Message Passing with MPI

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Hristo Iliev
IT Center / JARA-HPC

Agenda

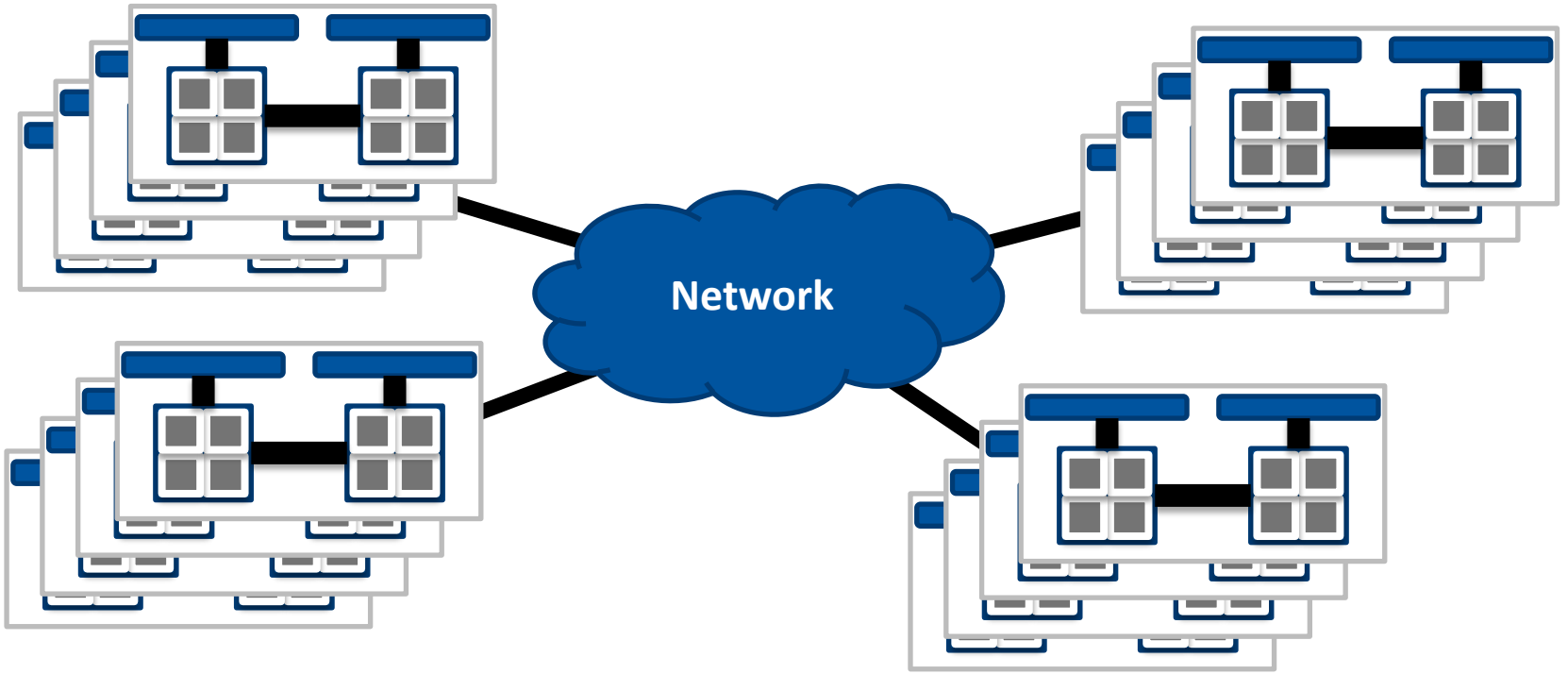
- Motivation
- Part 1
  - → Concepts
  - → Point-to-point communication
  - → Non-blocking operations
- Part 2
  - → Collective operations
  - → Communicators
  - → User datatypes
- **Part 3**
  - → Hybrid parallelisation
  - → Common parallel patterns

Hybrid Programming: Motivation

- **MPI is sufficiently abstract so it runs perfectly fine on a single node:**
  - → it doesn't care where processes are located as long as they can communicate
  - → message passing implemented using shared memory and IPC
    - →all details hidden by the MPI implementation;
    - →usually faster than sending messages over the network;
  - → but…
- **… this is far from optimal:**
  - → MPI processes are separate (heavyweight) OS processes
  - → portable data sharing is hard to achieve
  - → lots of program control / data structures have to be duplicated (uses memory)
  - → reusing cached data is practically impossible

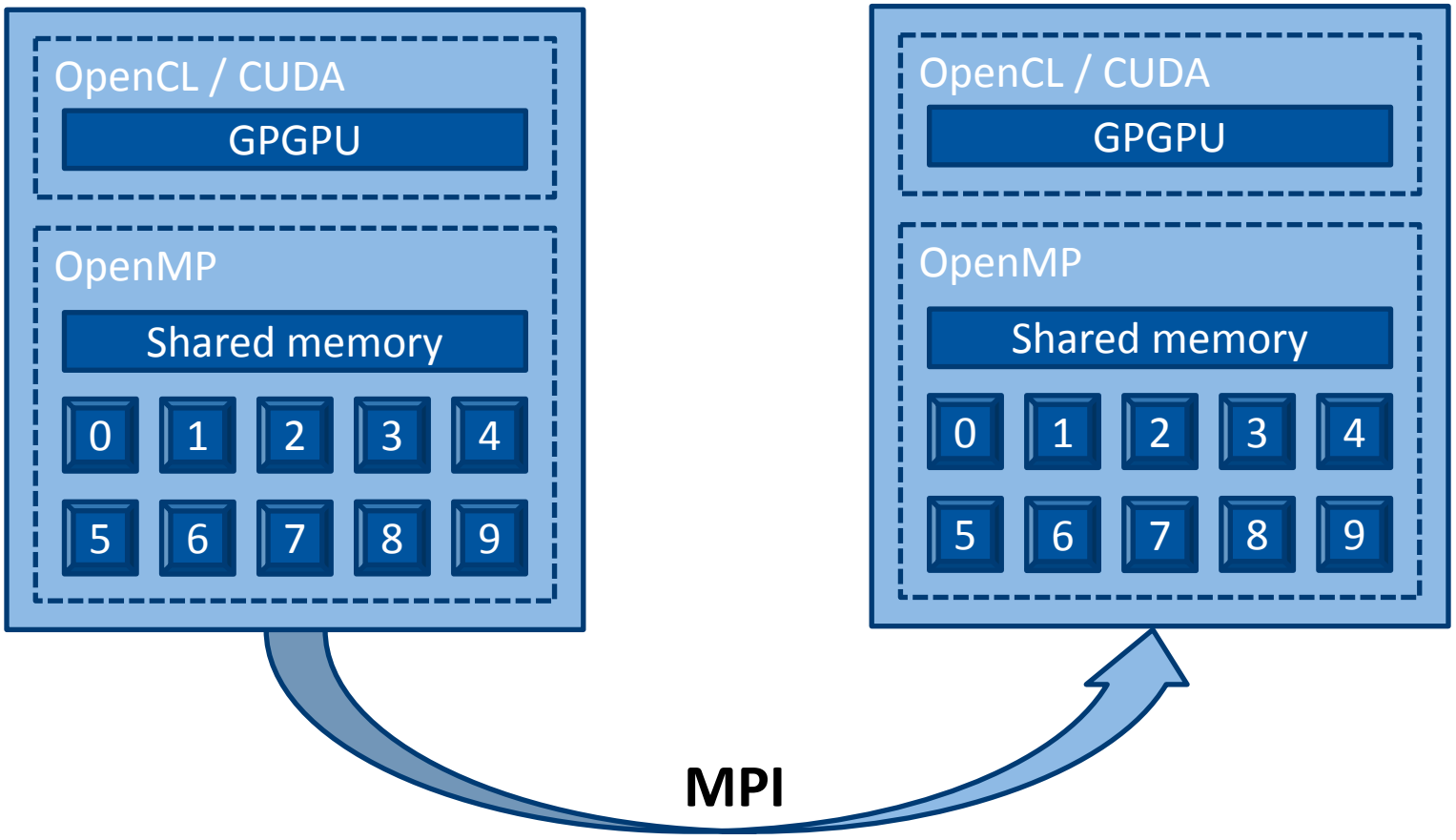
Clusters

- HPC market is at large dominated by distributed memory *multicomputers*: *clusters* and specialised *supercomputers*
- Nodes have no direct access to other nodes' memory and run a separate copy of the (possibly stripped down) OS



Basic Idea

- **Hierarchical mixing of different programming paradigms**



MPI – Threads Interaction

- **Most MPI implementation are threaded (e.g. for non-blocking requests) but not thread-safe.**

- **Four levels of threading support in increasing order:**

Level identifier	Description
`MPI_THREAD_SINGLE`	Only one thread may execute
`MPI_THREAD_FUNNELED`	Only the main thread may make MPI calls
`MPI_THREAD_SERIALIZED`	Only one thread may make MPI calls at a time
`MPI_THREAD_MULTIPLE`	Multiple threads may call MPI at once with no restrictions

- **All implementations support MPI_THREAD_SINGLE, but some does not support MPI_THREAD_MULTIPLE.**

Initialisation of MPI

- **Initialise MPI with thread support:**

```
MPI_Init_thread (int *argc, char ***argv, int required, int *provided)

SUBROUTINE MPI_INIT_THREAD (required, provided, ierr)
```

  - → **required** specifies what thread level support one requires from MPI
  - → **provided** is set to the actual thread level support provided
    - →could be lower or higher than the required level – always check!
  - → **MPI_Init** – equivalent to **required = MPI_THREAD_SINGLE**

- **The thread that calls MPI_Init_thread becomes the main thread**

- **The level of thread support cannot be changed later**

Query Functions

- **Obtain the provided level of thread support:**

```
MPI_Query_thread (int *provided)
```

  - → If MPI was initialised by **MPI_Init_thread**, then **provided** is set to the same value as the one returned by the initialisation call
  - → If MPI was initialised by **MPI_Init**, then **provided** is set to an implementation specific default value

- **Find out if running in the main thread:**

```
MPI_Is_thread_main (int *flag)
```

  - → **flag** set to **true** if the current thread is the main thread

MPI + OpenMP

- **The most common approach to hybrid programming**
  - → Coarse-grained parallelisation with MPI
  - → Fine-grained loop or task parallelisation with OpenMP
- **Different MPI implementations provide varying degree of support for threaded programs**
  - → MPI_THREAD_MULTIPLE rarely implemented completely for all transports
  - → Performance decrease due to locking overhead
- **Safest and most portable approach: Call MPI from the main thread only (and outside any OpenMP parallel region)**

MPI + OpenMP

- **Simple: Iterative processing with MPI only**

```
double data[], localData[];

for (int iter = 0; iter < maxIters; iter++) {

   MPI_Scatter(data, count, MPI_DOUBLE,
               localData, count, MPI_DOUBLE,
               0, MPI_COMM_WORLD);


   for (int i = 0; i < count; i++)
      localData[i] = exp(localData[i]);

   MPI_Gather(localData, count, MPI_DOUBLE,
              data, count, MPI_DOUBLE,
              0, MPI_COMM_WORLD);

}
```

MPI + OpenMP

- **Safe: MPI called outside any OpenMP parallel region**

```
double data[], localData[];

for (int iter = 0; iter < maxIters; iter++) {

   MPI_Scatter(data, count, MPI_DOUBLE,
               localData, count, MPI_DOUBLE,
               0, MPI_COMM_WORLD);

   #pragma omp parallel for
   for (int i = 0; i < count; i++)
      localData[i] = exp(localData[i]);

   MPI_Gather(localData, count, MPI_DOUBLE,
              data, count, MPI_DOUBLE,
              0, MPI_COMM_WORLD);

}
```

MPI + OpenMP

- **Advanced: MPI called by the master OpenMP thread only**

```
double data[], localData[];
#pragma omp parallel
for (int iter = 0; iter < maxIters; iter++) {
   #pragma omp master
   MPI_Scatter(data, count, MPI_DOUBLE,
               localData, count, MPI_DOUBLE,
               0, MPI_COMM_WORLD);
   #pragma omp barrier
   #pragma omp for
   for (int i = 0; i < count; i++)
      localData[i] = exp(localData[i]);
   #pragma omp master
   MPI_Gather(localData, count, MPI_DOUBLE,
              data, count, MPI_DOUBLE,
              0, MPI_COMM_WORLD);
   #pragma omp barrier
}
```

