

le Passing Interface benute le Schnittstelle für Mecsage Passing

· Am haufigsten

Kann selve nah aund HW programmiven

Verwendel für:

- Einselanwendungen mit trivièren komm auforderungen für HPC-sys. & cluther mit trivialen Komm. flot

- HPC (fast exclusively)

- Paradig mati'e Realisierung von message model

- Viele su terner fir ander inferfaces

Design Prinzipien, Ziell, etc.

· High-Performance -> wugen HWN she (100 probabl 8/ack overhead)

· Portability + Scalability (gab viell Porkulillab probleme)

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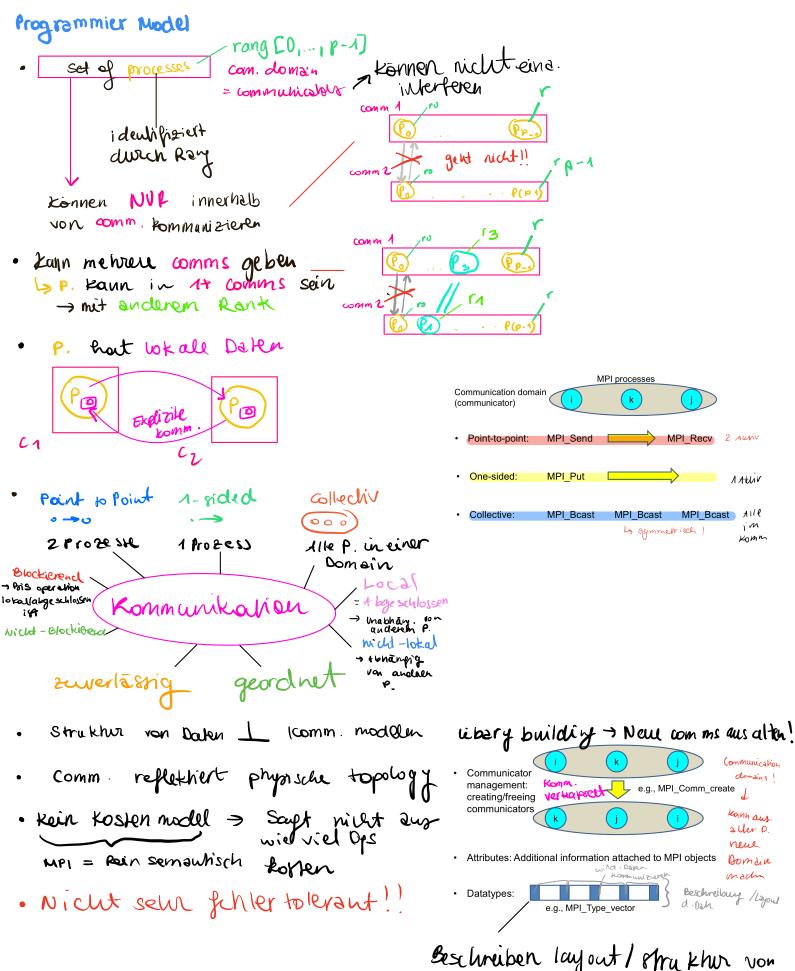
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Beschreiben layout/struktur von Outen, die Kom. werden

# MPI Programm

#### First MPI program

```
#include <mpi.h>
int main(int argc, char *argv[])
{
  int rank, size;

MPI_Init(&argc,&argv); \nd

MPI_Comm_size(MPI_COMM_WORLD,&size);
  MPI_Comm_rank(MPI_COMM_WORLD,&rank);

fprintf(stdout,"Here is %d out of %d\n",rank,size);

MPI_Finalize(); Endl
return 0;
}
```

#### The 6 basic functions (plus two)...

Get time (in micro-seconds with suitably high resolution) since some time in the past:

```
double point_in_time = MPI_Wtime();
```

Synchronize the processes (really: only semantically); often used for benchmarking applications

```
MPI_Barrier(MPI_COMM_WORLD);
```

Good SPMD practice: Write programs to work correctly for any number of processes

```
MPI_Comm_size(MPI_COMM_WORLD,&size);
MPI_Comm_rank(MPI_COMM_WORLD,&rank);
if (size<10||size>1000000) MPI_Abort(comm,errcode);
if (rank==0) {
   // code for rank 0; may be special
} else if (rank*2==0) {
   // remainder even ranks
} else if (rank==7) {
   // another special one
} else {
   // all other (odd) processes...
}

MPI_Comm_size(MPI_COMM_WORLD,&size);

MPI_Abort(comm,errcode);

Explicit assignment of work (code) to each process based on rank
}
```

<u>Dangerous C practice</u> (type error): Don't rely on C convention for Boolean expressions if (rank) {...}

#### The 6 basic functions

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

Who/where am I?" in communication context/set of processes.

Processes numbered (ranked) from 0 to size-1

MPI_Comm_rank(MPI_COMM_WORLD,&rank);
MPI_Comm_size(MPI_COMM_WORLD,&size);
```

### Point - to - Point

#### Process rank i:

```
int a[N];
float area;
MPI_Send(a,N,MPI_INT,j,TAG1,MPI_COMM_WORLD);
MPI_Send(&area,1,MPI_FLOAT,j,TAG2,MPI_COMM_WORLD);

Process rank j:

int b[N];
float area;
MPI_Recv(b,N,MPI_INT,i,TAG1,MPI_COMM_WORLD,&status);
MPI_Recv(&area,1,MPI_FLOAT,i,TAG2,MPI_COMM_WORLD,&status);

MPI_Recv(&area,1,MPI_FLOAT,i,TAG2,MPI_COMM_WORLD,&status);
```

#### Good practice for writing libraries

```
int my_library_init(comm,&libcomm)
{
   MPI_Comm_dup(comm,&libcomm); // store somewhere

