication
  - Collective Communication
  - One Sided Communication
  - (Collective) I/O Operations

- **Declarative Concepts:**
  - Groups and Communicators
  - Derived Datatypes
  - Process Topologies

- **Process Management**
  - Malleability, ensemble applications

- **Tool support**
  - Linking and runtime
MPI History

- An open standard library interface for message passing, ratified by the MPI Forum

- Versions: 1.0 ('94), 1.1 ('95), 1.2 ('97), 1.3 ('08)
  - Basic Message Passing Concepts
- 2.0 ('97), 2.1 ('08)
  - Added One Sided and I/O concepts
- 2.2 ('09)
  - Merging and smaller fixes
- 3.0 ('12)
  - Several additions to react to new challenges
- 3.1 ('15)
  - Several smaller issues and (hopefully) FT
- 4.0 ('??)
  - Unclear (come next week to Kobe!!)
What MPI is Not

- No explicit support for active messages
  - Can be emulated at the library level
- Not a programming language
  - But it’s close, semantics of library calls are clearly specified
  - MPI-aware compilers under development
- It’s not magic
  - Manual data decomposition (cf. libraries, e.g., ParMETIS)
    *Some MPI mechanisms (Process Topologies, Neighbor Colls.)*
  - Manual load-balancing (see libraries, e.g., ADLB)
- It’s neither complicated nor bloated
  - Six functions are sufficient for any program
  - 250+ additional functions that offer abstraction, performance portability and convenience for experts
What is this MPI Forum?

- An open Forum to discuss MPI
  - You can join! No membership fee, no perks either
- Since 2008 meetings every two months for three days (switching to four months and four days)
  - 5x in the US, once in Europe (with EuroMPI → next week)
- Votes by organization, eligible after attending two of the three last meetings, often unanimously
- Everything is voted twice in two distinct meetings
  - Tickets as well as chapters
Recommended Development Workflow

1. **Identify a scalable algorithm**
   - Analyze for memory and runtime

2. **Is there a library that can help me?**
   - Computational libraries
     - **PPM, PBGL, PETSc, PMTL, ScaLAPACK**
   - Communication libraries
     - **AM++, LibNBC**
   - Programming Model Libraries
     - **ADLB, AP**
   - Utility Libraries
     - **HDF5, Boost.MPI**

3. **Plan for modularity**
   - Writing (parallel) libraries has numerous benefits
Things to Keep in Mind

- MPI is an open standardization effort
  - Talk to us or join the forum
  - There will be a public comment period

- The MPI standard
  - Is free for everybody
  - Is not intended for end-users (no replacement for books and tutorials)
  - Is the last instance in MPI questions
Any Deeper Questions – Advanced MPI

includes all of MPI-3.0
to appear November 2014
Section II - Nonblocking and Collective Communication
Nonblocking and Collective Communication

- **Nonblocking communication**
  - Deadlock avoidance
  - Overlapping communication/computation

- **Collective communication**
  - Collection of pre-defined optimized routines

- **Nonblocking collective communication**
  - Combines both advantages
  - System noise/imbalance resiliency
  - Semantic advantages
  - Examples
Nonblocking Communication

- **Semantics are simple:**
  - Function returns no matter what
  - No progress guarantee!
- **E.g.,** `MPI_Isend(<send-args>, MPI_Request *req);`
- **Nonblocking tests:**
  - Test, Testany, Testall, Testsome
- **Blocking wait:**
  - Wait, Waitany, Waitall, Waitsome
Nonblocking Communication

- **Blocking vs. nonblocking communication**
  - Mostly equivalent, nonblocking has constant request management overhead
  - Nonblocking may have other non-trivial overheads

- **Request queue length**
  - Linear impact on performance
  - E.g., BG/P: 100ns/req

  *Tune unexpected Q length!*
Nonblocking Communication

- An (important) implementation detail
  - Eager vs. Rendezvous

- Most/All MPIs switch protocols
  - Small messages are copied to internal remote buffers
    
    And then copied to user buffer
    
    Frees sender immediately (cf. bsend)
  
  - Large messages wait until receiver is ready
    
    Blocks sender until receiver arrived

- Tune eager limits!
Software Pipelining - Motivation

```c
if(r == 0) {
    for(int i=0; i<size; ++i) {
        arr[i] = compute(arr, size);
    }
    MPI_Send(arr, size, MPI_DOUBLE, 1, 99, comm);
} else {
    MPI_Recv(arr, size, MPI_DOUBLE, 0, 99, comm, &stat);
}
```
Software Pipelining - Motivation

if(r == 0) {
    MPI_Request req=MPI_REQUEST_NULL;
    for(int b=0; b<nblocks; ++b) {
        if(b) {
            if(req != MPI_REQUEST_NULL) MPI_Wait(&req, &stat);
            MPI_Isend(&arr[(b-1)*bs], bs, MPI_DOUBLE, 1, 99, comm, &req);
        }
        for(int i=b*bs; i<(b+1)*bs; ++i) arr[i] = compute(arr, size);
    }
    MPI_Send(&arr[(nblocks-1)*bs], bs, MPI_DOUBLE, 1, 99, comm);
} else {
    for(int b=0; b<nblocks; ++b)
        MPI_Recv(&arr[b*bs], bs, MPI_DOUBLE, 0, 99, comm, &stat);
}
A Simple Pipeline Model

- **No pipeline:**
  \[ T = T_{comp}(s) + T_{comm}(s) + T_{startc}(s) \]

- **Pipeline:**
  \[ T = \text{nbloc}\text{k}\;\ast\; \left[ \max(T_{comp}(bs), T_{comm}(bs)) + T_{startc}(bs) \right] \]
2D Jacobi Example

- Many 2d electrostatic problems can be reduced to solving Poisson’s or Laplace’s equation
  - Solution by finite difference methods
  - $p_{\text{new}}(i,j) = \frac{p(i-1,j)+p(i+1,j)+p(i,j-1)+p(i,j+1)}{4}$
  - natural 2d domain decomposition
  - State of the Art:
    \begin{itemize}
    \item Compute, communicate
    \item Maybe overlap inner computation
    \end{itemize}
Simplified Serial Code

for(int iter=0; iter<niters; ++iter) {
    for(int i=1; i<n+1; ++i) {
        for(int j=1; j<n+1; ++j) {
            anew[ind(i,j)] = apply(stencil); // actual computation
            heat += anew[ind(i,j)]; // total heat in system
        }
    }
    for(int i=0; i<nsources; ++i) {
        anew[ind(sources[i][0],sources[i][1])] += energy; // heat source
    }
    tmp=anew; anew=aold; aold=tmp; // swap arrays
}
Simple 2D Parallelization

- Why 2D parallelization?
  - Minimizes surface-to-volume ratio
- Specify decomposition on command line (px, py)
- Compute process neighbors manually
- Add halo zones (depth 1 in each direction)
- Same loop with changed iteration domain
- Pack halo, communicate, unpack halo
- Global reduction to determine total heat
Source Code Example

- Browse through code (stencil_mpi.cpp)
Stencil Example - Overlap

- stencil_mpi_ddt_overlap.cpp

- Steps:
  - Start halo communication
  - Compute inner zone
  - Wait for halo communication
  - Compute outer zone
  - Swap arrays
Collective Communication

