

Advanced MPI

Hybrid programming, profiling and debugging of MPI applications

Hristo Iliev

RZ

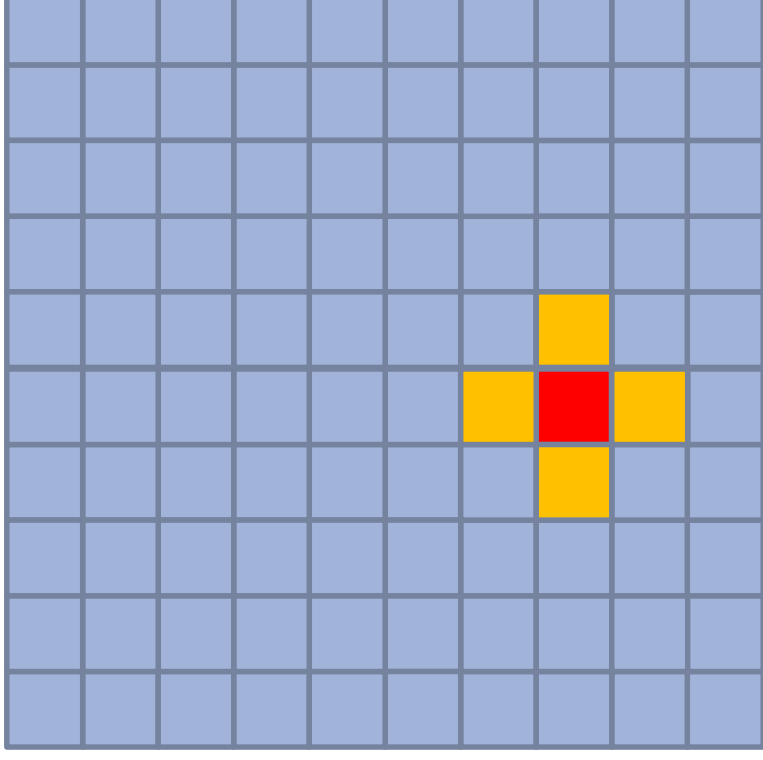
Agenda

- Halos (ghost cells)
- Hybrid programming
- Profiling of MPI applications
- Vampir
- Debugging of MPI applications
- TotalView
- ---
- Lab session

Halos (ghost cells)

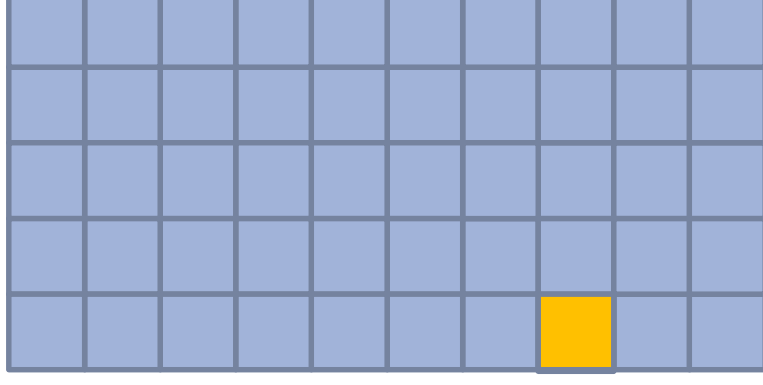
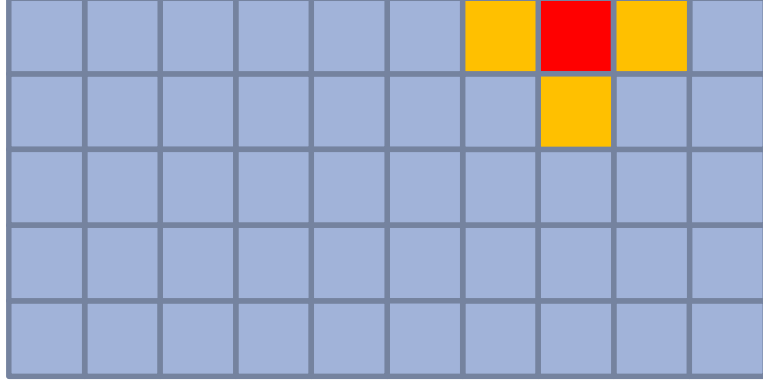
- Often as a result of domain decomposition interdependent data end in different processes

