EUROMPI/ASIA 2014

KYOTO JAPAN 9-12 SEPTEMBER, 2014

Kyoto International Community House

Advanced MPI: New Features of MPI-3

TORSTEN HOEFLER

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. Dataypes

- **All materials (slides, code examples) at:**

  http://htor.inf.ethz.ch/teaching/mpi_tutorials/eurompi14/

Used Techniques

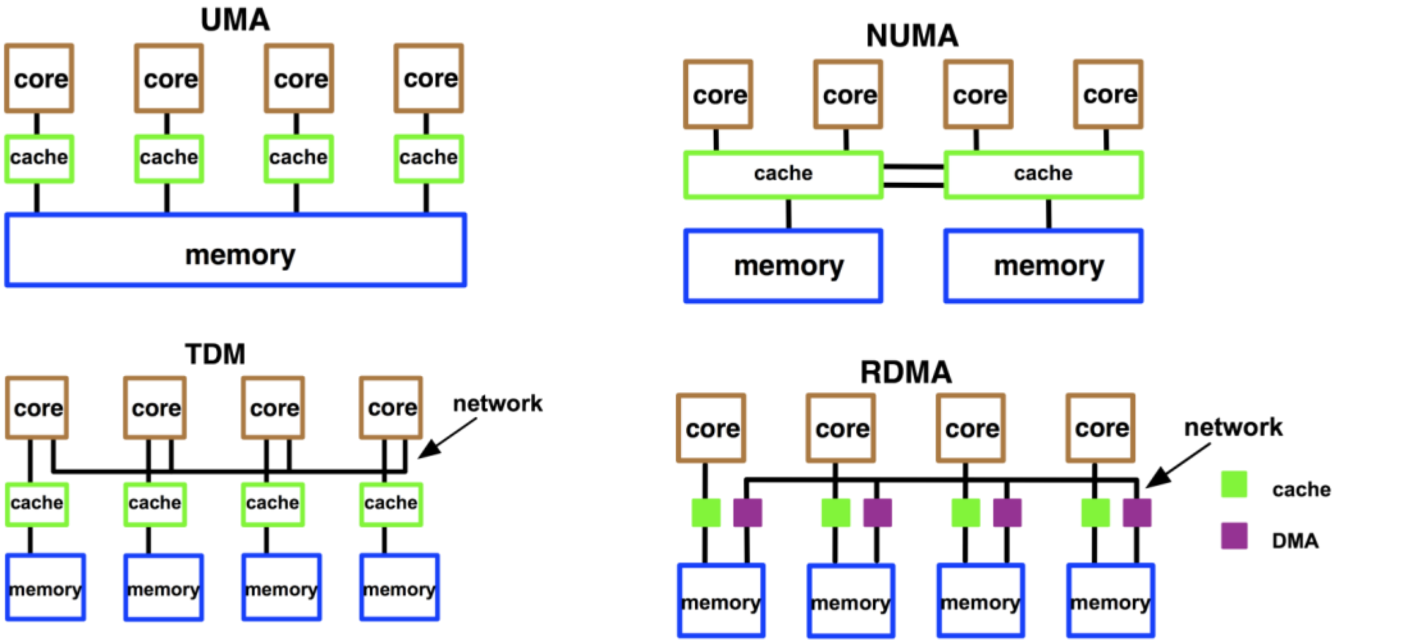
- **Benjamin Franklin *"Tell me, I forget, show me, I remember, involve me, I understand.“***
  - **Tell**: I will explain the abstract concepts and interfaces/APIs to use them
  - **Show**: I will demonstrate one or two examples for using the concepts
  - **Involve**: You will transform a simple MPI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

- **Please interrupt me with any question at any point!**

Section I - Introduction

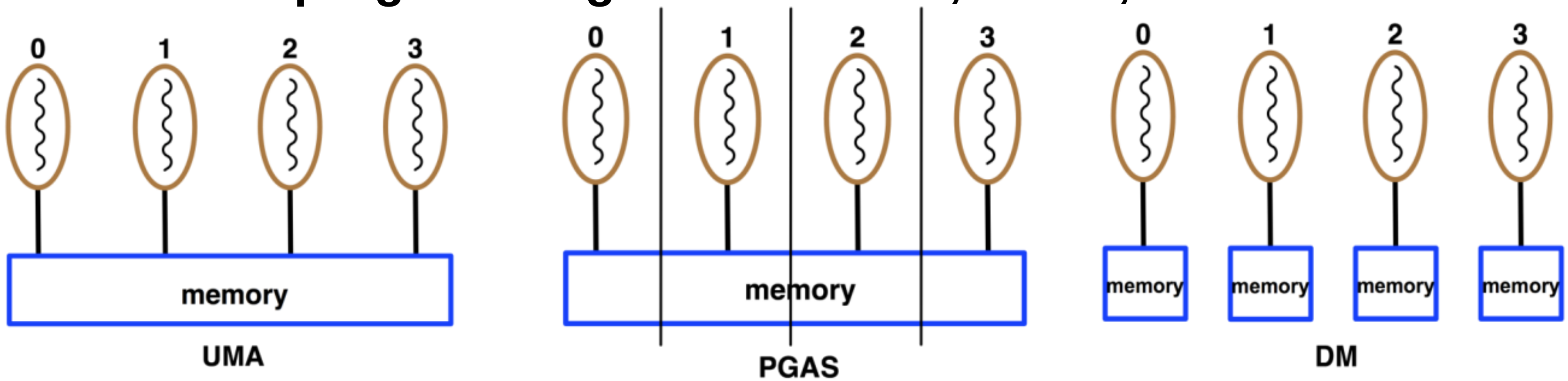
Introduction

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



Introduction

- **Different programming models: UMA, PGAS, DM**

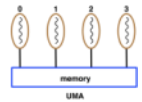


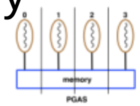
TBB, CILK, OpenMP, MPI-3 SM   UPC, CAF, MPI-2 OS   MPI-1, PVM

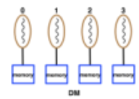
- **The question is all about memory consistency**

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

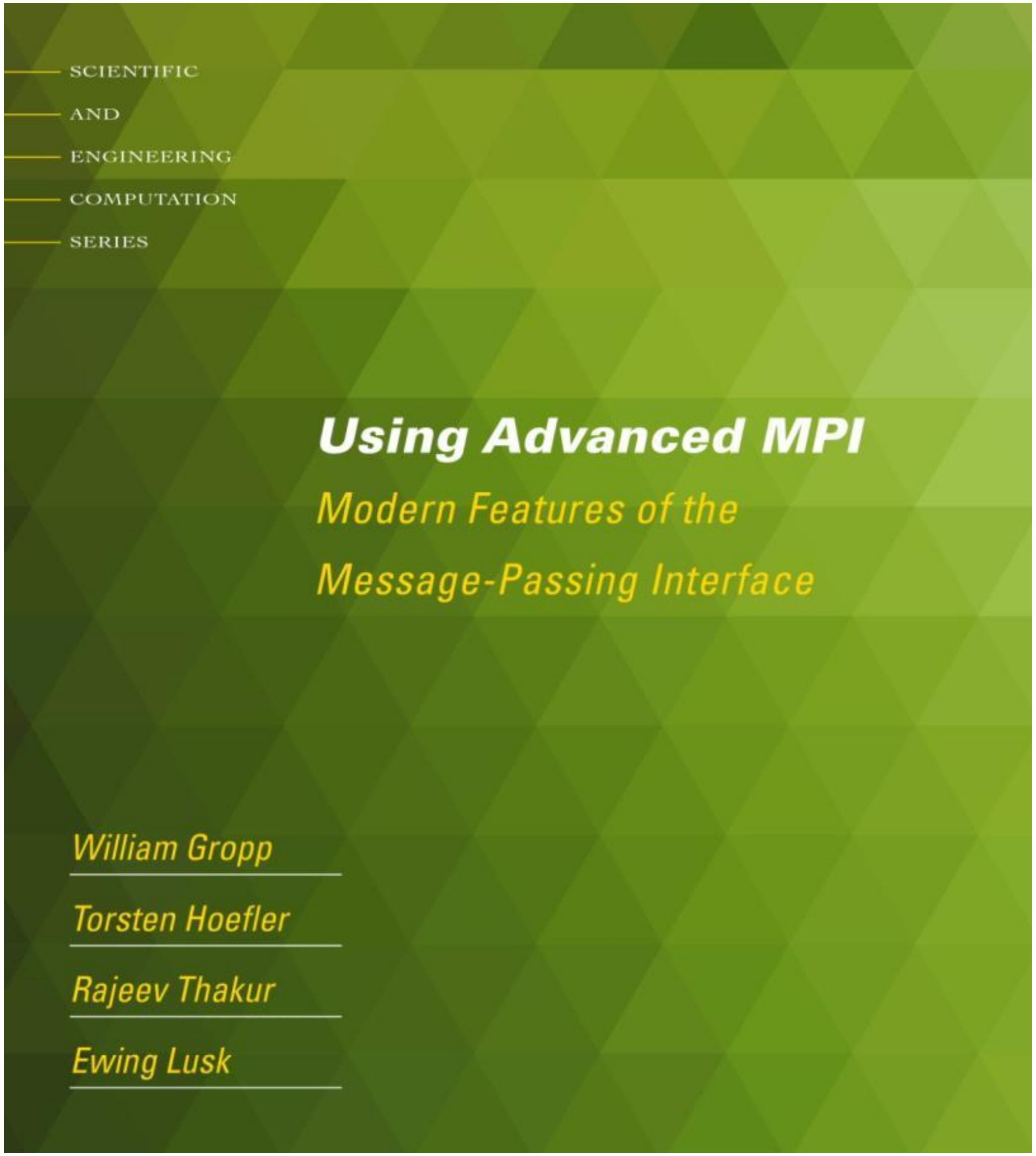
     ADLB, AP
   - Utility Libraries

     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

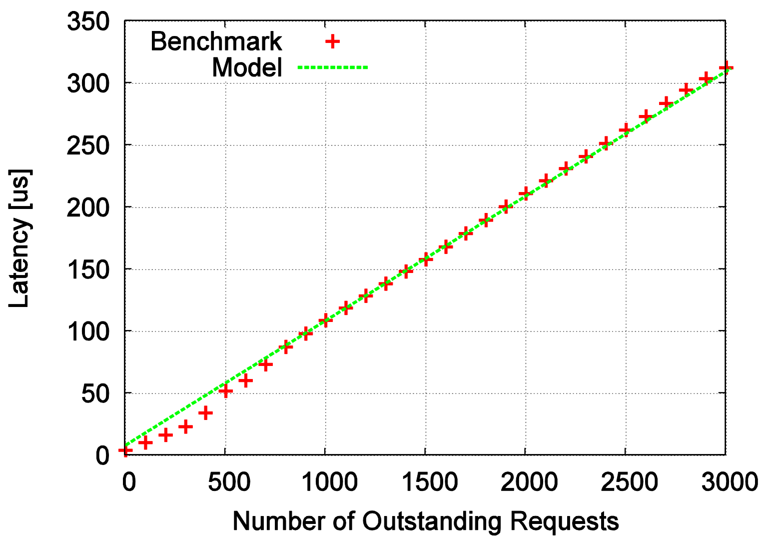
Nonblocking Communication

- **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

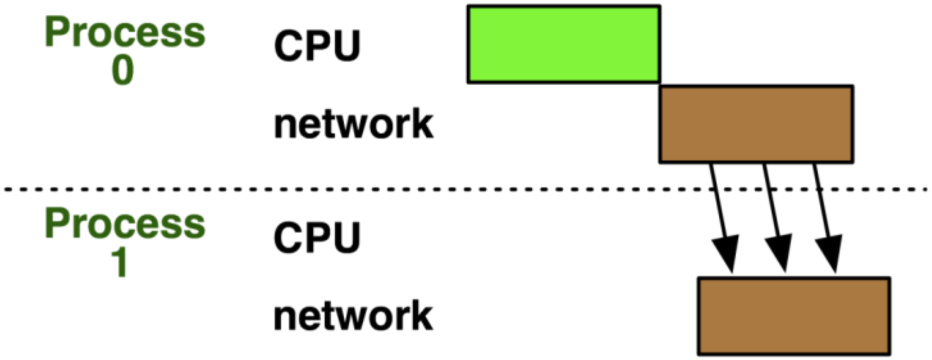
    And then copied to user buffer

    Frees sender immediately (cf. bsend)
  - Large messages wait until receiver is ready

    Blocks sender until receiver arrived
  - Tune eager limits!

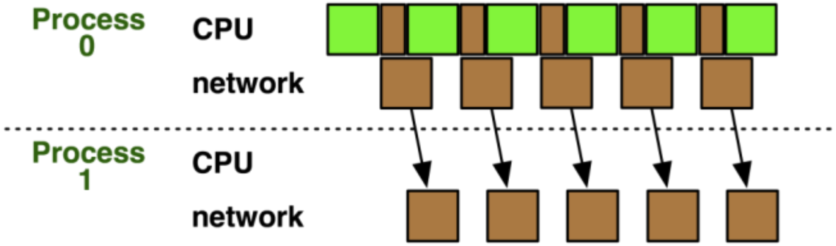
Software Pipelining - Motivation

```
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);
}
```



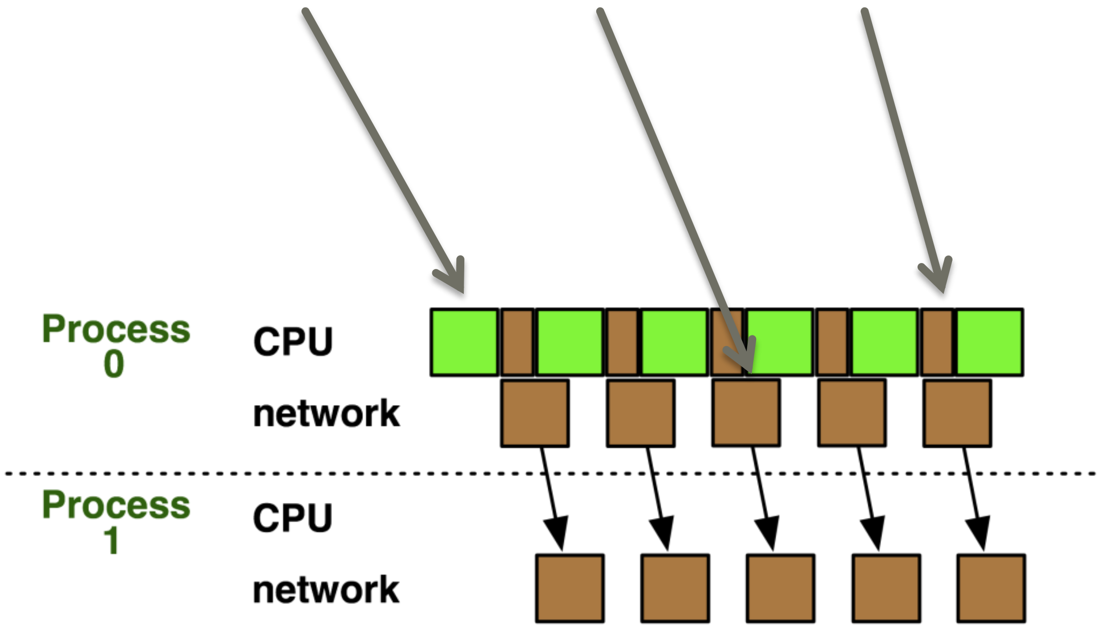
Software Pipelining - Motivation

```
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:**
  - $T = \text{nblocks} * \left[\max(T_{comp}(bs)\ ,\ T_{comm}(bs)) + T_{startc}(bs)\right]$

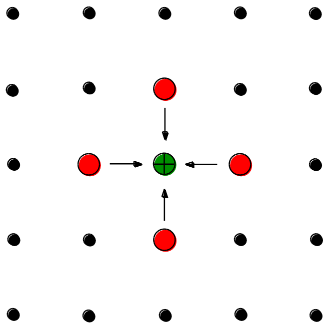


2D Jacobi Example

- **Many 2d electrostatic problems can be reduced to solving Poisson's or Laplace's equation**
  - Solution by finite difference methods
  - $p_{new}(i,j) = (p(i-1,j)+p(i+1,j)+p(i,j-1)+p(i,j+1))/4$
  - natural 2d domain decomposition
  - State of the Art:

    Compute, communicate

    Maybe overlap inner computation



Simplified Serial Code

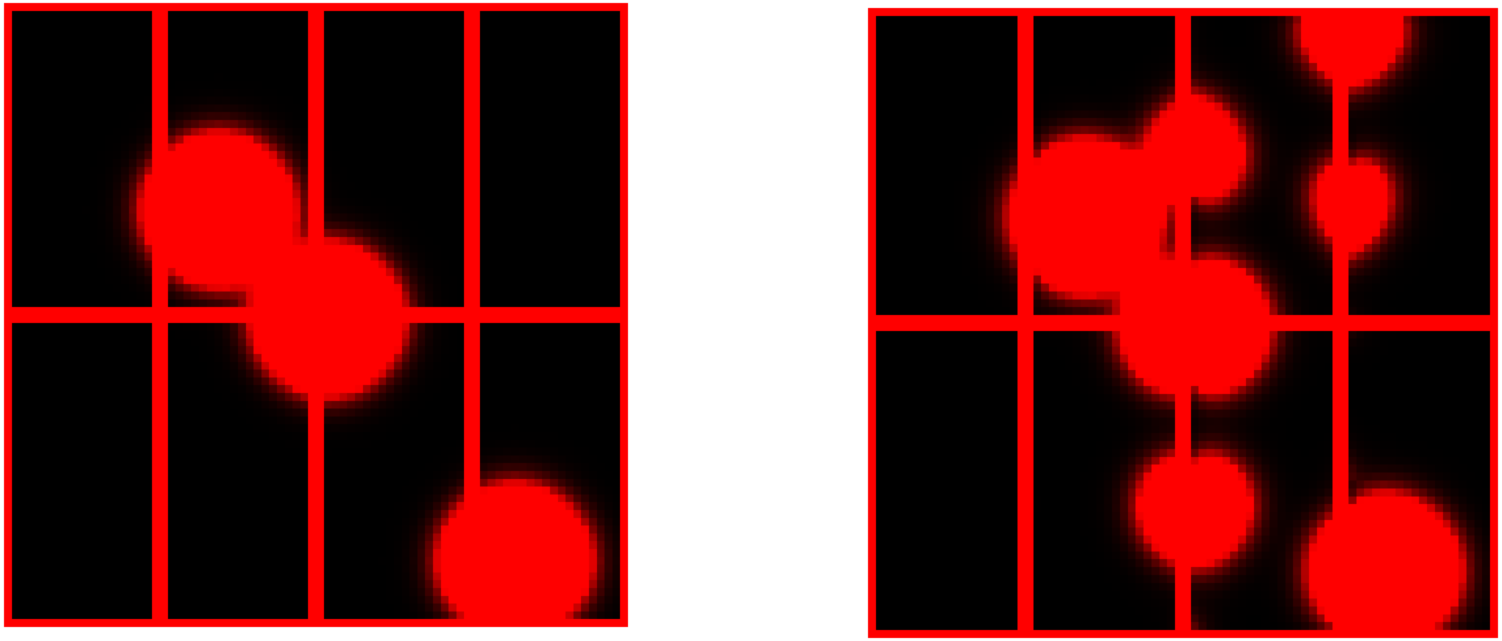
```
for(int iter=0; iter<niters; ++iter) {
    for(int i=1; i<n+1; ++i) {
        for(int j=1; j<n+1; ++j) {
            anew[ind(i,j)] = apply(stencil); // actual computation
            heat += anew[ind(i,j)]; // total heat in system
        }
    }
    for(int i=0; i<nsources; ++i) {
        anew[ind(sources[i][0],sources[i][1])] += 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**

