High Performance Computing – Programming Paradigms and Scalability Part 5: Distributed-Memory Programming

PD Dr. rer. nat. habil. Ralf-Peter Mundani
Computation in Engineering (CiE)
Scientific Computing (SCCS)

Summer Term 2015

Overview

- message passing paradigm
- collective communication
- programming with MPI
- MPI advanced

At some point…
we must have faith in the intelligence of the end user.
—Anonymous

Message Passing Paradigm

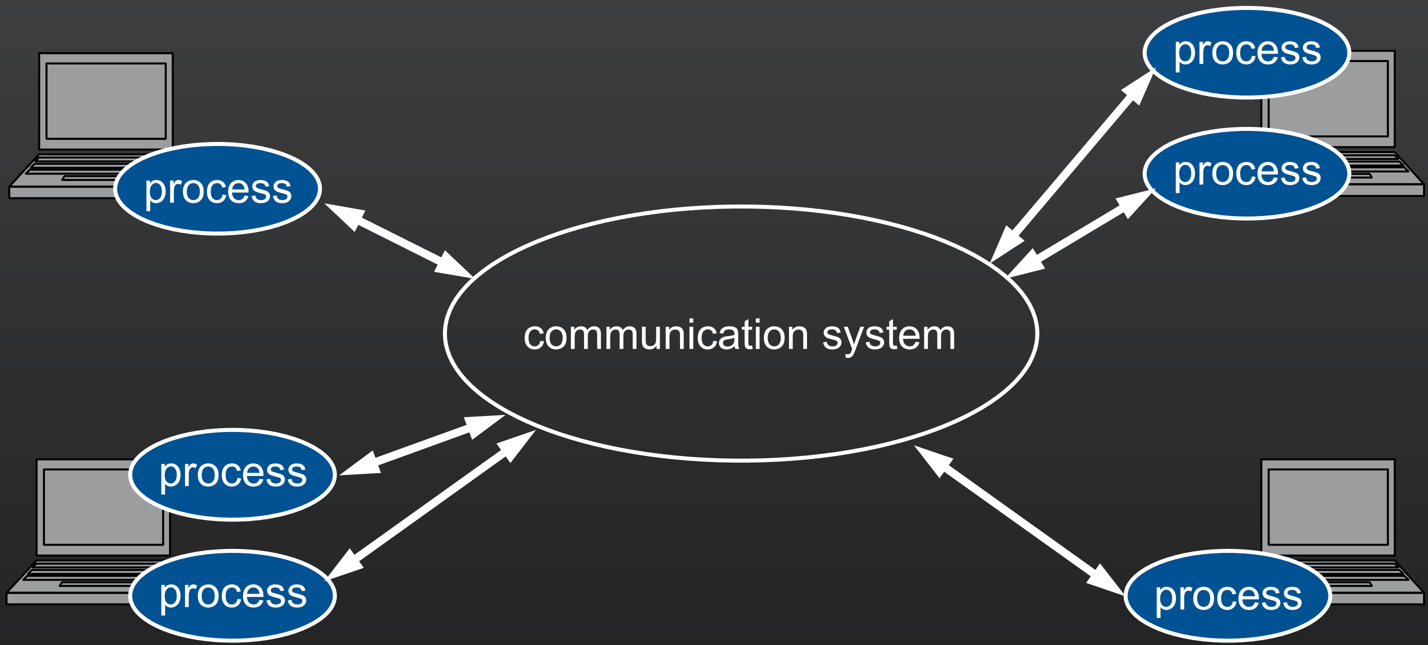
- message passing
  - very general principle, applicable to nearly all types of parallel architectures (message-coupled and memory-coupled)
  - standard programming paradigm for MesMS, i.e.
    - message-coupled multiprocessors
    - clusters of workstations (homogeneous architecture, dedicated use, high-speed network (InfiniBand, e.g.))
    - networks of workstations (heterogeneous architecture, non-dedicated use, standard network (Ethernet, e.g.))
  - several concrete programming environments
    - machine-dependent: MPL (IBM), PSE (nCUBE), …
    - machine-independent: EXPRESS, P4, PARMACS, PVM, …
  - machine-independent standards: PVM, MPI

Message Passing Paradigm

- underlying principle
  - parallel program with *P* processes with different address space
  - communication takes place via exchanging messages
    - header: target ID, message information (type of data, …)
    - body: data to be provided
  - exchanging messages via library functions that should be
    - designed without dependencies of
      - hardware
      - programming language
    - available for multiprocessors and standard monoprocessors
    - available for standard languages such as C/C++ or Fortran
    - linked to source code during compilation

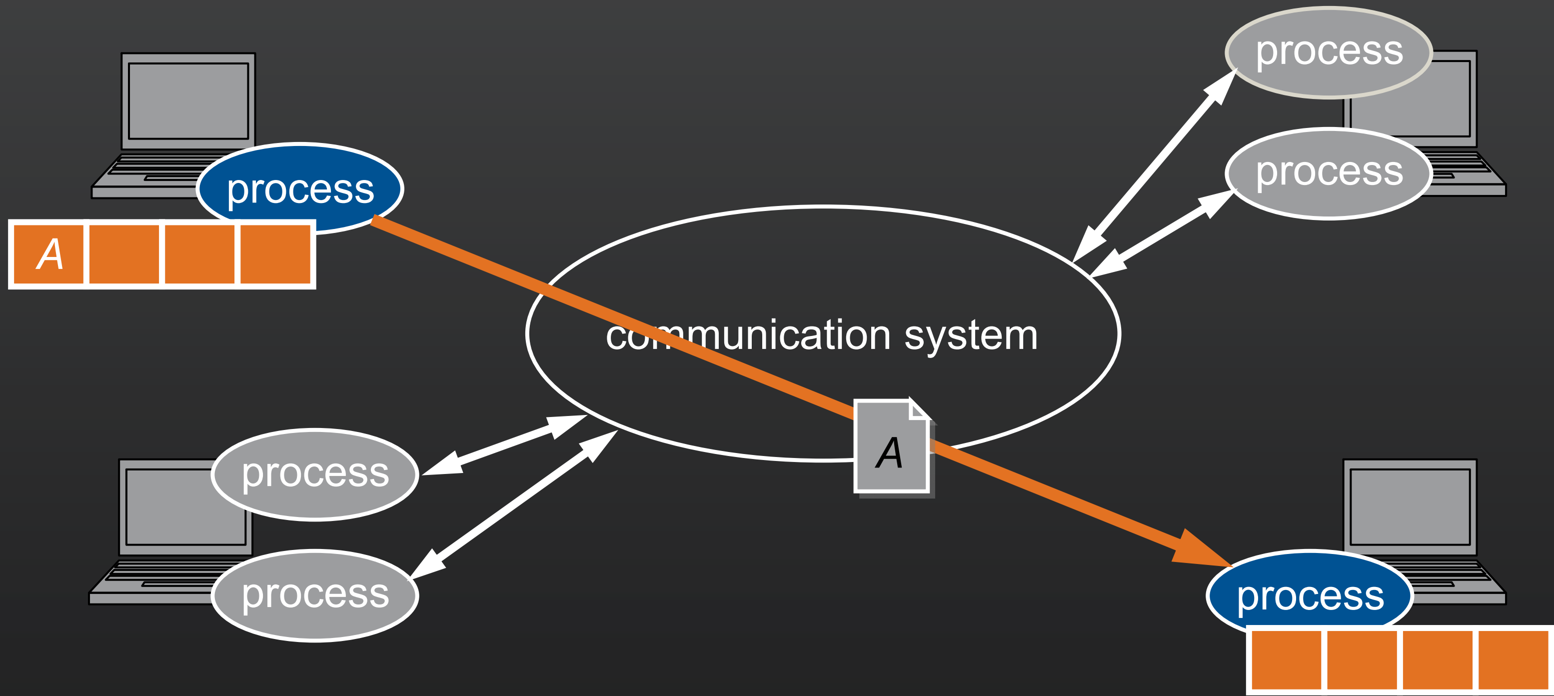
Message Passing Paradigm

- user's view
  - library functions are the only interface to communication system



Message Passing Paradigm

- user's view (cont'd)
  - library functions are the only interface to communication system
  - message exchange via **`send()`** and **`receive()`**



Message Passing Paradigm

- types of communication
  - point-to-point a.k.a. P2P (1:1-communication)
    - two processes involved: sender and receiver
    - way of sending interacts with execution of sub-program
      - *synchronous*: send is provided information about completion of message transfer, i.e. communication does not complete until message has been received (fax, e.g.)
      - *asynchronous*: send only knows when message has left; completes as soon as message is on its way (postbox, e.g.)
      - *blocking*: operations only finish when communication has completed (fax, e.g.)
      - *non-blocking*: operations return straight away and allow program to continue; at some later point in time program can test for completion (fax with memory, e.g.)

Message Passing Paradigm

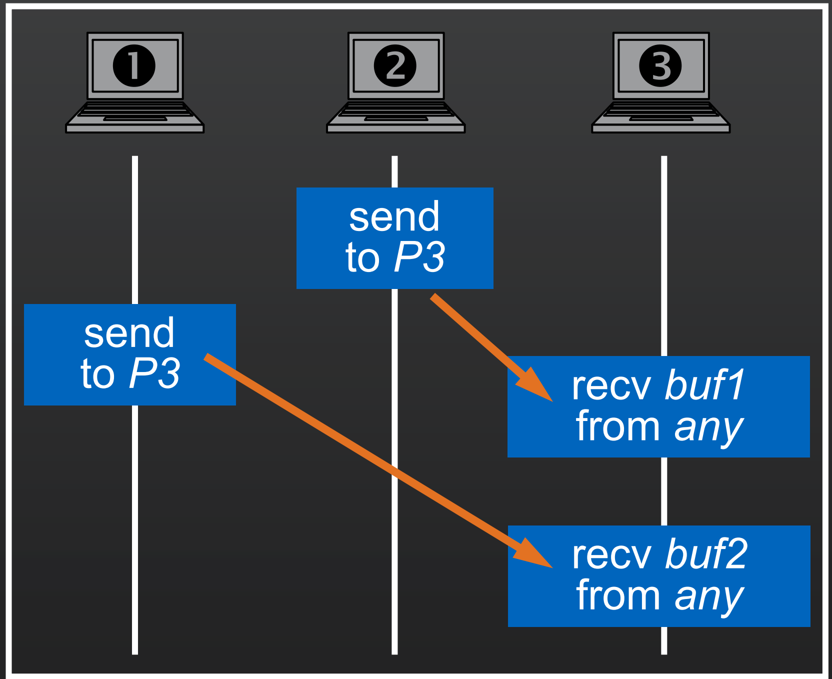
- types of communication (cont'd)
  - collective (1:M-communication, $M \leq P$, P number of processes)
    - all (some) processes involved
    - types of collective communication
      - *barrier*: synchronises processes (no data exchange), i.e. each process is blocked until all have called barrier routine
      - *broadcast*: one process sends same message to all (several) destinations with a single operation
      - *scatter / gather*: one process gives / takes data items to / from all (several) processes
      - *reduce*: one process takes data items from all (several) processes and reduces them to a single data item; typical reduce operations: sum, product, minimum / maximum, …