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



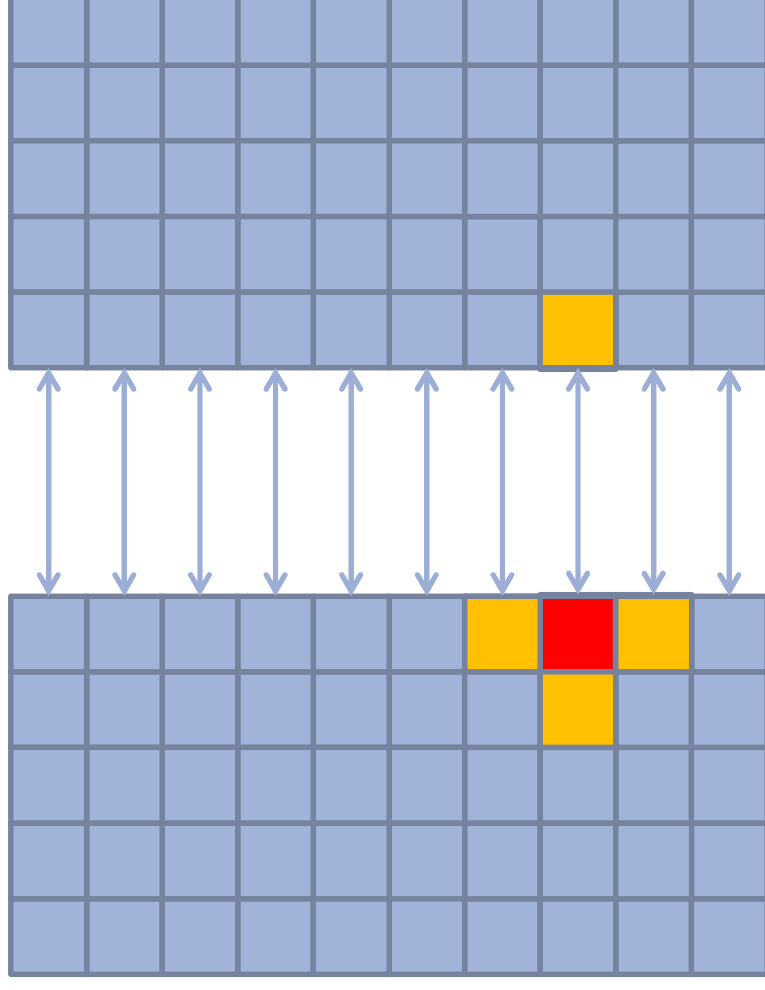
Halos (ghost cells)

- Often as a result of domain decomposition interdependent data end in different processes



- It makes no sense to request individually each neighbouring cell that one process needs to access

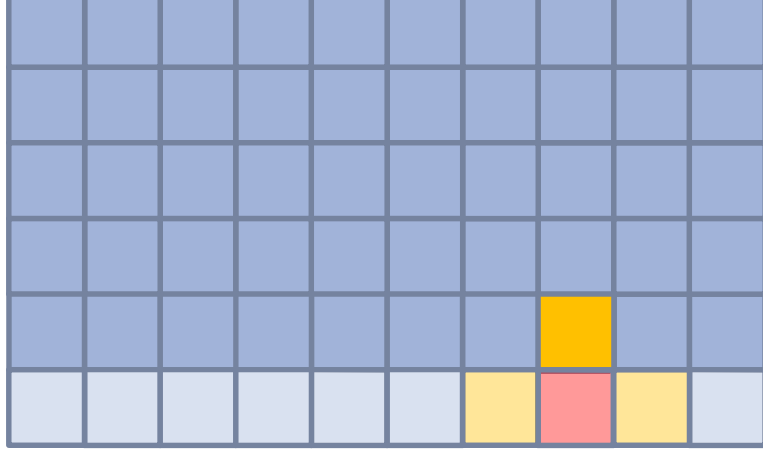
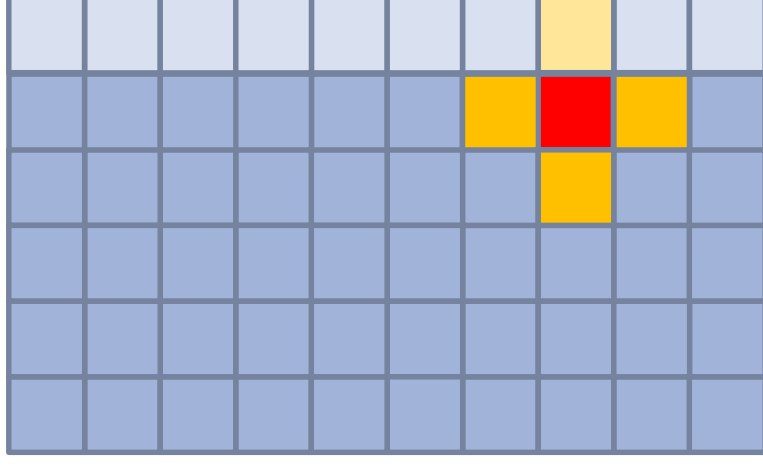
→ Better to transfer all cells in bulk, but where to store them?



Halos (ghost cells)