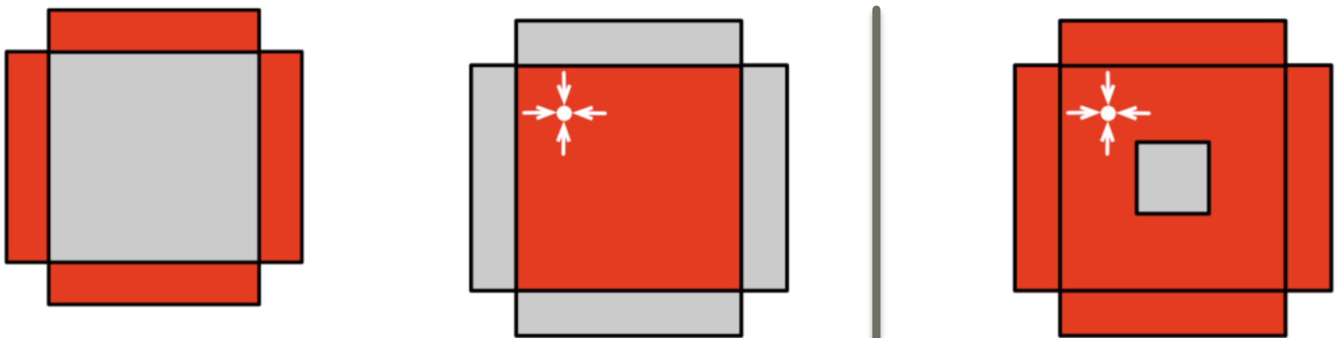
Source Code Example

- **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

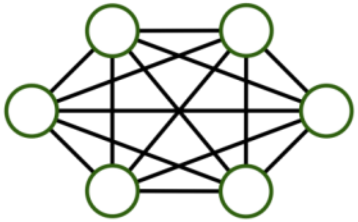
Collective Communication

- **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

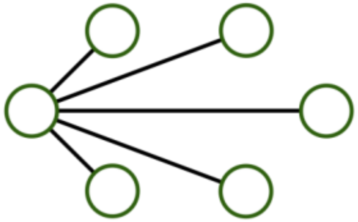
- **Barrier –**
  - Often α+β $\log_2 P$

$$\Theta(\log(P))$$



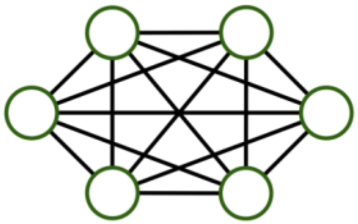
- **Scatter, Gather –**
  - Often αP+βPs

$$\Omega(\log(P) + Ps)$$



- **Alltoall, Allgather -**
  - Often αP+βPs

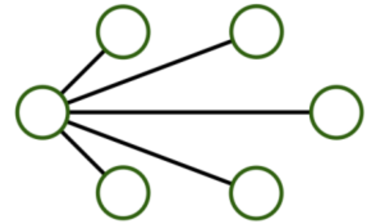
$$\Omega(\log(P) + Ps)$$



Collective Communication

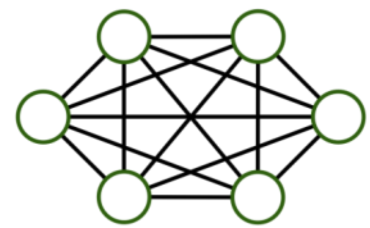
- **Reduce –**
  - Often $\alpha\log_2 P+\beta m+\gamma m$

$$\Omega(\log(P)+s)$$



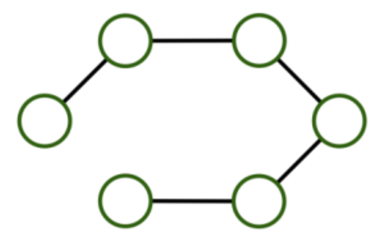
- **Allreduce –**
  - Often $\alpha\log_2 P+\beta m+\gamma m$

$$\Omega(\log(P)+s)$$



- **(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

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

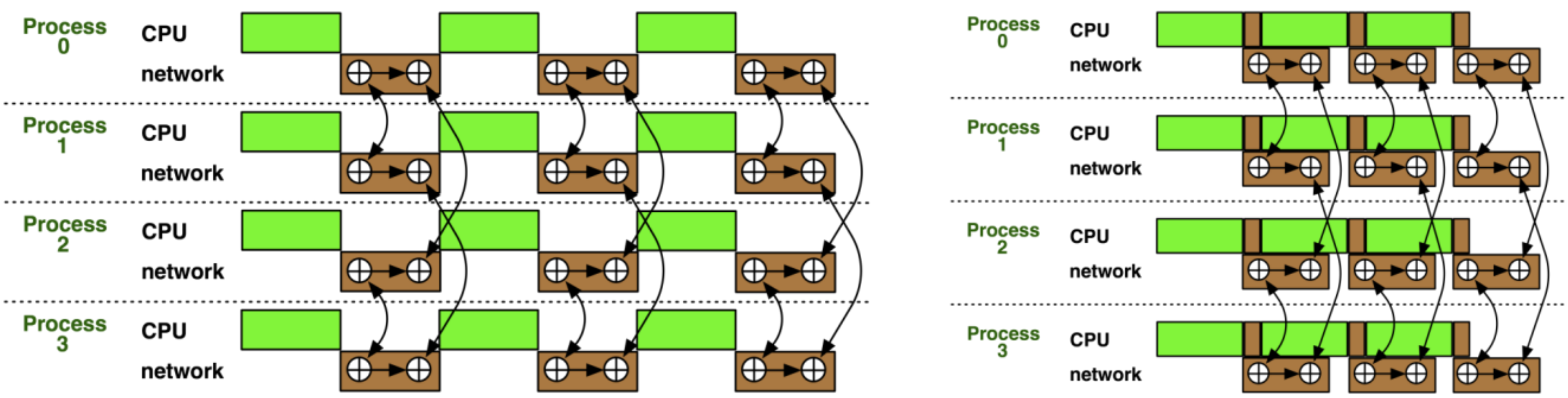
Nonblocking Collective Communication

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

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

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

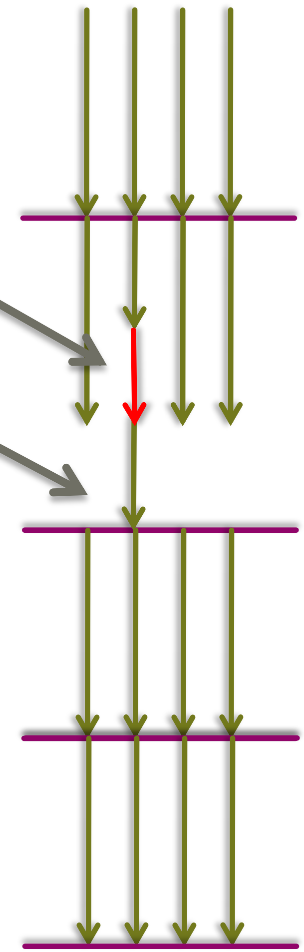
Nonblocking Collectives Overlap

- **Complex progression**
  - MPI’s global progress rule!
- **Higher CPU overhead (offloading?)**
- **Differences in asymptotic behavior**
  - Collective time often $\Omega(\log(P) + Ps)$
  - Computation $\mathcal{O}(\frac{N}{P})$
  - → Performance modeling ☺
  - One term often dominates and complicates overlap

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

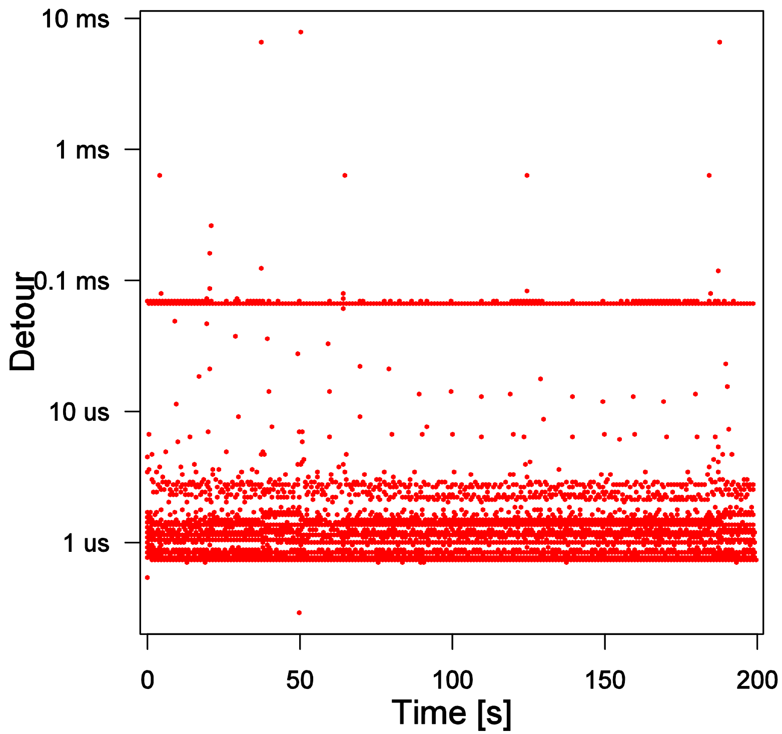
System Noise – Introduction

- **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)



TH, Schneider, Lumsadine: *Characterizing the Influence of System Noise on Large-Scale Applications by Simulation, SC10*

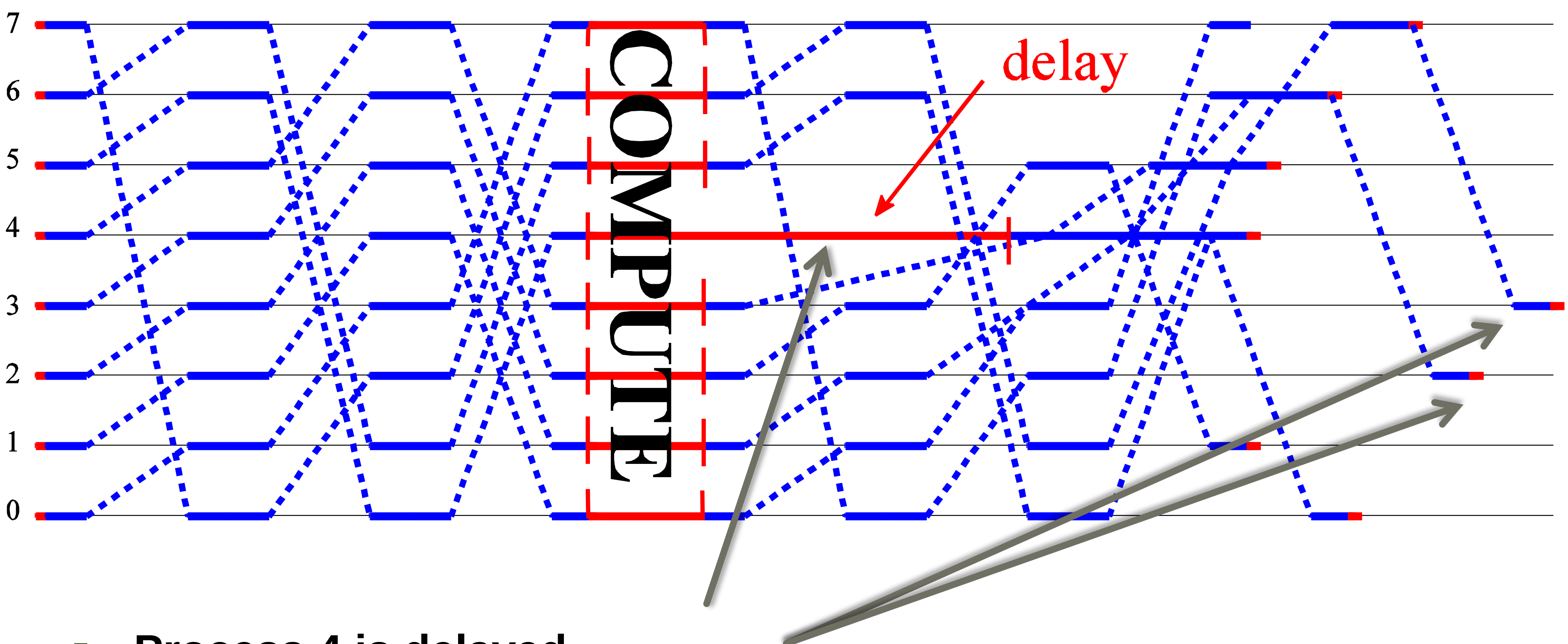
Measurement Results – Cray XE



- **Resolution: 32.9 ns, noise overhead: 0.02%**

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

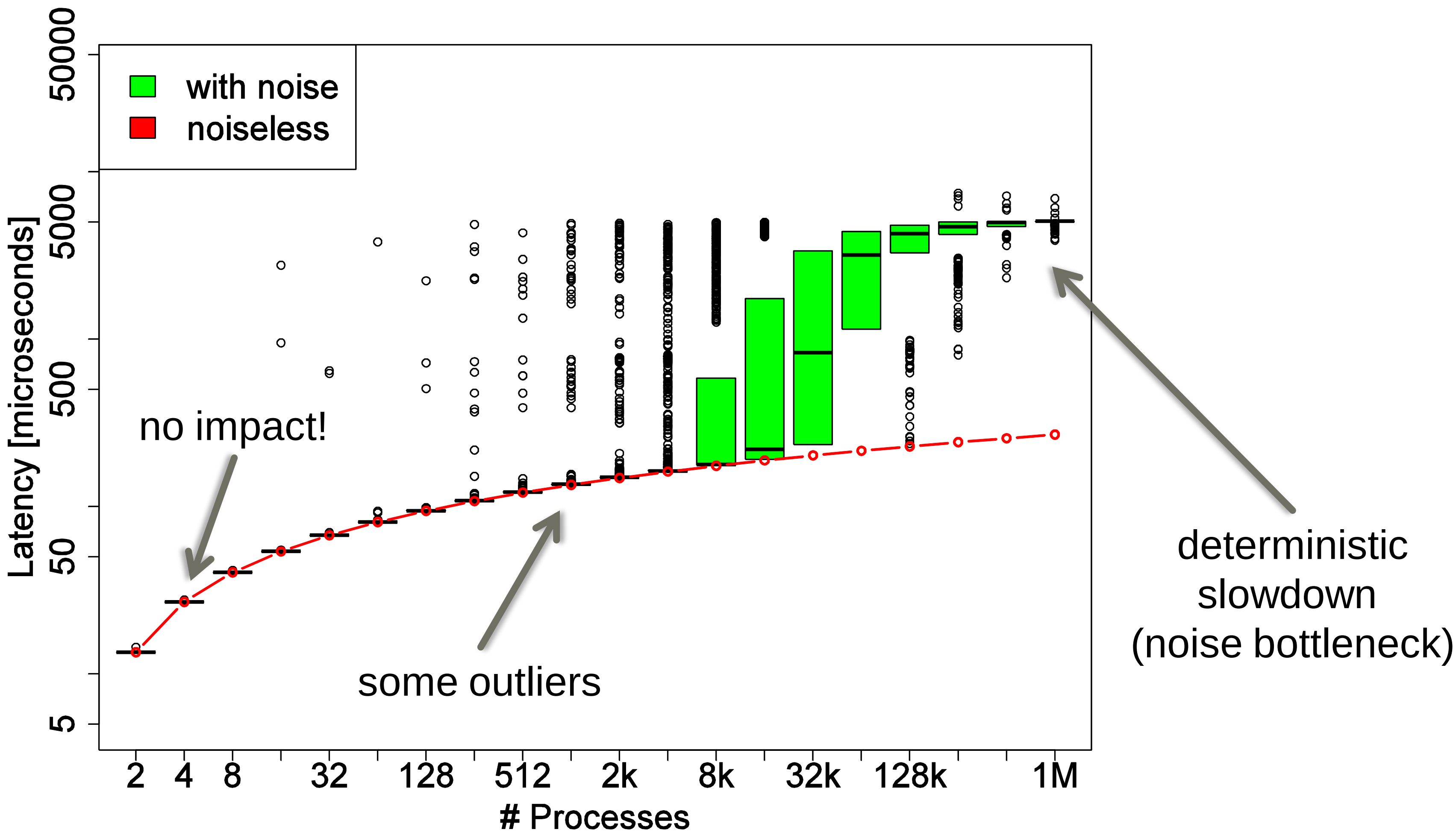
A Noisy Example – Dissemination



- **Process 4 is delayed**
  - Noise propagates "*wildly*" (of course deterministic)