- **Three types:**
  - Synchronization (Barrier)
  - Data Movement (Scatter, Gather, Alltoall, Allgather)
  - Reductions (Reduce, Allreduce, (Ex)Scan, Reduce_scatter)

- **Common semantics:**
  - no tags (communicators can serve as such)
  - Blocking semantics (return when complete)
  - Not necessarily synchronizing (only barrier and all*)

- **Overview of functions and performance models**
Collective Communication

- **Barrier** –
  - Often $\alpha + \beta \log_2 P$

- **Scatter, Gather** –
  - Often $\alpha P + \beta Ps$

- **Alltoall, Allgather** –
  - Often $\alpha P + \beta Ps$
Collective Communication

- **Reduce** –
  - Often $\alpha \log_2 P + \beta m + \gamma m$
  
  \[ \Omega(\log(P) + s) \]

- **Allreduce** –
  - Often $\alpha \log_2 P + \beta m + \gamma m$
  
  \[ \Omega(\log(P) + s) \]

- **(Ex)scan** –
  - Often $\alpha P + \beta m + \gamma m$
  
  \[ \Omega(\log(P) + s) \]
Nonblocking Collective Communication

- Nonblocking variants of all collectives
  - MPI_Ibcast(<bcast args>, MPI_Request *req);

- Semantics:
  - Function returns no matter what
  - No guaranteed progress (quality of implementation)
  - Usual completion calls (wait, test) + mixing
  - Out-of order completion

- Restrictions:
  - No tags, in-order matching
  - Send and vector buffers may not be touched during operation
  - MPI_Cancel not supported
  - No matching with blocking collectives
Nonblocking Collective Communication

- **Semantic advantages:**
  - Enable asynchronous progression (and manual)  
    *Software pipelining*
  - Decouple data transfer and synchronization  
    *Noise resiliency!*
  - Allow overlapping communicators  
    *See also neighborhood collectives*
  - Multiple outstanding operations at any time  
    *Enables pipelining window*
Nonblocking Collectives Overlap

- Software pipelining, similar to point-to-point
  - More complex parameters
  - Progression issues
  - Not scale-invariant

TH, Lumsdaine, Rehm: Implementation and Performance Analysis of Non-Blocking Collective Operations for MPI, SC07
Nonblocking Collectives Overlap

- Complex progression
  - MPI’s global progress rule!
- Higher CPU overhead (offloading?)
- Differences in asymptotic behavior
  - Collective time often $\Omega(\log(P) + Ps)$
  - Computation $O\left(\frac{N}{P}\right)$

  → Performance modeling 😊
  - One term often dominates and complicates overlap

TH, Gottschling, Lumsdaine: Leveraging Non-blocking Collective Communication in High-performance Applications, SPAA’08
System Noise – Introduction

- CPUs are time-shared
  - Deamons, interrupts, etc. steal cycles
  - No problem for single-core performance
    - Maximum seen: 0.26%, average: 0.05% overhead
  - “Resonance” at large scale (Petrini et al ’03)

- Numerous studies
  - Theoretical (Agarwal’05, Tsafrir’05, Seelam’10)
  - Injection (Beckman’06, Ferreira’08)
  - Simulation (Sottile’04)
Measurement Results – Cray XE

- **Resolution:** 32.9 ns, noise overhead: 0.02%
A Noisy Example – Dissemination

- Process 4 is delayed
  - Noise propagates “wildly” (of course deterministic)
Single Byte Dissemination on Jaguar

- no impact!
- some outliers
- deterministic slowdown (noise bottleneck)

TH, Schneider, Lumsdaine: Characterizing the Influence of System Noise on Large-Scale Applications by Simulation, SC10
Nonblocking Collectives vs. Noise

No Noise, blocking

Noise, blocking

Noise, nonblocking

TH, Schneider, Lumsdaine: Characterizing the Influence of System Noise on Large-Scale Applications by Simulation, SC10
A Non-Blocking Barrier?

- What can that be good for? Well, quite a bit!
- **Semantics:**
  - MPI_Ibarrier() – calling process entered the barrier, **no** synchronization happens
  - Synchronization **may** happen asynchronously
  - MPI_Test/Wait() – synchronization happens **if** necessary
- **Uses:**
  - Overlap barrier latency (small benefit)
  - Use the split semantics! Processes **notify** non-collectively but **synchronize** collectively!
A Semantics Example: DSDE

- Dynamic Sparse Data Exchange
  - Dynamic: comm. pattern varies across iterations
  - Sparse: number of neighbors is limited \( O(\log P) \)
  - Data exchange: only senders know neighbors

"TH, Siebert, Lumsdaine: Scalable Communication Protocols for Dynamic Sparse Data Exchange, PPoPP''10"
Dynamic Sparse Data Exchange (DSDE)

- Main Problem: metadata
  - Determine who wants to send how much data to me (I must post receive and reserve memory)

OR:

- Use MPI semantics:
  - Unknown sender
    - MPI_ANY_SOURCE
  - Unknown message size
    - MPI_PROBE

Reduces problem to counting the number of neighbors
Allow faster implementation!
Using Alltoall (PEX)

- Based on Personalized Exchange ($\Theta(P)$)
  - Processes exchange metadata (sizes) about neighborhoods with all-to-all
  - Processes post receives afterwards
  - Most intuitive but least performance and scalability!
Reduce\_scatter (PCX)

- **Bases on Personalized Census ($\Theta(P)$)**
  - Processes exchange metadata (counts) about neighborhoods with `reduce\_scatter`
  - Receivers checks with wildcard MPI\_IPROBE and receives messages
  - Better than PEX but non-deterministic!

*TH, Siebert, Lumsdaine: Scalable Communication Protocols for Dynamic Sparse Data Exchange, PPoPP’10*
MPI_Ibarrier (NBX)

- **Complexity - census (barrier):** \( \Theta(\log(P)) \)
  - Combines metadata with actual transmission
  - Point-to-point synchronization
  - Continue receiving until barrier completes
  - Processes start coll. synch. (barrier) when p2p phase ended
  - \textit{barrier} = \textit{distributed marker!}
- Better than PEX, PCX, RSX!

\[\text{TH, Siebert, Lumsdaine: Scalable Communication Protocols for Dynamic Sparse Data Exchange, PPoPP"'10}\]
Parallel Breadth First Search

- On a clustered Erdős-Rényi graph, weak scaling
  - 6.75 million edges per node (filled 1 GiB)

- HW barrier support is significant at large scale!

