Isomorphic, Sparse MPI-like Collective Communication Operations for Parallel Stencil Computations

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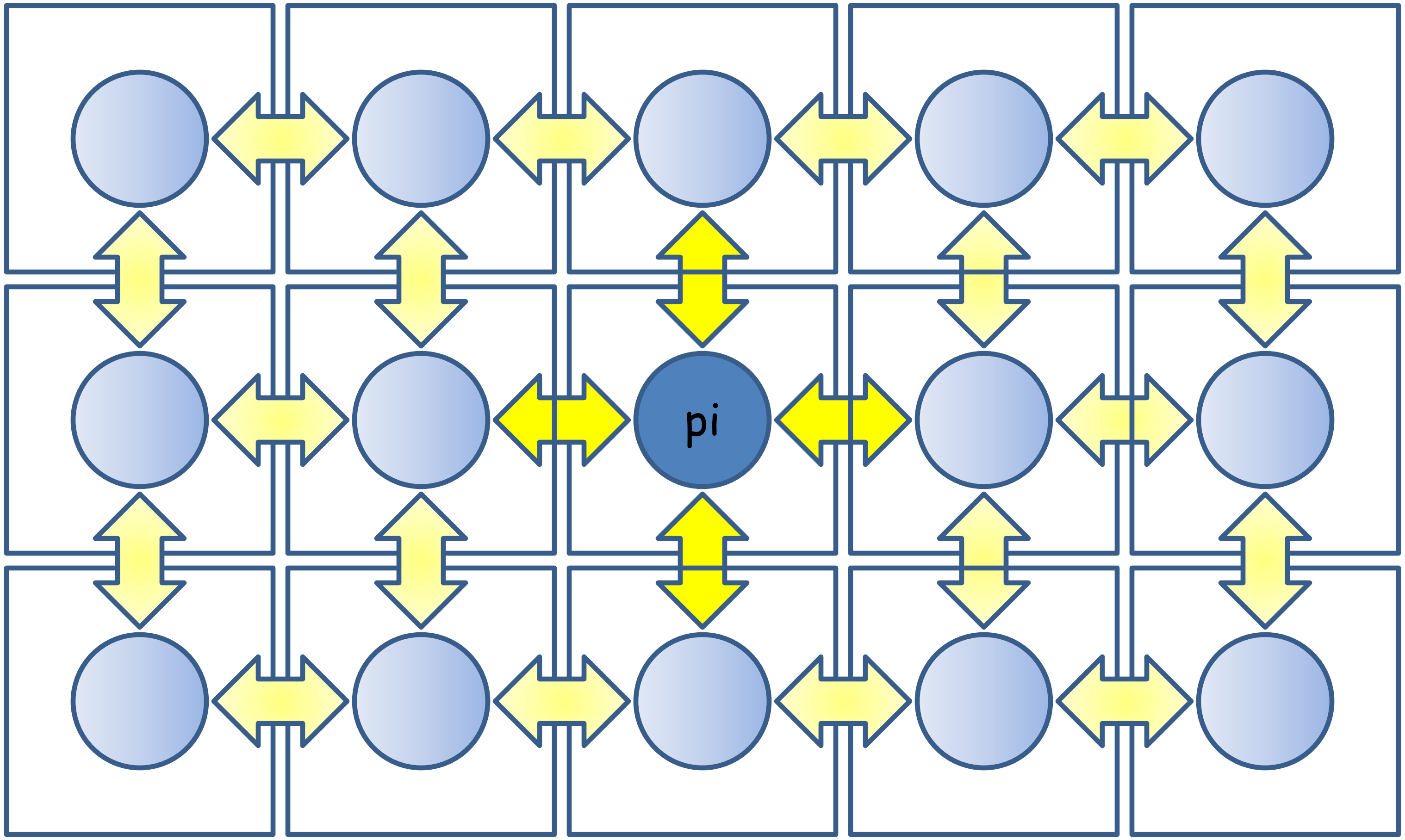

pi

Situation

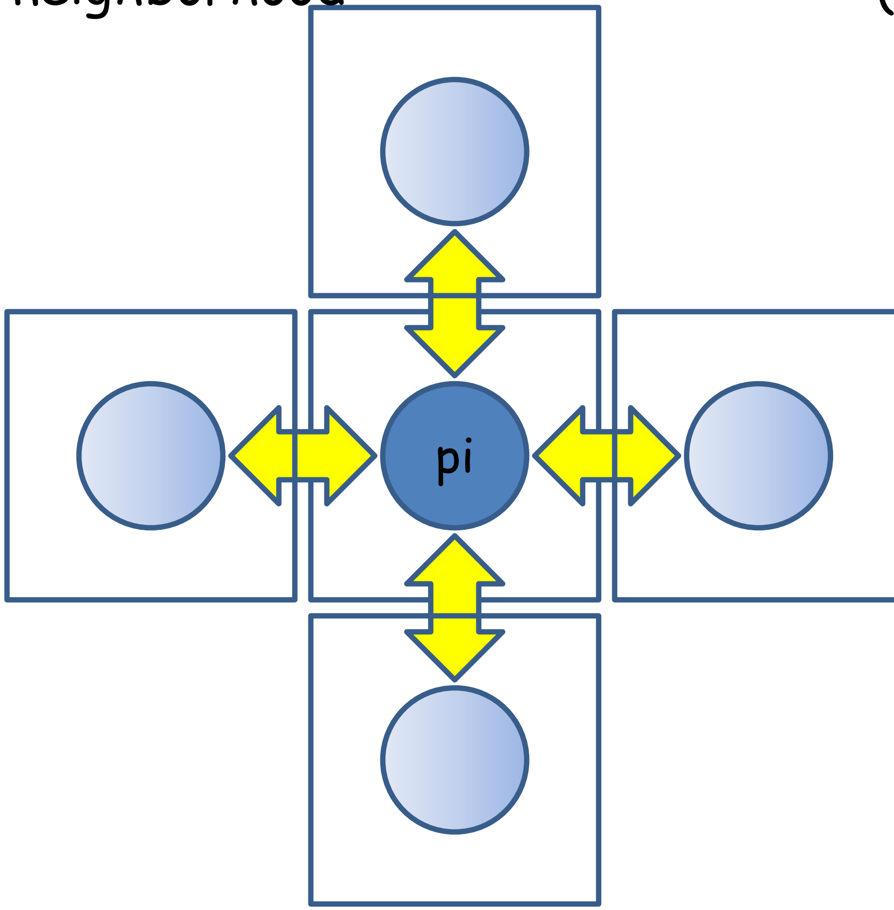
•Processes arranged in some regular structure (mesh, torus, …)
•Each process needs to communicate with a small neighborhood
•All processes have similar neighborhoods
•All processes involved: collective communication

Problem

•Is MPI support for this type of communication adequate/good?
•Can it potentially be supported better and more efficiently?

MPI 3.0 intention: non-blocking neighborhood collectives

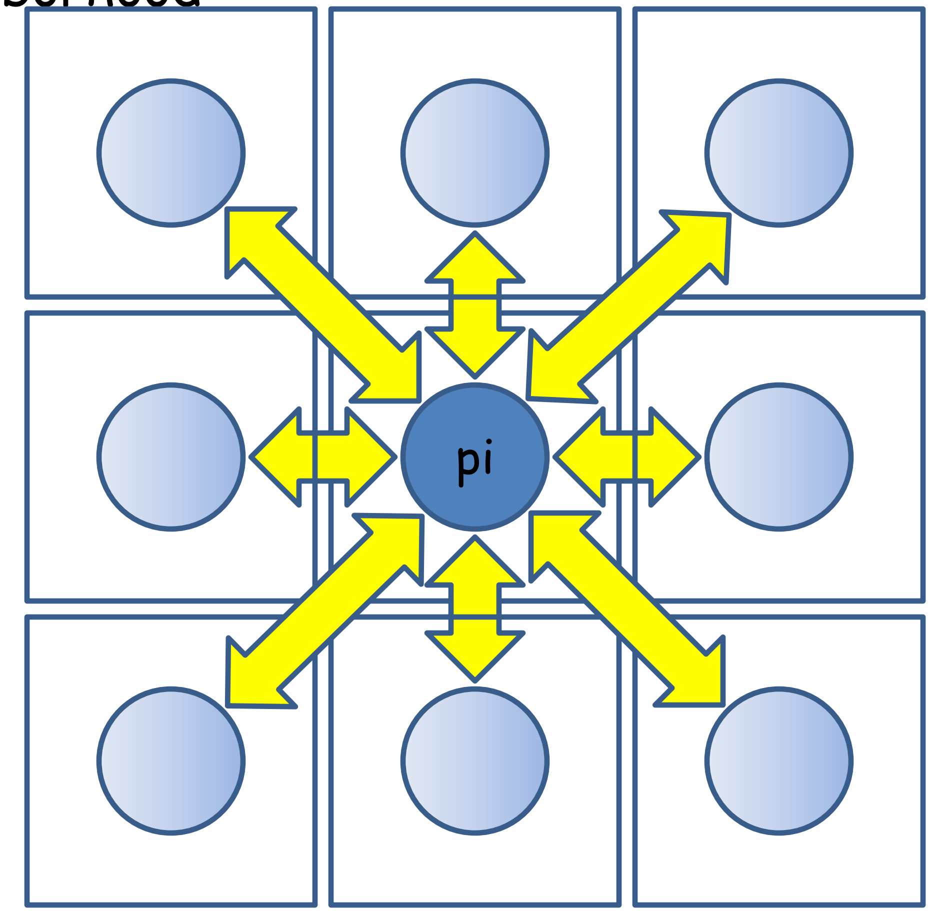
von Neumann neighborhood (5-point stencil)



Each process communicates with processes in mesh/torus that are exactly one "hop" away (Manhattan distance 1)