   // library communication wrt. libcomm
   // initialize other library data structures
   // could be cached with libcomm (attributes)
}
```

Communication inside library uses libcomm, and will never interfere with communication using other communicators

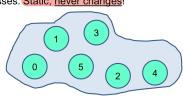
```
MPI Comm dup:
```

Collective operation, MUST be called by all processes in comm

## Communicator

MPI\_Init(&argc,&argv); // sets up internal data structures, incl: MPI Comm size (MPI COMM WORLD, &size);

MPI COMM WORLD: Initial communicator containing all started processes. Static, never changes!

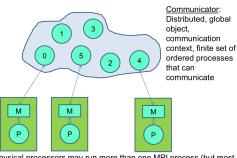


Communicator: distributed, global object with communication context, finite ordered set of processes that can communicate

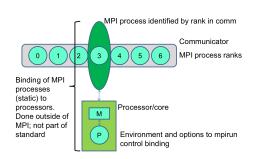
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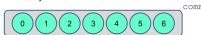
Also aus alter



Physical processors may run more than one MPI process (but most often only one)



Communicator object:



- All processes in a communicator can communicate
- All models (point-to-point, one-sided, collective; all other functionality)
- Has a size: number of processes
- Each process has a rank (0≤rank<size)

MPI\_Comm\_size(comm,&size); MPI\_Comm\_rank(comm,&rank);

MPI process: (normally) statically bound to some processor; can have different ranks in different communicators; canonically identified by rank in MPI COMM WORLD

MPI COMM\_WORLD, comm1, comm2, ...:

An MPI (predefined) handle used to access and perform operations on MPI objects (communicators, windows, datatypes, attributes)

ndurchsi chh

- Handles are (almost always) opaque: Internal MPI data structures cannot be accessed; but only manipulated through the operations defined on them
- MPI does not define how handles are represented (index into table, or pointer, or ...)
- · Handles in C and Fortran may be different

Example: MPI Comm f2c(comm):

Returns C handle of Fortran communicator (no error code here)

P. sind bestimmten Zupewiesen 1 MPI P. MA-1. I Was to Ben ? ausführer 1 MP1 P. Olphynischen Hozestor KI7 Him

### 1. Dublikat machen

Communicator object:

Fir bbs.



- All processes in a commun tor can communicate
- All models (point-to-point, c -sided, collective; all other functionality)
- Has a size: number of proc
- Each process has a rank (0 ank<size)
- es communicators at the same time اجا A process can belong to se

never Coms. MPI\_Comm\_dup(comm, &comm1);

• MPI Comm: Communicators (distributed object)

MPI\_Group: Process groups (local object)

MPI Win: Windows for one-sided communication (distributed)

• MPI Datatype: Description of data layouts (basic/primitive - or user-defined/derived; local)

Binary operators (built-in or user-defined) MPI Op:

MPI Request: Request handle for point-to-point

MPI Status: Communication status

• MPI Errhandler:

## To aus all machineus

#### Splitting communicators

Partition set of MPI processes (communicator) into disjoint sets (communicators) that can communicate independently

gibt rich MPI\_Comm\_split(comm1, color, key, &comm2); MPI\_Comm\_create(comm1,group,&comm2);

Calling MPI process may have different ranks in comm1 and comm2

- color, key: integers determine subsets and relative order, processes in comm2 will be in key order
- group: MPI\_Group of ordered processes

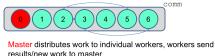


MPI\_Comm\_split (collective operation):

All processes with same color are grouped, order determined by key

- Calling processes are sorted into groups of same color
- In each group, processes are sorted according to key, ties broken by rank in calling communicator

#### Example: Master-worker (non-scalable) pattern



- results/new work to master
- Workers want to synchronize etc. independently of master

For workers: MPI\_Barrier(comm), MPI\_Allgather(comm), ... (collective operations, see later) would deadlock, if master is doing something else Solution: Split communicator, workers only communicator

Communicator (MPI Comm): A distributed, global object that can be manipulated through collective operations (MPI Comm split, MPI\_Comm\_dup, ...)

Process group (MPI Group): A process local object, ordered set of processes that can be manipulated locally by an MPI process

See later, one-sided

communication

- MPI Group\_union,
- MPI\_Group\_intersection
  MPI\_Group\_incl, MPI\_Group\_excl
  MPI\_Group\_translate\_ranks
- MPI\_Group\_compare

Use: Building special communicators, one-sided communication

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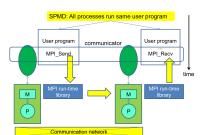
MPI\_Comm\_free(&comm);

frees created communicator comm

MPI COMM WORLD and MPI COMM SELF cannot be freed

#### Good MPI practice

Free any allocated MPI object after use (communicator, window, datatype, ...)



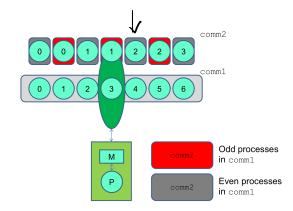
#### Example: Even-odd split

Even-numbered processes (in communicator comm1) shall work together, independently of the odd-numbered processes

General use: Divide-and-conquer type algorithms (Quicksort-like, see later)



Even numbered processes (in comm1) have color==0, odd





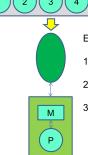
Solution 1: Splitting

Solution 2: Process groups Fiv .-workers

 $MPI\_Comm\_group(comm, \&group);$  // get processes in comm ranklist[0] = 0; // rank 0 to be excluded MPI Group excl(group), ranklist, &workgroup);
MPI Comm create(comm, workgroup, &workers);
// rank 0 (in comm) not in workers
// workers==MPI\_COMM\_NULL for rank 0 in co

→ Gruppen Operationen tokal -> 1 P. zann drauf arbeiten ohne, dass was parient

What is in a communicator (hidden in the implementation)?



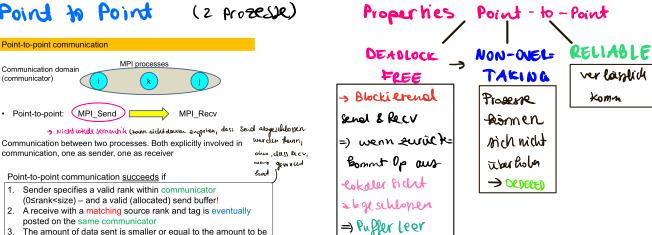
Each process locally maintains:

- List of processes (ordered set): The process group
- Mapping from rank to process to processor (implicit or explicit)
- Communication context: A tag to identify communication on . this communicator

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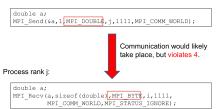
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- posted on the same communicator
- The amount of data sent is smaller or equal to the amount to be received (note: collective operations have different rule)
- The type signature of the data sent matches the type signature of the data to be received

- Mistakes normally caught by MPI\_Send: error (abort)
- If not, deadlock
- Otherwise, MPI\_ERR\_TRUNCATE or memory corruption (big trouble) at receiver!
- 4. MPI INT matches MPI INT, and so forth... rarely checked/enforced, user's responsibility

#### Process rank i:



Very bad practice: Type information (double) lost (process i and j could be on different types of processors, little/big endian)

#### Programmier Jehler

MPI macht KEINE Typkonversion Ipakakon version

Message in transit identified by "envelope" (meta-information):



- Communication context (identifier): Distinguishes communication on different communicators
- Source (implicit) 3. Destination
- Tag
- 5. Message type information (header, data block, error, ...)

Implementation: The "envelope" is not accessible to application programmer (and not specified by MPI standard)

Performance: MPI is designed to allow small message envelope

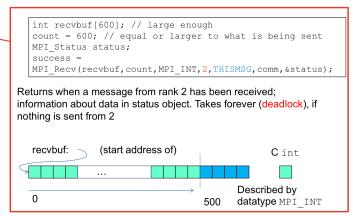
Implementation: The "envelope" is not accessible to application programmer (and not specified by MPI standard)

Performance: MPI is designed to allow small message envelope

#### Not part of envelope: TYP-1 wormanou

Type and structure of message: What is being sent is a sequence of basic datatypes (int, double, char, ...); and it is expected that receiving process has space for exactly the same sequence of basic datatypes

## Kann Deadlocks prog.



#### Point-to-point semantics

(Resourcen frei)

MPI Send(sendbuf, ..., rank, tag, comm):

Initiates and completes send to designated process rank:

- Completion is non-local: Call return may depend on receiving rank having initiated receive operation(\*)
- Operation is blocking: When call returns all of buffer can be
- Sent messages to same rank with same tag are non-overtaking (\*)but may also buffer message

MPI\_Recv(recvbuf,...,rank,tag,comm,&status):

Completes receive operation from specific rank, or ANY

Operation is blocking: Call returns when full message has been received

#### Status object (half opaque): Information on communication

MPI Status status; // status handle MPI Recv (..., &status);

Status contains information on what was received:

Fixed fields in C: status.MPI SOURCE: status.MPI TAG status.MPI ERROR

Why? Don't we know this??

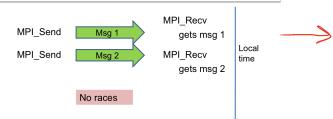
Fixed fields in FORTRAN: status(MPI SOURCE) status(MPI TAG) status(MPI ERROR)

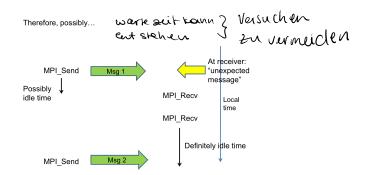
If so: Consider MPI STATUS IGNORE as status argument in MPI Recv

#### Reasoning about point-to-point communication

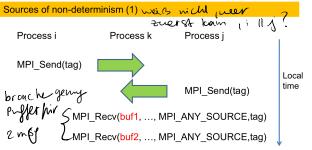
Deterministic messages are non-overtaking:

Messages sent to the same destination (rank) arrive in sent order at destination





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-> warregeit zu minimieren

Either message may be received first. Problems if messages have different count and/or type

#### Example: Synchronization with 0-count message

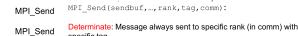


Can be used for process synchronization: Receiving process (with rank dest) cannot proceed before sending process (rank source) has reached send operation. For pairwise synchronization, send 0-message back

Alternative: MPI\_Ssend

Briefly, late

#### But MPI processes are not synchronized





receives from specific rank or some non-determined (ANY) rank, with specific or non-determined (ANY) tag

## um puller riddig suraleg

MPI\_Probe(source, tag, comm, &status);

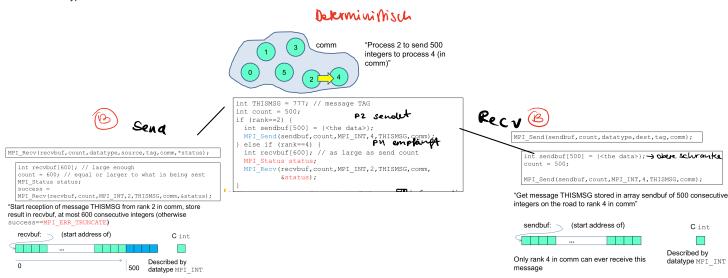
Return when a message with given source (or MPI\_ANY\_SOURCE) and tag (or MPI\_ANY\_TAG) in comm has arrived and is ready for reception; the count for message (and error code etc.) in status

After probe:

Receive message with MPI\_Recv(buffer,count,...,comm);

#### Advanced note:

Can cause problems in multi-threaded MPI applications, not "thread safe" (fix in MPI 3.0)



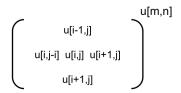
brat abgeschloren ⇒ konnen neuer reinschreiben →! Muss nicht empfage worden kin! Blockierench operation > vicht to tall semantik

## rokar I Abbe achlothen

#### Example: 2d-stencil, 5-point stencil hissen all with

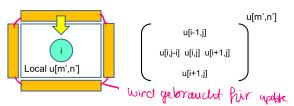
updates when 10p

Given mxn matrix u, for all 0≤i<m, 0≤j<n, update repeatedly  $u[i,j] <- \frac{1}{4}(u[i,j-1] + u[i,j+1] + u[i-1,j] + u[i+1,j] - h^2 f(i,j))$ 



Special conditions on borders, i=0, i=m-1, j=0, j=n-1

Per process (rank i) view of the parallelization



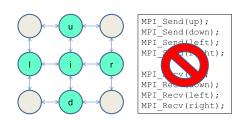
Before iteration, process needs to receive rows and columns of elements from the 4 neighboring processes

Per process (rank i) view of the parallelization



By symmetry, before iteration, process needs to send rows and columns of elements to the 4 neighboring processes

May deadlock: MPI\_Send has non-local completion semantics, each send may block until receive operation starts, and this may never happen



By symmetry, all processes (except processes on the border of the process mesh) need to send/receive rows/columns with all four neighbor processes

Für Jeden Nachbarn / Elem wird a. geniche op verwendet

towendunpfoll: Bildversibility -> g/sten

& Idee:

Teile man matrix in con gluich große n'xn' matrizen über p Prozesse

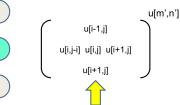
1 Jeder prozes hat eine Submatrix zum updater

G Problem Bei Grenzen nüben 2 P. mikinander kommunizieren

### Rom m

Arrange processes as a 2d mesh (process i needs to calculate ranks of its 4 neighboring processes I,r,u,d) recd

Send Becv 5 Symmetrisch



To update last row, values from first row of process d needed

& Problem: wicht

Konnen NictiTannehmen, dass send stage soldonen sein kann, bevor per generalet worden int

Send eigenerty

=> Non-what completion

### MPI\_Send

a Short mso Buffered at

-> Procested

ldler

MPI - Send

can return IMMEDIATE (Y may be buffered

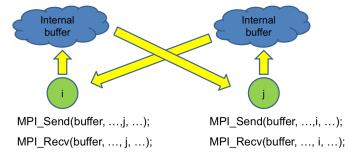
Medium msg

Seuder receiver sent when rec. has been posted

MPI\_send can rehun jest

range ms9 Par h cipation of receiving Process needed MPI \_Send cannot rehurn before Mf1-Recv becomes achine

Datensels giller -> bei großem Problem



Drawback: Extra copy – costly for large buffers

MPI design principle: Library should not allocate unbounded buffers

#### → deadlock

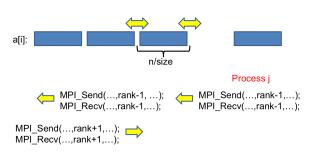
```
float *a = malloc((n/p+2)*sizeof(float));
a += 1; // offset, such that -1 and n/p can b addressed