MPI + OpenMP

- **Adventurous: MPI called by a single OpenMP thread at a time**

```
MPI_Init_thread(NULL, NULL, MPI_THREAD_SERIALIZED, &provided);

double data[], localData[];
#pragma omp parallel
for (int iter = 0; iter < maxIters; iter++) {
   #pragma omp single
   MPI_Scatter(data, count, MPI_DOUBLE,
               localData, count, MPI_DOUBLE,
               0, MPI_COMM_WORLD);
   #pragma omp for
   for (int i = 0; i < count; i++)
      localData[i] = exp(localData[i]);
   #pragma omp single
   MPI_Gather(localData, count, MPI_DOUBLE,
              data, count, MPI_DOUBLE,
              0, MPI_COMM_WORLD);
}
```

Addressing in Hybrid Programs

- **MPI was not designed initially with multithreading in mind**
  - → Single rank (end-point) per process per communicator
  - → Addressing individual threads is tricky (and mostly hacky)
- **MPI and OpenMP IDs live in orthogonal spaces**
  - → MPI rank ∈ [0, #procs-1] **MPI_Comm_rank()**
  - → OpenMP thread ID ∈ [0, #threads-1] **omp_get_thread_num()**
  - → Hybrid rank:thread ∈ [0, #procs-1] × [0, #threads-1]

Field	Value source	Remark
source rank	Sender process rank	Automatically copied, no control over it
destination rank	user-supplied	Only one rank per process
tag	user-supplied	Free to choose
communicator	user-supplied	Multiple communicators possible

Addressing in Hybrid Programs

- **Tags as thread IDs**
  - → Each MPI message carries a tag with at least 15 bits of user-supplied data
- **Simple idea: use tag value to address individual threads**
  - → (+) straightforward to implement
  - → (+) very large number of threads per process addressable
  - → (-) not possible to further differentiate the messages
  - → (-) no information about the sending thread retained

Addressing in Hybrid Programs

- **Tags as thread IDs**
  - → Each MPI message carries a tag with at least 15 bits of user-supplied data
- **Better idea: multiplex destination thread ID with tag value**
  - → e.g. 7 bits for tag value (0..127) and 8 bits for thread ID (0..255)
  - → (+) still possible to differentiate the messages
  - → (-) wildcard receives not trivial to implement
  - → (-) no information about the sending thread retained

Addressing in Hybrid Programs

- **Tags as thread IDs**
  - → Each MPI message carries a tag with at least 15 bits of user-supplied data
- **Even better idea: multiplex source and destination thread IDs with tag value**
  - → suitable for MPI implementations that allow more than 15 bits for tag value
    - → Open MPI and Intel MPI both allow tag values from 0 to 2^{31}-1
  - → (+) still possible to differentiate the messages
  - → (+) information about the sending thread retained
  - → (-) wildcard receives not trivial to implement
  - → (-) not portable to MPI implementations with smaller tag space

Addressing in Hybrid Programs

- **Multiplex source and destination thread IDs with tag value**

```
#define MAKE_TAG (tag,stid,dtid) \
    (((tag) << 16) | ((stid) << 8) | (dtid))

// Send data to drank:dtid with tag mytag

MPI_Send(data, count, MPI_FLOAT, drank,
         MAKE_TAG(mytag, omp_get_thread_num(), dtid),
         MPI_COMM_WORLD);

-------------------------------------------------------

// Receive data from srank:stid with a specific tag mytag

MPI_Recv(data, count, MPI_FLOAT, srank,
         MAKE_TAG(mytag, stid, omp_get_thread_num()),
         MPI_COMM_WORLD, MPI_STATUS_IGNORE);
```

Addressing in Hybrid Programs

- **Multiplex source and destination thread IDs with tag value**

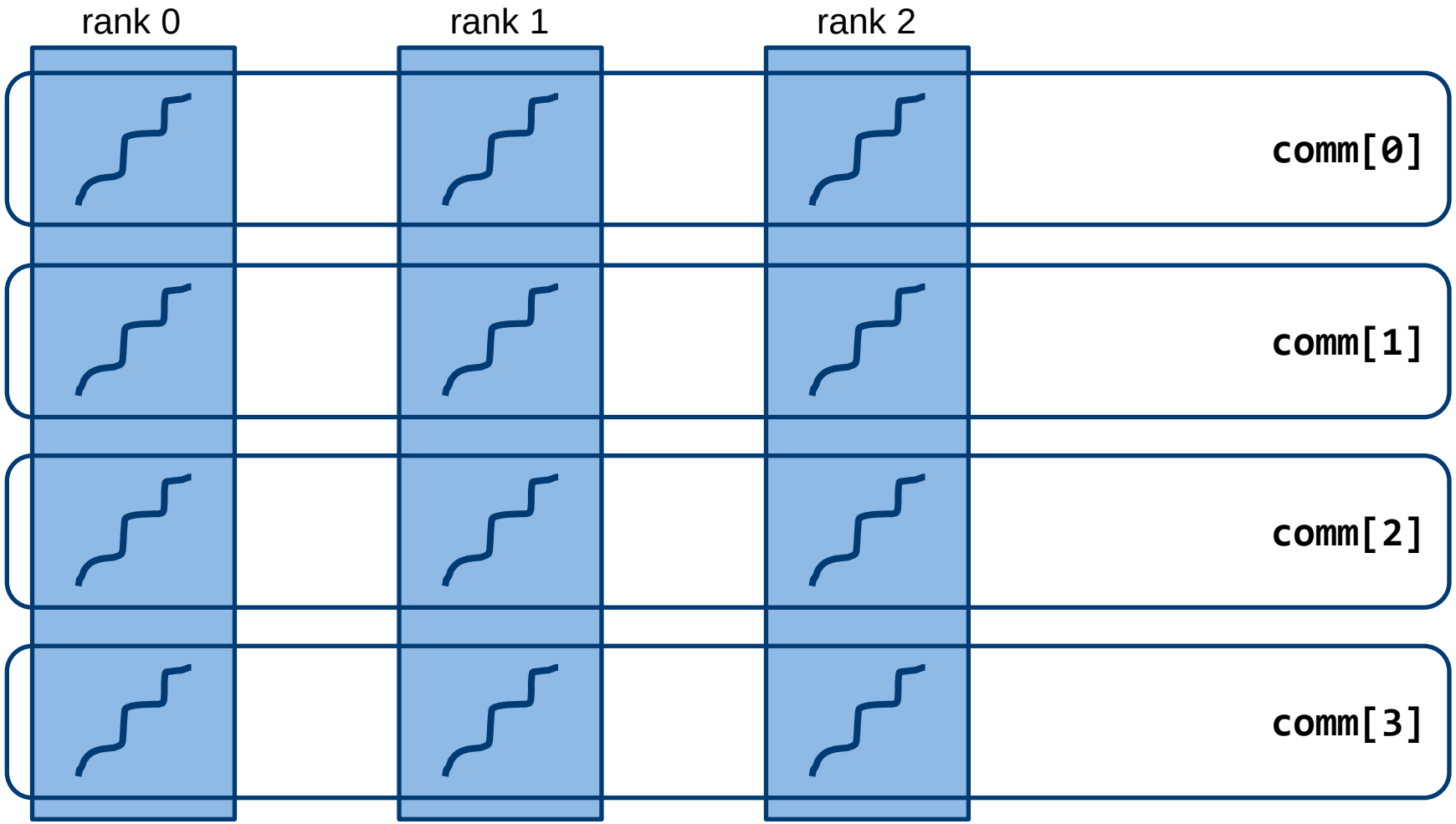
```
#define GET_TAG(val) \
    ((val) >> 16)
#define GET_SRC_TID(val) \
    (((val) >> 8) & 0xff)
#define GET_DST_TID(val) \
    ((val) & 0xff)

// Wildcard receive from srank:stid with any tag

MPI_Probe(srank, MPI_ANY_TAG, MPI_COMM_WORLD, &status);
if (GET_SRC_TID(status.MPI_TAG) == stid &&
    GET_DST_TID(status.MPI_TAG) == omp_get_thread_num())
{
    MPI_Recv(data, count, MPI_FLOAT, srank, status.MPI_TAG,
             MPI_COMM_WORLD, MPI_STATUS_IGNORE);
}
```

Addressing in Hybrid Programs

- **An alternative is the use of multiple communicators**



Addressing in Hybrid Programs

- **Multiple communicators**

```
MPI_Init_thread(NULL, NULL, MPI_THREAD_MULTIPLE, &provided);
MPI_Comm comm[nthreads], tcomm;
#pragma omp parallel private(tcomm) num_threads(nthreads)
{
   MPI_Comm_dup(MPI_COMM_WORLD, &comm[omp_get_thread_num()]);
   tcomm = comm[omp_get_thread_num()];
-------------------------------------------------------------
   // Sender
   MPI_Send(data, count, MPI_FLOAT, omp_get_thread_num(),
            drank, comms[dtid]);
-------------------------------------------------------------
   // Receiver
   MPI_Recv(data, count, MPI_FLOAT, stid, srank, tcomm,
            &status);
-------------------------------------------------------------
   MPI_Comm_free(&comm[omp_get_thread_num()]);
}
```

MPI Thread Support @ RWTH Cluster

- **Both official MPI libraries support threads:**

requested	Open MPI	Open MPI mt	Intel MPI w/o -mt_mpi	Intel MPI w/ -mt_mpi
SINGLE	SINGLE	SINGLE	SINGLE	SINGLE
FUNNELED	SINGLE	FUNNELED	SINGLE	FUNNELED
SERIALIZED	SINGLE	SERIALIZED	SINGLE	SERIALIZED
MULTIPLE	SINGLE	MULTIPLE	SINGLE	MULTIPLE

- **Open MPI**
  - → Switch to an MT version, e.g. **module switch openmpi openmpi/1.6.5mt**
  - → The InifiniBand BTL does not support **MPI_THREAD_MULTIPLE**!!!
- **Intel MPI**
  - → Compile with **-openmp**, **-parallel** or **-mt_mpi**

Hybrid Jobs @ RWTH Cluster

- **Sample hybrid job for Open MPI**

```
#!/usr/bin/env zsh
# 16 MPI procs x 6 threads = 96 cores
#BSUB -x
#BSUB -a openmpi
#BSUB -n 16
# 12 cores/node / 6 threads = 2 processes per node
#BSUB -R “span[ptile=2]”

module switch openmpi openmpi/1.6.5mt
# 6 threads per process
# Pass OMP_NUM_THREADS on to all MPI processes
$MPIEXEC $FLAGS_MPI_BATCH -x OMP_NUM_THREADS=6 \
         program.exe <args>
```

Hybrid Jobs @ RWTH Cluster

- **Sample hybrid job for Intel MPI**

```
#!/usr/bin/env zsh
# 16 MPI procs x 6 threads = 96 cores
#BSUB -x
#BSUB -a intelmpi
#BSUB -n 16
# 12 cores/node / 6 threads = 2 processes per node
#BSUB -R “span[ptile=2]”

module switch openmpi intelmpi
# 6 threads per process
# Pass OMP_NUM_THREADS on to all MPI processes
$MPIEXEC $FLAGS_MPI_BATCH –genv OMP_NUM_THREADS 6 \
         program.exe <args>
```

Caveats

- **Beware of possible data races:**
  - → messages, matched by **MPI_Probe** in one thread, can be received by a matching receive in another thread, stealing the message from the first one
  - → Problem solved in MPI-3 with **MPI_Mprobe** (see MPI documentation)
- **MPI provides no way to address specific threads in a process**
  - → clever use of message tags
  - → clever use of many communicators
  - → MPI-4 will (hopefully) provide a better solution – MPI Endpoints
- **In general, thread-safe MPI implementations perform worse than non-thread-safe because of the added synchronisation overhead**
- **Don’t use Open MPI on our cluster if full thread support is required!**

?

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- **Part 3**
  - → Hybrid parallelisation
  - → Common parallel patterns

No parallel program can outrun the sum of its sequential parts!

Keep this in mind for the rest of your (parallel) life!