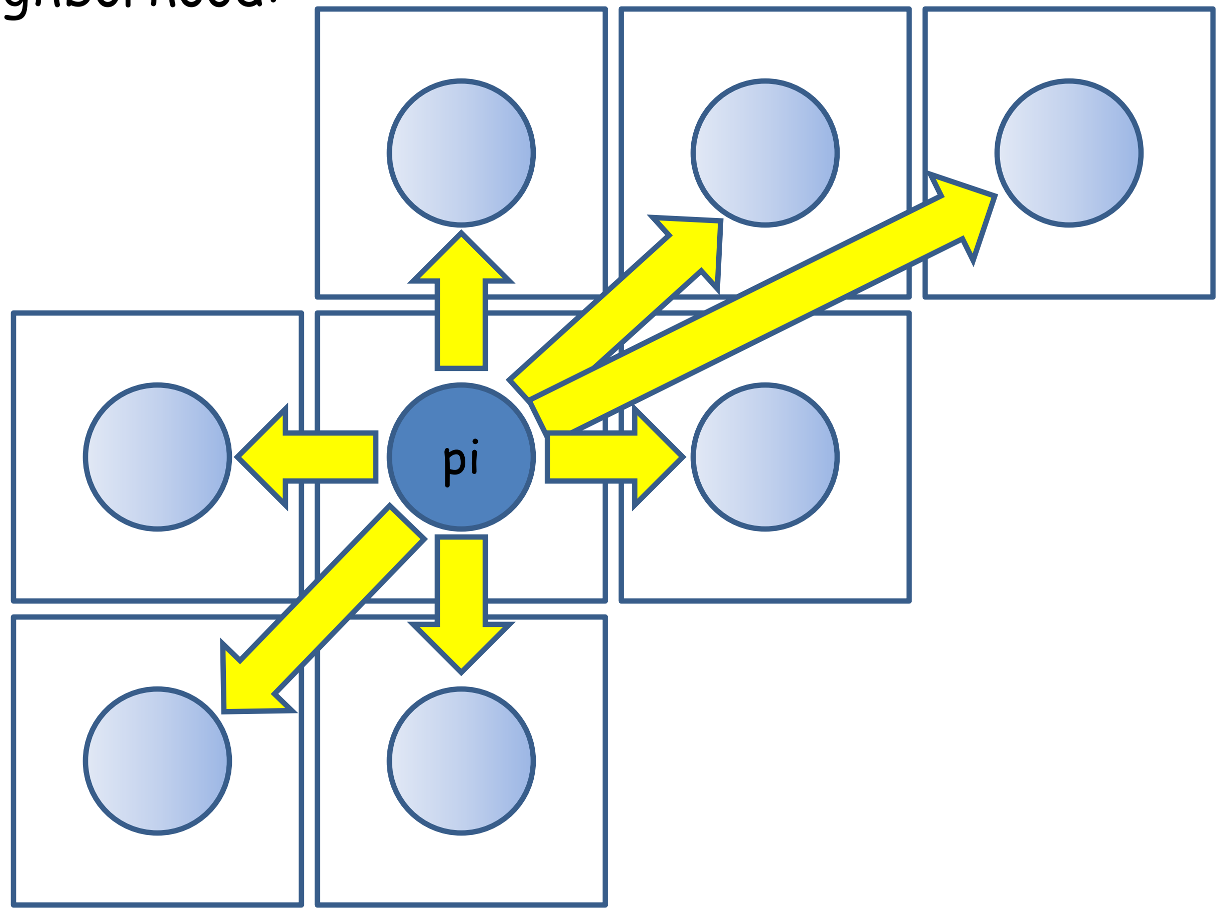
Moore neighborhood

(9-point stencil)



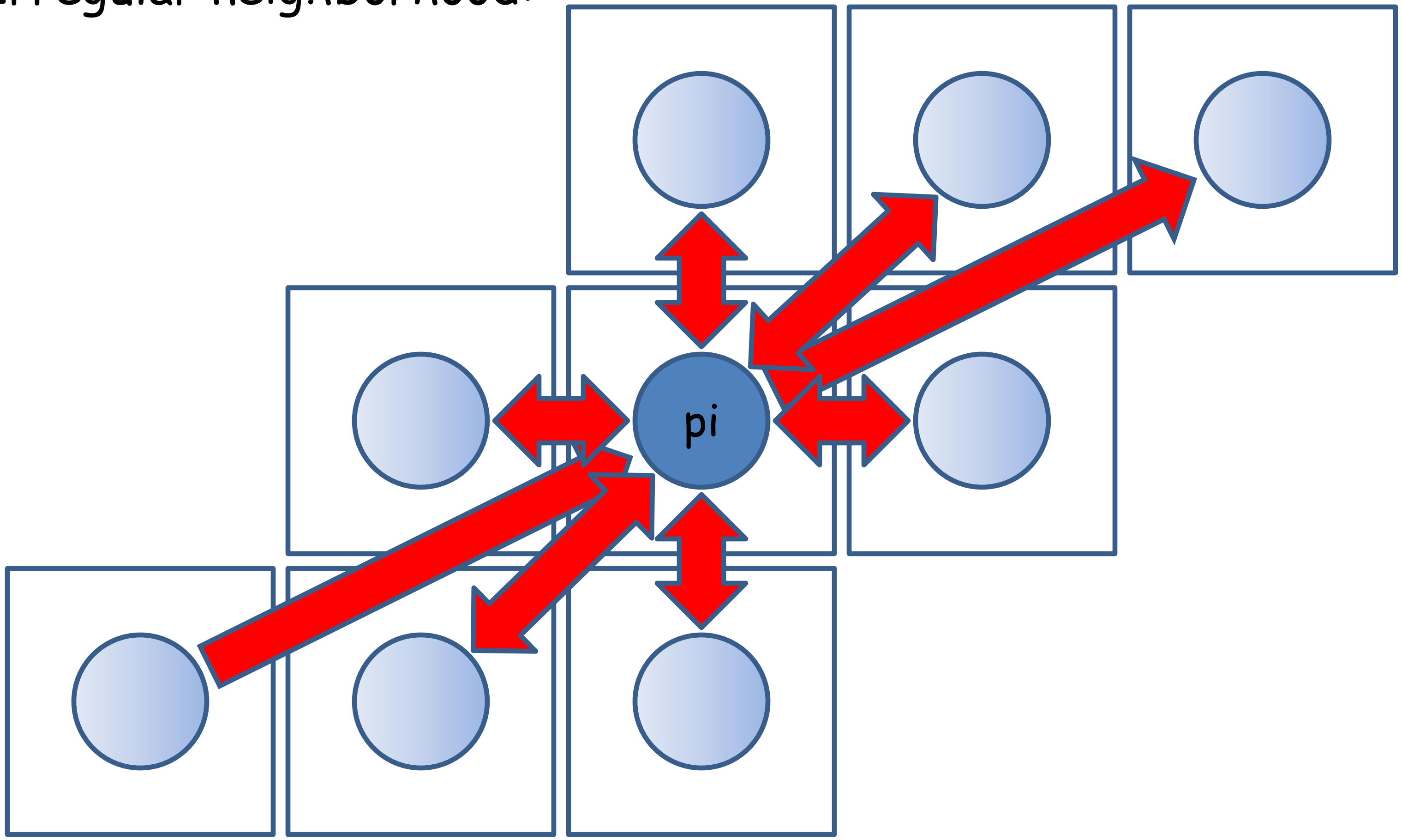
Each process communicates with processes in mesh/torus where at least one coordinate differs by one (Chebyshev distance 1)

Irregular neighborhood:



Each process sends data to s other processes. All processes use same pattern, per symmetry receives also from s processes

Irregular neighborhood:



Each process sends data to s other processes. All processes use same pattern, per symmetry receives also from s processes

Observations

- All processes use same collective communication pattern

Isomorphic, collective communication

- Convenient to describe neighborhoods relative to some underlying, regular structure (d-dimensional mesh, torus, …)

"Isomorphic" requirement easily fulfilled

MPI 3.0 solution

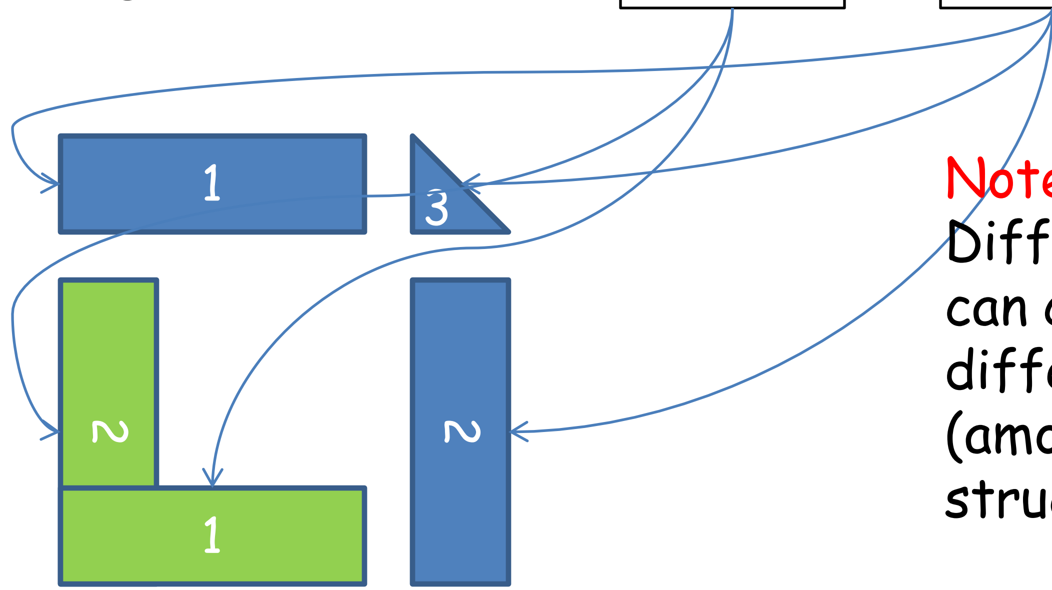
Use sparse, non-blocking collectives for neighborhood communication:

```
MPI_Ineighbor_alltoall()
MPI_Ineighbor_alltoallv()
MPI_Ineighbor_alltoallw()

MPI_Ineighbor_allgather()
MPI_Ineighbor_allgatherv()
```

Collective data exchange operations for some given, per process neighborhood


```
MPI_Neighbor_alltoallw(sendbuf,…,recvbuf,…,comm);
```



Note (-w collective): Different neighbors can communicate different data (amount and structure)

- Local neighborhood: implicit list of source (incoming) and destination (outgoing) neighbors (MPI processes)
- Order of neighbors determine order of communication buffers
- Correctness/deadlock freedom: Destinations and sources must match
- Neighborhoods are fixed and associated with communicator

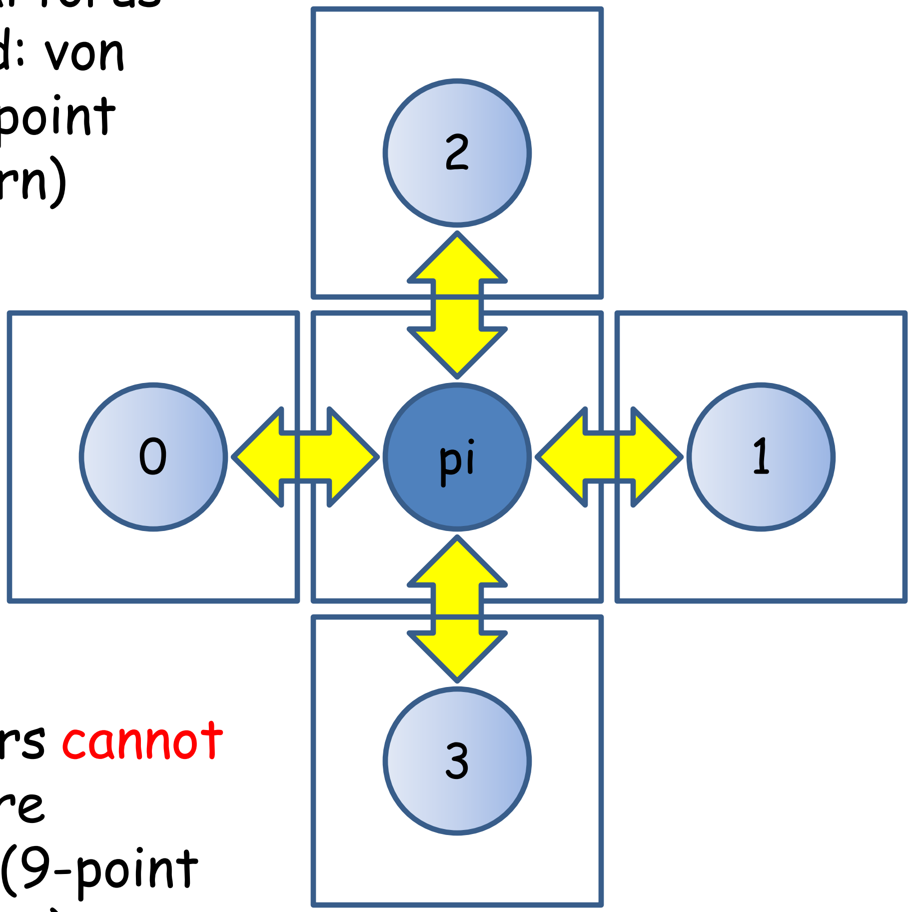
Implicit neighborhoods: Cartesian communicators

d-dimensional mesh/torus MPI process structures created with

```
MPI_Cart_create(comm,d,…,reorder,&cartcomm);
```