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

Single Byte Dissemination on Jaguar



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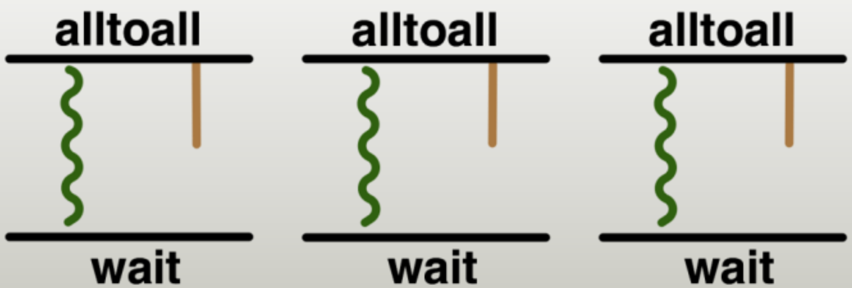
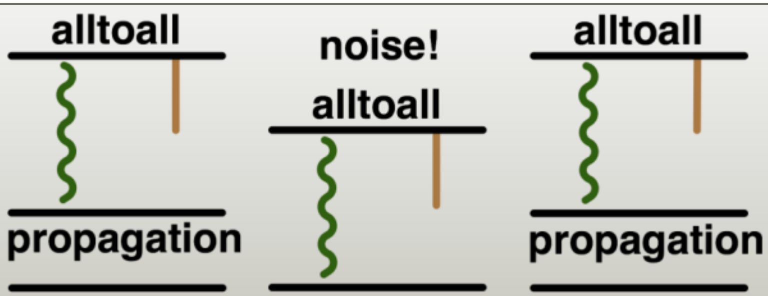
Nonblocking Collectives vs. Noise

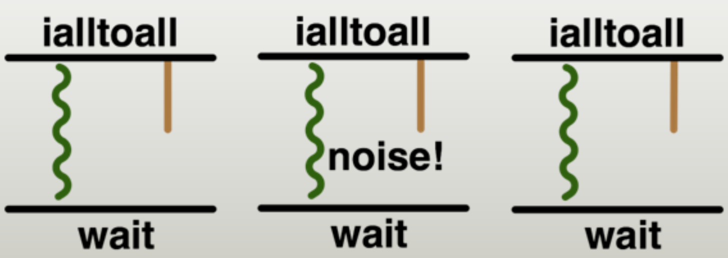
No Noise, blocking





Noise, blocking

Noise, nonblocking



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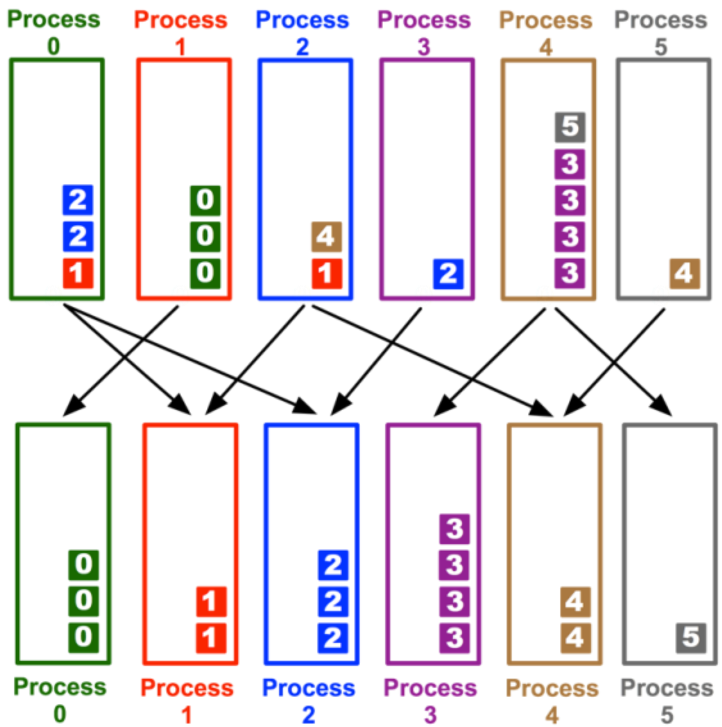
A Non-Blocking Barrier?

- **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 ($\mathcal{O}(\log P)$)
  - 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

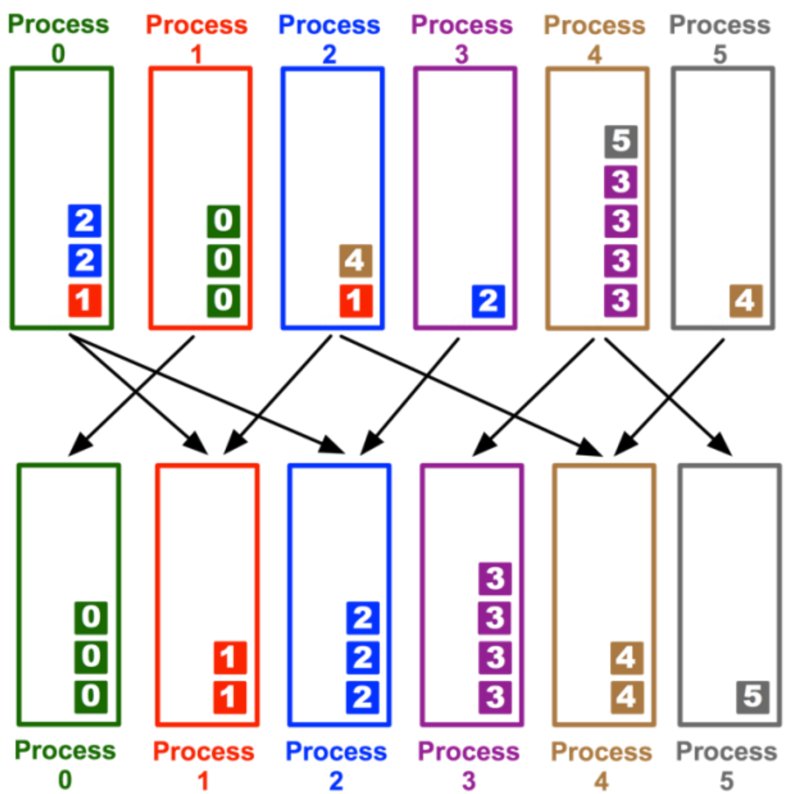
    MPI_ANY_SOURCE

    Unknown message size

    MPI_PROBE

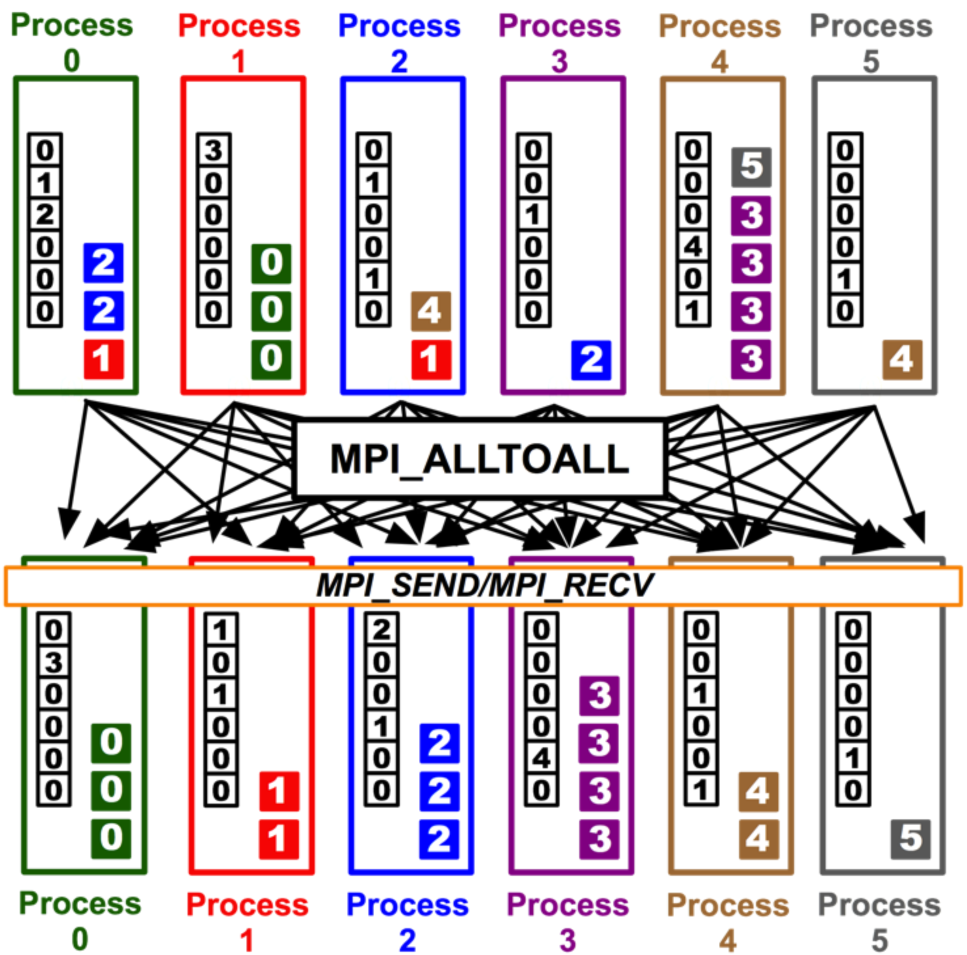
    Reduces problem to counting the number of neighbors

    Allow faster implementation!



Using Alltoall (PEX)

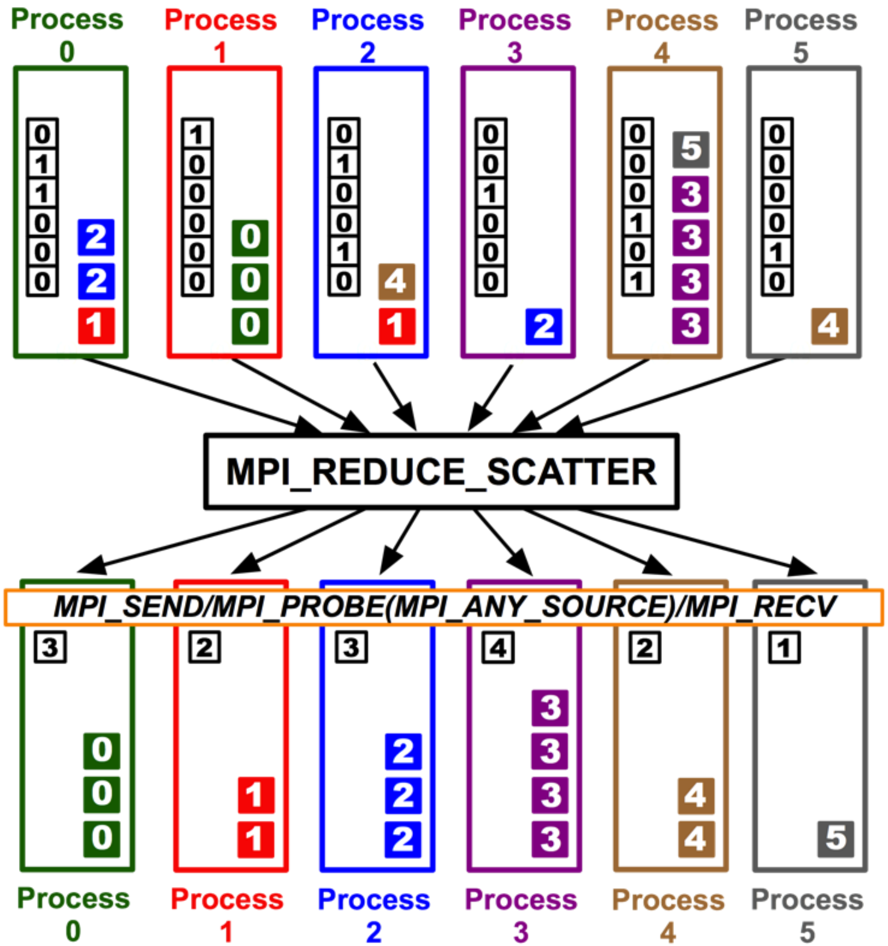
- **Based on Personalized Exchange ($\Theta(P)$)**
  - Processes exchange metadata (sizes) about neighborhoods with all-to-all
  - Processes post receives afterwards
  - Most intuitive but least performance and scalability!



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

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!

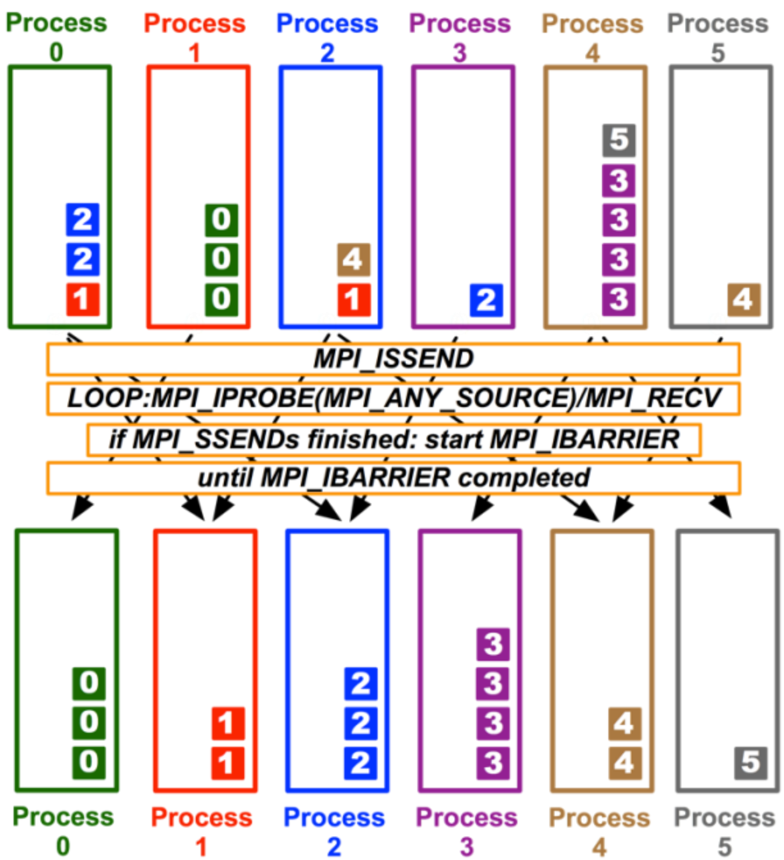


TH, Siebert, Lumsdaine: Scalable Communication Protocols for Dynamic Sparse Data Exchange, PPoPP"10

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

    barrier = distributed marker!
  - Better than PEX, PCX, RSX!



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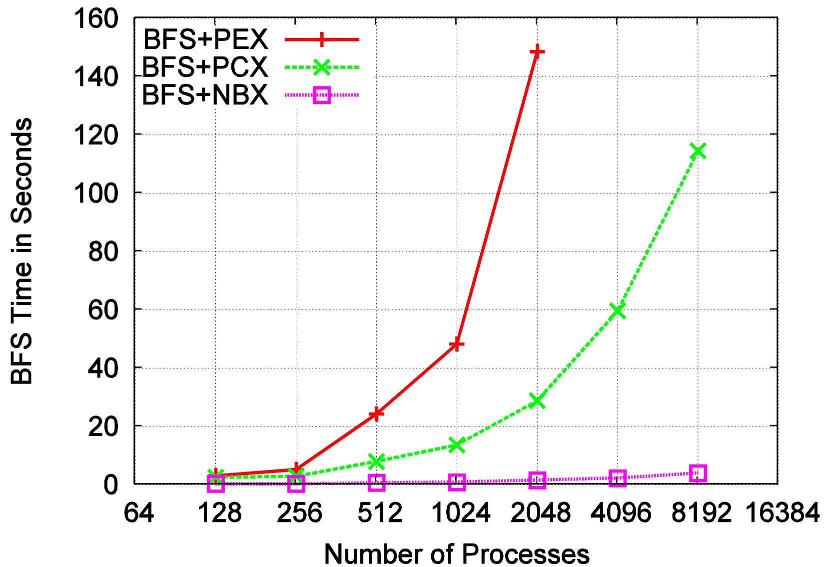
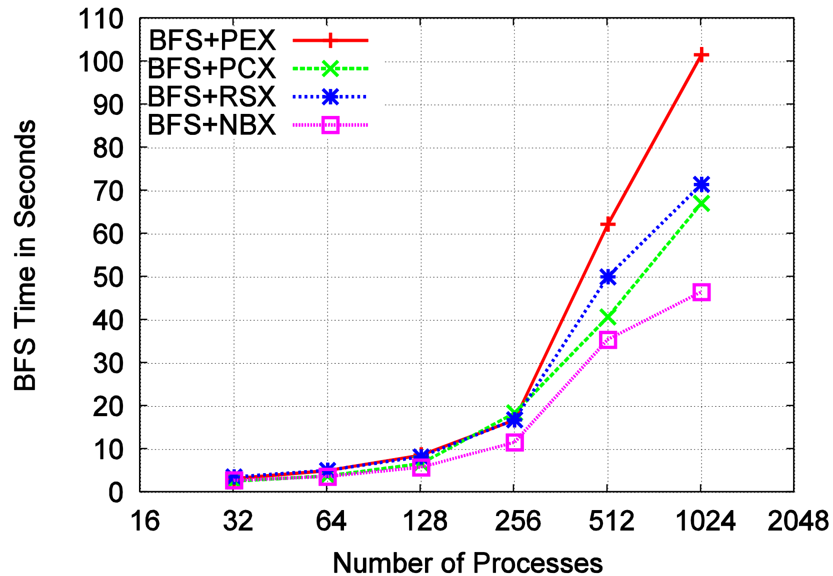
Parallel Breadth First Search

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

BlueGene/P – with HW barrier!