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**TH, Siebert, Lumsdaine: Scalable Communication Protocols for Dynamic Sparse Data Exchange, PPoPP’10**
Parallel Fast Fourier Transform

- 1D FFTs in all three dimensions
  - Assume 1D decomposition (each process holds a set of planes)
  - Best way: call optimized 1D FFTs in parallel \(\rightarrow\) alltoall

- Red/yellow/green are the (three) different processes!
A Complex Example: FFT

for(int x=0; x<n/p; ++x) 1d_fft(/* x-th stencil */);

// pack data for alltoall
MPI_Alltoall(&in, n/p*n/p, cplx_t, &out, n/p*n/p, cplx_t, comm);

// unpack data from alltoall and transpose

for(int y=0; y<n/p; ++y) 1d_fft(/* y-th stencil */);

// pack data for alltoall
MPI_Alltoall(&in, n/p*n/p, cplx_t, &out, n/p*n/p, cplx_t, comm);

// unpack data from alltoall and transpose

TH, Gottschling, Lumsdaine: Leveraging Non-blocking Collective Communication in High-performance Applications, SPAA’08
Parallel Fast Fourier Transform

- Data already transformed in y-direction
Parallel Fast Fourier Transform

- Transform first y plane in z
Parallel Fast Fourier Transform

- Start ialltoall and transform second plane
Parallel Fast Fourier Transform

- Start ialltoall (second plane) and transform third
Parallel Fast Fourier Transform

- Start alltoall of third plane and ...
Parallel Fast Fourier Transform

- Finish ialltoall of first plane, start x transform
Parallel Fast Fourier Transform

- Finish second `ialltoall`, transform second plane
Parallel Fast Fourier Transform

- Transform last plane → done
FFT Software Pipelining

MPI_Request req[nb];
for(int b=0; b<nb; ++b) { // loop over blocks
    for(int x=b*n/p/nb; x<(b+1)n/p/nb; ++x) 1d_fft(/* x-th stencil */);

    // pack b-th block of data for alltoall
    MPI_Ialltoall(&in, n/p*n/p/b, cplx_t, &out, n/p*n/p, cplx_t, comm, &req[b]);
}
MPI_Waitall(nb, req, MPI_STATUSES_IGNORE);

// modified unpack data from alltoall and transpose
for(int y=0; y<n/p; ++y) 1d_fft(/* y-th stencil */);
// pack data for alltoall
MPI_Alltoall(&in, n/p*n/p, cplx_t, &out, n/p*n/p, cplx_t, comm);
// unpack data from alltoall and transpose
Nonblocking And Collective Summary

- Nonblocking comm does two things:
  - Overlap and relax synchronization

- Collective comm does one thing
  - Specialized pre-optimized routines
  - Performance portability
  - Hopefully transparent performance

- They can be composed
  - E.g., software pipelining
Section III - One Sided Communication
One Sided Communication

- Terminology
- Memory exposure
- Communication
- Accumulation
  - Ordering, atomics
- Synchronization
- Shared memory windows
- Memory models & semantics 😊
One Sided Communication – The Shock

- The syntax is weird, really!
  - It grew – MPI-3.0 is backwards compatible!
- Think PGAS (with a library interface)
  - Remote memory access (put, get, accumulates)
- Forget locks 😊
  - Win_lock_all is not a lock, opens an epoch
- Think TM
  - That’s really what “lock” means (lock/unlock is like an atomic region, does not necessarily “lock” anything)
- Decouple transfers from synchronization
  - Separate transfer and synch functions
One Sided Communication – Terms

- **Origin process**: Process with the source buffer, initiates the operation
- **Target process**: Process with the destination buffer, does not explicitly call communication functions
- **Epoch**: Virtual time where operations are in flight. Data is consistent after new epoch is started.
  - **Access epoch**: rank acts as origin for RMA calls
  - **Exposure epoch**: rank acts as target for RMA calls
- **Ordering**: only for accumulate operations: order of messages between two processes (default: in order, can be relaxed)
- **Assert**: assertions about how One Sided functions are used, “fast” optimization hints, cf. Info objects (slower)
One Sided Overview

- **Creation**
  - Expose memory collectively - Win_create
  - Allocate exposed memory – Win_allocate
  - Dynamic memory exposure – Win_create_dynamic

- **Communication**
  - Data movement (put, get, rput, rget)
  - Accumulate (acc, racc, get_acc, rget_acc, fetch&op, cas)

- **Synchronization**
  - Active - Collective (fence); Group (PSCW)
  - Passive - P2P (lock/unlock); One epoch (lock_all)
Memory Exposure

MPI_Win_create(void *base, MPI_Aint size, int disp_unit, MPI_Info info, MPI_Comm comm, MPI_Win *win)

- Exposes consecutive memory (base, size)
- Collective call
- Info args:
  - no_locks – user asserts to not lock win
  - accumulate_ordering – comma-separated rar, war, raw, waw
  - accumulate_ops – same_op or same_op_no_op (default) – assert used ops for related accumulates

MPI_Win_free(MPI_Win *win)
Memory Exposure

MPI_Win_allocate(MPI_Aint size, int disp_unit, MPI_Info info, MPI_Comm comm, void *baseptr, MPI_Win *win)

- Similar to win_create but allocates memory
  - Should be used whenever possible!
  - May consume significantly less resources
- Similar info arguments plus
  - same_size – if true, user asserts that size is identical on all calling processes
- Win_free will deallocate memory!
  - Be careful 😊
Memory Exposure

Coll. memory exposure may be cumbersome
  - Especially for irregular applications

Win_create_dynamic creates a window with no memory attached

Register non-overlapping regions locally

Addresses are communicated for remote access!
  - MPI_Aint will be big enough on heterogeneous systems
One Sided Communication

Two similar communication functions:
- Put, Get
- Nonblocking, bulk completion at end of epoch

Conflicting accesses are not erroneous
- But outcome is undefined!
- One exception: polling on a single byte in the unified model (for fast synchronization)

MPI_Put(const void *origin_addr, int origin_count, MPI_Datatype origin_datatype, int target_rank, MPI_Aint target_disp, int target_count, MPI_Datatype target_datatype, MPI_Win win)
One Sided Communication

MPI_Rput(…, MPI_Request *request)

- **MPI_Rput, MPI_Rget for request-based completion**
  - Also non-blocking but return request
  - Expensive for each operation (vs. bulk completion)

- **Only for local buffer consistency**
  - Get means complete!
  - Put means buffer can be re-used, nothing known about remote completion
One Sided Accumulation

MPI_Accumulate(const void *origin_addr, int origin_count, MPI_Datatype origin_datatype, int target_rank, MPI_Aint target_disp, int target_count, MPI_Datatype target_datatype, MPI_Op op, MPI_Win win)

- Remote accumulations (only predefined ops)
  - Replace value in target buffer with accumulated
  - MPI_REPLACE to emulate MPI_Put
- Allows for non-recursive derived datatypes
  - No overlapping entries at target (datatype)
- Conflicting accesses are allowed!
  - Ordering rules apply
One Sided Accumulation

MPI_Get_accumulate(const void *origin_addr, int origin_count, MPI_Datatype origin_datatype, void *result_addr, int result_count, MPI_Datatype result_datatype, int target_rank, MPI_Aint target_disp, int target_count, MPI_Datatype target_datatype, MPI_Op op, MPI_Win win)

- MPI’s generalized fetch and add
  - 12 arguments 😊
  - MPI_REPLACE allows for fetch & set
  - New op: MPI_NO_OP to emulate get

- Accumulates origin into the target, returns content before accumulation in result
  - Atomically of course
One Sided Accumulation

MPI_Fetch_and_op(const void *origin_addr, void *result_addr, MPI_Datatype datatype, int target_rank, MPI_Aint target_disp, MPI_Op op, MPI_Win win)

- Get_accumulate may be very slow (needs to cover many cases, e.g., large arrays etc.)
  - Common use-case is single element fetch&op
  - Fetch_and_op offers relevant subset of Get_acc
- Very similar to Get_accumulate
  - Same semantics, just more limited interface
  - No request-based version
One Sided Accumulation

MPI_Compare_and_swap(const void *origin_addr, const void *compare_addr, void *result_addr, MPI_Datatype datatype, int target_rank, MPI_Aint target_disp, MPI_Win win)

- CAS for MPI (no CAS2 but can be emulated)
- Single element, binary compare (!)
- Compares compare buffer with target and replaces value at target with origin if compare and target are identical. Original target value is returned in result.
Accumulation Semantics

- Accumulates allow concurrent access!
  - Put/Get does not! They’re not atomic

- Emulating atomic put/get
  - Put = MPI_Accumulate(..., op=MPI_REPLACE, ...)
  - Get = MPI_Get_accumulate(..., op=MPI_NO_OP, ...)
  - Will be slow (thus we left it ugly!)