Amdahl's Law in Theory

- **The run time of a program consists of two parts:**
  - → serial (non-parallelisable) part: T_s
  - → parallelisable part: T_p
  - → total execution time: $T = T_s + T_p$
  - → serial share: $s = T_s / T$

- **An n-fold parallelisation yields:**
  - → total execution time: $T_n = T_s + T_p / n$
  - → parallel speedup: $S_n = T / T_n = n / [1 + (n-1).s]$
  - → parallel efficiency: $E_n = T / (n.T_n) = 1 / [1 + (n-1).s]$

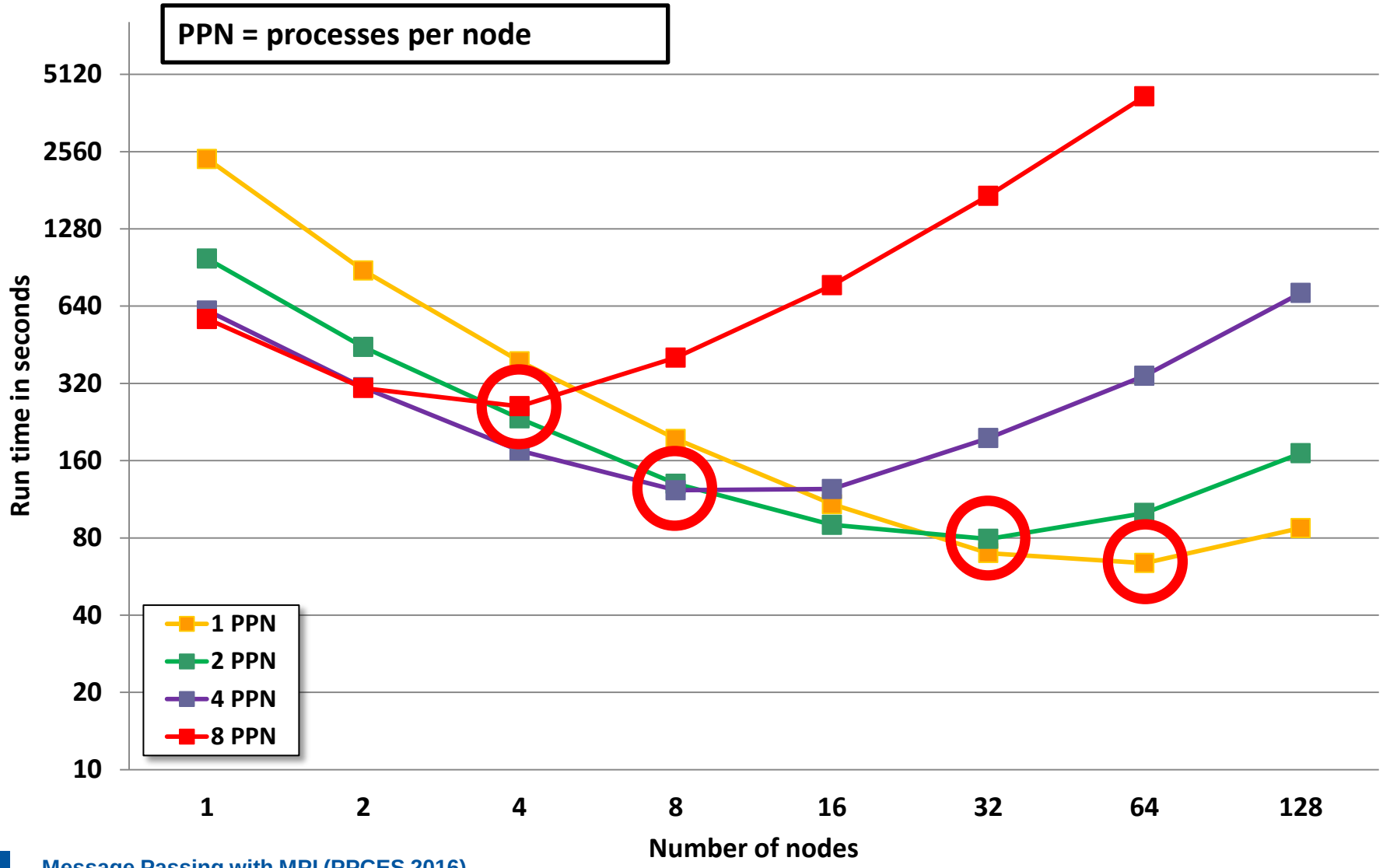
- **Asymptotic values in the limit of infinite number of processors:**
  - → total execution time: $T_\infty = T_s + T_p / \infty = T_s$
  - → parallel speedup: $S_\infty = T / T_\infty = T / T_s = 1 / s$
  - → parallel efficiency: $E_\infty = 1$ if $s = 0$; $E_\infty = 0$ otherwise

Amdahl's Law – The Ugly Truth™

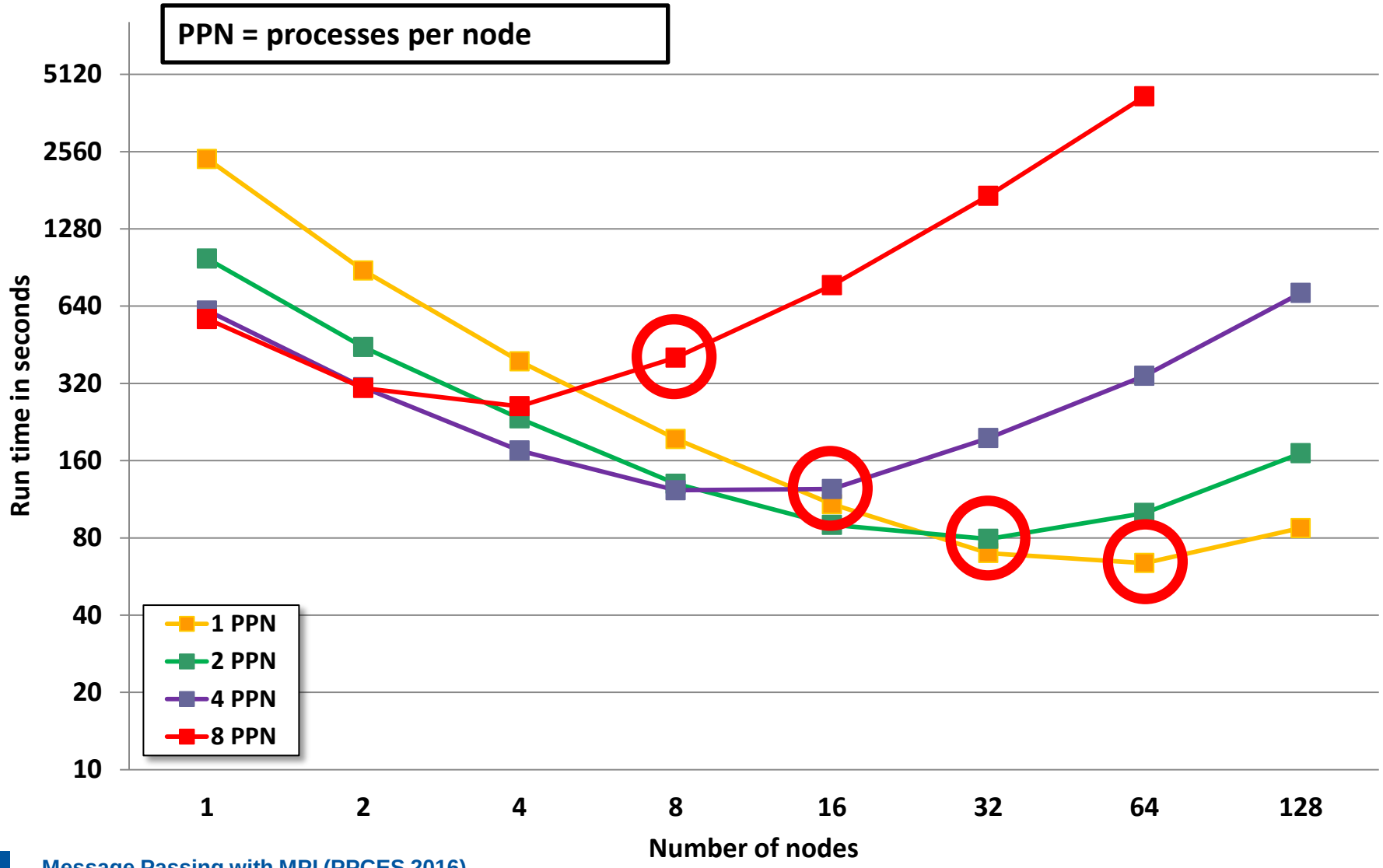
- **Parallelisation usually (if not always) introduces overhead:**
  - → communication is inherently serial → *s* increases
  - → usually $E_n < 1$ – you use more CPU time than if you run the serial program
  - → but sometimes cache effects result in $E_n > 1$ – superlinear speedup

- **Communication overhead increases with the number of processes:**
  - → more processes → more messages (depends on the communication pattern) especially true for the collective operations
    (you didn't re-implement them, did you?)
  - → more messages → more network latency → more serial time
  - → more serial time → lower parallel efficiency
  - → with large process counts the overhead could negate the parallelisation gain

Amdahl's Law – The Ugly Truth™



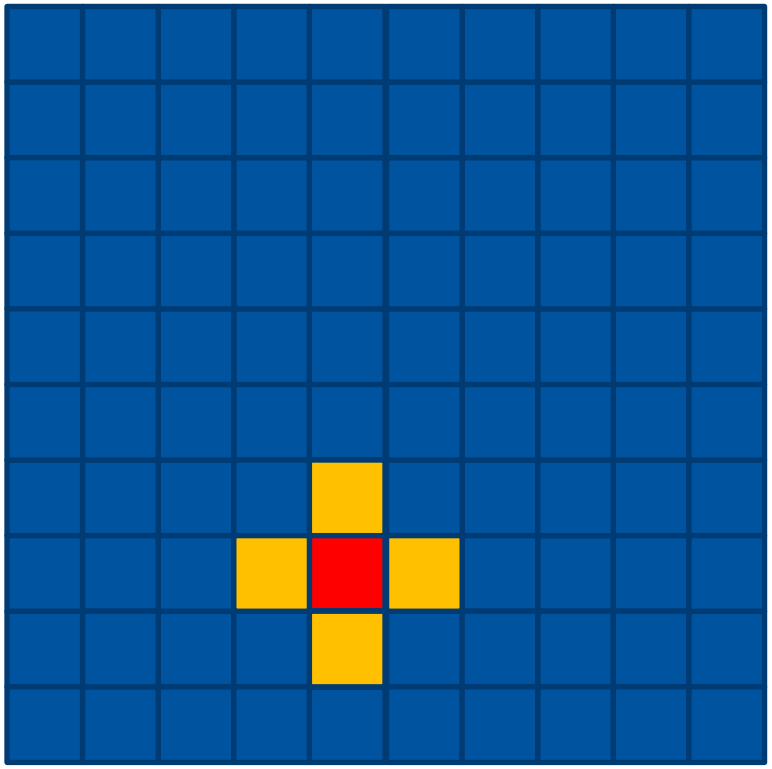
Amdahl's Law – The Ugly Truth™



Halos / Ghost Cells

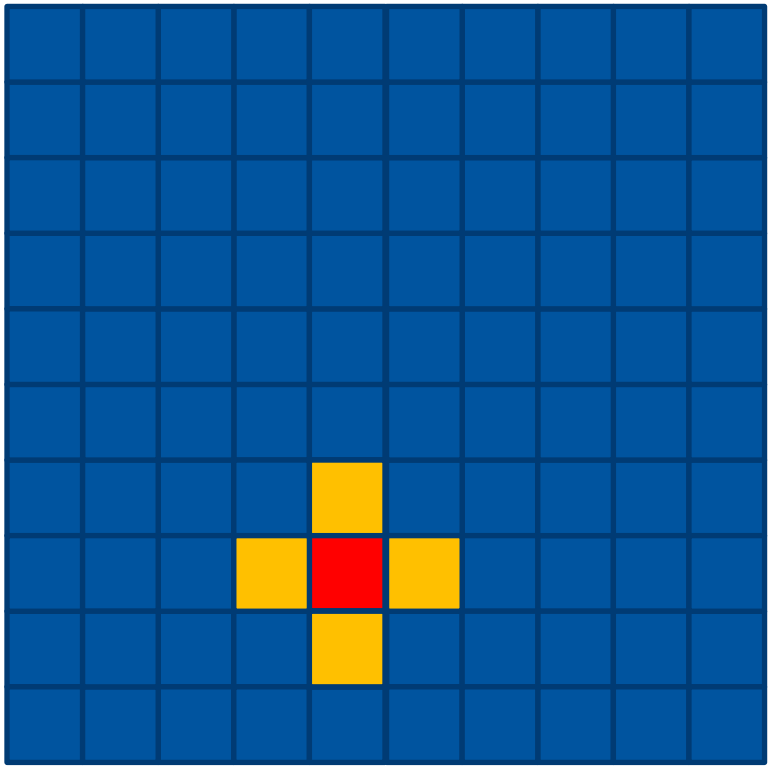
- **When decomposing a problem often interdependent data ends up in separate processes.**
- **Example: iterative matrix update in a PDE solver:**

$$cell_{i,j} = f\left(cell_{i,j}; cell_{i-1,j}, cell_{i+1,j}, cell_{i,j-1}, cell_{i,j+1}\right)$$