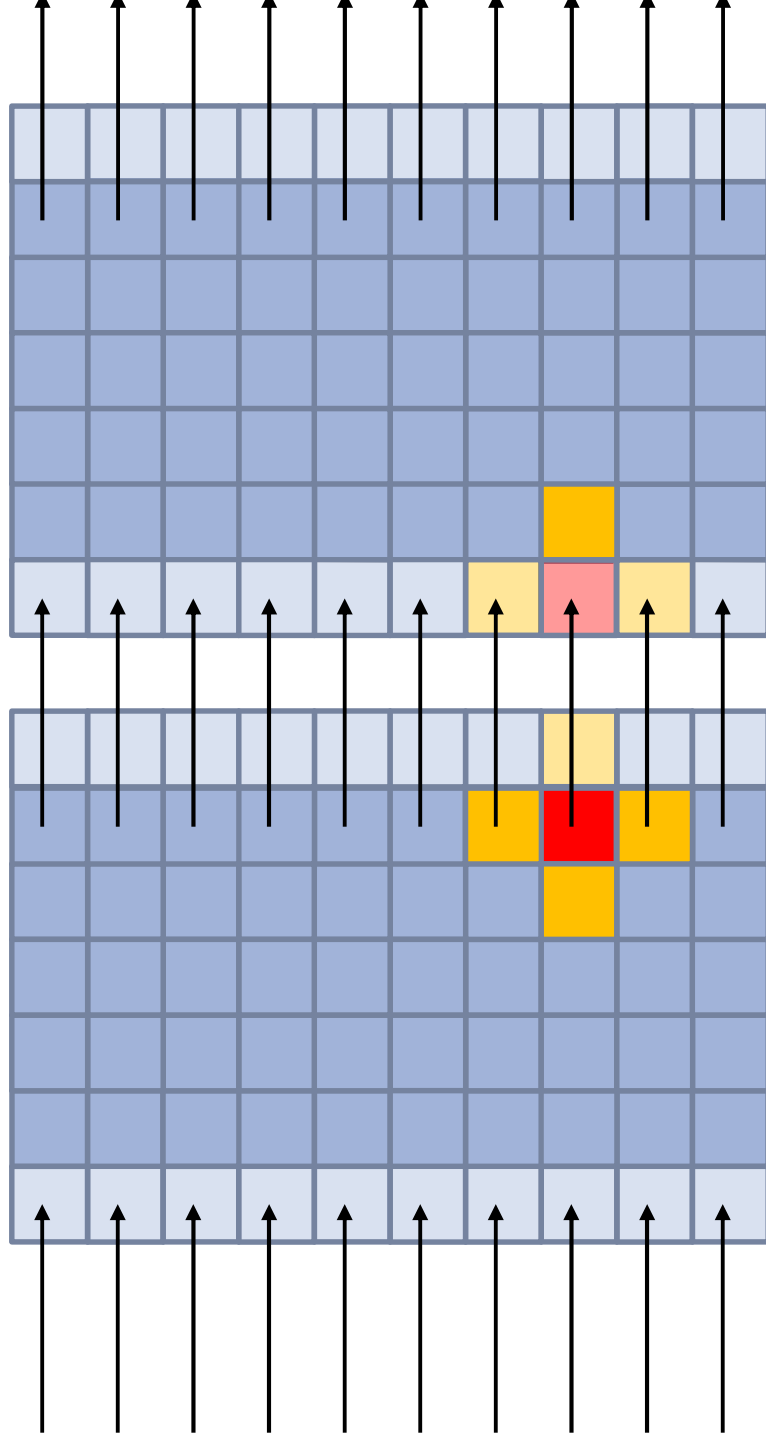
- Halos (ghost cells) are an additional layer of cells that duplicate the subset of neighbour cells that each iteration depends on

→ Not the real cells but temporary copies, hence “ghost” cells



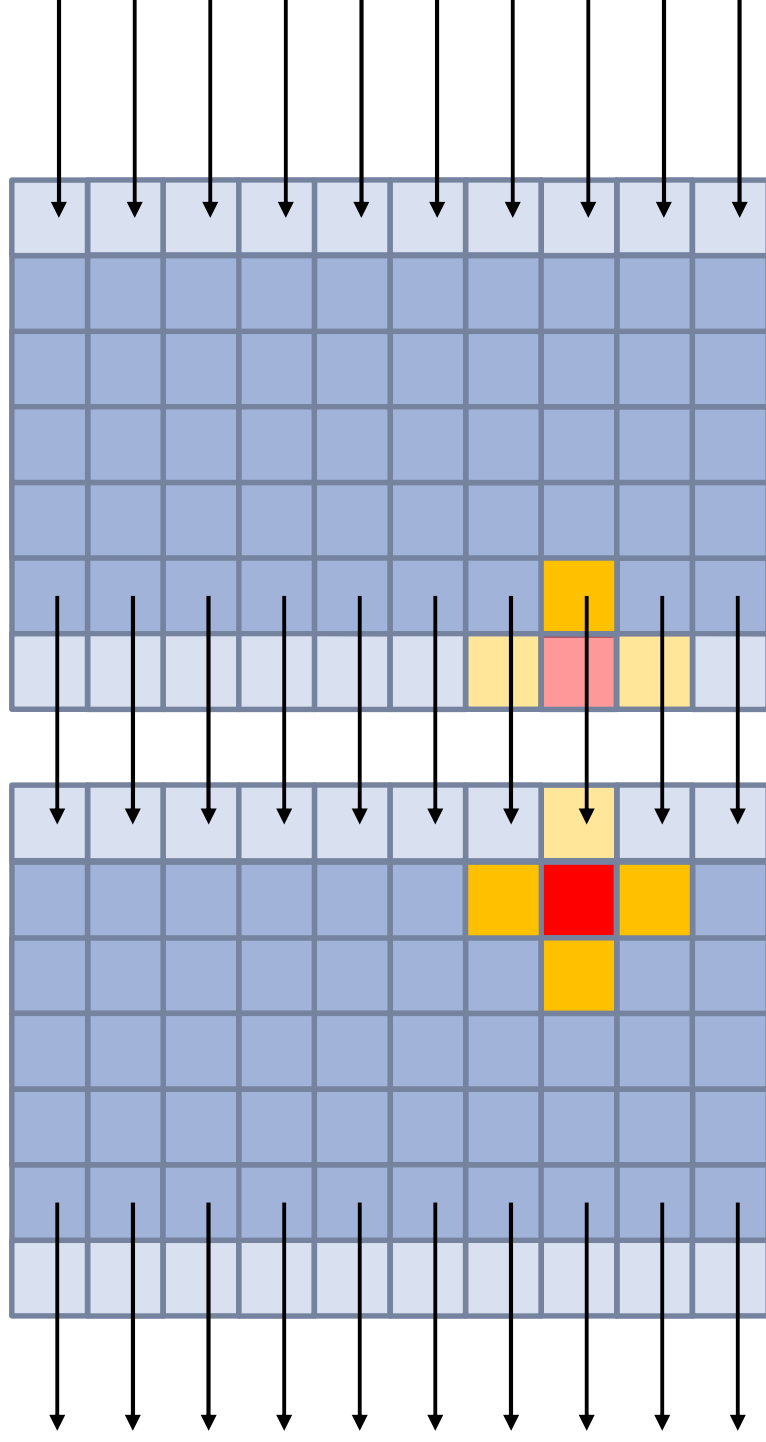
Halos (ghost cells)

