ADVANCED MPI 2.2 AND 3.0 TUTORIAL

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Hosted by: CSCS, Lugano, Switzerland

TUTORIAL OUTLINE

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

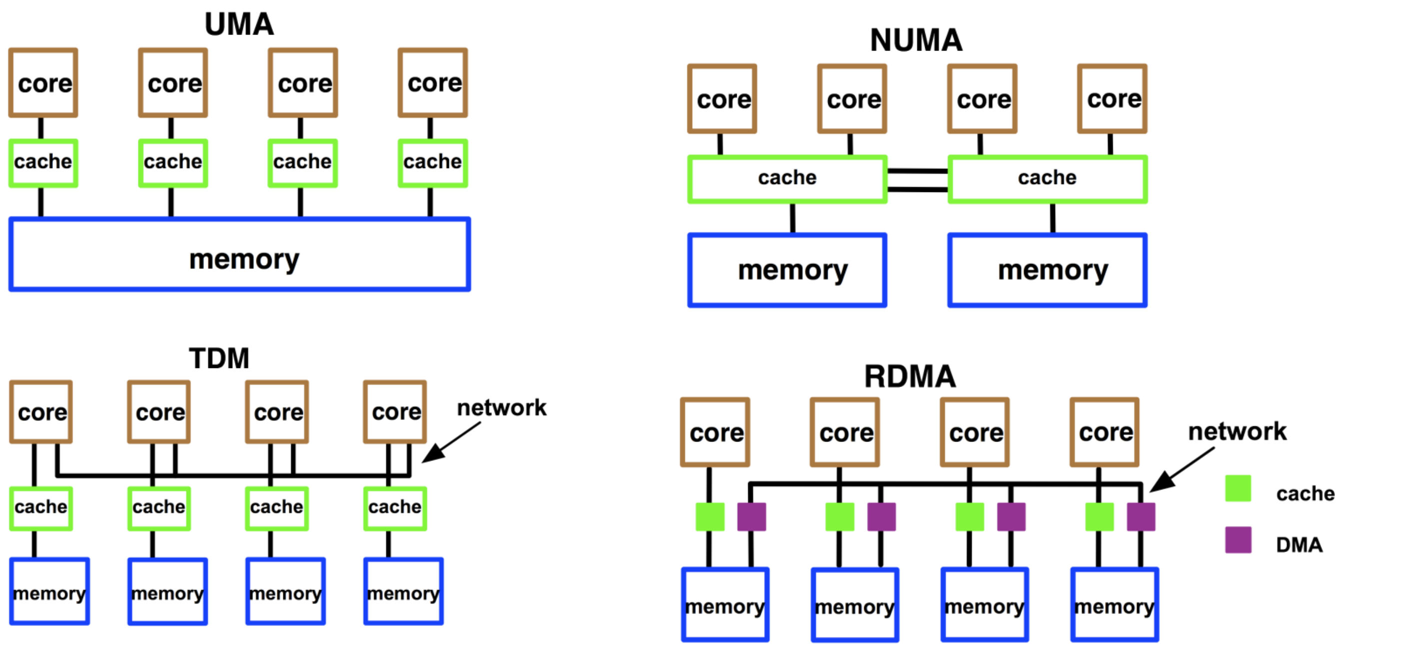
USED TECHNIQUES

- 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

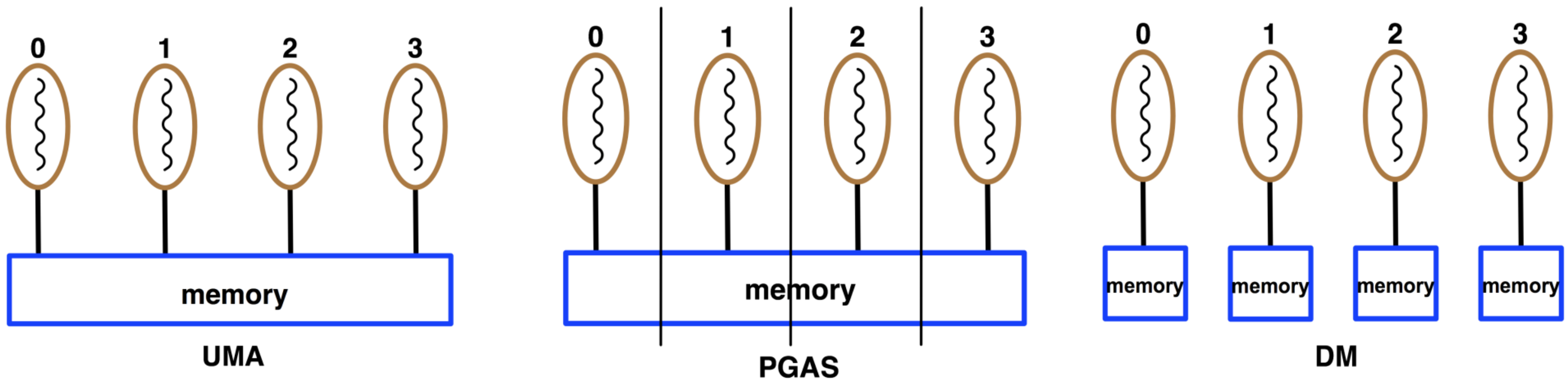
Introduction

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



Introduction

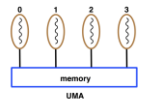
- Different programming models: UMA, PGAS, DM

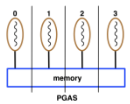


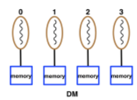
TBB, CILK, OpenMP, MPI-3 SM — UPC, CAF, MPI-2 OS — MPI-1, PVM

- The question is all about memory consistency

Programming Models

- Provide abstract machine models (contract)
  - Shared mem 

  - PGAS 

  - Distributed mem 

- 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 (probably '12)
  - Several additions to react to new challenges

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)
- 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

How does the MPI-3.0 process work

- Organization and Mantras:
  - Chapter chairs (convener) and (sub)committees
  - Avoid the “Designed by a Committee” phenomenon → standardize common practice
  - 99.5% backwards compatible
- Adding new things:
  - Review and discuss early proposals in chapter
  - Bring proposals to the forum (discussion)
  - Plenary formal reading (usually word by word)
  - Two votes on each ticket (distinct meetings)
  - Final vote on each chapter (finalizing MPI-3.0)

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

Performance Modeling

Nils Bohr: *"Prediction is very difficult, especially about the future."*

- Predictive models are never perfect
- They can help to drive action though
  - Back of the envelope calculations are valuable!
- This tutorial gives a rough idea about performance bounds of MPI functions.
  - Actual performance **will** vary across implementations and architectures

Section II – 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)

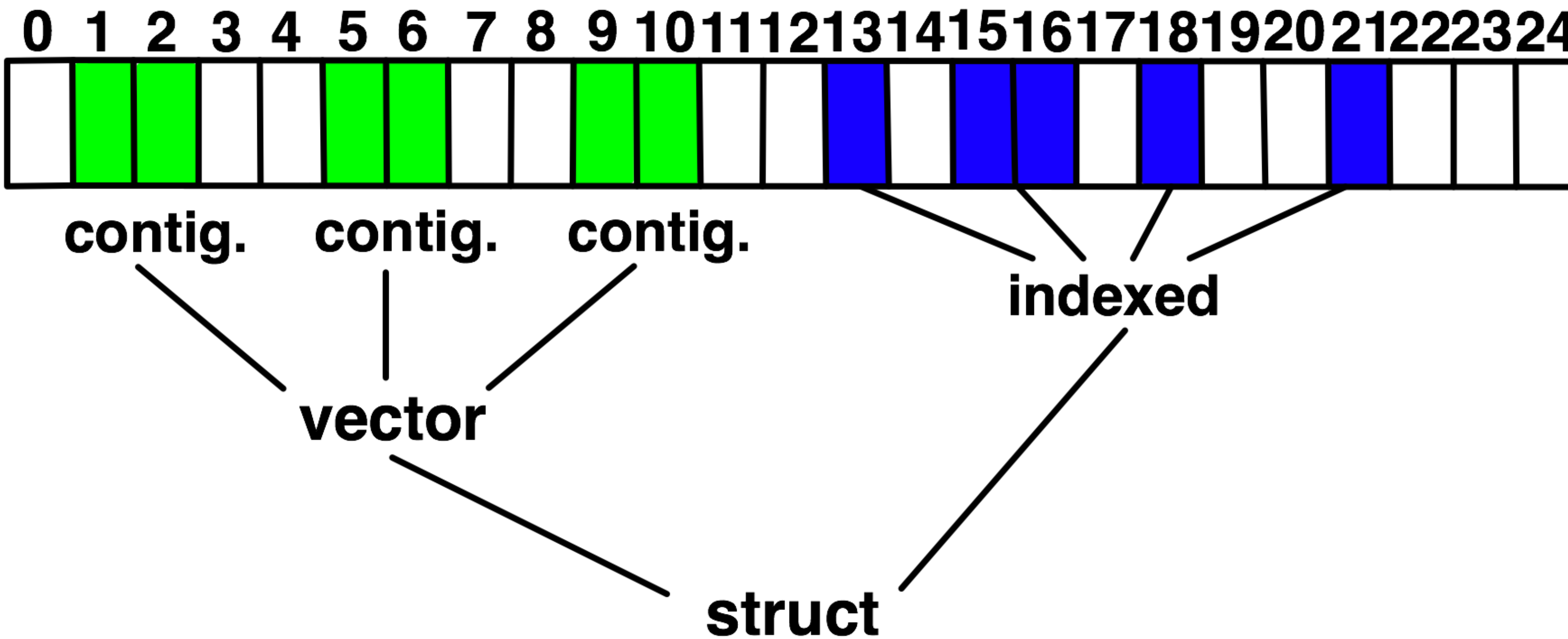
Quick MPI Datatype Introduction

- 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

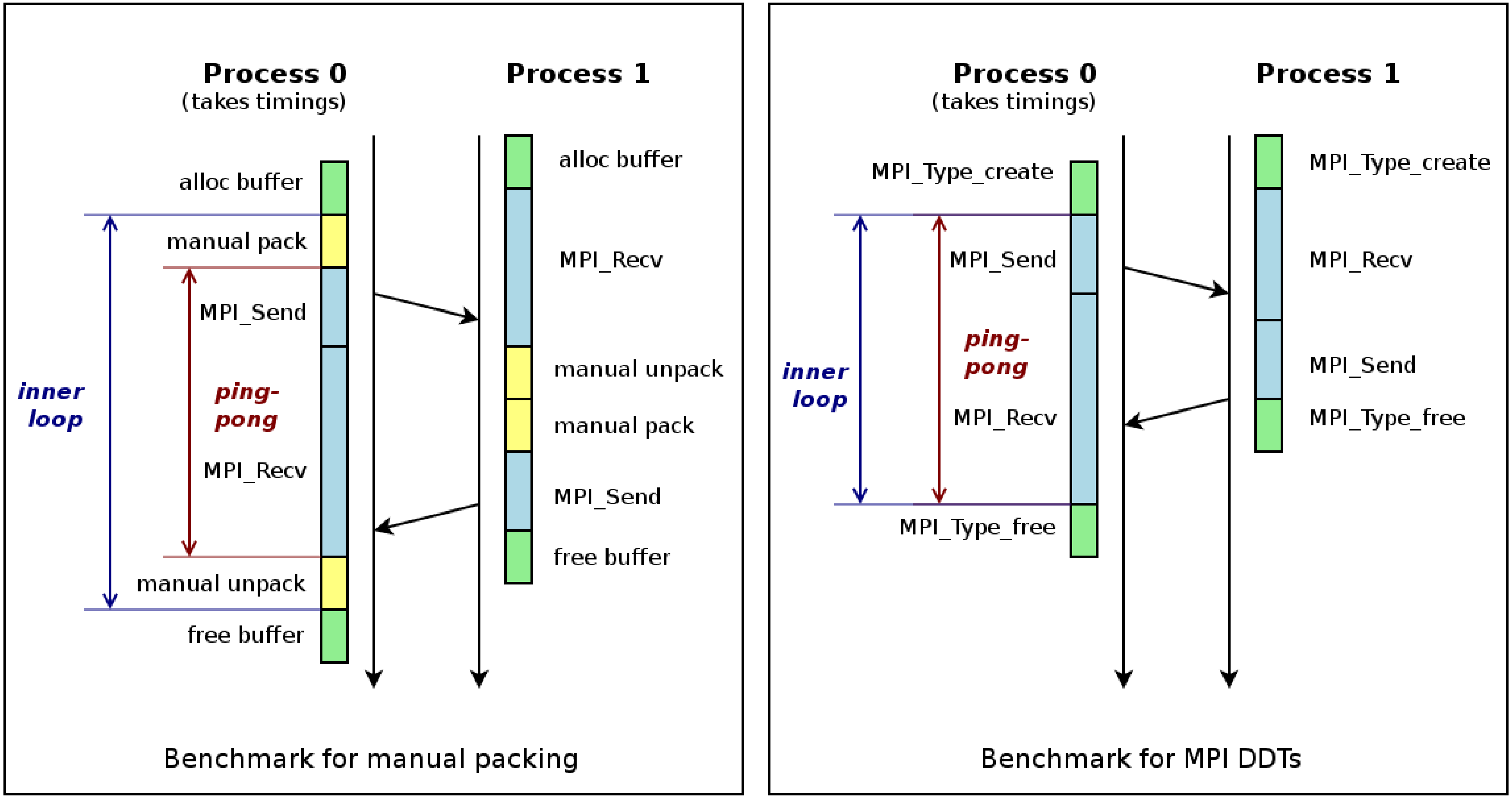
What is Zero Copy?