Myrinet 2000 with LibNBC

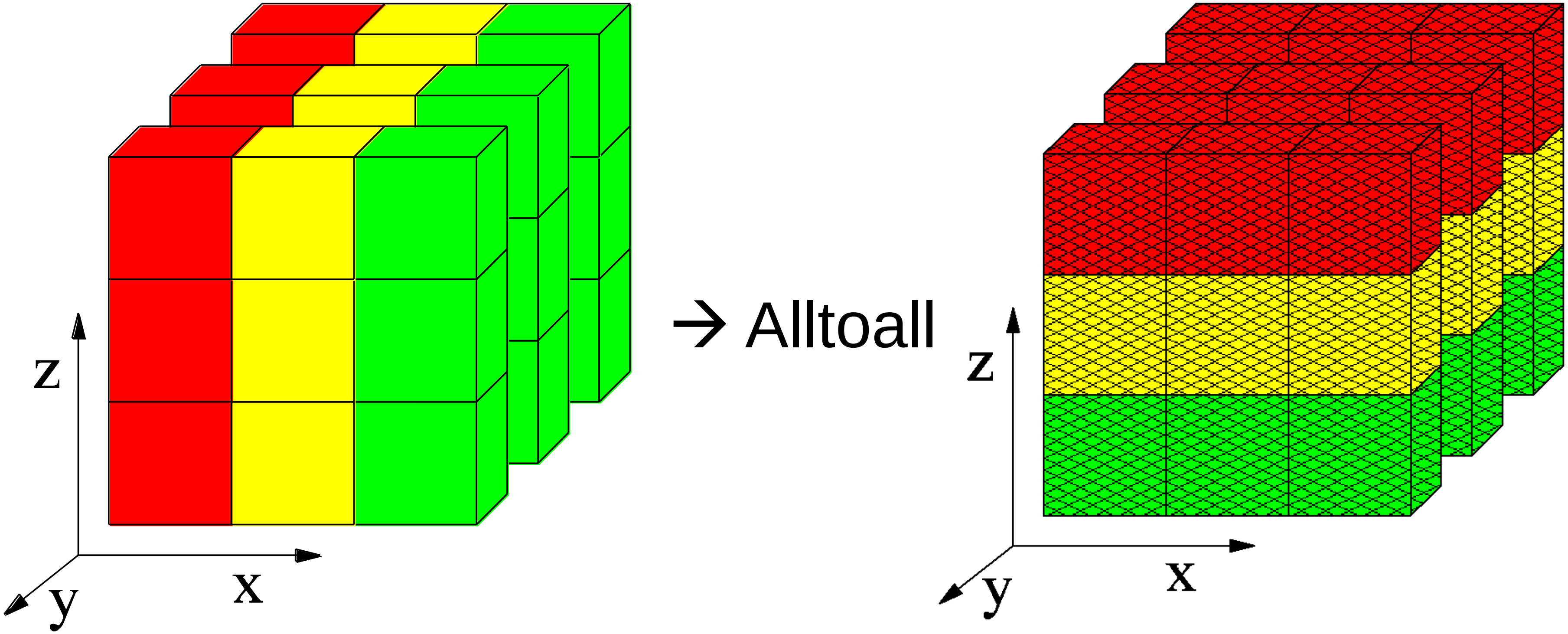


- **HW barrier support is significant at large scale!**

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 → 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

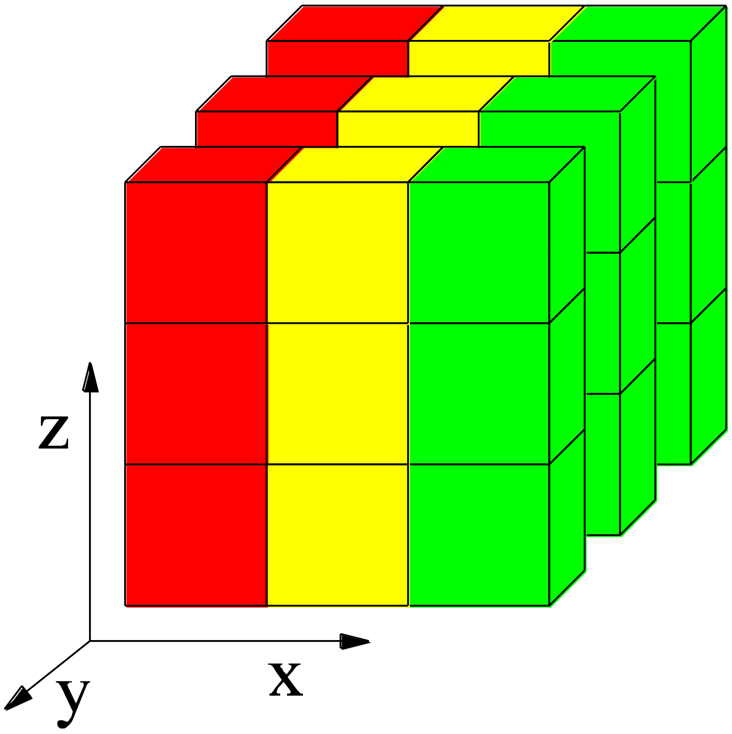
for(int y=0; y<n/p; ++y) 1d_fft(/* y-th stencil */);

// 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

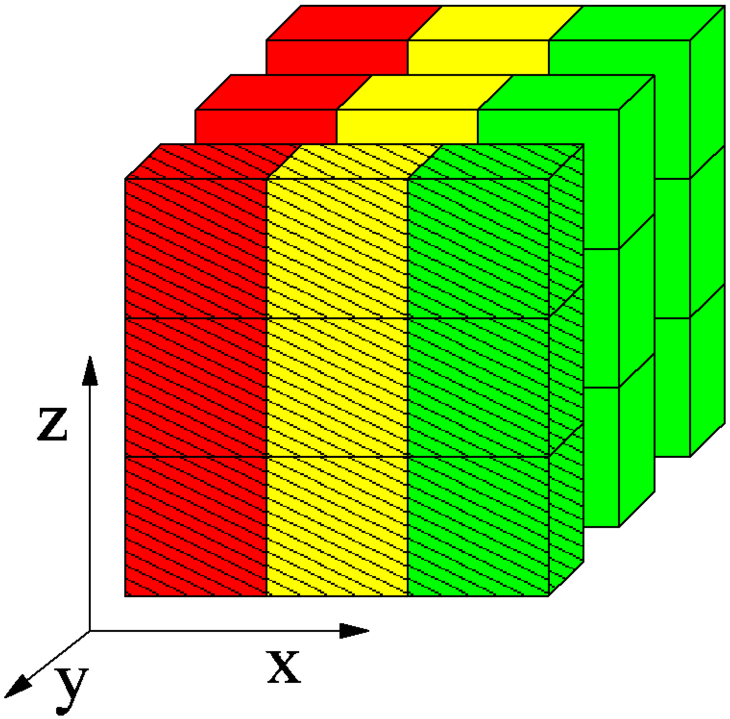
Parallel Fast Fourier Transform

- **Data already transformed in y-direction**



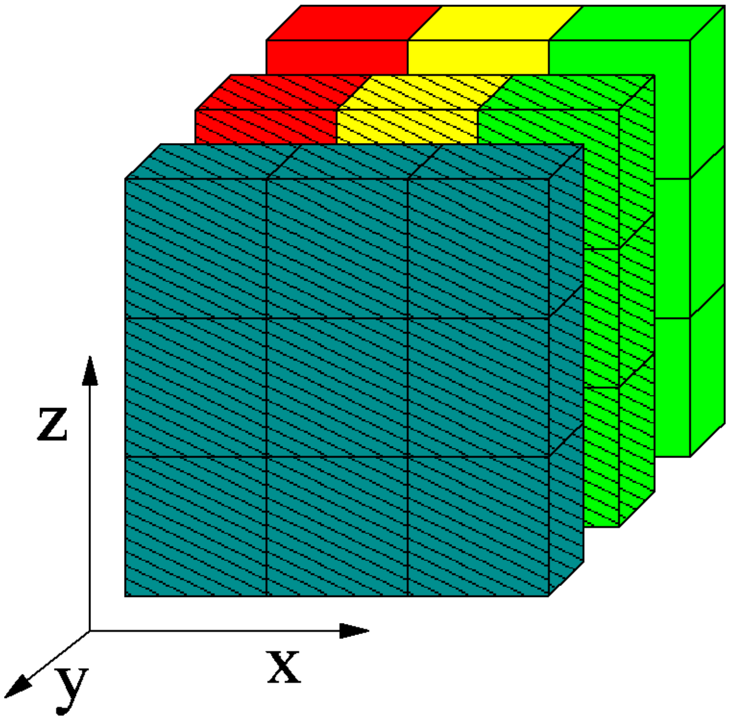
Parallel Fast Fourier Transform

- **Transform first y plane in z**



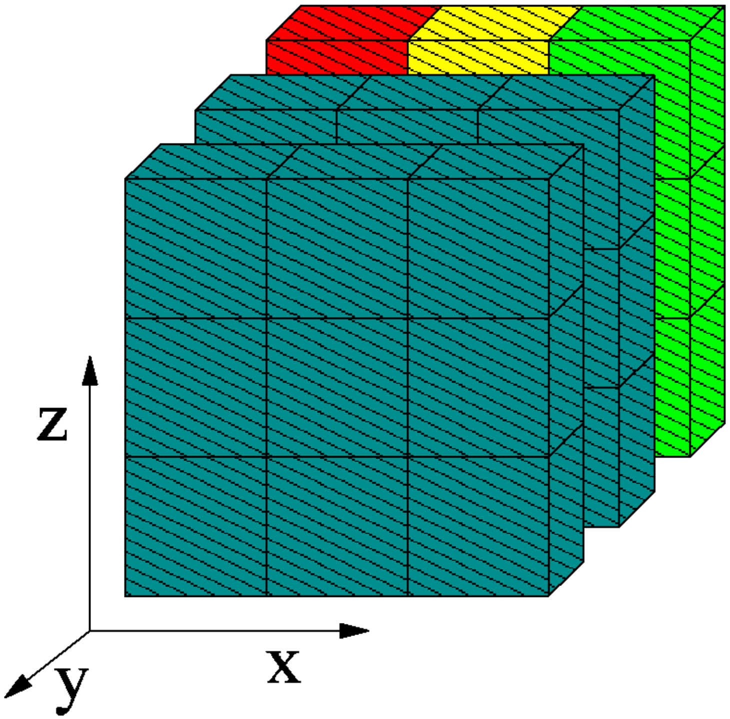
Parallel Fast Fourier Transform

- **Start ialltoall and transform second plane**



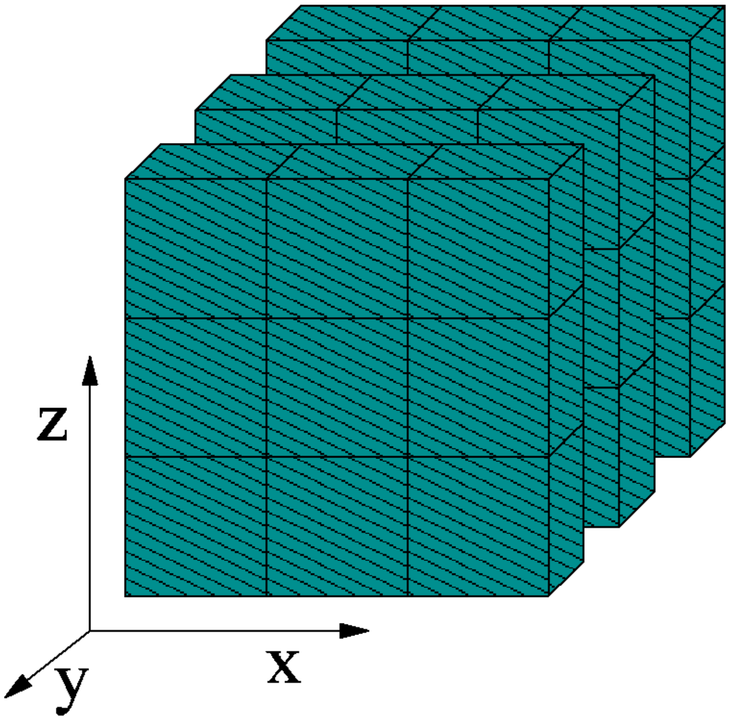
Parallel Fast Fourier Transform

- **Start ialltoall (second plane) and transform third**



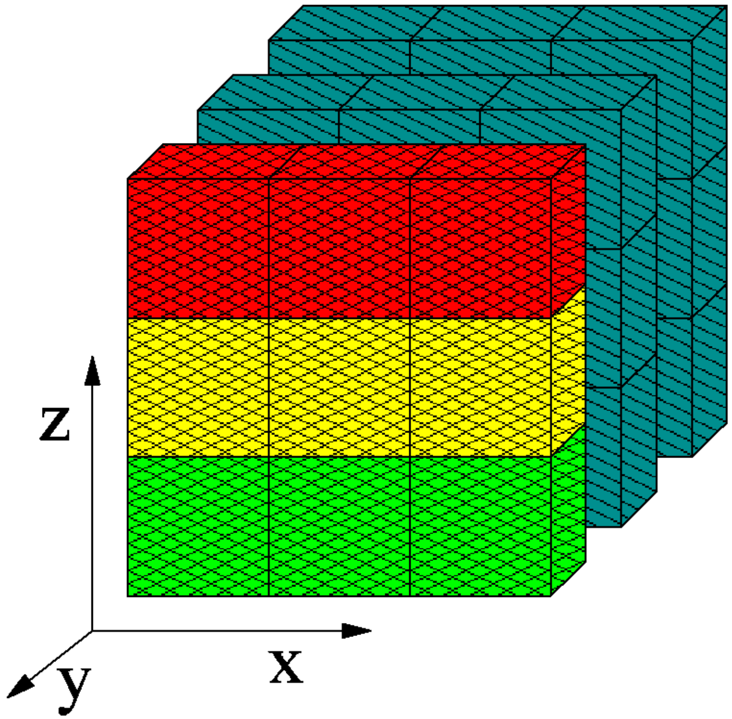
Parallel Fast Fourier Transform

- **Start ialltoall of third plane and …**



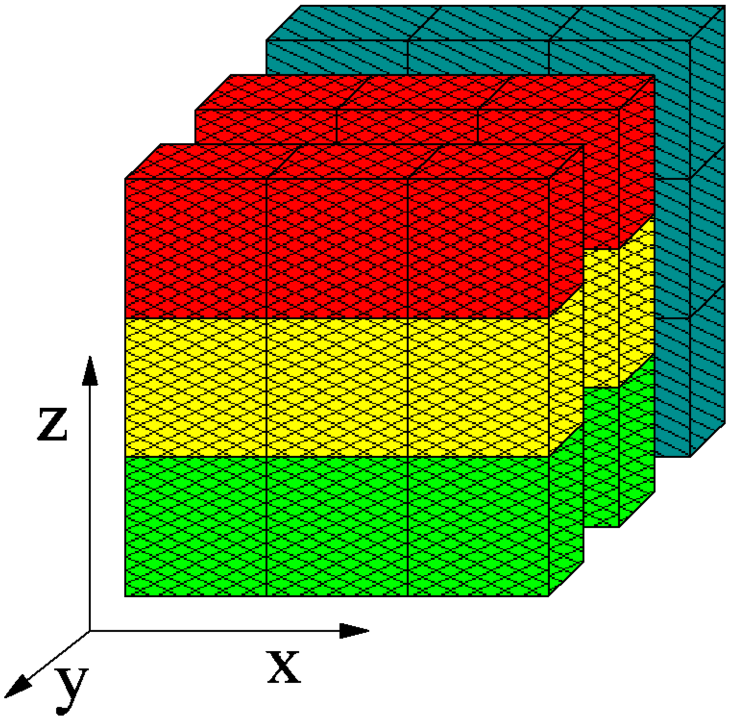
Parallel Fast Fourier Transform

- **Finish ialltoall of first plane, start x transform**



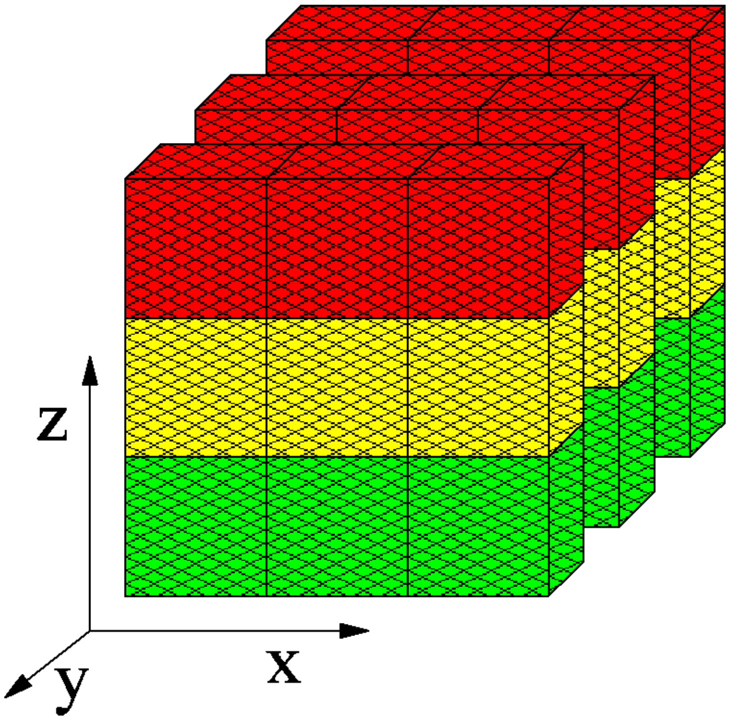
Parallel Fast Fourier Transform

- **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/bs, 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
```

TH, Gottschling, Lumsdaine: Leveraging Non-blocking Collective Communication in High-performance Applications, , SPAA'08

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

```
MPI_Win_create_dynamic(MPI_Info info, MPI_Comm comm, MPI_Win *win)
```

- **Coll. memory exposure may be cumbersome**
  - Especially for irregular applications
- **Win_create_dynamic creates a window with no memory attached**