- Ordering modes
  - Default ordering allows “no surprises” (cf. UPC)
  - Can (should) be relaxed with info (accumulate_ordering = raw, waw, rar, war) during window creation
Synchronization Modes

- **Active target mode**
  - Target ranks are calling MPI
  - Either BSP-like collective: MPI_Win_fence
  - Or group-wise (cf. neighborhood collectives): PSCW

- **Passive target mode**
  - Lock/unlock: no traditional lock, more like TM (without rollback)
  - Lockall: locking all processes isn’t really a lock 😊
MPI_Win_fence Synchronization

MPI_Win_fence(int assert, MPI_Win win)

- Collectively synchronizes all RMA calls on win
- All RMA calls started before fence will complete
  - Ends/starts access and/or exposure epochs
- Does not guarantee barrier semantics (but often synchronizes)
- Assert allows optimizations, is usually 0
  - MPI_MODE_NOPRECEDE if no communication (neither as origin or destination) is outstanding on win
PSCW Synchronization

- Specification of access/exposure epochs separately:
  - Post: start exposure epoch to group, nonblocking
  - Start: start access epoch to group, may wait for post
  - Complete: finish prev. access epoch, origin completion only (not target)
  - Wait: will wait for complete, completes at (active) target

- As asynchronous as possible

MPI_Win_post(MPI_Group group, int assert, MPI_Win win)
MPI_Win_start(MPI_Group group, int assert, MPI_Win win)
MPI_Win_complete(MPI_Win win)
MPI_Win_wait(MPI_Win win)
Lock/Unlock Synchronization

MPI_Win_lock(int lock_type, int rank, int assert, MPI_Win win)
MPI_Win_unlock(int rank, MPI_Win win)

- Initiates RMA access epoch to rank
  - No concept of exposure epoch
- Unlock closes access epoch
  - Operations have completed at origin and target
- Type:
  - Exclusive: no other process may hold lock to rank
    *More like a real lock, e.g., for local accesses*
  - Shared: other processes may hold lock
Lock_all Synchronization

- Starts a shared access epoch from origin to all ranks!
  - Not collective!
- Does not really lock anything
  - Opens a different mode of use, see following slides!

MPI_Win_lock_all(int assert, MPI_Win win)
MPI_Win_unlock_all(MPI_Win win)
Synchronization Primitives (passive)

- **Flush/Flush_all**
- Completes all outstanding operations at the target rank (or all) at origin and target
  - Only in passive target mode

- **MPI_Win_flush(int rank, MPI_Win win)**
- **MPI_Win_flush_all(MPI_Win win)**

- **Completes all outstanding operations at the target rank (or all) at origin (buffer reuse)**
  - Only in passive target mode

- **MPI_Win_flush_local(int rank, MPI_Win win)**
- **MPI_Win_flush_local_all(MPI_Win win)**
Synchronizing private and public window copies
- Same as closing and opening access and exposure epochs on the window
- Does not complete any operations though!

Cf. memory barrier
Memory Models

- MPI offers two memory models:
  - Unified: public and private window are identical
  - Separate: public and private window are separate
- Type is attached as attribute to window
  - MPI_WIN_MODEL

![Diagram of MPI_UNIFIED](image1)

- Store and load operations
- Put and get operations

![Diagram of MPI_SEPARATE](image2)

- Synchronization between processes
- Separate public and private copies
## Separate Semantics

- Very complex, rules-of-thumb at target:

<table>
<thead>
<tr>
<th></th>
<th>Load</th>
<th>Store</th>
<th>Get</th>
<th>Put</th>
<th>Acc</th>
</tr>
</thead>
<tbody>
<tr>
<td>Load</td>
<td>OVL+NOV L</td>
<td>OVL+NOV L</td>
<td>OVL+NOV L</td>
<td>NOVL</td>
<td>NOVL</td>
</tr>
<tr>
<td>Store</td>
<td>OVL+NOV L</td>
<td>OVL+NOV L</td>
<td>NOVL</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>Get</td>
<td>OVL+NOV L</td>
<td>NOVL</td>
<td>OVL+NOV L</td>
<td>NOVL</td>
<td>NOVL</td>
</tr>
<tr>
<td>Put</td>
<td>NOVL</td>
<td>X</td>
<td>NOVL</td>
<td>NOVL</td>
<td>NOVL</td>
</tr>
<tr>
<td>Acc</td>
<td>NOVL</td>
<td>X</td>
<td>NOVL</td>
<td>NOVL</td>
<td>OVL+NOV L</td>
</tr>
</tbody>
</table>

- OVL – overlapping
- NOVL - non-overlapping
- X - undefined

Credits: RMA Working Group, MPI Forum
**Unified Semantics**

- Very complex, rules-of-thumb at target:

<table>
<thead>
<tr>
<th></th>
<th>Load</th>
<th>Store</th>
<th>Get</th>
<th>Put</th>
<th>Acc</th>
</tr>
</thead>
<tbody>
<tr>
<td>Load</td>
<td>OVL+NOVL</td>
<td>OVL+NOVL</td>
<td>OVL+NOVL</td>
<td>NOVL+BOVL</td>
<td>NOVL+BOVL</td>
</tr>
<tr>
<td>Store</td>
<td>OVL+NOVL</td>
<td>OVL+NOVL</td>
<td>NOVL</td>
<td>NOVL</td>
<td>NOVL</td>
</tr>
<tr>
<td>Get</td>
<td>OVL+NOVL</td>
<td>NOVL</td>
<td>OVL+NOVL</td>
<td>NOVL</td>
<td>NOVL</td>
</tr>
<tr>
<td>Put</td>
<td>NOVL+BOVL</td>
<td>NOVL</td>
<td>NOVL</td>
<td>NOVL</td>
<td>NOVL</td>
</tr>
<tr>
<td>Acc</td>
<td>NOVL+BOVL</td>
<td>NOVL</td>
<td>NOVL</td>
<td>NOVL</td>
<td>OVL+NOVL</td>
</tr>
</tbody>
</table>

- OVL – Overlapping operations
- NOVL – Nonoverlapping operations
- BOVL – Overlapping operations at a byte granularity
- X – undefined