- Processes organized into d-dimensional torus pattern (with given size of dimensions)
- Isomorphic: neighborhoods defined for all processes as immediate torus neighbors (-/+ 1 hop in each dimension)
- Symmetric: all neighbors both source and destination
- Order of neighbors is fixed, dimensionwise (0 to d-1), -/+
- Number of neighbors is always 2*d (for meshes, some non-existent, MPI_PROC_NULL)

2-dimensional torus neighborhood: von Neumann (5-point stencil pattern)

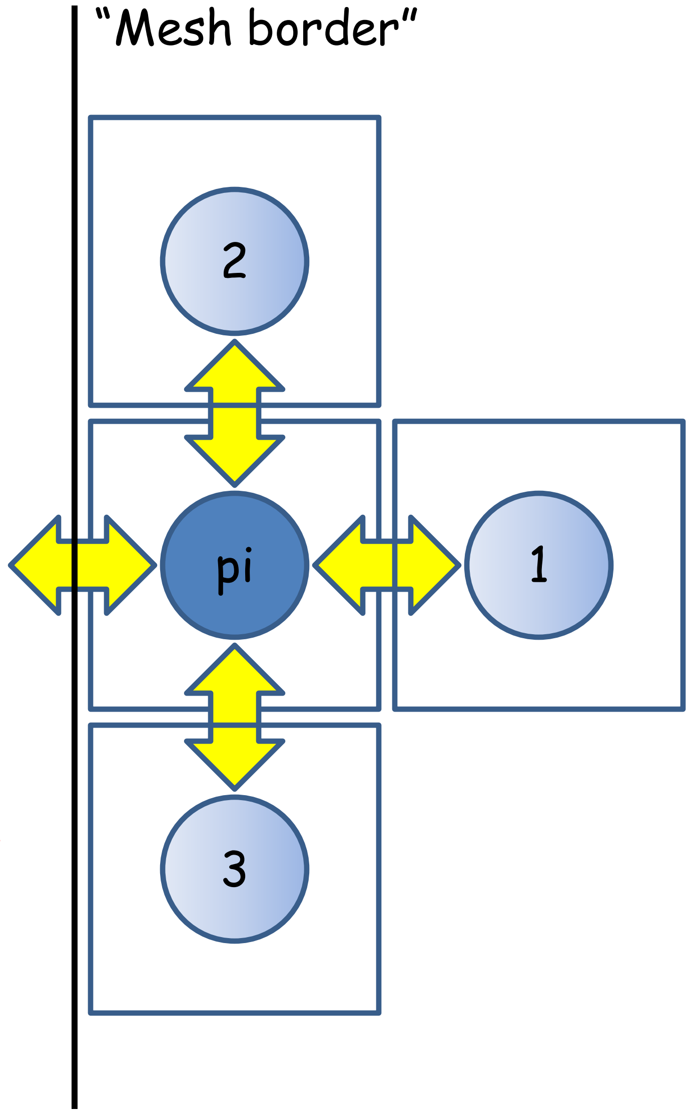


Cartesian communicators cannot express Moore neighborhod (9-point stencil pattern)

2-dimensional mesh neighborhood

MPI_PROC_NULL neighbor

Cartesian communicators cannot express Moore neighborhod (9-point stencil pattern)



```
MPI_Cart_create(comm,d,…,reorder,&cartcomm);
```

Makes it possible for MPI library to map torus communication topology to actual network topology

Contrast to explicit graph communicators:

- No weights on communication edges (could help mapping)
- No MPI_Info object (could pass information on how to map)

- No query functions for neighborhood: Cart_neighborhood_get()

Get neighbors with MPI_Cart_shift()

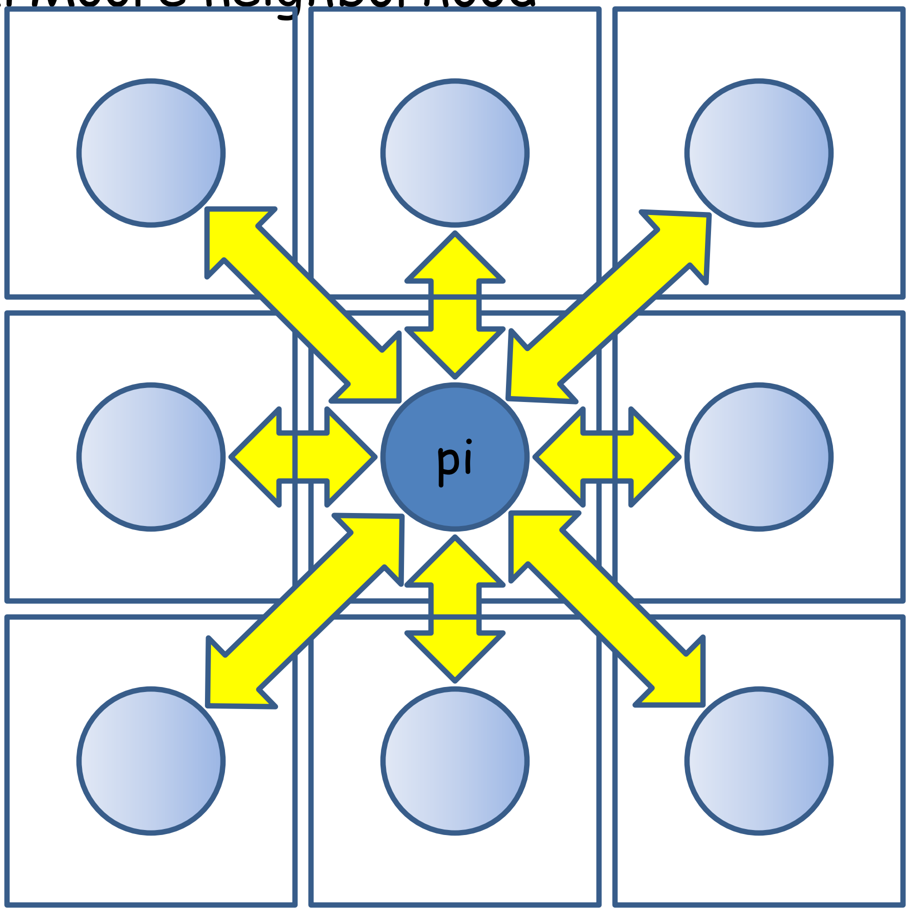
Explicit neighborhoods: general graph communicators

Arbitrary directed communication (multi-)graph created with

```
MPI_Dist_graph_create(_adjacent)(comm,
                                 <edges>,<weights>,
                                 info,reorder,
                                 &graphcomm);
```

- Communication edges between "real" MPI processes only (no MPI_PROC_NULL)
- Local neighborhoods consist of adjacent processes: sources and destinations (not necessarily symmetric)
- Not necessarily isomorphic neighborhoods
- Neighborhood query functions: MPI_Dist_graph_neighbors()
- Edge weights and MPI_Info object to guide mapping

2-dimensional Moore neighborhood



… must be specified as general graph topology. User must determine explicit ranks of all 8 neighbors, must use query function to later determine order of neighbors

Summary: MPI 3.0 implicit and explicit neighborhoods

- Cartesian communicators severely limited: express only von Neumann type neighborhoods

- General graph topologies perhaps too general for many common situations, no information on global graph structure

- Unfortunate differences between Cartesian and general graph communicator functionalities (info/weights, query functionality, MPI_PROC_NULL)

Same neighborhood set up in two different ways can have quite different properties

"Isomorphic neighborhoods" a valuable assertion for sparse collective communication algorithms

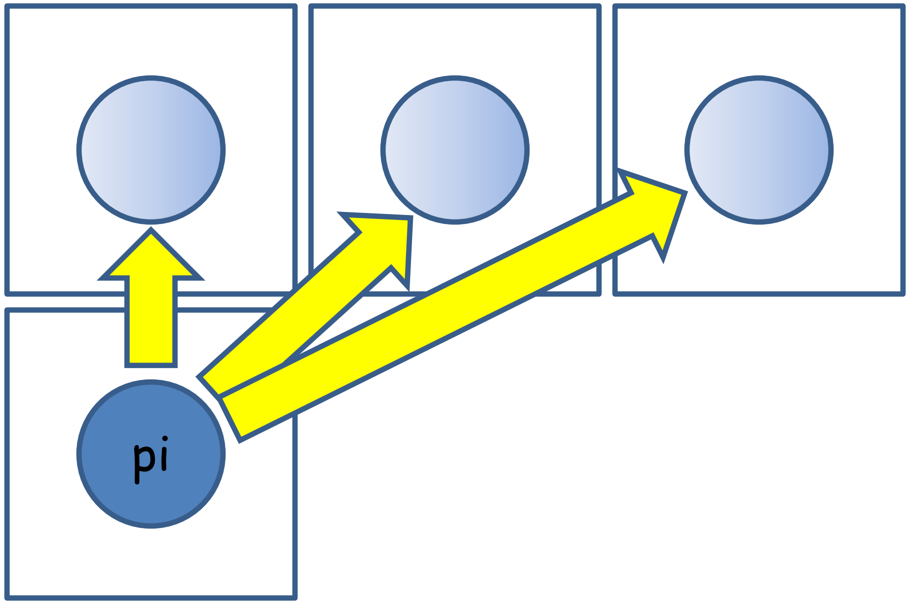
An extension and a restriction: isomorphic, sparse collectives

Given d-dimensional Cartesian communicator: mesh (periodic in some dimensions), torus

Isomorphic (sparse) neighborhoods

- Neighborhood given by (ordered) list of relative coordinates (d-vectors)
- Only destination coordinates listed (sources implied by isomorphic requirement)
- Isomorphic: all processes use (exactly!) same neighborhood (same coordinates, same order)