```
MPI_Win_attach(MPI_Win win, void *base, MPI_Aint size)
MPI_Win_detach(MPI_Win win, const void *base)
```

- **Register non-overlapping regions locally**
- **Addresses are communicated for remote access!**
  - MPI_Aint will be big enough on heterogeneous systems

One Sided Communication

```
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)
```

- **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)

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

```
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)
```

- **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**

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

```
MPI_Win_lock_all(int assert, MPI_Win win)
MPI_Win_unlock_all(MPI_Win win)
```

- **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!

Synchronization Primitives (passive)

```
MPI_Win_flush(int rank, MPI_Win win)
MPI_Win_flush_all(MPI_Win win)
```

- **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_local(int rank, MPI_Win win)
MPI_Win_flush_local_all(MPI_Win win)
```

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

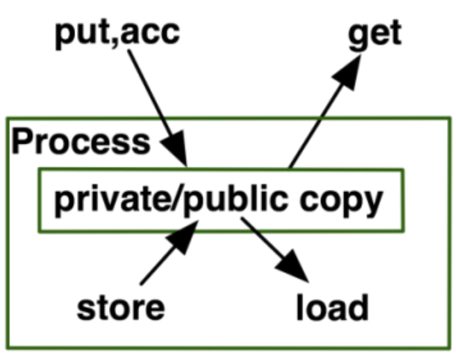
Synchronization Primitives (passive)

```
MPI_Win_sync(MPI_Win win)
```

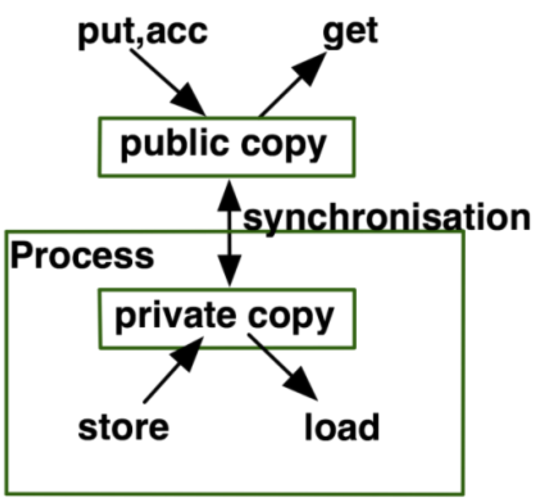
- **Synchronizes private and public window copies**
  - Same as closing and opening access and exposure epochs on the window
  - Does not complete any operations though!
- **Cf. memory barrier**

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



MPI_UNIFIED



MPI_SEPARATE

Separate Semantics

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

	Load	Store	Get	Put	Acc
Load	OVL+NOVL	OVL+NOVL	OVL+NOVL	NOVL	NOVL
Store	OVL+NOVL	OVL+NOVL	NOVL	X	X
Get	OVL+NOVL	NOVL	OVL+NOVL	NOVL	NOVL
Put	NOVL	X	NOVL	NOVL	NOVL
Acc	NOVL	X	NOVL	NOVL	OVL+NOVL

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

Credits: RMA Working Group, MPI Forum

Unified Semantics

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

	Load	Store	Get	Put	Acc
Load	OVL+NOVL	OVL+NOVL	OVL+NOVL	NOVL+BOVL	NOVL+BOVL
Store	OVL+NOVL	OVL+NOVL	NOVL	NOVL	NOVL
Get	OVL+NOVL	NOVL	OVL+NOVL	NOVL	NOVL
Put	NOVL+BOVL	NOVL	NOVL	NOVL	NOVL
Acc	NOVL+BOVL	NOVL	NOVL	NOVL	OVL+NOVL

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

Credits: RMA Working Group, MPI Forum

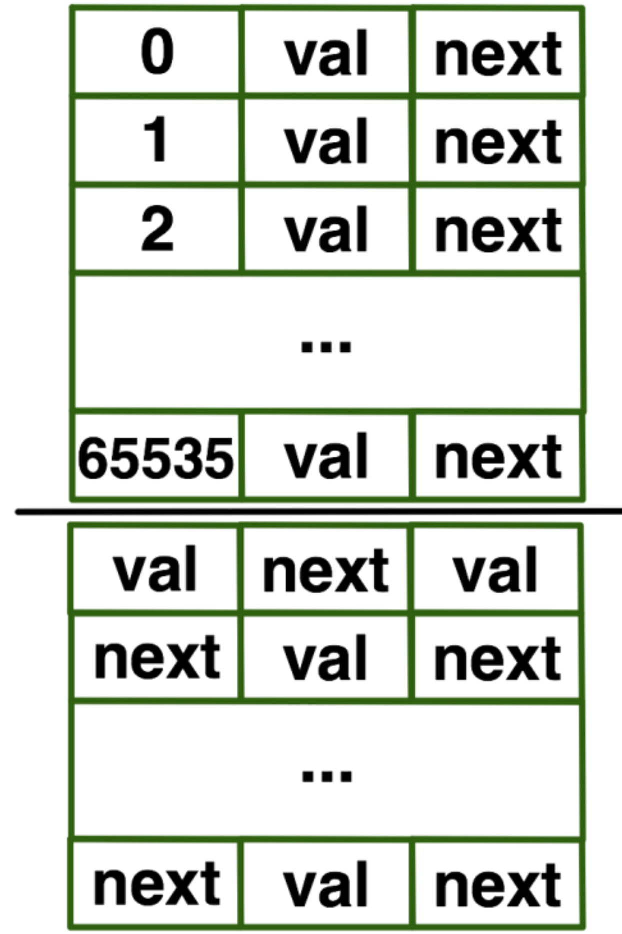
Stencil One-Sided Example

- **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



Distributed Hashtable Example

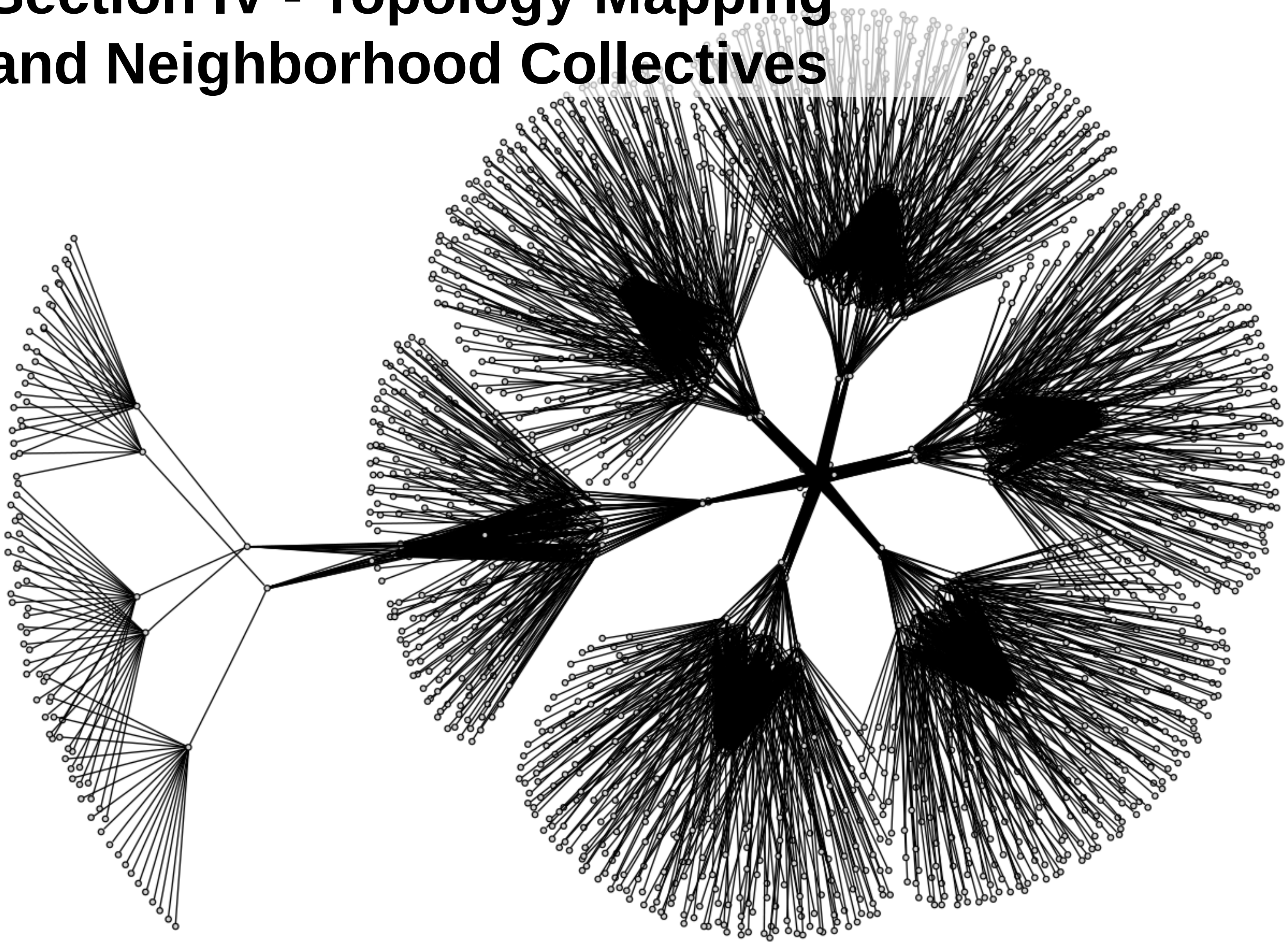
```
int insert(t_hash *hash, int elem) {
  int pos = hashfunc(elem);
  if(hash->table[pos].value == -1) { // direct value in table
    hash->table[pos].value = elem;
  } else { // put on heap
    int newelem=hash->nextfree++; // next free element
    if(hash->table[pos].next == -1) { // first heap element
      // 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

```
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

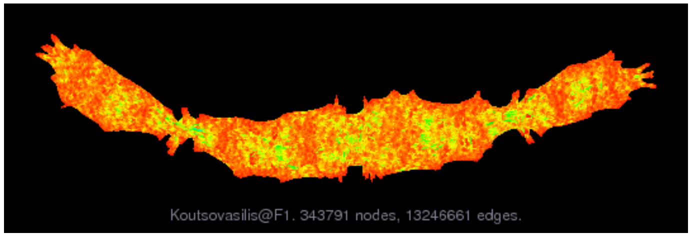
Topology Mapping Basics

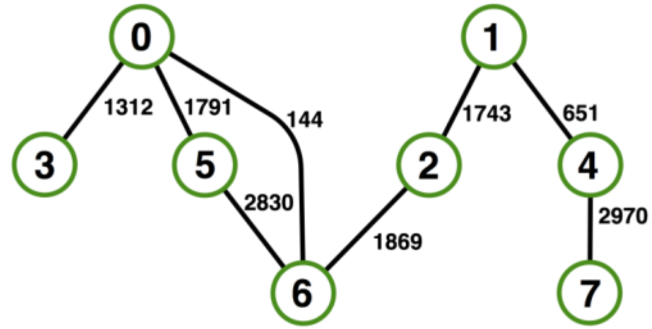
- **First type: Allocation mapping**
  - Up-front specification of communication pattern
  - Batch system picks good set of nodes for given topology
- **Properties:**
  - Not supported by current batch systems
  - Either predefined allocation (BG/P), random allocation, or “global bandwidth maximation”
  - Also problematic to specify communication pattern upfront, not always possible (or static)

Topology Mapping Basics

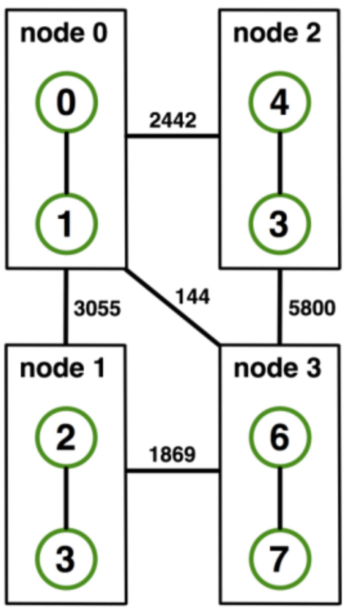
- **Rank reordering**
  - Change numbering in a given allocation to reduce congestion or dilation
  - Sometimes automatic (early IBM SP machines)
- **Properties**
  - Always possible, but effect may be limited (e.g., in a bad allocation)
  - Portable way: MPI process topologies
    Network topology is not exposed
  - Manual data shuffling after remapping step

On-Node Reordering



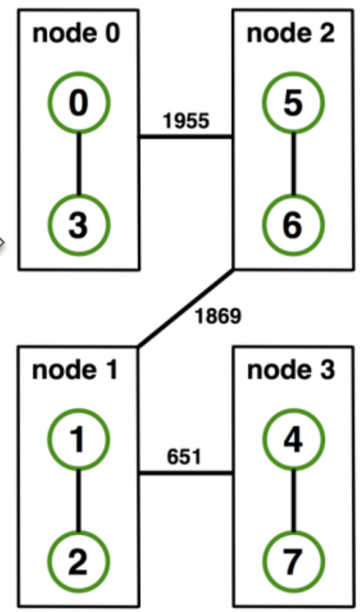


Naïve Mapping



Topomap

Optimized Mapping



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

```
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 <= 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

```
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

```
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

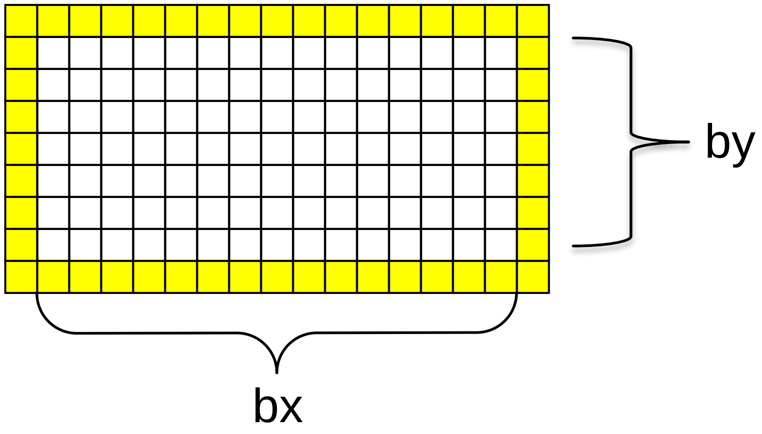
Cartesian Communication Helpers

```
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

```
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const int *edges, int reorder, MPI_Comm *comm_graph)
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  - 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

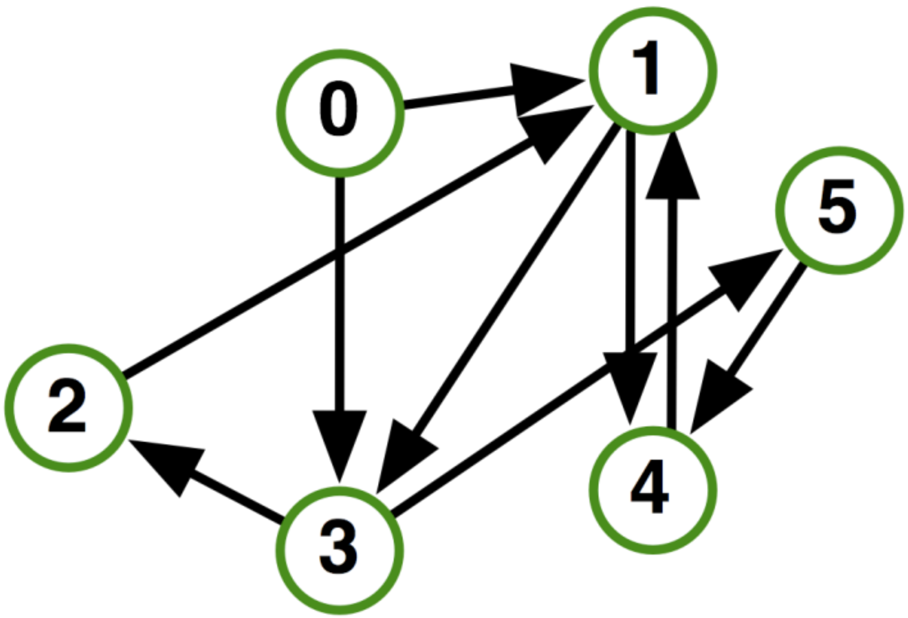
MPI_Dist_graph_create_adjacent

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)

- **indegree, sources, ~weights – source proc. Spec.**
- **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)
```