**Credits:** RMA Working Group, MPI Forum
Stencil One-Sided Example

- stencil_mpi_ddt_rma.cpp
Distributed Hashtable Example

- hashtable_mpi.cpp
- Use first two bytes as hash
  - Trivial hash function ($2^{16}$ values)
- Static $2^{16}$ table size
  - One direct value
  - Conflicts as linked list
- Static heap
  - Linked list indexes into heap
  - Offset as pointer
int insert(t_hash *hash, int elem) {
    int pos = hashfunc(elem);
    if(hash->table[pos].value == -1) { // direct value in table
        hash->table[pos].value = elem;
    } else { // put on heap
        int newelem=hash->nextfree++; // next free element
        if(hash->table[pos].next == -1) { // first heap element
            // link new elem from table
            hash->table[pos].next = newelem;
        } else { // direct pointer to end of collision list
            int newpos=hash->last[pos];
            hash->table[newpos].next = newelem;
        }
        hash->last[pos]=newelem;
        hash->table[newelem].value = elem; // fill allocated element
    }
}
DHT Example – In MPI-3.0

```c
int insert(t_hash *hash, int elem) {
    int pos = hashfunc(elem);
    if(hash->table[pos].value == -1) { // direct value in table
        hash->table[pos].value = elem;
    } else { // put on heap
        int newelem=hash->nextfree++; // next free element
        if(hash->table[pos].next == -1) { // first heap element
            // link new elem from table
            hash->table[pos].next = newelem;
        } else {
            // direct pointer to end of collision list
            int newpos=hash->last[pos];
            hash->table[newpos].next = newelem;
        }
        hash->last[pos]=newelem;
        hash->table[newelem].value = elem; // fill allocated element
    }
}
```

Which function would you choose?
Section IV - Topology Mapping and Neighborhood Collectives
Topology Mapping and Neighborhood Collectives

- **Topology mapping basics**
  - Allocation mapping vs. rank reordering
  - Ad-hoc solutions vs. portability

- **MPI topologies**
  - Cartesian
  - Distributed graph

- **Collectives on topologies – neighborhood colls**
  - Use-cases
Topology Mapping Basics

- **First type: Allocation mapping**
  - Up-front specification of communication pattern
  - Batch system picks good set of nodes for given topology

- **Properties:**
  - Not supported by current batch systems
  - Either predefined allocation (BG/P), random allocation, or “global bandwidth maximization”
  - Also problematic to specify communication pattern upfront, not always possible (or static)
Topology Mapping Basics

- **Rank reordering**
  - Change numbering in a given allocation to reduce congestion or dilation
  - Sometimes automatic (early IBM SP machines)

- **Properties**
  - Always possible, but effect may be limited (e.g., in a bad allocation)
  - Portable way: MPI process topologies
    - *Network topology is not exposed*
  - Manual data shuffling after remapping step
On-Node Reordering

Naïve Mapping

Optimized Mapping

Topomap

Gottschling, TH: Productive Parallel Linear Algebra Programming with Unstructured Topology Adaption, CCGrid'11
MPI Topology Intro

- Convenience functions (in MPI-1)
  - Create a graph and query it, nothing else
  - Useful especially for Cartesian topologies
    - Query neighbors in n-dimensional space
  - Graph topology: each rank specifies full graph 😞

- Scalable Graph topology (MPI-2.2)
  - Graph topology: each rank specifies its neighbors or arbitrary subset of the graph

- Neighborhood collectives (MPI-3.0)
  - Adding communication functions defined on graph topologies (neighborhood of distance one)
**MPI_Cart_create**

```c
MPI_Cart_create(MPI_Comm comm_old, int ndims, const int *dims, const int *periods, int reorder, MPI_Comm *comm_cart)
```

- **Specify ndims-dimensional topology**
  - Optionally periodic in each dimension (Torus)
- **Some processes may return MPI_COMM_NULL**
  - Product sum of dims must be \( \leq P \)
- **Reorder argument allows for topology mapping**
  - Each calling process may have a new rank in the created communicator
  - Data has to be remapped manually
MPI_Cart_create Example

```c
int dims[3] = {5,5,5};
int periods[3] = {1,1,1};
MPI_Comm topocomm;
MPI_Cart_create(comm, 3, dims, periods, 0, &topocomm);
```

- Creates logical 3-d Torus of size 5x5x5
- But we’re starting MPI processes with a one-dimensional argument (-p X)
  - User has to determine size of each dimension
  - Often as “square” as possible, MPI can help!
MPI_Dims_create

MPI_Dims_create(int nnodes, int ndims, int *dims)

- Create dims array for Cart_create with nnodes and ndims
  - Dimensions are as close as possible (well, in theory)
- Non-zero entries in dims will not be changed
  - nnodes must be multiple of all non-zeroes
**MPI_Dims_create Example**

```c
int p;
MPI_Comm_size(MPI_COMM_WORLD, &p);
MPI_Dims_create(p, 3, dims);

int periods[3] = {1,1,1};
MPI_Comm topocomm;
MPI_Cart_create(comm, 3, dims, periods, 0, &topocomm);
```
Cartesian Query Functions

- Library support and convenience!
- **MPI_Cartdim_get()**
  - Gets dimensions of a Cartesian communicator
- **MPI_Cart_get()**
  - Gets size of dimensions
- **MPI_Cart_rank()**
  - Translate coordinates to rank
- **MPI_Cart_coords()**
  - Translate rank to coordinates
Cartesian Communication Helpers

MPI_Cart_shift(MPI_Comm comm, int direction, int disp, int *rank_source, int *rank_dest)

- **Shift in one dimension**
  - Dimensions are numbered from 0 to ndims-1
  - Displacement indicates neighbor distance (-1, 1, …)
  - May return MPI_PROC_NULL

- **Very convenient, all you need for nearest neighbor communication**
  - No “over the edge” though
Code Example

- stencil_mpi_ddt_overlap_carttopo.cpp
- Adds calculation of neighbors with topology
MPI_Graph_create

MPI_Graph_create(MPI_Comm comm_old, int nnodes, const int *index, const int *edges, int reorder, MPI_Comm *comm_graph)

- nnodes is the total number of nodes
- index i stores the total number of neighbors for the first i nodes (sum)
  - Acts as offset into edges array
- edges stores the edge list for all processes
  - Edge list for process j starts at index[j] in edges
  - Process j has index[j+1]-index[j] edges
MPI_Graph_create

MPI_Graph_create(MPI_Comm comm_old, int nnodes, const int *index, const int *edges, int reorder, MPI_Comm *comm_graph)

- **nnodes** is the total number of nodes
- **index** \( i \) stores the total number of neighbors for the first \( i \) nodes (sum)
  - Acts as offset into edges array
- **edges** stores the edge list for all processes
  - Edge list for process \( j \) starts at index[\( j \)] in edges
  - Process \( j \) has index[\( j + 1 \)]-index[\( j \)] edges
Distributed graph constructor

- MPI_Graph_create is discouraged
  - Not scalable
  - Not deprecated yet but hopefully soon

- New distributed interface:
  - Scalable, allows distributed graph specification
    - Either local neighbors or any edge in the graph
  - Specify edge weights
    - Meaning undefined but optimization opportunity for vendors!
  - Info arguments
    - Communicate assertions of semantics to the MPI library
      - E.g., semantics of edge weights

Hoefler et al.: The Scalable Process Topology Interface of MPI 2.2, CCPE’10
MPI_Dist_graph_create_adjacent

MPI_Dist_graph_create_adjacent(MPI_Comm comm_old, int indegree, const int sources[], const int sourceweights[], int outdegree, const int destinations[], const int destweights[], MPI_Info info, int reorder, MPI_Comm *comm_dist_graph)

- outdegree, destinations, ~weights – dest. proc. spec.
- info, reorder, comm_dist_graph – as usual
- directed graph
- Each edge is specified twice, once as out-edge (at the source) and once as in-edge (at the dest)
MPI_Dist_graph_create_adjacent

- **Process 0:**
  - Indegree: 0
  - Outdegree: 2
  - Dests: \{3,1\}

- **Process 1:**
  - Indegree: 3
  - Outdegree: 2
  - Sources: \{4,0,2\}
  - Dests: \{3,4\}

- ...

