

High Performance Computing

Advanced MPI: Topologies

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High Performance Computing: MPI topics and algorithms

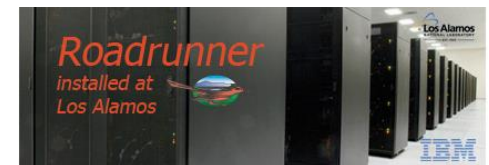
- “Advanced” features of MPI (Message-Passing Interface): **Collective operations**, non-blocking collectives, sparse collectives, **datatypes**, one-sided communication, **process topologies**, MPI I/O, ...
- **Efficient implementation of MPI collectives**: Algorithms under (simplified) network assumptions
- Useful for implementation of own algorithms, libraries, etc.

MPI: the "Message-Passing Interface"

- Library with C and Fortran bindings that implements a message-passing model
- Current *de facto* standard in HPC and distributed memory parallel computing



PGAS competitors:
UPC, CaF, OpenSHMEM, ...



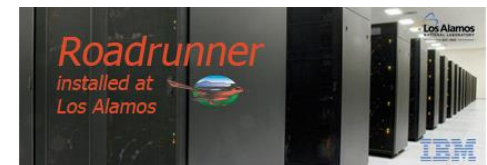
MPI: the "Message-Passing Interface"

- Library with C and Fortran bindings that implements a message-passing model
- Current *de facto* standard in HPC and distributed memory parallel computing

Open source implementations:

- `mpich` from Argonne National Laboratory (ANL)
- `mvapich` from Ohio State
- OpenMPI, community effort

from which many special purpose/vendor implementations are derived



mpich(2) canonical references

William Gropp, Ewing L. Lusk, Nathan E. Doss, Anthony Skjellum: A High-Performance, Portable Implementation of the MPI Message Passing Interface Standard. *Parallel Computing* 22(6): 789-828 (1996)

William Gropp, Ewing L. Lusk: Sowing mpich: a Case Study in the Dissemination of a Portable Environment for Parallel Scientific Computing. *IJHPCA* 11(2): 103-114 (1997)

William Gropp, Ewing L. Lusk: A High-Performance MPI Implementation on a Shared-Memory Vector Supercomputer. *Parallel Computing* 22(11): 1513-1526 (1997)

Rajeev Thakur, Rolf Rabenseifner, William Gropp: Optimization of Collective Communication Operations in MPICH. *IJHPCA* 19(1): 49-66 (2005)

Open MPI canonical references

Richard L. Graham, Brian Barrett, Galen M. Shipman, Timothy S. Woodall, George Bosilca: Open MPI: a High Performance, Flexible Implementation of MPI Point-to-Point Communications. *Parallel Processing Letters* 17(1): 79-88 (2007)

Edgar Gabriel, Graham E. Fagg, George Bosilca, Thara Angskun, Jack J. Dongarra, Jeffrey M. Squyres, Vishal Sahay, Prabhanjan Kambadur, Brian Barrett, Andrew Lumsdaine, Ralph H. Castain, David J. Daniel, Richard L. Graham, Timothy S. Woodall: Open MPI: Goals, Concept, and Design of a Next Generation MPI Implementation. *PVM/MPI 2004*: 97-104

Richard L. Graham, Timothy S. Woodall, Jeffrey M. Squyres: Open MPI: A Flexible High Performance MPI. *PPAM 2005*: 228-239

Message-passing model

- Processors (in **MPI**: processes - something executed by a physical processor/core) execute program on local data
- Processors exchange data and synchronize by **explicit communication**; only way to exchange information ("shared nothing")

Program: MIMD, SPMD

Communication:

- Asynchronous (non-blocking) or synchronous (blocking)
- In-order, out of order
- One-to-one, one-to-many, many-to-one, many-to-many

Strict message-passing (theoretical model):

Synchronous, in-order, one-to-one communication: Enforces event order, easier to reason about correctness, mostly deterministic execution, no race-conditions

Hoare: CSP

Practical advantages:

- Enforces locality (no cache sharing, less memory per process)
- Synchronous communication can be implemented space efficiently (no intermediate buffering)

Recent: GO

May: OCCAM

C. A. R. Hoare: Communicating Sequential Processes. Comm. ACM 21(8): 666-677 (1978)

MPI message-passing model

Three main communication models:

MPI_Send



MPI_Recv



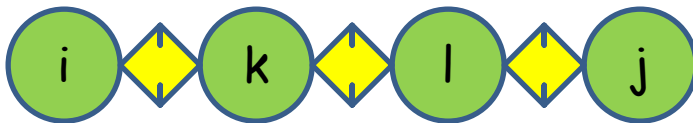
Point-to-point: Two processes explicitly involved

MPI_Put/Get/Accumulate



One-sided: One process explicitly involved

MPI_Bcast



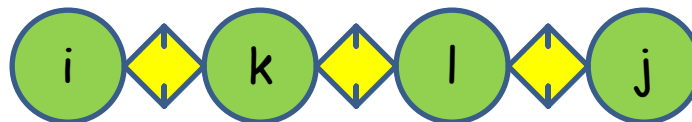
Collective: $p \geq 1$ processes explicitly involved

MPI message-passing model

All communication between **named processes** in same communication domain:

Communication domain ("communicator"): Ordered set of processes that can communicate (e.g., `MPI_COMM_WORLD`)

Name: For domain of p processes, rank between 0 and $p-1$



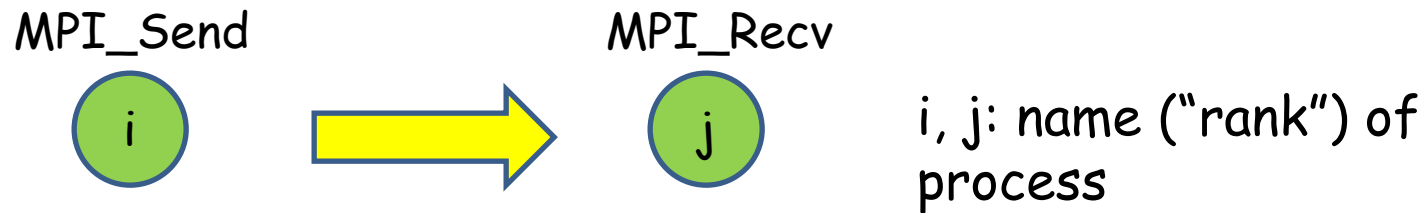
Note:

MPI is a **specification**; **not an implementation** (term “MPI library” refers to specific implementation of the standard)

MPI specification/standard prescribes (almost) nothing about the implementation, in particular:

- **No performance model** (thus no assumptions on communication network)
- **No performance guarantees**
- No prescribed algorithms (for collective communication, synchronization, datatypes etc.)
- But: Some assumptions about “High Quality implementation”

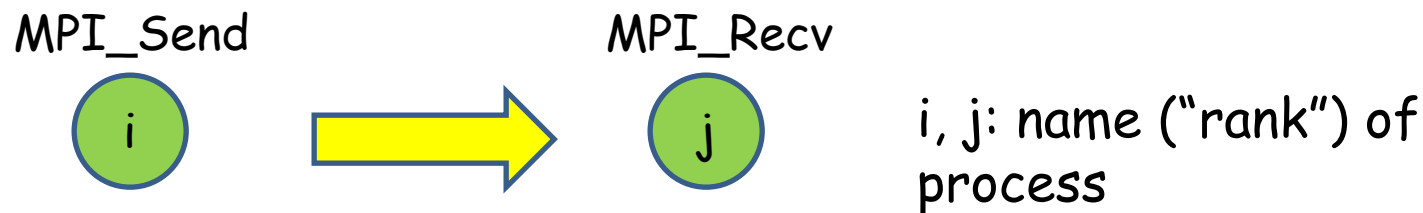
Point-to-point communication



- Both sender and receiver explicitly involved in communication
- Communication is **reliable** (implementation and underlying communication infrastructure must guarantee this)
- Communication is **ordered**: Messages with same destination and same tag arrive in order sent (implementation must guarantee this)

(*) Whether MPI_Send can complete may depend on MPI implementation

Point-to-point communication



- Largely asynchronous model: MPI_Send has semi-local completion semantics, when call completes buffer can be reused (*)
- Blocking and **non-blocking** ("immediate") semantics

Blocking MPI call:

Returns when operation locally complete, buffer can be reused, **may or may not depend** on actions of other processes, no guarantee regarding state of other processes

Point-to-point communication

MPI_Isend



MPI_Irecv



i, j: name ("rank") of process

- Largely asynchronous model: MPI_Send has semi-local completion semantics, when call completes buffer can be reused
- Blocking and **non-blocking** ("immediate") semantics

Non-blocking MPI call:

Returns immediately, independent of actions of other processes, buffer may be in use. Completion as in blocking call must be enforced (MPI_Wait, MPI_Test, ...)

Point-to-point communication

MPI_Isend



MPI_Irecv



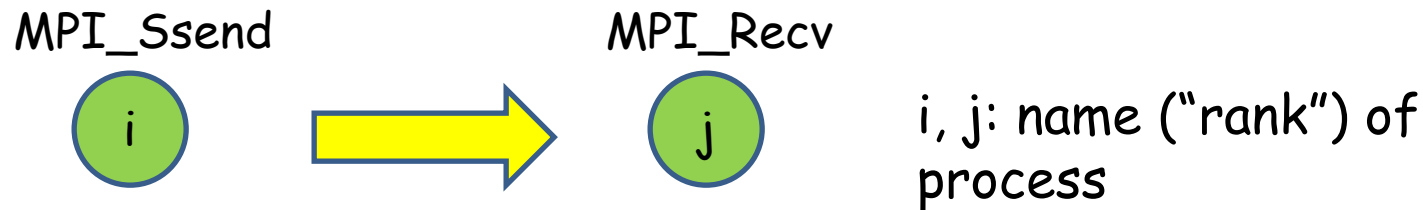
i, j: name ("rank") of process

- Largely asynchronous model: MPI_Send has semi-local completion semantics, when call completes buffer can be reused
- Blocking and **non-blocking** ("immediate") semantics

Terminology note:

Non-blocking in MPI is **not** a non-blocking **progress condition**, but means that the calling process can continue; progress of communication eventually depends on progress of other process

Point-to-point communication



- Largely asynchronous model: MPI_Send has semi-local completion semantics, when call completes buffer can be reused
- Blocking and **non-blocking** ("immediate") semantics
- Many send "modes": MPI_Ssend (MPI_Bsend, MPI_Rsend)

```
int x[count];  
MPI_Ssend(x, count, MPI_INT, dest, tag, comm);
```


Point-to-point communication

MPI_Issend



MPI_Irecv

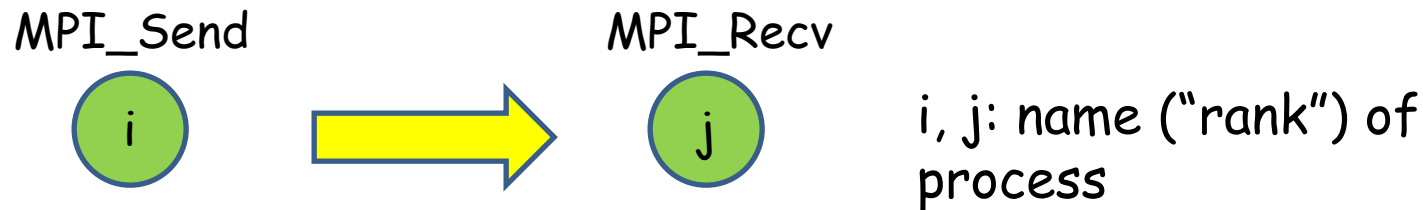


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- Many send "modes": MPI_Ssend (MPI_Bsend, MPI_Rsend)

```
int x[count];  
MPI_Issend(x, count, MPI_INT, dest, tag, comm,  
           &request);
```

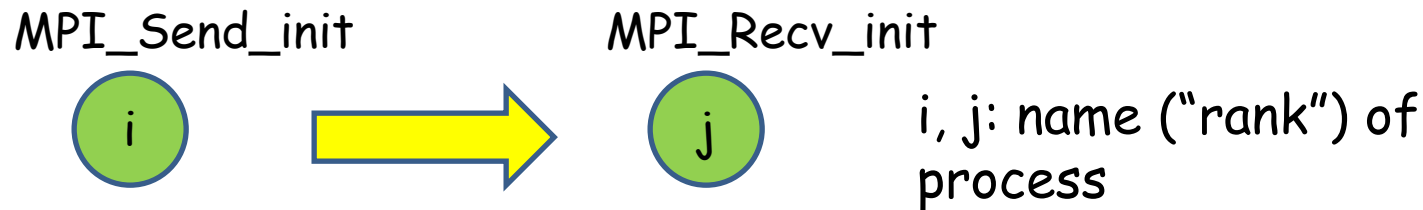
Point-to-point communication



- Largely asynchronous model: MPI_Send has semi-local completion semantics, when call completes buffer can be reused
- Blocking and **non-blocking** ("immediate") semantics
- Non-determinism only through "wildcards" in MPI_Recv

```
int x[count];  
MPI_Recv(x, count, MPI_INT, MPI_ANY_SOURCE,  
         MPI_ANY_TAG, comm, &status);
```

Point-to-point communication

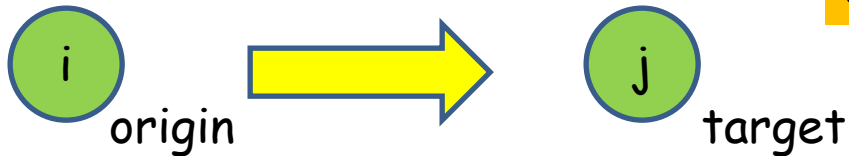


- Persistent versions of all blocking point-to-point operations
- Optimization potential: All parameters bound at initialization call (in `MPI_Request` object), can be reused, algorithm can be adapted to use case (parameters, process mapping, etc.)

```
MPI_Request request[2];
MPI_Recv_init(x, count, MPI_INT, MPI_ANY_SOURCE,
              MPI_ANY_TAG, comm, &request[0]);
MPI_Ssend_init(y, count, MPI_INT, j, TAG, comm,
               &request[1]);
MPI_Startall(2, request);
```

One-sided communication

MPI_Put/Get/Accumulate

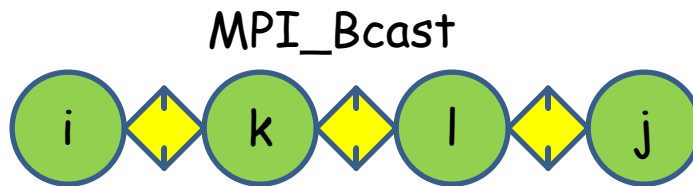


Introduced with MPI 2.0

News in MPI 3.0

- Only one process explicitly involved in communication; origin supplies all information
- Communication is **reliable**, but **not ordered**
- Non-blocking communication, completion at synchronization point
- Different types of synchronization (active/passive; collective/localized)
- Target memory in exposed/accessible window

Collective communication

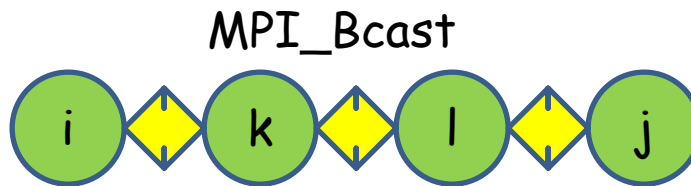


News in MPI 3.0

- All processes explicitly involved in data exchange or compute operation (one-to-many, many-to-one, many-to-many)
- All collective operations blocking in the MPI sense: Return when operation is locally complete, buffers can be reused
- Operations are **reliable**
- Collectives (except for MPI_Barrier) are **not synchronizing**

```
float *buffer = malloc(count*sizeof(float));  
MPI_Bcast(buffer, count, MPI_FLOAT, root, comm);
```

Collective communication



Synchronizing:

MPI_Barrier

Exchange, regular, rooted

MPI_Bcast

MPI_Gather/MPI_Scatter

Non-rooted (symmetric)

MPI_Allgather

MPI_Alltoall

Reduction, regular, rooted

MPI_Reduce

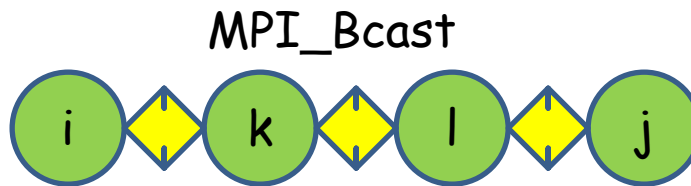
Non-rooted (symmetric)

MPI_Allreduce

MPI_Reduce_scatter_block

MPI_Scan/MPI_Exscan

Collective communication



Exchange, irregular (vector)

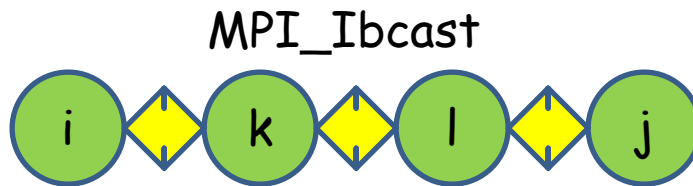
MPI_Gatherv/MPI_Scatterv
MPI_Allgatherv
MPI_Alltoallv/MPI_Alltoallw

Reduction, irregular (vector)

MPI_Reduce_scatter

Irregular collective: Size and basetype (technically: type signature) of buffers must match pairwise between processes, but can differ between different pairs

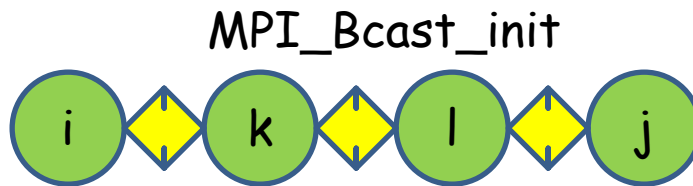
Collective communication



With MPI 3.0

- All 17 collectives in **non-blocking** versions
- Call returns immediately, independent of actions of other processes
- Completion with same semantics as blocking counterpart must be explicitly enforced (MPI_Wait, MPI_Waitall, ...)