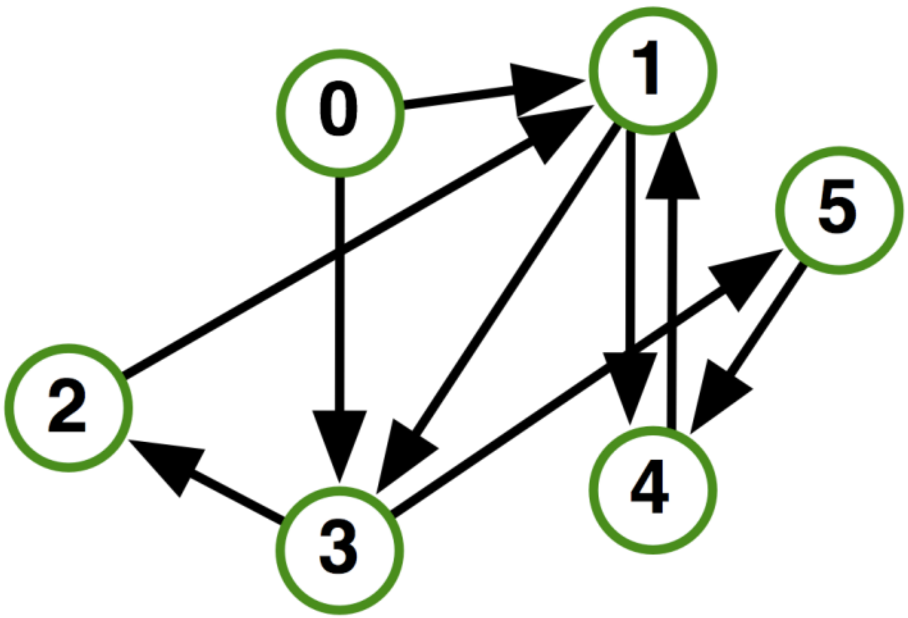
n – number of source nodes

- **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

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

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**

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

Further Graph Queries

MPI_Topo_test(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!**

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

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

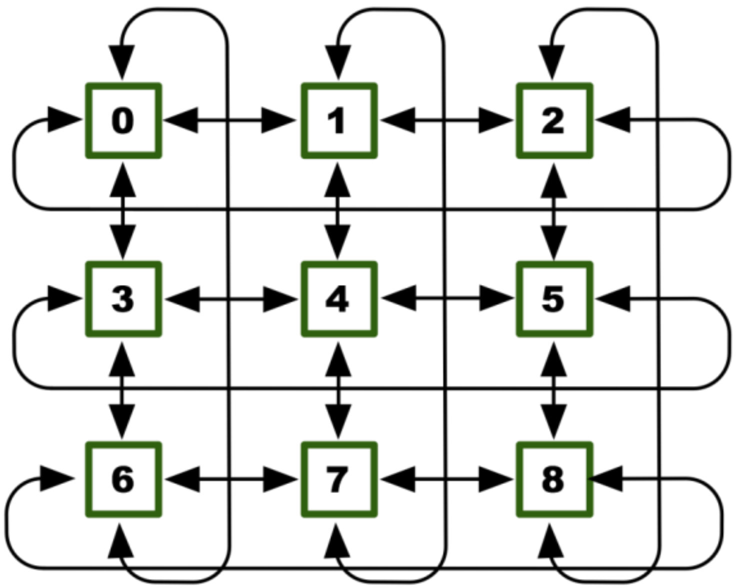
    *2*ndims sources and destinations*

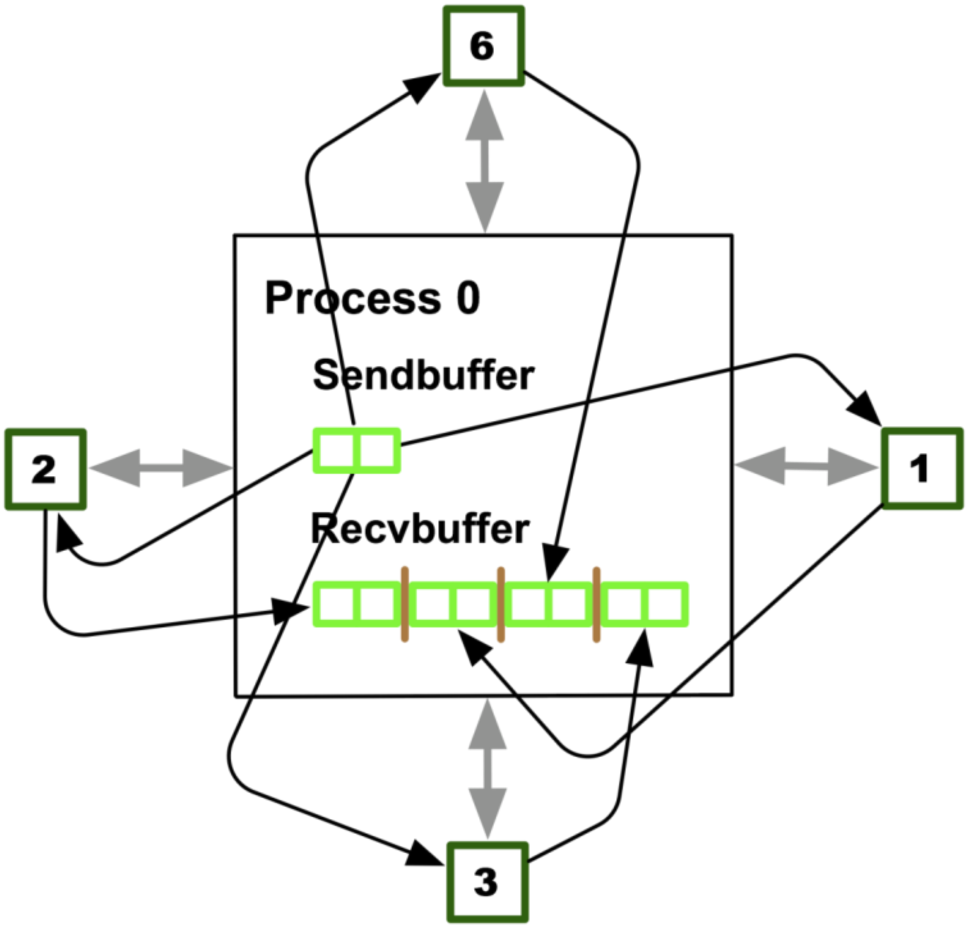
    Processes at borders (MPI_PROC_NULL) leave holes in buffers (will not be updated or communicated)!

TH and J. L. Traeff: Sparse Collective Operations for MPI, HIPS'09

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!

TH and J. L. Traeff: Sparse Collective Operations for MPI, HIPS'09

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

```
MPI_Ineighbor_allgather(…, MPI_Request *req); MPI_Ineighbor_alltoall(…,
MPI_Request *req);
```