*Hoefler et al.: The Scalable Process Topology Interface of MPI 2.2, CCPE’10*
MPI_Dist_graph_create

MPI_Dist_graph_create(MPI_Comm comm_old, int n,
const int sources[], const int degrees[],
const int destinations[], const int weights[], MPI_Info info,
int reorder, MPI_Comm *comm_dist_graph)

n – number of source nodes
- sources – n source nodes
- degrees – number of edges for each source
- destinations, weights – dest. processor specification
- info, reorder – as usual
- More flexible and convenient
  - Requires global communication
  - Slightly more expensive than adjacent specification

Hoefler et al.: The Scalable Process Topology Interface of MPI 2.2, CCPE’10
MPI_Dist_graph_create

- **Process 0:**
  - N: 2
  - Sources: \{0,1\}
  - Degrees: \{2,1\} *
  - Dests: \{3,1,4\}

- **Process 1:**
  - N: 2
  - Sources: \{2,3\}
  - Degrees: \{1,1\}
  - Dests: \{1,2\}

- …

* Note that in this example, process 0 specifies only one of the two outgoing edges of process 1; the second outgoing edge needs to be specified by another process
Distributed Graph Neighbor Queries

MPI_Dist_graph_neighbors_count(MPI_Comm comm,
   int *indegree, int *outdegree, int *weighted)

- Query the number of neighbors of calling process
- Returns indegree and outdegree!
- Also info if weighted

MPI_Dist_graph_neighbors(MPI_Comm comm, int maxindegree,
   int sources[], int sourceweights[], int maxoutdegree,
   int destinations[], int destweights[])

- Query the neighbor list of calling process
- Optionally return weights
Further Graph Queries

\[
\text{MPI\_Topo\_test}(\text{MPI\_Comm\ comm, int *status})
\]

- **Status is either:**
  - MPI\_GRAPH (ugs)
  - MPI\_CART
  - MPI\_DIST\_GRAPH
  - MPI\_UNDEFINED (no topology)
- **Enables to write libraries on top of MPI topologies!**
Neighborhood Collectives

- Topologies implement no communication!
  - Just helper functions

- Collective communications only cover some patterns
  - E.g., no stencil pattern

- Several requests for “build your own collective” functionality in MPI
  - Neighborhood collectives are a simplified version
  - Cf. Datatypes for communication patterns!
Cartesian Neighborhood Collectives

- Communicate with direct neighbors in Cartesian topology
  - Corresponds to cart_shift with disp=1
  - Collective (all processes in comm must call it, including processes without neighbors)
  - Buffers are laid out as neighbor sequence:
    *Defined by order of dimensions, first negative, then positive*
    *2*ndims sources and destinations

Processes at borders (MPI_PROC_NULL) leave holes in buffers (will not be updated or communicated)!
Cartesian Neighborhood Collectives

- Buffer ordering example:
Graph Neighborhood Collectives

- Collective Communication along arbitrary neighborhoods
  - Order is determined by order of neighbors as returned by (dist_)graph_neighbors.
  - Distributed graph is directed, may have different numbers of send/recv neighbors.
  - Can express dense collective operations 😊
  - Any persistent communication pattern!
MPI_Neighbor_allgather

MPI_Neighbor_allgather(const void* sendbuf, int sendcount,
                        MPI_Datatype sendtype, void* recvbuf, int recvcount,
                        MPI_Datatype recvtype, MPI_Comm comm)

- Sends the same message to all neighbors
- Receives indegree distinct messages
- Similar to MPI_Gather
  - The all prefix expresses that each process is a “root” of his neighborhood
- Vector version for full flexibility
MPI_Neighbor_alltoall

MPI_Neighbor_alltoall(const void* sendbuf, int sendcount,
MPI_Datatype sendtype, void* recvbuf, int recvcount,
MPI_Datatype recvtype, MPI_Comm comm)

- Sends outdegree distinct messages
- Received indegree distinct messages
- Similar to MPI_Alltoall
  - Neighborhood specifies full communication relationship
- Vector and w versions for full flexibility
Nonblocking Neighborhood Collectives

- Very similar to nonblocking collectives
- Collective invocation
- Matching in-order (no tags)
  - No wild tricks with neighborhoods! In order matching per communicator!

MPI_Ineighbor_allgather(…, MPI_Request *req); MPI_Ineighbor_alltoall(…, MPI_Request *req);
Walkthrough of 2D Stencil Code with Neighborhood Collectives

- stencil_mpi_carttopo_neighcolls.cpp
Why is Neighborhood Reduce Missing?

- Was originally proposed (see original paper)
- High optimization opportunities
  - Interesting tradeoffs!
  - Research topic
- Not standardized due to missing use-cases
  - My team is working on an implementation
  - Offering the obvious interface

MPI_Ineighbor_allreducev(…);
Topology Summary

- Topology functions allow to specify application communication patterns/topology
  - Convenience functions (e.g., Cartesian)
  - Storing neighborhood relations (Graph)
- Enables topology mapping (reorder=1)
  - Not widely implemented yet
  - May requires manual data re-distribution (according to new rank order)
- MPI does not expose information about the network topology (would be very complex)
Neighborhood Collectives Summary

- Neighborhood collectives add communication functions to process topologies
  - Collective optimization potential!
- Allgather
  - One item to all neighbors
- Alltoall
  - Personalized item to each neighbor
- High optimization potential (similar to collective operations)
  - Interface encourages use of topology mapping!
Section Summary

- **Process topologies enable:**
  - High-abstraction to specify communication pattern
  - Has to be relatively static (temporal locality)
  - *Creation is expensive (collective)*
  - Offers basic communication functions

- **Library can optimize:**
  - Communication schedule for neighborhood colls
  - Topology mapping
Section V - Hybrid Programming Primer
Hybrid Programming Primer

- No complete view, discussions not finished
  - Considered very important!
- Modes: shared everything (threaded MPI) vs. shared something (SHM windows)
  - And everything in between!
- How to deal with multicore and accelerators?
  - OpenMP, Cuda, UPC/CAF, OpenACC?
  - Very specific to actual environment, no general statements possible (no standardization)
  - MPI is generally compatibly, minor pitfalls
Threads in MPI-2.2

- Four thread levels in MPI-2.2
  - Single – only one thread exists
  - Funneled – only master thread calls MPI
  - Serialized – no concurrent calls to MPI
  - Multiple – concurrent calls to MPI