if (rank>0) {
    MPI_Recv(&a[-1],1,MPI_FLOAT,rank-1,999,comm,&status);
    MPI_Send(&a[0],1,MPI_FLOAT,rank-1,999,comm);
}

if (rank<size-1) {
    MPI_Recv(&a[n/p],1,MPI_FLOAT,rank+1,999,comm,&status);
    MPI_Send(&a[n/p-1],1,MPI_FLOAT,rank+1,999,comm;
}

for (i=0; i<n/p; i++) {
    b[i] = a[i-1]+a[i]+a[i+1];
}</pre>
```

DEADLOCK! All processes attempt to receive, no progress, since receive operations cannot complete



All processes trying to send, looks like deadlock

In MPI: <u>Unsafe programming</u>, if behavior (deadlock) depends on concrete implementation of send in MPI library.

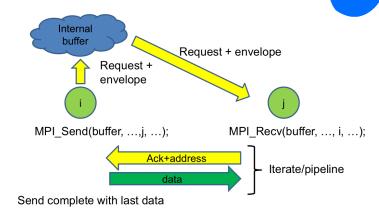
#### Safe(r) programming



Unsafe! Can be made safe by symmetry breaking (scheduling)



#### Template MPI\_Send implementation, long messages



```
float *a = malloc((n/p+2)*sizeof(float));
a += 1; // offset, such that -1 and n/p can b addressed

if (rank>0) {
    MPI_Send(&a[0],1,MPI_FLOAT,rank-1,999,comm);
    MPI_Recv(&a[-1],1,MPI_FLOAT,rank-1,999,comm,&status);
}
if (rank<size-1) {
    MPI_Send(&a[n/p-1],1,MPI_FLOAT,rank+1,999,comm;
    MPI_Recv(&a[n/p],1,MPI_FLOAT,rank+1,999,comm,&status);
}
for (i=0; i<n/p; i++) {
    b[i] = a[i-1]+a[i]+a[i+1];
}</pre>
```

## DEADLOCK? be thingt you serol a 6! Clibrary 0. larged. map)

All processes attempt to send. Can a send complete without a matching receive operation? Depends on semantics and implementation of send operation

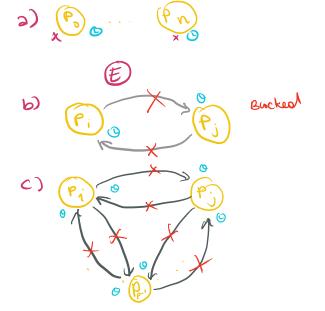
#### DEADLOCK:

- a. All processes waiting for event that cannot happen
- Process i waiting for action by process j, process j waiting for action by process i
- Process i0 waiting for action by process i1, process i1 waiting for action by process i2, ... process i(p-1) waiting for action by process i0

All deadlock forms are possible with MPI programs

Particularly problematic: Some deadlocks are context and MPI library implementation dependent. Such programs are called unsafe

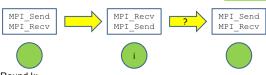
<u>Definition</u>: MPI program is <u>unsafe</u> if termination depends on whether messages are internally buffered by MPI\_Send (or other MPI implementation properties).



Problem: What if the number of processes is odd?

Example: Hillis-Steele prefix-sums algorithm

Recall from algorithms lecture



Round k:

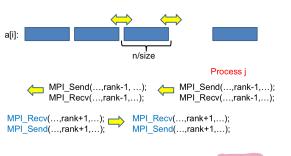
Each process i receives partial sum from process i-2k, and sends partial result to process i+2k

Is process i odd or even in round k?

#### Next attempt to parallelize data parallel loop

```
float *a = malloc((n/p+2)*sizeof(float));
a += 1;
if (rank>0) {
 MPI_Send(&a[0],1,MPI_FLOAT,rank-1,999,comm);
MPI_Recv(&a[-1],1,MPI_FLOAT,rank-1,999,comm,&status);
  MPI_Recv(&a[n/p],1,MPI_FLOAT,rank+1,999,comm);
 MPI_Send(&a[n/p-1],1,MPI_FLOAT,rank+1,999,comm,
            &status);
for (i=0; i<n/p; i++)
   b[i] = a[i-1]+a[i]+a[i+1];
```

Symmetry breaking: Processes 0 and size-1 are special



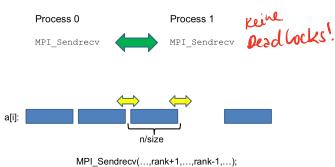
Unfortunate even-odd scheduling leads to serialization. Last process size-1 receives after p=size steps!

# wollken dar nicht!

#### Safe(r) programming

Process 0	Process 1
MPI_Send	MPI_Send
MPI Recv	MPI Recv

Unsafe. Can be made safe safe by combined send-receive



MPI\_Sendrecv(...,rank-1,...,rank+1,...);