- 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

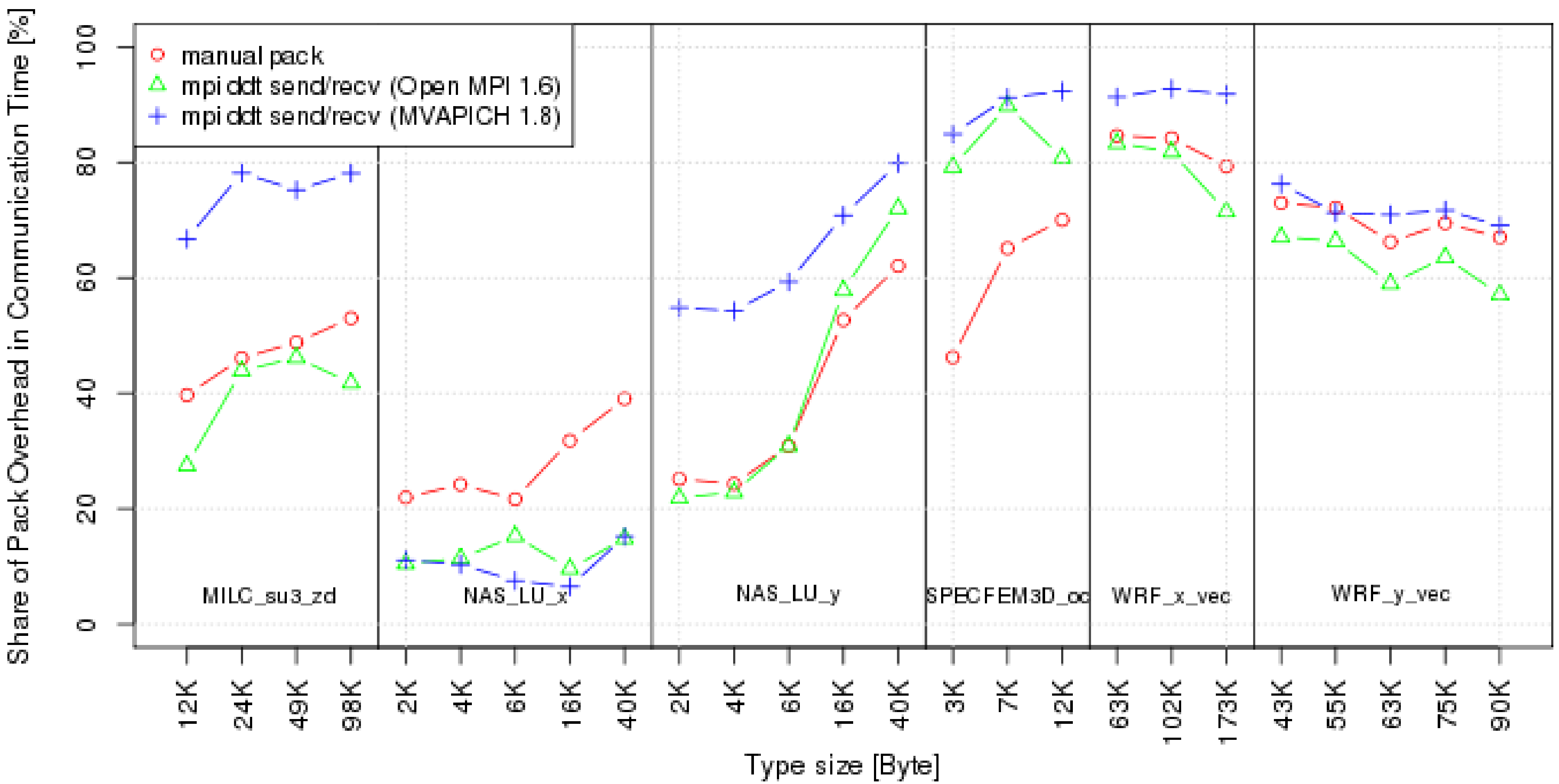
- Demonstrate utility of DDT in practice
  - Early implementations were bad → folklore
  - Some are still bad → chicken egg problem
- Show creative use of DDTs
  - Encode local transpose for FFT
  - Enable you to create more!
- Gather input on realistic benchmark cases
  - Guide optimization of DDT implementations

A NEW WAY OF BENCHMARKING



Schneider, Gerstenberger, Hoefler: Micro-Applications for Communication Data Access Patterns

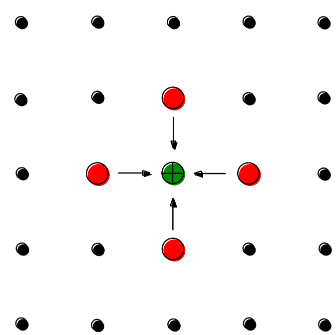
MOTIVATION



Schneider, Gerstenberger, Hoefler: Micro-Applications for Communication Data Access Patterns

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

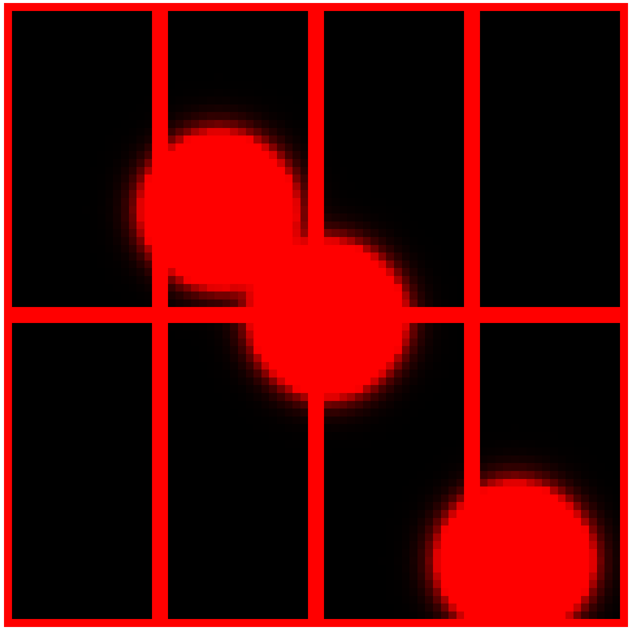
```
for(int iter=0; iter<niters; ++iter) {
  for(int i=1; i<n+1; ++i) {
    for(int j=1; j<n+1; ++j) {
      anew[ind(i,j)] = apply(stencil); // actual computation
      heat += anew[ind(i,j)]; // total heat in system
    }
  }
  for(int i=0; i<nsources; ++i) {
    anew[ind(sources[i][0],sources[i][1])]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

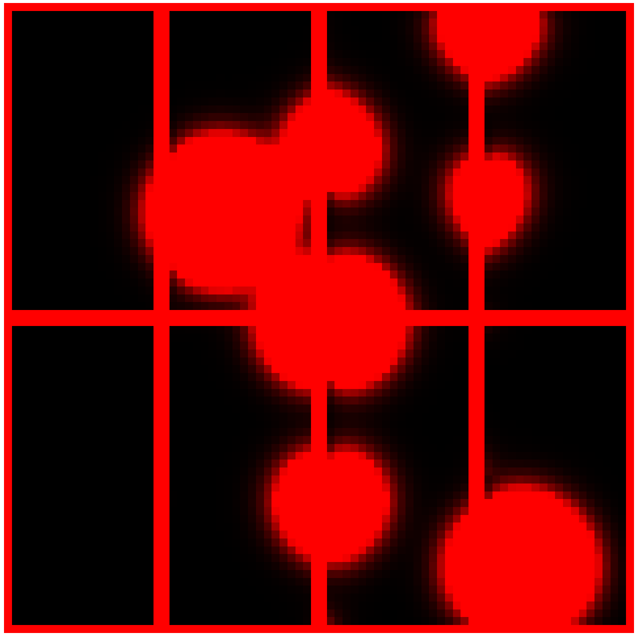
Simple 2D Parallelization

- 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

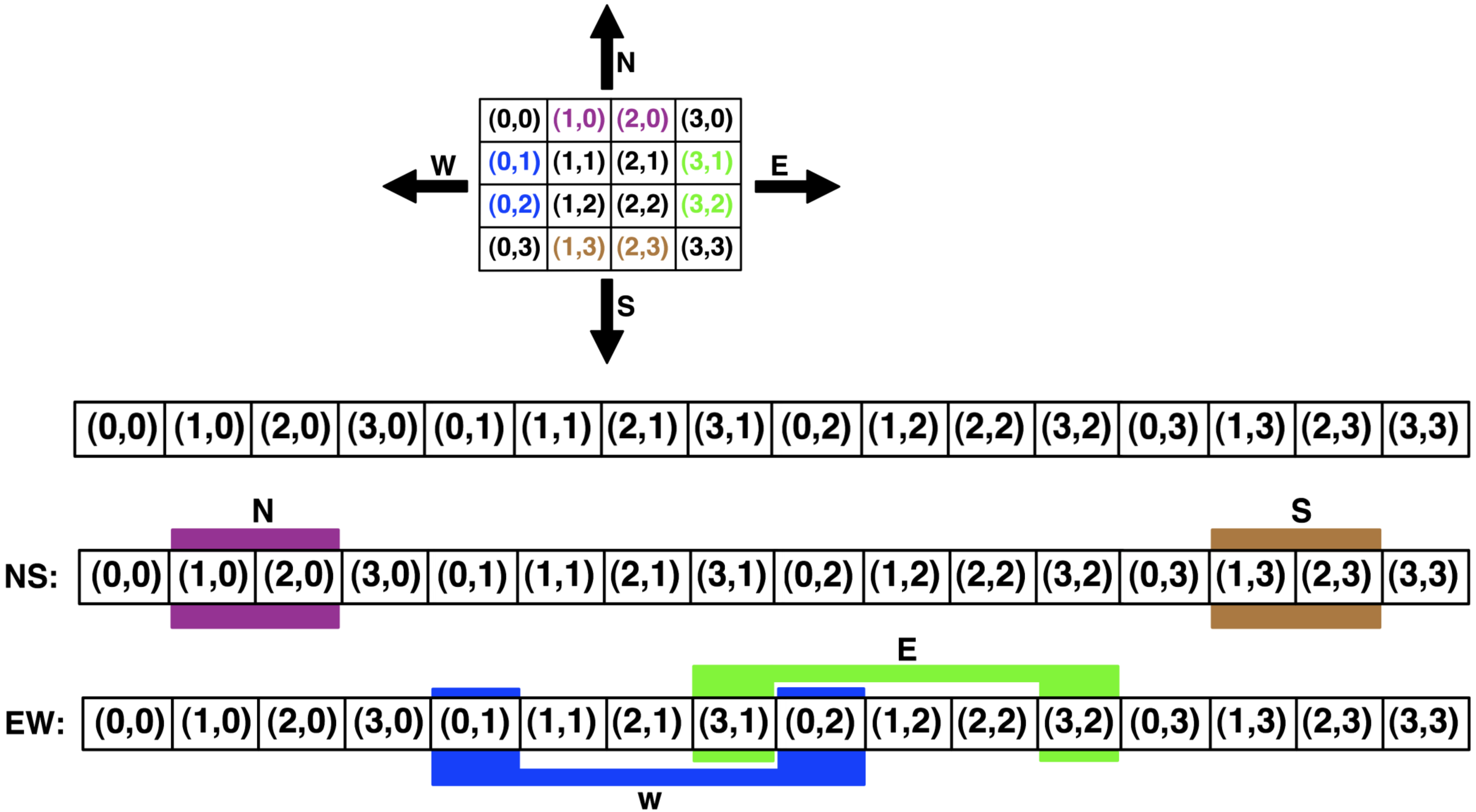
Source Code Example

- Browse through code (stencil_mpi.cpp)
- Show how to run and debug (visualize) it





DATATYPES FOR THE STENCIL



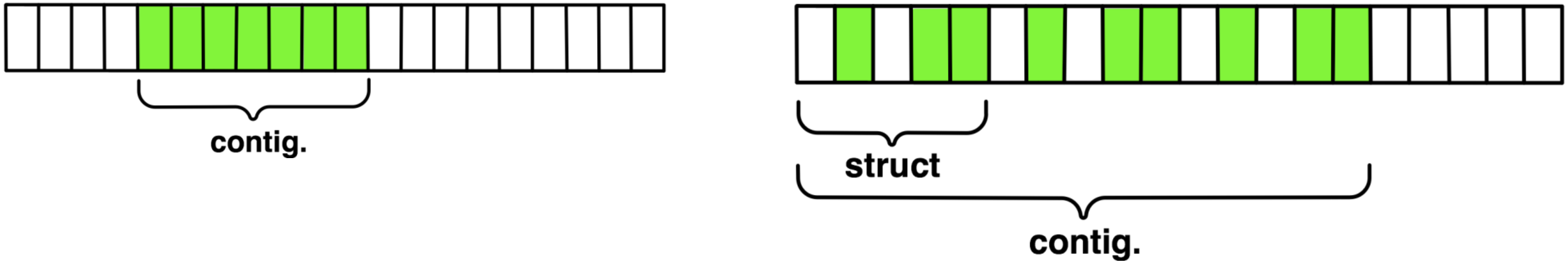
MPI's Intrinsic Datatypes

- 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)

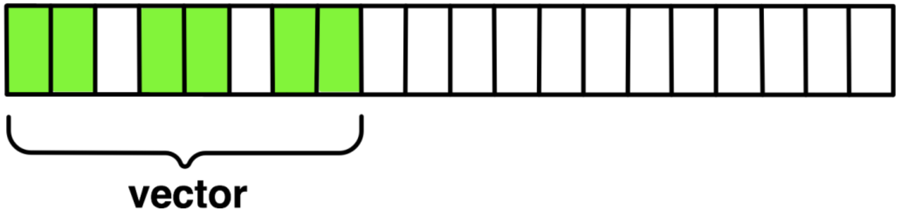
- Contiguous array of oldtype
- Should not be used as last type (can be replaced by count)

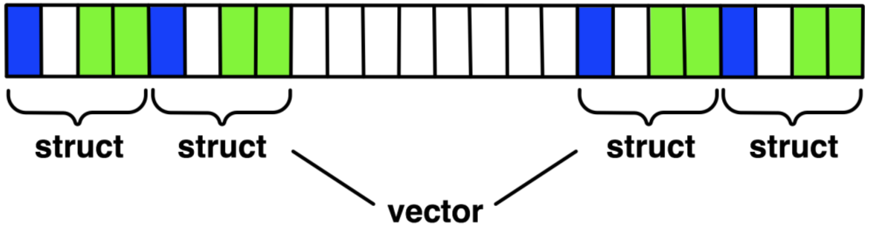


MPI_TYPE_VECTOR

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

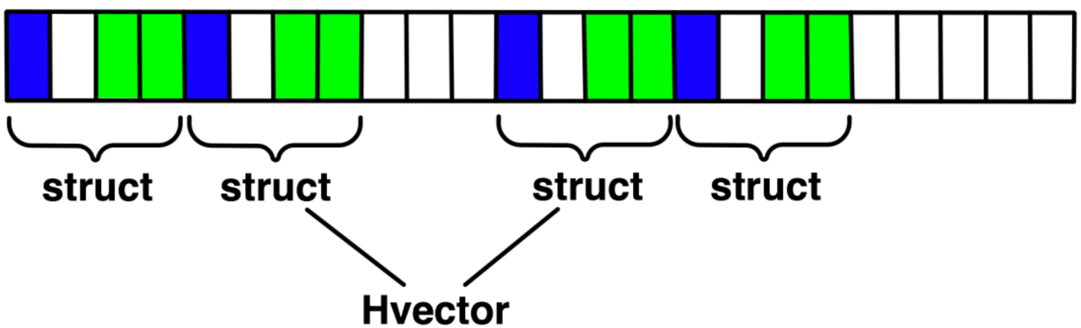




MPI_TYPE_CREATE_HVECTOR

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

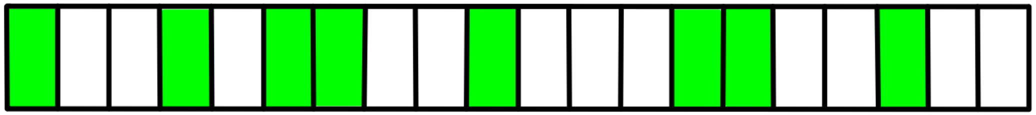
- Create non-unit strided vectors
- Useful for composition, e.g., vector of structs



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!

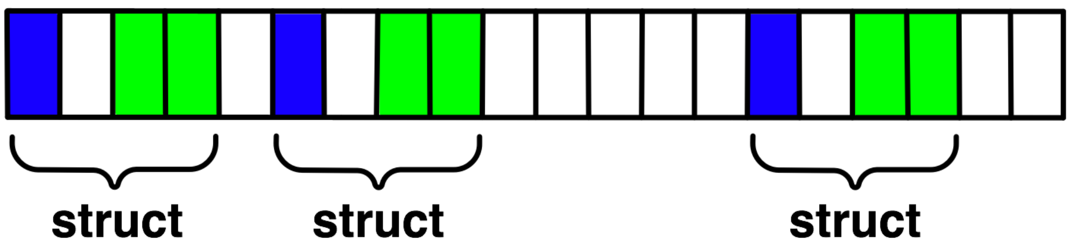


  - blen={1,1,2,1,2,1}
  - displs={0,3,5,9,13,17}

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)

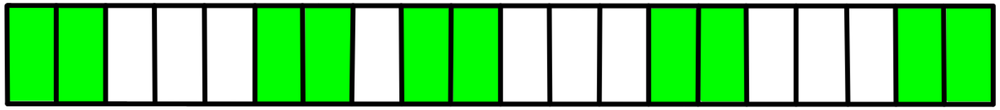
- Indexed with non-unit displacements, e.g., pulling types out of different arrays



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

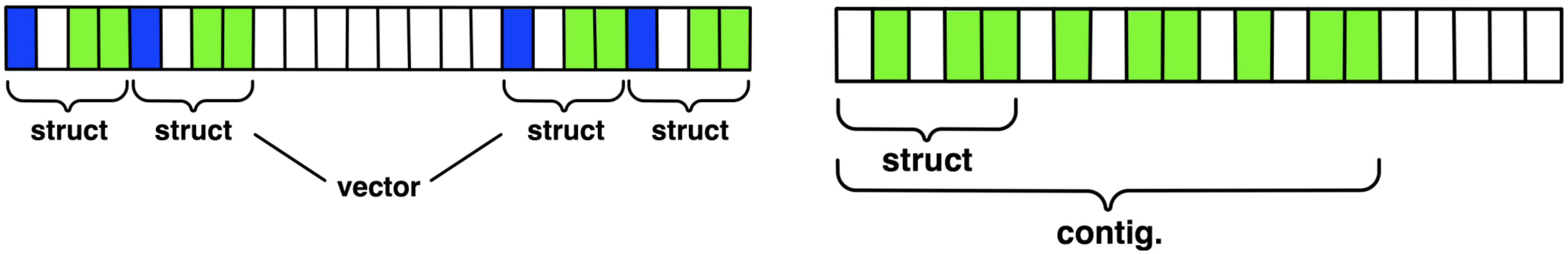


  - blen=2
  - displs={0,5,9,13,18}

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)
```