- Halos are updated regularly using halo swap operations
 - ➔ Conveniently performed using two `MPI_SENDRECV` per dimension



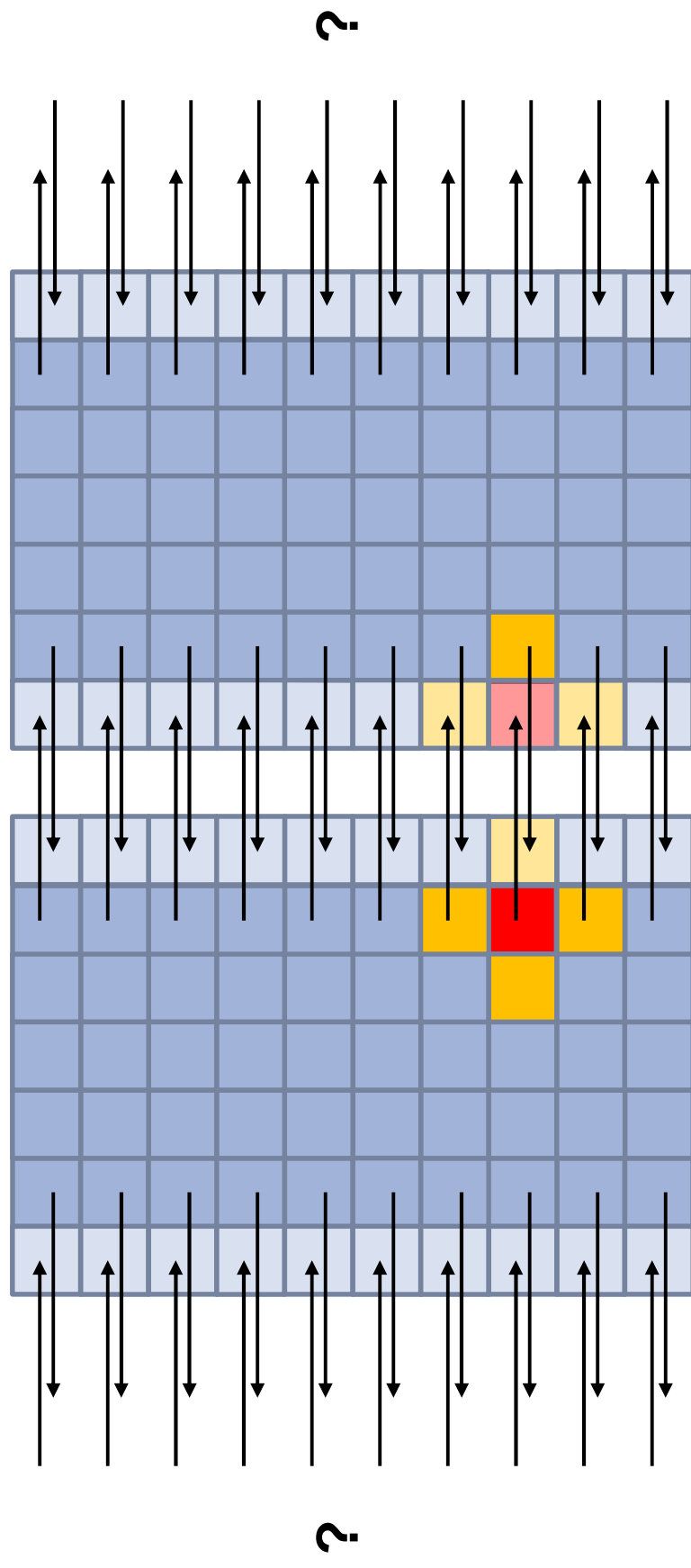
Halos (ghost cells)

- Halos are updated regularly using halo swap operations
 - Conveniently performed using two `MPI_SENDRECV` per dimension