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

Walkthrough of 2D Stencil Code with Neighborhood Collectives

- **stencil_mpi_carttopo_neighcolls.cpp**

Why is Neighborhood Reduce Missing?

```
MPI_Ineighbor_allreducev(…);
```

- **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

TH and J. L. Traeff: Sparse Collective Operations for MPI, HIPS'09

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)**

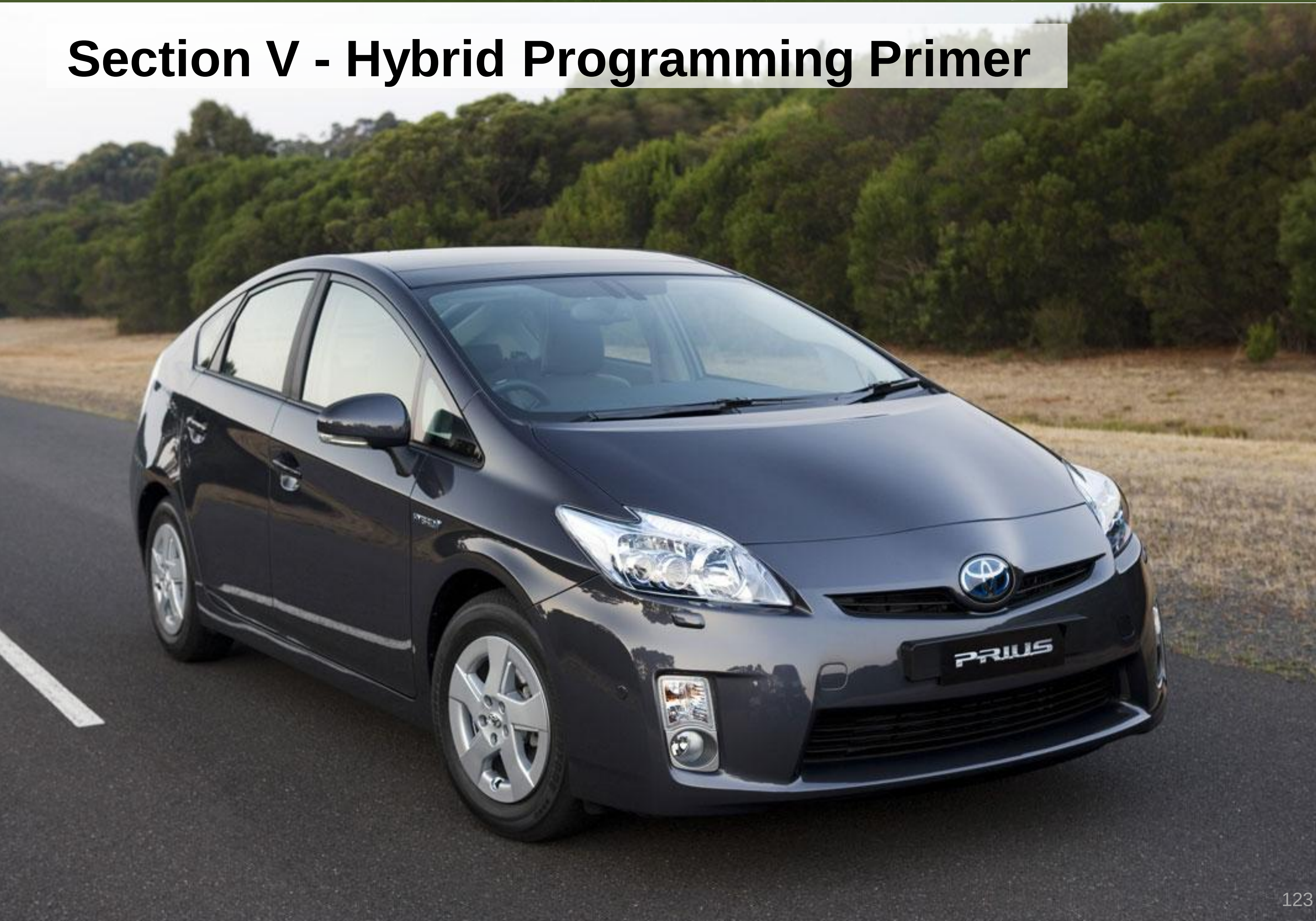
Neighborhood Collectives Summary

- **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

```
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

J. Dinan et al.: Noncollective Communicator Creation in MPI, EuroMPI'11
T. Hoefler: Writing Parallel Libraries with MPI - Common Practice, Issues, and Extensions, Keynote, IMUDI'11

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

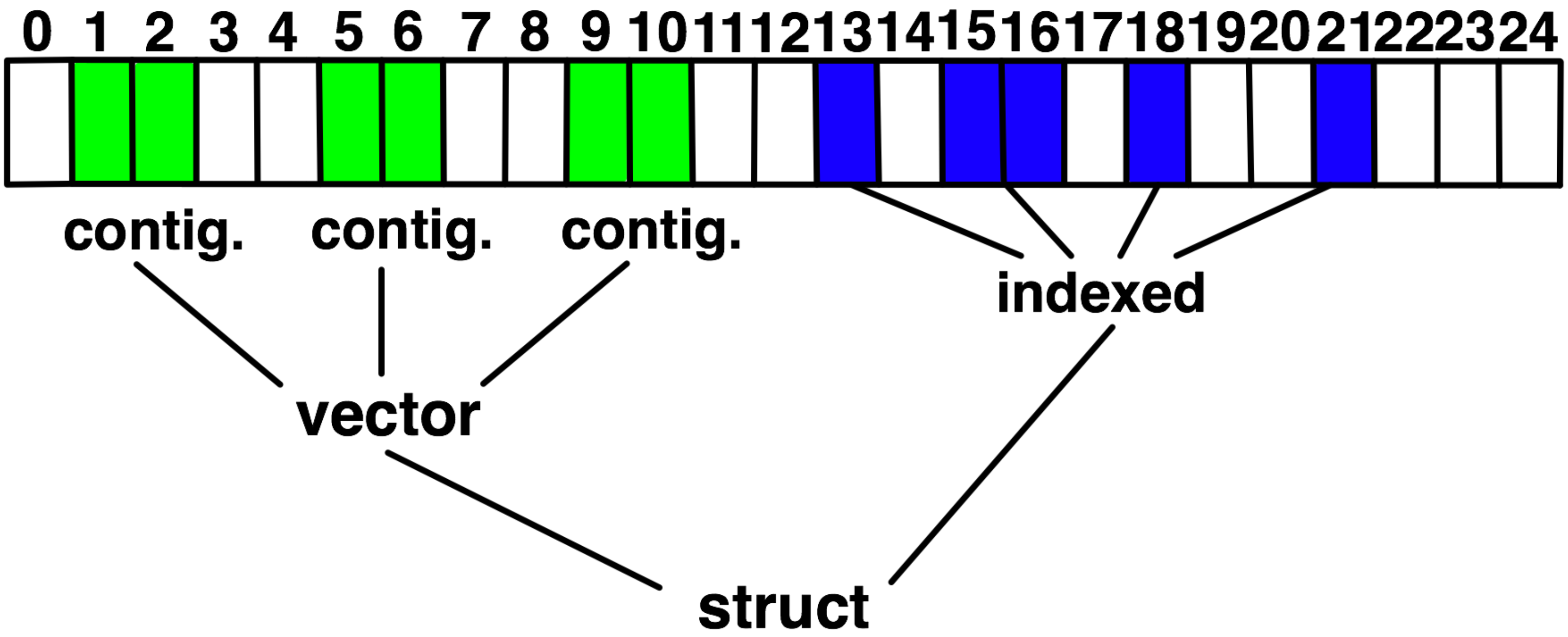
- **Datatypes allow to (de)serialize arbitrary data layouts into a message stream**
  - Networks provide serial channels
  - Same for block devices and I/O
- **Several constructors allow arbitrary layouts**
  - Recursive specification possible
  - *Declarative* specification of data-layout

    "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

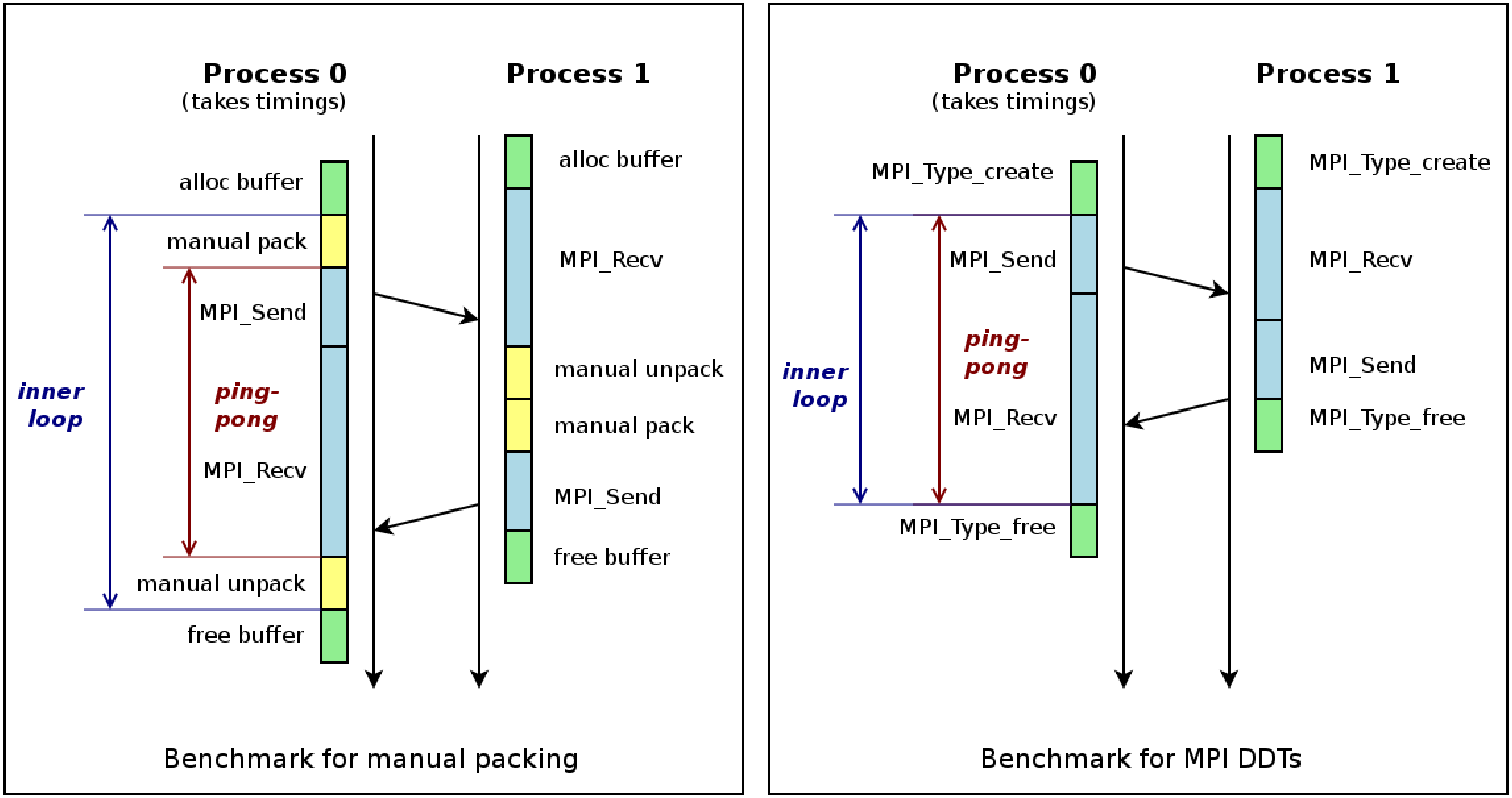
    E.g., manual pack, unpack or data rearrangement

    DDT can do both!

Purpose of this Section

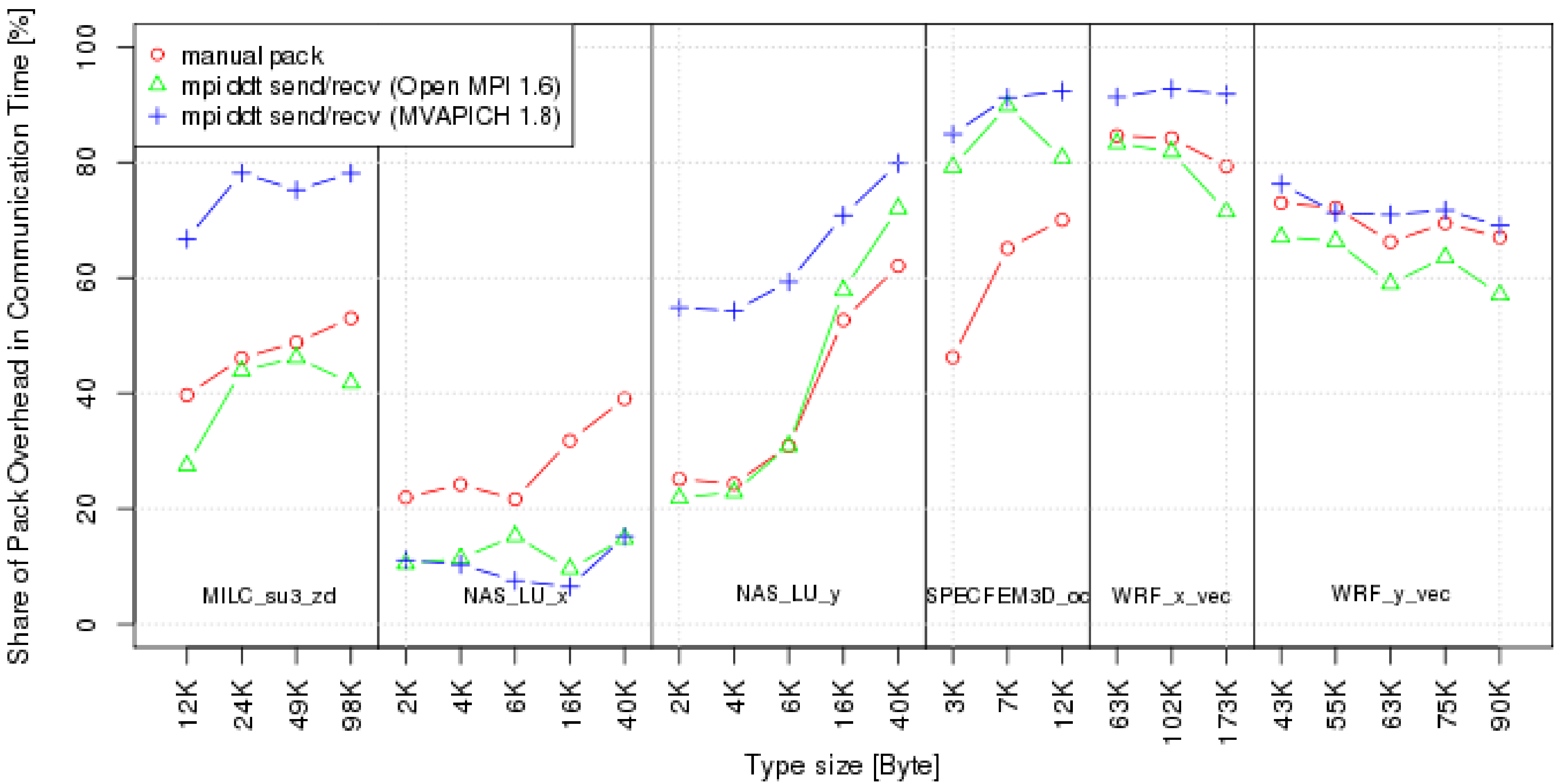
- **Demonstrate utility of DDT in practice**
  - Early implementations were bad → folklore
  - Some are still bad → chicken egg problem
- **Show creative use of DDTs**
  - Encode local transpose for FFT
  - Enable you to create more!
- **Gather input on realistic benchmark cases**
  - Guide optimization of DDT implementations

A new Way of Benchmarking



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

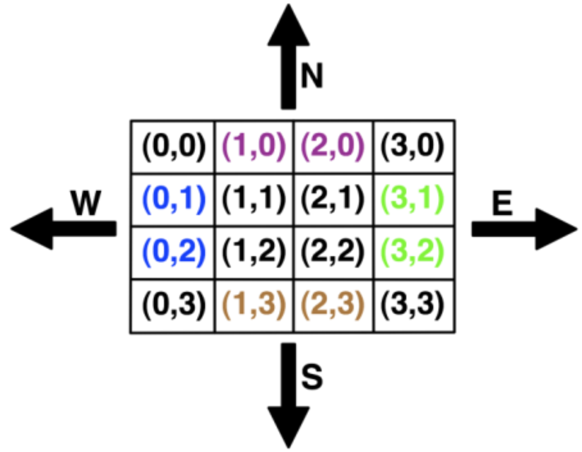
Motivation

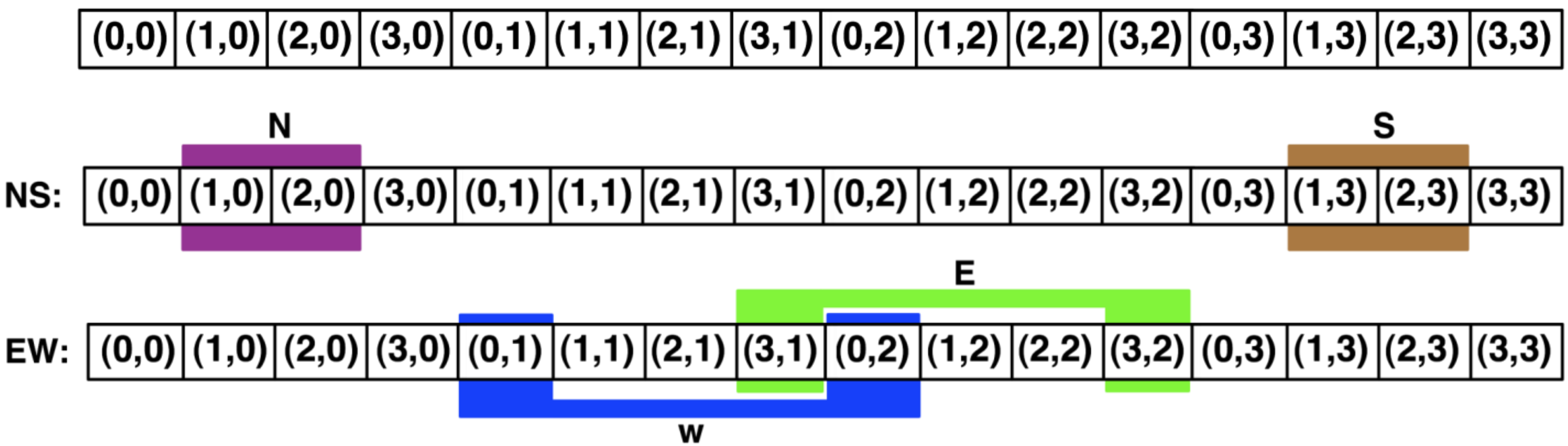


Schneider, Gerstenberger, TH: Micro-Applications for Communication Data Access Patterns, EuroMPI'13

Datatypes for the Stencil

- **stencil_mpi_ddt.cpp**





MPI's Intrinsic Datatypes

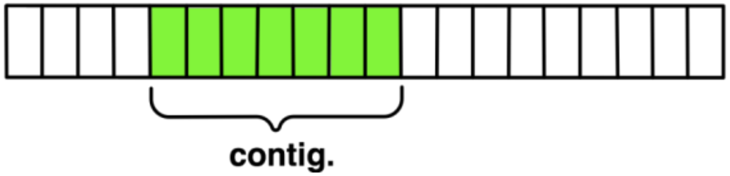
- **Why intrinsic types?**
  - Heterogeneity, nice to send a Boolean from C to Fortran
  - Conversion rules are complex, not discussed here
  - Length matches to language types

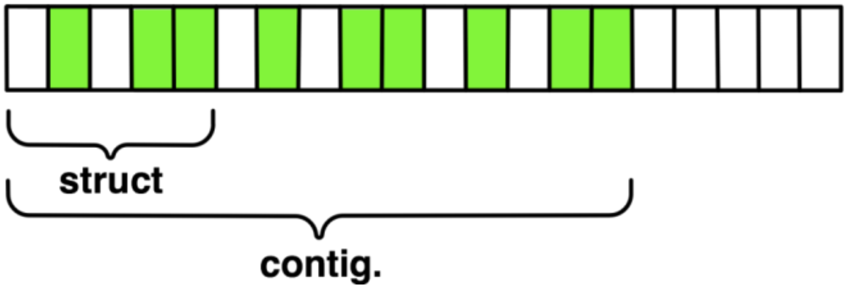
    Avoid sizeof(int) mess
- **Users should generally use intrinsic types as basic types for communication and type construction!**
  - MPI_BYTE should be avoided at all cost
- **MPI-2.2 adds some missing C types**
  - E.g., unsigned long long

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)**

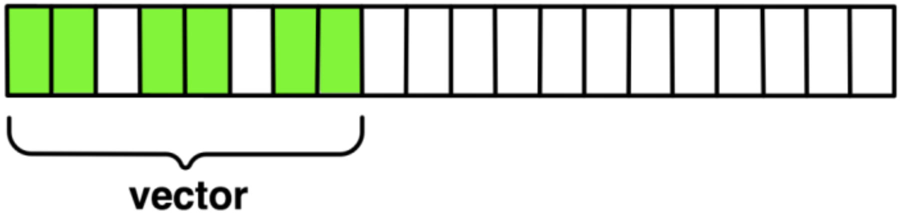


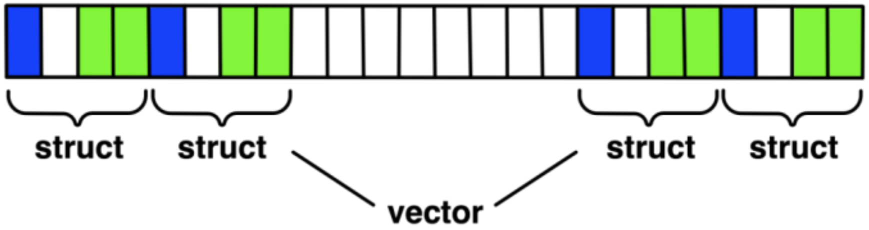


MPI_Type_vector

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**

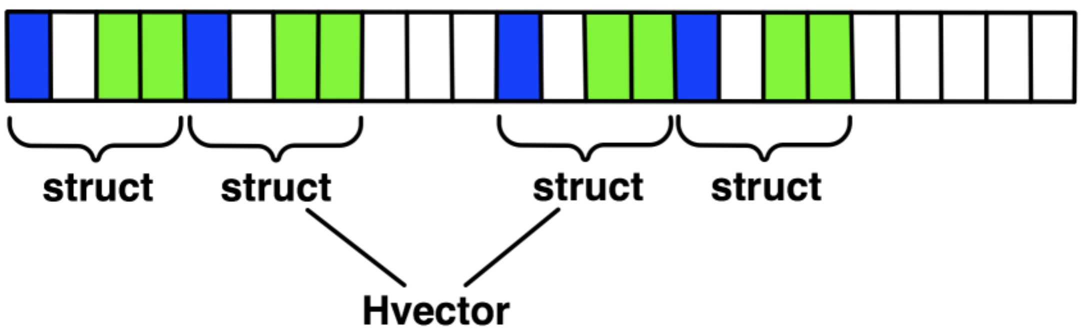




MPI_Type_create_hvector

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)
```

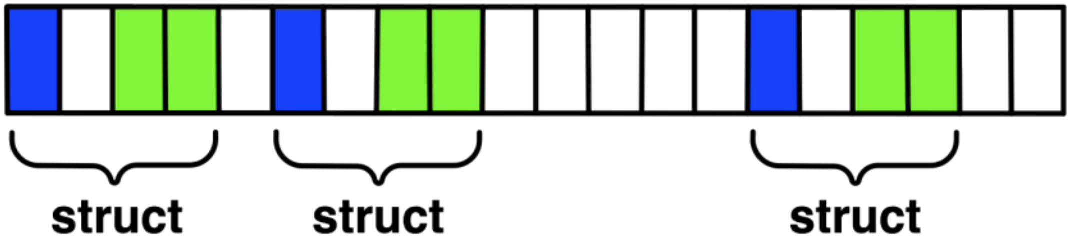
- **Pulling irregular subsets of data from a single array (cf. vector collectives)**
  - dynamic codes with index lists, expensive though!

  - 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**



MPI_Type_create_indexed_block

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

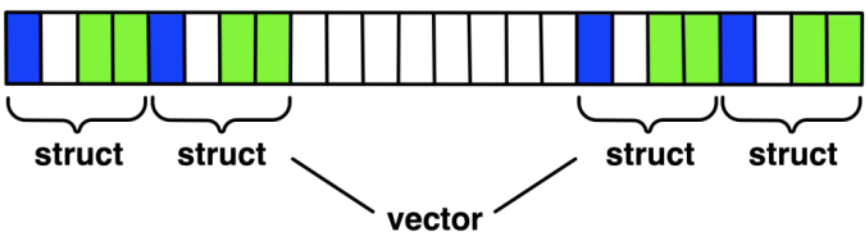
- **Like Create_indexed but blocklength is the same**