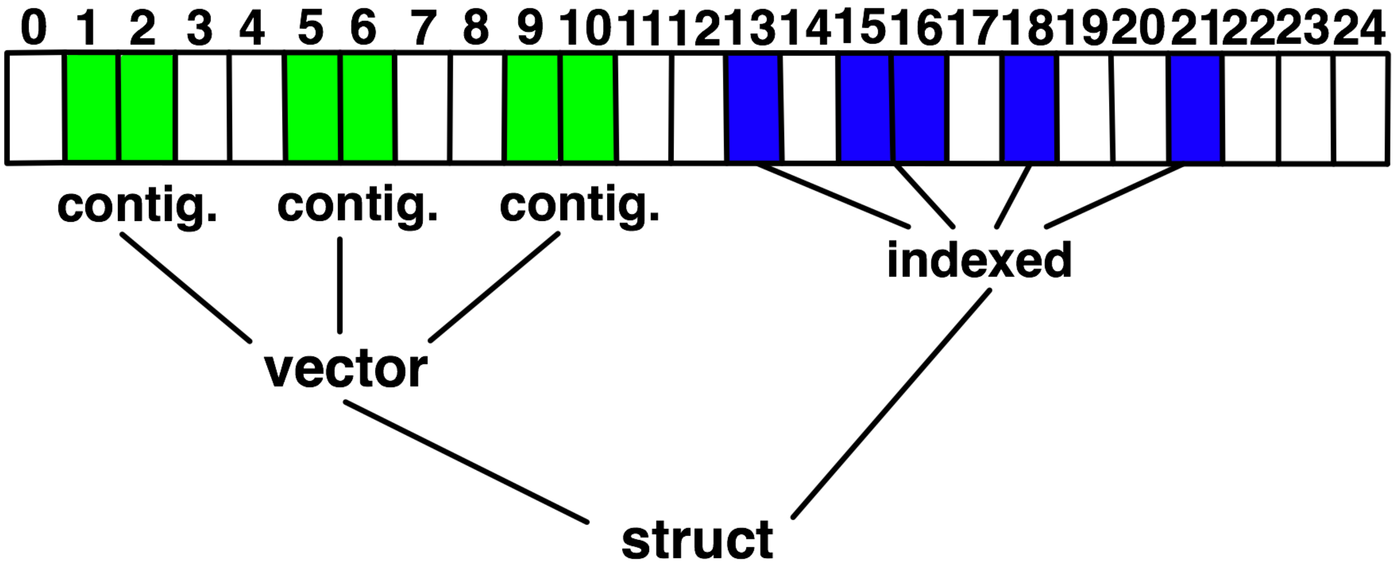
- Create distributed array, supports block, cyclic and no distribution for each dimension
  - Very useful for I/O

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/

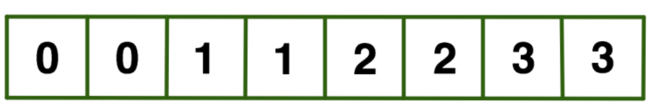
DATATYPE SELECTION TREE

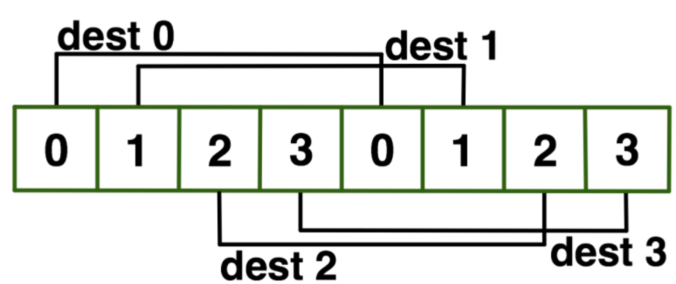
- Simple and effective performance model:
  - More parameters == slower
- **contig < vector < index_block < index < struct**
- Some (most) MPIs are inconsistent
  - But this rule is portable
- Advice to users:
  - Try datatype “compression” bottom-up

W. Gropp et al.:Performance Expectations and Guidelines for MPI Derived Datatypes

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)



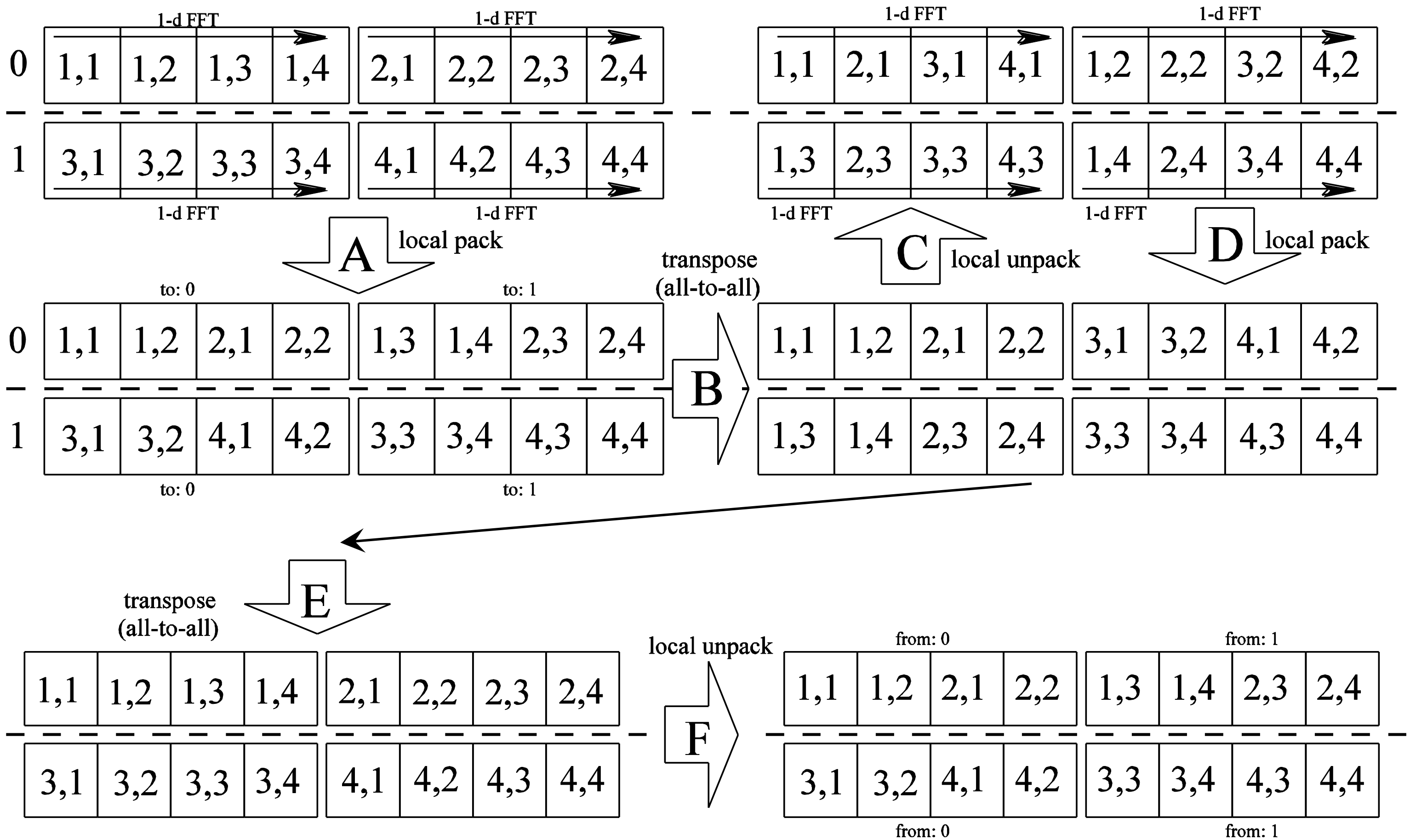


A Complex Example - FFT

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)

Hoefler, Gottlieb: Parallel Zero-Copy Algorithms for Fast Fourier Transform and Conjugate Gradient using MPI Datatypes

A Complex Example - FFT



Hoefler, Gottlieb: Parallel Zero-Copy Algorithms for Fast Fourier Transform and Conjugate Gradient using MPI Datatypes

2D-FFT Optimization Possibilities

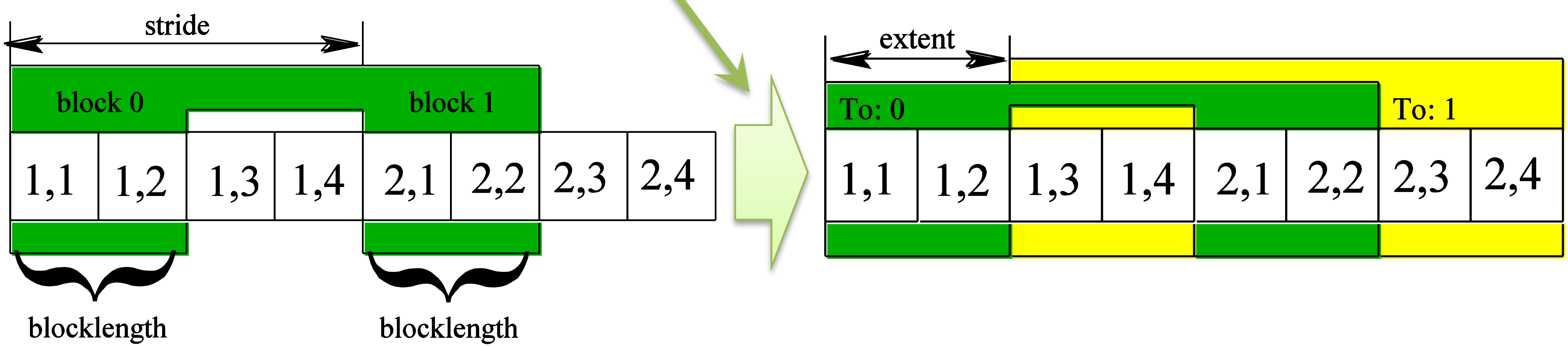
1. Use DDT for pack/unpack (obvious)
   - Eliminate 4 of 8 steps
     - Introduce local transpose

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

Hoefler, Gottlieb: Parallel Zero-Copy Algorithms for Fast Fourier Transform and Conjugate Gradient using MPI Datatypes

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)

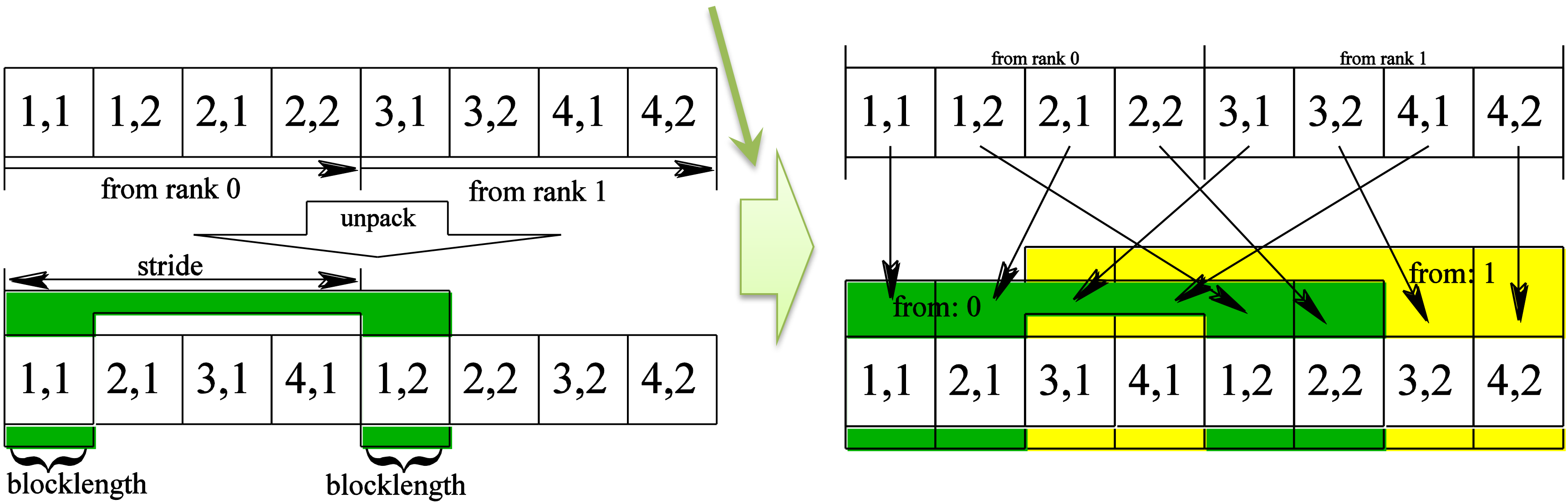


- Three hierarchy-layers

Hoefler, Gottlieb: Parallel Zero-Copy Algorithms for Fast Fourier Transform and Conjugate Gradient using MPI Datatypes