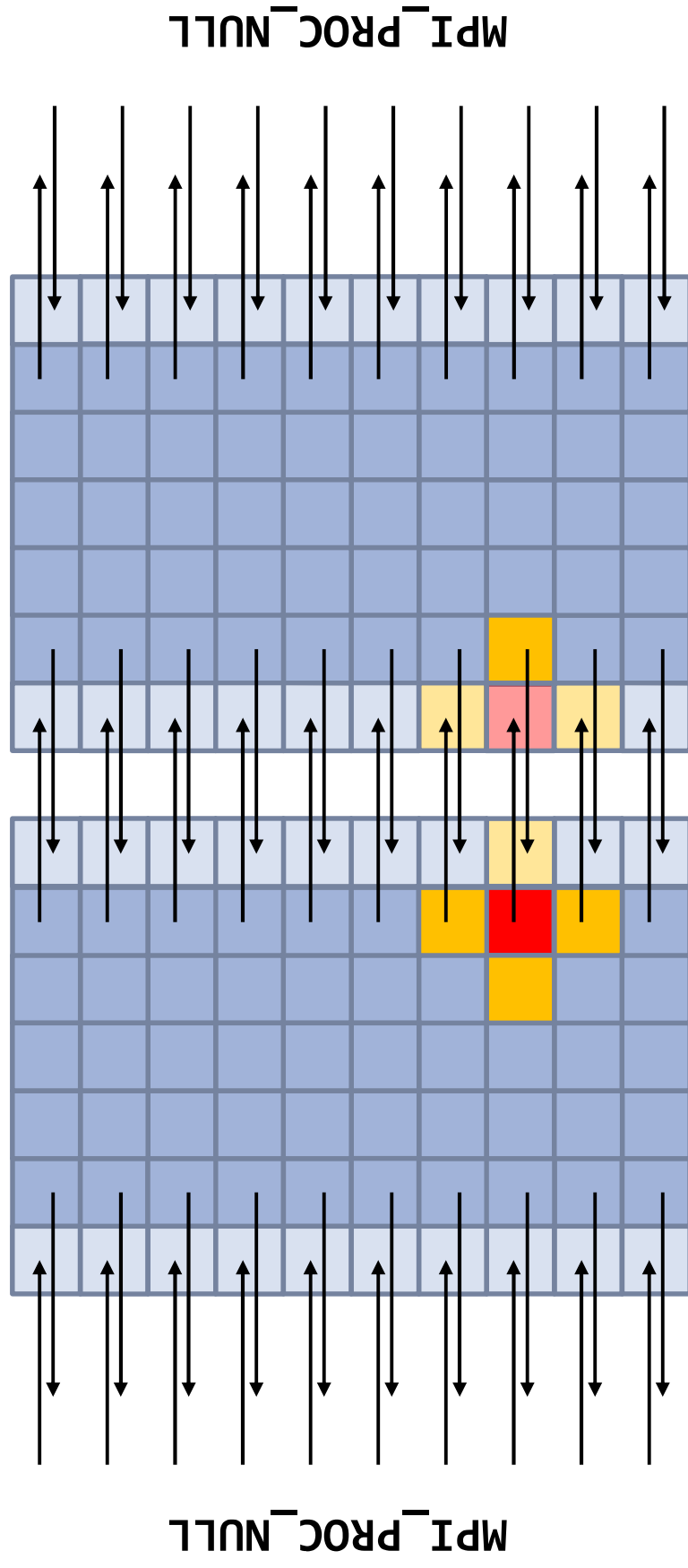
Halos (ghost cells)

- Halos are updated regularly using halo swap operations
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Halos (ghost cells)

- Halos are updated regularly using halo swap operations
 - Conveniently performed using two `MPI_SENDRECV` per dimension



Halos (ghost cells)

- **Could be performed in multiple dimensions**

- Independent swaps on each dimension
- Order is not important in most cases
- Diagonal elements in 2D-, 3D-, 4D-, etc. cases move automatically to their correct positions in the halos