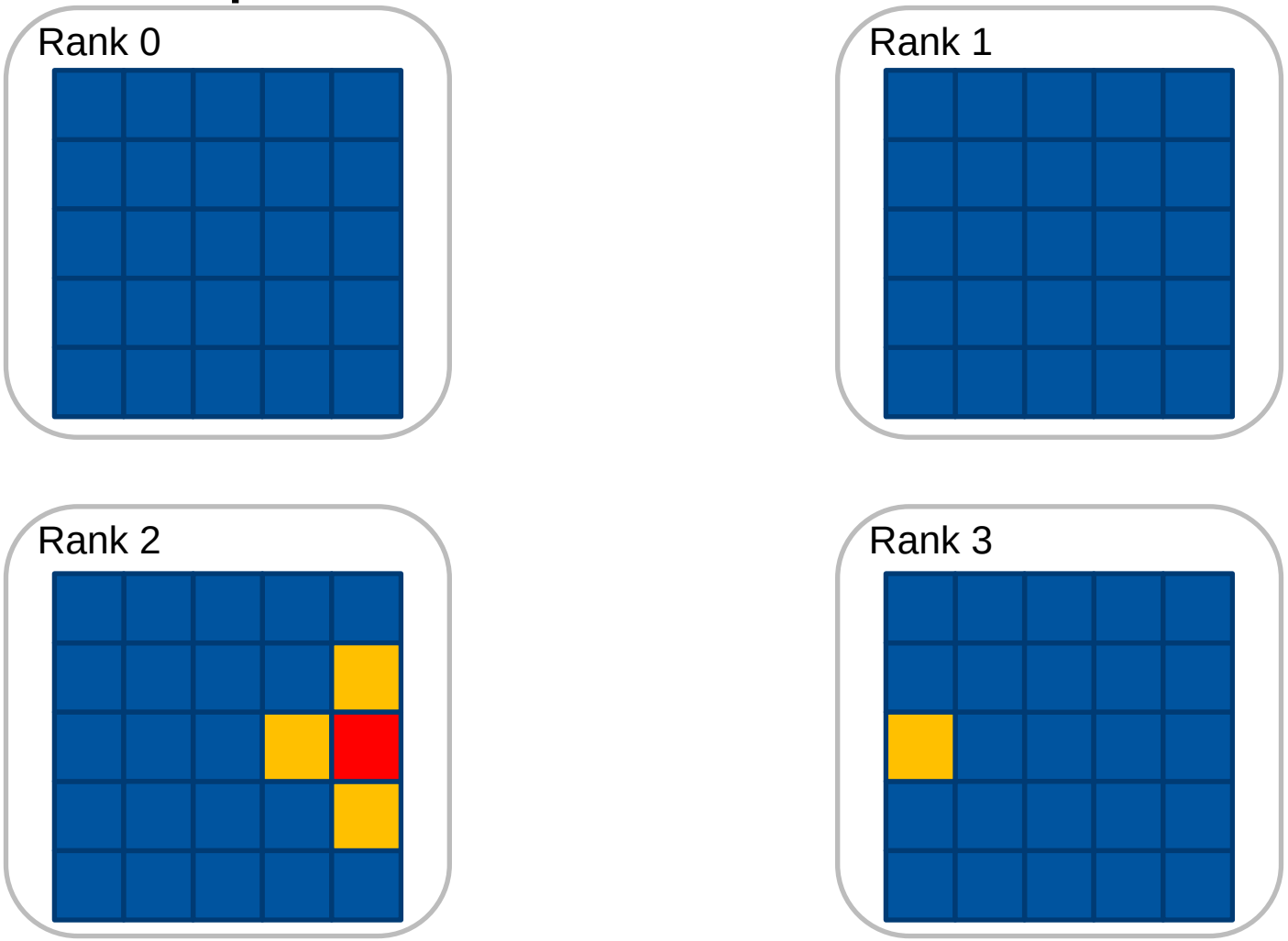
Halos / Ghost Cells

- **Domain decomposition strategy:**
  - → Partition the domain into parts.
  - → Each process works on one part only.



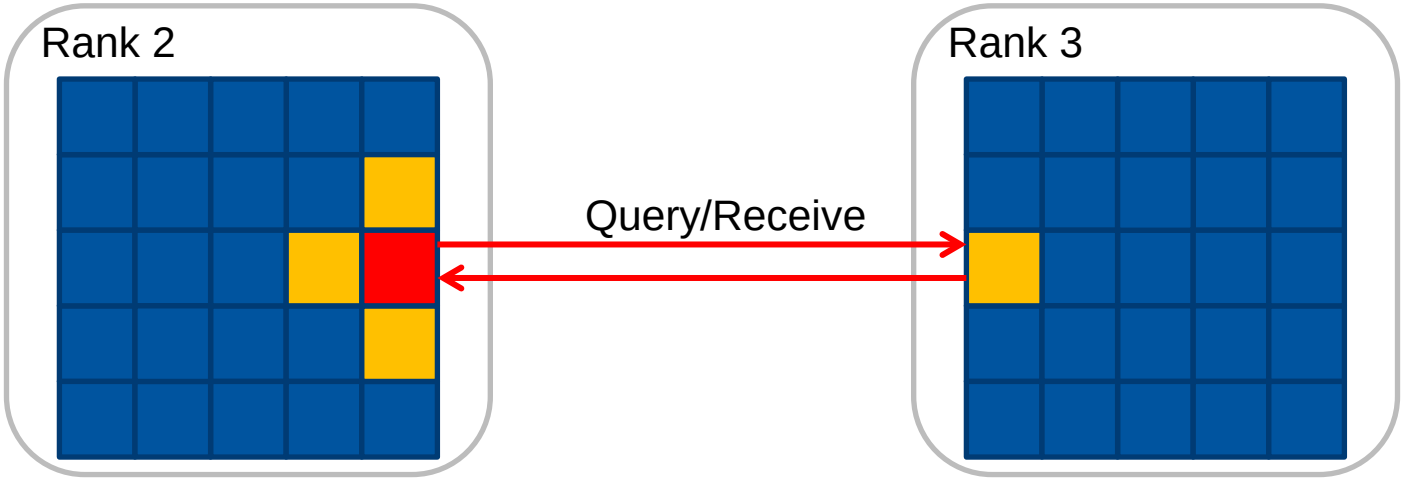
Halos / Ghost Cells

- **Domain decomposition**



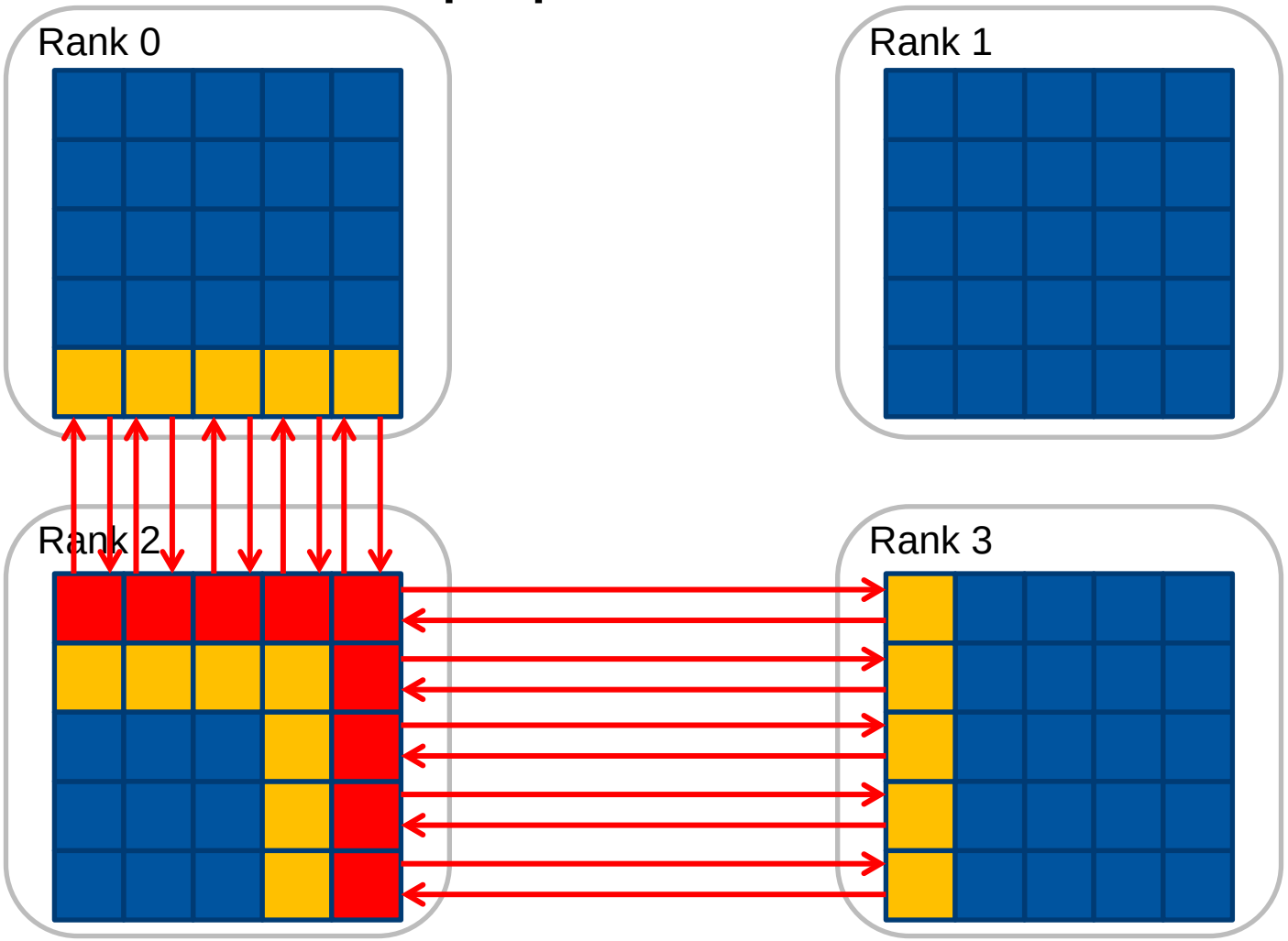
Halos / Ghost Cells

- **Communication**
  - → For every border cell communication with a neighbour rank is needed
- **Problems:**
  - → Introduces synchronisation on a very fine level
  - → Lots of communication calls – highly inefficient
  - → Performance can (and will) drastically suffer