Collective communication



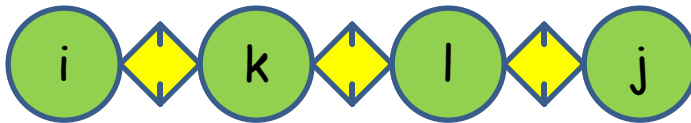
With MPI 4.0

- All 17 collectives in persistent versions
- Optimization potential: All parameters bound at initialization call (in `MPI_Request` object), can be reused, algorithm can be adapted to use case (parameters, process mapping, etc.)

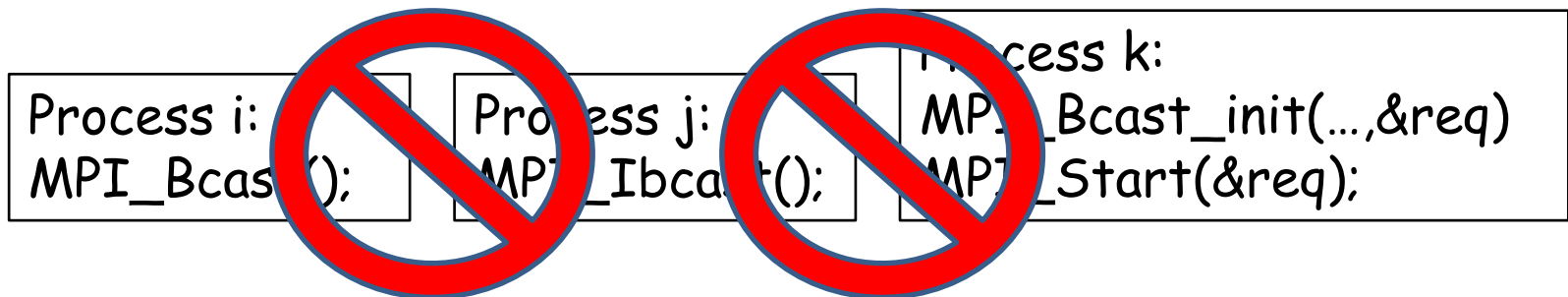
```
MPI_Barrier_init(comm, MPI_INFO_NULL, &request);
while (1) {
    MPI_Start(&request); // start the barrier
    MPI_Wait(&request);  // now enforce the barrier
}
MPI_Request_free(&request);
```

Collective communication

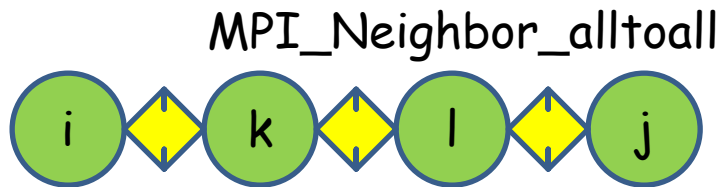
MPI_Bcast, MPI_Ibcast, MPI_Bcast_init



- Although semantically equivalent, blocking, non-blocking, and persistent collective cannot be used together
- Different from persistent point-to-point: modes can be mixed



Collective communication



With MPI 3.0 and
MPI 4.0

- 5 sparse (neighbor) collective operations, in blocking, non-blocking and persistent versions

Non-rooted (symmetric)

MPI_Neighbor_allgather
MPI_Neighbor_alltoall

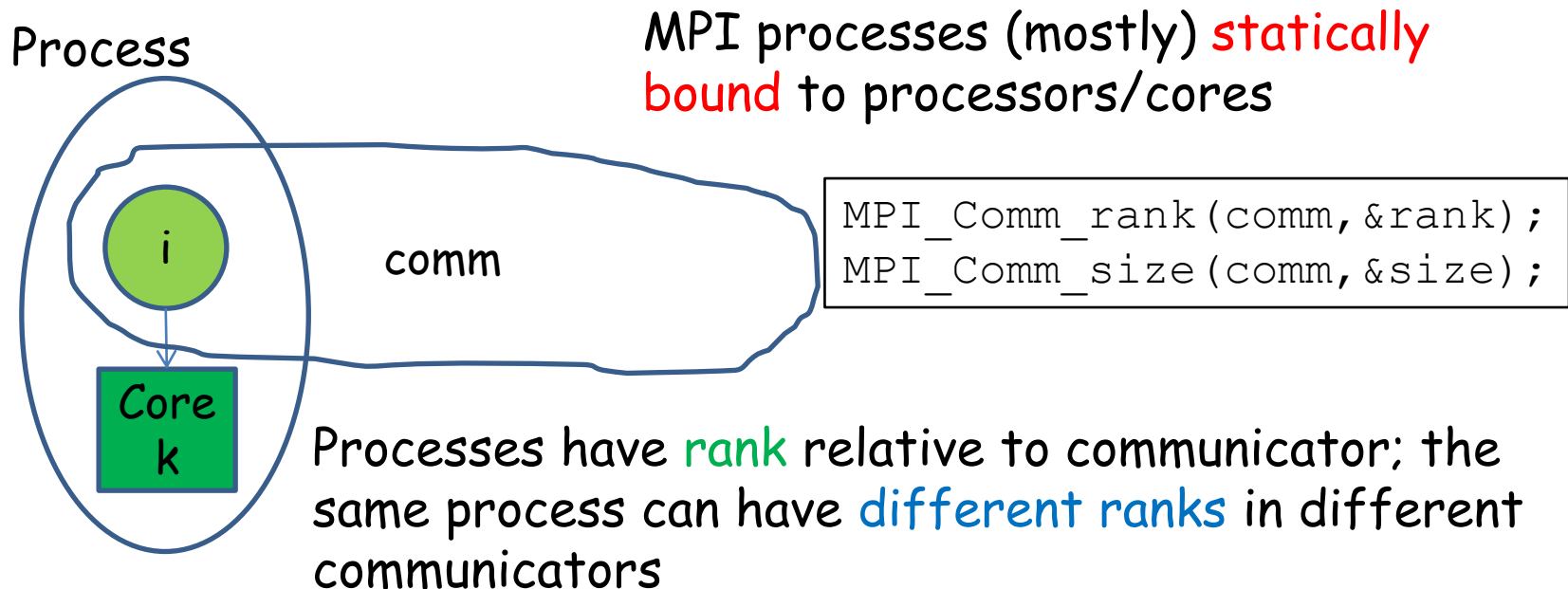
Exchange, irregular (vector)

MPI_Neighbor_allgatherv
MPI_Neighbor_alltoallv
MPI_Neighbor_alltoallw

All models

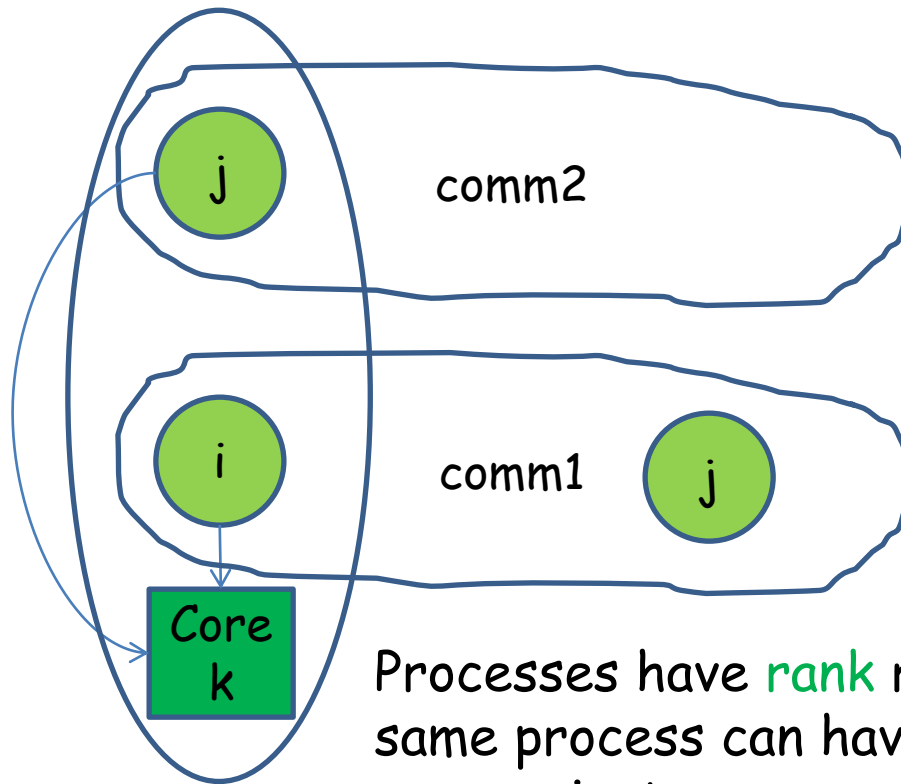
Communication is wrt. **communicator**: Ordered set of processes, mapped to physical nodes/processors/cores

In one-sided model, communicator is part of **memory-window**



MPI has multi-purpose (collective) operations for creating new communicators out of old ones. If a different mapping is needed, new communicator must be created (**MPI objects are static**)

Process



Process with rank j in comm1 may have to send state/data to the process with rank j in comm2

Processes have **rank** relative to communicator; the same process can have **different ranks** in different communicators

For discussion on collective interfaces, sparse (neighbor) and global communication, and the relation to communicators, see

Jesper Larsson Träff, Sascha Hunold, Guillaume Mercier, Daniel J. Holmes: MPI collective communication through a single set of interfaces: A case for orthogonality. *Parallel Comput.* 107: 102826 (2021)

Many interesting things to do for (paid) Master's thesis...

All models

- Data in buffers can be arbitrarily structured, not necessarily only consecutive elements
- Data structure/layout communicated to MPI implementation by datatype handle
- Communication buffers: Buffer start (address), element count, element datatype



e.g. indexed datatype

MPI terms: Derived datatypes, user-defined datatypes, ... (MPI 3.1 standard, Chapter 4)

Beyond message-passing MPI features

- MPI-IO: Serial and parallel IO, heavy use of derived datatypes in specification
- MPI process management (important concept: intercommunicators): Coarse grained management (spawn, connect) of additional processes
- Topologies: Mapping application communication patterns to communication system
- Tools support: Profiling interface and library information

Concrete example (MPI code recap)

- C code (could also be “mild” C++)
- What to include, what to define
- Using assertions
- Good SPMD style: program works for all numbers of processes
- Compiling and running (environment dependent)

```
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
```

```
#include <mpi.h>
// #define NDEBUG
#include <assert.h>
```



Good practice: Make assertions

```
#define SRTAG 777
```

```
int main(int argc, char *argv[])
{
    MPI_Comm comm;
    int rank, size;
    int root;
```

```
MPI_Init(&argc, &argv);
```



MPI library must be initialized

```
// [...] Here comes the code
```

```
MPI_Finalize();
```



... and finalized

```
return 0;
```

```
}
```

The code, part 1: Two processes communicate (first and last)

```
MPI_Comm_dup(MPI_COMM_WORLD, &comm);
MPI_Comm_rank(comm, &rank);
MPI_Comm_size(comm, &size);
assert(rank < size);
```

New comm for this

Assert simple assumptions

```
int r;
```

Buffers always have this structure: Address, count, type

```
if (rank == 0) {
    MPI_Sendrecv(&rank, 1, MPI_INT, size-1, SRTAG,
                 &r, 1, MPI_INT, size-1, SRTAG,
                 comm, MPI_STATUS_IGNORE);
```

```
    assert(r == size-1);
```

```
} else if (rank == size-1) {
```

```
    MPI_Sendrecv(&rank, 1, MPI_INT, 0, SRTAG,
                 &r, 1, MPI_INT, 0, SRTAG,
                 comm, MPI_STATUS_IGNORE);
```

```
    assert(r == 0);
```

```
}
```

Good SPMD style: All sizes

The code, part 2: All processes communicate collectively

```
int *allrank;  
allrank = (int*)malloc(size*sizeof(int));  
for (root=0; root<size; root++) {  
    allrank[root] = rank;  
    MPI_Bcast(&allrank[root],1,MPI_INT,root,comm);  
    assert(allrank[root]==root);  
}  
int *ar;  
ar = (int*)malloc(size*sizeof(int));  
MPI_Allgather(&rank,1,MPI_INT,  
              ar,    1,MPI_INT,comm);  
for (root==0; root<size; root++)  
    assert(ar[root]==allrank[root]);  
  
free(allrank);  
free(ar);
```

No stack allocation

Buffer structure, but beware: one block

Allgather is Bcast from all

Free after use, don't forget

Running the code (on hydra):

```
> scp mpiintro.c <account>@hydra:~/  
> ssh hydra  
> module avail  
> module load mpi/openmpiS  
> mpicc -o intro -O3 mpiintro.c  
> srun -N 10 --tasks-per-node=32 ./intro  
>
```

Now on hydra

See doku.par.tuwein.ac.at for more

Example: Three algorithms for matrix-vector multiplication

$m \times n$ matrix A and n -element vector x distributed evenly across p MPI processes: compute

$$y = Ax$$

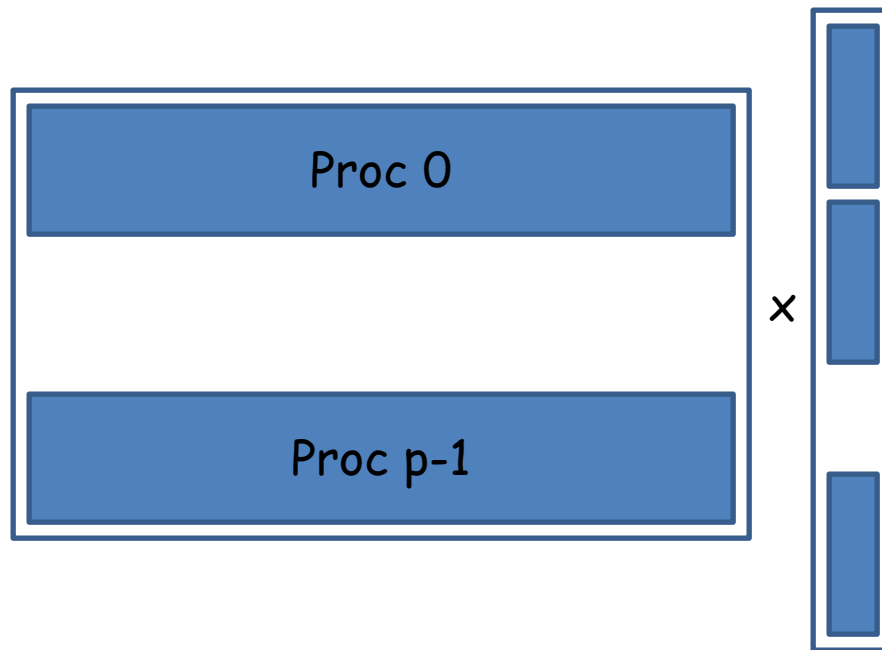
with y the m -element result vector

Even distribution:

- Each of p processes has an $m \cdot n/p$ element submatrix, an n/p element subvector, and computes an m/p element result vector.
- Algorithms should respect/preserve distribution

$$\begin{pmatrix} y_0 \\ y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} A_0 \\ A_1 \\ A_2 \end{pmatrix} \begin{pmatrix} x_0 \\ x_1 \\ x_2 \end{pmatrix}$$

A_i : $(m/p) \times n$ matrix



Algorithm 1:

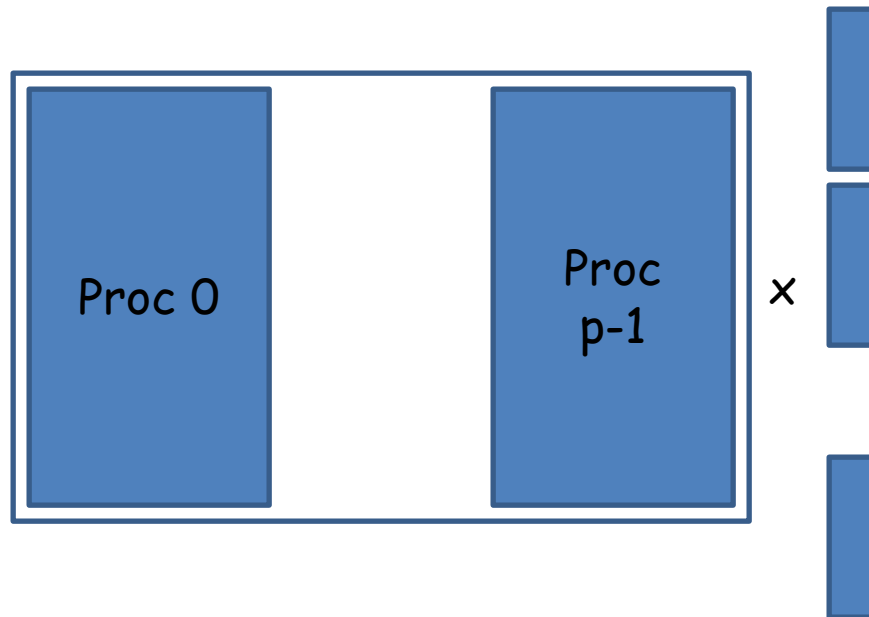
- Row-wise matrix distribution
- Each process needs full vector:
`MPI_Allgather(v)`
- Compute blocks of result vector locally

Conjecture: $T(m,n,p) = O((m/p)n + n + \log p)$, $p \leq m$

Why?

$$\begin{bmatrix} y_0 \\ y_1 \\ y_2 \end{bmatrix} = A_0 x_0 + A_1 x_1 + A_2 x_2$$

$A = (A_0 \mid A_1 \mid A_2)$, A_i $m \times (n/p)$ matrix



Algorithm 2:

- Column-wise matrix distribution
- Compute local partial result vector
- [`MPI_Reduce_scatter`](#) to sum and distribute partial results

Conjecture: $T(m,n,p) = O(m(n/p) + m + \log p)$, $p \leq n$

Why?

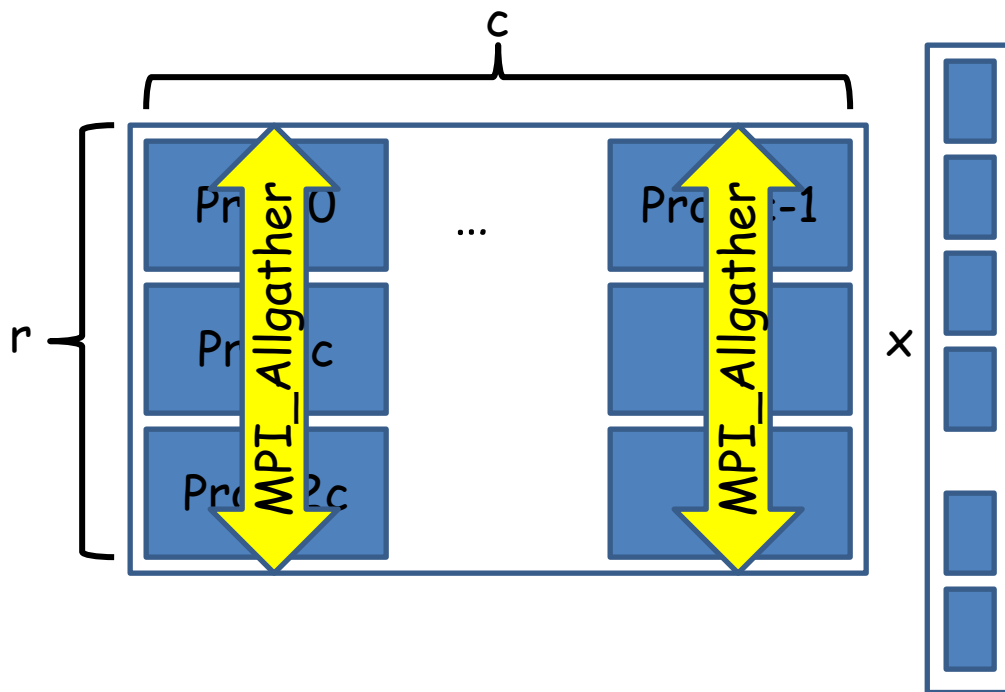
Conjecture:

- $\text{MPI_Allgatherv}(n)$ can be done in $O(n + \log p)$ communication steps
- $\text{MPI_Reduce_scatter}(n)$ can be done in $O(n + \log p)$ communication steps

for certain types of networks, and not better (regardless of network)

This lecture:
Will substantiate the conjectures (constructions and proofs)

Factor $p = rc$, each process has $m/r \times n/c$ submatrix and $n/rc = n/p$ subvector

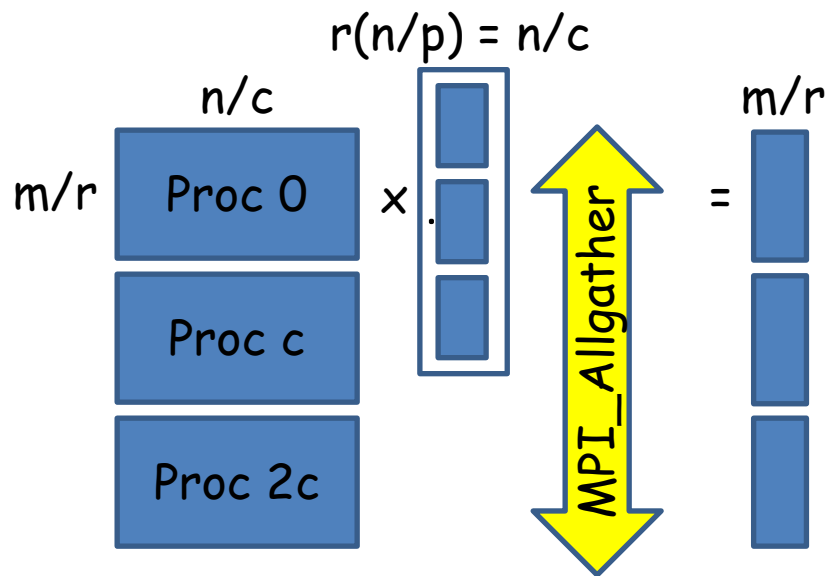


Algorithm 3:

- Matrix distribution into blocks of $m/r \times n/c$ elements
- Algorithm 1 on columns
- Algorithm 2 on rows

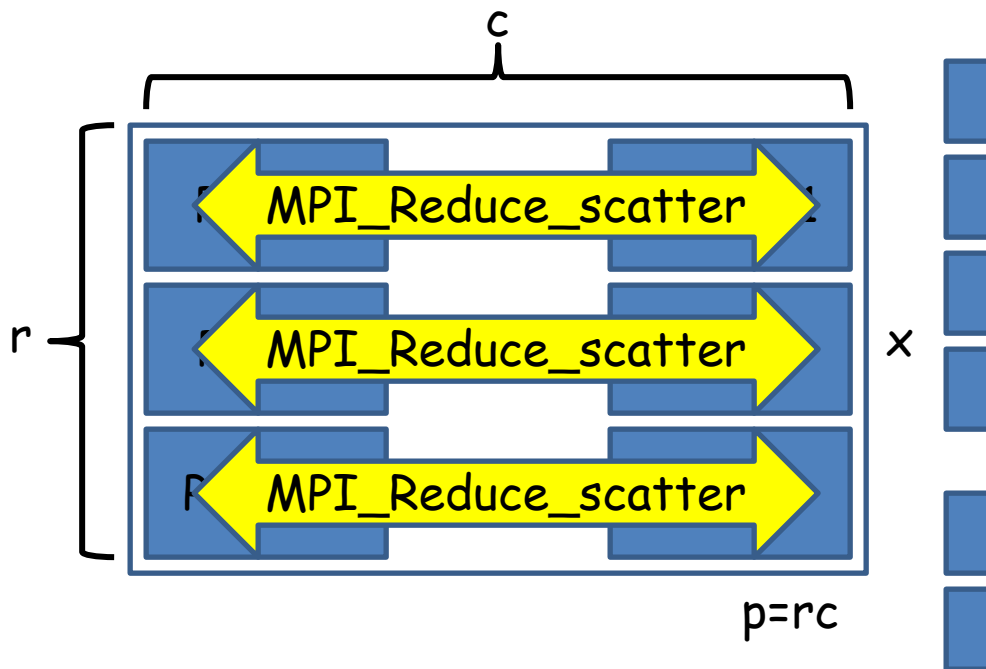
Step 1: Simultaneous $\text{MPI_Allgather}(v)$ on all c process columns

Factor $p = rc$, each process has $m/r \times n/c$ submatrix and $n/rc = n/p$ subvector



Step 1: Simultaneous `MPI_Allgather(v)` on all c process columns

Factor $p = rc$, each process has $m/r \times n/c$ submatrix and $n/rc = n/p$ subvector

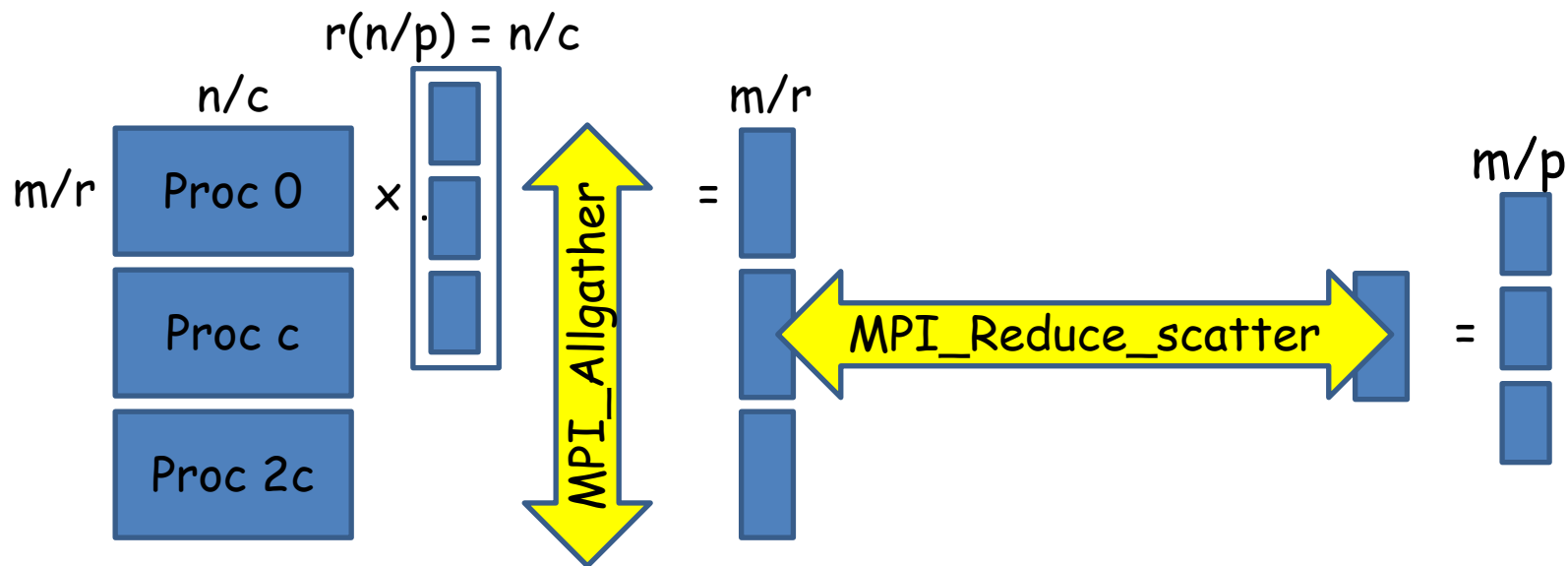


Algorithm 3:

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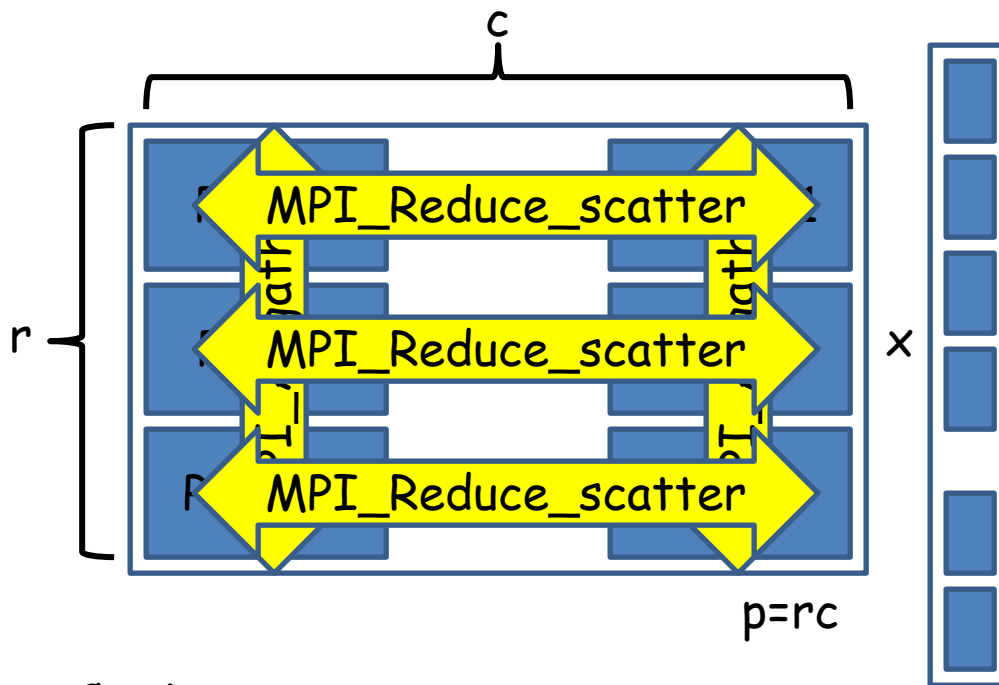
Step 4: Simultaneous `MPI_Reduce_Scatter(_block)` on process row communicators

Factor $p = rc$, each process has $m/r \times n/c$ submatrix and $n/rc = n/p$ subvector



Step 4: Simultaneous `MPI_Reduce_Scatter(_block)` on process row communicators

Factor $p = rc$, each process has $m/r \times n/c$ submatrix and $n/rc = n/p$ subvector