3-neighborhood:
(1,0),(1,1),(1,2)
relative destinations



3-neighborhood:
(1,0),(1,1),(1,2)
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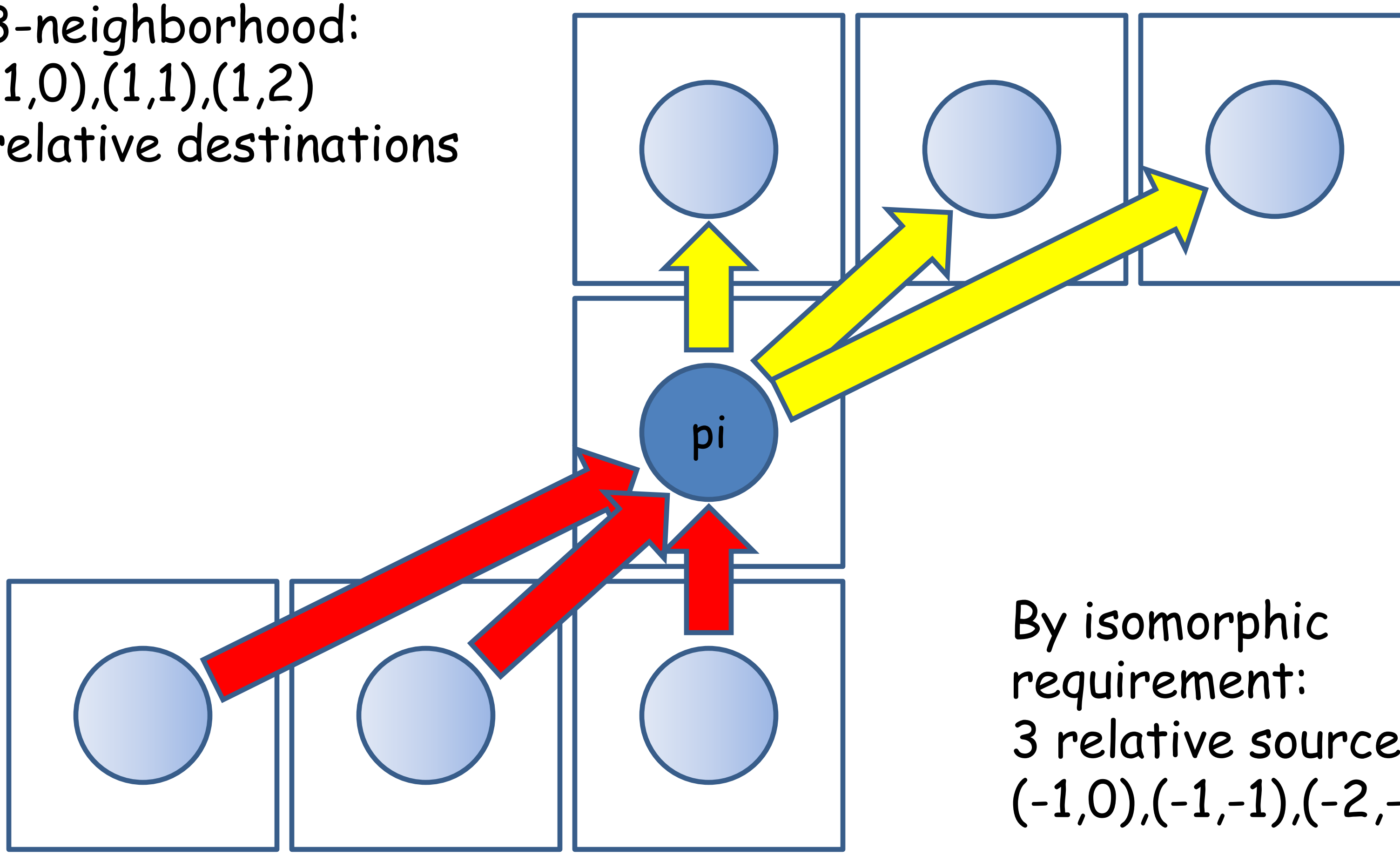
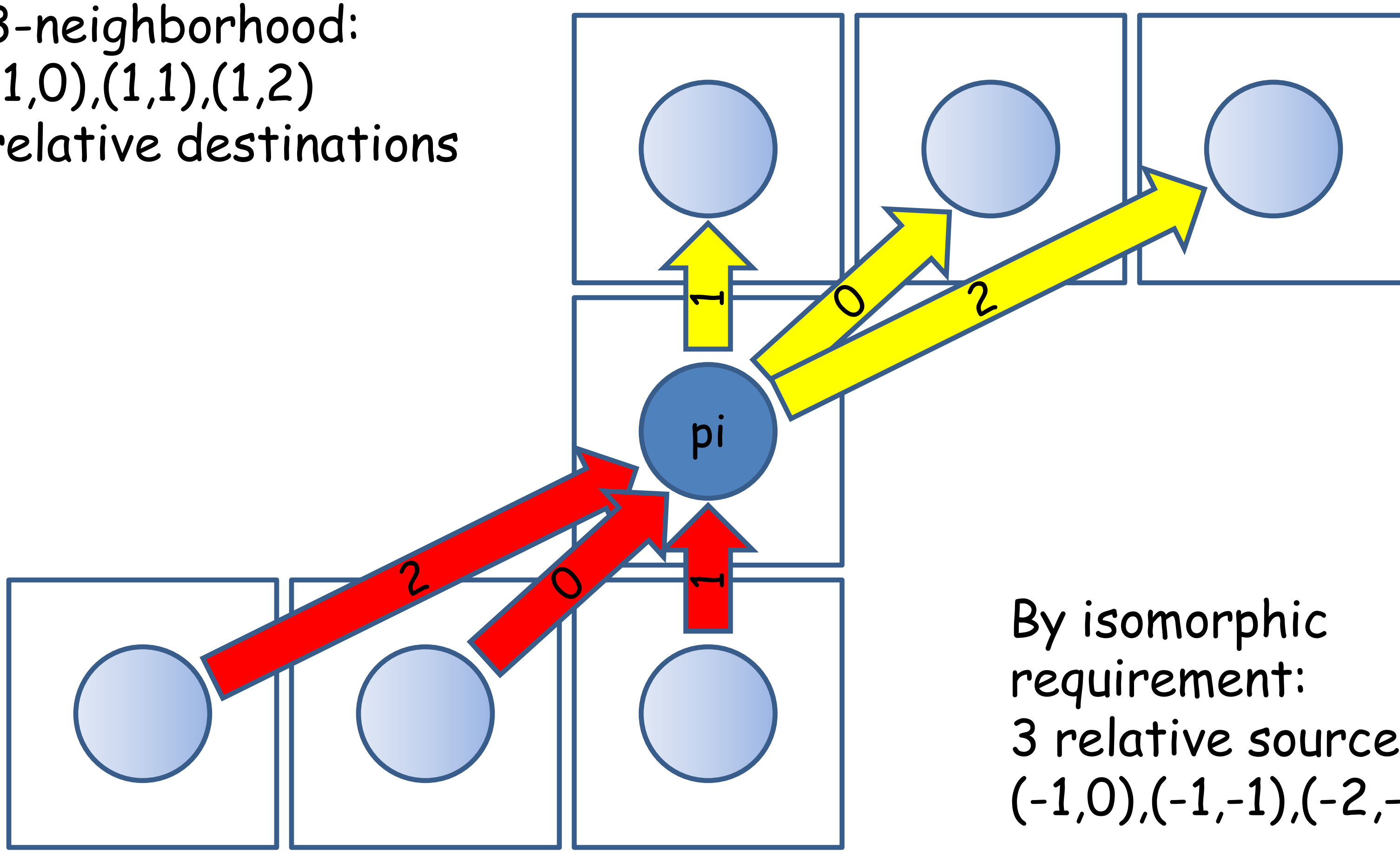


By isomorphic requirement:
3 relative sources
(-1,0),(-1,-1),(-2,-1)

3-neighborhood:
(1,0),(1,1),(1,2)
relative destinations



By isomorphic requirement:
3 relative sources
(-1,0),(-1,-1),(-2,-1)

Repetitions allowed

s-neighborhood: list of s relative coordinates [C0, C1, C2, C3, …]

Example, 5-dimensions: [(0,1,1,3,1), (1,1,0,1,2), (-2,-2,-2,-2,-2), (0,1,1,3,1), …] (C-style: flattened into simple array)

•s destination neighbors for rank R in absolute coordinates: R+C0, R+C1, R+C2, R+C3, …

•s source neighbors for rank R: R-C0, R-C1, R-C2, R-C3, …

```
Iso_neighborhood_create(MPI_Comm cartcomm,
                        int s,
                        int relative_coordinates[],
                        MPI_Comm *isocomm)
```

isocomm still Cartesian

```
Iso_neighborhood_create(MPI_Comm cartcomm,
                        int s,
                        int relative_coordinates[],
                        MPI_Comm *isocomm)
```

Implementation (very cheap):
Attaches neighborhood list to cartcomm, precomputes absolute ranks, etc.

(a "real" implementation would need to create new isocomm, but this can partly be precomputed with cartcomm and amortized)

Design decision: no reorder possibility, no weights, no MPI_Info. Process mapping done by Cart_create()

Convenience functions: navigation

```
Cart_relative_rank(MPI_Comm cartcomm, int relative[],
                   int *rank)
Cart_relative_coord(MPI_Comm cartcomm, int rank,
                    int relative)
Cart_relative_shift(MPI_Comm cartcomm,
                    int relative_shift[],
                    int *source, int *target)
```

Implementation: easy, on top of MPI Cartesian functionality

Convenience functions: query

Similar functions for Cartesian communicators

```
Iso_neighborhood_count(MPI_Comm isocomm,
                       int *s,
                       int *indegree, int *outdegree)
Iso_neighborhood_get(MPI_Comm isocomm, int max_s,
                     int sources[], int destinations[])

Iso_neighborhood_graph_get(MPI_Comm isocomm, int max_s,
                           int sources[],
                           int destinations[])
```

1. First get function: return all neighbors, including MPI_PROC_NULL ones
2. Second get function: return only "real" neighbors, no MPI_PROC_NULL
3. Output format for MPI_Dist_graph_create_adjacent()

Convenience functions: query

Similar functions for Cartesian communicators

```
Iso_neighborhood_count(MPI_Comm isocomm,
                       int *s,
                       int *indegree, int *outdegree)
Iso_neighborhood_get(MPI_Comm isocomm, int max_s,
                     int sources[], int destinations[])

Iso_neighborhood_graph_get(MPI_Comm isocomm,   t max_s,
                           int sources[],
                           int destinations[])
```

Implementation: easy, return attached, precomputed r k information

List of absolute process ranks

Isomorphic blocking collectives

```
Iso_neighbor_alltoall(void *sendbuf, …
                      void *recvbuf, …,
                      MPI_Comm isocomm)
Iso_neighbor_alltoallv(void *sendbuf, …
                       void *recvbuf, …,
                       MPI_Comm isocomm)
Iso_neighbor_alltoallw(void *sendbuf, …,
                       void *recvbuf, …,
                       MPI_Comm isocomm)
```

Probably most useful alltoall variant: different neighbors have different structure (datatype) and volume

Interface scalablity not an issue for sparse neighborhoods

Isomorphic blocking collectives

```
Iso_neighbor_allgather(void *sendbuf, …
                       void *recvbuf, …,
                       MPI_Comm isocomm)
Iso_neighbor_allgatherv(void *sendbuf, …
                        void *recvbuf, …,
                        MPI_Comm isocomm)
Iso_neighbor_allgatherw(void *sendbuf, …,
                        void *recvbuf, …,
                        MPI_Comm isocomm)
```