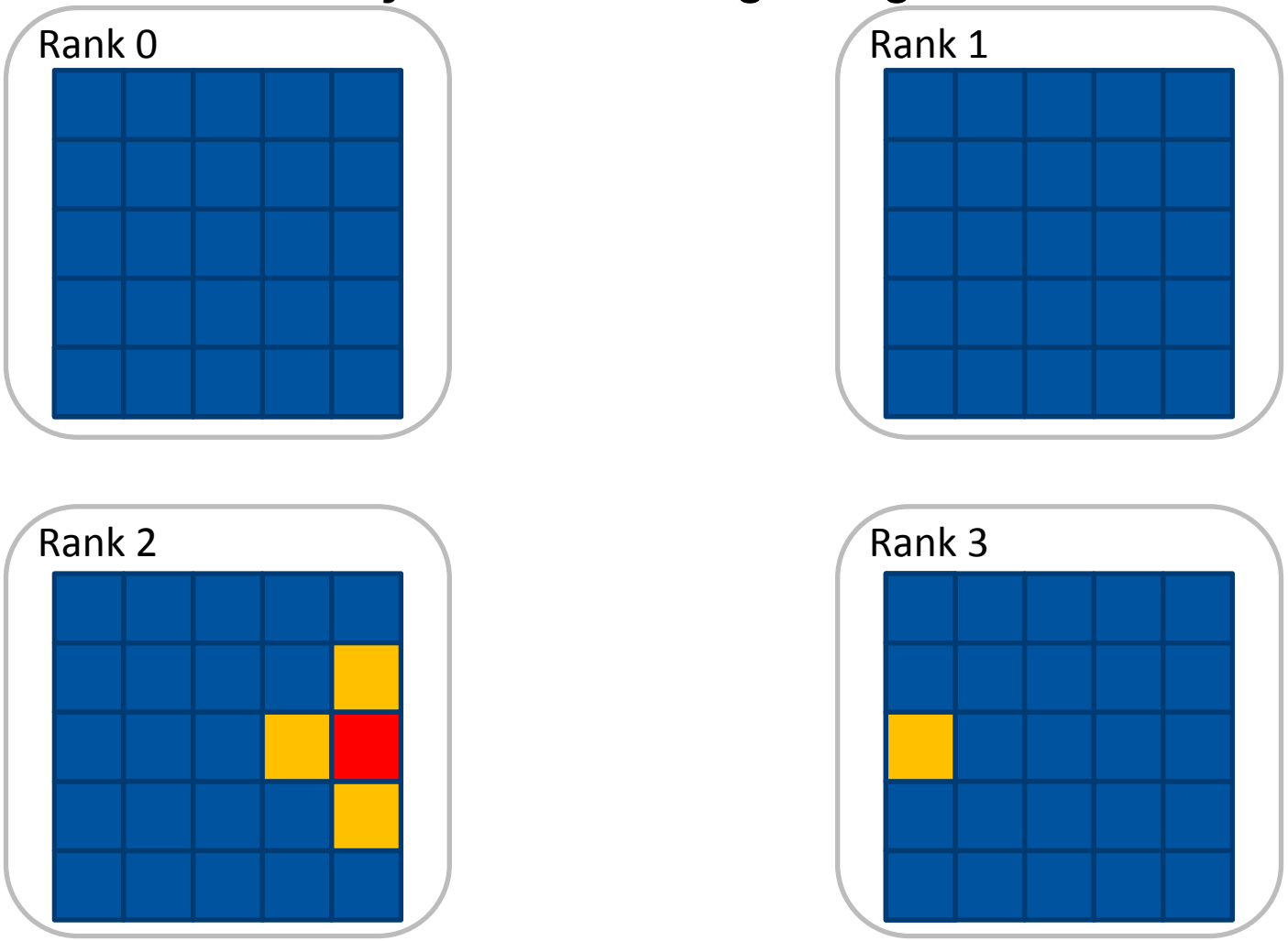
Halos / Ghost Cells

- **10 communication calls per process**



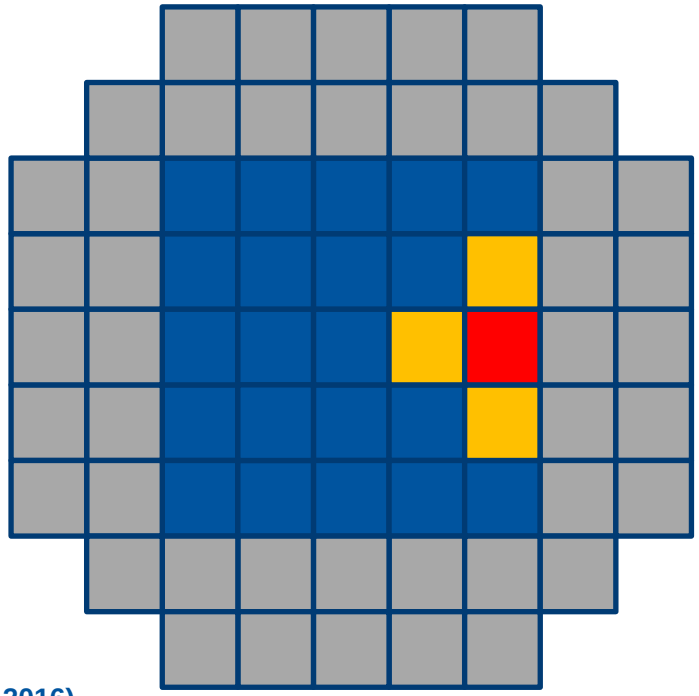
Halos / Ghost Cells

- **Copy all the necessary data at the beginning of each iteration**



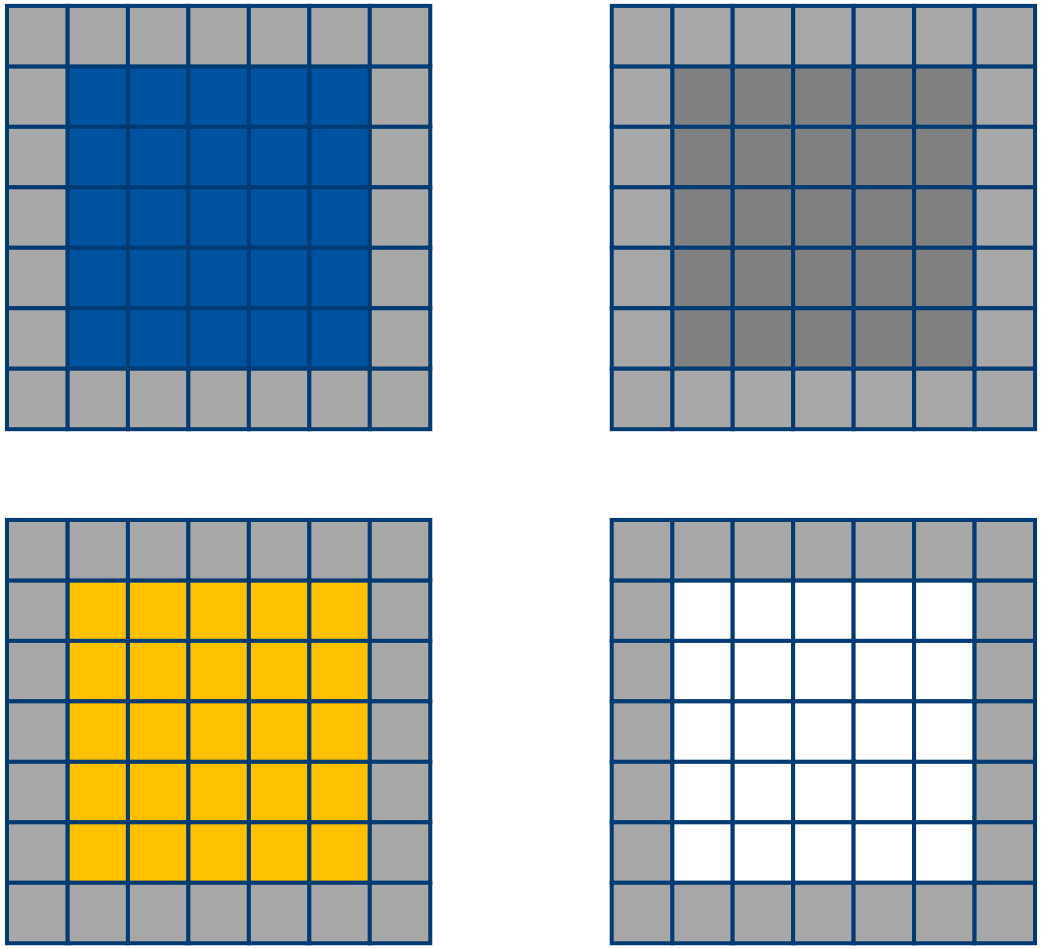
Halos / Ghost Cells

- **Copies around the host domain are called *halos* or *ghost cells***
- **Multi-level halos are also possible:**
  - → if required by the stencil
  - → to reduce the number of communications