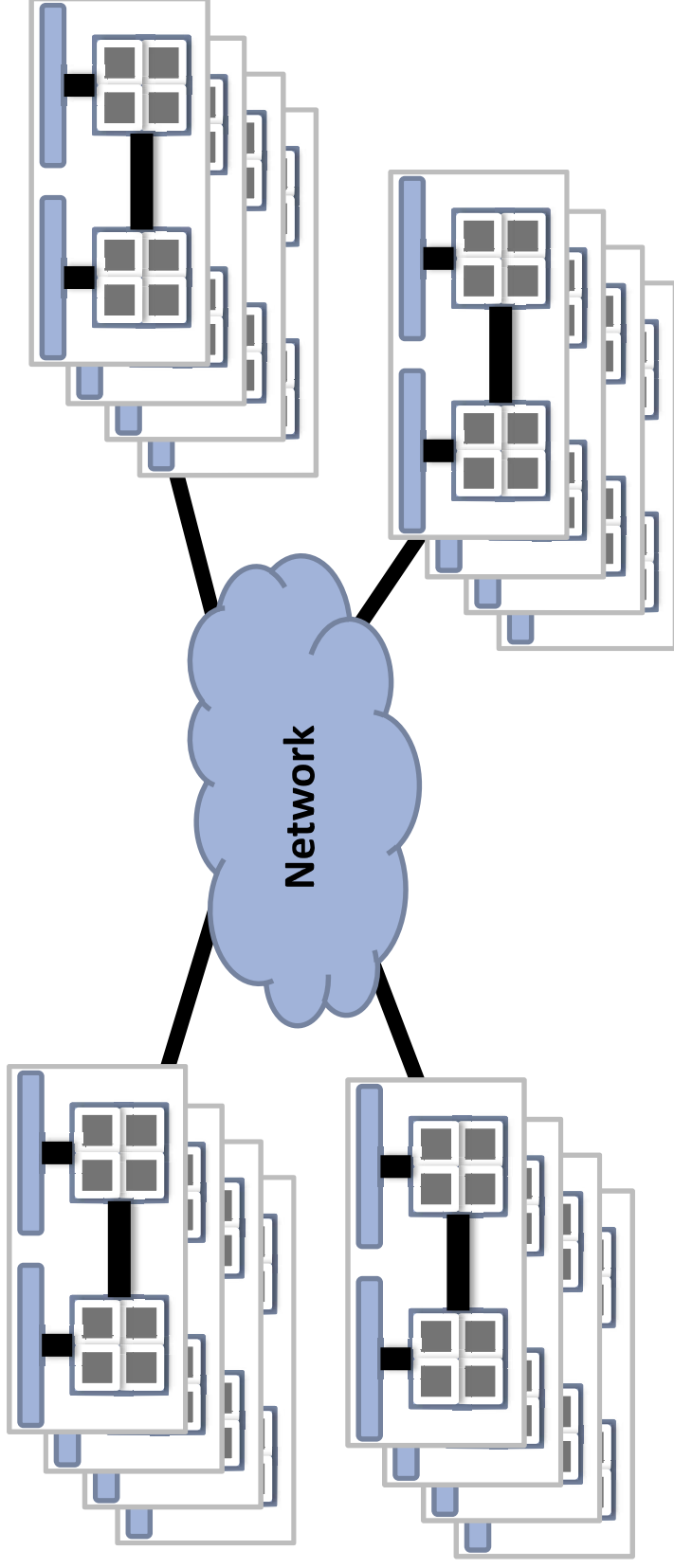
- **If communication is expensive**

- Multilevel halos
- More data during halo swaps but less frequent communication
- Use halo data from level n to compute halo data from level $n-1$ and so on

Hybrid programming

■ Clusters of small supercomputers

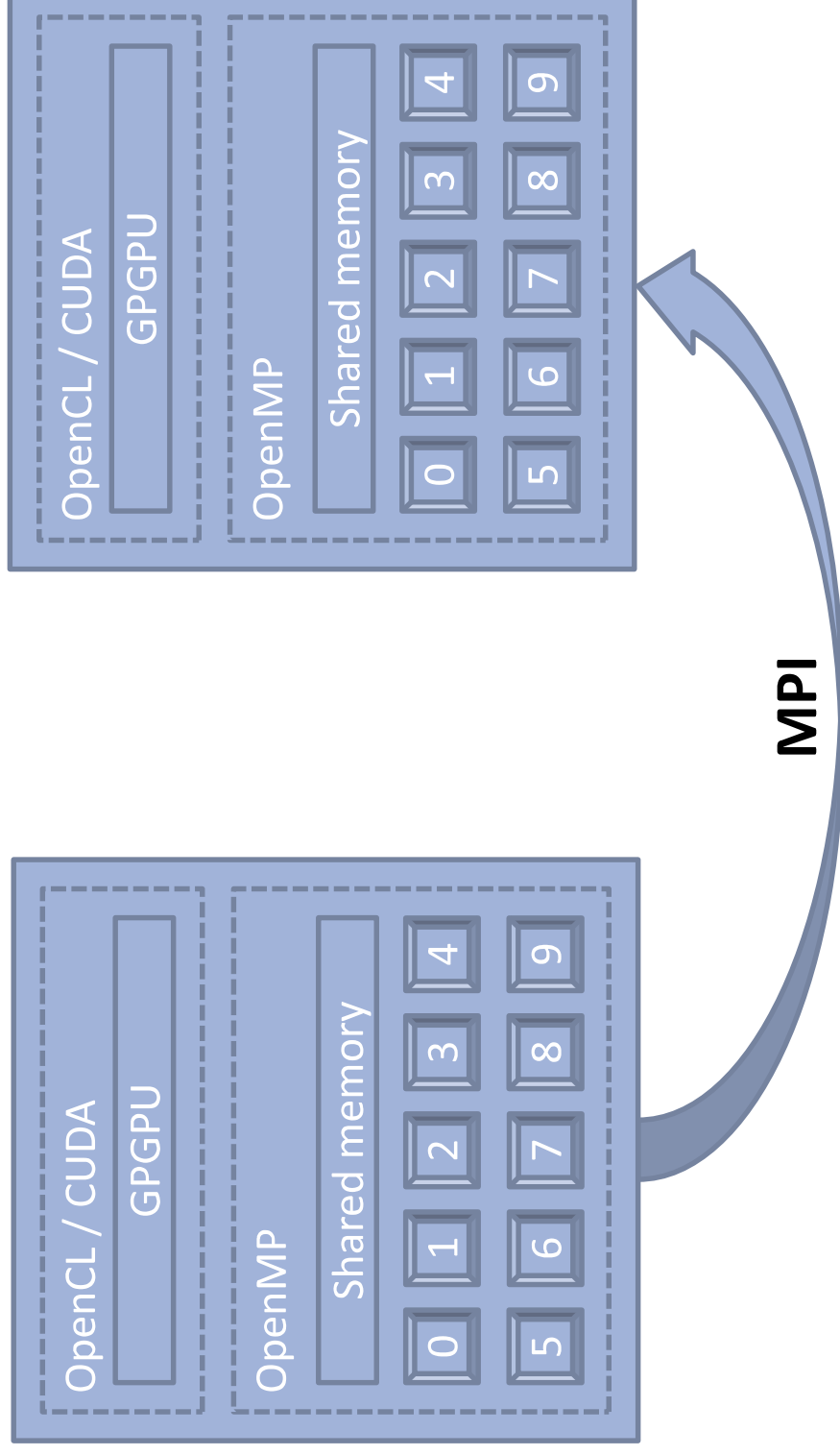
- Increasingly complex nodes – many cores, GPUs, Intel MIC, etc.
- Green computing will make things even more complex



MPI on a single node

- **MPI is sufficiently abstract to run on a single node**
 - It doesn't care where its processes are located
 - Message passing implemented using shared memory and IPC
 - The MPI library takes care
 - Usually faster than sending messages over the network
 - but...
- **... it is far from optimal**
 - MPI processes are implemented as separate OS processes
 - Portable data sharing is hard to achieve
 - Lots of control / problem data has to be duplicated
 - Reusing cached data is practically impossible