Not in MPI 3.0 but equally useful

Isomorphic blocking collectives

```
Iso_neighbor_reduce (void *sendbuf, void *recvbuf, …,
                     MPI_Comm isocomm)
Iso_neighbor_reduce_scatter(void *sendbuf, …
                            void *recvbuf, …,
                            MPI_Comm isocomm)
```

Reduction neighbor collectives dropped for MPI 3.0

And non-blocking variants: Iiso_neighbor_alltoallw(), …

Prototype library implementation at
www.par.tuwien.ac.at/Downloads/TUWMPI/tuwisosparse.tgz

Algorithms' observations

Isomorphic property makes deadlock-free implementations trivial

```
// pseudo: negate all coordinates
minusrelative = -relative

for (i=0; i<s; i++) {
  Cart_relative_rank(isocomm,relative+i*d,&destrank);
  Cart_relative_rank(isocomm,minusrelative+i*d,
                     &sourcerank);
  MPI_Sendrecv(sendbuf[i],…,destrank,ISOTAG,
               recvbuf[i],…,sourcerank,ISOTAG,
               comm,MPI_STATUS_IGNORE);
}
```

Does not work with graph neighborhoods: not known that i'th destination matches i'th source

Key observation:

By isomorphic condition (a global graph property), communication schedules can be computed locally and still be deadlock free processes will compute same schedule

Idea 1: Dimension-wise message combining

Write C as linear combination of coordinate basis vectors

$C = \{a0\ V0\}+\{a1\ V1\}+\{a2\ V2\}+\ldots+\{ad\ Vd\}$, $Vi = (0,0,\ldots 0,1,0,\ldots 0)$

Send (and receive) in d' rounds, in round i combine all messages with same {ai Vi} component

Key observation:

By isomorphic condition (a global graph property), communication schedules can be computed locally and still be deadlock free processes will compute same schedule

Idea 2: Logarithmic round message combining (Bruck)

Assume all neighbors Ci are linearly dependent, Ci = i*a*K for some relative coordinate K.

With message-combining, log s rounds suffice, s/2 blocks per round

Not yet implemented

Experimental work

Implementations:

•Iso_neighborhood_create() by attaching information to Cartesian communicator

•Iso_neighbor_alltoallw() with non-blocking send-recive operations

Towards a systematic benchmark for neighborhood communication

Questions:

•How expensive is neighborhood creation in comparison to Cartesian and graph communicators? Do Cartesian and graph communicator setup times differ? Does the communication graph play a role?

•How well does the simple alltoallw implementation compare to MPI 3.0 functionality?

Systems

Small, 36-node InfiniBand cluster, each node with two 8-core AMD 6134 Opteron processors at 2.3GHz, Mellanox IB MT4036 QDR

Three different MPI libraries:
necMPI (1.3.1), mvapich (2.2.1), OpenMPI (1.8.4)

Not here/not in paper:
Experiments also on 64 32-core nodes of Cray XC40 system with Cray-mpich (7.0.4) at KTH, Sweden

Communicator creation times

von Neumann and Moore neighborhoods with different radii

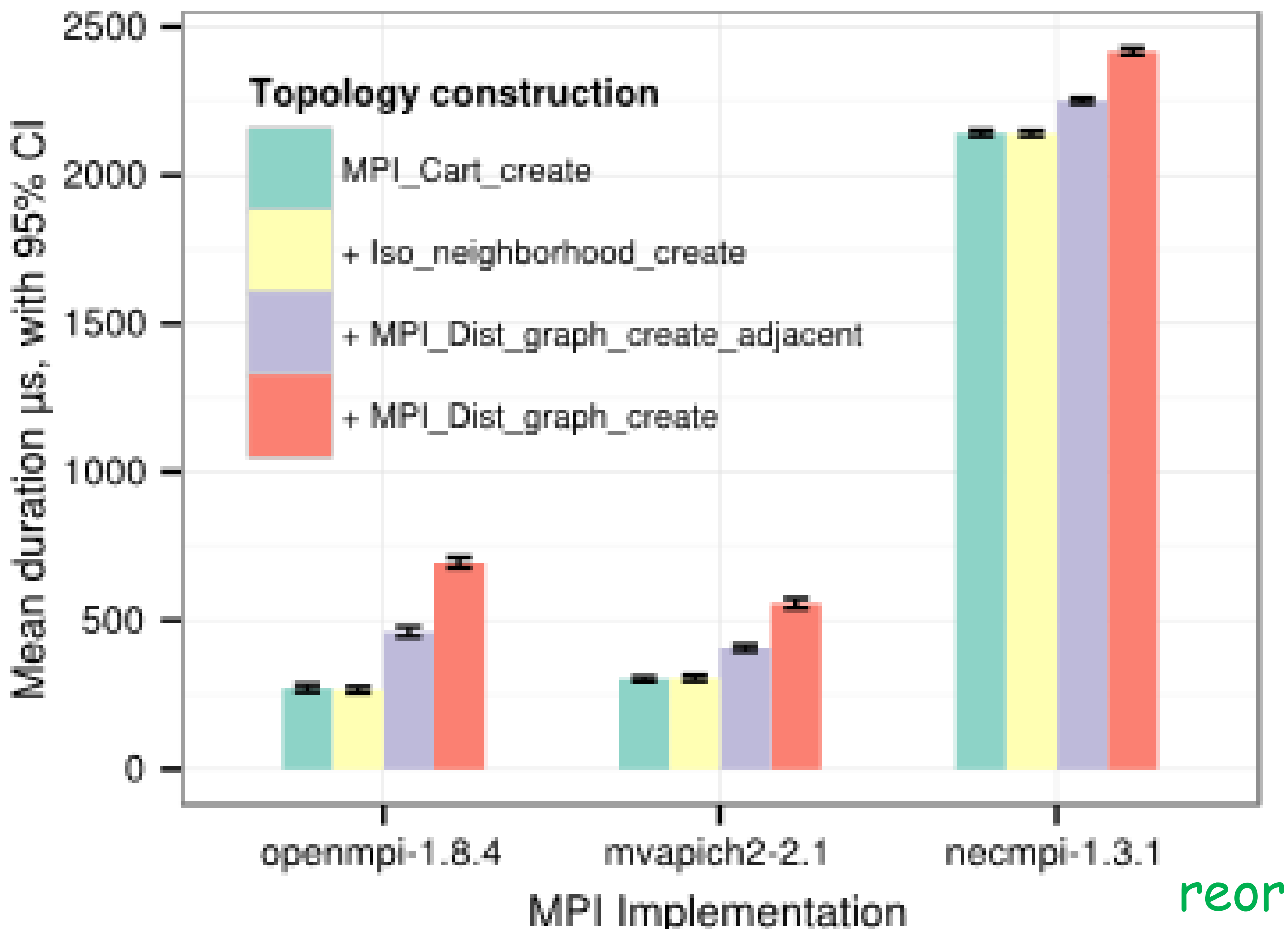
Setup times:

- MPI_Cart_create()
- MPI_Dist_graph_create_adjacent()

Attachment time:

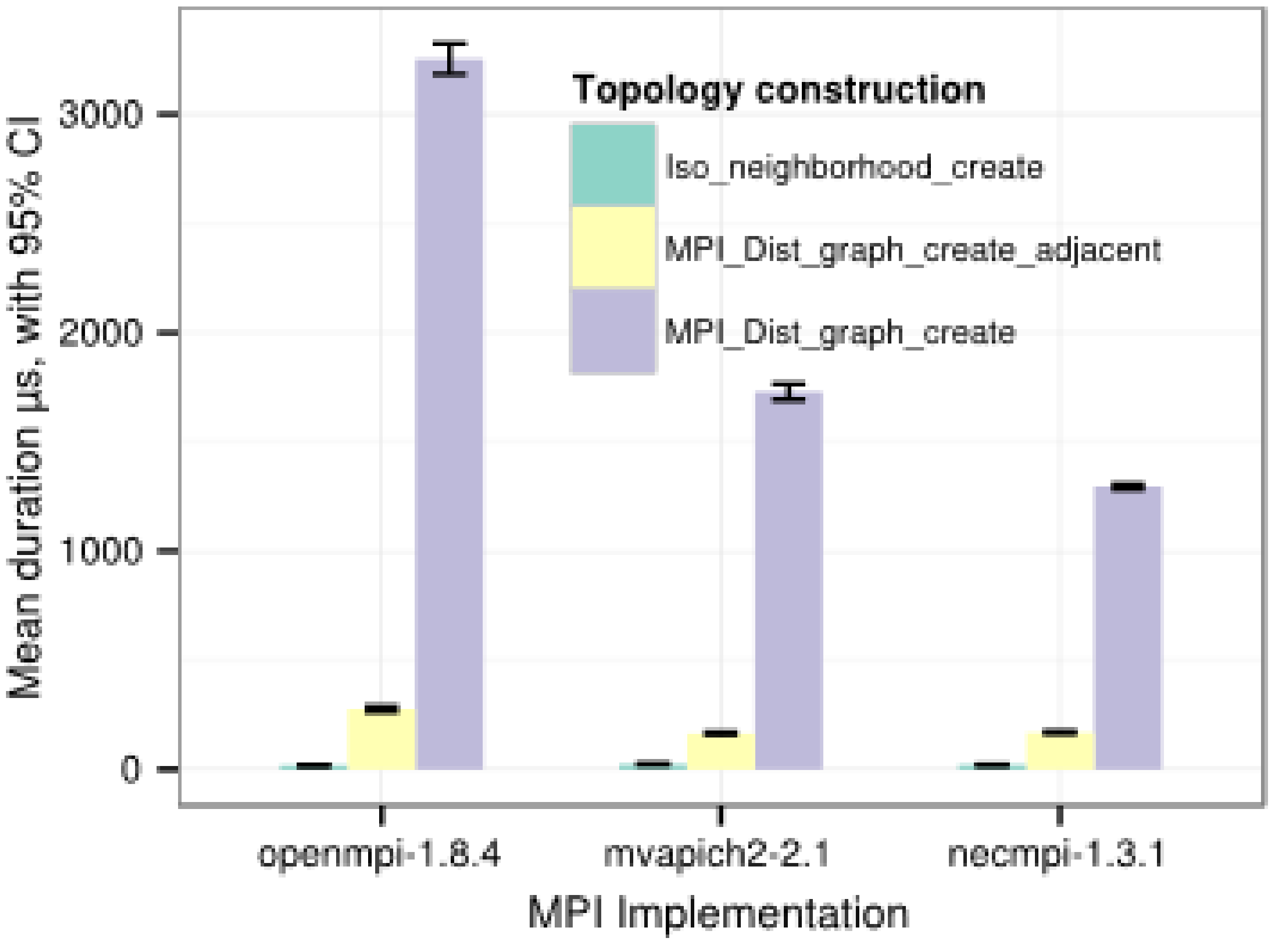
- Iso_neighborhood_create()

d=2, 24x20 virtual torus, r=1 von Neumann neighborhood



Note: reorder=true in MPI_Cart_create

d=2, 24x20 virtual torus, r=3 Moore neighborhood



Findings:

- MPI libraries differ

- Use MPI_Dist_graph_create_adjacent() where possible! Not MPI_Dist_graph_create()

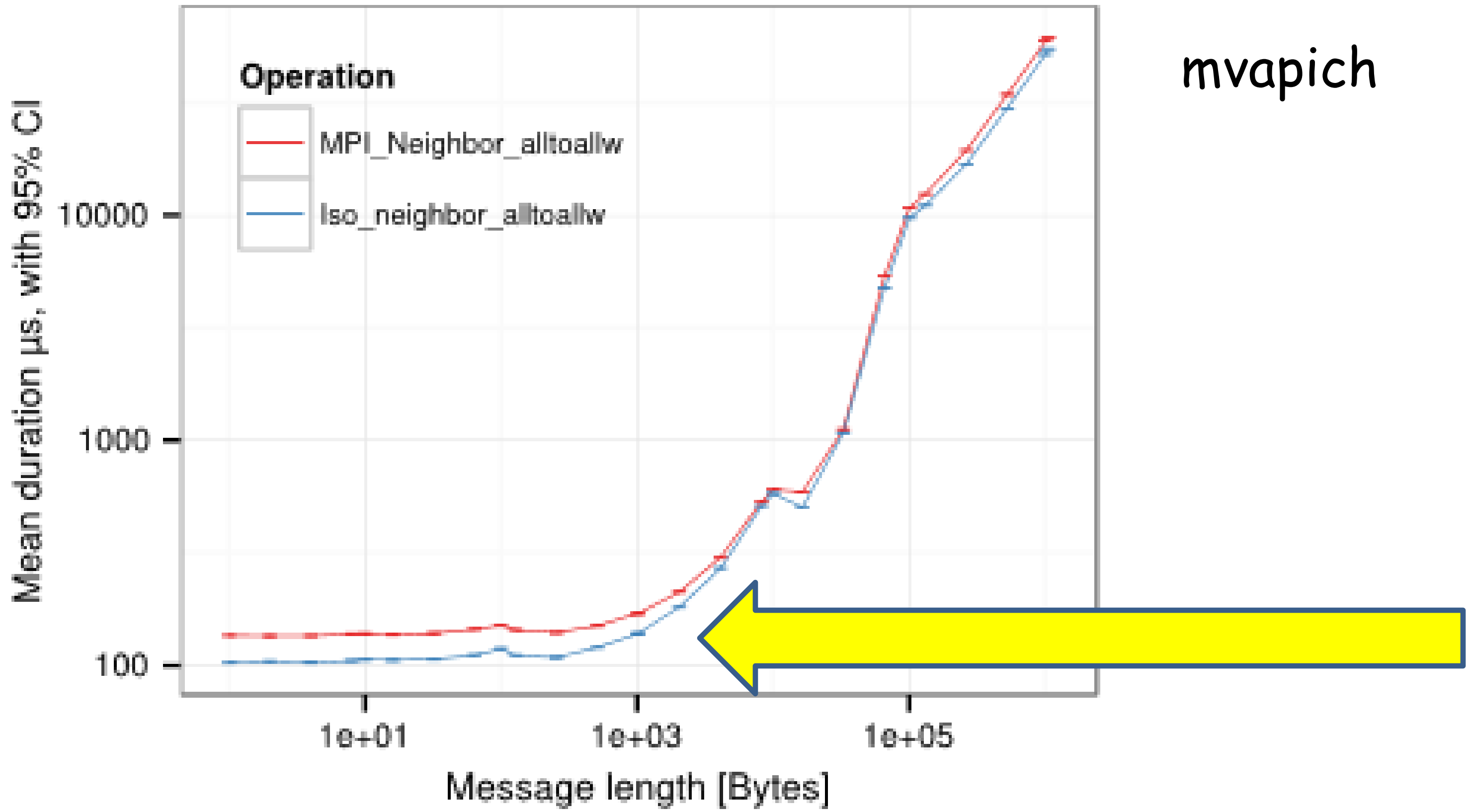
Sparse alltoall(w) communication times

Different neighborhoods:
•structure
•order

•Iso_neighbor_alltoallw() vs.
•MPI_Neighbor_alltoallw()