The Receive Datatype

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



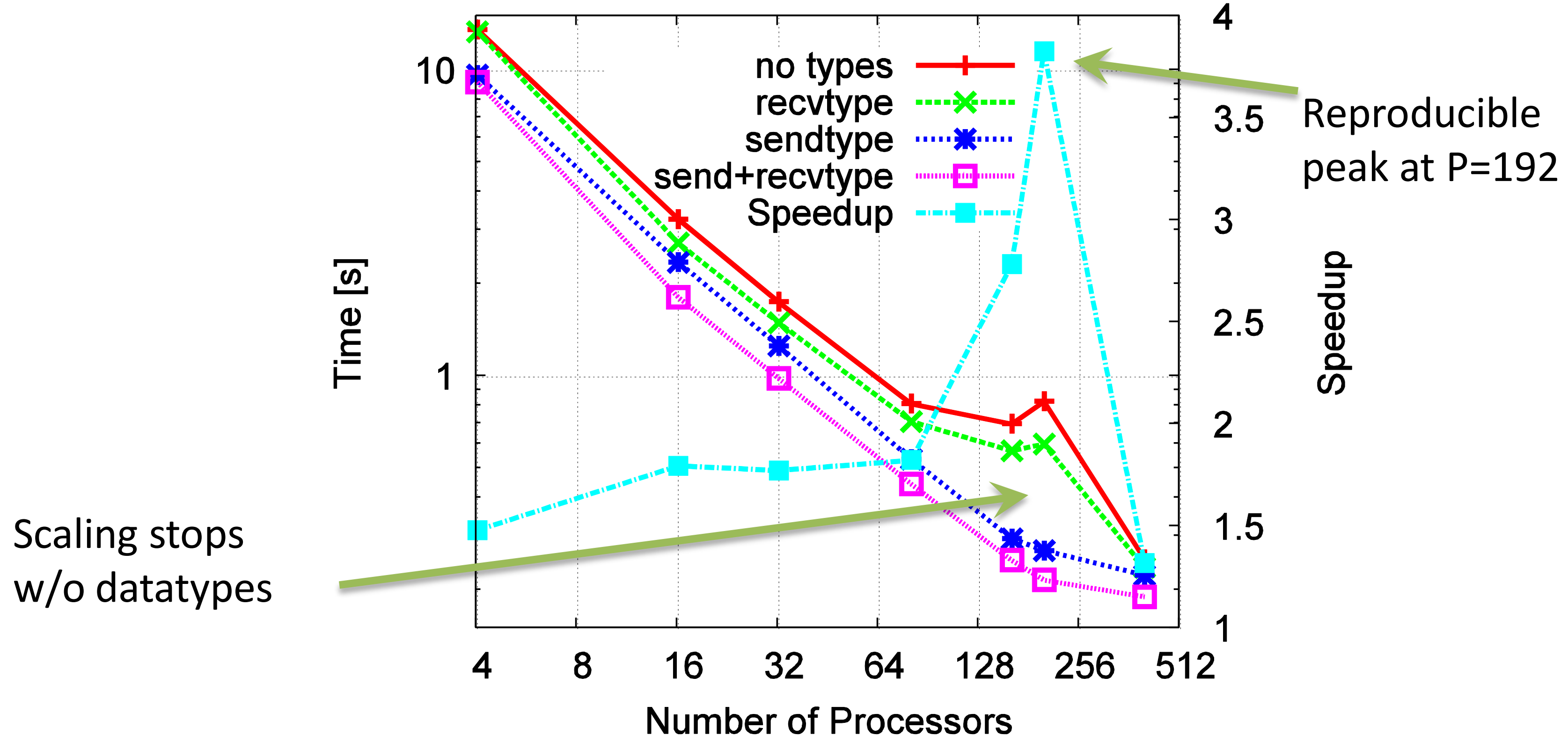
Hoefler, Gottlieb: Parallel Zero-Copy Algorithms for Fast Fourier Transform and Conjugate Gradient using MPI Datatypes

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"

Hoefler, Gottlieb: Parallel Zero-Copy Algorithms for Fast Fourier Transform and Conjugate Gradient using MPI Datatypes

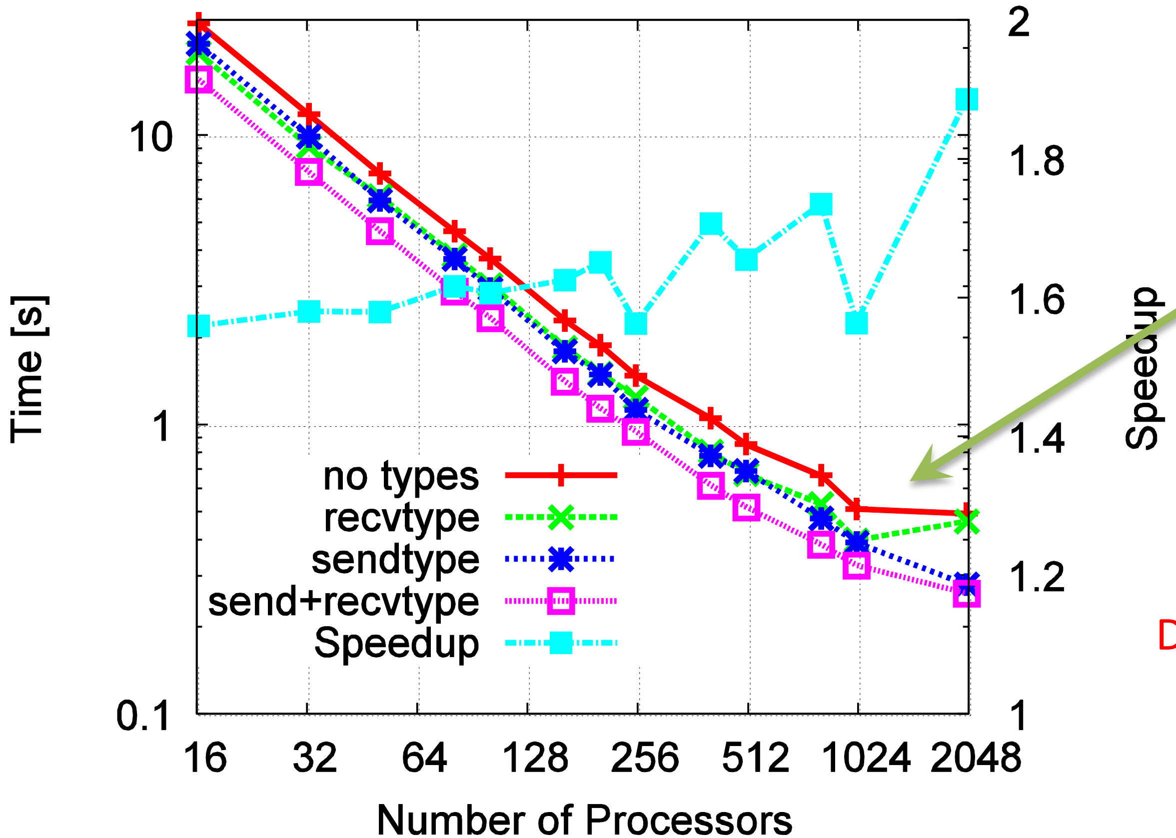
STRONG SCALING - ODIN (8000^2)



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

Hoefler, Gottlieb: Parallel Zero-Copy Algorithms for Fast Fourier Transform and Conjugate Gradient using MPI Datatypes

Strong Scaling – Jaguar (20k²)



Scaling stops w/o datatypes

DDT increase scalability

Hoefler, Gottlieb: Parallel Zero-Copy Algorithms for Fast Fourier Transform and Conjugate Gradient using MPI Datatypes

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!

Section III - Nonblocking and Collective Communication

NONBLOCKING AND COLLECTIVE COMMUNICATION

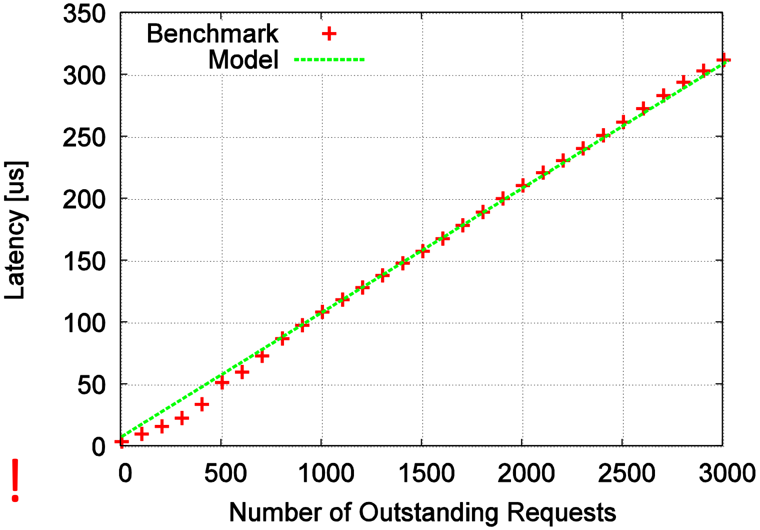
- Nonblocking communication
  - Deadlock avoidance
  - Overlapping communication/computation
- Collective communication
  - Collection of pre-defined optimized routines
- Nonblocking collective communication
  - Combines both advantages
  - System noise/imbalance resiliency
  - Semantic advantages
  - 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!

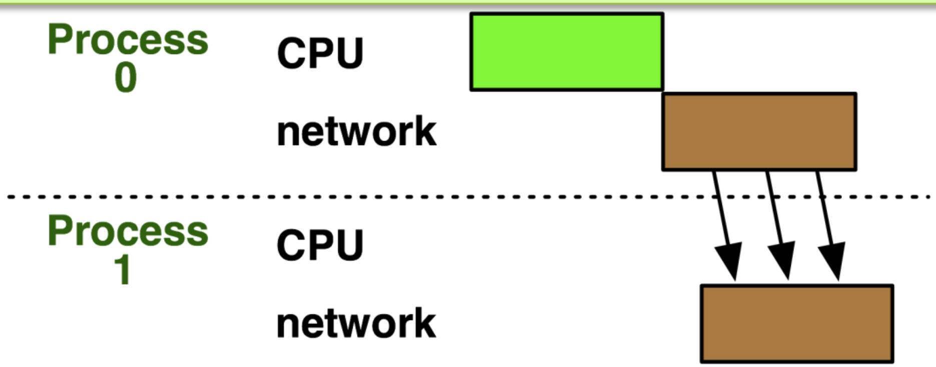


Nonblocking Communication

- 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!

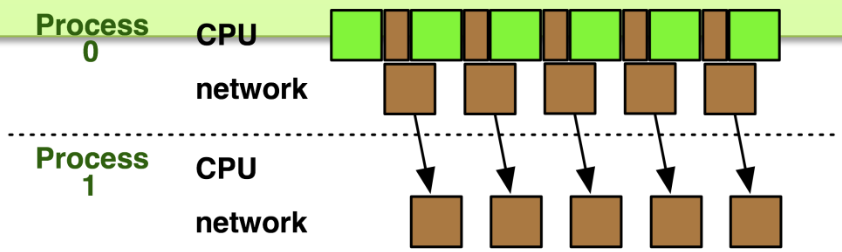
SOFTWARE PIPELINING - MOTIVATION

```
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);
}
```



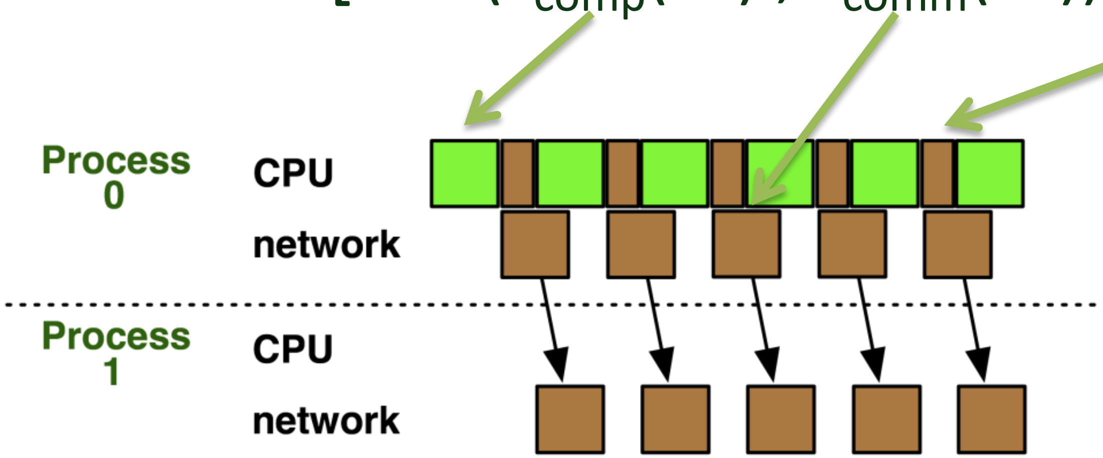
Software Pipelining - Motivation

```
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);
}
```