- Hierarchical mixing of different programming paradigms



Best of all worlds

■ OpenMP / pthreads

- Cache reuseage, data sharing
- Simple programming model (not so simple with POSIX threads)
- Threaded libraries (e.g. MKL)

■ OpenCL / CUDA

- Massively parallel GPGPU accelerators

■ MPI

- Fast transparent networking
- Scalability

■ Downsides

- Only benefits truly multiscale hierarchical problems
- Code could be hard to maintain

MPI – threads interaction

- Most MPI implementations are threaded (e.g. for non-blocking requests) but not thread-safe
- Four levels of threading support

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

■ Initialise MPI with thread support

```
C/C++:  int MPI_Init_thread (int *argc, char ***argv,  
                             int required, int *provided)  
Fortran: SUBROUTINE MPI_INIT_THREAD (required, provided,  
                                      ierr)
```

- **required** tells MPI what level of thread support is required
- **provided** tells us what level of threading MPI actually supports
 - could be less than the required level
- **MPI_INIT** – same as a call with **required = MPI_THREAD_SINGLE**
- The thread that has called **MPI_INIT_THREAD** becomes the *main thread*
- The level of thread support is fixed by this call and cannot be changed later

■ Obtain current level of thread support

```
MPI_Init_thread (provided)
```

- **provided** is filled with the current level of thread support
- If **MPI_INIT_THREAD** was called, **provided** will equal the value returned by the MPI initialisation call
- If **MPI_INIT** was called, **provided** will equal an implementation specific value

■ Find out if current thread is the main one

```
MPI_Is_thread_main (flag)
```

■ Thread support in various MPI libraries

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

- Use module versions ending with **mt** (e.g. **openmpi/1.6mt**)
- The InfiniBand BTL is not fully thread safe!

■ Intel MPI

- Enabled when compiling with **-openmp**, **-parallel**, or **-mt_mpi**

■ Modern MPI libraries provide some degree of CUDA interoperation

- Device pointers as buffer arguments in many MPI calls
- Direct device to device RDMA transfers over InfiniBand
- Implemented by Open MPI and MVAPICH2

■ Experimental CUDA build of Open MPI 1.7 in the BETA modules category

```
gpu-cluster$ module load BETA  
gpu-cluster$ module switch openmpi/1.7cuda
```

- You would need first to obtain access to the GPU cluster
(ask RZ ServiceDesk)

■ Sample hybrid job script (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]"

# 6 threads per process
export OMP_NUM_THREADS=6
# Pass OMP_NUM_THREADS on to all MPI processes
$MPIEXEC $FLAGS_MPI_BATCH -x OMP_NUM_THREADS \
    program.exe <args>
```

■ For the most up to date information refer to the HPC Primer

■ Sample hybrid job script (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>
```

■ For the most up to date information refer to the HPC Primer

Profiling of MPI applications

VampirTrace and Vampir

■ Profiling – collecting performance data about an application

- Number of calls
- Time spent in specific calls
- MPI messages – volume, speed, latency, etc.

■ Challenges

- Many interdependent processes running on many nodes
- Measurement overhead
- Accurate vs. realistic profile
- Scalability of performance data collection
- Analysis of performance data

- **MPI defines a very lightweight “black box” tools interface – PMPI**

- `MPI_Some_call` is not a real function but a weak symbol synonym to...
- The true MPI call is `PMPI_Some_call`
- Weak symbols can be overridden at link time

```
int MPI_Some_call (int arg1, MPI_Comm arg2)
{
    measure_enter("MPI_Some_call", arg1, arg2);
    int ierr = PMPI_Some_call(arg1, arg2);
    measure_exit();
    return ierr;
}
```

- **Can be abused e.g. for testing different collective algorithms**

- Link with the rest of the code and all `MPI_Some_call()` calls get redirected

■ Instrumentation

- Insertion of data and event collection points into the program code
- Automatic (by the compiler) or by hand

■ Trace – collection of timestamped events, gathered through the means of instrumentation

- enter into and exit from subroutines
- IO and network events
- performance counters
- user-defined events

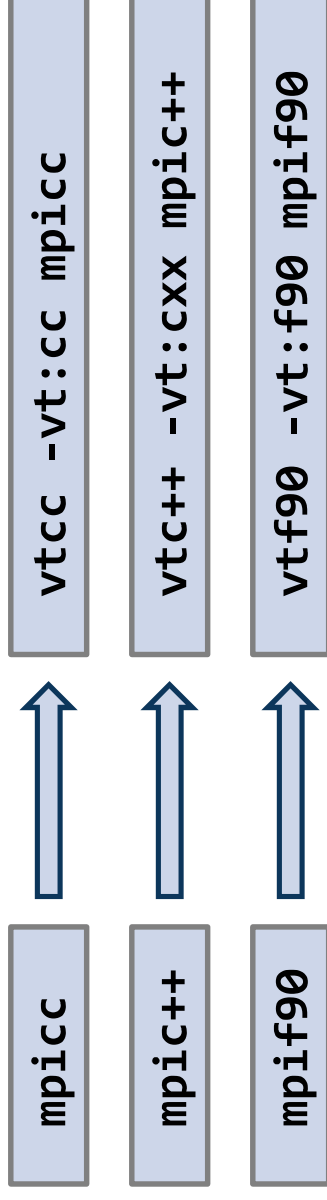
■ Traces are collected separately for each rank (and then merged)