Message Passing Paradigm

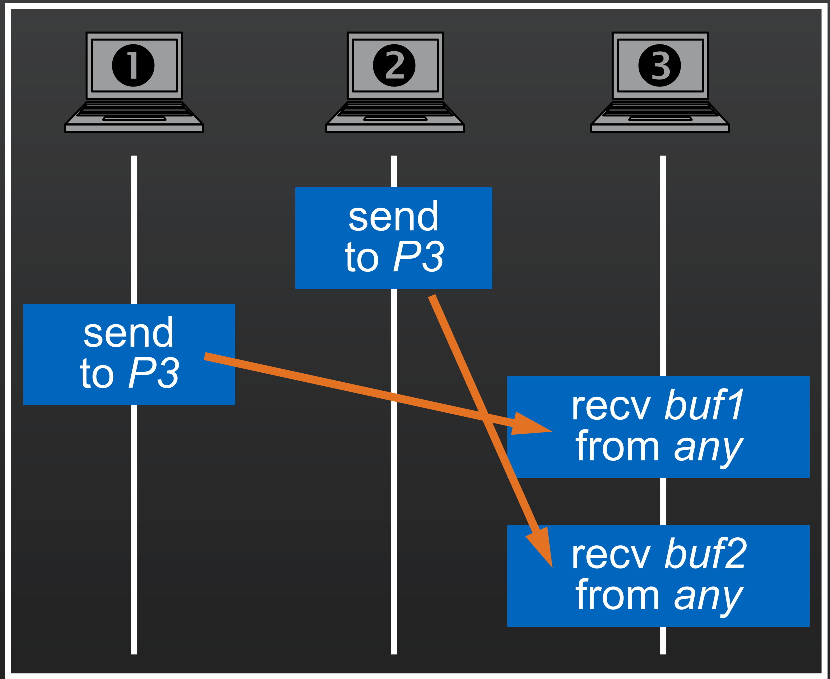
- message buffering
  - message buffering decouples send and receive operations ➔ a send can complete even if a matching receive hasn't been posted
  - buffering can be expensive
    - requires the allocation of memory for buffers
    - entails additional memory-to-memory copying
  - types of buffering
    - *send buffer*: in general allocated by the application program or by the message passing system for temporary usage (➔ system buffer)
    - *receive buffer*: allocated by the message passing system
  - problem: buffer space maybe not available on all systems

Message Passing Paradigm

- order of transmission
  - problem: there is no global time in a distributed system
  - hence, wrong send-receive assignments may occur (in case of more than two processes and the usage of wildcards)



or

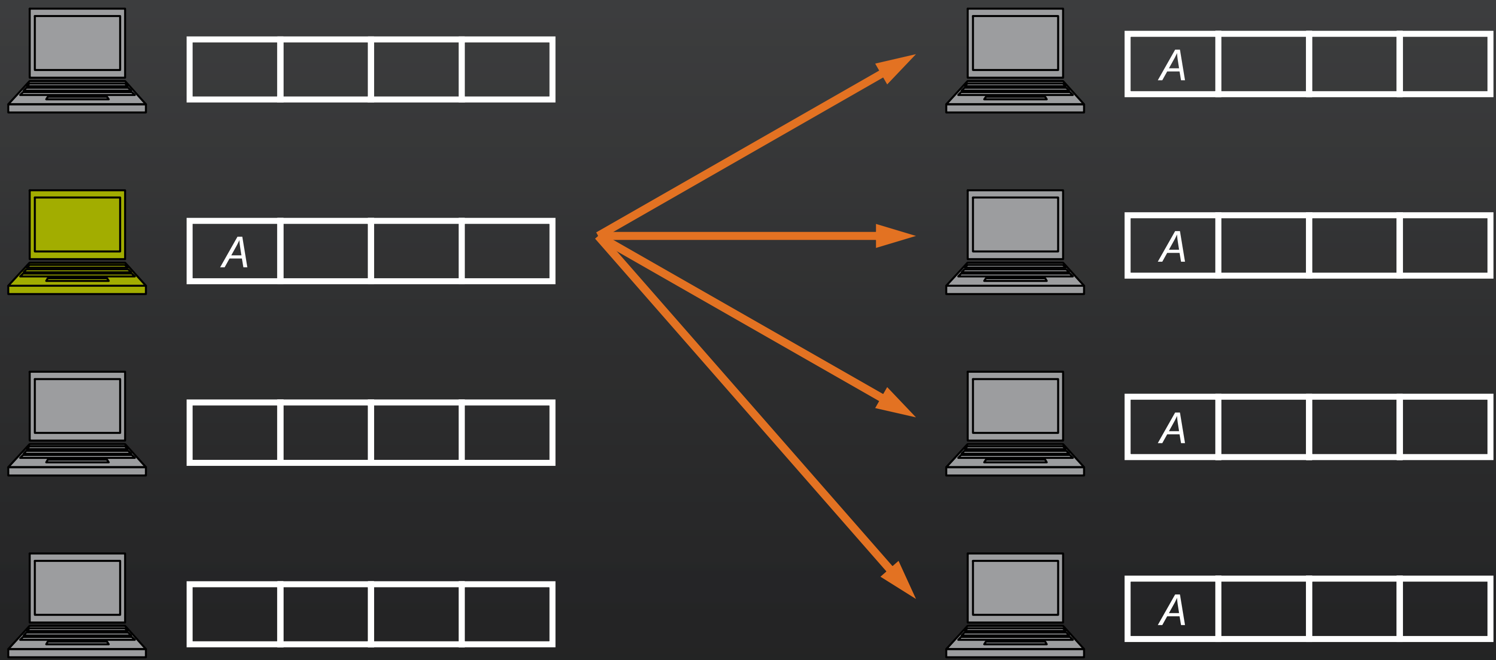


Overview

- message passing paradigm
- collective communication
- programming with MPI
- MPI advanced

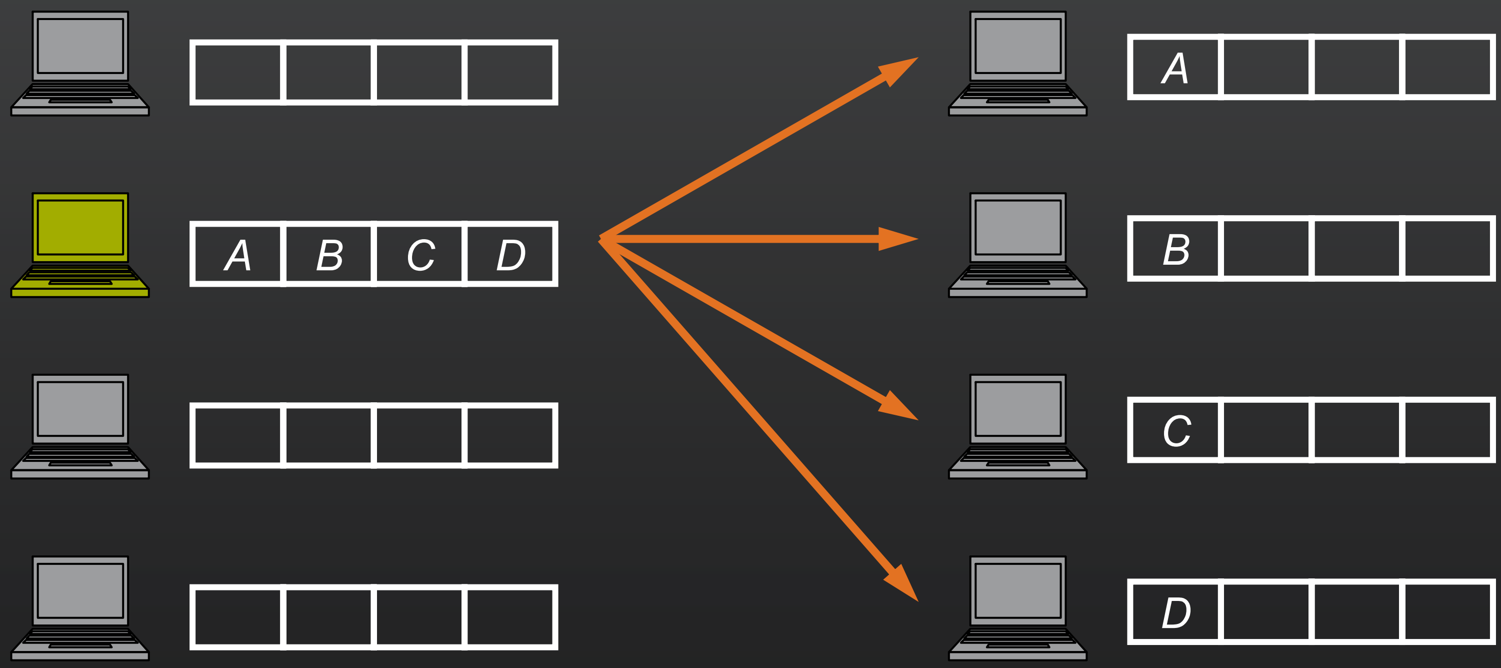
Collective Communication

- broadcast
  - sends same message to all participating processes
  - example: first process in competition informs others to stop



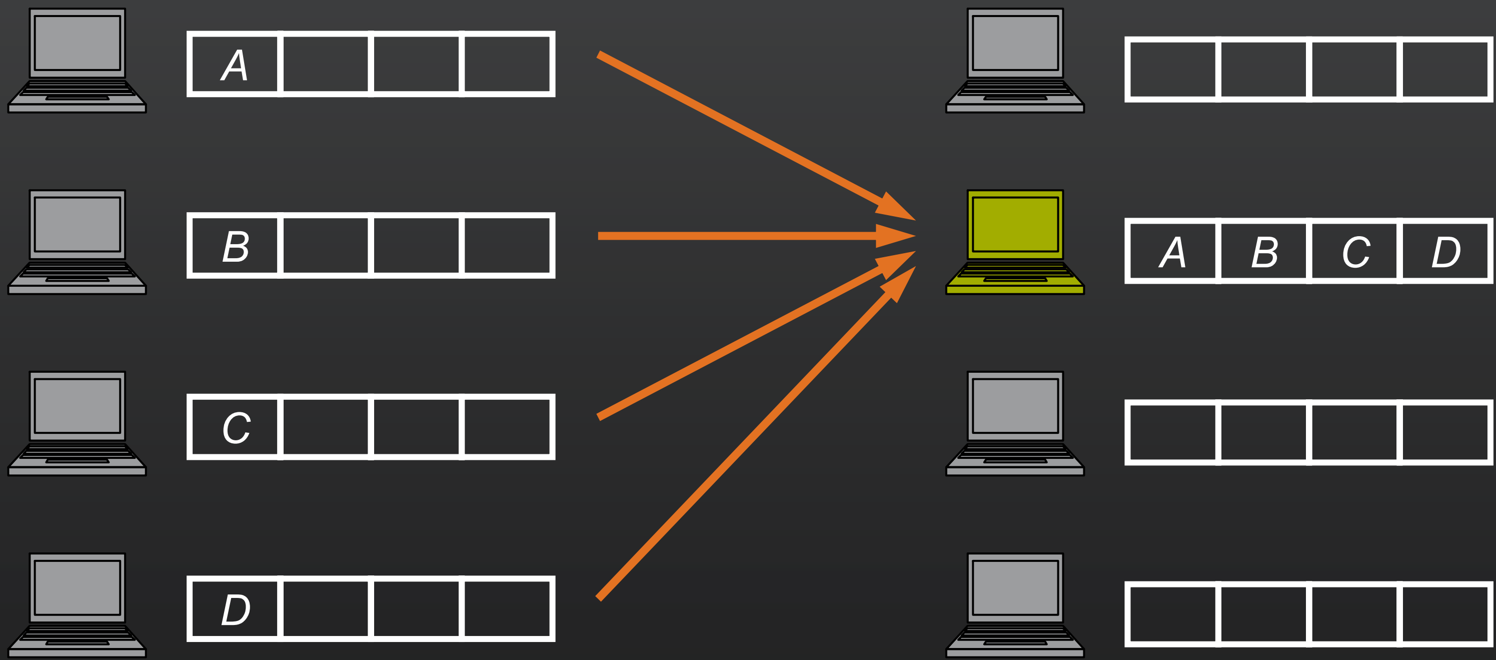
Collective Communication

- scatter
  - data from one process are distributed among all processes
  - example: rows of a matrix for a parallel solution of SLE