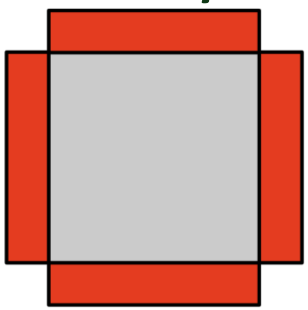
A Simple Pipeline Model

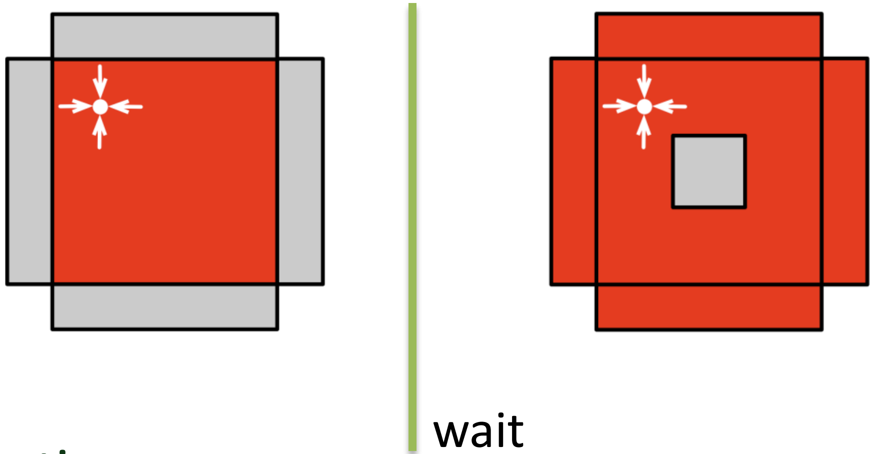
- No pipeline:
  - $T = T_{comp}(s) + T_{comm}(s) + T_{startc}(s)$
- Pipeline:
  - $T = nblocks * [\max(T_{comp}(bs) , T_{comm}(bs)) + T_{startc}(bs)]$



Stencil Example - Overlap

- Necessary code transformation – picture





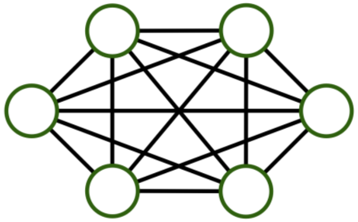
- Steps:
  - Start halo communication
  - Compute inner zone
  - Wait for halo communication
  - Compute outer zone
  - Swap arrays

Collective Communication

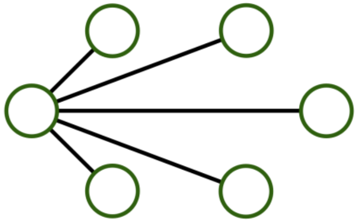
- Three types:
  - Synchronization (Barrier)
  - Data Movement (Scatter, Gather, Alltoall, Allgather)
  - Reductions (Reduce, Allreduce, (Ex)Scan, Red_scat)
- Common semantics:
  - no tags (communicators can serve as such)
  - Blocking semantics (return when complete)
  - Not necessarily synchronizing (only barrier and all*)
- Overview of functions and performance models

COLLECTIVE COMMUNICATION

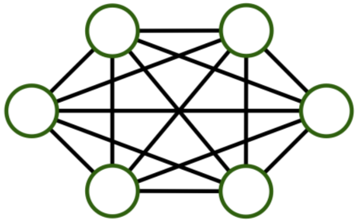
- Barrier – $\Theta(\log(P))$
  - Often $\alpha+\beta \log_2 P$



- Scatter, Gather – $\Omega(\log(P) + Ps)$
  - Often $\alpha P+\beta Ps$

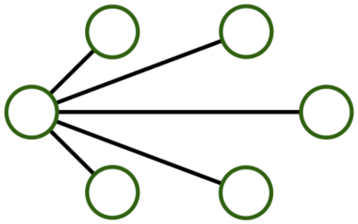


- Alltoall, Allgather - $\Omega(\log(P) + Ps)$
  - Often $\alpha P+\beta Ps$

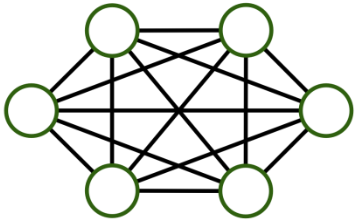


Collective Communication

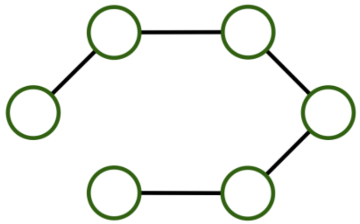
- Reduce – $\Omega(\log(P) + s)$
  - Often $\alpha \log_2 P + \beta m + \gamma m$



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



- (Ex)scan – $\Omega(\log(P) + s)$
  - Often $\alpha P + \beta m + \gamma m$



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

Hoefler et al.: Implementation and Performance Analysis of Non-Blocking Collective Operations for MPI

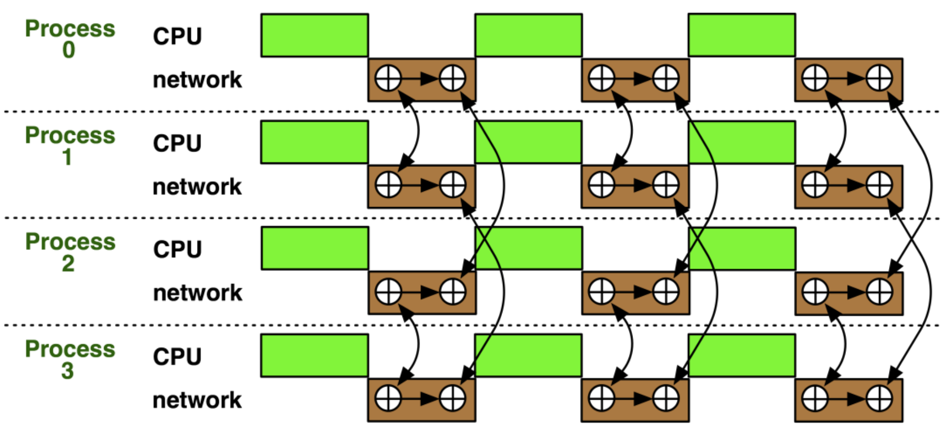
Nonblocking Collective Communication

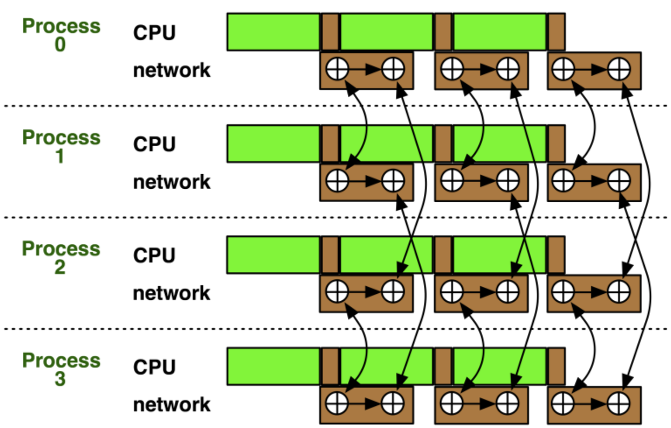
- Semantic advantages:
  - Enable asynchronous progression (and manual)
    - Software pipelinling
  - Decouple data transfer and synchronization
    - Noise resiliency!
  - Allow overlapping communicators
    - See also neighborhood collectives
  - Multiple outstanding operations at any time
    - Enables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

Hoefler et al.: Implementation and Performance Analysis of Non-Blocking Collective Operations for MPI

NONBLOCKING COLLECTIVES OVERLAP

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





Hoefler: Leveraging Non-blocking Collective Communication in High-performance Applications

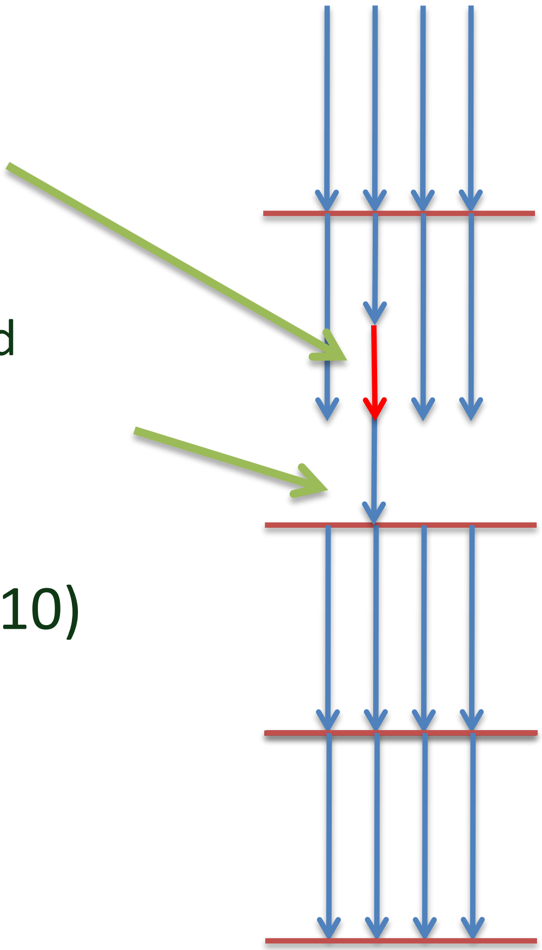
Nonblocking Collectives Overlap

- 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

Hoefler: Leveraging Non-blocking Collective Communication in High-performance Applications

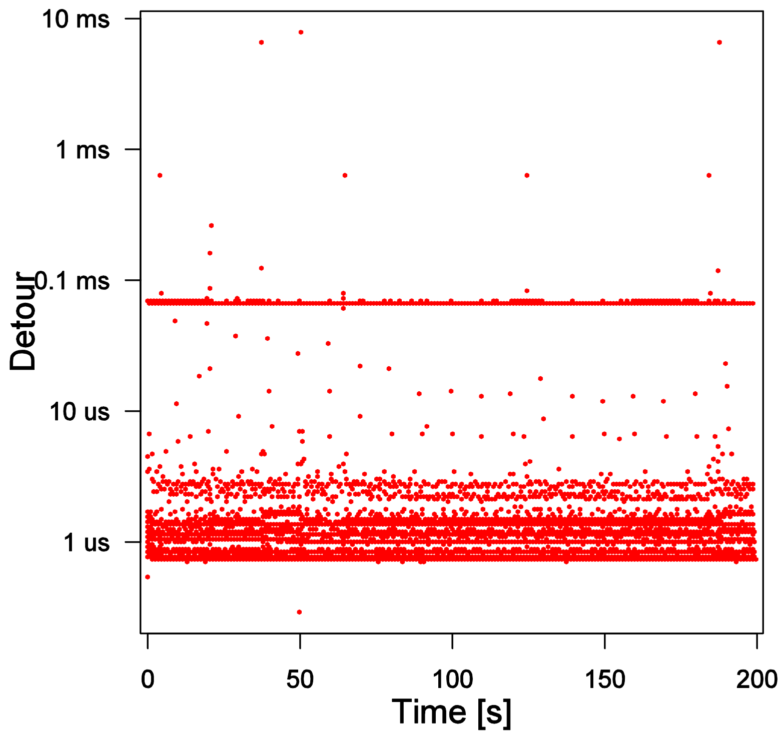
System Noise – Introduction

- 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)



Hoefler et al.: Characterizing the Influence of System Noise on Large-Scale Applications by Simulation

Measurement Results – Cray XE



- Resolution: 32.9 ns, noise overhead: 0.02%

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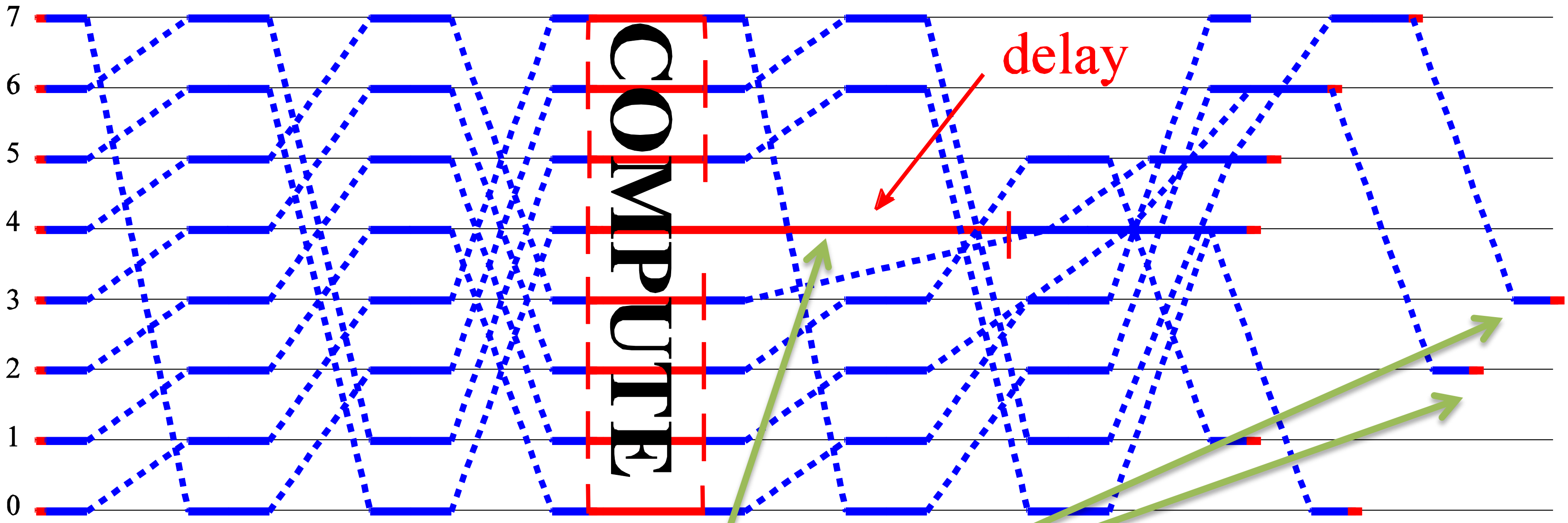
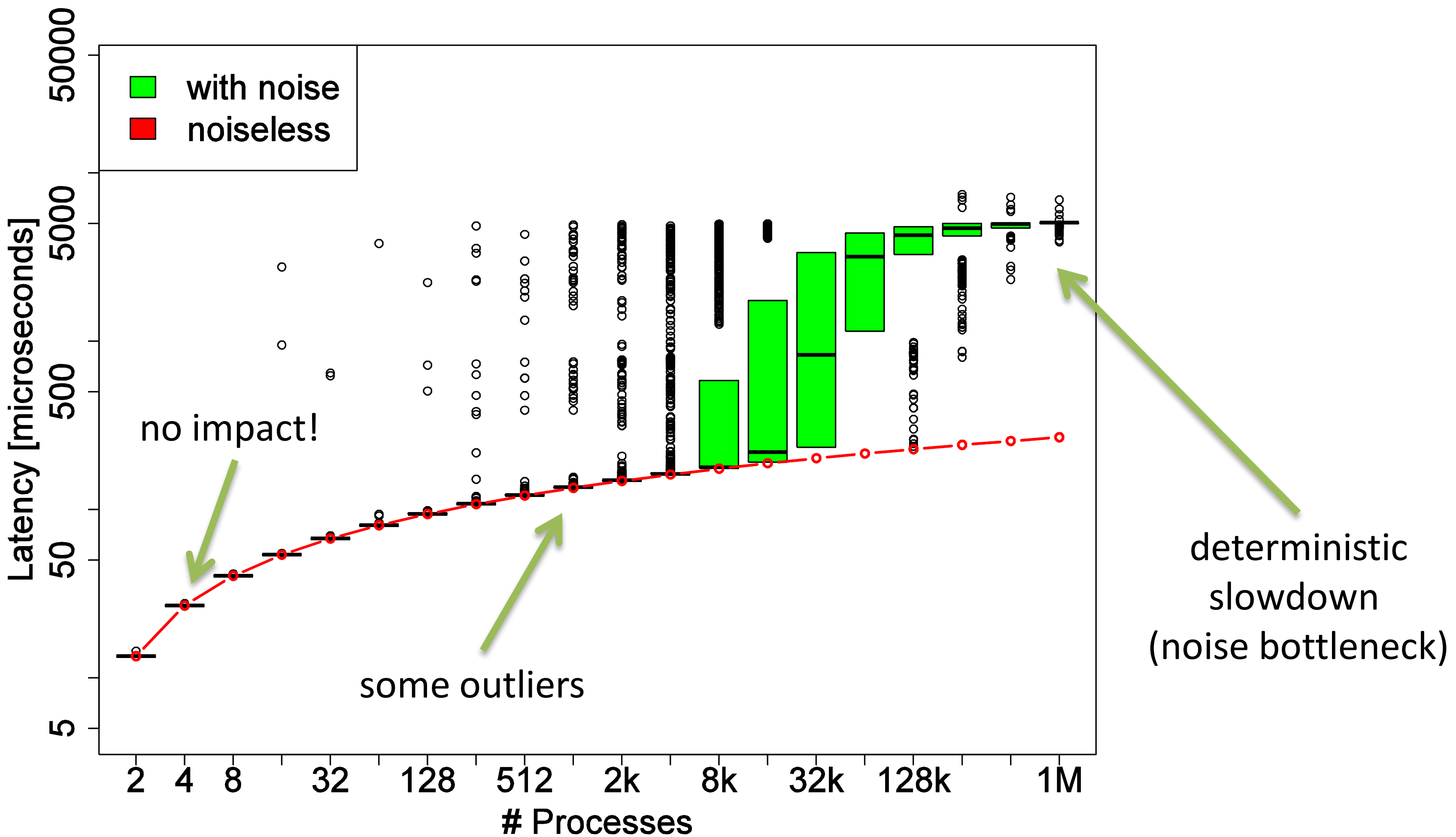
A Noisy Example – Dissemination