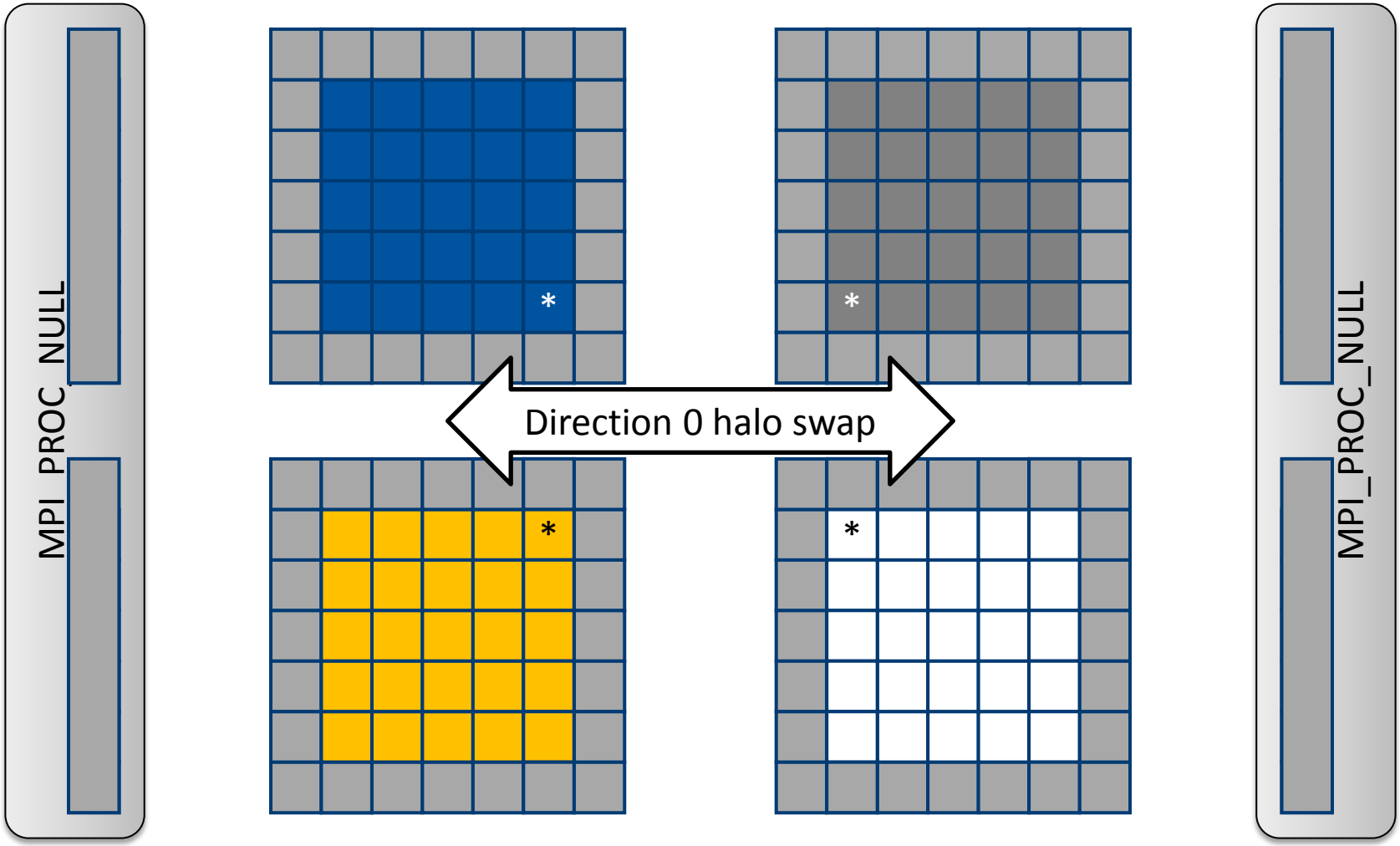
Halos / Ghost Cells

- **Halo Swap**



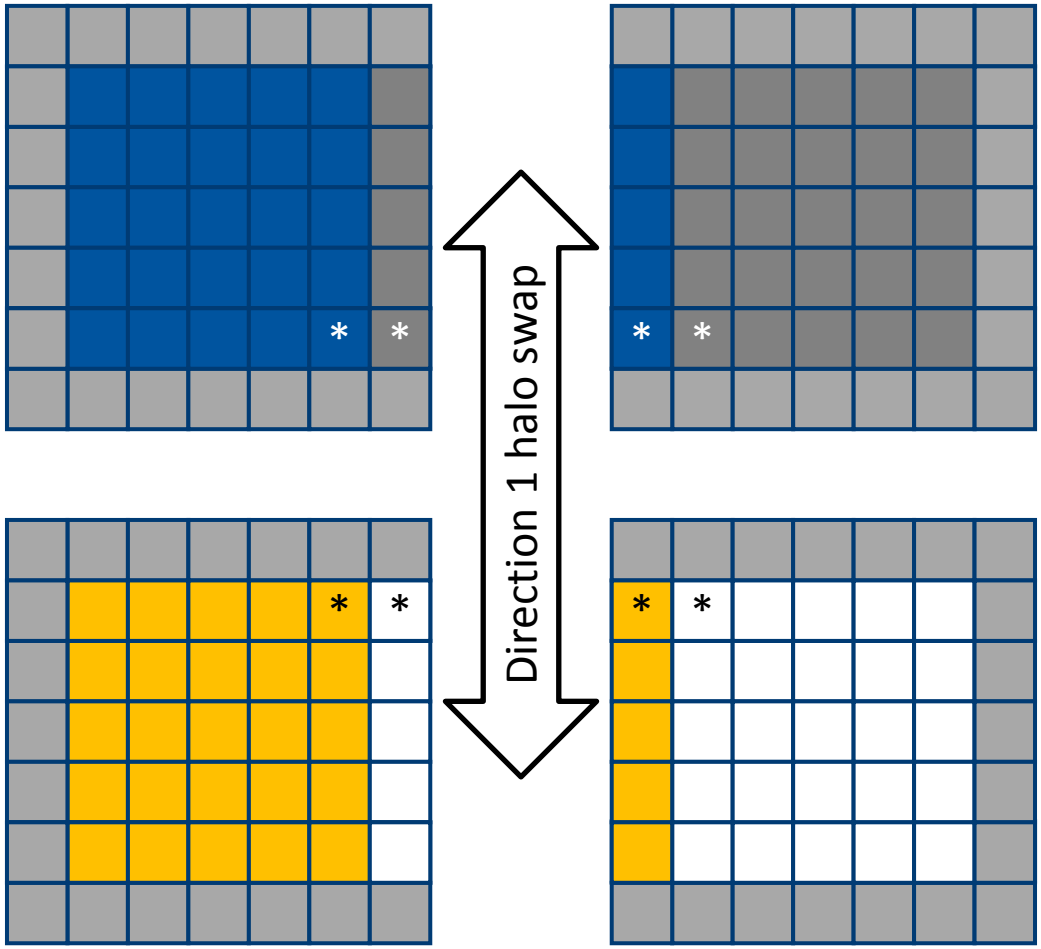
Halos / Ghost Cells

- **Halo Swap**



Halos / Ghost Cells

- **Halo Swap**



Halos / Ghost Cells

- **Halo Swaps are locally synchronous, but combined they make a globally synchronous operation:**
  - → initial process synchronisation is critical for the performance
  - → one late process delays all the other processes
  - → sensitivity to OS jitter
- **Pros:**
  - → idea comes naturally
  - → simple to implement (two MPI send-receive calls per direction)
- **Cons:**
  - → not suitable for problems where load imbalance may occur

Irregular Problems

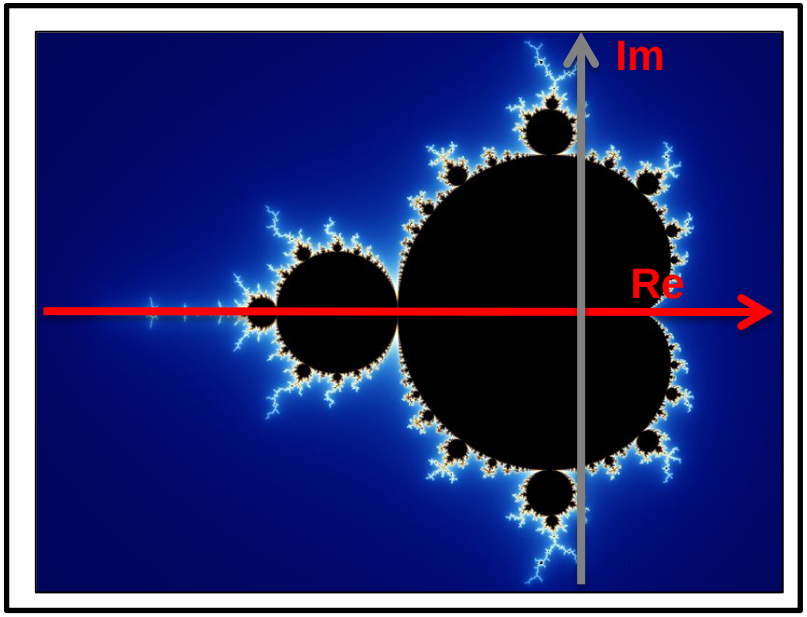
- **Escape time colouring algorithm for the Mandelbrot set**

```
For each image pixel (x, y):
// (x, y) – scaled pixel coords
c = x + i*y
z = 0
iteration = 0
maxIters = 1000
while (|z|² <= 2² &&
       iteration < maxIters)
{
   z = z² + c
   iteration = iteration + 1
}
if (iteration == maxIters)
   color = black
else
   color = iteration
plot(x, y, color)
```

Does the complex series

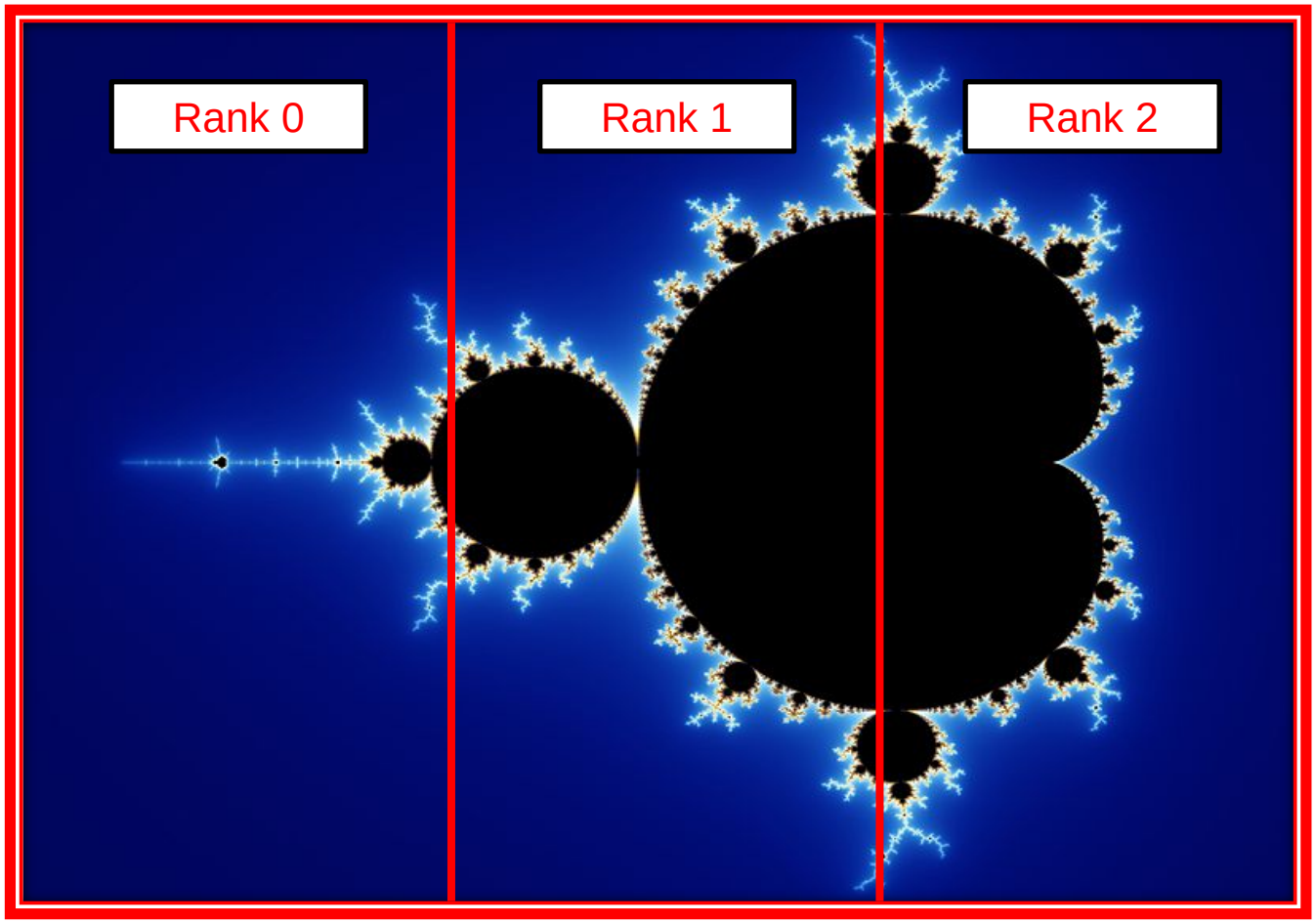
$$z_0 = 0;\ z_{n+1} = {z_n}^2 + c \quad z, c \in \mathbb{C}$$

remain bounded?



Irregular Problems

- **Static work distribution:**
  - → Every MPI rank works on 1/Nth of the problem (N – number of MPI ranks)



Irregular Problems

Mandelbrot set

```
For each image pixel (x, y):
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c = x + i*y
z = 0
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maxIters = 1000
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{
   z = z² + c
   iteration = iteration + 1
}
if (iteration == maxIters)
   color = black
else
   color = iteration
plot(x, y, color)
```
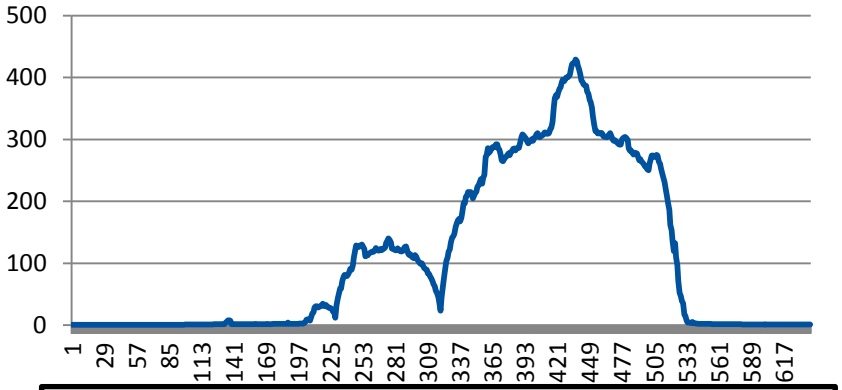
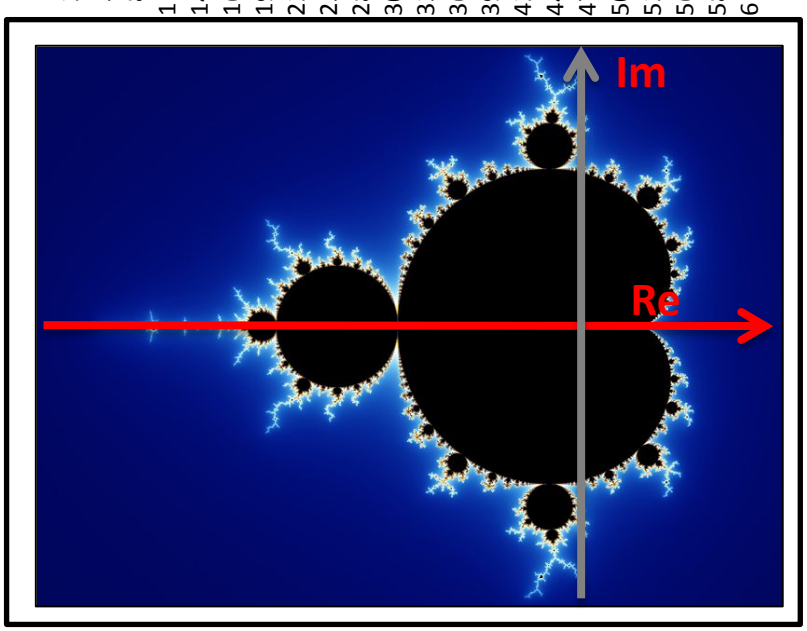
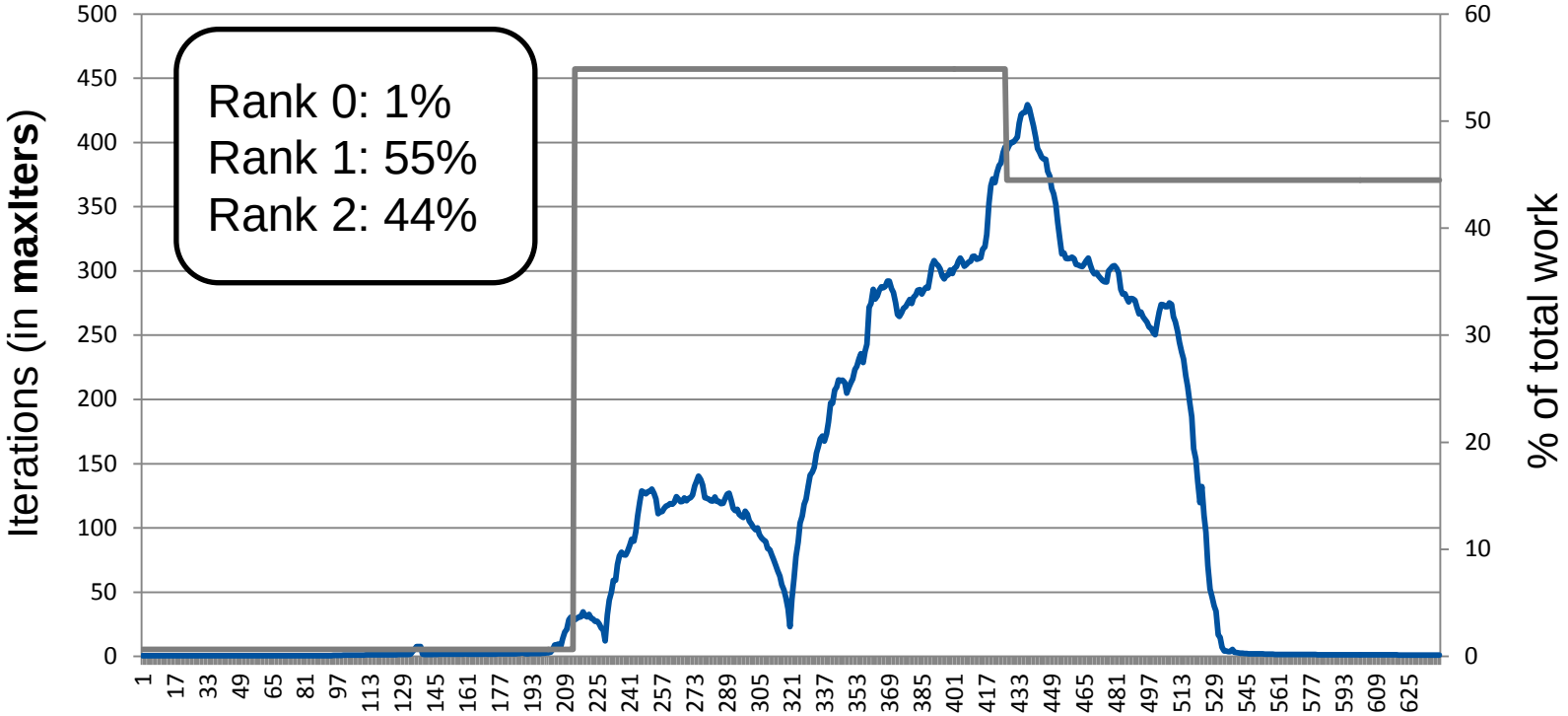