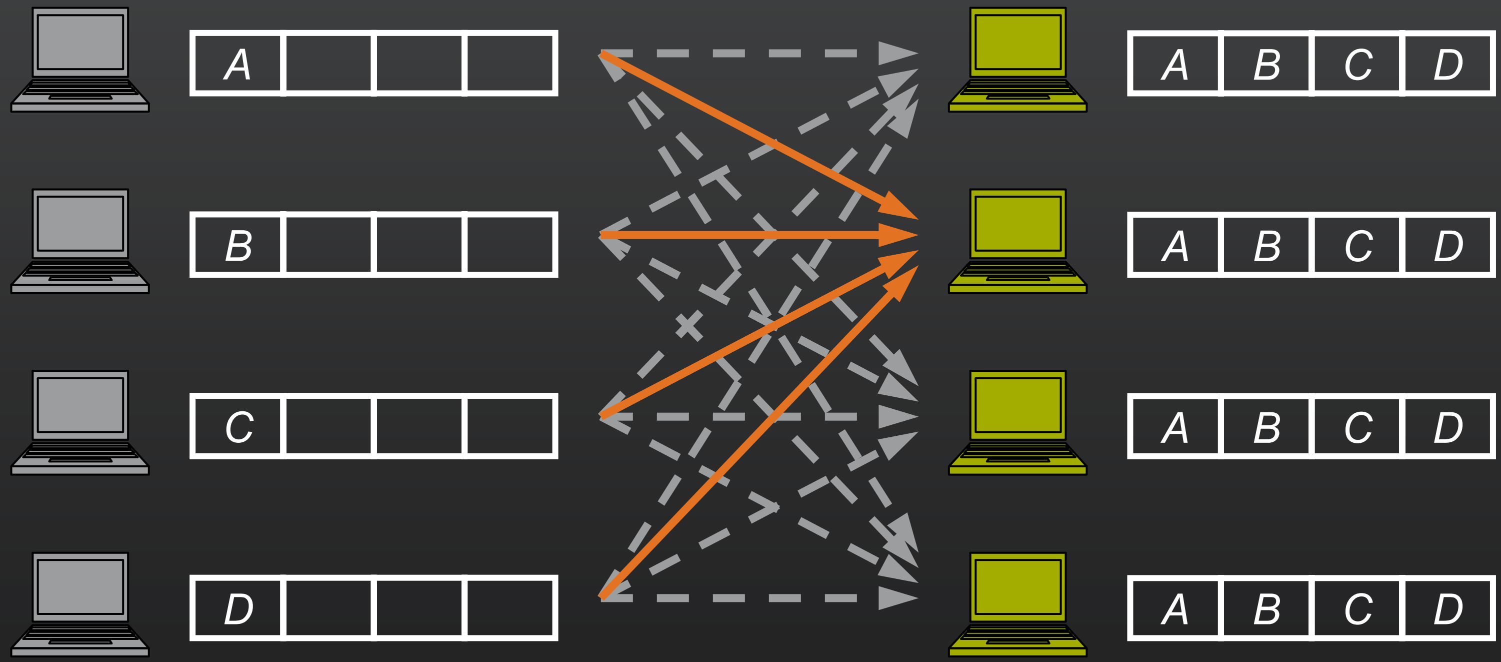
Collective Communication

- gather
  - data from all processes are collected by a single process
  - example: assembly of solution vector from parted solutions



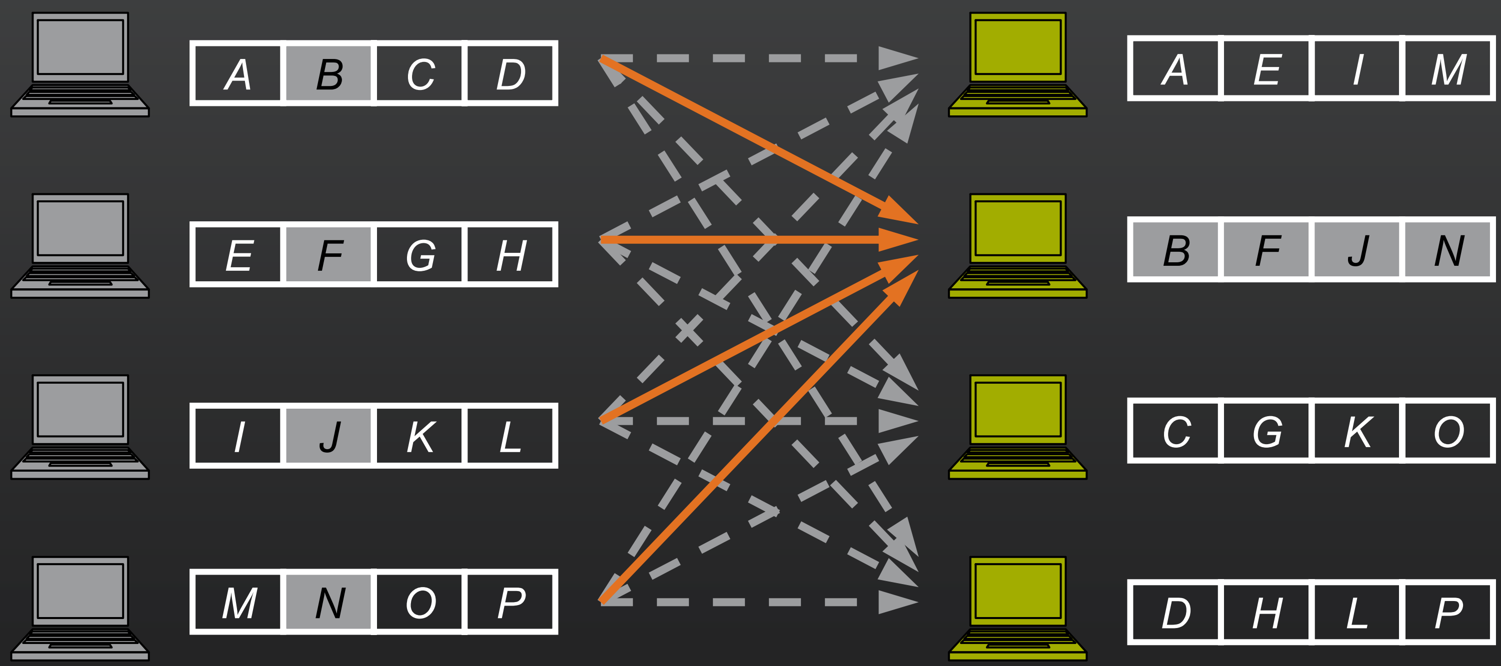
Collective Communication

- gather-to-all
  - all processes collect distributed data from all others
  - example: as before, but now all processes need global solution for continuation



Collective Communication

- all-to-all
  - data from all processes are distributed among all others
  - example: any ideas?



Collective Communication

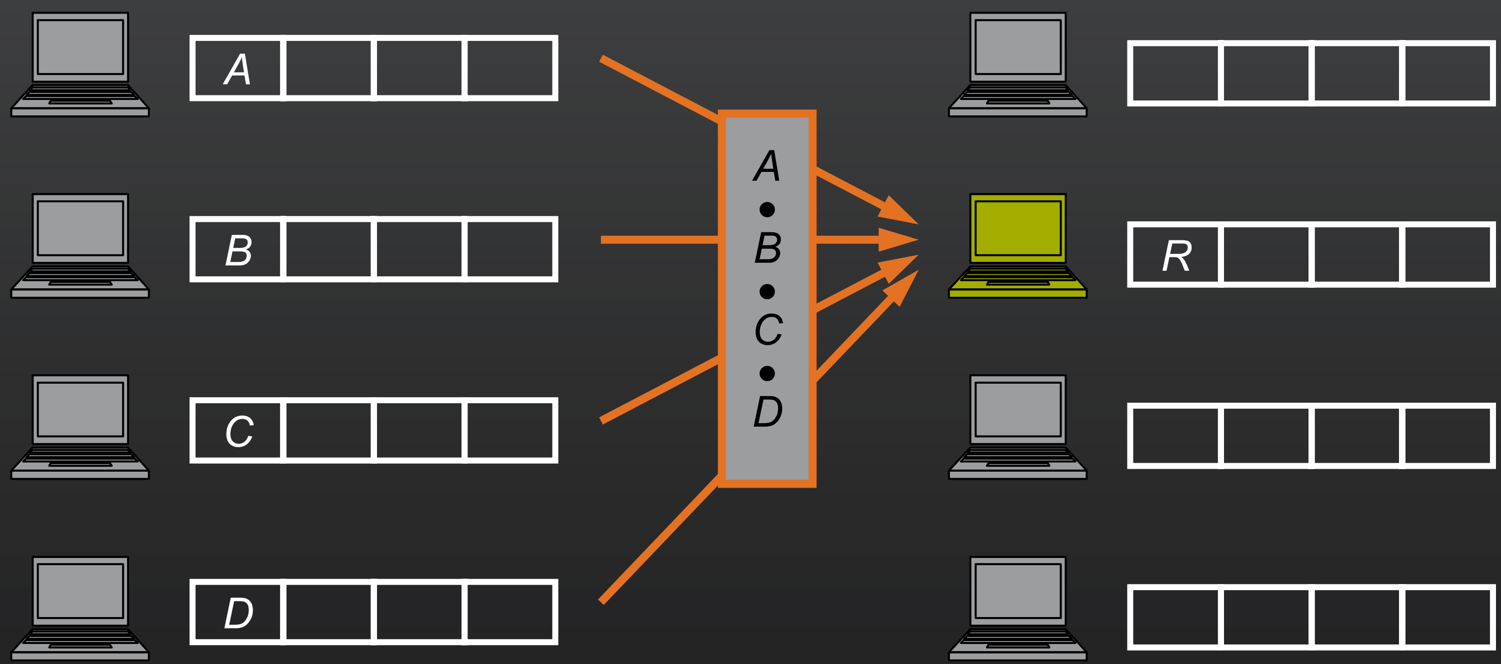
- all-to-all (cont'd)
  - also referred to as *total exchange*
  - example: transposition of matrix A (stored row-wise in memory)
    - total exchange of blocks B_{ij}
    - afterwards, each process computes transposition of its blocks

$$A = \begin{pmatrix} B_{11} & B_{12} & B_{13} & B_{14} \\ B_{21} & B_{22} & B_{23} & B_{24} \\ B_{31} & B_{32} & B_{33} & B_{34} \\ B_{41} & B_{42} & B_{43} & B_{44} \end{pmatrix} \rightarrow A^T = \begin{pmatrix} B_{11} & B_{21} & B_{31} & B_{41} \\ B_{12} & B_{22} & B_{32} & B_{42} \\ B_{13} & B_{23} & B_{33} & B_{43} \\ B_{14} & \boxed{B_{24}} & B_{34} & B_{44} \end{pmatrix}$$

$$\boxed{\begin{matrix} b_{11}^{(24)} & \cdots & b_{1N}^{(24)} \\ \vdots & \ddots & \vdots \\ b_{N1}^{(24)} & \cdots & b_{NN}^{(24)} \end{matrix}}$$