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

Hoefler et al.: Characterizing the Influence of System Noise on Large-Scale Applications by Simulation

SINGLE BYTE DISSEMINATION ON JAGUAR



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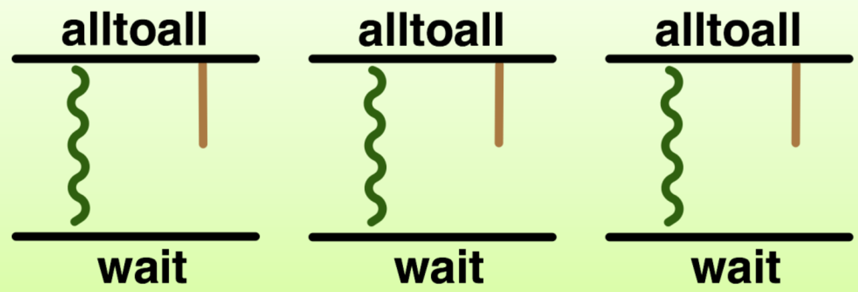
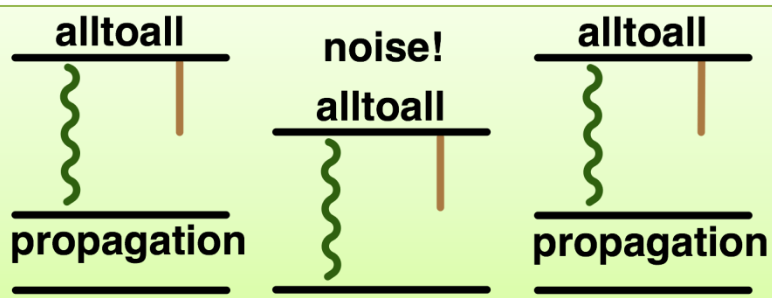
Nonblocking Collectives vs. Noise

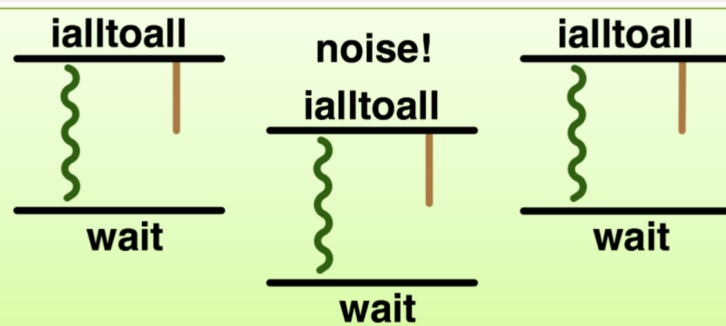
No Noise, blocking





Noise, blocking

Noise, nonblocking



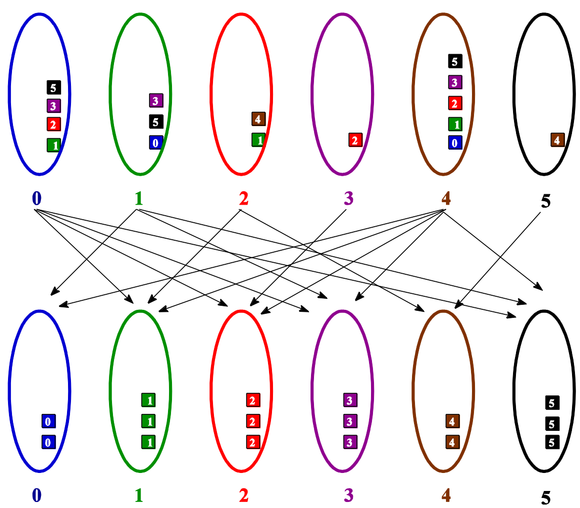
Hoefler et al.: Characterizing the Influence of System Noise on Large-Scale Applications by Simulation

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



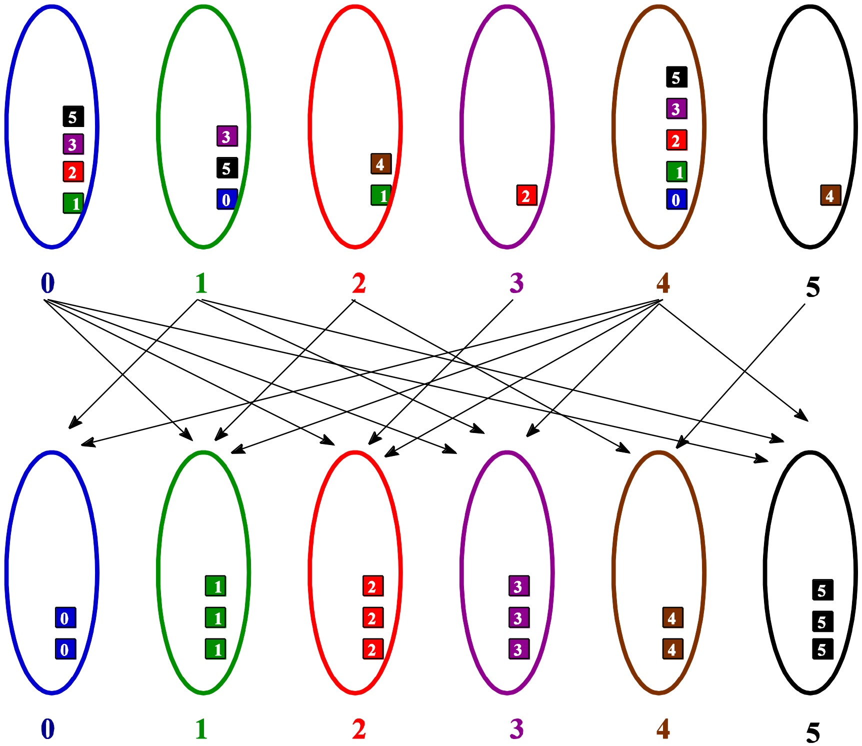
T. Hoefler et al.:Scalable Communication Protocols for Dynamic Sparse Data Exchange

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:

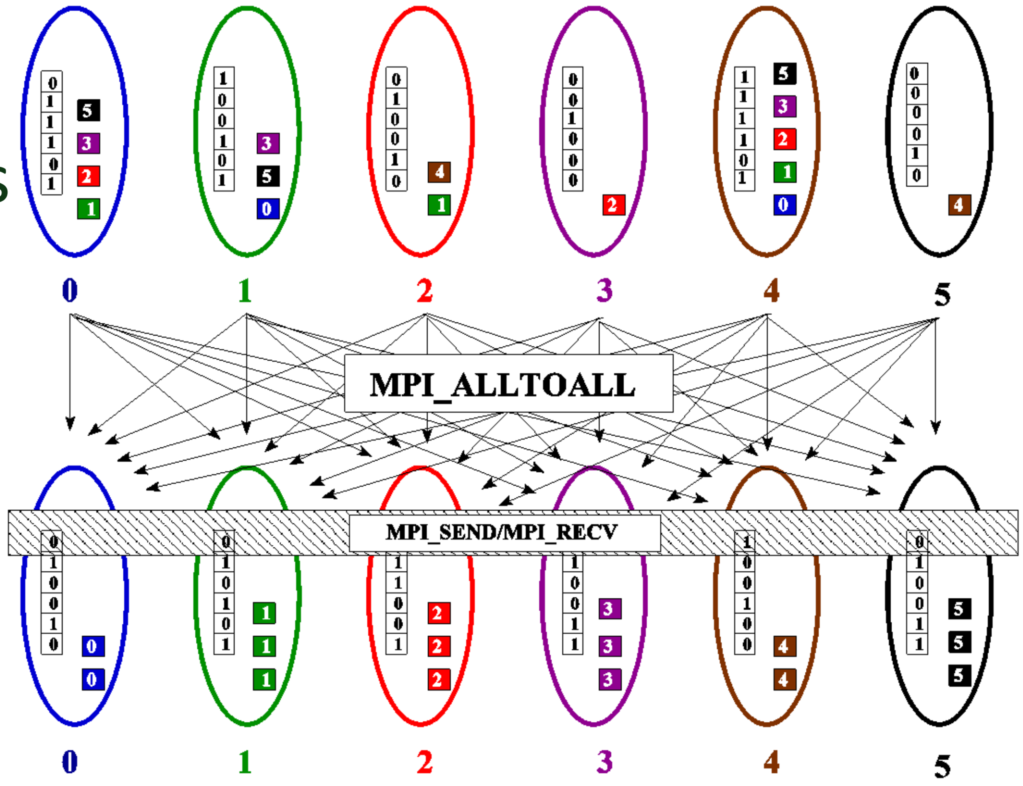
  - Use MPI semantics:
    - Unknown sender
      - MPI_ANY_SOURCE
    - Unknown message size
      - MPI_PROBE
    - Reduces problem to counting the number of neighbors
    - Allow faster implementation!



T. Hoefler et al.:Scalable Communication Protocols for Dynamic Sparse Data Exchange

USING ALLTOALL (PEX)

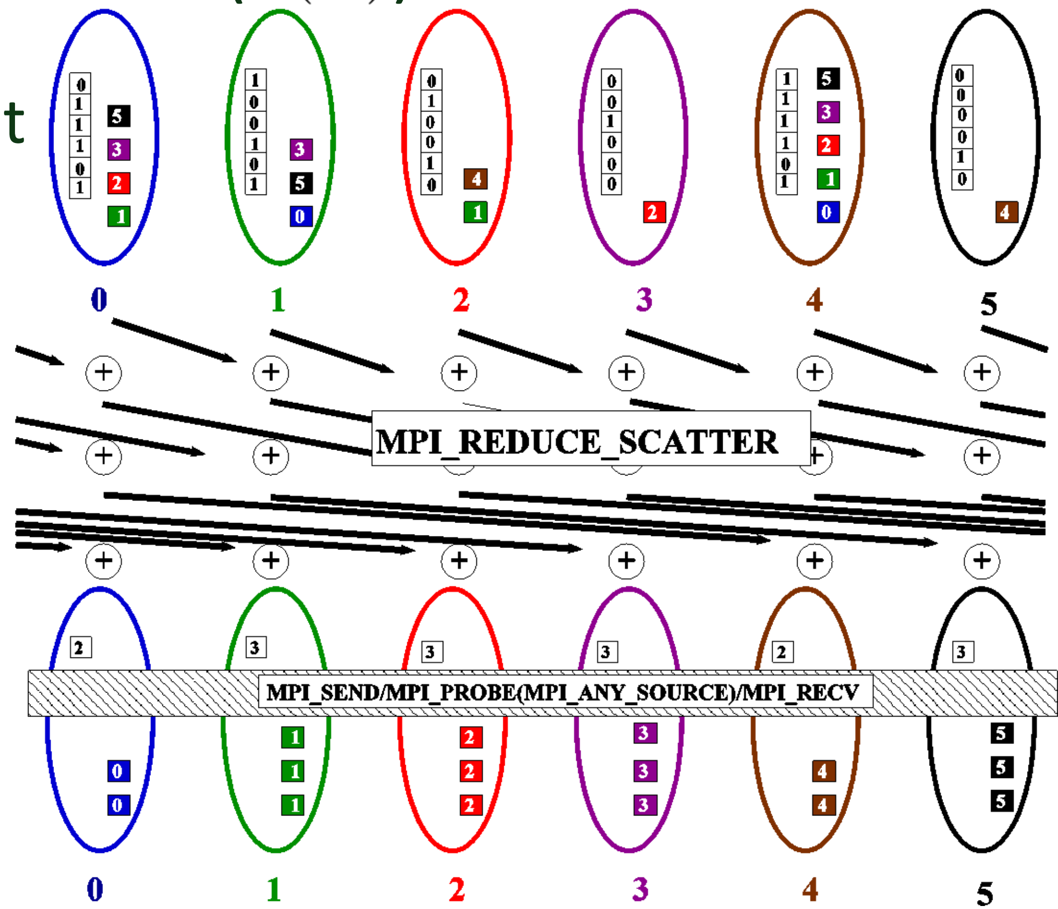
- Bases on Personalized Exchange ($\Theta(P)$)
  - Processes exchange metadata (sizes) about neighborhoods with all-to-all
  - Processes post receives afterwards
  - Most intuitive but least performance andscalability!