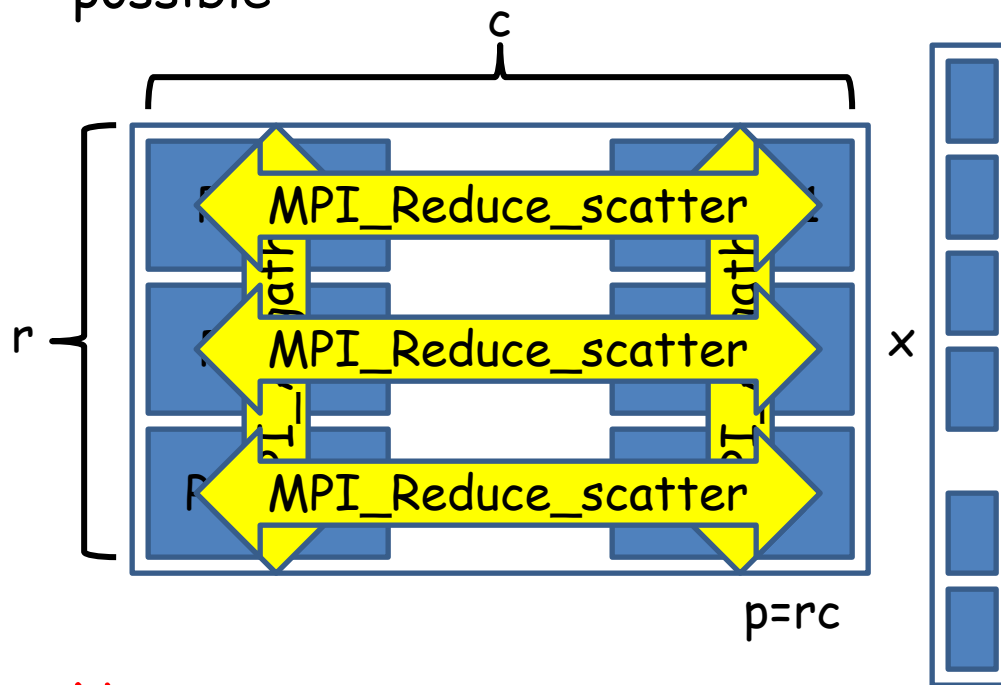
Algorithm 3:

- Matrix distribution into blocks of $m/r \times n/c$ elements
- Algorithm 1 on columns
- Algorithm 2 on rows

Conjecture:

$$T(m,n,p) = O(mn/p + n/c + m/r + \log p), p \leq \min(mc, nr)$$

Algorithm 3 is more **scalable**. To implement the algorithm, **essential** that independent, simultaneous, collective communication on (column and row) subsets of processes is possible



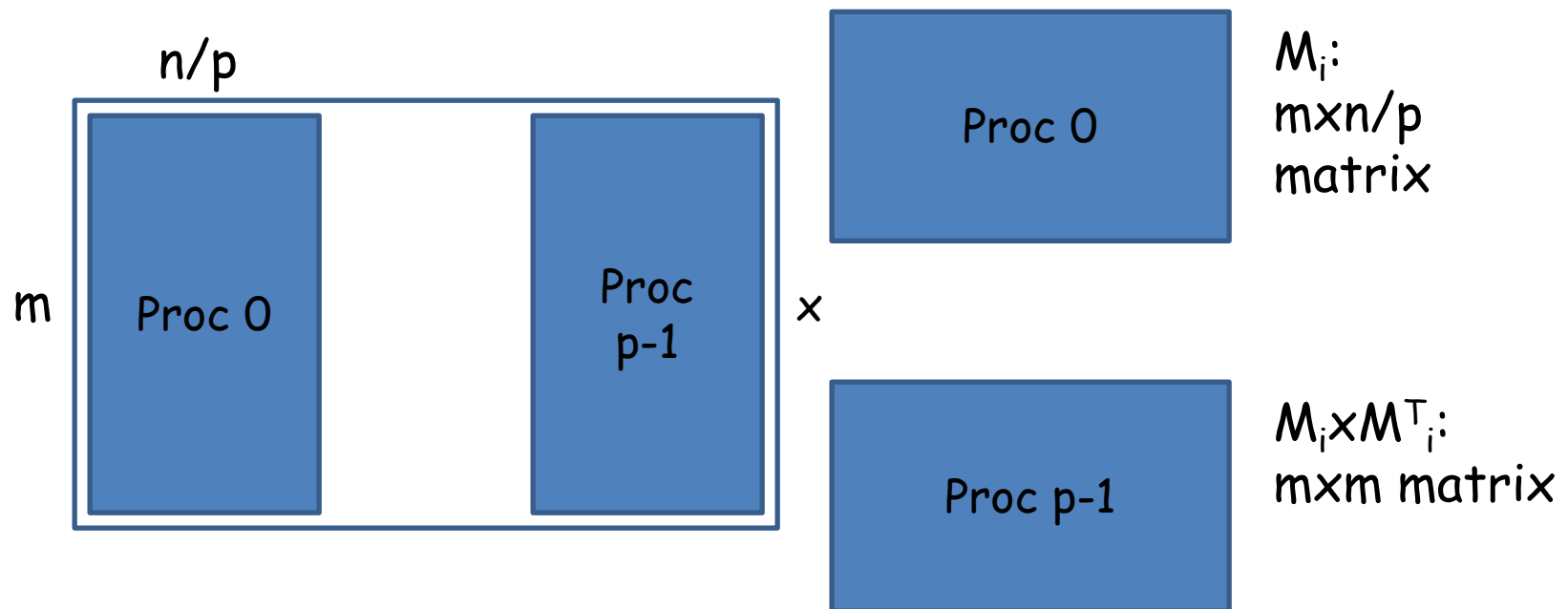
Algorithm 3:

- Matrix distribution into blocks of $m/r \times n/c$ elements
- Algorithm 1 on columns
- Algorithm 2 on rows

Note:

Interfaces that do not support collectives on subsets of processes **cannot express** Algorithm 3 (e.g., UPC, CaF)

Algorithm 2 can also be used for computing $M \times M^T$, the product of $m \times n$ matrix M with its own transpose (also called **SYRK**: Symmetric Rank K update); result is a symmetric $m \times m$ matrix



Compute for processor i :
 $(M \times M^T)_i = \sum_{0 \leq j < p} M_i \times M_j^T$ with local SYRK and MPI_Reduce_scatter,
 result distributed column- or row-wise (use-case for datatypes)

This algorithm is good (optimal) for $m \leq n$ (short, wide matrices) and smaller p , $p \leq n/\sqrt{m(m-1)}$

Cost analysis (conjecture): $T(m,n,p) = O(m^2n/p + m^2 + \log p)$



Real communication volume is $m(m+1)/2 (p-1)/p$

MPI Process topologies (MPI 3.1, Chapter 7)

Observation:

For Algorithm 3, row and column subcommunicators are needed; must support concurrent collective operations

Convenient to organize processors into a Cartesian $r \times c$ mesh with MPI processes in row-major.

Use this Cartesian (x,y) **naming** to create subcommunicators for the matrix-vector example

Cartesian naming useful for torus/mesh algorithms, e.g., for d-dimensional stencil computations (Jacobi, Life, ...)

```
rcdim[0] = c;   rcdim[1] = r;  
period[0] = 0; period[1] = 0; // no wrap around  
  
reorder = 0; // no attempt to reorder  
  
MPI_Cart_create(comm, 2, rcdim, period, reorder, &rccomm);
```



Collective communicator creation call:

All processes belonging to old communicator (`comm`) must perform call, each process becomes new communicator (`rccomm`, or `MPI_COMM_NULL`), possibly with new rank and size

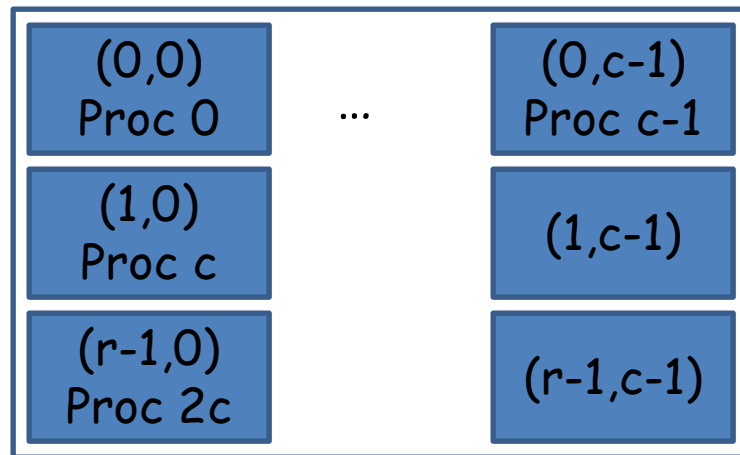
```

rcdim[0] = c;   rcdim[1] = r;
period[0] = 0; period[1] = 0; // no wrap around

reorder = 0; // no attempt to reorder

MPI_Cart_create(comm, 2, rcdim, period, reorder, &rccomm);

```



Row major process numbering

Same processes in rccomm communicator as in comm (rc must be **at most** size(comm)). But in rccomm, processes also have a d-dimensional coordinate as "name".

But: Ranks may **not** be bound to the same processors (if reorder=1)

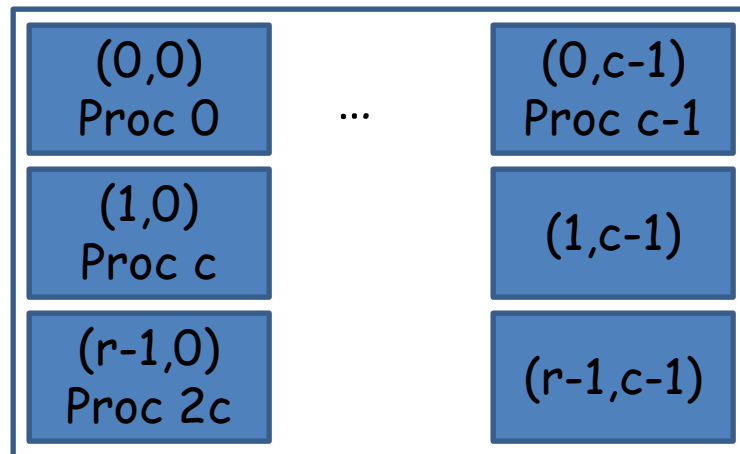
```

rcdim[0] = c;  rcdim[1] = r;
period[0] = 0; period[1] = 0; // no wrap around

reorder = 0; // no attempt to reorder

MPI_Cart_create(comm, 2, rcdim, period, reorder, &rccomm);

```



$$\text{rank} = \sum_{0 \leq i < d} (\text{coord}[i] \prod_{0 \leq j < i} d[j])$$

Translation functions

```

int rccoord[2];
MPI_Cart_coords(rccomm,
                rcrank,
                2, rccoord);

```

```

MPI_Cart_rank(rccomm,
              rccoord,
              &rcrank);

```

E.g., $\text{rank}(2, c-2) = c-2 + 2c = 3c-2$

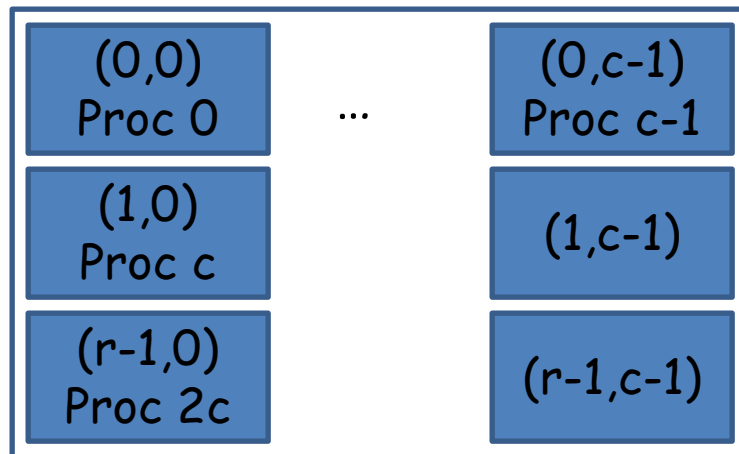
```

rcdim[0] = c;   rcdim[1] = r;
period[0] = 0; period[1] = 0; // no wrap around

reorder = 0; // no attempt to reorder

MPI_Cart_create(comm, 2, rcdim, period, reorder, &rccomm);

```



Communication in rccomm uses ranks (not coordinates).

Communication between any ranks possible/allowed.

Processes are neighbors if they are adjacent in Cartesian mesh/torus

```

rcdim[0] = c;   rcdim[1] = r;
period[0] = 0; period[1] = 0; // no wrap around

reorder = 0; // no attempt to reorder

MPI_Cart_create(comm, 2, rcdim, period, reorder, &rccomm);

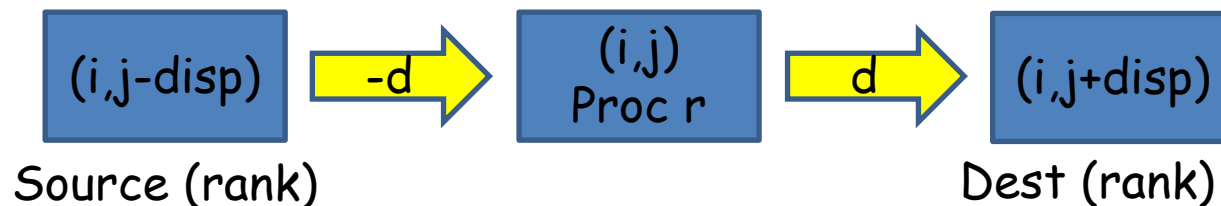
```

Rank "shifting" function (no communication)

```

MPI_Cart_shift(rccomm, dimension, displacement,
               &source, &dest);

```



Shift along dimension 0, displacement 2 (e.g.). What if $j\text{-disp} < 0$ or $j\text{+disp} \geq \text{size}$? Answer: `MPI_PROC_NULL` if `(!period[0])`, otherwise cyclic shift

MPI convenience functionality for factoring p into “best” (closest??) r and c ... (in d dimensions)

```
int dimensions[d] = {0, ..., 0}; // all dimensions free
MPI_Dims_create(p,d,dimensions);
```

Factor p into d dimensions with order (size) as close to each other as possible... (MPI 3.1, p.293)

Much natural functionality is not in MPI (what can you think of?)

Jesper Larsson Träff, Sascha Hunold, Guillaume Mercier, Daniel J. Holmes: MPI collective communication through a single set of interfaces: A case for orthogonality. *Parallel Comput.* 107: 102826 (2021)


```
int dimensions[d] = {0, ..., 0}; // all dimensions free
MPI_Dims_create(p,d,dimensions);
```

Factor p into d dimensions with order (size) as close to each other as possible... (MPI 3.1, p.293). **Why should this be best?**

Note: Seemingly innocent interface entails **integer factorization**. Complexity of factorization is unknown (probably high)

Note: This algorithm for 2-dimensional balancing is **exponential**:

```
f = (int) sqrt((double)p);
while (p%f!=0) f--;
```

Pseudo-polynomial: Polynomial in the magnitude, but **not** the size of p . It takes only $\log p$ bits to represent p .

But... factorization of small numbers (p in the order of millions) that fulfill the MPI specification (dimension sizes in increasing order) is **not** expensive (for p up to millions):

Jesper Larsson Träff, Felix Donatus Lübbecke: Specification Guideline Violations by MPI_Dims_create. EuroMPI 2015: 19:1-19:2

Ca. 2015:

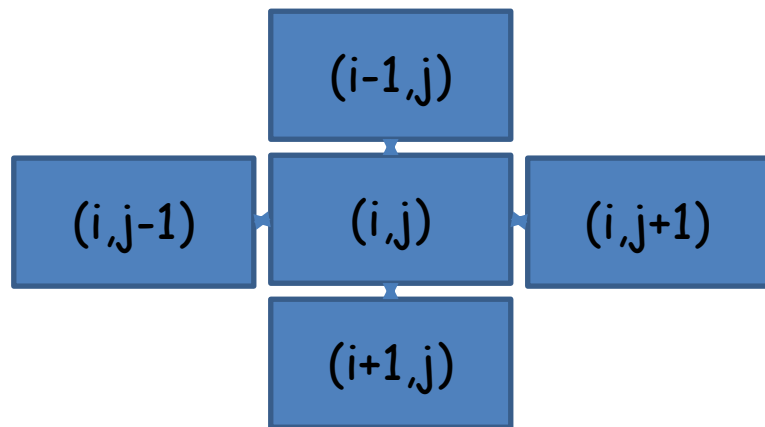
Many (all?) MPI libraries had (severely) broken implementations of MPI_Dims_create

(SE) Problem: How can quality of MPI library implementation be assessed? Ensured?