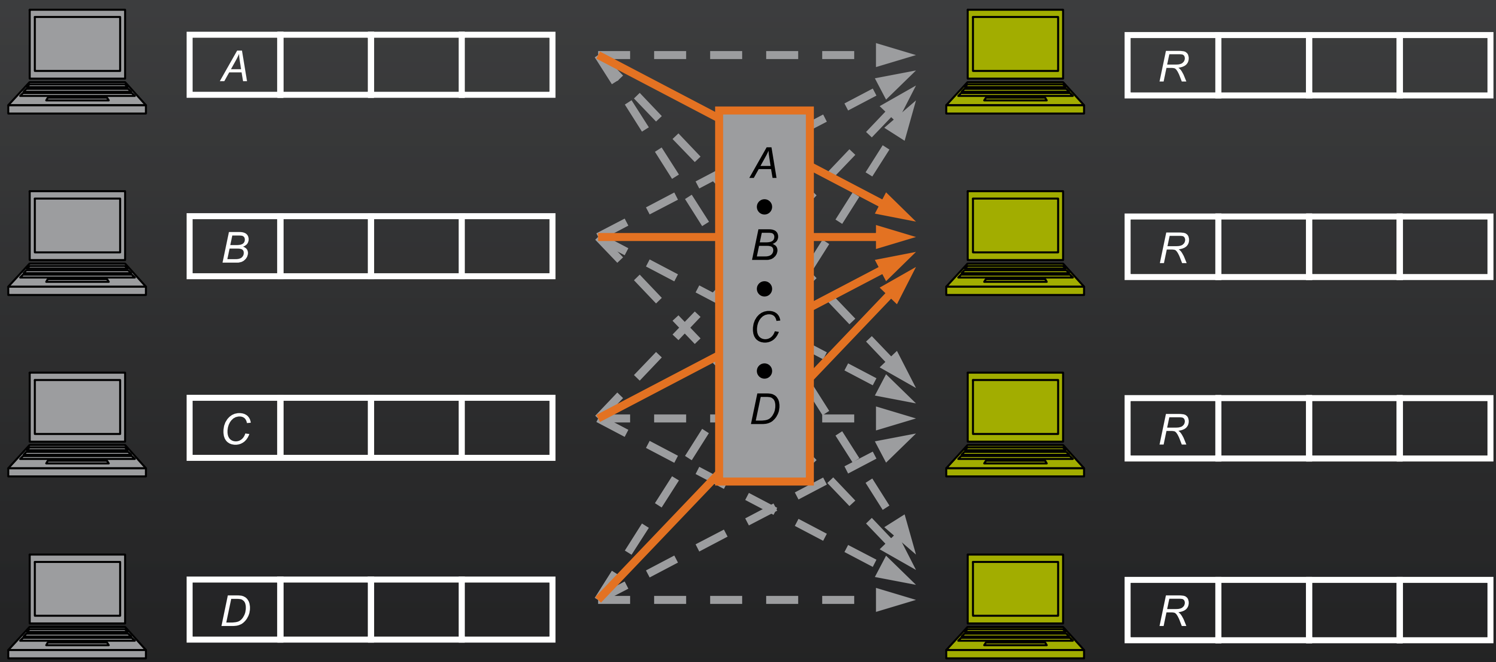
Collective Communication

- reduce
  - data from all processes are reduced to single data item(s)
  - example: global minimum / maximum / sum / product / …



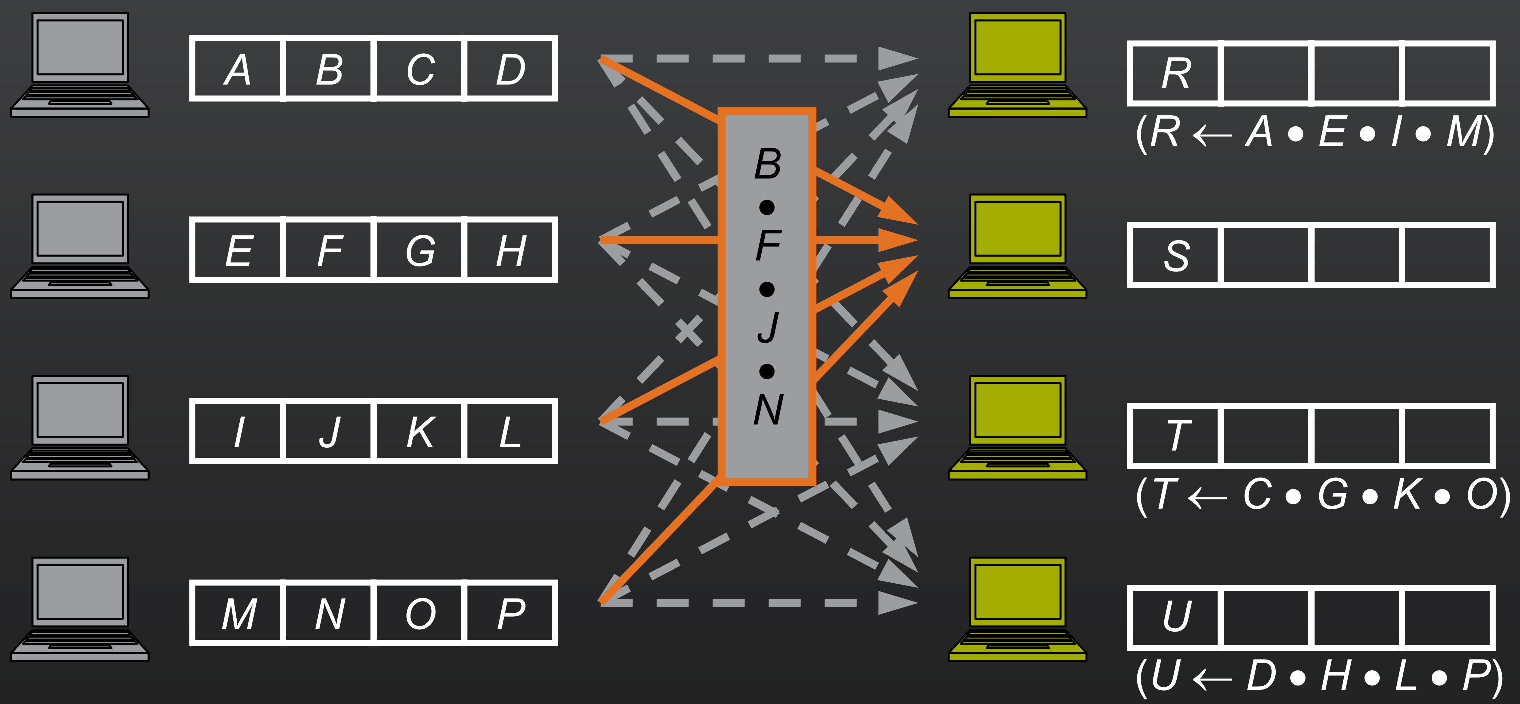
Collective Communication

- all-reduce
  - all processes are provided reduced data item(s)
  - example: finding prime numbers with “Sieve of ERATOSTHENES” ➔ processes need global minimum for deleting multiples of it



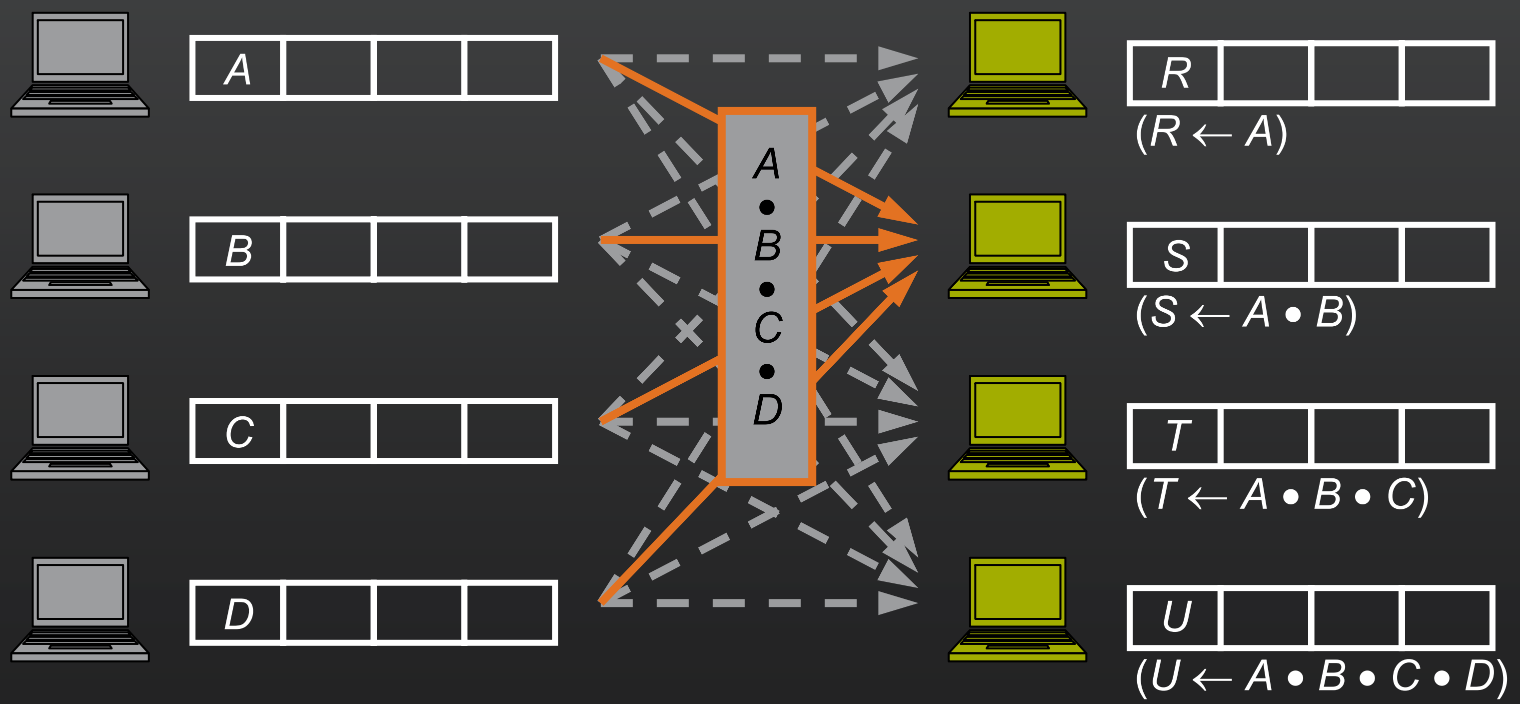
Collective Communication

- reduce-scatter
  - data from all processes are reduced and distributed
  - example: any ideas?