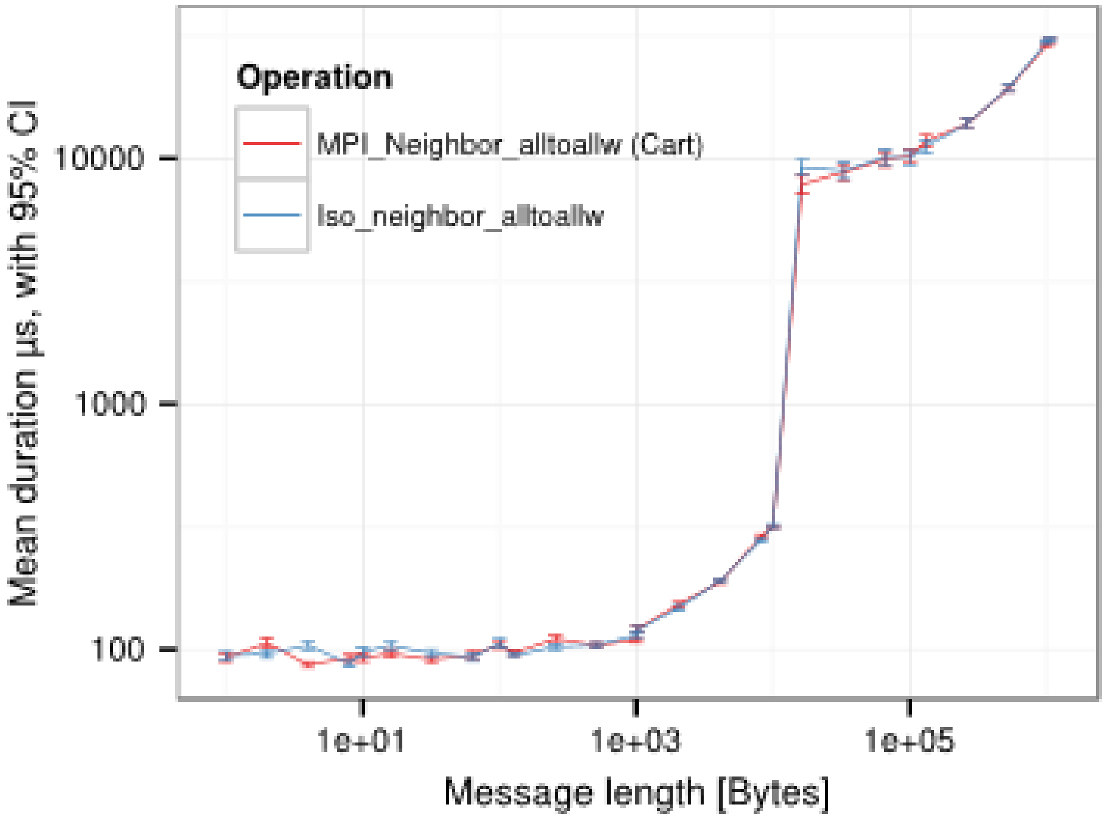
•Different MPI libraries

2=2, 6x5 virtual torus, r=3 Moore neighborhood



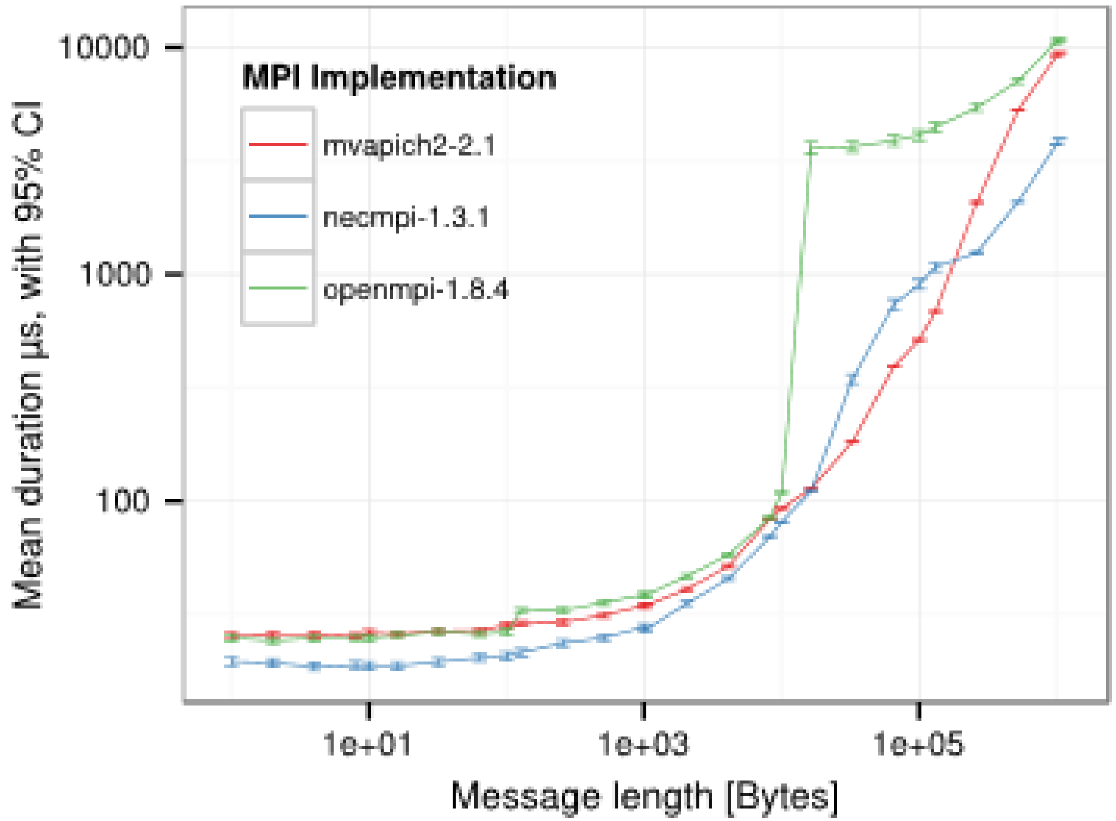
mvapich

d=2, 24x20 virtual torus, r=1 von Neumann neighborhood

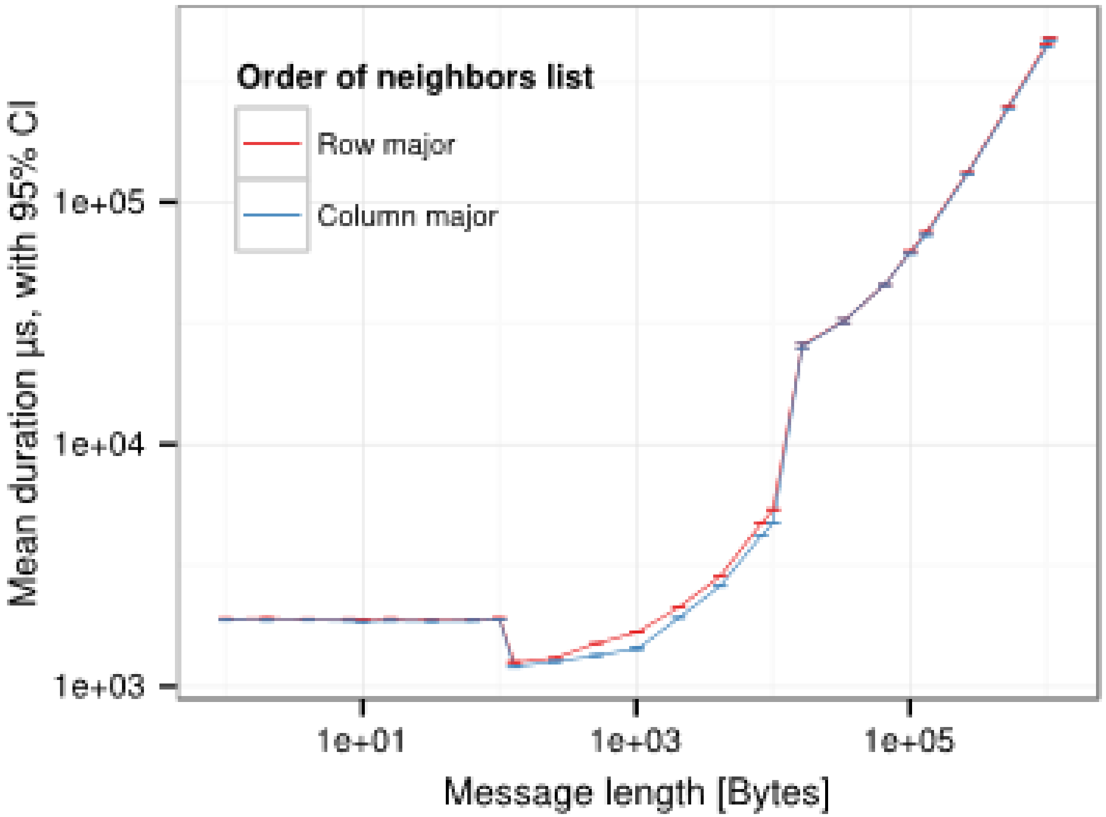


OpenMPI

d=2, 6x5 virtual torus, r=1 Moore neighborhood



d=2, 24x20 virtual mesh, r=3 Moore neighborhood



OpenMPI

Findings:

Preliminary: there are many, many combinations to try out. Automatic benchmark guided by performance guidelines could make more systematic assessment possible

- Basic communication performance between Iso_neighbor_alltoallw() and MPI_Neighbor_alltoallw() comparable. MPI libraries do not seem to have invested in non-trivial optimizations?

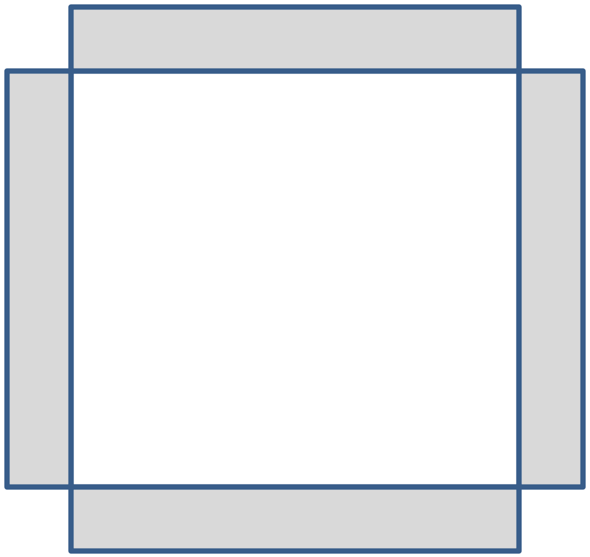
- Neighbor order does not seem to play a large role

- Sometimes notable differences between MPI libraries

Stencil computations

- 5-point (von Neumann) and 9-point (Moore) d=2 stencil computation with halo of depth k, k≥1
- Only communication here, no actual stencil update, 100 iterations of communication loop
- Matrix order n (per process)
- Total time, including time to set up neighborhood
- Iso_neighbor_alltoallw() vs. MPI_Neighbor_alltoallw()

5-point stencil, k=1 halo

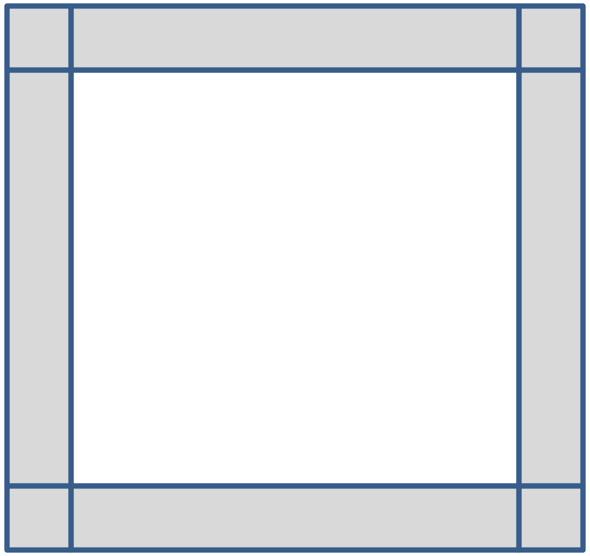


•Halo has same structure as stencil

•Different data layout in the two dimensions

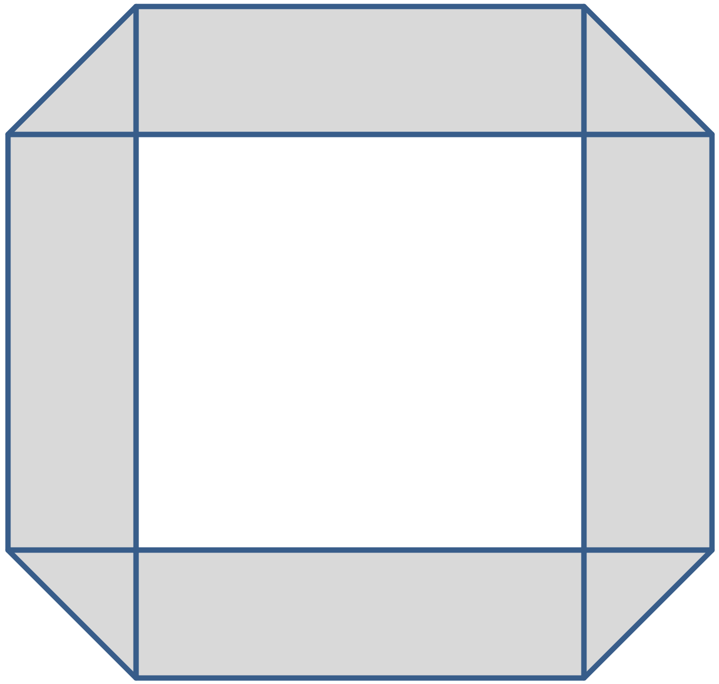
•Need for alltoallw-functionality: different datatypes for different dimensions

9-point stencil, k=1 halo



- Halo has same structure as stencil
- Different data layout in the two dimensions
- Need for alltoallw-functionality: different datatypes for different dimensions

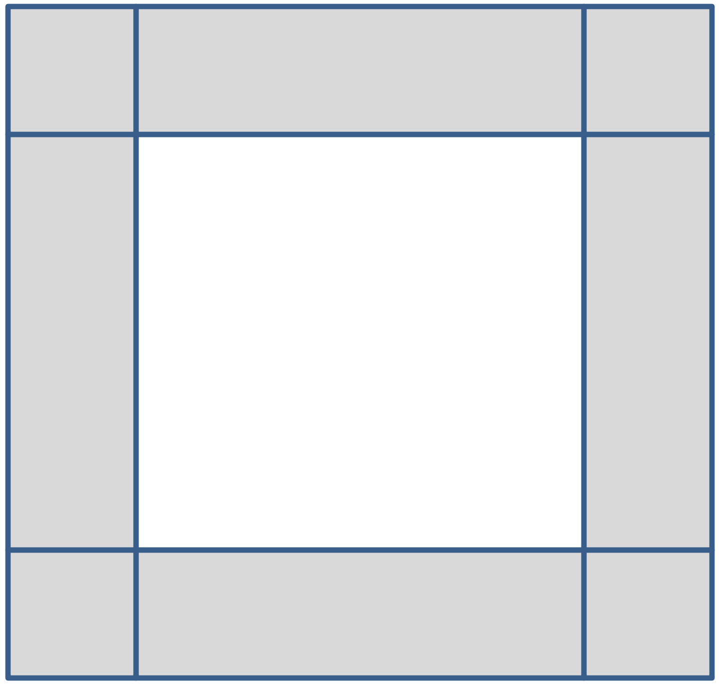
5-point stencil, k>1 halo



- Halo has different structure from stencil: Moore neighborhood needed, all 8 neighbors
- Different data layout in the two dimensions
- Need for alltoallw-functionality: different datatypes for different dimensions

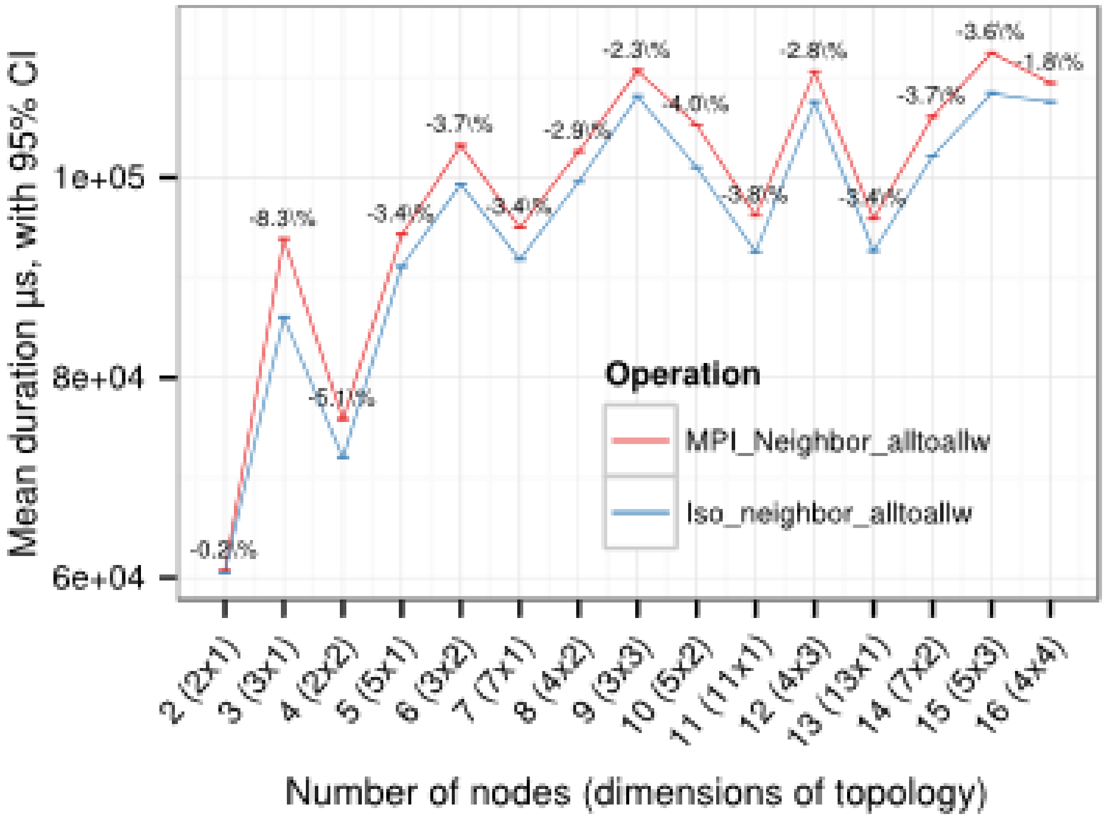
MPI Cartesian neighborhood does not suffice even for simple 5-point stencil with deeper halo