```
MPI Sendrecv (void *sendbuf,
             int sendcount, MPI_Datatype sendtype,
             int dest, int sendtag,
             void *recvbuf,
             int recvcount, MPI_Datatype recvtype,
             int source, int recvtag,
              MPI_Comm comm, MPI_Status *status);
```

Combined send-receive operation, in one operation send to some process and receive from some (possibly different) process

Requirement: sendbuf and recybuf must be disjoint

#### Performance advantage:

Can possibly better utilize (fully) bidirectional communication network

Example: Hillis-Steele prefix-sums algorithm (solution)



#### Round k:

Each process i receives partial sum from process i-2k, and sends partial result to process i+2k

#### Safe programming: Non-blocking communication MPI\_Request req[8]; MPI Status stats[8]; MPI\_Isend(up,&req[0]); MPI\_Isend(down,&req[1]); MPI Isend(left, &req[2]); MPI\_Isend(right,&req[3]); MPI Irecv(up, reg[4]); MPI\_Irecv(down,&req[5]); MPI\_Irecv(left, &req[6]);

MPI Irecv(right, &req[7]);

MPI\_Waitall(8, req, stats);

Safe: I(mmediate), non-blocking operations with local completion semantics

#### Point-to-point semantics: Immediate operations

MPI\_lsend(sendbuf,...,rank,tag,comm,request):

Locally initiates send to designated process rank

- Completion is local: Returns immediately, send has been initiated
- Operation is non-blocking: Buffers cannot be reused before completion has been checked/enforced
- Sent messages to same rank with same tag are non-overtaking

MPI\_Irecv(recvbuf,...,rank,tag,comm,request):

Initiates receive operation from specific rank, or ANY

Operation is non-blocking: Call returns immediately, message received after completion



MPI\_Status status;
MPI\_Request request;
MPI\_Isend(sendbuf,...,comm,&request);

starts ("posts") send operation, returns immediately – local completion semantics, independent of receiving side – sendbuf must NOT be modified before operation is complete

"progress" information in request object:

MPI\_Test(&request,flag,&status);

If flag==1 operation has completed, information in status

MPI\_Wait(&request,&status);

Wait: Returns when operation has completed, information in status

#### 

#### is equivalent to

#### Test and completion calls

Completion checked/enforced for all non-blocking operations by

- MPI\_Wait
- MPI Test
- MPI\_Waitall(number,array\_of\_requests,array\_of\_st atuses)
- MPI Testall
- MPI Waitany
- MPI\_Testany
- MPI\_Waitsome

Details, see MPI Standard

MPI Testsome

#### Sources of non-determinism (2)



tag1 message has matched MPI ANY TAG

#### Point-to-point communication performance rules

Send operations: Creating envelope in local buffer, initiating communication (e.g.,  $\alpha$ + $\beta$ m transfer time)



Rule-of-thumb: Avoid many small messages, group into fewer, larger messages ( $\alpha$  may be large)

Performance: MPI\_Send may or may not have to wait for acknowledgement; can sometimes be faster than other send operations

Semantics: MPI\_Send may (for large messages) depend on activity of receiving process

Summary: Send modes, send semantics			
Mode		Remark	Semantics
MPI_Send	Standard Returns when sendbuf can be reused		Non-local (poten- tially)
MPI_Ssend	Synchronous Returns when sendbuf can be reused AND receiver has started reception		Strictly non-local
MPI_Bsend	Buffered, returns immediately, data may be copied into intermediate buffer	Intermediate buffer from user space must have been attached with MPI_Buffer_attach	local
MPI_Rsend	Ready, standard	Precondition: matching receive MUST have been posted	Non-local

Only one receive mode (blocking and nonblocking)

MPI Recv/MPI Irecv

Blocking/non-blocking and modes are orthogonal, and can be arbitrarily combined



MPI\_Iprobe(source, tag, comm, &flag, &status);

Non-blocking probe,  ${\tt flag}{=}{=}1~$  means message with source and tag ready for reception in comm

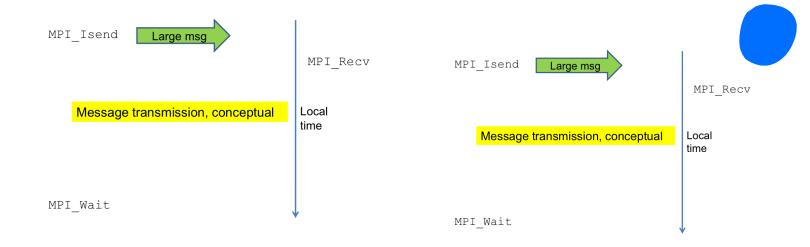
Information in status only when flag==1

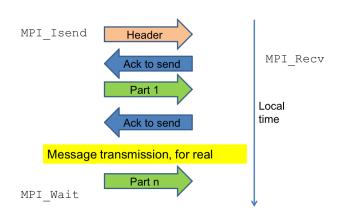
#### Point-to-point communication performance rules

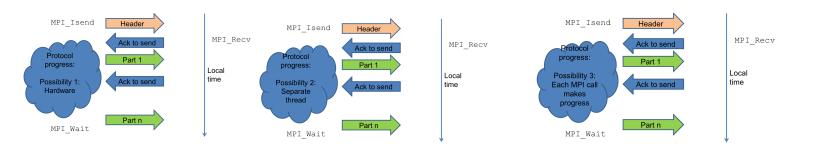
MPI\_Isend: Can return immediately; progress and completion depends on activity of receiver AND often on activity/MPI calls by sender



Again: Completion of MPI\_Send and MPI\_Isend does not imply anything about receiving process

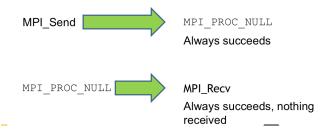






#### Other point-to-point communication features

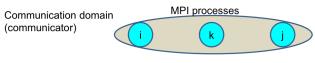
- MPI\_PROC\_NULL "empty" process to send to and receive from
- (MPI\_Ssend, MPI\_Bsend)
- Persistent requests
- MPI\_Cancel dangerous!
- MPI\_Sendrecv\_replace



# 1 sided 1

# (1 Prosess) 1 synchron

### One-sided communication



One-sided:



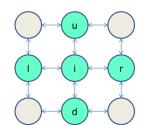
) Blockierence

teil von

Communication between two processes, but only one process is explicitly involved with communication calls

#### One-sided communication by example

Safe neighbor exchange with one-sided (put) communication



MPI_Put(up);	Process i actively puts data to
<pre>MPI_Put(down);</pre>	actively puts
<pre>MPI_Put(left);</pre>	data to
MPI_Put(right);	neighbors

#### Issues:

- Where is the memory put to (and gotten from)?
- When are data ready/operations complete? or au chen synd.

One-sided communication decouples communication and synchronization

#### Communication window:

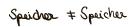
Distributed, global object containing memory for each process that can be accessed in one-sided communication operations

MPI\_Win\_create(base, size, dispunit, info, comm, &win);

Collective operation, all processes in comm provide a base address (size in Bytes may be 0), displacement unit

info (special MPI (key,value) object) can influence window properties (use MPI\_INFO\_NULL)

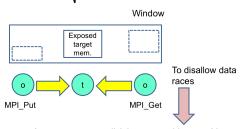
MPI\_Alloc\_mem: Special MPI memory allocator, sometimes
beneficial (performance) for windows \





### Vermeiden von Beadlock

2 x Put -> digunhet adresser



#### <u>Rules</u>:

Concurrent gets/puts must access <u>disjoint target addresses</u>. Very strict rules, violation is undefined (and usually not checked)

MPI\_Accumulate: Atomic (at level of basic datatype) update at target, concurrent accumulates allowed (www wie (cond recv)

#### MPI one-sided communication terminology



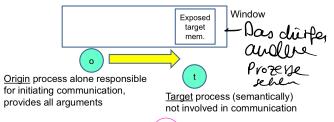
Origin process alone responsible for initiating communication, provides all arguments

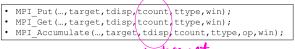
Target process (semantically) not involved in communication

```
    MPI_Put(obuf,ocount,otype,...,win)
    MPI_Get(obuf,ocount,otype,...,win)
    MPI_Accumulate(obuf,ocount,otype,...,op,win);
```

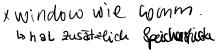
Communication calls are non-blocking, local completion semantics: no guarantee that data have arrived before synchronization operation

Origin puts/get data from standard MPI buffer (buf,count,type)





Data on target exposed in window structure, addressed with relative displacement



MPI\_Put(obuf,...,target,targetdisp,...,win);

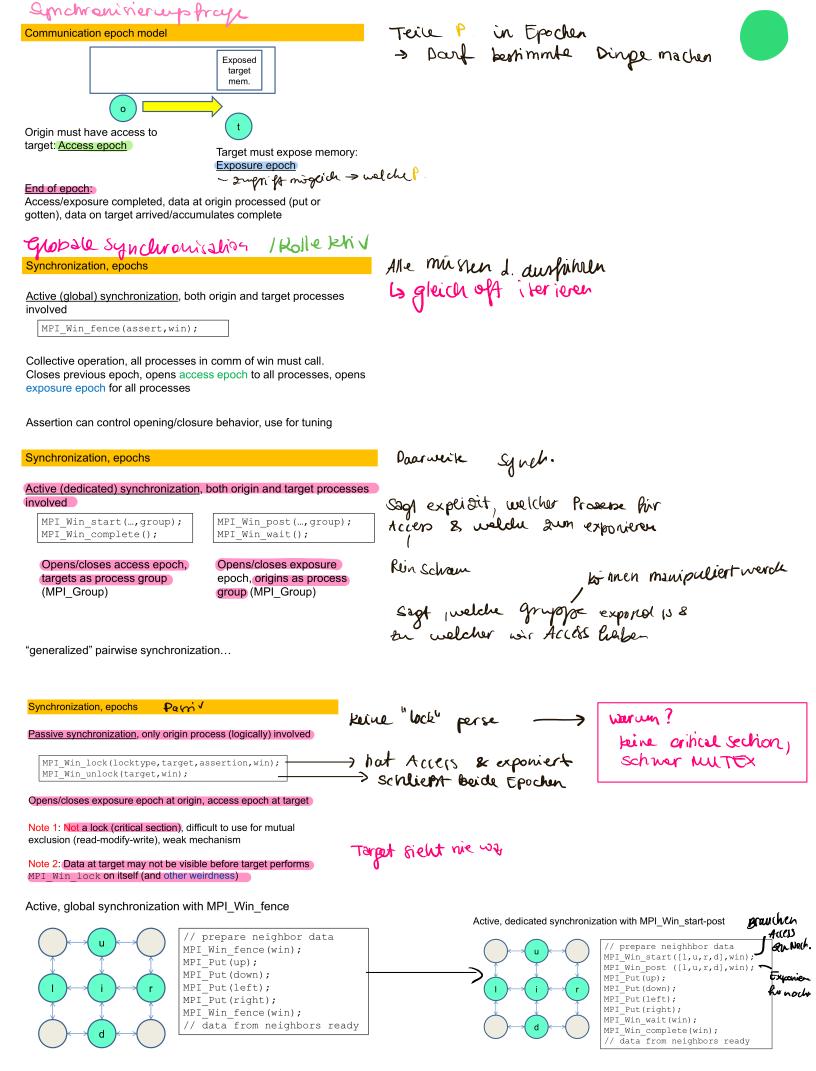
Data from obuf into target base+targetdispunit\*targetdisp



Requirements: Origin data must fit into target buffer, type signatures must match, i.e., length of origin data at most length of target data, same sequence of basic types

#### Note

Same rules as for point-to-point communication,  ${\tt MPI\_PROC\_NULL} \ is a \ valid \ target \ process \ (nothing \ happens)$ 



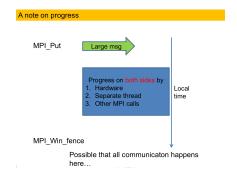
MPI\_Win\_free(win);

Free after use... (like other MPI objects); freeing the memory per process is  ${\hbox{NOT}}$  handled by MPI