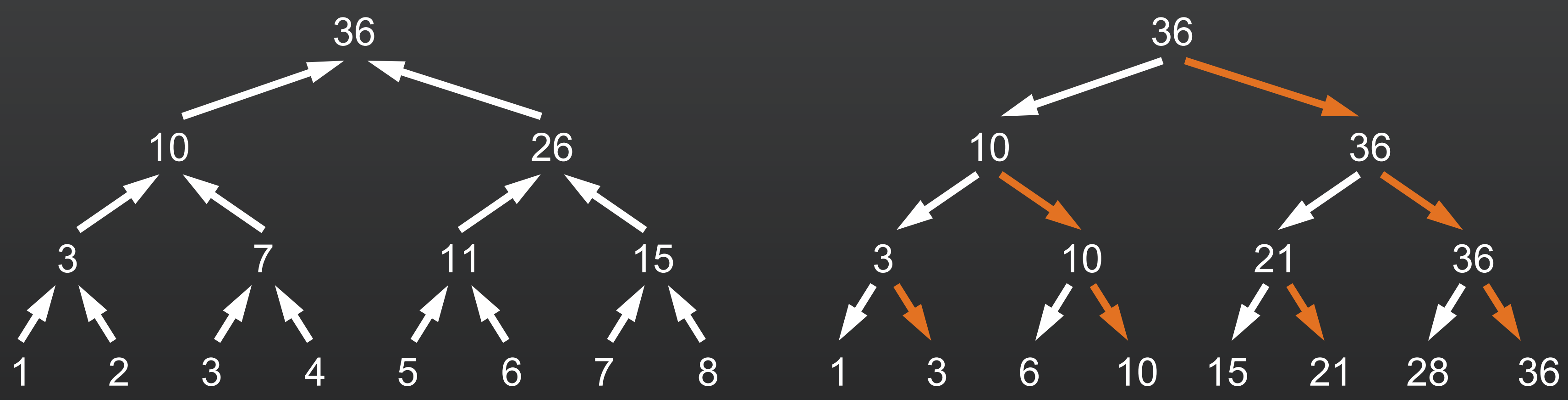
Collective Communication

- parallel prefix
  - processes receive partial result of reduce operation
  - example: matrix multiplication in quantum chemistry



Collective Communication

- parallel prefix (cont'd)
  - problem: finding all (partial) results within $\mathrm{O}(\log N)$ steps
  - implementation: two stages (up and down) using binary trees, e.g.
  - example: computing partial sums of N numbers



ascend:

$val_P \leftarrow val_{C\_left} + val_{C\_right}$

descend (level-wise):

even index (→): $val_C \leftarrow val_P$

odd index (→): $val_C \leftarrow val_C + val_{P-1}$

Overview

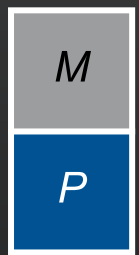
- message passing paradigm
- collective communication
- programming with MPI
- MPI advanced

Programming with MPI

- brief overview
  - de facto standard for writing parallel programs
  - both free available and vendor-supplied implementations
  - supports most interconnects
  - available for C / C++, Fortran 77, and Fortran 90
  - target platforms: SMPs, clusters, massively parallel processors
  - useful links
    - http://www.mpi-forum.org
    - http://www.hlrs.de/mpi/
    - http://www-unix.mcs.anl.gov/mpi/

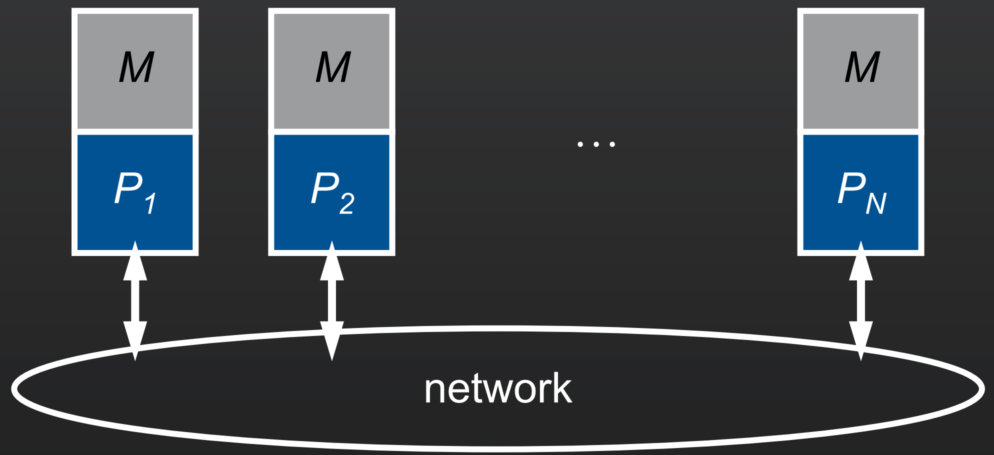
Programming with MPI

- programming model
  - sequential programming paradigm
    - one processor (*P*)
    - one memory (*M*)



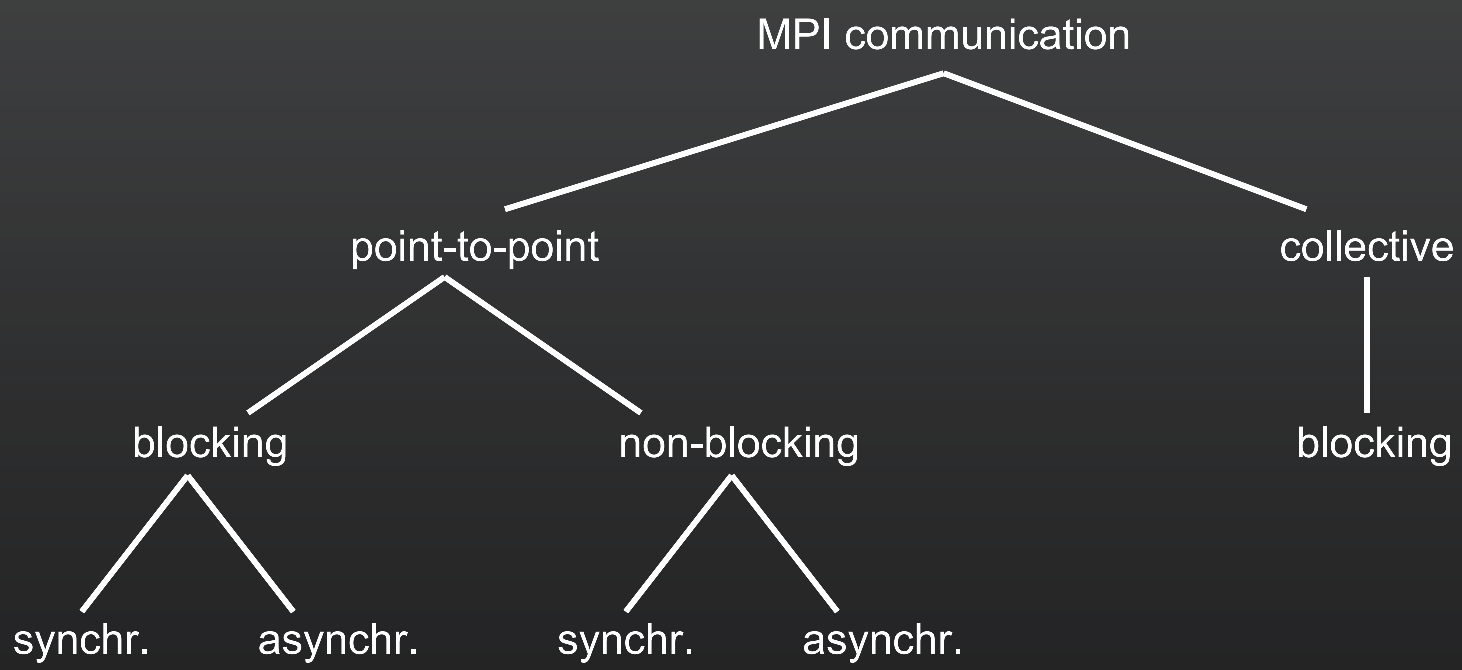
Programming with MPI

- programming model (cont'd)
  - message-passing programming paradigm
    - several processors / memories
    - each processor runs one or more processes
    - all data are private
    - communication between processes via messages



Programming with MPI

- types of communication
  - communication hierarchy (≤ MPI-2)



Programming with MPI

- writing and running MPI programs
  - header file to be included: mpi.h
  - all names of routines and constants are prefixed with MPI_
  - first routine called in any MPI program must be for initialisation

```
MPI_Init (int *argc, char ***argv)
```

  - clean-up at the end of program when all communications have been completed

```
MPI_Finalize (void)
```

  - `MPI_Finalize()` does not cancel outstanding communications
  - `MPI_Init()` and `MPI_Finalize()` are mandatory

Programming with MPI

- writing and running MPI programs (cont'd)
  - processes can only communicate if they share a communicator
    - predefined / standard communicator MPI_COMM_WORLD
    - contains list of processes
      - consecutively numbered from 0 (referred to as *rank*)
      - *rank* identifies each process within communicator
      - *size* identifies amount of all processes within communicator
    - why creating a new communicator
      - restrict collective communication to subset of processes
      - creating a virtual topology (torus, e.g.)
      - …

Programming with MPI

- writing and running MPI programs (cont'd)
  - determination of *rank*

```
MPI_Comm_rank (communicator comm, int &rank)
```

  - determination of *size*

```
MPI_Comm_size (communicator comm, int &size)
```

  - remarks
    - *rank* $\in$ [0, *size*–1]
    - *size* has to be specified at program start
      - MPI-1: *size* cannot be changed during runtime
      - MPI-2 and further: spawning of processes during runtime possible

Programming with MPI

- writing and running MPI programs (cont'd)
  - compilation of MPI programs: mpicc, mpicxx, mpif77, or mpif90

```
$ mpicc [ –o my_prog ] my_prog.c
```

  - available nodes for running an MPI program have to be stated explicitly via so called machinefile (list of hostnames or FQDNs)

```
node01
node02:2
lx64ia1.lrz-muenchen.de
```

  - running an MPI program (depends on distribution)

```
$ mpirun -machinefile <file> -np <#procs> my_prog
```

Programming with MPI

- writing and running MPI programs (cont'd)
  - example

```
include <mpi.h>

int main (int argc, char **argv) {
    int rank, size;

    MPI_Init (&argc, &argv);
    MPI_Comm_rank (MPI_COMM_WORLD, &rank);
    MPI_Comm_size (MPI_COMM_WORLD, &size);

    if (rank == 0) printf ("%d processes alive\n", size);
    else printf ("Slave %d: Hello world!\n", rank);

    MPI_Finalize ();
    return 0;
}
```

Programming with MPI

- messages
  - information that has to be provided for the message transfer
    - ranks of processes sending / receiving the message
    - memory location (send buffer) of data to be transmitted
    - type of data to be transmitted
    - amount of data to be transmitted
    - memory location (receive buffer) for data to be stored
  - in general, message is a (consecutive) array of elements of a particular MPI data type
  - data type must be specified both for sender and receiver → type conversion on heterogeneous parallel architectures done by the system (big-endian vs. little-endian, e.g.)

Programming with MPI

- messages (cont'd)
  - MPI data types (1)
    - basic types (see tabular)
    - derived types built up from basic types (vector, e.g.)