- But how do I call this function – oh well 😊

- To add more confusion: MPI processes may be OS threads!
Threads in MPI-3.x

- Make threaded programming explicit
  - Not standardized yet, but imagine
    `mpiexec -n 2 -t 2 ./binary`
  - Launches two processes with two threads each
  - MPI managed, i.e., threads are MPI processes and have shared address space
- Question: how does it interact with OpenMP and PGAS languages (open)?
Matched Probe

- **MPI_Probe** to receive messages of unknown size
  - MPI_Probe(…, status)
  - size = get_count(status)*size_of(datatype)
  - buffer = malloc(size)
  - MPI_Recv(buffer, …)

- **MPI_Probe** peeks in matching queue
  - Does not change it → stateful object
Matched Probe

- Two threads, A and B perform probe, malloc, receive sequence
  - $A_P \rightarrow A_M \rightarrow A_R \rightarrow B_P \rightarrow B_M \rightarrow B_R$

- Possible ordering
  - $A_P \rightarrow B_P \rightarrow B_M \rightarrow B_R \rightarrow A_M \rightarrow A_R$
  - Wrong matching!
  - Thread A’s message was “stolen” by B
  - Access to queue needs mutual exclusion 😞
MPI_Mprobe to the Rescue

- Avoid state in the library
  - Return handle, remove message from queue

```c
MPI_Message msg; MPI_Status status;
/* Match a message */
MPI_Mprobe(MPI_ANY_SOURCE, MPI_ANY_TAG, MPI_COMM_WORLD,
           &msg, &status);
/* Allocate memory to receive the message */
int count; MPI_get_count(&status, MPI_BYTE, &count);
char* buffer = malloc(count);
/* Receive this message. */
MPI_Mrecv(buffer, count, MPI_BYTE, &msg, MPI_STATUS_IGNORE);
```
Shared Memory Use-Cases

- **Reduce memory footprint**
  - E.g., share static lookup tables
  - Avoid re-computing (e.g., NWCHEM)

- **More structured programming than MPI+X**
  - Share what needs to be shared!
  - Not everything open to races like OpenMP

- **Speedups (very tricky!)**
  - Reduce communication (matching, copy) overheads
  - False sharing is an issue!
Shared Memory Windows

MPI_Win_allocate_shared(MPI_Aint size, MPI_Info info, MPI_Comm comm, void *baseptr, MPI_Win *win)

- Allocates shared memory segment in win
  - Collective, fully RMA capable
  - All processes in comm must be in shared memory!
- Returns pointer to start of own part
- Two allocation modes:
  - Contiguous (default): process i’s memory starts where process i-1’s memory ends
  - Non Contiguous (info key alloc_shared_noncontig) possible ccNUMA optimizations
Shared Memory Comm Creation

MPI_Comm_split_type(MPI_Comm comm, int split_type, int key, MPI_Info info, MPI_Comm *newcomm)

- Returns disjoint comms based on split type
  - Collective
- Types (only one so far):
  - MPI_COMM_TYPE_SHARED – split into largest subcommunicators with shared memory access
- Key mandates process ordering
  - Cf. comm_split
SHM Windows Address Query

MPI_Win_shared_query(MPI_Win win, int rank, MPI_Aint *size, void *baseptr)

- User can compute remote addresses in contig case but needs all sizes
  - Not possible in noncontig case!
  - Processes **cannot** communicate base address, may be different at different processes!
- Base address query function!
  - MPI_PROC_NULL as rank returns lowest offset
New Communicator Creation Functions

- **Noncollective communicator creation**
  - Allows to create communicators without involving all processes in the parent communicator
  - Very useful for some applications (dynamic sub-grouping) or fault tolerance (dead processes)

- **Nonblocking communicator duplication**
  - MPI_Comm_idup(…, req) – like it sounds
  - Similar semantics to nonblocking collectives
  - Enables the implementation of nonblocking libraries
Section VI – Derived Datatypes
Derived Datatypes

Abelson & Sussman: “Programs must be written for people to read, and only incidentally for machines to execute.”

- Derived Datatypes exist since MPI-1.0
  - Some extensions in MPI-2.x and MPI-3.0
- Why do I talk about this really old feature?
  - It is a very advanced and elegant declarative concept
  - It enables many elegant optimizations (zero copy)
  - It falsely has a bad reputation (which it earned in early days)
Quick MPI Datatype Introduction

- Datatypes allow to (de)serialize arbitrary data layouts into a message stream
  - Networks provide serial channels
  - Same for block devices and I/O
- Several constructors allow arbitrary layouts
  - Recursive specification possible
  - *Declarative* specification of data-layout
    - “what” and not “how”, leaves optimization to implementation (many unexplored possibilities!)
  - Choosing the right constructors is not always simple
Derived Datatype Terminology

- **Type Size**
  - Size of DDT signature (total occupied bytes)
  - Important for matching (signatures must match)

- **Lower Bound**
  - Where does the DDT start
  - Allows to specify “holes” at the beginning

- **Extent**
  - Complete size of the DDT
  - Allows to interleave DDT, relatively “dangerous”
Derived Datatype Example

- Explain Lower Bound, Size, Extent
What is Zero Copy?

- Somewhat weak terminology
  - MPI forces “remote” copy, assumed baseline

- But:
  - MPI implementations copy internally
    - *E.g.*, networking stack (TCP), packing DDTs
    - Zero-copy is possible (RDMA, I/O Vectors, SHMEM)
  - MPI applications copy too often
    - *E.g.*, manual pack, unpack or data rearrangement
    - *DDT can do both!*
Purpose of this Section

- **Demonstrate utility of DDT in practice**
  - Early implementations were bad → folklore
  - Some are still bad → chicken egg problem

- **Show creative use of DDTs**
  - Encode local transpose for FFT
  - Enable you to create more!

- **Gather input on realistic benchmark cases**
  - Guide optimization of DDT implementations
A new Way of Benchmarking

Schneider, Gerstenberger, TH: Micro-Applications for Communication Data Access Patterns, EuroMPI'13
Datatypes for the Stencil

- stencil_mpi_ddt.cpp

```
(0,0) (1,0) (2,0) (3,0) (0,1) (1,1) (2,1) (3,1) (0,2) (1,2) (2,2) (3,2) (0,3) (1,3) (2,3) (3,3)
```

NS:
```
(0,0) (1,0) (2,0) (3,0) (0,1) (1,1) (2,1) (3,1) (0,2) (1,2) (2,2) (3,2) (0,3) (1,3) (2,3) (3,3)
```

EW:
```
(0,0) (1,0) (2,0) (3,0) (0,1) (1,1) (2,1) (3,1) (0,2) (1,2) (2,2) (3,2) (0,3) (1,3) (2,3) (3,3)
```
MPI’s Intrinsic Datatypes

- Why intrinsic types?
  - Heterogeneity, nice to send a Boolean from C to Fortran
  - Conversion rules are complex, not discussed here
  - Length matches to language types

  *Avoid sizeof(int) mess*

- Users should generally use intrinsic types as basic types for communication and type construction!
  - MPI_BYTE should be avoided at all cost

- MPI-2.2 adds some missing C types
  - E.g., unsigned long long
MPI_Type_contiguous

MPI_Type_contiguous(int count, MPI_Datatype oldtype, MPI_Datatype *newtype)

- Contiguous array of oldtype
- Should not be used as last type (can be replaced by count)
MPI_Type_vector