MPI_Cart_create operation

- Defines Cartesian naming, creates new communicator, and caches information with this (number and sizes of dimensions ...)
- Row-major ordering of processes (dimension order 0, 1, 2, ...)
- Neighbors: The 2d adjacent processes in each dimension
- Defines order of neighbors (dimension-wise), important for MPI 3.0 neighborhood collectives See later
- May (reorder=1) attempt to remap processes, such that processes that are **neighbors in virtual application topology** are **neighbors in physical system**

Cartesian neighborhoods in two dimensions

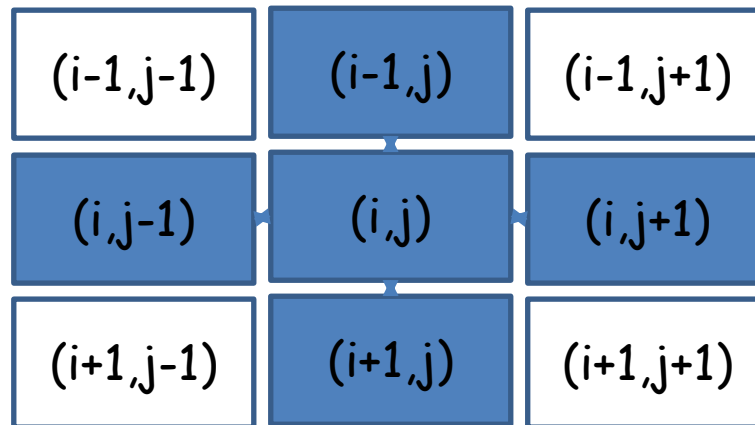


Pattern aka 5-point stencil

Process with coordinates (i,j) has 2d direct neighbors (for Cartesian communicator in d dimensions) with which it is implicitly supposed to communicate. This is the neighborhood (graph) used with MPI neighborhood collectives

Process $(0,j)$ neighbor of process $(r-1,j)$ if periodic in dimension

Cartesian neighborhoods in two dimensions



MPI restrictions:

- Not possible to specify other patterns, e.g., 9-point stencil
- Neighborhood is unweighted

Process with coordinates (i, j) has 2d direct neighbors (for Cartesian communicator in d dimensions) with which it is implicitly supposed to communicate. This is the neighborhood (graph) used with MPI neighborhood collectives

Process $(0, j)$ neighbor of process $(r-1, j)$ if periodic in dimension

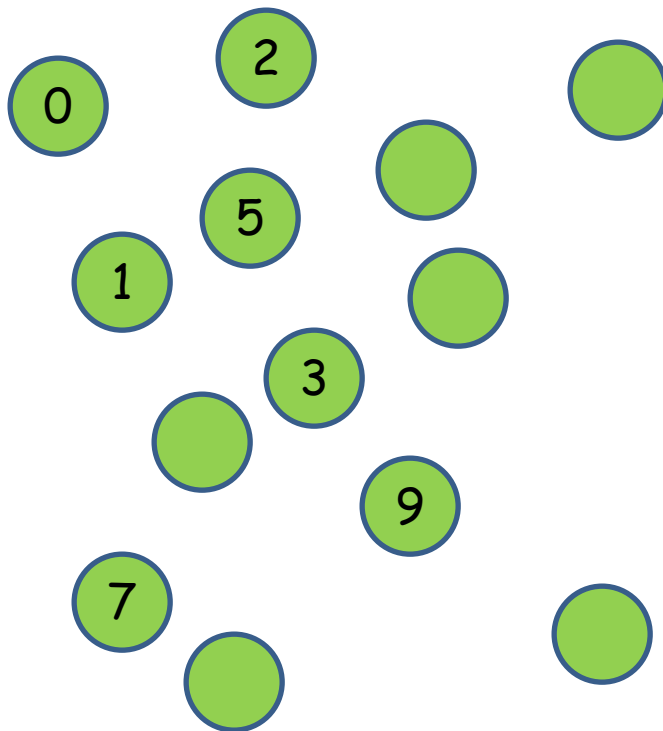
For discussion on communicators, naming schemes and topological information associated with communicators, see again

Jesper Larsson Träff, Sascha Hunold, Guillaume Mercier, Daniel J. Holmes: MPI collective communication through a single set of interfaces: A case for orthogonality. *Parallel Comput.* 107: 102826 (2021)

Many interesting things to do for (paid) Master's thesis...

Reordering processes via new communicators

oldcomm

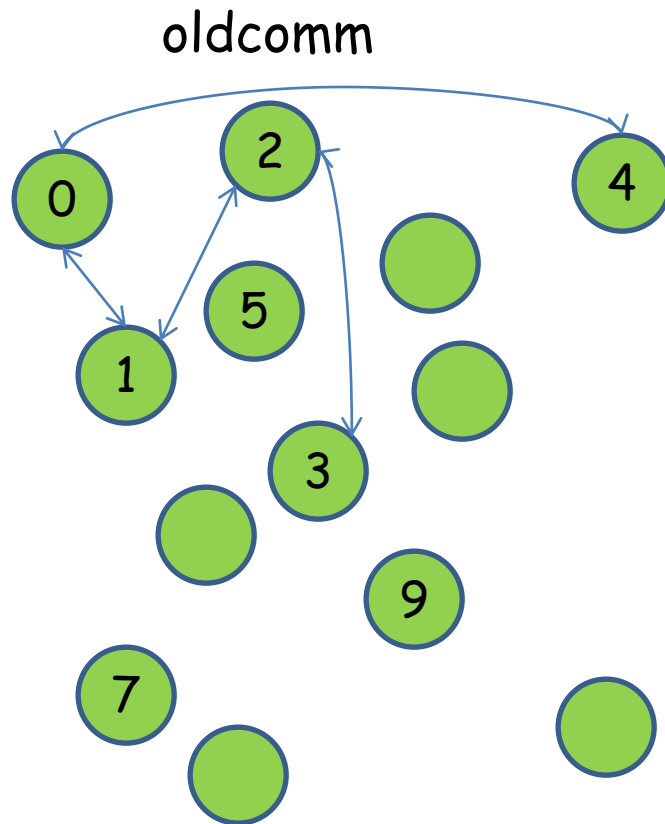


MPI assumption:

Application programmer knows which processes will communicate (heaviest communication, most frequent communication): **Virtual topology**

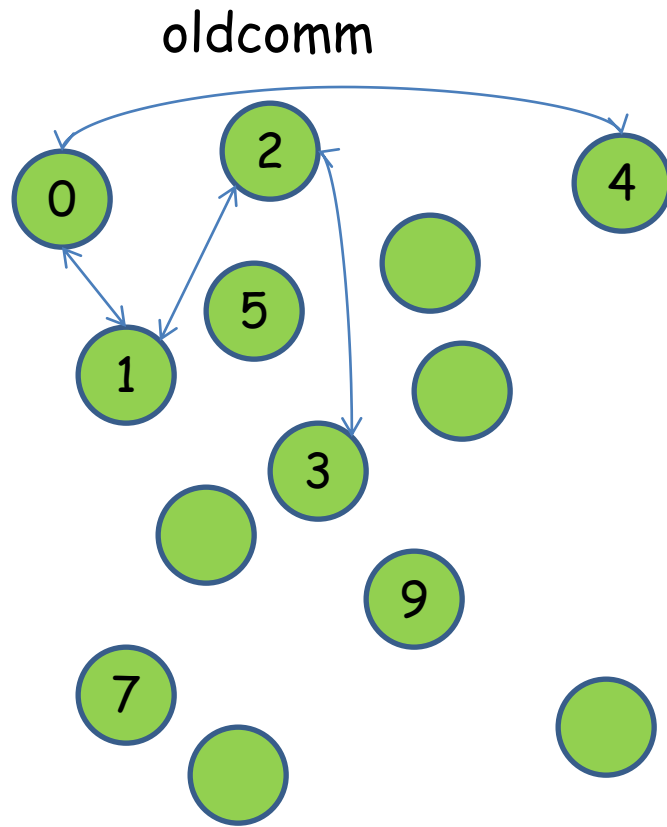
Idea:

Convey this information to MPI library; library can suggest a good mapping of MPI processes to processors that fits communication system



`MPI_Cart_create:`

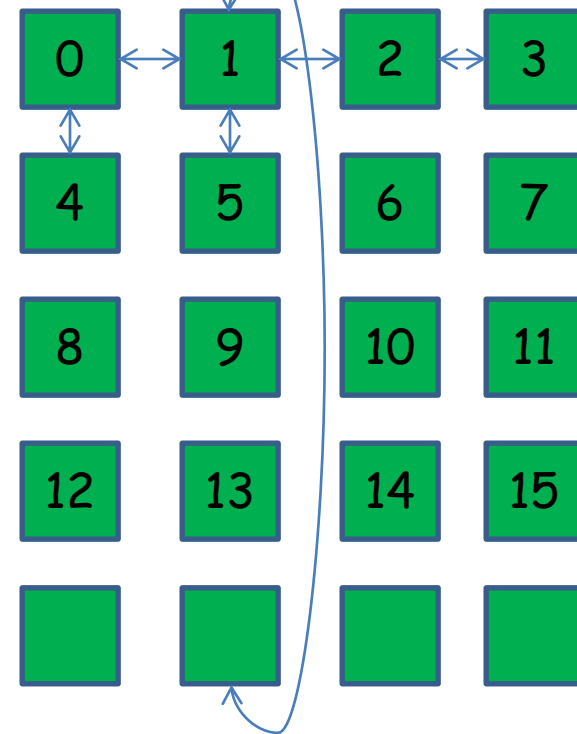
Implicit assumption: Process with rank i in old communicator will likely communicate with neighboring processes in implicit Cartesian neighborhood



If $\text{period}[1]=1$



newcomm



Torus network ...

If period[1]=1

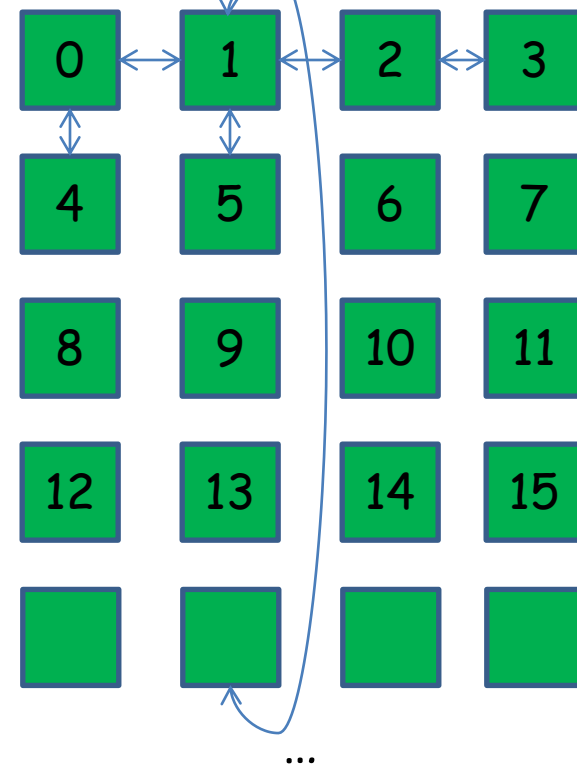


newcomm

Ranks in newcomm are organized in a (virtual) d-dimensional mesh/torus

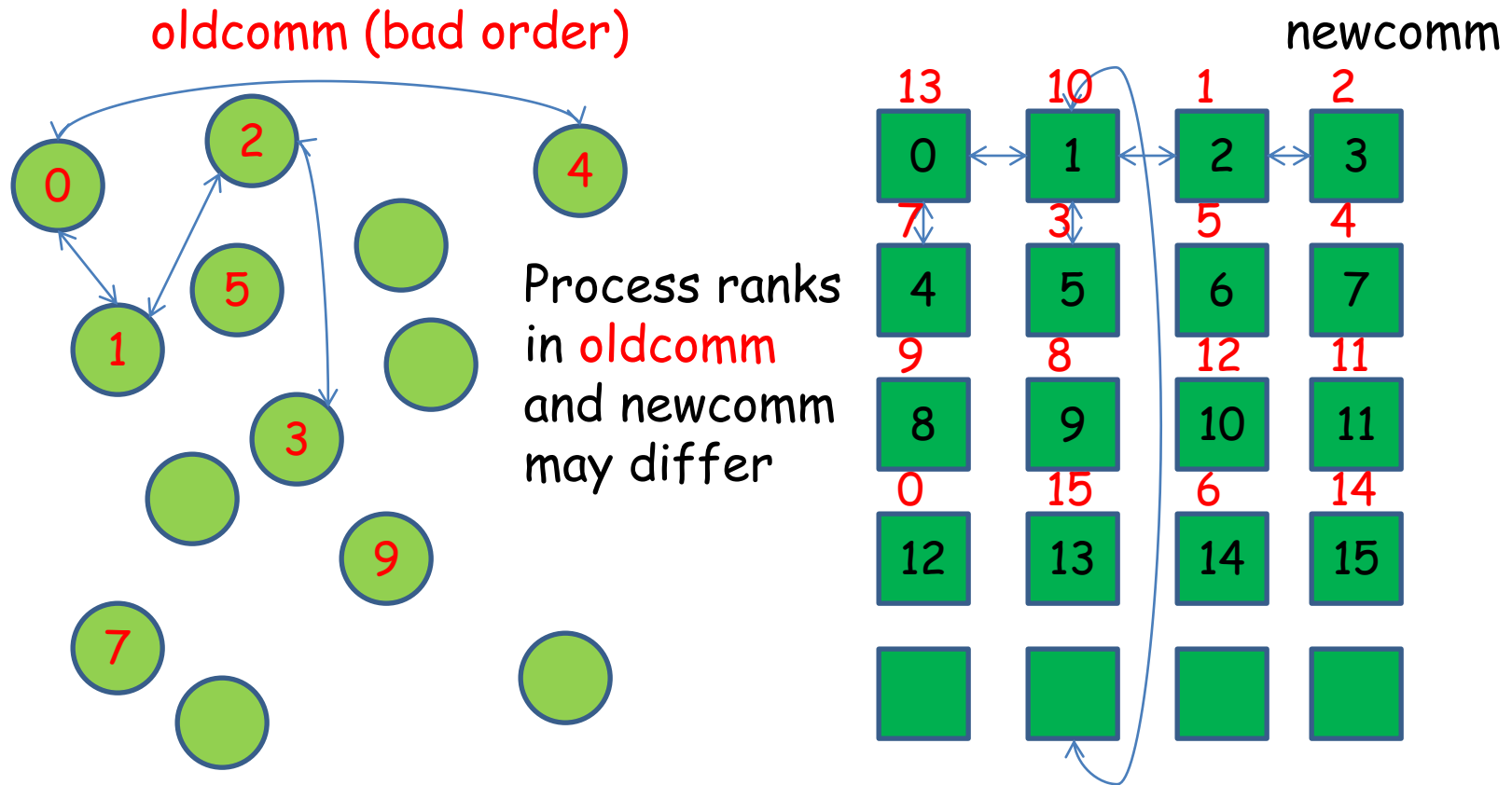
Good order: Ranks correspond to processor id's in physical torus system

Physical torus systems:
3-dim, 5-dim, 6-dim; BlueGene,
Cray, Fujitsu K, Fugaku



Torus network

Topology creation with reorder=1: MPI library may attempt to map virtual topology to physical topology: newcomm