MPI data type	C / C++ data type
MPI_CHAR	signed char
MPI_SHORT	signed short int
MPI_INT	signed int
MPI_LONG	signed long int
MPI_UNSIGNED_CHAR	unsigned char
MPI_UNSIGNED_SHORT	unsigned short int

Programming with MPI

- messages (cont'd)
  - MPI data types (2)

MPI data type	C / C++ data type
MPI_UNSIGNED	unsigned int
MPI_UNSIGNED_LONG	unsigned long int
MPI_FLOAT	float
MPI_DOUBLE	double
MPI_LONG_DOUBLE	long double
MPI_BYTE	represents eight binary digits
MPI_PACKED	for matching any other type

Programming with MPI

- point-to-point communication (P2P)
  - different communication modes
    - *synchronous send*: completes when receive has been started
    - *buffered send*: always completes (even if receive has not been started); conforms to an asynchronous send
    - *standard send*: either buffered or unbuffered
    - *ready send*: always completes (even if receive has not started)
    - *receive*: completes when a message has arrived
  - all modes exist in both blocking and non-blocking form
    - *blocking*: return from routine implies completion of message passing stage
    - *non-blocking*: modes have to be tested (manually) for completion of message passing stage

Programming with MPI

- blocking P2P communication
  - neither sender nor receiver are able to continue the program execution during the message passing stage
  - sending a message (generic)

```
MPI_Send (buf, count, data type, dest, tag, comm)
```

  - receiving a message

```
MPI_Recv (buf, count, data type, src, tag, comm, status)
```

  - *tag*: marker to distinguish between different sorts of messages (i.e. communication context)
  - *status*: sender and tag can be queried for received messages (in case of wildcard usage)

Programming with MPI

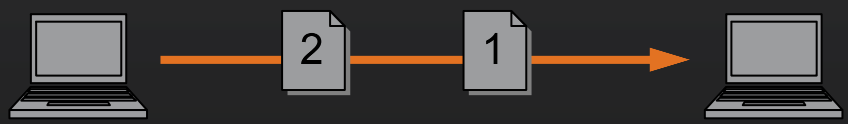
- blocking P2P communication (cont'd)
  - synchronous send: `MPI_Ssend( arguments )`
    - start of data reception finishes send routine, hence, sending process is idle until receiving process catches up
    - *non-local operation*: successful completion depends on the occurrence of a matching receive
  - buffered send: `MPI_Bsend( arguments )`
    - message is copied to send buffer for later transmission
    - user must attach buffer space first (one buffer per process); size should be at least the sum of all outstanding sends
    - buffered send guarantees to complete immediately ➔ *local operation*: independent from occurrence of matching receive
    - non-blocking version has no advantage over blocking version

Programming with MPI

- blocking P2P communication (cont'd)
  - standard send: `MPI_Send( arguments )`
    - MPI decides (depending on message size, e.g.) to send
      - *buffered*: completes immediately
      - *unbuffered*: completes when matching receive has been posted
  - ready send: `MPI_Rsend( arguments )`
    - completes immediately
    - matching receive must have already been posted, otherwise outcome is undefined
    - performance may be improved by avoiding handshaking and buffering between sender and receiver
    - non-blocking version has no advantage over blocking version

Programming with MPI

- blocking P2P communication (cont'd)
  - receive: `MPI_Recv( arguments )`
    - completes when message has arrived
    - usage of wildcards possible
      - MPI_ANY_SOURCE: receive from arbitrary source
      - MPI_ANY_TAG: receive with arbitrary tag
      - MPI_STATUS_IGNORE: don't care about state
  - general rule: messages from one sender (to one receiver) do not overtake each other, message from different senders (to one receiver) might arrive in different order than being sent



Programming with MPI

- blocking P2P communication (cont'd)
  - example: a simple ping-pong

```
int rank, buf;
MPI_Status status;

MPI_Comm_rank (MPI_COMM_WORLD, &rank);

if (rank == 0) {
    MPI_Send (&rank, 1, MPI_INT, 1, 0, MPI_COMM_WORLD);
    MPI_Recv (&buf, 1, MPI_INT, 1, 0, MPI_COMM_WORLD, &status);
} else {
    MPI_Recv (&buf, 1, MPI_INT, 0, 0, MPI_COMM_WORLD, &status);
    MPI_Send (&rank, 1, MPI_INT, 0, 0, MPI_COMM_WORLD);
}
```

Programming with MPI

- blocking P2P communication (cont'd)
  - example: buffered send

```
int intsize, charsize, buffersize;
void *buffer;

MPI_Pack_size (MAX, MPI_INT, MPI_COMM_WORLD, &intsize);
MPI_Pack_size (MAX, MPI_CHAR, MPI_COMM_WORLD, &charsize);

buffersize = intsize + charsize + 2*MPI_BSEND_OVERHEAD;
buffer = (void *)malloc (buffersize*sizeof (void *));
MPI_Buffer_attach (buffer, buffersize);

if (rank == 0) {
    MPI_Bsend (msg1, MAX, MPI_INT, 1, 0, MPI_COMM_WORLD);
    MPI_Bsend (msg2, MAX, MPI_CHAR, 2, 0, MPI_COMM_WORLD);
}
```

Programming with MPI

- blocking P2P communication (cont'd)
  - example: communication in a ring – does this work?

```
int rank, size, buf, next, prev;
MPI_Status status;

MPI_Init (&argc, &argv);
MPI_Comm_rank (MPI_COMM_WORLD, &rank);
MPI_Comm_size (MPI_COMM_WORLD, &size);

next = (rank+1)%size;
prev = (rank-1+size)%size;
MPI_Recv (&buf, 1, MPI_INT, prev, 0, MPI_COMM_WORLD, &status);
MPI_Send (&rank, 1, MPI_INT, next, 0, MPI_COMM_WORLD);

MPI_Finalize();
```

Programming with MPI

- non-blocking P2P communication
  - problem: blocking communication does not return until it has been completed ➔ risk of idly waiting and / or deadlocks
  - hence, usage of non-blocking communication
  - communication is separated into three phases

    1) initiate non-blocking communication
    2) do some work (involving other communications, e.g.)
    3) wait for non-blocking communication to complete

  - non-blocking routines have identical arguments to blocking counterparts, except for an extra argument *request*
  - request handle is important for testing if communication has been completed

Programming with MPI

- non-blocking P2P communication (cont'd)
  - sending a message (generic)

```
MPI_Isend (buf, count, data type, dest, tag, comm, request)
```

  - receiving a message

```
MPI_Irecv (buf, count, data type, src, tag, comm, request)
```

  - communication modes
    - synchronous send: `MPI_Issend(` ***arguments*** `)`
    - buffered send: `MPI_Ibsend(` ***arguments*** `)`
    - standard send: `MPI_Isend(` ***arguments*** `)`
    - ready send: `MPI_Irsend(` ***arguments*** `)`

Programming with MPI

- non-blocking P2P communication (cont'd)
  - testing communication for completion is essential before
    - making use of the transferred data
    - re-using the communication buffer
  - tests for completion are available in two different types
    - *wait*: blocks until communication has been completed

```
MPI_Wait (request, status)
```

    - *test*: returns TRUE or FALSE depending whether or not communication has been completed; it does not block

```
MPI_Test (request, flag, status)
```

  - what's an `MPI_Isend()` with an immediate `MPI_Wait()`

Programming with MPI

- non-blocking P2P communication (cont'd)
  - waiting / testing for completion of multiple communications

`MPI_Waitall()`	blocks until all have been completed
`MPI_Testall()`	TRUE if all, otherwise FALSE
`MPI_Waitany()`	blocks until one or more have been completed, returns (arbitrary) index
`MPI_Testany()`	returns flag and (arbitrary) index
`MPI_Waitsome()`	blocks until one ore more have been completed, returns index of all completed ones
`MPI_Testsome()`	returns flag and index of all completed ones

  - blocking and non-blocking forms can be combined

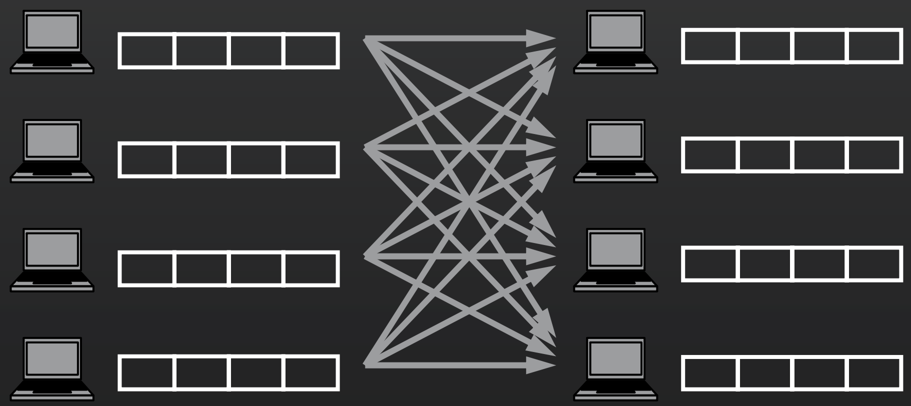
Programming with MPI

- non-blocking P2P communication (cont'd)
  - example: communication in a ring

```
int rank, size, buf, next, prev;
MPI_Request request;

MPI_Init (&argc, &argv);
MPI_Comm_rank (MPI_COMM_WORLD, &rank);
MPI_Comm_size (MPI_COMM_WORLD, &size);

next = (rank+1)%size;
prev = (rank-1+size)%size;
MPI_Irecv (&buf, 1, MPI_INT, prev, 0, MPI_COMM_WORLD, &request);
MPI_Send (&rank, 1, MPI_INT, next, 0, MPI_COMM_WORLD);
MPI_Wait (&request, MPI_STATUS_IGNORE);

MPI_Finalize ();
```

Programming with MPI

- collective communication
  - characteristics (< MPI-3)
    - all processes (within communicator) communicate
    - synchronisation may or may not occur
    - all collective operations are blocking operations
    - no tags allowed
    - all receive buffers must be exactly of the same size



Programming with MPI

- collective communication (cont'd)
  - barrier synchronisation
    - blocks calling process until all other processes have called barrier routine
    - hence, `MPI_Barrier()` always synchronises

```
MPI_Barrier (comm)
```

  - broadcast
    - has a specified root process
    - every process receives one copy of the message from root
    - all processes must specify the same root

```
MPI_Bcast (buf, count, data type, root, comm)
```

Programming with MPI

- collective communication (cont'd)
  - gather and scatter
    - has a specified root process
    - all processes must specify the same root
    - send and receive details must be specified as arguments

```
MPI_Gather (sbuf, scount, data type send, rbuf, rcount,
            data type recv, root, comm)

MPI_Scatter (sbuf, scount, data type send, rbuf, rcount,
             data type recv, root, comm)
```

  - variants
    - `MPI_Allgather()`: all processes collect data from all others
    - `MPI_Alltoall()`: total exchange

Programming with MPI

- collective communication (cont'd)
  - global reduction
    - has a specified root process
    - all processes must specify the same root
    - all processes must specify the same operation
    - reduction operations can be predefined or user-defined
    - root process ends up with an array of results

```
MPI_Reduce (sbuf, rbuf, count, data type, op, root, comm)
```

  - variants (no specified root)
    - **`MPI_Allreduce()`**: all processes receive result
    - **`MPI_Reduce_Scatter()`**: resulting vector is distributed to all
    - **`MPI_Scan()`**: processes receive partial result (➔ parallel prefix)