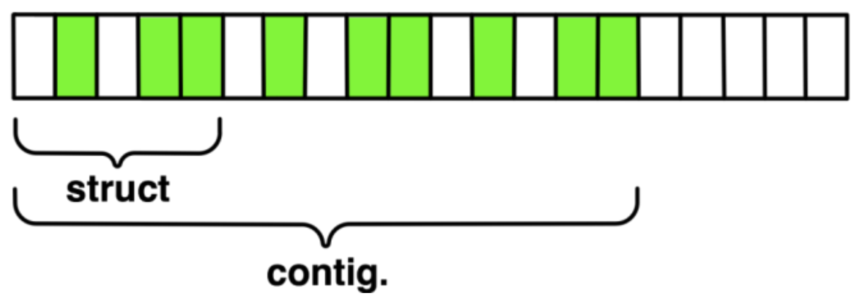
  - blen=2
  - displs={0,5,9,13,18}

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)**

(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_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)
```

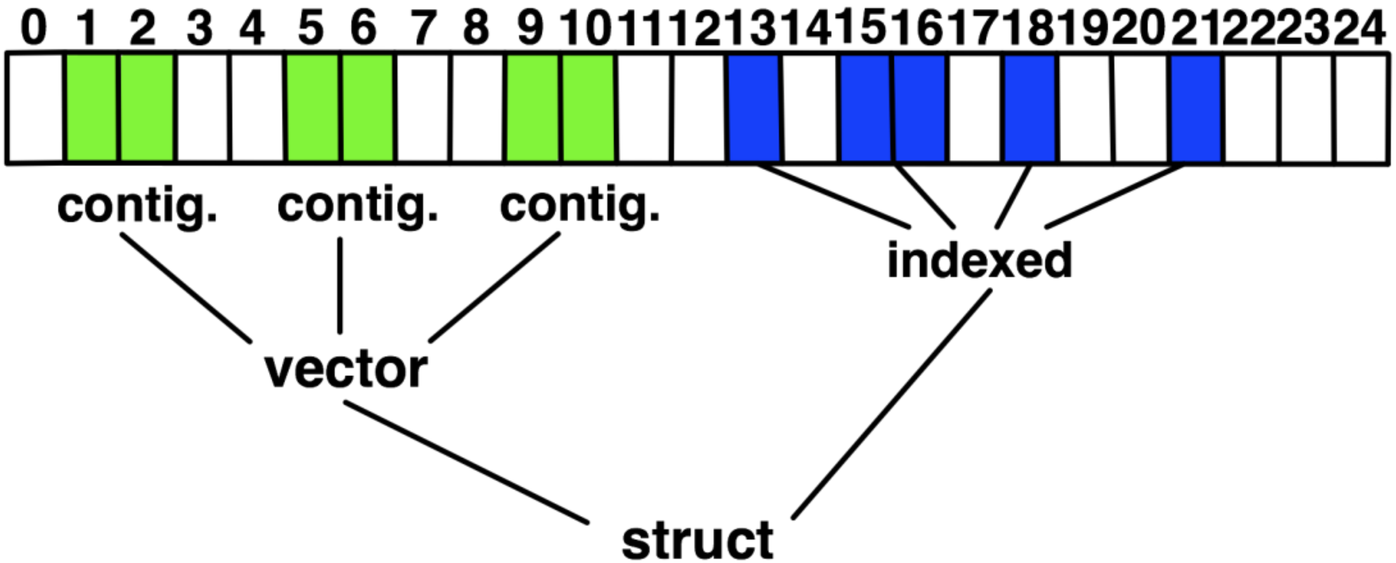
- **Create distributed array, supports block, cyclic and no distribution for each dimension**
  - Very useful for I/O

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 comitted 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)

1: http://www.mcs.anl.gov/mpitypes/

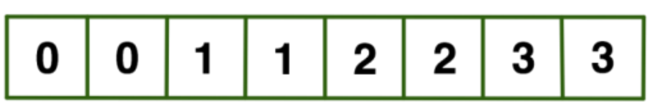
Datatype Selection Tree

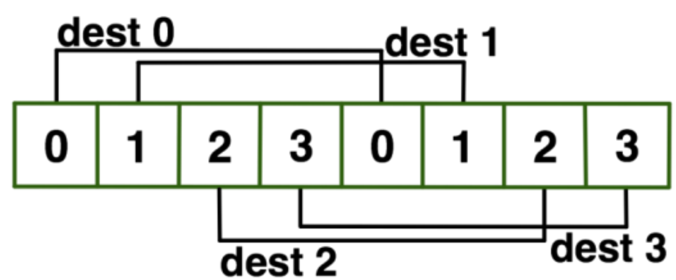
- **Simple and effective performance model:**
  - More parameters == slower
- **contig < vector < index_block < index < struct**
- **Some (most) MPIs are inconsistent**
  - But this rule is portable
- **Advice to users:**
  - Try datatype “compression” bottom-up

W. Gropp et al.:Performance Expectations and Guidelines for MPI Derived Datatypes, EuroMPI’12

Datatypes and Collectives

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



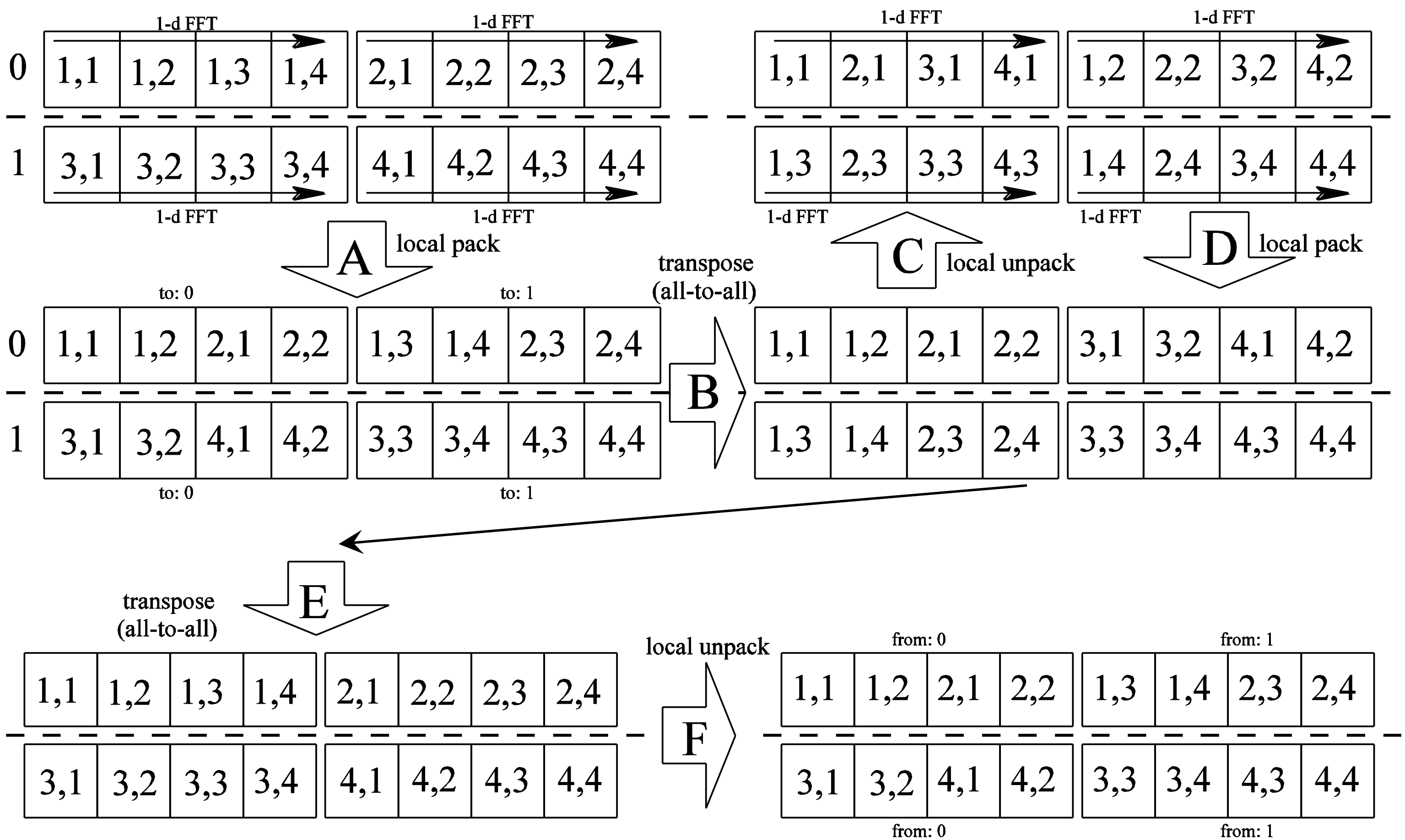


A Complex Example - FFT

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)

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

A Complex Example - FFT



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

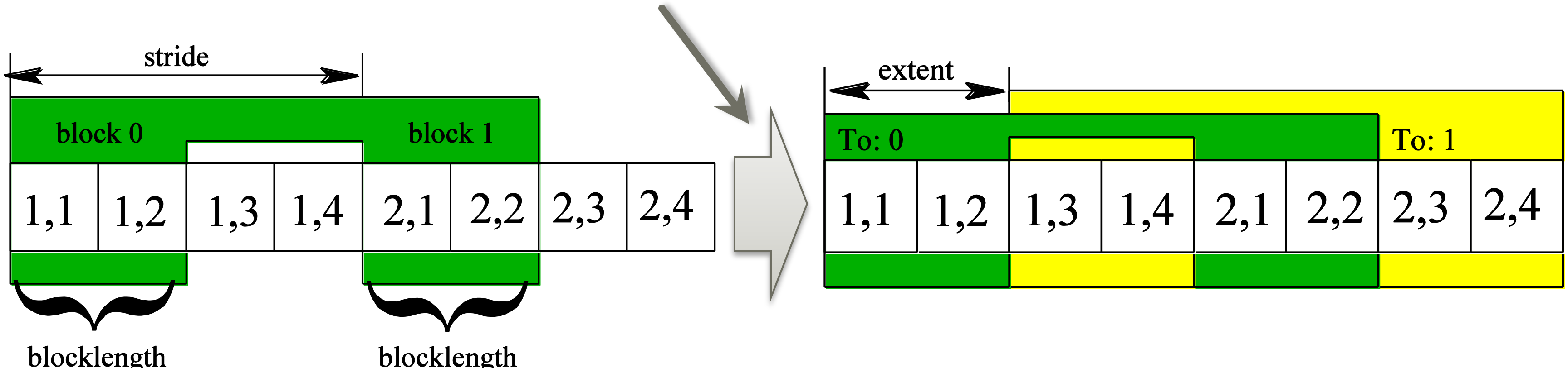
     Eliminate local transpose

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

The Send Datatype

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

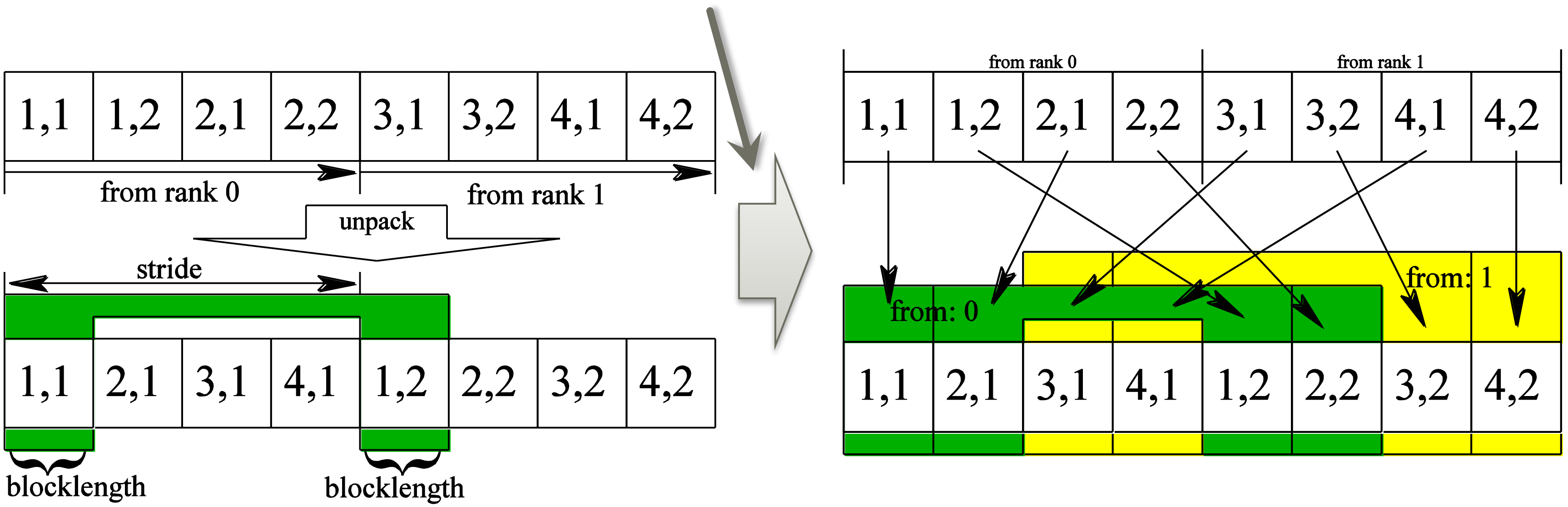
Need to change extent to allow overlap (create_resized)



- Three hierarchy-layers

The Receive Datatype

- Type_struct (complex)
- Type_vector (no contiguous, local transpose)
  Needs to change extent (create_resized)

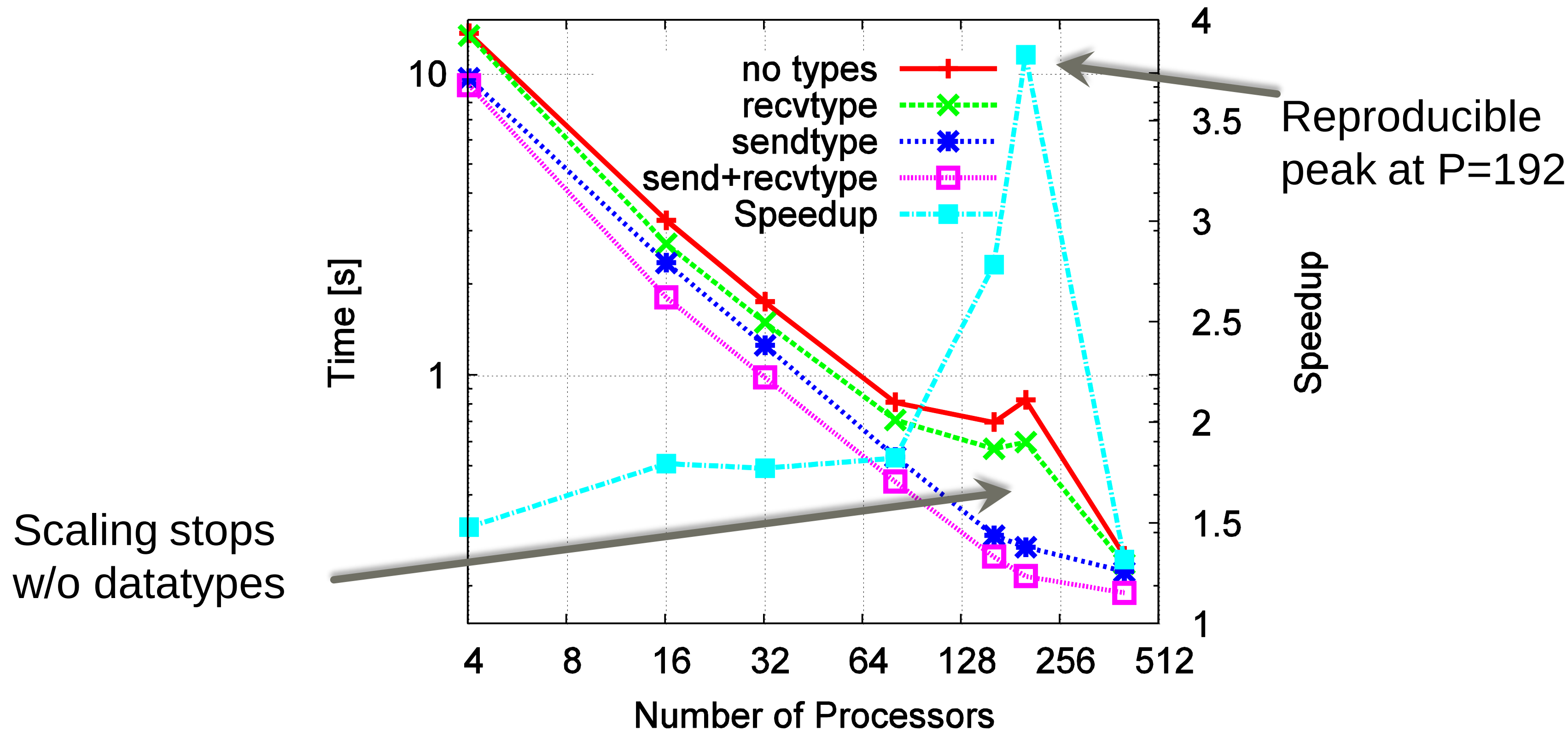


TH, Gottlieb: Parallel Zero-Copy Algorithms for Fast Fourier Transform and Conjugate Gradient using MPI Datatypes, EuroMPI'12

Experimental Evaluation

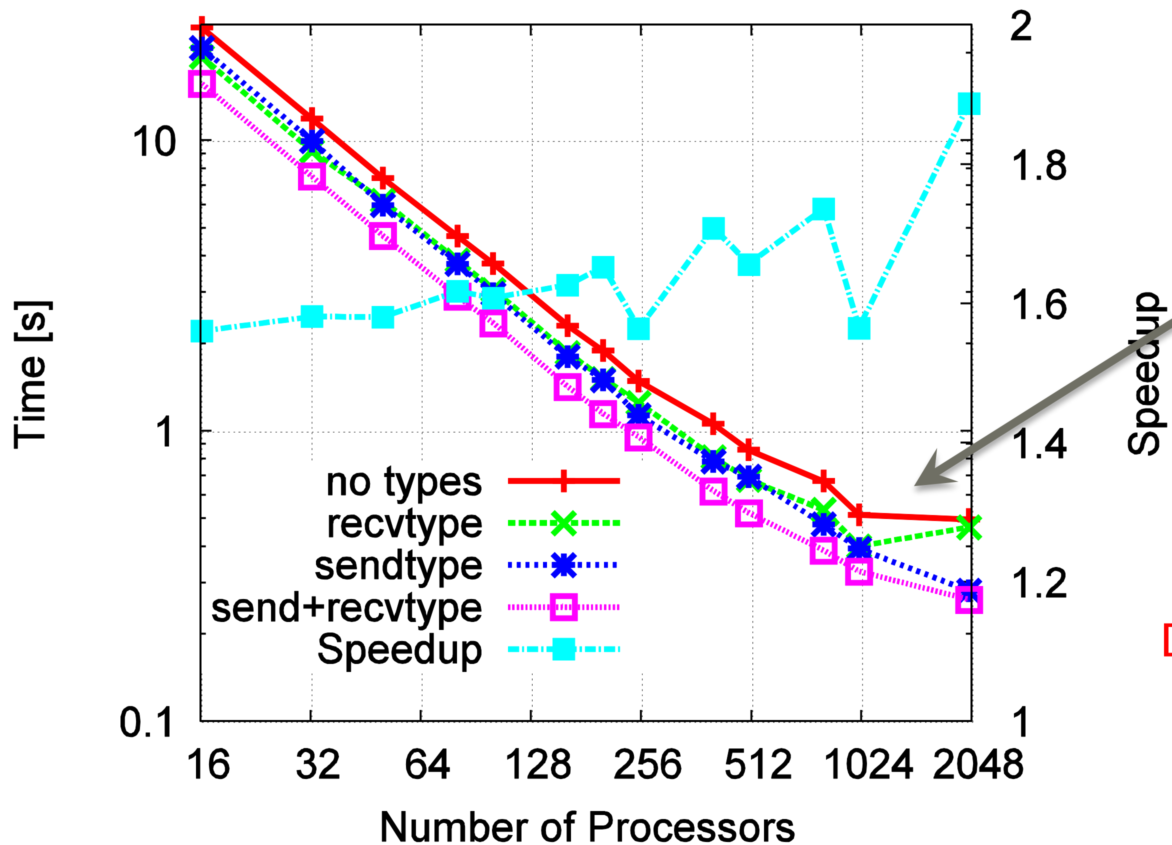
- **Odin @ IU**
  - 128 compute nodes, 2x2 Opteron 1354 2.1 GHz
  - SDR InfiniBand (OFED 1.3.1).
  - Open MPI 1.4.1 (openib BTL), g++ 4.1.2
- **Jaguar @ ORNL**
  - 150152 compute nodes, 2.1 GHz Opteron
  - Torus network (SeaStar).
  - CNL 2.1, Cray Message Passing Toolkit 3
- **All compiled with "-O3 –mtune=opteron"**

Strong Scaling - Odin (8000²)



- **4 runs, report smallest time, <4% deviation**

Strong Scaling – Jaguar (20k²)



Scaling stops w/o datatypes

DDT increase scalability

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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!

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

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:

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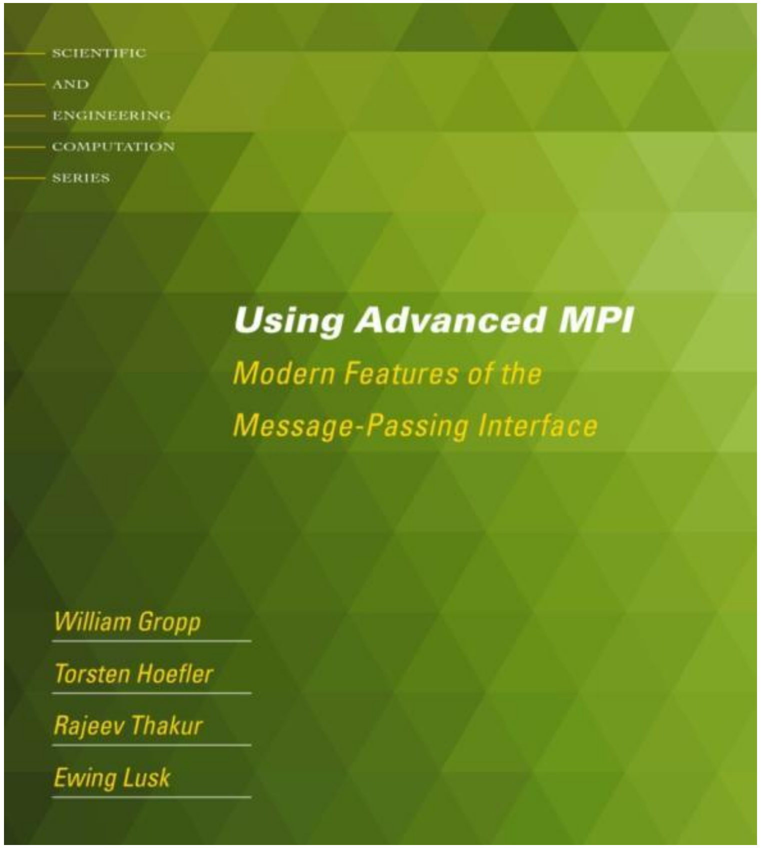

  - All materials (slides, code examples) at: *http://htor.inf.ethz.ch/teaching/mpi_tutorials/eurompi14/*