Iterations per image column (in **maxIters**)





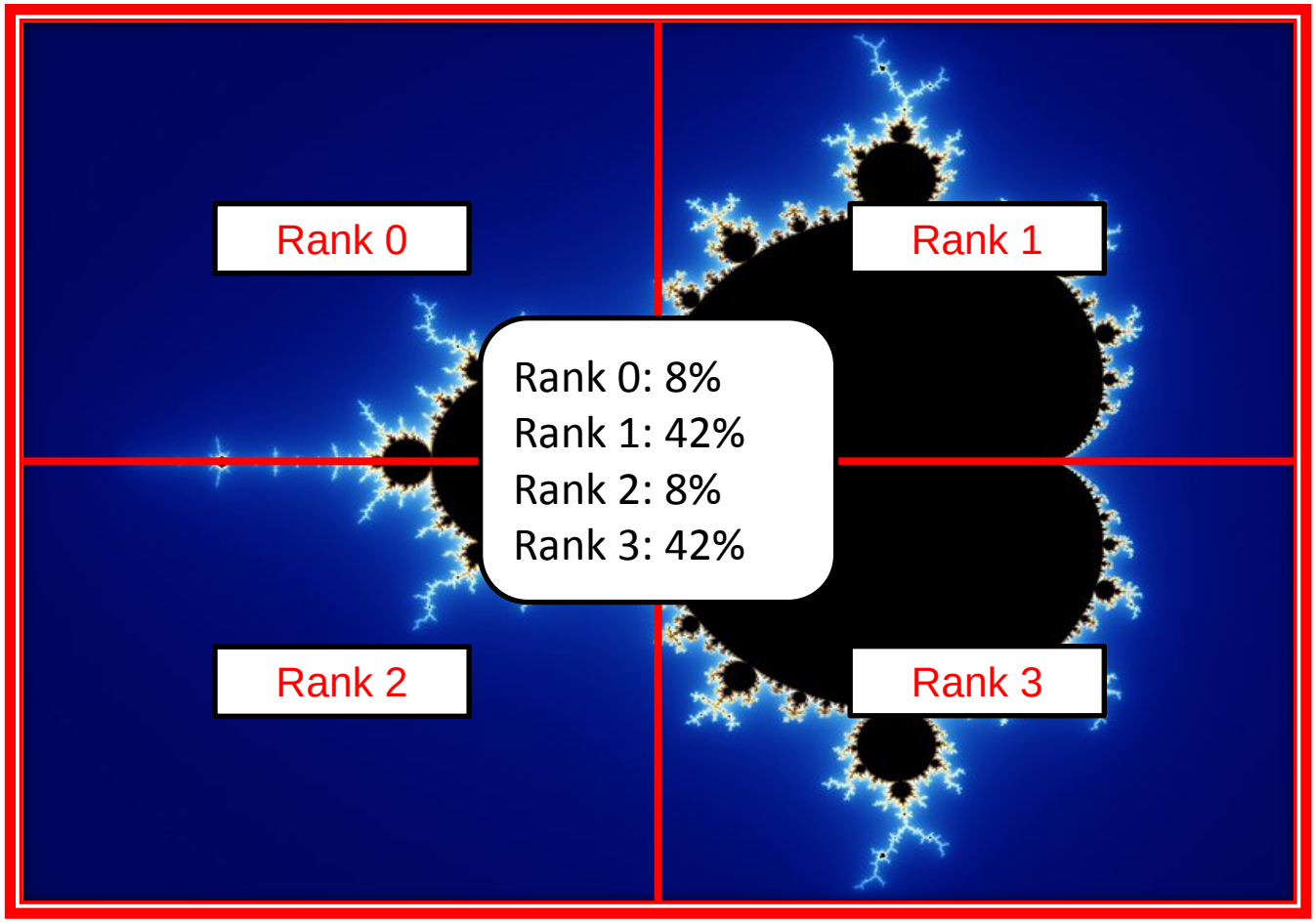
Work Imbalance

- **Computation complexity mapped to ranks**



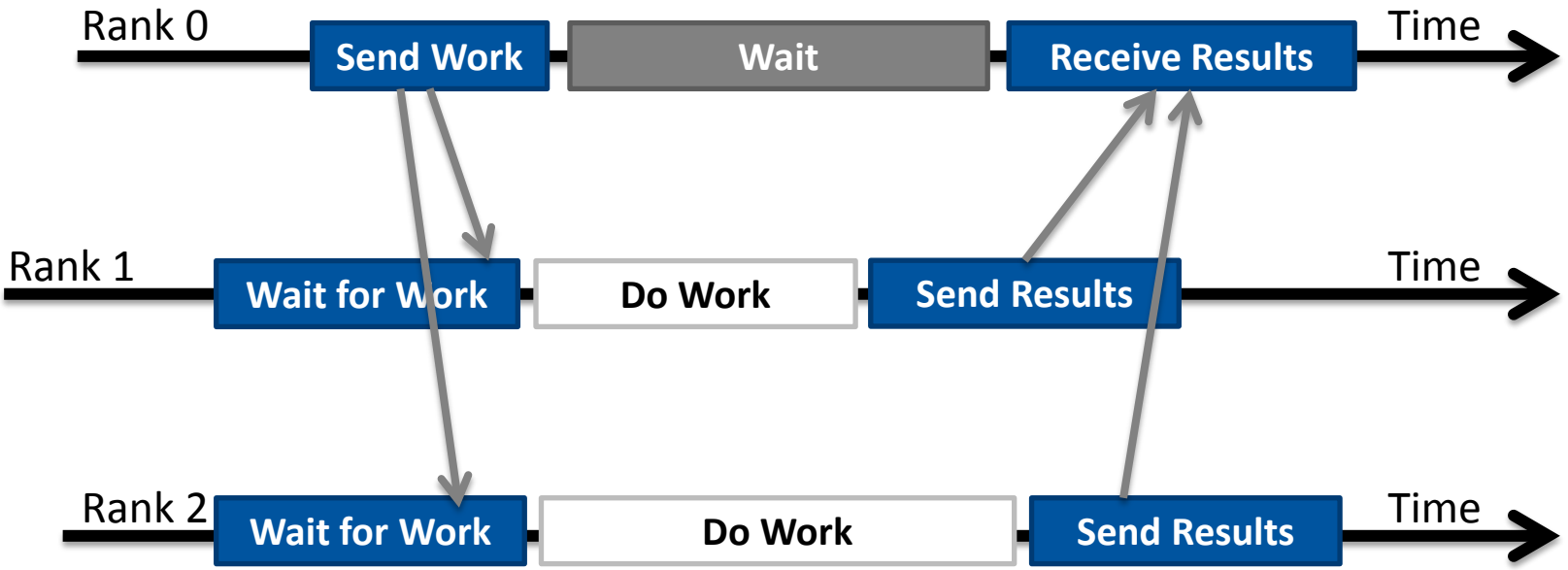
Work Imbalance

- **May be a different decomposition?**



Controller – Worker

- **One process (controller) manages the work**
  - → Work is split into many relatively small work items
- **Many other processes (workers) compute over the work items:**

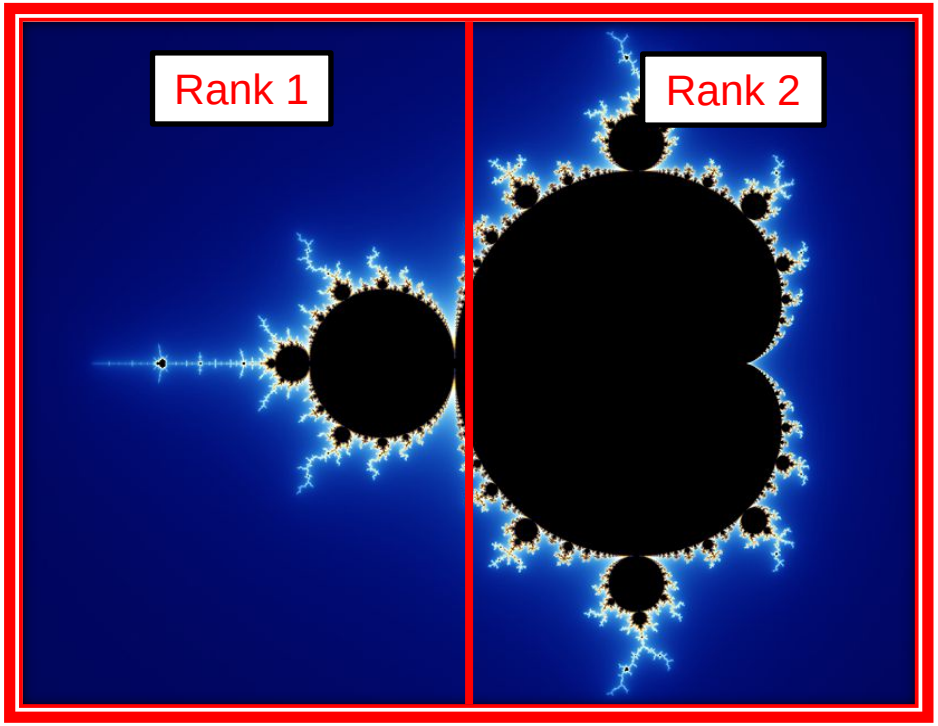


- **Above steps are repeated until all work items are processed**
- **Sometimes called “bag of jobs” pattern**