Programming with MPI

- collective communication (cont'd)
  - possible reduction operations (1)

operator	result
MPI_MAX	find global maximum
MPI_MIN	find global minimum
MPI_SUM	calculate global sum
MPI_PROD	calculate global product
MPI_LAND	make logical AND
MPI_BAND	make bitwise AND
MPI_LOR	make logical OR

Programming with MPI

- collective communication (cont'd)
  - possible reduction operations (2)

operator	result
MPI_BOR	make bitwise OR
MPI_LXOR	make logical XOR
MPI_BXOR	make bitwise XOR
MPI_MAXLOC	find global minimum and its position
MPI_MINLOC	find global maximum and its position

Programming with MPI

- example
  - finding prime numbers with the "Sieve of ERATOSTHENES" (*)
    - given: set of (integer) numbers A ranging from 2 to N

      1) find minimum value a_{MIN} of A → next prime number
      2) delete all multiples of a_{MIN} within A
      3) continue with step 1) until $a_{MIN} > \lfloor \sqrt{N} \rfloor$
      4) hence, A contains only prime numbers

    - parallel approach
      - distribute A among all processes (→ data parallelism)
      - find local minimum and compute global minimum
      - delete all multiples of global minimum in parallel

(*) Greek mathematician, born 276 BC in Cyrene (in modern-day Lybia), died 194 BC in Alexandria

Programming with MPI

- example (cont'd)
  - finding prime numbers with the "Sieve of ERATOSTHENES"

```
min ← 0
A[] ← 2 … MAX

MPI_Init (&argc, &argv)
MPI_Comm_size (MPI_COMM_WORLD, &size);

divide A into size parts Ai
while (min ≤ sqrt(MAX)) do
    find local minimum mini from Ai
    MPI_Allreduce (mini, min, MPI_MIN)
    delete all multiples of min from Ai
od

MPI_Finalize();
```

Overview

- message passing paradigm
- collective communication
- programming with MPI
- MPI advanced (*)

(*) not to be covered within this lecture

MPI Advanced

- persistent communication
  - overhead through repeated communication calls (several `send()` or `receive()` within a loop, e.g.)
  - idea of re-casting the communication
  - persistent communication requests may reduce the overhead
  - freely compatible with normal point-to-point communication

```
MPI_Send_init (buf, count, data type, dest, tag, comm, request)

MPI_Recv_init (buf, count, data type, src, tag, comm, request)
```

  - one routine for each send mode: Ssend, Bsend, Send, Rsend
  - each routine returns immediately, creating a request handle

MPI Advanced

- persistent communication (cont'd)
  - request handle to execute communication as often as required

```
MPI_Start (request)
```

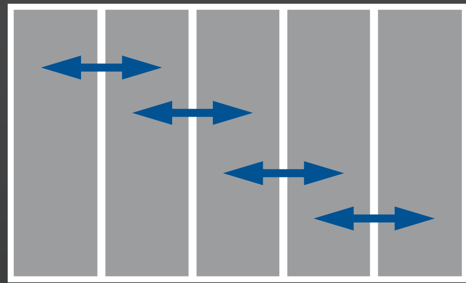
  - `MPI_Start()` initiates respective non-blocking communication
  - completion to be tested with known routines (test / wait)
  - request handle must be de-allocated explicitly when finished

```
MPI_Request_free (request)
```

  - variant: `MPI_Startall()` to activate multiple request

MPI Advanced

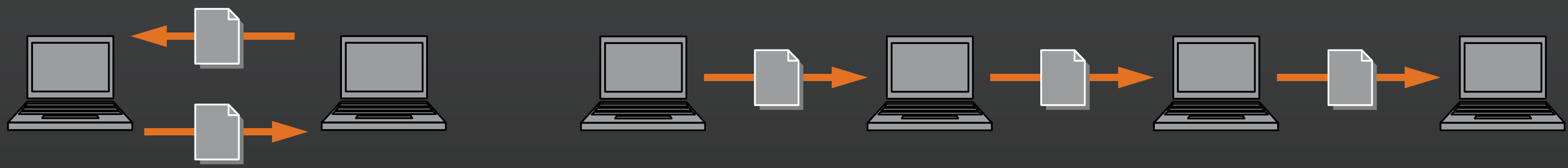
- persistent communication (cont'd)
  - example: column-wise data distribution
    - communication among direct neighbours
    - several communication stages



```
call MPI_Send_init() for sending request handles
call MPI_Recv_init() for receiving request handles

while (…) do
    update boundary cells
    call MPI_Start() for sending updates left / right
    call MPI_Start() for receiving updates left / right
    update non-boundary cells
    wait for completion of send / receive operation
od

call MPI_Request_free() to de-allocate request handles
```

MPI Advanced

- shift
  - passes data among processes in a “chain-like” fashion
  - each process sends and receives a maximum of one message



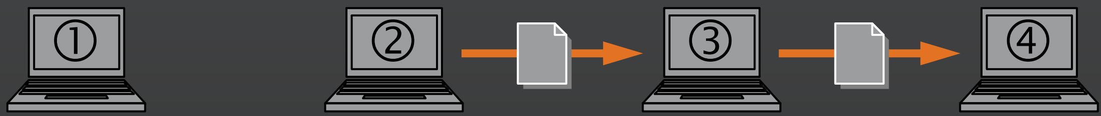
  - one routine for sending / receiving, i.e. atomic communication

```
MPI_Sendrecv (sbuf, scount, send data type, dest, stag,
              rbuf, rcount, recv data type, src, rtag,
              comm, status)
```

  - hence, blocking communication, but no risk of deadlocks
  - usage of MPI_NULL_PROC for more “symmetric” code

MPI Advanced

- shift (cont'd)
  - example



process	source	destination
1	MPI_NULL_PROC	MPI_NULL_PROC
2	MPI_NULL_PROC	3
3	2	4
4	3	MPI_NULL_PROC

  - variant: **`MPI_Sendrecv_replace()`** to use same buffer for sending and receiving

MPI Advanced

- timers
  - useful routine for timing programs

```
double MPI_Wtime (void)
```

  - returns elapsed wall-clock time in seconds
  - timer has no defined starting point ➔ two calls are necessary for computing difference (in general within master process)

```
double time1, time2;

MPI_Init (&argc, &argv);
time1 = MPI_Wtime ();
        ⋮
time2 = MPI_Wtime () – time1;
MPI_Finalize ();
```

MPI Advanced

- derived data types
  - basic types only consist of (arrays of) variables of same type
  - not sufficient for sending mixed and / or non-contiguous data
  - hence, creation of derived data types

`MPI_Type_contiguous()`	elements of same type stored in contiguous memory
`MPI_Type_vector()`	blocks of elements of same type with displacement (number of elements) between blocks
`MPI_Type_hvector()`	same as above; displacement in bytes
`MPI_Type_indexed()`	different sized blocks of elements of same type with different displacements (number of elements)
`MPI_Type_hindexed()`	same as above; displacements in bytes
`MPI_Type_struct()`	different sized blocks of elements of different type with different displacements (bytes)

MPI Advanced

- derived data types (cont'd)
  - derived data types are created at runtime
  - creation is done in two stages
    - construction of new data type definition from existing ones (either derived or basic)
    - commitment of new data type definition to be used in any number of communications

```
MPI_Type_commit (data type)
```

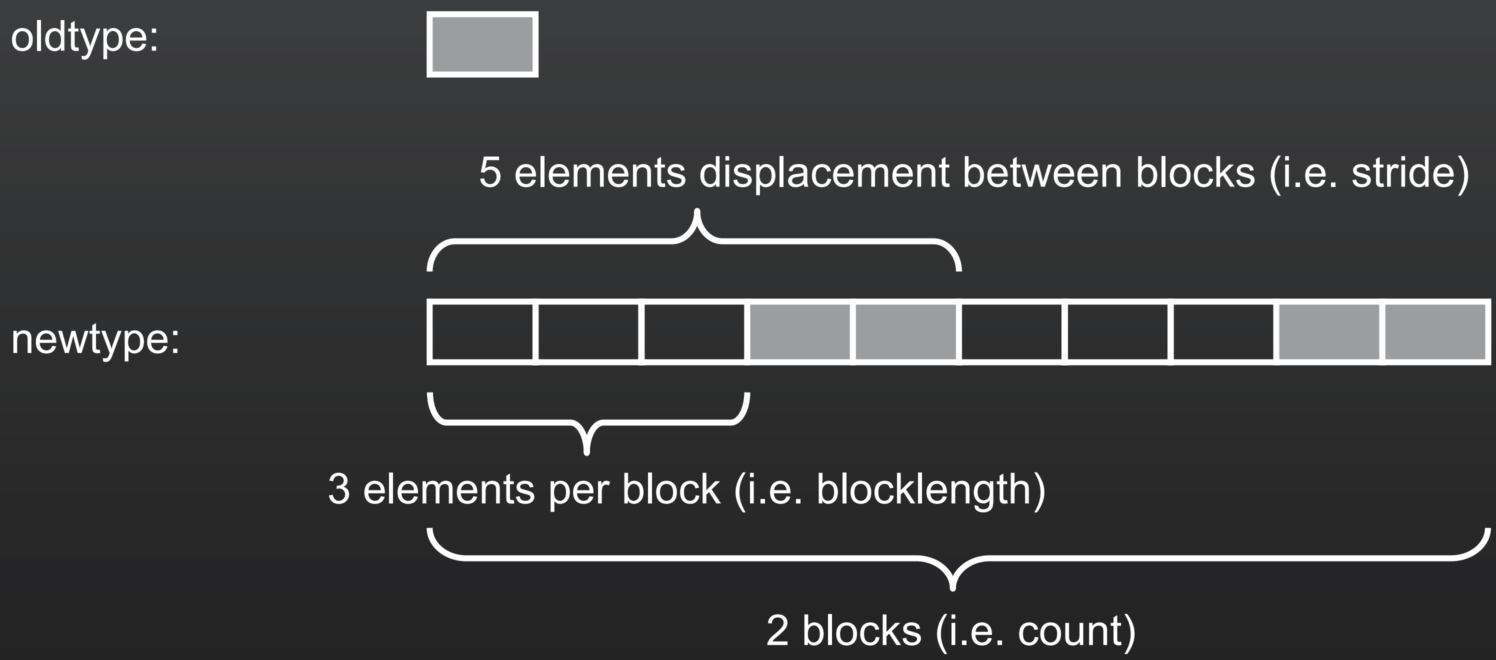
  - complementary routine to `MPI_Type_commit()` for de-allocation

```
MPI_Type_free (data type)
```

MPI Advanced

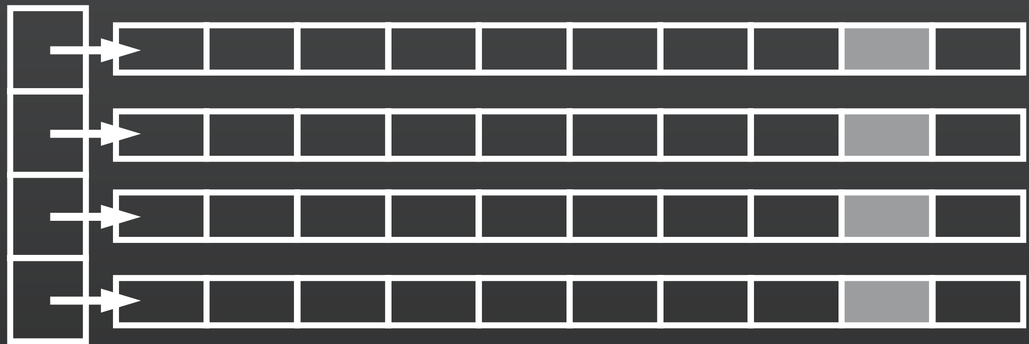
- derived data types (cont'd)
  - `MPI_Type_vector()`

```
MPI_Type_vector (count, blocklength, stride, oldtype, newtype)
```