MPI_Type_vector(int count, int blocklength, int stride, MPI_Datatype oldtype, MPI_Datatype *newtype)

- Specify strided blocks of data of oldtype
- Very useful for Cartesian arrays

Diagram showing vector and struct representations.
MPI_Type_create_hvector

MPI_Type_create_hvector(int count, int blocklength, MPI_Aint stride, MPI_Datatype oldtype, MPI_Datatype *newtype)

- Create non-unit strided vectors
- Useful for composition, e.g., vector of structs
MPI_Type_indexed

MPI_Type_indexed(int count, int *array_of_blocklengths, int *array_of_displacements, MPI_Datatype oldtype, MPI_Datatype *newtype)

- Pulling irregular subsets of data from a single array (cf. vector collectives)
  - dynamic codes with index lists, expensive though!
    - blen={1,1,2,1,2,1}
    - displs={0,3,5,9,13,17}
MPI_Type_create_hindexed

MPI_Type_create_hindexed(int count, int *arr_of_blocklengths, MPI_Aint *arr_of_displacements, MPI_Datatype oldtype, MPI_Datatype *newtype)

- Indexed with non-unit displacements, e.g., pulling types out of different arrays

```
struct

struct

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```
MPI_Type_create_indexed_block

MPI_Type_create_indexed_block(int count, int blocklength, int *array_of_displacements, MPI_Datatype oldtype, MPI_Datatype *newtype)

- Like Create_indexed but blocklength is the same
  - blen=2
  - displs={0,5,9,13,18}
MPI_Type_create_struct

MPI_Type_create_struct(int count, int array_of_blocklengths[], MPI_Aint array_of_displacements[], MPI_Datatype array_of_types[], MPI_Datatype *newtype)

- Most general constructor (cf. Alltoallw), allows different types and arbitrary arrays
MPI_Type_create_subarray

MPI_Type_create_subarray(int ndims, int array_of_sizes[], int array_of_subsizes[], int array_of_starts[], int order, MPI_Datatype oldtype, MPI_Datatype *newtype)

- Specify subarray of n-dimensional array (sizes) by start (starts) and size (subsize)

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MPI_Type_create_darray

MPI_Type_create_darray(int size, int rank, int ndims, int array_of_gsizes[], int array_of_distribs[], int array_of_dargs[], int array_of_psizes[], int order, MPI_Datatype oldtype, MPI_Datatype *newtype)

- Create distributed array, supports block, cyclic and no distribution for each dimension
  - Very useful for I/O
MPI_BOTTOM and MPI_Get_address

- **MPI_BOTTOM** is the absolute zero address
  - Portability (e.g., may be non-zero in globally shared memory)

- **MPI_Get_address**
  - Returns address relative to MPI_BOTTOM
  - Portability (do not use "&" operator in C!)

- **Very important to**
  - build struct datatypes
  - If data spans multiple arrays
Recap: Size, Extent, and Bounds

- MPI_Type_size returns size of datatype
- MPI_Type_get_extent returns lower bound and extent
Commit, Free, and Dup

- **Types must be committed before use**
  - Only the ones that are used!
  - `MPI_Type_commit` may perform heavy optimizations (and will hopefully)

- **MPI_Type_free**
  - Free MPI resources of datatypes
  - Does not affect types built from it

- **MPI_Type_dup**
  - Duplicated a type
  - Library abstraction (composability)
Other DDT Functions

- **Pack/Unpack**
  - Mainly for compatibility to legacy libraries
  - You should not be doing this yourself

- **Get_envelope/contents**
  - Only for expert library developers
  - Libraries like MPITypes\(^1\) make this easier

- **MPI_Create_resized**
  - Change extent and size (dangerous but useful)

Datatype Selection Tree

- Simple and effective performance model:
  - More parameters == slower
- contig < vector < index_block < index < struct
- Some (most) MPIs are inconsistent
  - But this rule is portable
- Advice to users:
  - Try datatype “compression” bottom-up
Datatypes and Collectives

- Alltoall, Scatter, Gather and friends expect data in rank order
  - 1\textsuperscript{st} rank: offset 0
  - 2\textsuperscript{nd} rank: offset <extent>
  - i\textsuperscript{th} rank: offset: i*<extent>
- Makes tricks necessary if types are overlapping \rightarrow use extent (create_resized)

![Diagram of data distribution]
A Complex Example - FFT

1. perform $N_x/P$ 1-d FFTs in $y$-dimension ($N_y$ elements each)
2. pack the array into a sendbuffer for the all-to-all (A)
3. perform global all-to-all (B)
4. unpack the array to be contiguous in $x$-dimension (each process has now $N_y/P$ $x$-pencils) (C)
5. perform $N_y/P$ 1-d FFTs in $x$-dimension ($N_x$ elements each)
6. pack the array into a sendbuffer for the all-to-all (D)
7. perform global all-to-all (E)
8. unpack the array to its original layout (F)
A Complex Example - FFT

TH, Gottlieb: Parallel Zero-Copy Algorithms for Fast Fourier Transform and Conjugate Gradient using MPI Datatypes, EuroMPI'12
2d-FFT Optimization Possibilities

1. Use DDT for pack/unpack (obvious)
   - Eliminate 4 of 8 steps
     - Introduce local transpose

2. Use DDT for local transpose
   - After unpack
   - Non-intuitive way of using DDTs
     - Eliminate local transpose
The Send Datatype

1. Type_struct for complex numbers
2. Type_contiguous for blocks
3. Type_vector for stride

Need to change extent to allow overlap (create_resized)

Three hierarchy-layers
The Receive Datatype

- Type_struct (complex)
- Type_vector (no contiguous, local transpose)

*Needs to change extent (create_resized)*
Experimental Evaluation

- **Odin @ IU**
  - 128 compute nodes, 2x2 Opteron 1354 2.1 GHz
  - SDR InfiniBand (OFED 1.3.1).
  - Open MPI 1.4.1 (openib BTL), g++ 4.1.2

- **Jaguar @ ORNL**
  - 150152 compute nodes, 2.1 GHz Opteron
  - Torus network (SeaStar).
  - CNL 2.1, Cray Message Passing Toolkit 3

- All compiled with “-O3 –mtune=opteron”
Strong Scaling - Odin (8000^2)

- 4 runs, report smallest time, <4% deviation
Strong Scaling – Jaguar (20k²)

- Scaling stops w/o datatypes
- DDT increase scalability

TH, Gottlieb: Parallel Zero-Copy Algorithms for Fast Fourier Transform and Conjugate Gradient using MPI Datatypes, EuroMPI'12
Datatype Conclusions

- MPI Datatypes allow zero-copy
  - Up to a factor of 3.8 or 18% speedup!
  - Requires some implementation effort
- Declarative nature makes debugging hard
  - Simple tricks like index numbers help!
- Some MPI DDT implementations are slow
  - Some nearly surreal (IBM) 😊
  - Complain to your vendor if performance is not consistent!
Tutorial Conclusion

- Thanks for attending!
  - Ask any questions you have – anytime
  - The book contains all advanced topics (not datatypes, which are included in the “Using MPI” book)
  - Enjoy:

- All materials (slides, code examples) at:
  http://htor.inf.ethz.ch/teaching/mpi_tutorials/eurompi14/