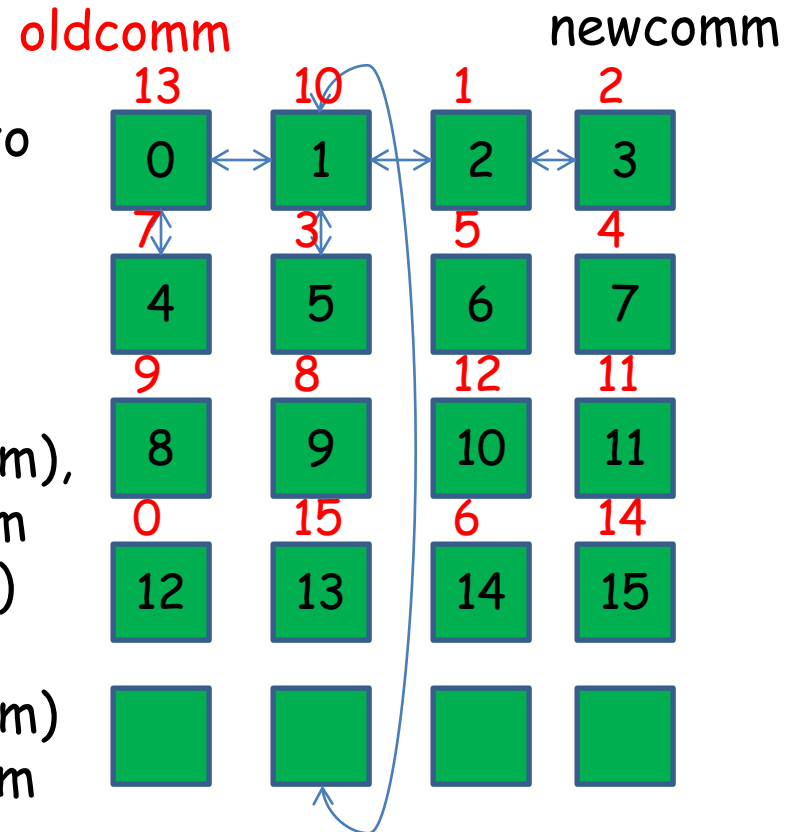


Torus network

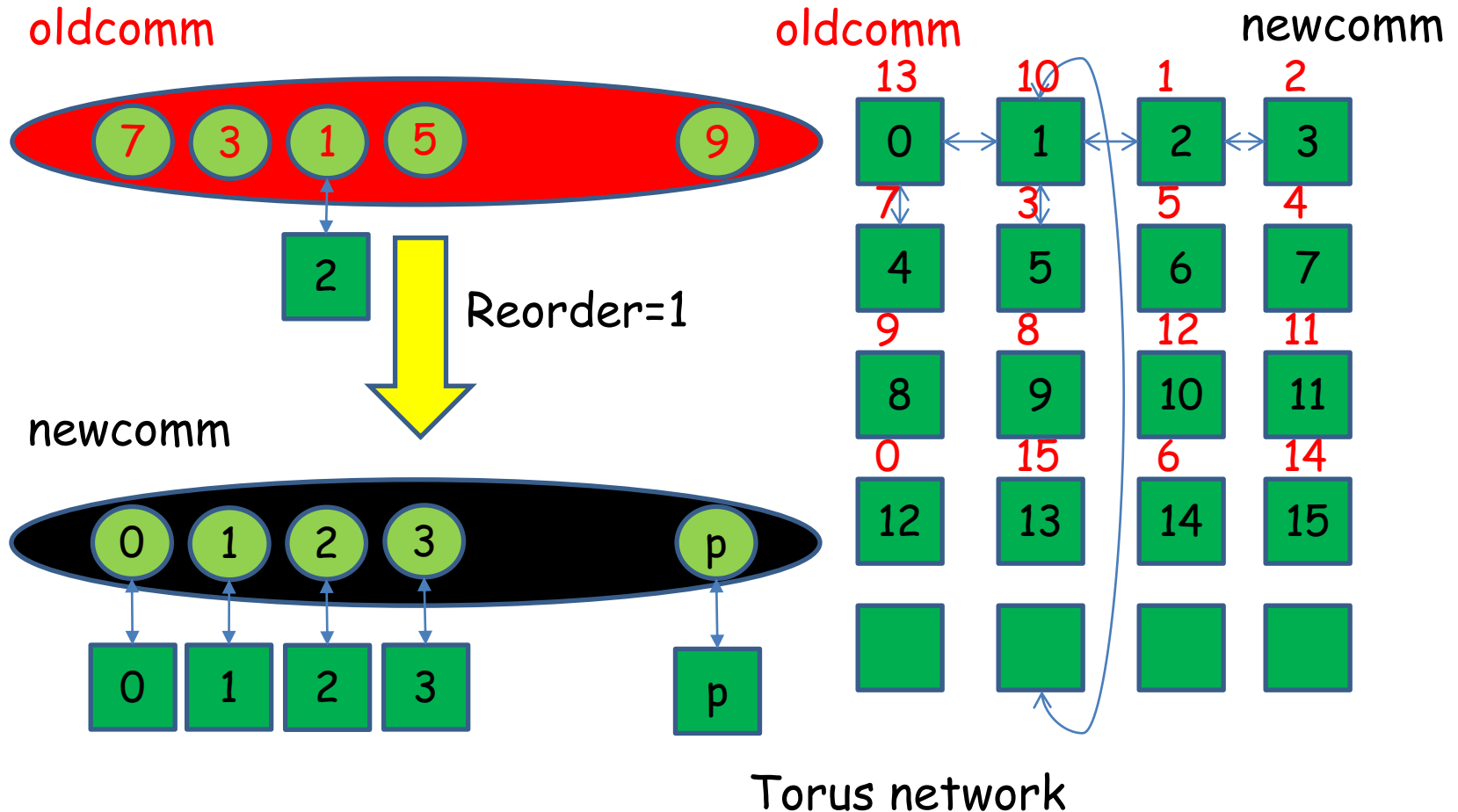
Processes in **oldcomm** remapped to other processes in newcomm

Example:

- **Rank 1** in **oldcomm** mapped to processor 2 (rank 2 in newcomm), **remapped** to rank 1 in newcomm (which was **rank 10** in **oldcomm**)
- **Rank 4** in **oldcomm** mapped to processor 7 (rank 7 in newcomm) **remapped** to rank 4 in newcomm



Torus network



If reordering has been done (ranks in newcomm \neq ranks in oldcomm)

- Has reordering been done? All processes: Check whether rank in the two communicators differ, allreduce to inform all (or use `MPI_Comm_compare`)
- Application may have to transfer data to same rank in new communicator; no MPI support for this
- Need to be able to translate between ranks in different communicators

Cartesian communicators can capture only limited Cartesian communication patterns: 2d neighborhoods

```
MPI_Comm_compare(comm1, comm2, &result)
```

Result either of

- `MPI_IDENT` (communicators identical, same)
- `MPI_CONGRUENT` (same processes in same order, nevertheless different communicator)
- `MPI_SIMILAR` (same processes, different order)
- `MPI_UNEQUAL` (otherwise)

Interface ideas for general stencil patterns

Jesper Larsson Träff, Felix Donatus Lübbe, Antoine Rougier, Sascha Hunold: Isomorphic, Sparse MPI-like Collective Communication Operations for Parallel Stencil Computations. EuroMPI 2015: 10:1-10:10

Jesper Larsson Träff, Sascha Hunold: Cartesian Collective Communication. ICPP 2019: 48:1-48:11

Jesper Larsson Träff, Sascha Hunold, Guillaume Mercier, Daniel J. Holmes: MPI collective communication through a single set of interfaces: A case for orthogonality. Parallel Comput. 107: 102826 (2021)

Interesting Master thesis projects here

Recent improvements to MPI implementations

- Remapping for network topology: Place links in communication graph (e.g. Cartesian neighborhoods) on links in hardware network
- Remapping for hierarchical systems: Map as many neighbors as possible inside compute nodes

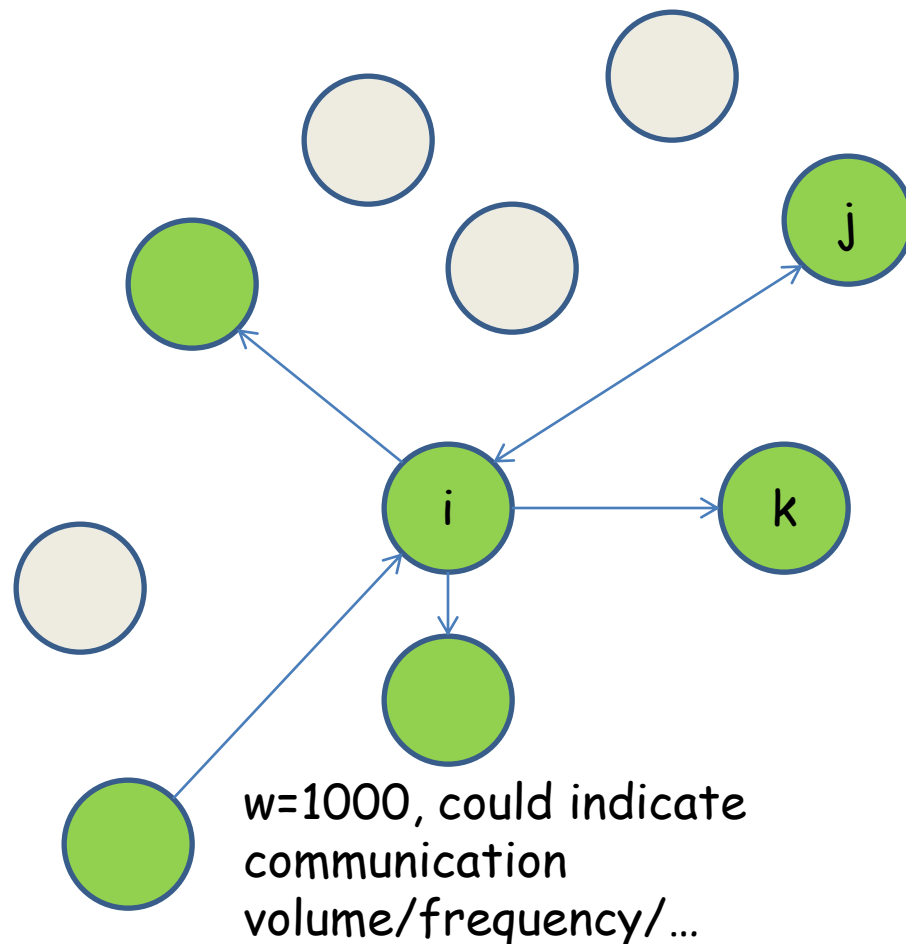
William D. Gropp: Using node and socket information to implement MPI Cartesian topologies. *Parallel Computing* 85: 98-108 (2019)

- Remapping for hierarchical systems: Heuristically map as many neighbors as possible inside compute nodes
- **Challenge:** balance bandwidth inside nodes with (multi-lane) bandwidth across nodes

Konrad von Kirchbach, Markus Lehr, Sascha Hunold, Christian Schulz, Jesper Larsson Träff: Efficient Process-to-Node Mapping Algorithms for Stencil Computations. CLUSTER 2020: 1-11

TU Wien: New FWF project on process mapping

Fully general application communication patterns



- Weighted, directed (multi)graph to specify application communication pattern (whom with whom, how much)
- Hints can be provided (info)
- Distributed description, any MPI process can specify any edges

```
MPI_Dist_graph_create(comm,
                      n, sources, degrees, destinations,
                      weights,
                      info, reorder, &graphcomm)
```

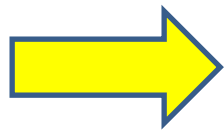
Example: Process i may specify (what it knows):

sources:	[0,5,7,2,...]
(out)degrees:	[2,2,2,2,...]
destinations:	[1,2,18,36,4,5,8,117,...]
weights:	[100,1000,10,10,1000,1000,100,100,...]

MPI (3.0) uses graph structure for descriptive purposes (neighborhood collectives). MPI library can attempt to remap communication graph to fit target communication system. Other optimizations are possible.

```
int reorder = 1;
MPI_Dist_graph_create(comm,
                      n, sources, degrees, destinations,
                      weights,
                      info, reorder, &graphcomm)
```

If reordering is requested, rank i in new graphcomm **may** be bound to different processor than rank i in comm



Data redistribution (from rank i in comm to rank i in graphcomm) can be necessary; must be done **explicitly by application** (first: Check if reordering has taken place)

Note:

It is legal for an MPI library to return a graphcomm with the same mapping as comm

If each process knows its incoming and outgoing communication edges

```
MPI_Dist_graph_create_adjacent(comm,  
    indeg, sources, sourceweights,  
    outdeg, destinations, destweights,  
    info, reorder, &graphcomm)
```

may be more convenient and efficient

Furthermore, the operation does not require communication in order to support the neighborhood query functions:

```
MPI_Dist_graph_neighbors_count(graphcomm, ...)  
MPI_Dist_graph_neighbors(graphcomm, ...)
```

MPI 3.1 Virtual topologies

- “info” can be provided; not (yet) specified in MPI standard, implementation dependent
- Interpretation of weights unspecified (when? How much? How often? ...)
- Differences between Cartesian and distributed graph topologies: Cartesian creation function (`MPI_Cart_create`) takes no weights, no info

Do MPI libraries perform non-trivial mapping?

Try it

Distributed graph interface since MPI 2.2.

Old MPI 1.0 interface is **badly non-scalable**: Full graph required at each process

Don't use `MPI_Graph_create`!

Definition:

An MPI construct is non-scalable if it entails $\Omega(p)$ memory or time **overhead**(*)

(*): that cannot be accounted for/amortized in the application

T. Hoefler, R. Rabenseifner, H. Ritzdorf, B. R. de Supinski, R. Thakur, Jesper Larsson Träff: The scalable process topology interface of MPI 2.2. *Concurrency and Computation: Practice and Experience* 23(4): 293-310 (2011)

Implementing topology mapping

Step 1:

Application specifies communication patterns as weighted directed (**guest**) graph (implicitly: Unweighted, d-dimensional Cartesian pattern)

Step 2:

MPI library knows physical communication structure; model subgraph of system spanned by communicator as weighted, directed (**host**) graph

Step 3:

Map/**embed** communication (**guest**) graph onto system (**host**) graph, subject to... The map (embedding) is an injective function Γ from guest graph vertices to host graph vertices

Mapping function can be injective, surjective, bijective

Some optimization criteria:

- As many heavy communication edges on physical edges as possible
- Minimize communication costs (volume)
- Small congestion (bandwidth)
- Small dilation (latency)
- ...

Meta-Theorem: Most graph embedding problems are NP-hard

Depending on physical system (e.g., clustered, hierarchical), problem can sometimes be formulated as a **graph partitioning** problem (e.g., clusters, partition into nodes, minimize weight of inter-node edges), ...

Guest graph $G=(V,E)$, let $w(u,v)$ denote the volume of data from process (vertex) u to process (vertex) v

Host graph $H=(V',E')$, let $c(u',v')$ denote the network capacity between processors u' and v' . Let $R(u',v')$ be a function determining the path from processor u' to v' in the system (Routing algorithm)

Let $\Gamma: V \rightarrow V'$ be an injective mapping (embedding). The **congestion** of link e in E' wrt. Γ is defined as

$$\text{Cong}(e) = [\sum w(u,v) \text{ over } (u,v) \text{ in } E \text{ where } e \text{ in } R(\Gamma(u),\Gamma(v))]/c(e)$$

The congestion of Γ is defined as the maximum congestion of any link e

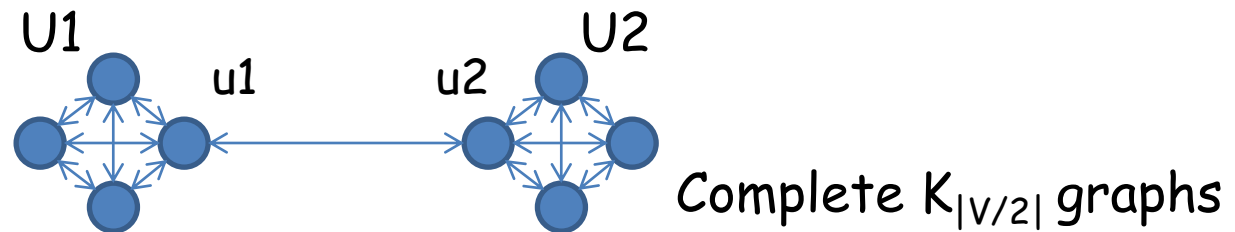
Call the problem of determining whether an embedding exists that has congestion less than C for **CONG**

Concrete Theorem: For given guest and host graphs G and H , determining whether an embedding exists that has congestion at most C is NP-complete.