MPI Advanced

- derived data types (cont'd)
  - example: matrix A stored row-wise in memory

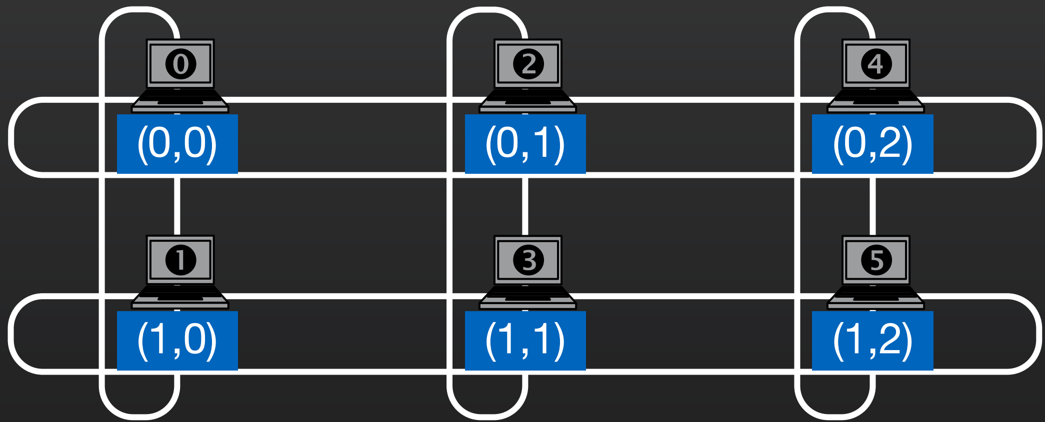


  - sending a row is no problem, but sending a column
  - hence, definition of new data type via **`MPI_Type_vector()`**

```
MPI_Datatype newtype;
MPI_Type_vector (4, 1, 10, MPI_DOUBLE, &newtype);
MPI_Type_commit (&newtype);
MPI_Send (&(A[0][8]), 1, newtype, dest, 0, comm);
```

MPI Advanced

- virtual topologies
  - allows for a convenient process naming
  - naming scheme to fit the communication pattern
  - simplifies writing of code
  - example: communication only with nearest neighbours
    - virtual topology to reflect this fact (2D grid, e.g.)
    - hence, simplified communication based on grid coordinates



MPI Advanced

- virtual topologies (cont'd)
  - creating a topology produces a new communicator
  - MPI allows generation of
    - Cartesian topologies
      - each process is "connected" to its neighbours
      - boundaries can be cyclic
      - processes are identified by Cartesian coordinates
    - graph topologies
      - arbitrary connections between processes
      - see MPI document for more details

MPI Advanced

- virtual topologies (cont'd)
  - Cartesian topology

```
MPI_Cart_create (old_comm, ndims, dims[], periods[],
                 reorder, cart_comm)
```

- *ndims*: number of dimensions
- *dims*: number of processes in each dimension
- *periods*: dimension has cyclic boundaries (TRUE or FALSE)
- *reorder*: choose dependent if data is yet distributed or not
  - FALSE: process ranks remain the same
  - TRUE: MPI may renumber (to match physical topology)

MPI Advanced

- virtual topologies (cont'd)
  - mapping functions to convert between rank and grid coordinates
    - converting given grid coordinates to process rank (returns MPI_NULL_PROC for rank if coordinates are off-grid in case of non-periodic boundaries)

```
MPI_Cart_rank (cart_comm, coords[], rank)
```

    - converting given process rank to grid coordinates

```
MPI_Cart_coords (cart_comm, rank, ndims, coords[])
```

MPI Advanced

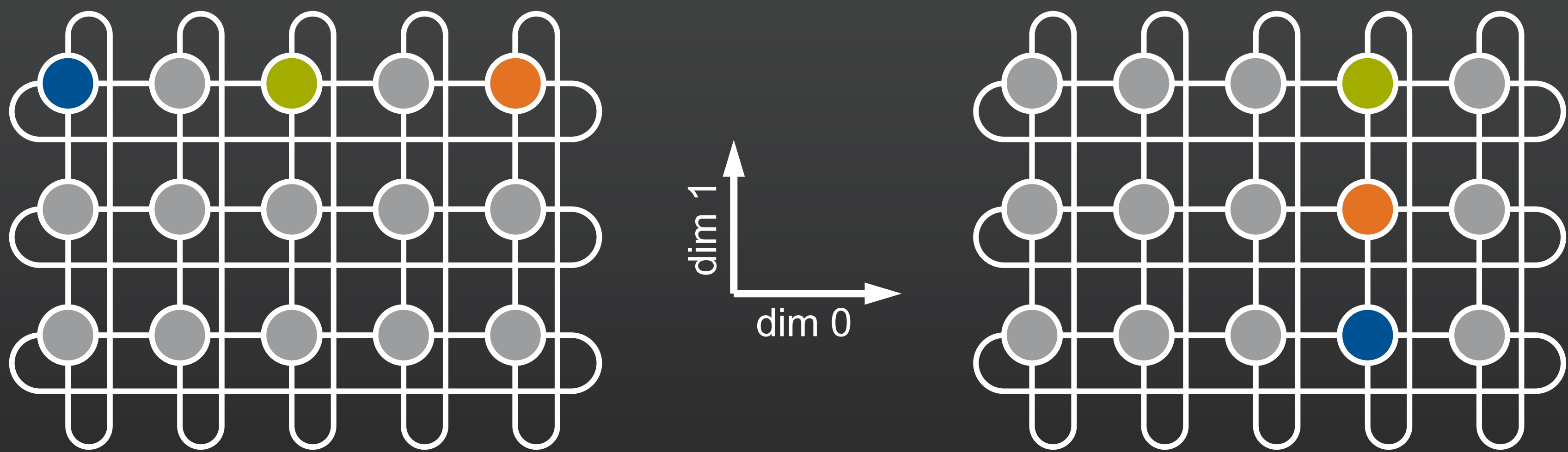
- virtual topologies (cont'd)
  - computing correct ranks for a shift

```
MPI_Cart_shift (cart_comm, direction, disp, src, dest)
```

- *direction* $\in$ [0, *ndims*–1]: dimension to perform the shift
- *disp*: displacement in that direction (positive or negative)
- returns two results
  - *src*: rank of process from which to receive a message
  - *dest*: rank of process to which to send a message
  - otherwise: MPI_NULL_PROC if coordinates are off-grid
- **`MPI_Cart_shift()`** does not perform the shift itself ➔ to be done separately via **`MPI_Send()`** or **`MPI_Sendrecv()`**

MPI Advanced

- virtual topologies (cont'd)
  - example



direction = 0
disp = 2

direction = 1
disp = –1

process calling `MPI_Cart_shift()` source destination

MPI Advanced

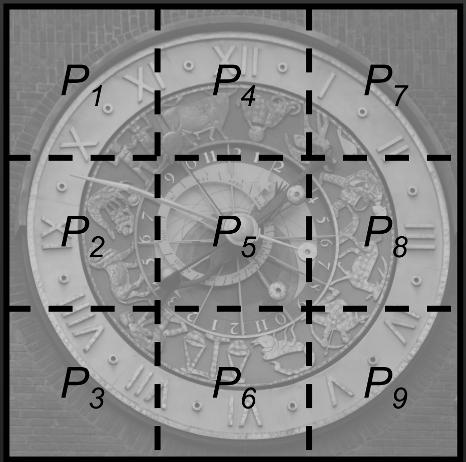
- case study
  - task: two-dimensional smoothing of grayscale pictures
  - pictures stored as (quadratic) matrix P of type integer
  - elements $p(i, j) \in [0, 255]$ of P stored row-wise in memory
  - linear smoothing of each pixel (i.e. matrix element) via

$$p(i, j) = 1/5*(p(i+1, j) + p(i-1, j) + p(i, j+1) + p(i, j-1) - 4 \cdot p(i, j))$$

  - several smoothing stages to be applied on P

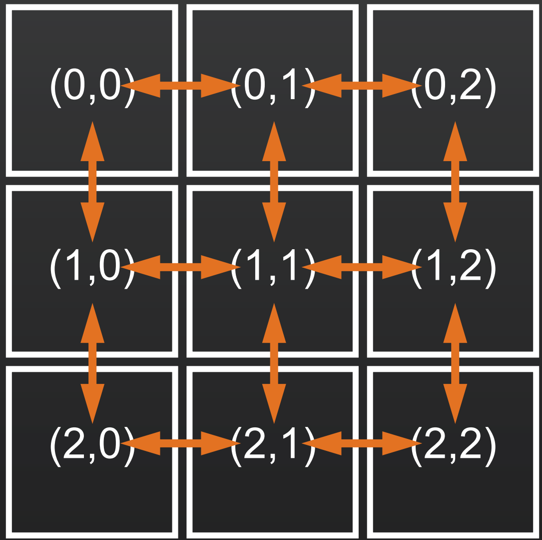
MPI Advanced

- case study (cont'd)
  - data parallelism ➔ domain decomposition, i.e. subdivision of *P* into equal parts (stripes, blocks, …)
  - hence, processes organised via virtual Cartesian topology (grid)
  - boundary values of direct neighbours needed by each process for its local computations (simplified data exchange via shifts ⟷)



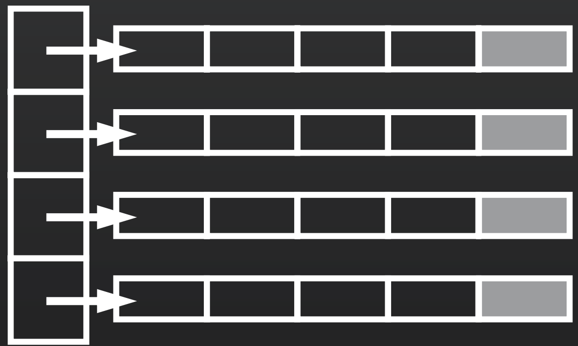
`MPI_Cart_create()`

→



MPI Advanced

- case study (cont'd)
  - communication
    - exchange of updated boundaries with neighbours in each iteration ➔ `MPI_Cart_shift()` and `MPI_Sendrecv()` due to virtual topology (2D grid)
    - usage of MPI_NULL_PROC for nodes at the borders of domain
    - problem for vertical boundaries (data stored row-wise in memory) ➔ definition of derived data type (vector)



`MPI_Type_vector()`

`MPI_Type_commit()`

MPI Advanced

- case study (cont'd)

```
MPI_Comm_rank ();
MPI_Comm_size ();

MPI_Cart_Create ();
distribute data among processes (MPI_Scatter, e.g.)


MPI_Type_vector ();
MPI_Type_commit ();

while (condition) do
    compute new values for interior p(i,j) in subdomain
    exchange interface values with all neighbours
        MPI_Cart_shift ();
        MPI_Sendrecv ();
    update interface values
od

gather data and assemble result
```