Controller – Worker

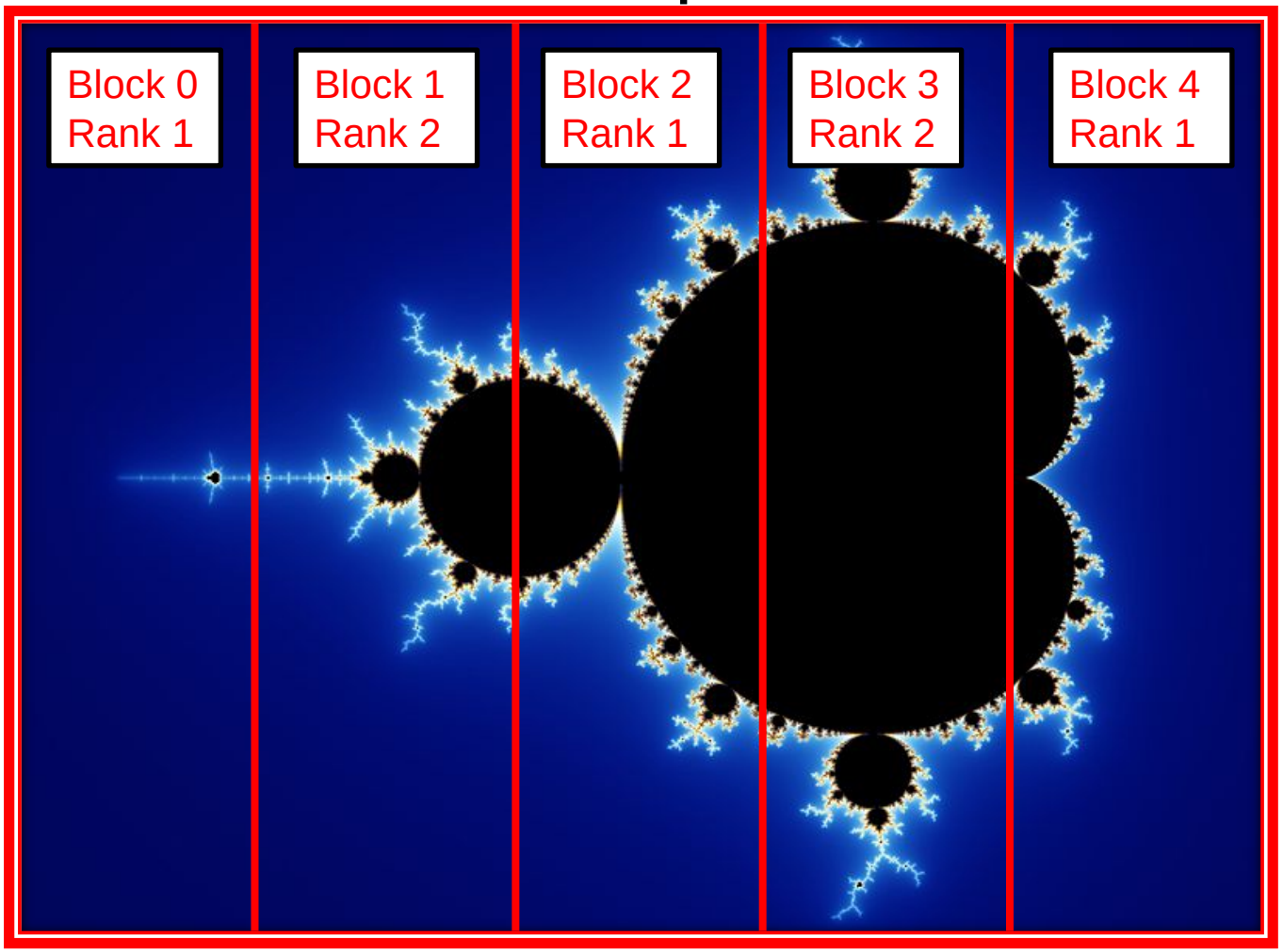
- **The algorithm:**

```
START
if (rank == 0)
{
   splitDomain;
   sendWorkItems;
   receiveItemResults;
   assembleResult;
   output;
}
else
{
   receiveWorkItems;
   processWorkItems;
   sendItemResults;
}
DONE
```



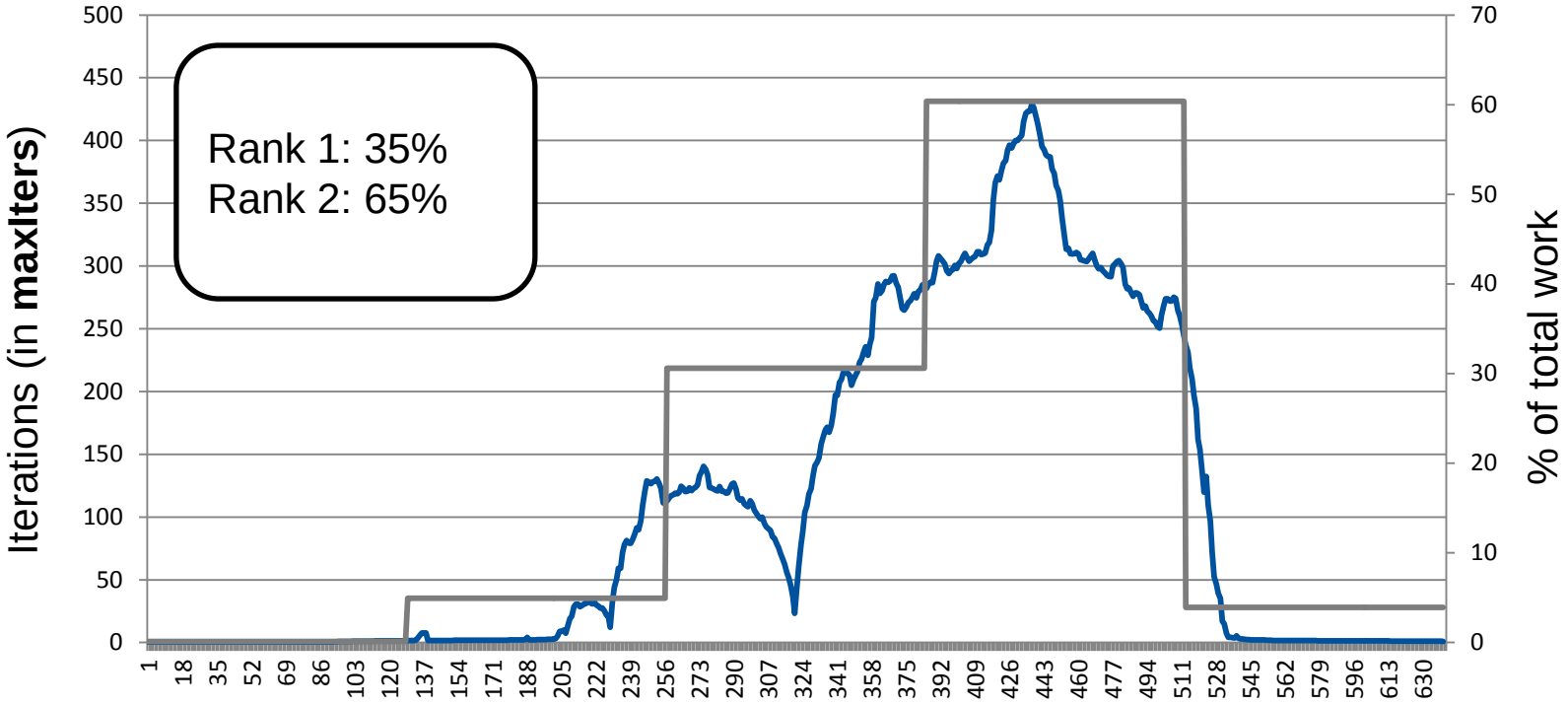
Controller – Worker

- **Controller – Worker with 3 worker processes**



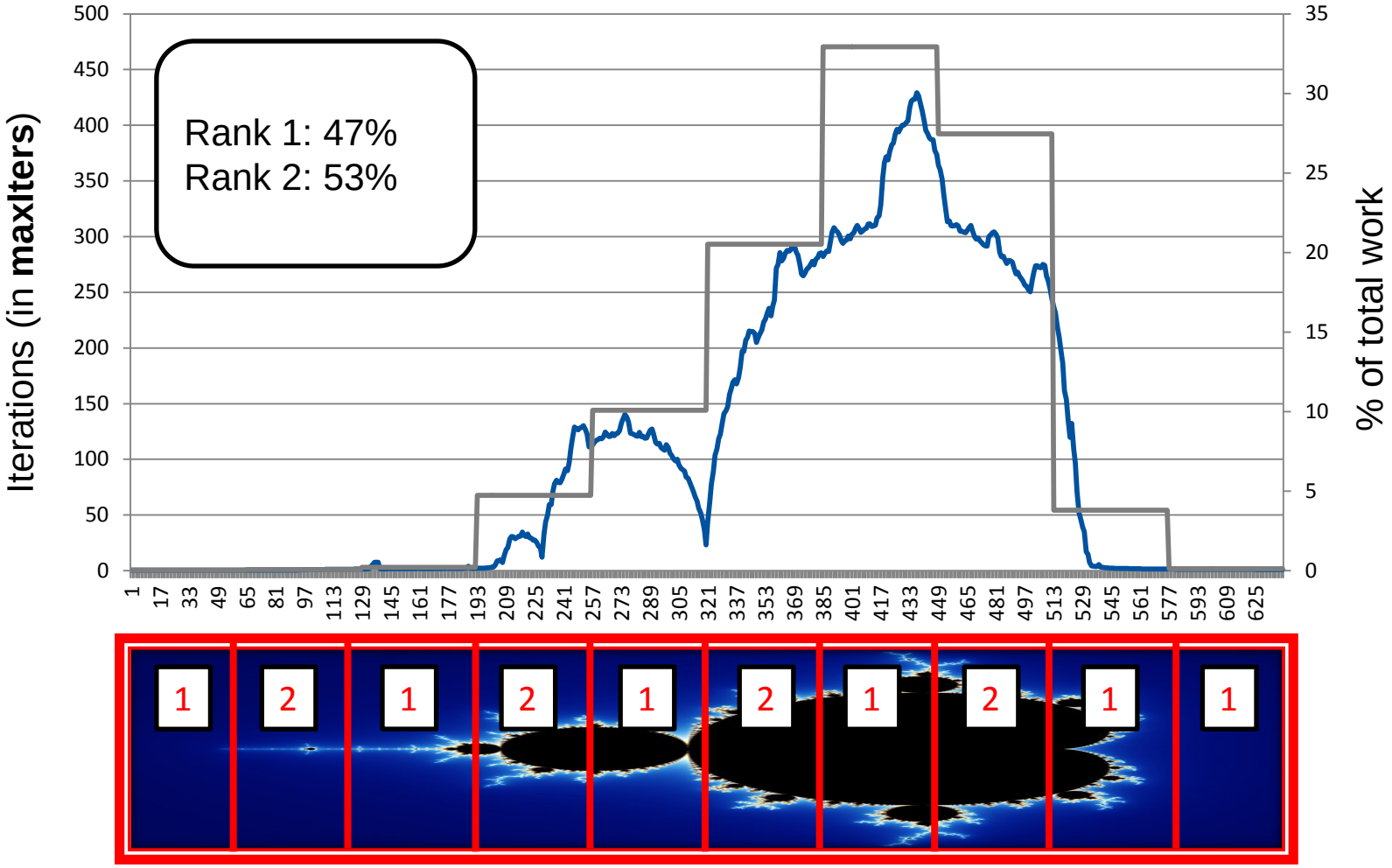
Work Balancing

- **Computational complexity mapped to ranks**



Work Balancing

- **Computational complexity mapped to ranks**



Work Balancing

- **Static work distribution:**
  - → Works best for regular problems
  - → Very simple to implement (e.g. nothing really to implement)
  - → Irregular problems result in work imbalance (e.g. Mandelbrot)
  - → Not usable for dynamic workspace problems (e.g. adaptive integration)

- **Controller – Worker approach:**
  - → Allows for great implementation flexibility
  - → Automatic work balancing if work units are properly sized
  - → Can be used for problems with dynamic workspaces
  - → Performs well on heterogeneous systems (e.g. CoWs)

Parallel Patterns

?

Now What?

- **Here is a list of important MPI topics not covered by this course:**
  - → Parallel I/O
  - → Neighbour (Sparse) Collectives (MPI-3 feature)
  - → Non-blocking Collectives (MPI-3 feature)

- **And a list of more exotic topics:**
  - → Dynamic process control
  - → Client/server relations
  - → One-sided operations (RMA)

Thank you for your attention!