T. Hoefler et al.:Scalable Communication Protocols for Dynamic Sparse Data Exchange

REDUCE_SCATTER (PCX)

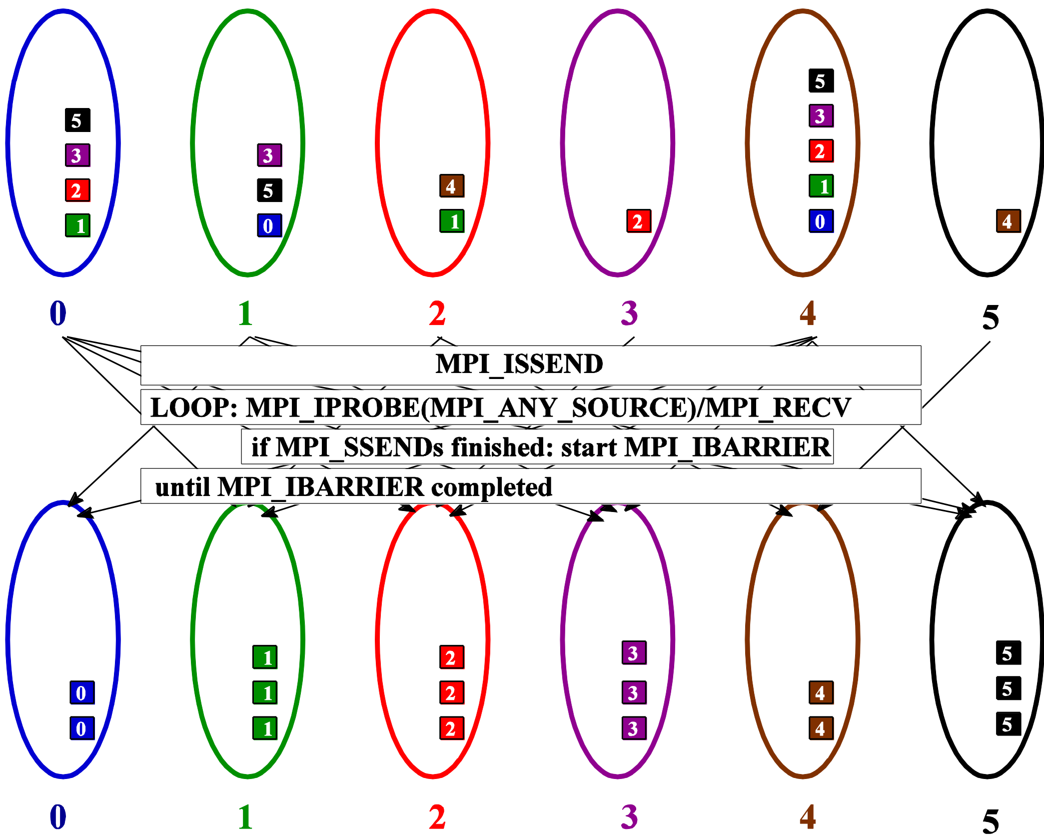
- Bases on Personalized Census ($\Theta(P)$)
  - Processes exchange metadata (counts) about neighborhoods with reduce_scatter
  - Receivers checks with wildcard MPI_IPROBE and receives messages
  - Better than PEX but non-deterministic!



T. Hoefler et al.:Scalable Communication Protocols for Dynamic Sparse Data Exchange

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!

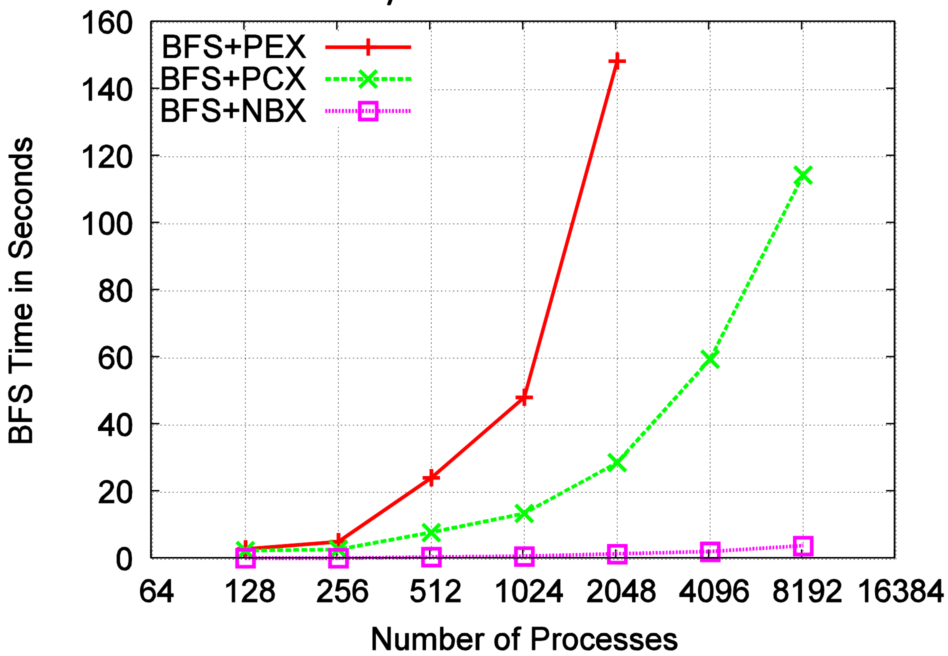


T. Hoefler et al.:Scalable Communication Protocols for Dynamic Sparse Data Exchange

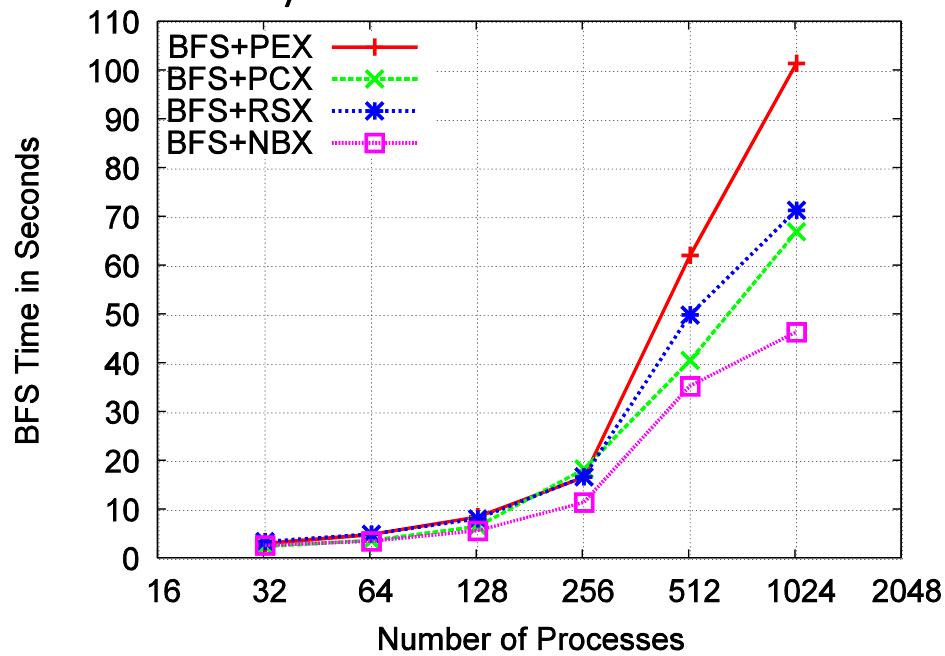
PARALLEL BREADTH FIRST SEARCH

- 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!

T. Hoefler et al.:Scalable Communication Protocols for Dynamic Sparse Data Exchange

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
```

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FFT Software Pipelining

```
NBC_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
  NBC_Ialltoall(&in, n/p*n/p/bs, cplx_t, &out, n/p*n/p, cplx_t, comm, &req[b]);
}
NBC_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
```

Hoefler: Leveraging Non-blocking Collective Communication in High-performance Applications

A Complex Example: FFT

- Main parameter: nb vs. n → blocksize
- Strike balance between k-1st alltoall and kth FFT stencil block
- Costs per iteration:
  - Alltoall (bandwidth) costs: $T_{a2a} \approx n^2/p/nb * \beta$
  - FFT costs: $T_{fft} \approx n/p/nb * T_{1DFFT}(n)$
- Adjust blocksize parameters to actual machine
  - Either with model or simple sweep

Hoefler: Leveraging Non-blocking Collective Communication in High-performance Applications

Nonblocking And Collective Summary

- Nonblocking comm does two things:
  - Overlap and relax synchronization
- Collective does one thing
  - Specialized pre-optimized routines
  - Performance portability
  - Hopefully transparent performance
- They can be composed
  - E.g., software pipelining

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

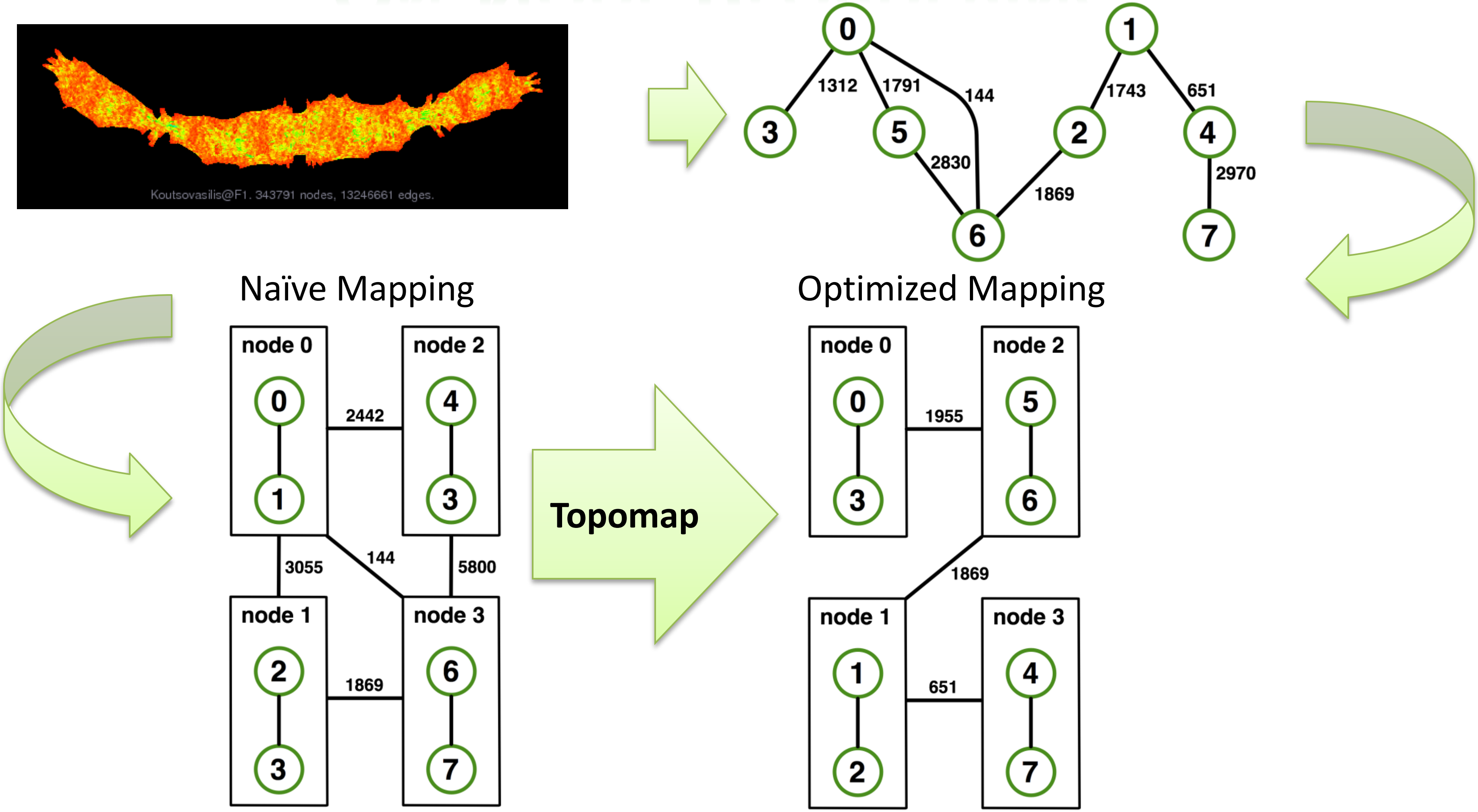
Topology Mapping Basics

- 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

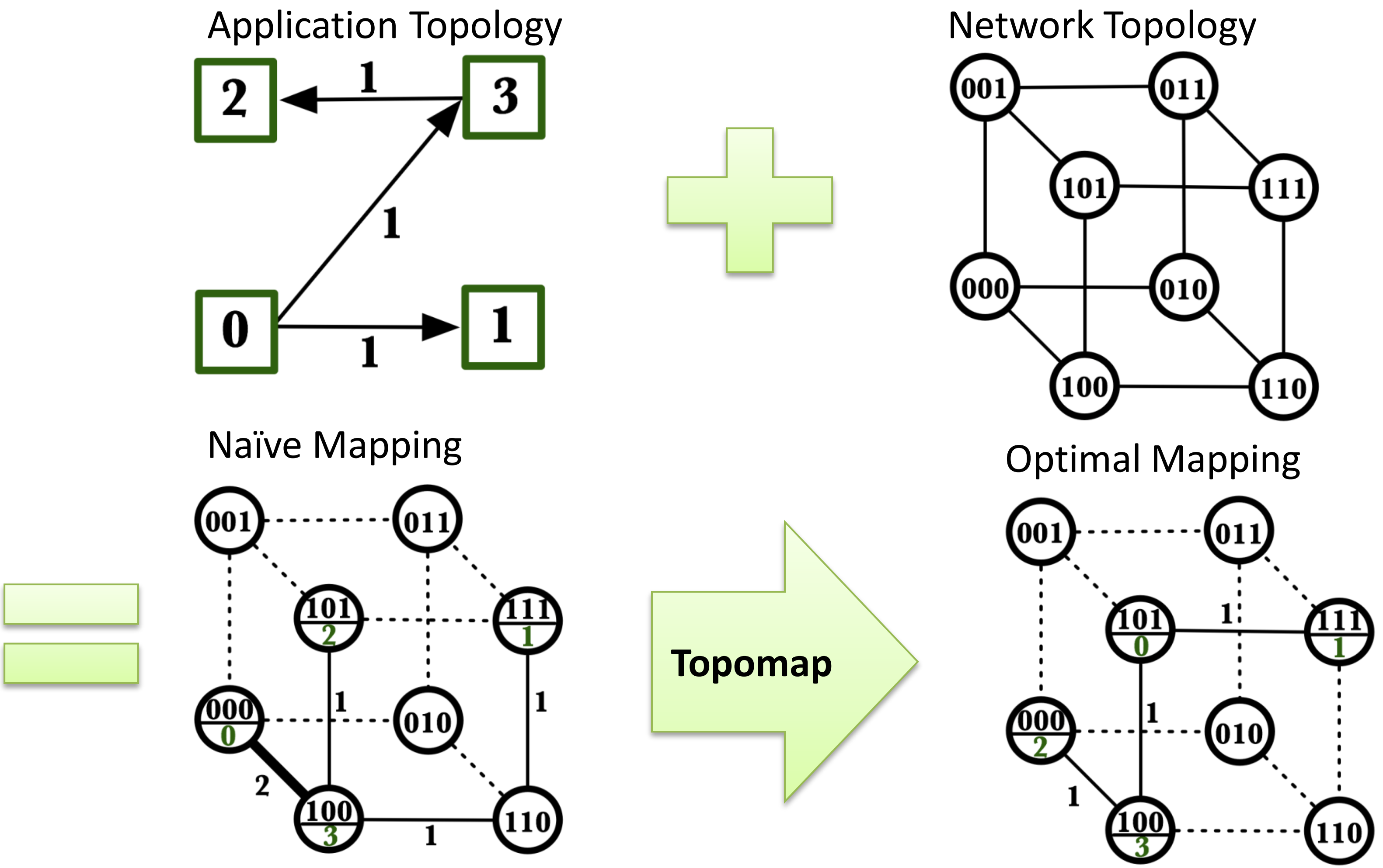
- Rank reordering
  - Change numbering in a given allocation to reduce congestion or dilation
  - Sometimes automatic (early IBM SP machines)
- Properties
  - Always possible, but effect may be limited (e.g., in a bad allocation)
  - Portable way: MPI process topologies
    - Network topology is not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

On-Node Reordering



Gottschling and Hoefler: Productive Parallel Linear Algebra Programming with Unstructured Topology Adaption

Off-Node (Network) Reordering



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);
```