```
base = (void*)malloc(size);
// or: MPI_Alloc_mem(size,MPI_INFO_NULL,&base);
MPI_Win_create(base,size,dispunit,info,comm,&win);
... // one sided communication epochs
MPI_Win_free(&win);
free(base);
// or: MPI_free_mem(base);
```

window is ker aber milted.

spulu!



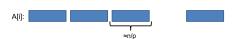
Schouren, dans Epochen nicht zulzug sien

#### Example: Binary search with one-sided communication

```
 \begin{aligned} & \text{A[i]:} \\ & \\ & \text{II} = -1; \ u = n; \\ & \text{do } \{ \\ & \text{m} = (1+u)/2; \\ & \text{if } (x < A[m]) \ u = m; \ \text{else } 1 = m; \\ & \text{j while } (1+1 < u); \\ & \text{i} = 1; \end{aligned} \end{aligned} \end{aligned}  Binary search for key x in array A[0,...,n-1] in at most ceil(log n) steps. Upon termination A[i] \leq x < A[i+1]
```

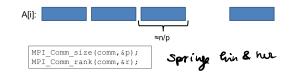
Task: Implement sequential binary search in MPI (distributed memory, message passing), many processes search simultaneously

Side note: Binary search cannot be sped up (much) by parallel processing (Snir lower bound)

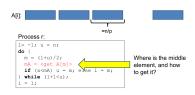


Process r can compute where A[m] is, but this process cannot know that r want to read an element: Fits one-sided model

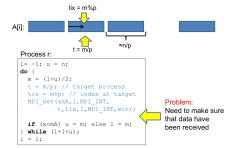
All processes make their block of A accessible to other processes in communication window

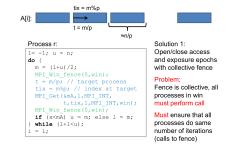


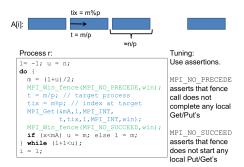
Array A distributed (roughly) evenly over p MPI processes, process r,  $0 \le r < p$ , has block of (roughly) n/p elements

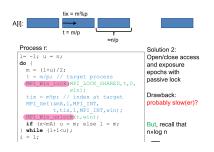


Process r can compute where A[m] is, but this process cannot know that r want to read an element: Fits one-sided model

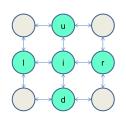








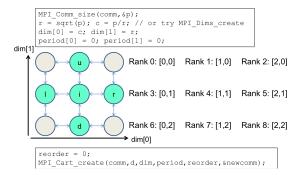
#### Convenience functionality: d-dimensional MPI process naming



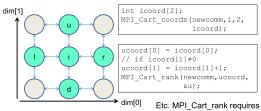
For d-dimensional stencil computation:

MPI processes are organized into a d-dimensional mesh: Each process rank needs to be able to compute efficiently in O(1) operations its 2d neighbor ranks

By-hand solution: Row-order numbering. Assume d=2, let p=rc (row-column), rank i,  $0 \le i < p$ , has coordinate (i/c,i%c), coordinate (a,b),  $0 \le a < r$ ,  $0 \le b < c$ , has rank a\*c+b



Computing coordinates of u, d, I, r (Solution 1)



Etc. MPI\_Cart\_rank requires coordinate in dimension i to be in range, when period[i] ==0

MPI functionality: Cartesian communicators

MPI\_Cart\_create(comm,d,dim,period,reorder,&newcomm);

creates new communicator with helper functionality for ddimensional Cartesian coordinate addressing. Collective operation, all processes in comm must call

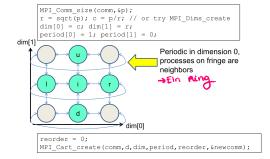
d: number of dimensions (1, 2, 3, ...)

dim : d-element array, dim[i] is size in i'th dimension, must hold that  $\prod \texttt{dim}[\texttt{i}] \leq p$ 

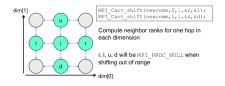
period: d-dimensional flag-array, if period[i] ==1 (true) the Cartesian grid is periodic in the i'th dimension

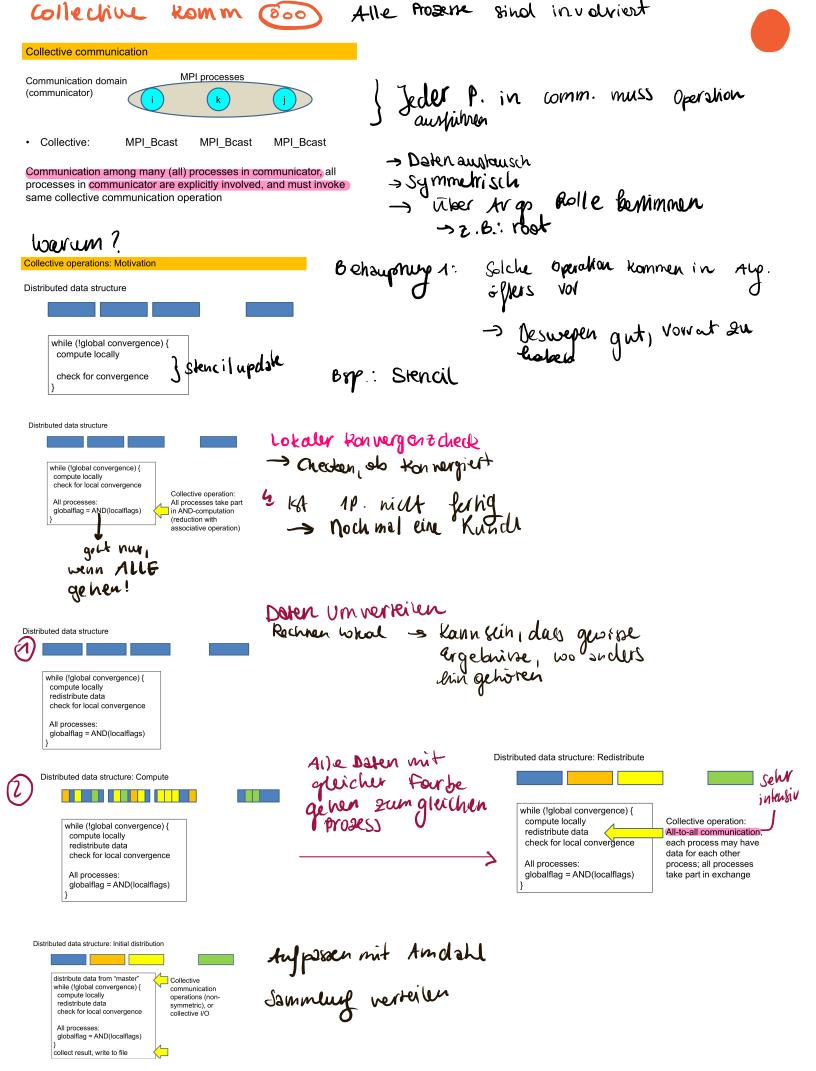
Here: Let reorder=0 (false), otherwise MPI library may attempt to rerank processes to let virtual, Cartesian topology fit better with communication network topology

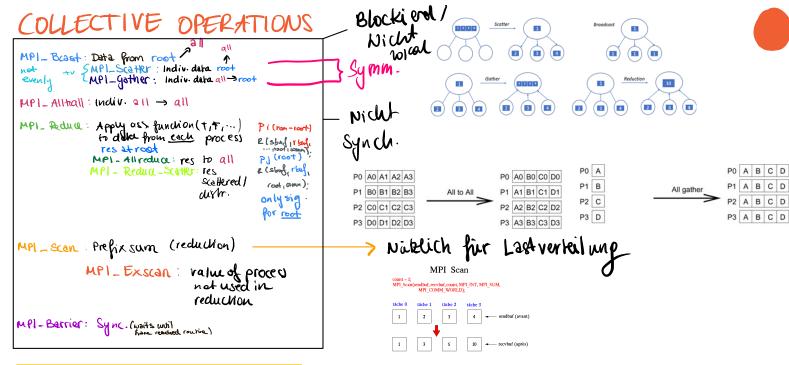
gist # P. in Dimension Periodisth Vinordnen



Computing coordinates of u, d, I, r (Solution 2)





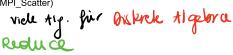


#### Collective operations: Motivation, why these?

Fit many applications (MPI\_Allreduce for convergence tests, MPI\_Scan for load balancing, MPI\_Bcast for initialization, ...)

Parallel, <u>dense linear algebra</u> (matrices, vectors) algorithms can be constructed from exactly these operations

Good symmetry and completeness properties (MPI\_Gather, MPI\_Scatter)



Example: MPI\_Reduce

- MPI\_Op: different operators (+, -, \*, ... even user-defined), must be <u>associative</u> (but not necessarily commutative)
- MPI\_Datatype: Many different basic datatypes (MPI\_INT, MPI\_DOUBLE, ...), even user-defined for user-defined op
- Any process can be root, communicator arbitrary
- count: Input per process is a vector, operation applied elementwise

Better idea: Use properties of "+" to improve performance

Since "+" is associative

$$x_0 + x_1 + x_2 + \dots + x_{p-1} = y$$

can be computed as

$$(x_0+x_1)+(x_2+x_3)+...+x_{p-1}=y$$
  
 $((x_0+x_1)+(x_2+x_3))+...((x_{p-2}+x_{p-1})=y$ 

and etc.

#### Complexity of collective operations (fully connected network)

MPI Collective	Complexity	Important to find	
MPI_Barrier	O(log p)	algorithms with small	
MPI_Bcast	O(n+log p)	constants: See HPC	
MPI_Gather/Scatter	O(n+log p)	lecture	
MPI_Allgather	O(n+log p)		
MPI_Alltoall	O(n+p) (*)	(*) interesting tradeoffs	
MPI_Reduce	O(n+log p)	possible	
MPI_Allreduce	O(n+log p)	MPI_Bcast complexity i NOT O(n log p)	
MPI_Scan/Exscan	O(n+log p)		

- p MPI processes (on p processors), n is total amount of data per process
- Strong (fully connected) network, linear communication cost

#### Collective operations: Motivation

Difficult to implement, need:

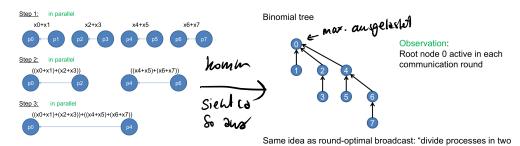
- Good performance on any given network, MPI library must work for any network and system
- Correctness, correct results for all possible (allowed) inputs, (communicators, datatypes, etc.)
- <u>Safety</u>, different collective operations must never interfere with each other and other communication

For many/most of the MPI collective operations, good algorithms exist, at least for fully connected networks

Implementing them well is not trivial



set of numbers worden durch



equal-sized sets, local reduction to local root in each, send result

from one set to the set in which the global root is...

Complexity of collective operations (general)

MPI Collective	Complexity	Important to find
MPI_Barrier	O(d)	algorithms with small constants: See HPC
MPI_Bcast	O(n+d)	
MPI_Gather/Scatter	O(n+d)	lecture
MPI_Allgather	O(n+d)	(*) interesting tradeoff possible
MPI_Alltoall	O(n+p) (*)	
MPI_Reduce	O(n+d)	
MPI_Allreduce	O(n+d)	
MPI_Scan/Exscan	O(n+d)	

- p MPI processes (on p processors), n is total amount of data per process
- d = max(log p, diameter of network), determines latency

#### Collective operation semantics

#### Requirement:

If a process calls collective MPI\_<A> on communicator C, then eventually all other processes in C must call MPI\_<A> and no other collective inbetween (on that communicator)

Collective operations are safe: Collective communication on communicator C will not interfere with other communication on C

#### Requirement:

Collective operations must be called with consistent arguments: same root, same op, exactly matching amounts of data (see individual functions)

#### Collective operation semantics

If a process calls collective MPI <A> on communicator C, then eventually all other processes in C must call MPI\_<A> and no other collective inbetween (on that communicator)

Collective functions are blocking. A process returns when locally complete, buffers etc. can be reused. Completion semantics are non-local (most likely dependent on what other processes do) (\*)

Collective functions are not synchronizing. A process may leave MPI\_<A> as soon as it is locally complete (required local data sent Like and received)

MPI Send

(\*) nonblocking collectives from MPI 3.0

Exception: MPI\_Barrier(comm);

Blockietend

quiche root operation

#### Incorrect:

Process i: MPI\_Bcast(buffer,...,root,comm); MPI\_Reduce(sbuf,rbuf,...,root,comm); Process j:

MPI\_Reduce(sbuf,rbuf,...,root,comm); \$ might underly

#### Process local time

#### Note:

"incorrect" means that MPI may crash, deadlock, give wrong results! Or even work (for small counts): unsafe

Unsafe: comm1: {i,j} comm2: {i,j,k} Process in MPI\_Bcast(buffer,...,root,comm2)
MPI\_Gather(sbuf,...,root,comm1); MPI Bcast(buffer, ..., root, comm2); Process j: Process local time MPI\_Gather(sbuf,...,root,comm1);
MPI\_Bcast(buffer,...,root,comm2); May work for small

komen night richer sein, dan Boat; abopschloren it bevor wir to guttur op kommen lunn Pj

## Kolleluhiv mit Anderen Romm ops Arter

counts, hang for large



### Correct:

```
MPI_Bcast(buffer,...,root,co
                            MPI_Bcast(buffer, ..., root, comm)
                      MPI Boast is blocking:
Process local time
```

#### Correct:

```
Process i:
 MPI_Bcast(buffer,...,root,comm);
                            Process j:
                            MPI_Bcast(buffer,...,root,comm);
                      MPI Bcast is not synchro
                       root: may return as soon as data have left
Process local time
                      buffer (independent of non-roots)
                       Non-root: may return as soon as data from
                      root have been received in buffer
                      (independent of other non-roots)
```

Correct: comm1: {i,j} comm2: {i,k} Process i: MPI\_Bcast (buffer, ..., root, comm2); MPI\_Gather(sendbuf, ..., comm1); MPI\_Bcast(buffer, ..., root, comm2); Process j: Process local time

Process involvement in/blocking behavior of collective call MPI\_<A> is implementation dependent

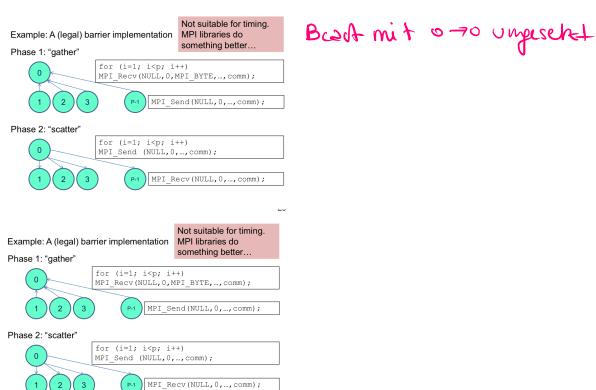
MPI Gather (sendbuf, ..., comm1);

Unsafe collective programming: Relying on synchronization properties

#### Observation:

Explicit MPI\_Barrier calls are never (should never be) needed for correctness of MPI programs

If it seems so, there's probably something wrong



#### MPI "collectives" classification

	Class	regular	Irregular, vector
	Symmetric, no data	MPI_Barrier	
	Rooted	MPI_Bcast	
	Rooted	MPI_Scatter	MPI_Scatterv
	Rooted	MPI_Gather	MPI_Gatherv
	Symmetric, non-rooted	MPI_Allgather	MPI_Allgatherv
	Symmetric, non-rooted	MPI_Alltoall	MPI_Alltoallv, MPI_Alltoallw
	Rooted	MPI_Reduce	
(*)	Non-rooted	MPI_Reduce_scatter_block	MPI_Reduce_scatter
	Symmetric, non-rooted	MPI_Allreduce	
	Non-rooted	MPI_Scan	
	Non-rooted	MPI_Exscan	

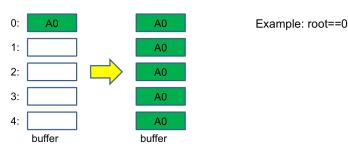
(\*) MPI\_Reduce\_scatter\_block: MPI 2.2 extension

<u>Symmetric</u> vs. <u>non-symmetric</u>: all processes have the same role in collective vs. one/some process (root) is special

Regular vs. irregular: each process contributes or receives the same amount of data from/to each other process vs. different pairs of processes may exchange different amounts of data



MPI Bcast(buffer,count,datatype,root,comm);



<u>Semantics</u>: Data from root buffer is transferred to buffer of all non-root processes

<u>Use</u>: All processes broadcast with same root, buffer with same type signature (e.g., same count for basic datatypes like MPI FLOAT)

#### MPI requirement

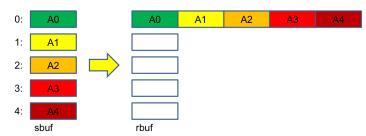
Collective functions MUST be called with consistent arguments:

- Same root
- Matching type signatures (in particular: pairwise same size)
- Note: Number of elements sent and received must match exactly (unlike Send-Recv: sent≤recv and Get/Put)
- Same op (MPI\_Reduce etc.)