Proof: CONG is in NP. Non-deterministically choose an embedding, and check whether its congestion is at most C ; this can be done in polynomial time

Completeness is by reduction from MINIMUM CUT INTO BOUNDED SETS (Garey&Johnson ND17): Given a graph $G=(V,E)$, two vertices s,t in V , integer L , determine whether there is a partition of V into subsets V_1 and V_2 with s in V_1 , t in V_2 , $|V_1|=|V_2|$, such that the number of edges between V_1 and V_2 is at most L

Let (G, s, t, L) be an instance of MINIMUM CUT INTO BOUNDED SETS. Let the **host graph** H be constructed as follows



$c(u_1, u_2) = |V|$, $c(e) = 1$ for all other edges of H . The routing function R selects for u, v in V' a shortest path from u to v

Let the **guest graph** be G with $w(e) = 1$ for e in E , except for the edge (s, t) for which $w(s, t) = |V|^4$ if (s, t) is not in E , and $w(s, t) = |V|^4 + 1$ if (s, t) in E . That is, the guest graph may have one edge not in G , namely (s, t) , and each edge in G contributes a volume of at least 1

Any injective mapping Γ from G to H determines a partition of V into V_1 and V_2 with $|V_1|=|V_2|$, namely $V_i = \{v \mid \Gamma(v) \text{ in } U_i\}$

Any mapping that minimizes the congestion must map (s,t) to (u_1,u_2) . This gives a congestion of at most $|V|^3+|V|$ (the volume on (u_1,u_2) is at most $|V|^4+|V|^2/4$); any other mapping has congestion at least $|V|^4$.

In such a mapping, the most congested edge is (u_1,u_2) , with congestion

$$C = |V|^3 + |\{(v_1,v_2) \text{ in } E \mid v_1 \text{ in } V_1 \text{ and } v_2 \text{ in } V_2\}| / |V|$$

fractional

Thus, a solution to CONG with congestion at most $|V|^3 + L/|V|$ gives a solution to the MINIMUM CUT INTO BOUNDED SETS instance

A nicer construction (15.11.2021)

Host graph H as before (dumbbell)

Let the **guest graph** be G with $w(e) = |V|$ for e in E , except for the edge (s,t) for which $w(s,t) = |V|^4$ if (s,t) is not in E , and $w(s,t) = |V|^4 + |V|$ if (s,t) in E . That is, the guest graph may have one edge not in G , namely (s,t) , and each edge in G contributes a volume of at least $|V|$

Any injective mapping Γ from G to H determines a partition of V into V_1 and V_2 with $|V_1|=|V_2|$, namely $V_i = \{v \mid \Gamma(v) \text{ in } U_i\}$

Any mapping that minimizes the congestion must map (s,t) to (u_1,u_2) . This gives a congestion of at most $|V|^3+|V|^2$ (the volume on (u_1,u_2) is at most $|V|^4+|V||V|^2/4$); any other mapping has congestion at least $|V|^4$.

In such a mapping, the most congested edge is (u_1,u_2) , with congestion

$$C = |V|^3 + |\{(v_1,v_2) \text{ in } E \mid v_1 \text{ in } V_1 \text{ and } v_2 \text{ in } V_2\}|$$

Thus, a solution to CONG with congestion at most $|V|^3+L$ gives a solution to the MINIMUM CUT INTO BOUNDED SETS instance

Conversely, from a solution to the MINIMUM CUT INTO BOUNDED SETS an embedding with this congestion can easily be constructed (check!)

Proof (simplified) from

T. Hoefler, M. Snir: *Generic topology mapping strategies for large-scale parallel architectures*. ICS 2011: 75-84

ND17, see

M. R. Garey, D. S. Johnson: *Computer and Intractability. A guide to the theory of NP-Completeness*. W. H. Freeman, 1979 (update 1991)

CONG is a special case of the **simple graph embedding problem**

For given (complete) guest graph $G=(V,E)$ with edge weights $w(u,v)$, and host graph $H=(V',E')$ with edge costs $c(u',v')$, find an injective mapping (embedding) $\Gamma: V \rightarrow V'$ that minimizes

$$\sum_{(u,v) \in E} w(u,v)c(\Gamma(u), \Gamma(v))$$

This is the quadratic assignment problem (QAP), which is NP-complete (Garey&Johnson ND43)

$w(u,v)$: volume of data to be transferred between processes u and v

$c(u,v)$: cost per unit; could model pairwise communication costs (without congestion) in network

Some MPI relevant solutions to the topology mapping problem

S. H. Bokhari: On the Mapping Problem. IEEE Trans. Computers (TC) 30(3):207-214 (1981)

T. Hatazaki: Rank Reordering Strategy for MPI Topology Creation Functions. PVM/MPI 1998: 188-195

J. L. Träff: Implementing the MPI process topology mechanism. SC 2002:1-14

H. Yu, I-Hsin Chung, J. E. Moreira: Blue Gene system software - Topology mapping for Blue Gene/L supercomputer. SC 2006: 116

A. Bhatele: Topology Aware Task Mapping. Encyclopedia of Parallel Computing 2011: 2057-2062

A. Bhatele, L. V. Kalé: Benefits of Topology Aware Mapping for Mesh Interconnects. Parallel Processing Letters 18(4): 549-566 (2008)

Emmanuel Jeannot, Guillaume Mercier, Francois Tessier: Process Placement in Multicore Clusters: Algorithmic Issues and Practical Techniques. IEEE Trans. Parallel Distrib. Syst. 25(4): 993-1002 (2014)

Heuristics for Cartesian topology mapping (with arbitrary neighborhoods)

Sascha Hunold, Konrad von Kirchbach, Markus Lehr, Christian Schulz, Jesper Larsson Träff: Efficient Process-to-Node Mapping Algorithms for Stencil Computations. IEEE Cluster (2020)

William D. Gropp: Using node and socket information to implement MPI Cartesian topologies. Parallel Comput. 85: 98-108 (2019)

Graph partitioning software for process topology embedding

KaHIP, Karlsruhe High Quality Partitioning, recent, state-of-the-art graph partitioning (heuristic, multi-level) for large graphs; see <http://algo2.iti.kit.edu/documents/kahip/>

Peter Sanders, Christian Schulz:
Think Locally, Act Globally: Highly Balanced Graph Partitioning.
SEA 2013: 164-175

VieM, Vienna Mapping and Quadratic Assignment, solves the embedding problem for hierarchical systems as a special quadratic assignment problem; see <http://viem.taa.univie.ac.at/>

Christian Schulz, Jesper Larsson Träff: Better Process Mapping and Sparse Quadratic Assignment. SEA 2017: 4:1-4:15

Graph partitioning software for process topology embedding

METIS, ParMETIS, ... : Well-known (early) software packages for (hyper)graph and mesh partitioning; see <http://glaros.dtc.umn.edu/gkhome/projects/gp/products?q=view/s/metis>

George Karypis: METIS and ParMETIS. Encyclopedia of Parallel Computing 2011: 1117-1124

Scotch, a "software package and libraries for sequential and parallel graph partitioning, static mapping and clustering, sequential mesh and hypergraph partitioning, and sequential and parallel sparse matrix block ordering"; see <http://www.labri.fr/perso/pelegrin/scotch/>

Cédric Chevalier, François Pellegrini: PT-Scotch. Parallel Computing 34(6-8): 318-331 (2008)

Graph partitioning software for process topology embedding

Jostle, originally for partitioning and load balancing for unstructured meshes; no longer open source (2017); see <http://staffweb.cms.gre.ac.uk/~wc06/jostle/>

C. Walshaw and M. Cross. JOSTLE: Parallel Multilevel Graph-Partitioning Software - An Overview. In F. Magoules, editor, Mesh Partitioning Techniques and Domain Decomposition Techniques, pages 27-58. Civil-Comp Ltd., 2007. (Invited chapter)

Lots of possibilities for projects/Master's Thesis

Topology mapping: Discussion

- For scalability, distributed specification of communication graph
- Requires distributed algorithm (**heuristic**) to solve/approximate hard optimization problem
- Can the mapping overhead be amortized?
- Does it make sense to look for an optimum? Is the MPI interface sufficiently rich to provide all relevant information? Does the application have this information?
- Is the application programmer prepared to use the complex interface?

Creating the communicators for MV example (Method 1)

```
int rcrank;  
int rccoord[2];  
  
MPI_Comm_rank(rccomm, &rcrank);  
MPI_Cart_coords(rccomm, rcrank, 2, rccoord);  
  
MPI_Comm_split(rccomm, rccoord[0], rccoord[1], &ccomm);  
MPI_Comm_split(rccomm, rccoord[1], rccoord[0], &rcomm);
```

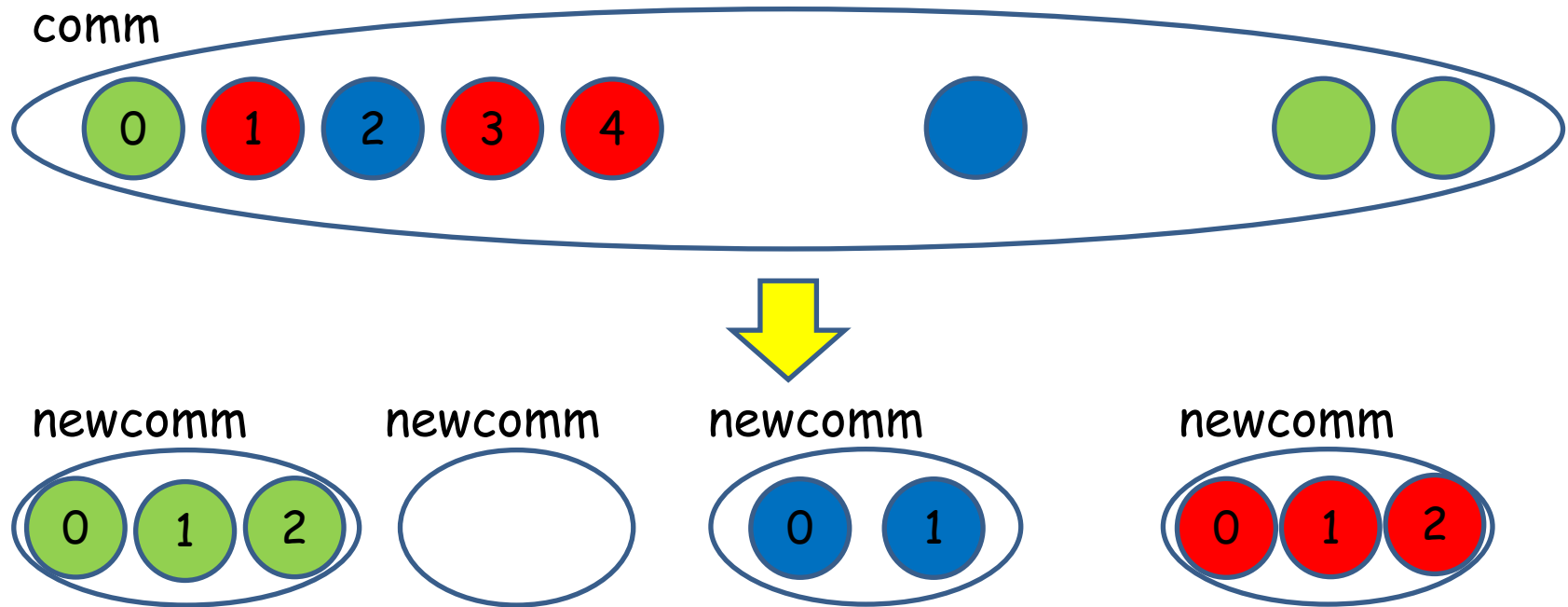


color: all processes calling with same color, will belong to same communicator



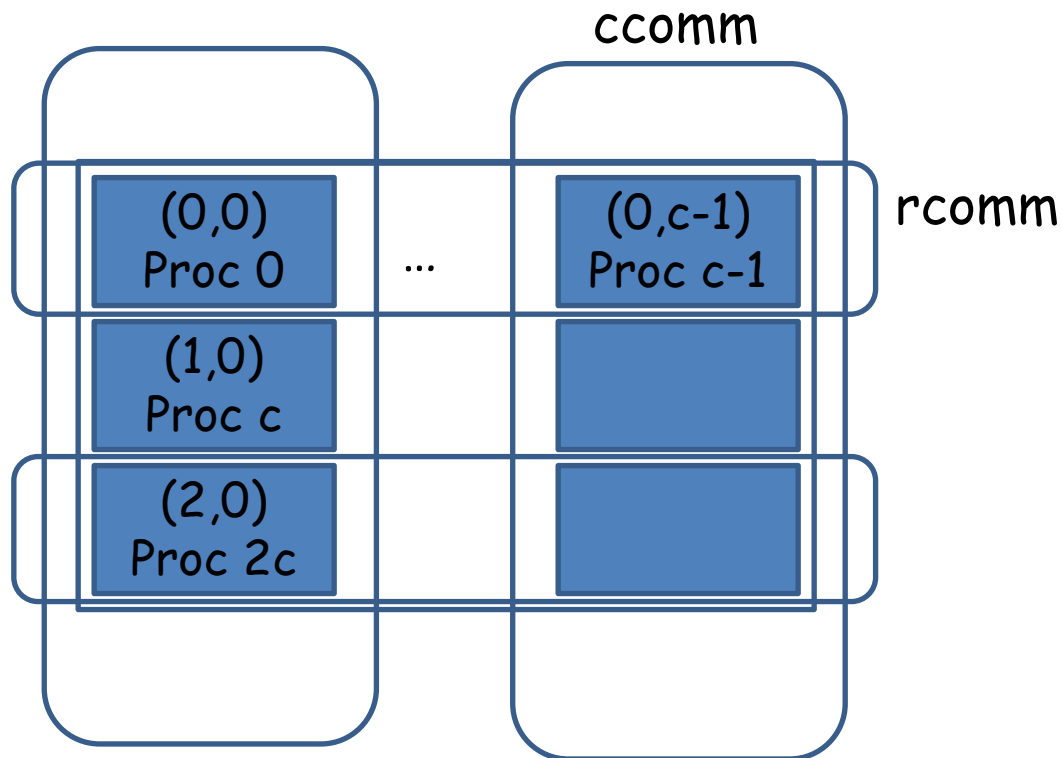
key: determines relative process ordering in new communicator

```
MPI_Comm_split(comm, color, key, &newcomm);
```



Processes in comm are sorted after **key**; determines relative order in newcomm

```
MPI_Comm_split (color=rccoord[0]);  
MPI_Comm_split (color=rccoord[1]);
```



Creating the communicators for MV example (Method 2)

`MPI_Comm_split()` is an expensive collective operation. MPI process groups can be used for possibly more efficient communicator creation

```
MPI_Comm_group(rccomm, &rcgroup); // get group out
MPI_Comm_rank(rccomm, &rcrank);
MPI_Cart_coords(rccomm, rcrank, 2, rccoord);

for (i=0; i<rcsize; i++) {
    MPI_Cart_coords(rccomm, i, 2, coord);
    if (coord[0]==rccoord[0]) cranks[c++] = i;
    if (coord[1]==rccoord[1]) rranks[r++] = i;
}
MPI_Group_include(rcgroup, c, cranks, &cgroup);
MPI_Group_include(rcgroup, r, rranks, &rgroup);
MPI_Comm_create(rccomm, cgroup, &ccomm);
MPI_Comm_create(rccomm, rgroup, &rcomm);
```

Process
group
operations

Better?

MPI process groups (MPI 3.1, Chapter 6)

Process local MPI objects representing ordered sets of processes

`MPI_Comm_group`: Get group of processes associated with communicator

Processes in group ranked from 0 to size of group-1, a process can locally determine if it's a member of some group, and its rank in this group

Operations:

- Comparing groups (same processes, in same order)
- Group union, intersection, difference, ...
- Inclusion and exclusion of groups
- Range groups
- Translation of ranks between groups

Creating the communicators (Method 2')

`MPI_Comm_split()` is an expensive collective operation. MPI process groups can be used for possibly more efficient communicator creation

```
MPI_Comm_group(rccomm, &rcgroup); // get group out
MPI_Comm_rank(rccomm, &rcrank);
MPI_Cart_coords(rccomm, rcrank, 2, rccoord);

for (i=0; i<rcsize; i++) {
    MPI_Cart_coords(rccomm, i, 2, coord);
    if (coord[0]==rccoord[0]) cranks[c++] = i;
    if (coord[1]==rccoord[1]) rranks[r++] = i;
}
```

Even better?

```
MPI_Group_include(rcgroup, c, cranks, &cgroup);
MPI_Group_include(rcgroup, r, rranks, &rgroup);
MPI_Comm_create_group(rccomm, cgroup, tag, &ccomm);
MPI_Comm_create_group(rccomm, rgroup, tag, &rcomm);
```

MPI 3.1 standard: Many variations, many subtleties: Read it

- `MPI_Comm_create(comm, ...)`: Collective over all processes in `comm`
- `MPI_Comm_create_group(comm, group, ...)`: Collective over all processes in `group`, processes in `group` subset of processes in `group of comm`

`MPI_Comm_create_group`: Smaller groups can work independently to create their communicator. Tag arguments for multi-threaded uses (many news in MPI 3.1)

Why should MPI_Comm_create be better than MPI_Comm_split?