- Makes life a little bit easier
  - Some problems may be better with a non-square layout though

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

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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  - 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

MPI_DIST_GRAPH_CREATE_ADJACENT

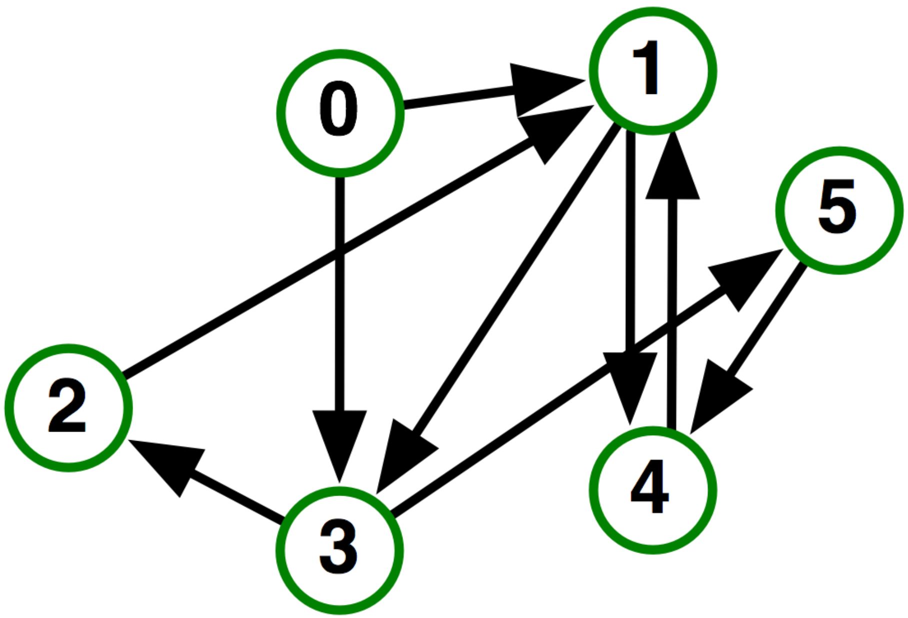
```
MPI_Dist_graph_create_adjacent(MPI_Comm comm_old, int indegree, const int sources[], const int sourceweights[], int outdegree, const int destinations[], const int destweights[], MPI_Info info,int reorder, MPI_Comm *comm_dist_graph)
```

- 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)

Hoefler et al.: The Scalable Process Topology Interface of MPI 2.2

MPI_DIST_GRAPH_CREATE_ADJACENT

- Process 0:
  - Indegree: 0
  - Outdegree: 1
  - 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

MPI_DIST_GRAPH_CREATE

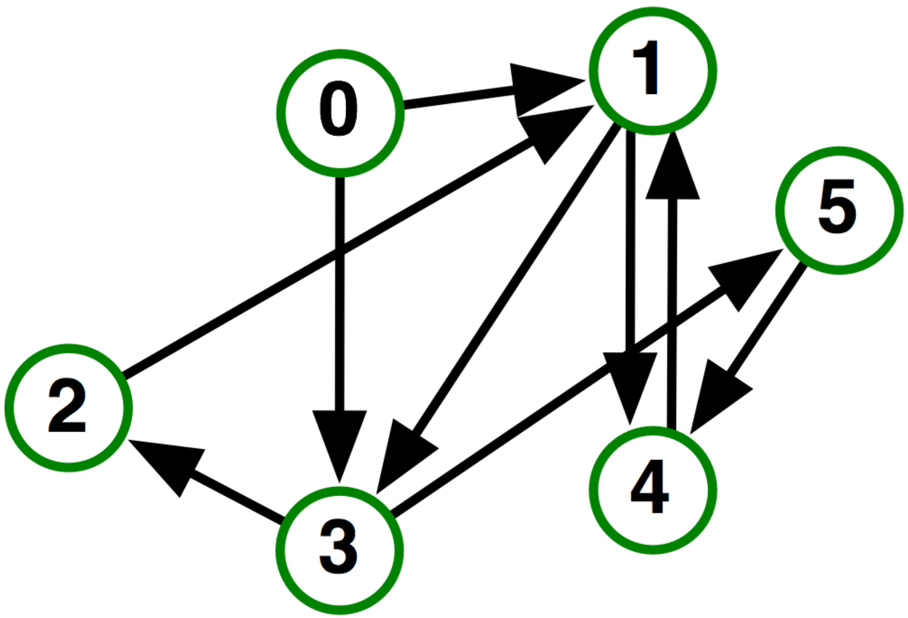
MPI_Dist_graph_create(MPI_Comm comm_old, int n, const int sources[], const int degrees[], const int destinations[], const int weights[], MPI_Info info, int reorder, MPI_Comm *comm_dist_graph)

- 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

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}
- …



Hoefler et al.: *The Scalable Process Topology Interface of MPI 2.2*

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

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!

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!

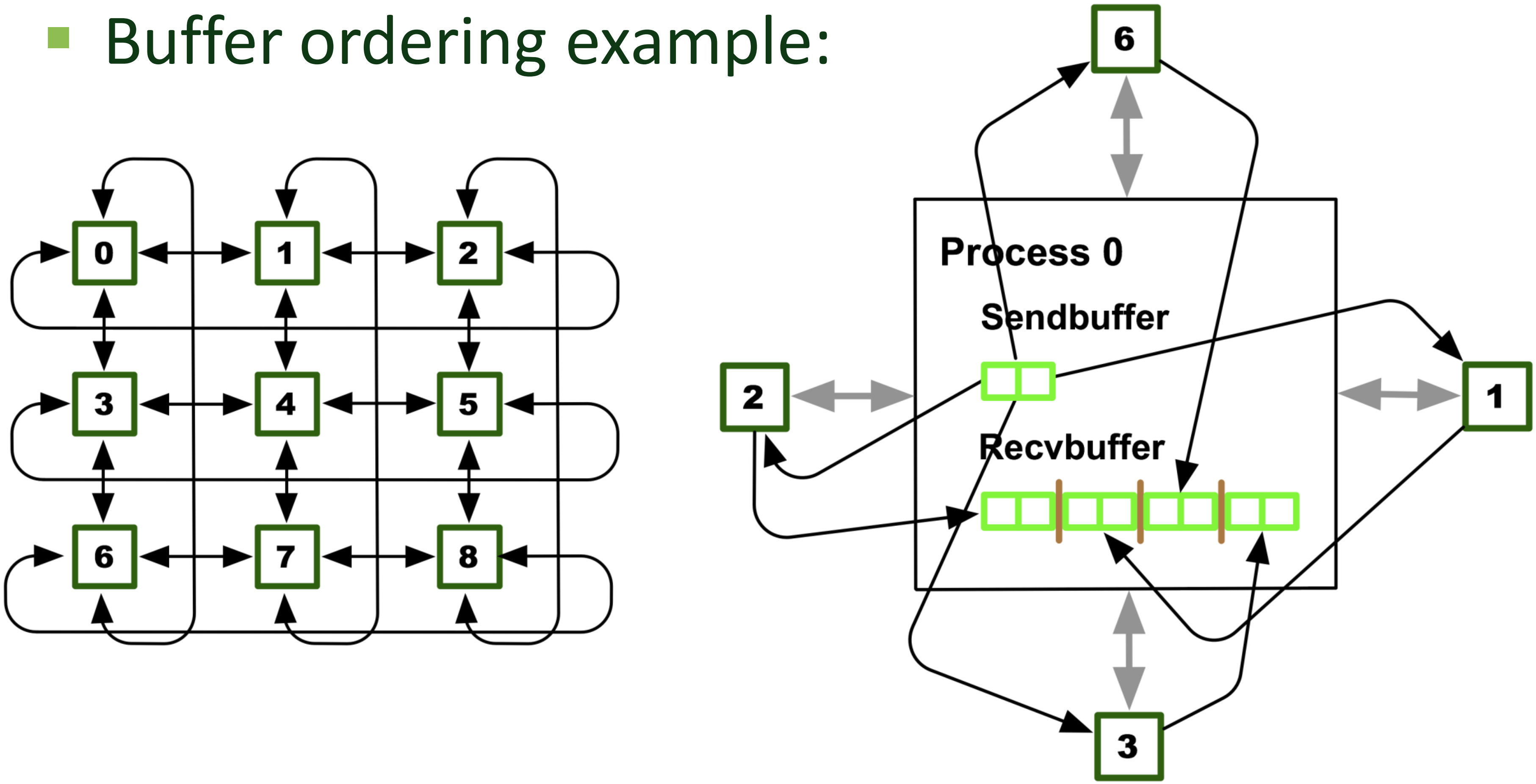
Cartesian Neighborhood Collectives

- 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)!

T. Hoefler and J. L. Traeff: Sparse Collective Operations for MPI

Cartesian Neighborhood Collectives

- Buffer ordering example:



T. Hoefler and J. L. Traeff: Sparse Collective Operations for MPI

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!

T. Hoefler and J. L. Traeff: Sparse Collective Operations for MPI

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 and w versions 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!

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

T. Hoefler and J. L. Traeff: Sparse Collective Operations for MPI

Stencil Example

- Two options: use DDTs or not
- Without DDTs:
  - Change packing loops to pack into one buffer
  - Use alltoallv along Cartesian topology
- Using DDTs:
  - Use alltoallw with correct offsets and types
  - Even more power to MPI
    - Complex DDT optimizations possible

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 - 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

- It's 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)
```

- 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

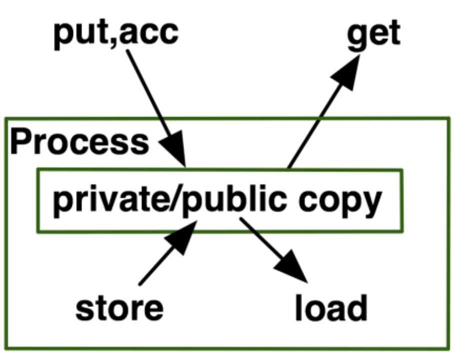
SYNCHRONIZATION PRIMITIVES (PASSIVE)

MPI_Win_sync(MPI_Win win)

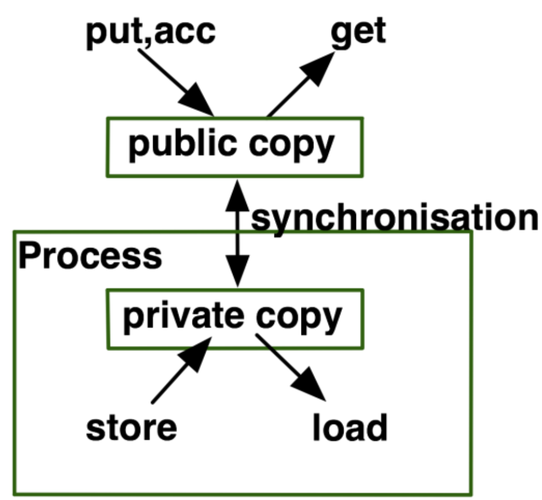
- Synchronizes private and public window copies
  - Same as closing and opening access and exposure epochs on the window
  - Does not complete any operations though!
- Cf. memory barrier

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:

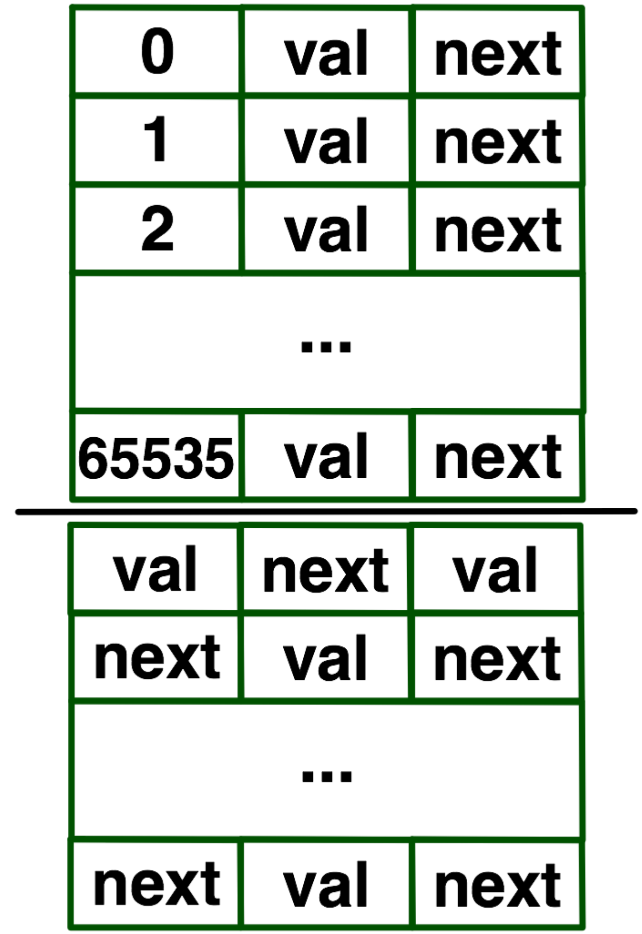
	Load	Store	Get	Put	Acc
Load	OVL+NOVL	OVL+NOVL	OVL+NOVL	NOVL+BOVL	NOVL+BOVL
Store	OVL+NOVL	OVL+NOVL	NOVL	NOVL	NOVL
Get	OVL+NOVL	NOVL	OVL+NOVL	NOVL	NOVL
Put	NOVL+BOVL	NOVL	NOVL	NOVL	NOVL
Acc	NOVL+BOVL	NOVL	NOVL	NOVL	OVL+NOVL

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

Credits: RMA Working Group, MPI Forum

Distributed Hashtable Example

- 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 VI - 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

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