```
int matrixdims[3]; // 3 dimensional matrix
if (rank==0) {
  MPI_Bcast(matrixdims,3,MPI_INT,0,comm);
} else {
  // do something on non-root first
  MPI_Bcast(matrixdims,2,MPI_INT,0,comm);
  // uhuh, Bcast probably works, but later...
}
```



MPI Gather(sbuf, scount, stype, rbuf, rcount, rtype, root, comm);

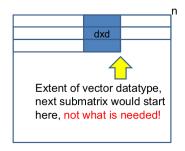


<u>Semantics</u>: Each process contributes a block of data to rbuf at root, blocks end up stored consecutively in rank order at root

Block from process i is stored at rbuf+i\*rcount\*extent(rtype)

Note: rcount is count of one block, not of whole rbuf

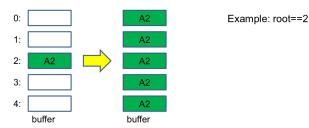
Challenge: Scattering submatrices of large input matrix



- Describe submatrix as vector, block of d elements, stride n
- 2. MPI\_Scatter will not
   work... (why?)
- 3. MPI\_Type\_create\_res ize with MPI\_Scatterv can solve this problem

Advanced datatype use in HPC lecture

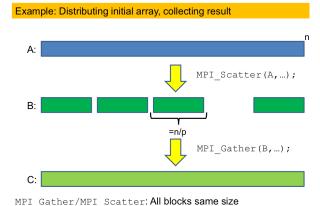
MPI\_Bcast(buffer,count,datatype,root,comm);



 $\underline{\textbf{Semantics}}.$  Data from root buffer is transferred to buffer of all non-root processes

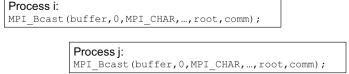
 $\underline{\text{Use}}$ : All processes broadcast with same root, buffer with same type signature (e.g., same count for basic datatypes like MPI FLOAT)



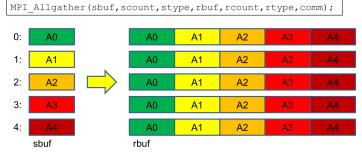


Further differences to point-to-point communication:

- Collective communication functions do not have tag argument
- Amount of data from process i to process j must equal amount of data expected by process j from process i
- Buffers of size 0 do not have to be sent



Correct! May be implemented as no-op, nothing broadcast



<u>Semantics</u>: Each process contributes a block of data to rbuf at all processes, blocks end up stored consecutively in rank order

Block from process i is stored at rbuf+i\*rcount\*extent(rtype)

#### Fact:

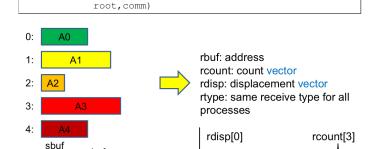
Much better algorithms for MPI\_Allgather than MPI\_Gather+MPI\_Bcast exist

A good MPI implementation will ensure that "best possible" algorithm is implemented, and that indeed MPI\_Allgather always (all other things being equal) performs better than MPI\_Gather+MPI\_Bcast

#### Golden MPI rule

- Use collectives for conciseness and performance whereever possible
- Complain to MPI library implementer if performance anomalies are discovered

MPI\_Gatherv(sbuf, scount, stype, rbuf, rcount, rdisp, rtype,



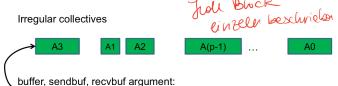
Block from process i stored at rbuf+disp[i]\*extent(rtype)

A2

rbuf

Α1

Displacement in extent(rtype) units; same for all processes (one rtype only)



buffer, sendbuf, recybuf argument:
Start address of buffer for all data to be transferred (sent or received)

Segments to be transferred to/from different ranks may have different size (count[i]), and different displacement (displ[i]) relative to start address. Displacement is in datatype units

MPI Allgather (sbuf, ... rbuf, rcount, rtype, ... comm);

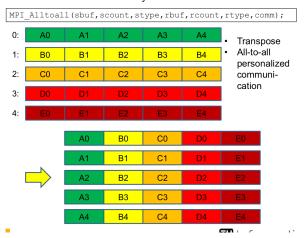
#### is equivalent to

```
MPI_Gather(sbuf,...,rbuf,...,0,comm);
MPI_Bcast(rbuf,size*rcount,rtype,...,0,comm);
```

#### and