Reasonable to expect



"not slower than"

$\text{MPI_Comm_create}(\dots, \text{group}, \dots) \leq \text{MPI_Comm_split}(\dots, \text{color} \dots)$

all other things (communicator) being equal

- MPI_Comm_create() straightforward by MPI_Comm_split(): take color as first process in group, key as rank in group, for processes in group (MPI_UNDEFINED otherwise). More specialized operation

Exercise: Implement

Reasonable to expect MPI_Comm_create() in $O(\log p)$? Or $O(\log p + p)$? **Probably not! Recall:** MPI has no performance model or

guarantee

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$\text{MPI_Comm_create}(\dots, \text{group}, \dots) \leq \text{MPI_Comm_split}(\dots, \text{color} \dots)$

Example of **performance guideline** that can be verified by benchmarking.

If not fulfilled, something wrong with MPI library

Jesper Larsson Träff, William D. Gropp, Rajeev Thakur: Self-Consistent MPI Performance Guidelines. IEEE Trans. Parallel Distrib. Syst. 21(5): 698-709 (2010)

All group operations can be implemented in $O(s)$ operations, where s is the size of the largest group in the operation. Space consumption is $O(U)$, where U is the maximum number of MPI processes in the system (size of `MPI_COMM_WORLD`)

Questions:

- Group (and communicator) operations permit construction of unrestricted rank->process mappings; this is costly in space. Possible to define a useful set of more restricted operations?
- Which group operations can be implemented in $o(s)$ operations?

Jesper Larsson Träff: Compact and Efficient Implementation of the MPI Group Operations. EuroMPI 2010: 170-178

Problem still to be solved:

Finding out where data from some rank (in oldcomm) have to be sent to: Where is the rank in newcomm?

```
MPI_Group_translate_ranks(MPI_Group group1,  
                           int n, const int ranks1[],  
                           MPI_Group group2,  
                           int ranks2[])
```

Problem: Find `fromrank`, `torank`, such that process in (in `oldcomm`) can receive data from `fromrank`, and send its own data to `torank`

Recall: Cannot send from rank in `oldcomm` to rank in `newcomm`; communication is always relative to one, same communicator

```
int torank, fromrank; // to be computed, in oldcomm
int oldrank, newrank;

MPI_Group oldgroup, newgroup;
MPI_Comm_group(oldcomm, &oldgroup);
MPI_Comm_group(newcomm, &newgroup);

// where has rank been mapped to?
MPI_Comm_rank(oldcomm, &oldrank); // rank in old
MPI_Group_translate_rank(newgroup, 1, &oldrank,
                        oldgroup, &torank);

// torank may be MPI_UNDEFINED
// if newcomm smaller than oldcomm

MPI_Comm_rank(newcomm, &newrank);
MPI_Group_translate_ranks(newgroup, 1, &newrank,
                        oldgroup, &fromrank);
```

Scalability of MPI communicator concept

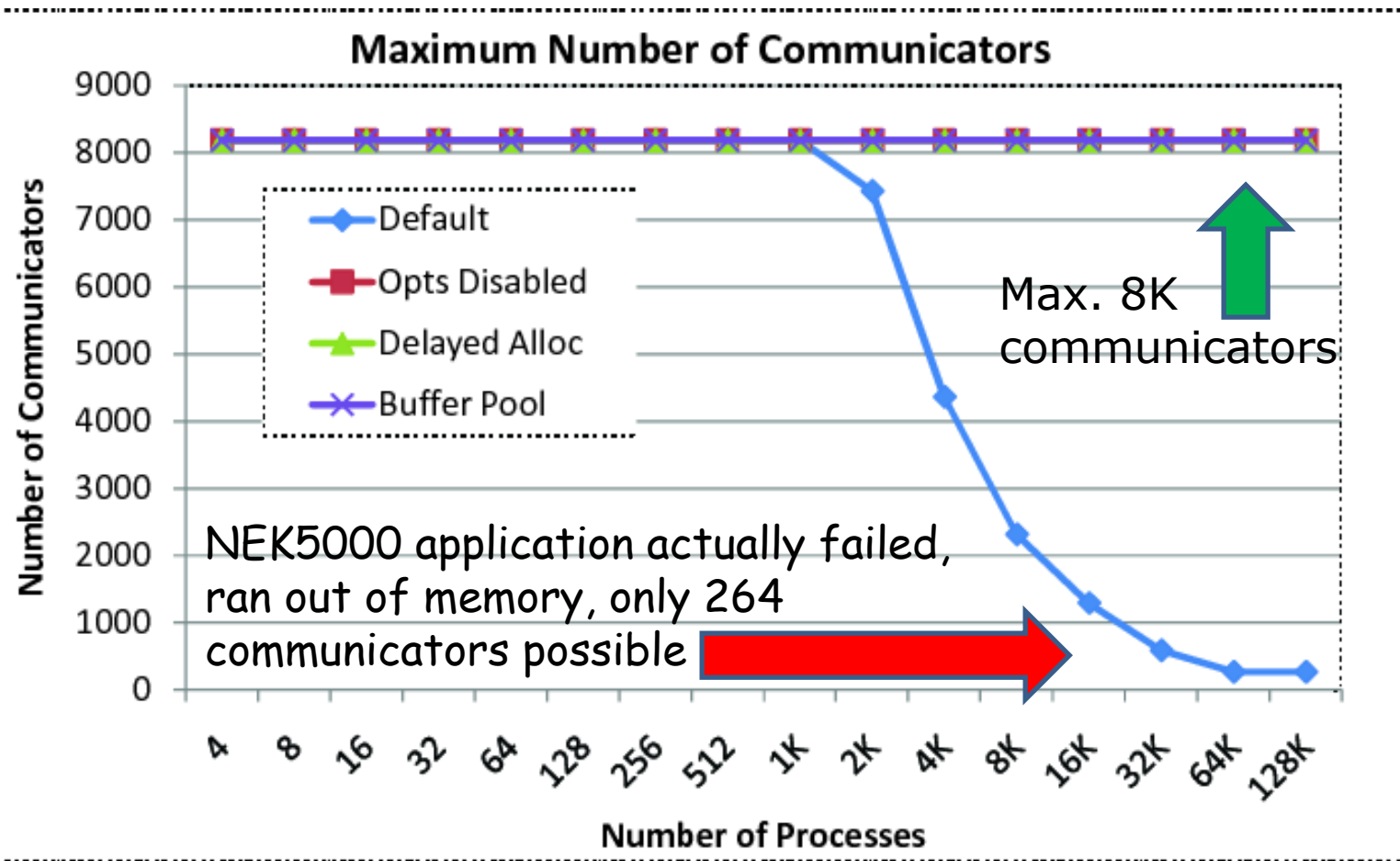
- A communicator must support translation from MPI rank to physical core in system
- Storing translations explicitly as p-element lookup array (per core) is a **non-scalable implementation**. But still the most common

Example: 250.000 cores, 4-Byte integers \approx 1MByte space per communicator (per core). Applications on systems with limited memory, and many communicators can be trouble

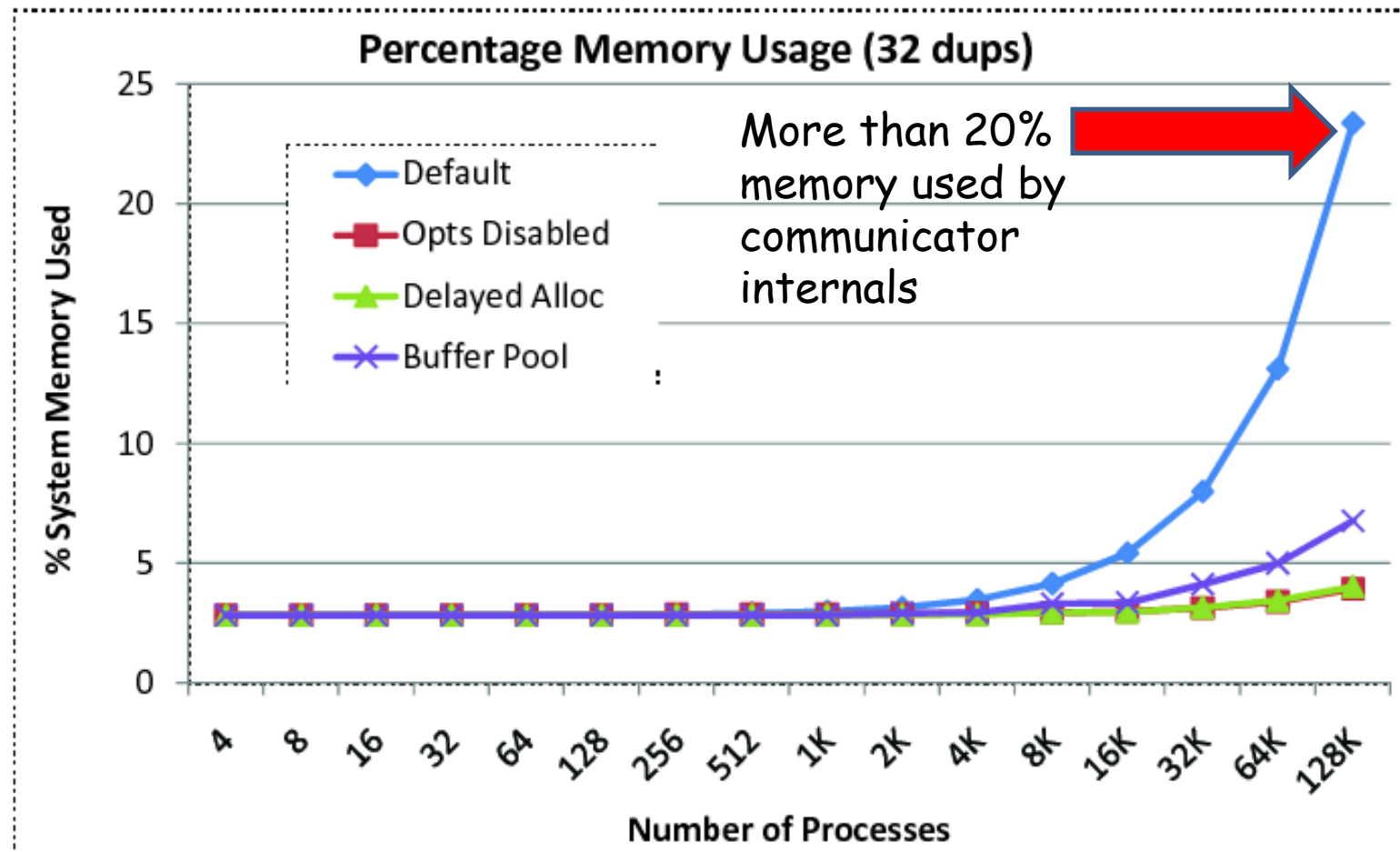
Note:

MPI specification puts no restrictions on the number and kind of communicators that can be created

Experiment (1) at Argonne National Lab BlueGene system, 2011



Experiment (2) at Argonne National Lab BlueGene system, 2011



NEK5000: Computational fluid dynamics code, often used
(benchmark variant: NEKBONE), see
<https://nek5000.mcs.anl.gov/>

On scalability of MPI, especially communicators and interface

P. Balaji, D. Buntinas, D. Goodell, W. Gropp, T. Hoefler, S. Kumar, E. L. Lusk, R. Thakur, Jesper Larsson Träff: MPI on millions of Cores. *Parallel Processing Letters* 21(1): 45-60 (2011)

H. Kamal, S. M. Mirtaheri, A. Wagner: Scalability of communicators and groups in MPI. *HPDC 2010*: 264-275

Somewhat recent (now routine) result with many, many MPI processes (little detail): MPI has so far been able to scale

P. Barnes, C. Carothers, D. Jefferson, J. LaPre: Warp speed: executing Time Warp on 1,966,080 cores. *ACM SIGSIM-PADS*, 2013

Topological awareness

Orthogonal idea:

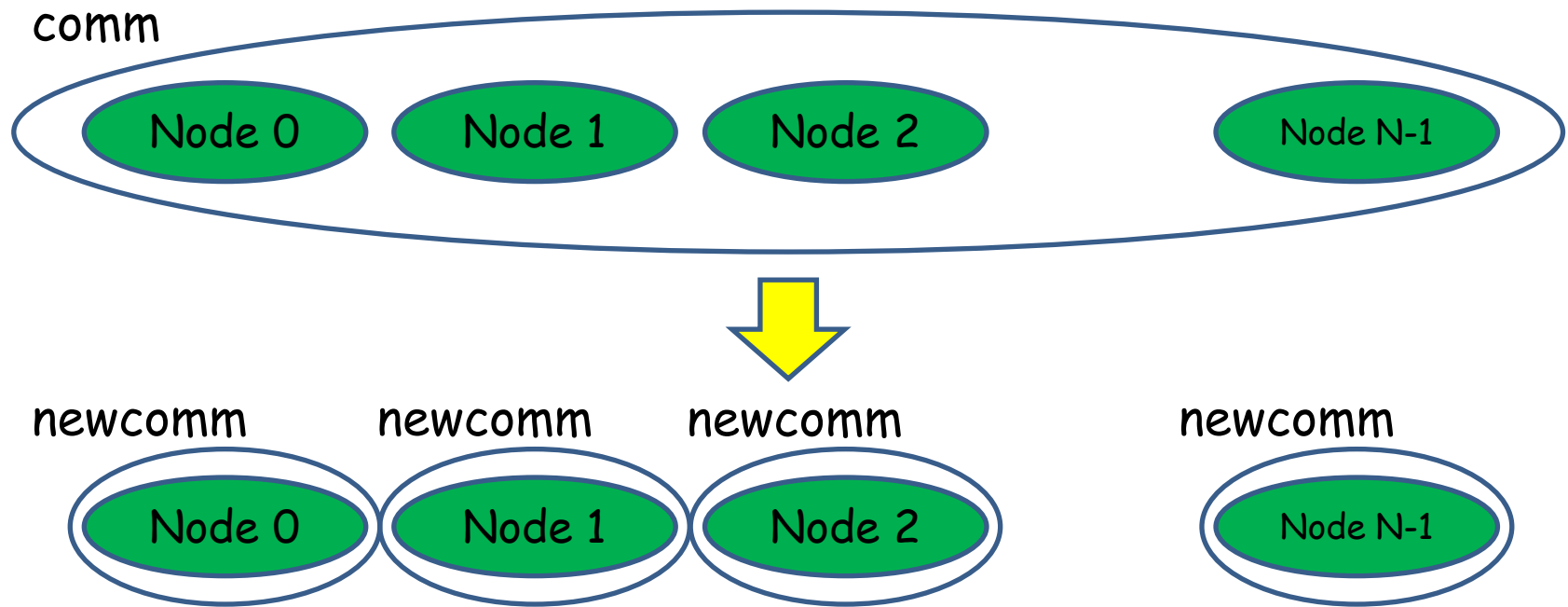
Instead of letting user specify communication requirements (communication topology), let system suggest good communicators subject to specified constraints

New in **MPI 3.0**, some support for better exploiting hierarchical systems/shared memory nodes

```
MPI_Comm_split_type(comm, MPI_COMM_TYPE_SHARED, key,  
                    info, &newcomm);
```

MPI_COMM_TYPE_SHARED: *Creates communicator for processes where a shared memory region can be created (processes on same shared-memory node)*

```
MPI_Comm_split_type(comm, MPI_COMM_TYPE_SHARED, key,  
                    info, &newcomm);
```



More to come with MPI 4.0

New split types with MPI 4.0

`MPI_COMM_TYPE_HW_UNGUIDED`, `MPI_COMM_TYPE_HW_GUIDED`:
Splitting according to other hardware characteristics (NUMA nodes), either per default, or as specified in `MPI_Info` object