9-point stencil, k>1 halo



- Halo has same structure as stencil
- Different data layout in the two dimensions
- Need for alltoallw-functionality: different datatypes for different dimensions

10.000x10.000 matrix, 5-point stencil, halo depth k=10

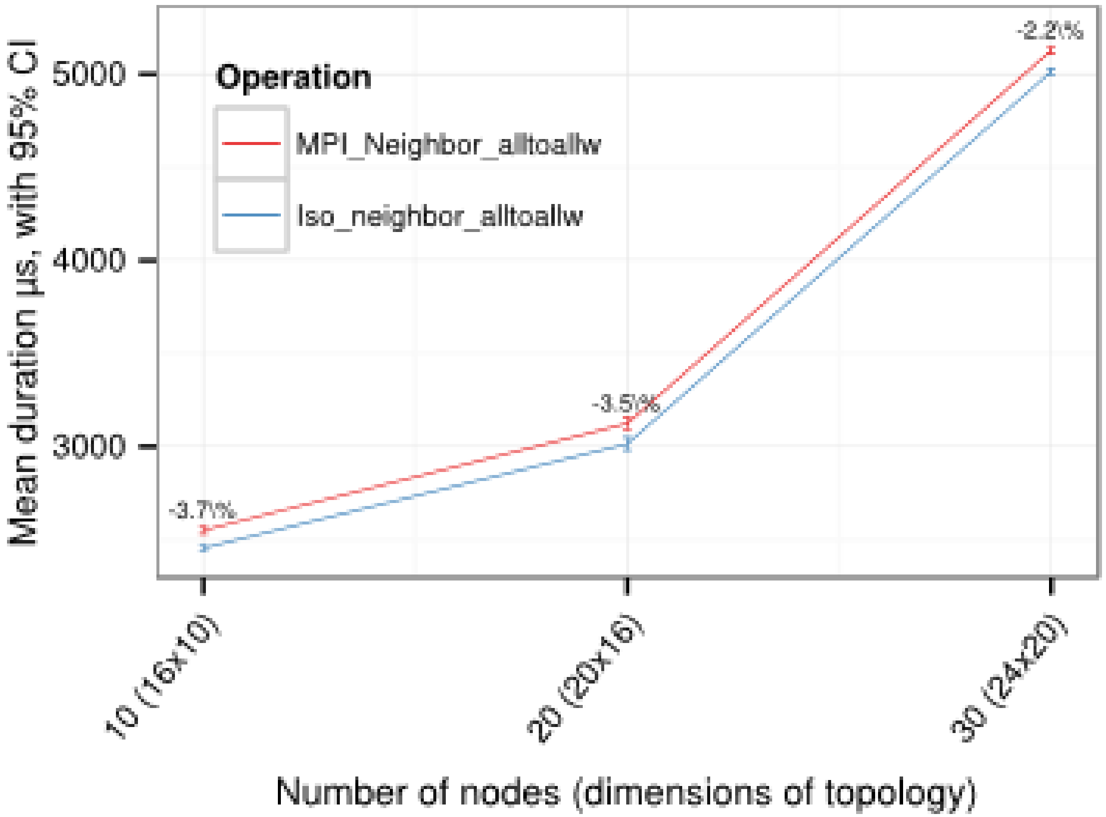


mvapich

First attempt: MPI_Dims_create() to factor p into “best” 2 dimension sizes.

MPI libraries differ badly, and sometimes fail miserably. See POSTER

100x100 matrix, 9-point stencil, halo depth k=2



necMPI

Findings:

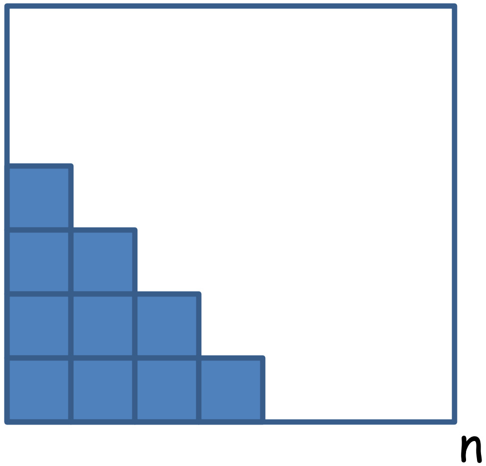
- Due to smaller set up time, Iso_neighbor_alltoallw() can be faster

- Problems with MPI_Dims_create()

Not really MPI function (no communicator): deprecate

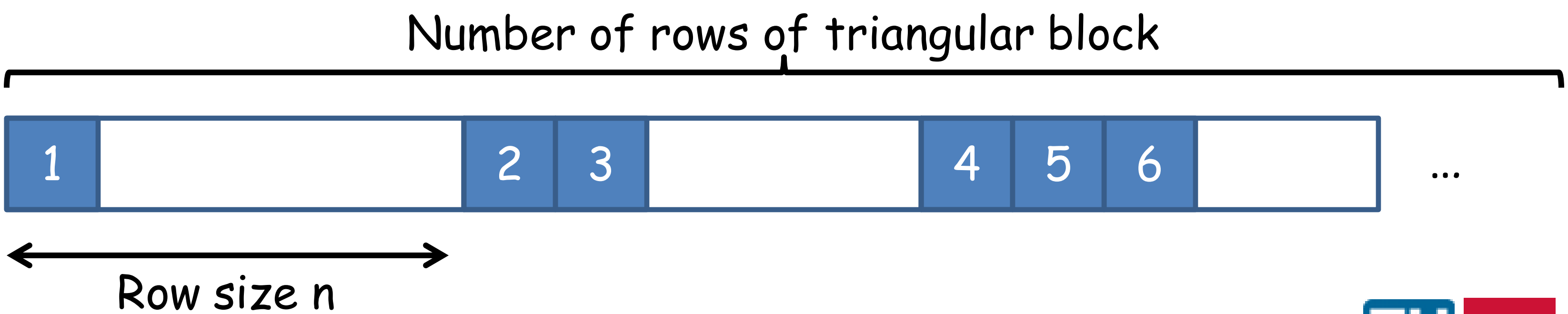
A useful datatype

Here:
Corners for 5-point stencil with halo k>1

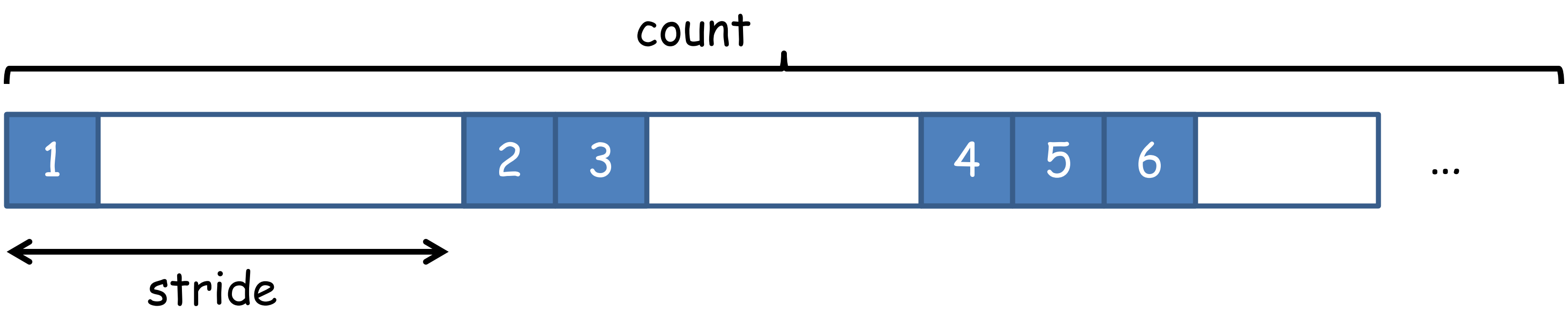


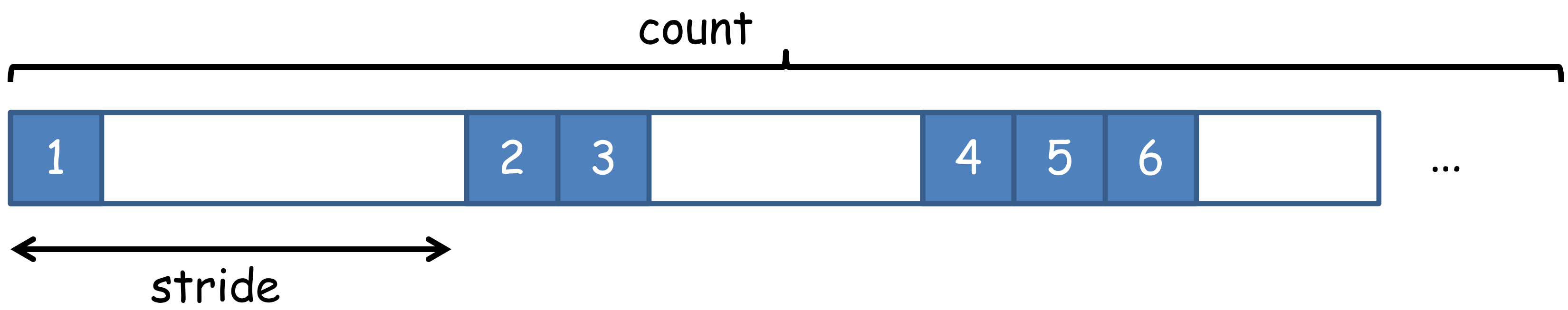
Common structure:

Triangular block of d=2 matrix



```
Create_triangular(count,
                  firstblock,blockincrement,
                  stride,strideincrement,
                  oldtype,*newtype);
```





Can trivially be implemented with MPI_Type_indexed() constructor, but

- Indexed requires storing and processing count, non-O(1) offsets

BUT:

Pattern is regular, can be represented with O(1) information, and presumably processed efficiently

Yesterday's talk

Strong (enough) case for considering additional datatype constructors for MPI?

Summary

- A more structured interface for stencil-like, sparse collective communication, easy to implement on top of MPI

- Isomorphic communication provides many possibilities for local schedule computations for efficient collective communication

Analogy with regular collectives: what can be asserted about global structure that will assist algorithms development?

- Some steps toward systematic benchmarking of neighborhood collectives

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EPiGRAM

FWF

Der Wissenschaftsfonds.