```
for (i) { // all-to-all broadcast
  if (i==rank) MPI_Bcast(sbuf,...,i,comm); else
  MPI_Bcast(rbuf+i*rcount*extent(rtype),...,i,comm);
}
memcpy(rbuf+rank*rcount*extent(rtype),sbuf,...);
```

#### But: Performance of library function should be better!



Irregular (vector, v-) collectives:

Possibly different amounts of data destined to different processes

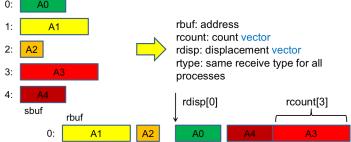
## untersch. große Block

- MPI Gatherv, MPI Scatterv
- MPI Allgatherv
- MPI Alltoallv, MPI Alltoallw

Data sizes and signatures must match pairwise, amount destined to a process must match what is required by that process

Processes can use different datatypes (data need not have the same structure, but signature must match)

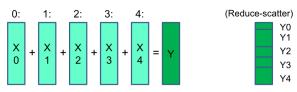




Received data must not overlap. Displacement and count vectors significant only at root. Size/signature match pairwise

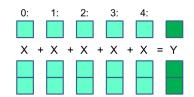
# Zusammen gpiel

#### Reduction collectives

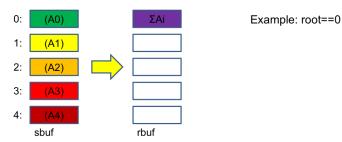


- Each process has vector of data X (same size, same type)
- · Associative operation + (MPI builtin, MPI\_SUM,..., user def)
- Element-wise reduction result Y=X0+X1+X2+ ... + X(p-1) is stored at
- 1. Root: MPI Reduce
- 2. All processes: MPI Allreduce
- Scattered in blocks (Y0 to 0, Y1 to 1, ...): MPI Reduce Scatter

Reductions are performed elementwise on the input vectors



MPI\_Reduce(sbuf,rbuf,count,type,op,root,comm);



<u>Semantics</u>: All processes contribute sbuf (vector) of same size, elementwise result stored in rbuf at root. With  $\texttt{MPI\_IN\_PLACE}$  as sbuf, input is taken from rbuf

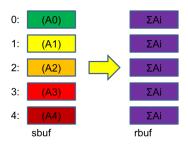
MPI Reduce\_scatter\_block(sbuf,rbuf,count,type,op,comm);



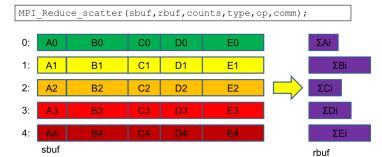
 $\underline{Semantics} : All \ processes \ contribute \ sbuf \ (vector) \ of \ same \ size, \\ elementwise \ result \ is \ scattered \ in \ same \ sized \ blocks \ and \ stored \ in \\ rbuf \ at \ each \ process. \ With \ \texttt{MPI_IN_PLACE} \ as \ sbuf, \ input \ is \ taken \\ from \ rbuf$ 

MPI_Op	function	Operand type
MPI_MAX	max	Integer, Floating
MPI_MIN	min	Integer, Floating
MPI_SUM	sum	Integer, Floating
MPI_PROD	product	Integer, Floating
MPI_LAND	logical and	Integer, Logical
MPI_BAND	bitwise and	Integer, Byte
MPI_LOR	logical or	Integer, Logical
MPI_BOR	bitwise or	Integer, Byte
MPI_LXOR	logical exclusive or	Integer, Logical
MPI_BXOR	bitwise exclusive or	Integer, Byte
MPI_MAXLOC	max value and location of max	Special pair type
MPI_MINLOC	min value and location of min	Special pair type

MPI\_Allreduce(sbuf,rbuf,count,type,op,comm);



<u>Semantics</u>: All processes contribute sbuf (vector) of same size, elementwise result stored in rbuf at all processes. With MPI IN PLACE as sbuf, input is taken from rbuf



<u>Semantics</u>: All processes contribute sbuf (vector) of same size, elementwise result is scattered in blocks and stored in rbuf at each process. With MPI\_IN\_PLACE as sbuf, input is taken from rbuf. Since rbuf may have different size at different processes, counts[] is a vector. All processes provide <u>same</u> counts[] vector

makes it possible to define/register own, "user-defined", binary, associative operators that can even work on derived datatypes

Free it again after use...

## mussen sapen wie verteilt

#### Solution 2: Matrix-vector multiplication

Assume p divides n, distribute M column-wise, each process has n/p columns of M, n/p elements of V

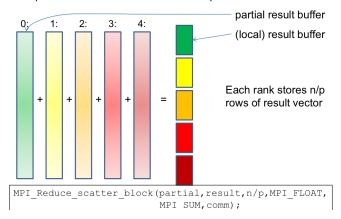
For process k,  $0 \le k < p$ , columns  $c_i \le j < c_{i+1}$ , where  $c_i = k(n/p)$ 

$$\begin{split} W[j] &= \sum_{c0 \leq i < c1} M'[j][i]^* V'[i] + \sum_{c1 \leq i < c2} M'[j][i]^* V'[i] + \ldots + \\ &\sum_{c(p-1)0 \leq i < cp} M'[j][i]^* V'[i] \end{split}$$

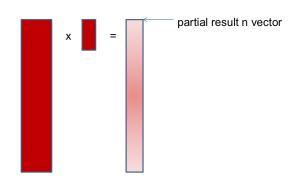
Correct since "+" is associative. Here i is index in global matrix, i-ck index in local column-matrix M' and local vector V'

Solution: distribute M column-wise, perform local M'V, sum partial results

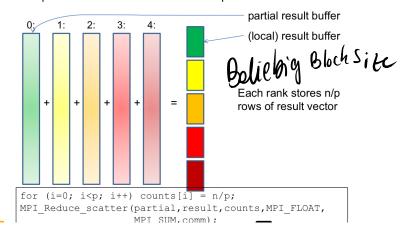
#### 2. Sum partial result n vectors and scatter n/p blocks



#### 1. Locally compute (nxn/p) matrix n/p vector product, M'V'

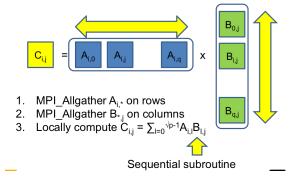


#### 2. Sum partial result n vectors and scatter n/p blocks



#### Folklore: Blockwise algorithm

Process (i,j) computes  $C_{i,j}$  as  $(A_{i,0},A_{i,1},\ldots A_{i,q})x(B_{0,j},B_{1,j},\ldots ,B_{q,j})$ , notation  $q=\sqrt{p-1}$ 



#### SUMMA: Scalable Universal Matrix-Multiplication Algorithm

Idea: Pipeline allgather (Recall: allgather = "p times bcast")

To compute  $C_{i,j} = \sum_{l=0}^{\sqrt{p-1}} A_{i,l} B_{l,j}$ ,  $\sqrt{p}$  communication rounds, in round I,  $0 \le l < \sqrt{p}$ , broadcast of  $A_{i,l}$  on row communicator, broadcast of  $B_{l,j}$  on column communicator

Note: This algorithm performs all sums in order, does not exploit commutativity of matrix addition

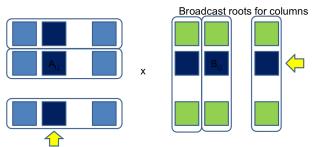
#### Main algorithm

C = 0

for  $\sqrt{p}$  rounds, I=0,..., $\sqrt{p}$ -1

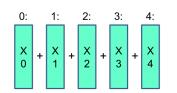
- 1. Broadcast A<sub>i,l</sub> to all processes on row i from process (i,l)
- 2. Broadcast B<sub>I,j</sub> to all processes on column j from process (I,j)
- 3. Update C = C+AB

#### Main algorithm, round 1



Broadcast roots for rows

#### Scan collectives



wie ville Mind vormit?

- Each process has vector of data X (same size, same type)
- Associative operation + (MPI builtin, MPI SUM,..., user def)
- All prefix sums Yi=X0+...+Xi are computed and stored
- Yi at rank i: MPI Scan
- Yi at rank i+1: MPI Exscan (rank 0 undefined)

### Quicksort

Step 1: Choose pivot, distribute to all processes

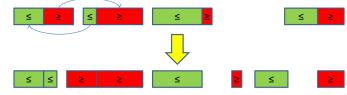


- 1. Process 0 chooses pivot, MPI Bcast
- Better, perhaps: Each process chooses pivot, MPI\_Allgather, median of p as pivot

Step 2: Local partition



Step 3: Global partition, pairwise (hypercube) exchange



Even numbered process i sends larger than pivot elements to process i+1, and receives smaller than pivot elements from process i+1. Odd numbered process i receives larger than pivot elements from process i-1 and sends smaller than pivot elements to process i: MPI\_Sendrecv

Implementation: May need to exchange number of elements first

#### Drawbacks:

- Only for powers-of-two numbers of processors (hypercube algorithm)
- Load balance might be arbitrarily bad, one process could do all the work if pivot is bad

Analysis, assuming exact median pivot and Bcast:

 $T(n,p) = O(\log p)+O(n/p)+T(n/2,p/2)$  $T(n,1) = O(n \log n)$ 

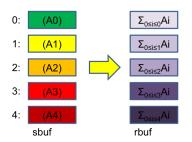
But what does
MPI\_Comm\_split
cost?

Since (n/2)/(p/2) = n/p, and  $2^{\log p} = p$ , we get  $T(n,p) = O(\log^2 p + (\log p)(n/p)) + O(n/p \log(n/p)) =$ 

 $O(\log^2 p) + O((\log p)(n/p) + (n/p)(\log n) - (n/p)(\log p)) = O(\log^2 p) + O(n/p \log n)$ 

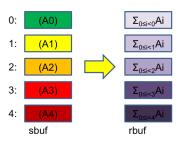
Speedup:  $O((n \log n)/(n/p \log n)) = O(p)$  for n»p

MPI Scan(sbuf, rbuf, count, type, op, comm);



<u>Semantics</u>: Elementwise, inclusive prefix sums over sbuf vectors. Rank i stores sum from rank 0 to rank i (included)

MPI Exscan(sbuf,rbuf,count,type,op,comm);



<u>Semantics</u>: Elementwise, exclusive prefix sums over sbuf vectors. Rank i stores sum from rank 0 to rank i (excluded)

Step 4: Split communicator and recurse



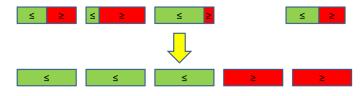
Use MPI\_Comm\_split with color rank%2: Even numbered processes will work on smaller than pivot elements, odd numbered processes on larger than pivot elements



After  $\log_2 p$  steps, each process is in communicator by itself: Sort locally

Youran Lan, Magdi A. Mohamed: Parallel Quicksort in hypercubes. SAC 1992: 740-746

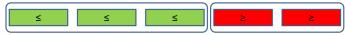
Improved step 3: Global partition by compaction



Smaller than pivot elements:

- For process i, compute how many smaller than pivot elements there are at process 0, 1, ..., i-1: MPI\_Exscan with result m<sub>i</sub>
- Elements have to be sent to process m<sub>i</sub>/(n/p) and (possibly) process m<sub>i</sub>/(n/p)+1
- All processes need to inform their receiving processes (at most two) how many elements to receive: MPI Alltoall
- Redistribution by MPT\_Alltoally or send and receive

#### Step 4: Split communicator and recurse



Use MPI\_Comm\_split with color=(rank<middle ? 0 : 1) to divide the processes into those with smaller than and those with larger than pivot elements

After log₂p steps, each process is in communicator by itself: Sort locally

Same analysis applies, but good better balance irrespective of pivot choice

Given n integers in range [0,R[ (=[0,1,2,...,R-1]) stored in array A

3. Distribute elements of A into buckets (in new array B)

4. Copy B back to A, if needed

#### Note:

As implemented, this bucket-sort is stable: Relative order or elements in A with same key is preserved

n integers in a given range [0,R[, distributed evenly across p MPI processes: m= n/p integers per process

$$A = \begin{bmatrix} 0 & 1 & 3 & 0 & 0 & 2 & 0 & 1 & \dots \\ 0 & 1 & 3 & 0 & 0 & 2 & 0 & 1 & \dots \end{bmatrix} \qquad B = \begin{bmatrix} 4 & 2 & 1 & 1 \\ 1 & 3 & 1 & 1 \\ 3 & 1$$

Step 1: Bucket sort locally, B[i] number of elements with key i

#### Now:

Vector AllB contains the sizes of all buckets over all processes; RelB is for process rank the relative position of rank's elements in the buckets

n integers in a given range [0,R[, distributed evenly across p MPI processes: m= n/p integers per process

Step 5: compute number of elements to be sent to each other process, sendelts[i], i=0,...,p-1

#### Step 6:

#### Step 7: redistribute elements

#### Example: Integer (bucket, counting) sorting

Given n integers in range [0,R[ (=[0,1,2,...,R-1]) stored in array A

#### Bucket sort:

1. Count number of elements of each magnitude ("key")

2. Compute start index of each bucket: exclusive prefix-sums operation

#### Example: Integer (bucket, counting) sorting in parallel

n integers in a given range [0,R[, distributed evenly across p MPI processes: m= n/p integers per process

$$B = \begin{bmatrix} 4 \\ 2 \\ 1 \\ 3 \end{bmatrix}$$

Input array distributed over p processes, A and B process local arrays of input elements and bucket sizes

n integers in a given range [0,R[, distributed evenly across p MPI processes: m= n/p integers per process

$$B = \begin{bmatrix} 4 \\ 2 \\ 1 \\ 3 \end{bmatrix}$$

Step 1: Bucket sort locally, B[i] number of elements with key i

Step 2: MPI\_Allreduce(B, AllB, R, MPI\_INT, MPI\_SUM, comm);

Step 3: MPI\_Exscan(B, RelB, R, MPI\_INT, MPI\_SUM, comm);

#### Now

Vector AllB contains the sizes of all buckets over all processes; RelB is for process rank the relative position of rank's elements in the buckets

n integers in a given range [0,R[, distributed evenly across p MPI processes: m= n/p integers per process

$$A = \begin{bmatrix} 0 & 1 & 3 & 0 & 0 & 2 & 0 & 1 & \dots \\ 0 & 1 & 3 & 0 & 0 & 2 & 0 & 1 & \dots \end{bmatrix} \qquad B = \begin{bmatrix} 4 & 2 & 1 & 1 \\ 1 & 3 & 1 & 1 \\ 3 & 1$$

#### Step 7: Redistribute elements

Step 8: Reorder elements from C back to A

Possible optimization: Replace MPI\_Allreduce by MPI\_Bcast

#### Example: Integer (bucket, counting) sorting in parallel

The algorithm is stable



Choice of radix R depends on properties of network (fully connected, fat tree, mesh/torus, ...) and quality of reduction/scan-algorithms

The algorithm is portable (by virtue of the MPI collectives), but tuning depends on systems: Concrete performance model needed, but analysis outside scope of MPI

Note: On strong network T(MPI\_Allreduce(m)) = O(m+log p)

NOT: O(mlog p)

#### Quicksort and bucketsort data redistribution

In both cases, the redistribution has special structure, and it may be possible to do better with special algorithm than with MPI\_Alltoallv

#### Worth trying:

- MPI\_Exscan over block sizes; compute where data goes
- MPI\_Win\_lock(MPI\_LOCK\_SHARED); MPI\_Put; MPI\_Win\_unlock to deliver data