- **Open-source tracing library, part of the Vampir suite, developed at TU Dresden**
- **Supports many different events**
 - Full call tracing (very data-intensive, doesn't scale)
 - MPI events
 - IO events
 - Hardware performance counters (via PAPI)

■ **Collected traces stored in Open Trace Format (OTF)**

- master file <name>.otf
- global definition file <name>.0.def
- events for each MPI rank <name>.<1-#procs>.events
- ZLIB compression

■ More compiler wrappers



■ Instrumentation type selected via `-vt:inst <type>`

- `compinst` compiler assisted instrumentation (default)
 - all function calls traced; very detailed; huge trace files
- `manual` manual tracing using VampirTrace API
 - traces only MPI events and user-specified events;
 - significantly reduced trace file size

■ VampirTrace is controlled by many environment variables

- VT_BUFFER_SIZE internal trace buffer size; flushed to the disk when full (default: 32M)
- VT_FILE_PREFIX OTF file prefix (default: executable name)
- VT_MAX_FLUSHES number of trace buffer flushes before tracing is disabled (0 – no limit)
- VT_SYNC_FLUSH synchronised buffer flushes (default: no)

■ Things to be aware of:

- By default buffers are flushed asynchronously and it takes time
- Significant skew in program's performance profile possible
- No trace written after abnormal program termination

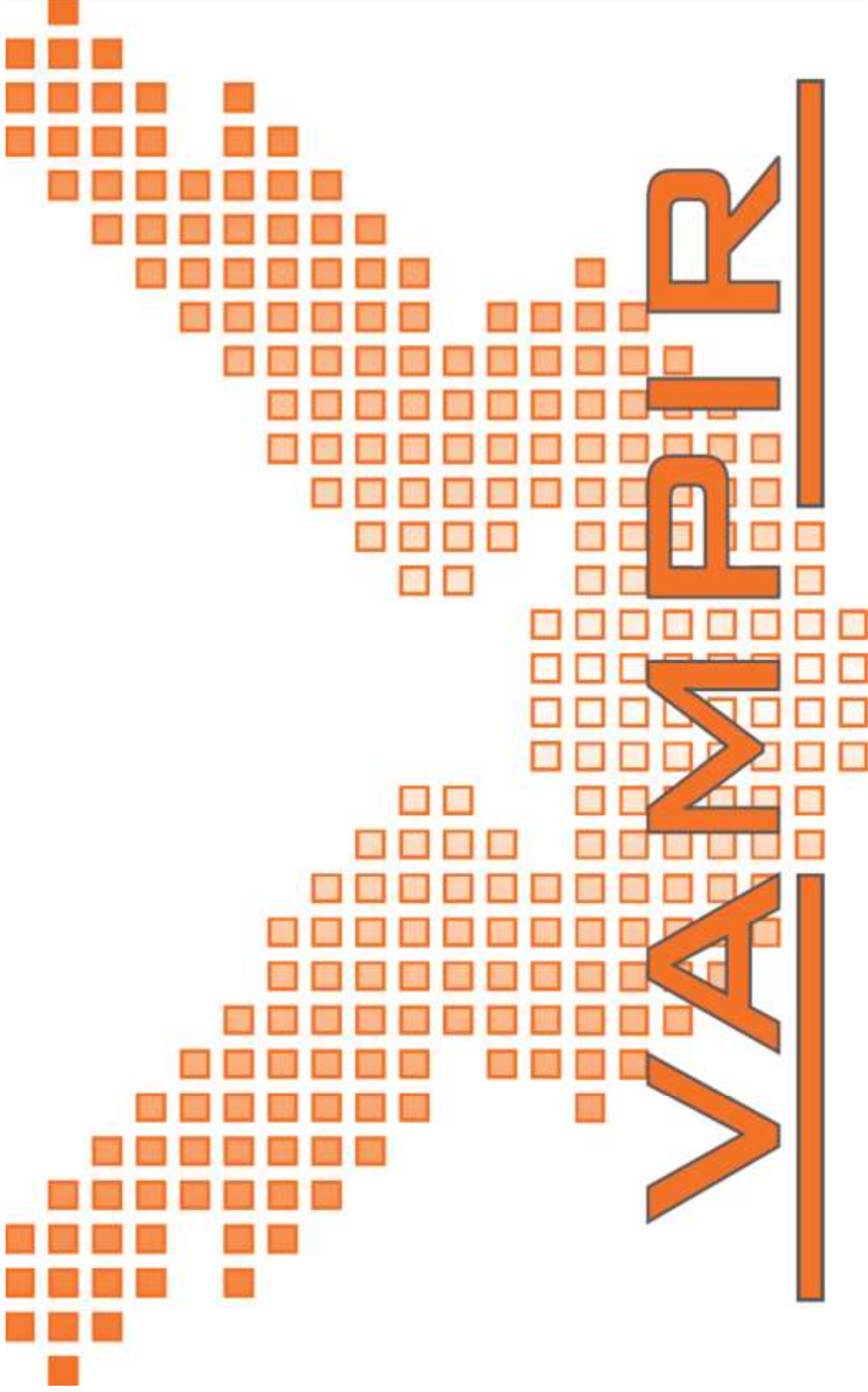
Using VampirTrace – running

■ Open MPI

```
module load UNITE vampirtrace
export VT_BUFFER_SIZE=128M
$MPIEXEC -x VT_BUFFER_SIZE -x LD_LIBRARY_PATH \
    <program> <args>
```

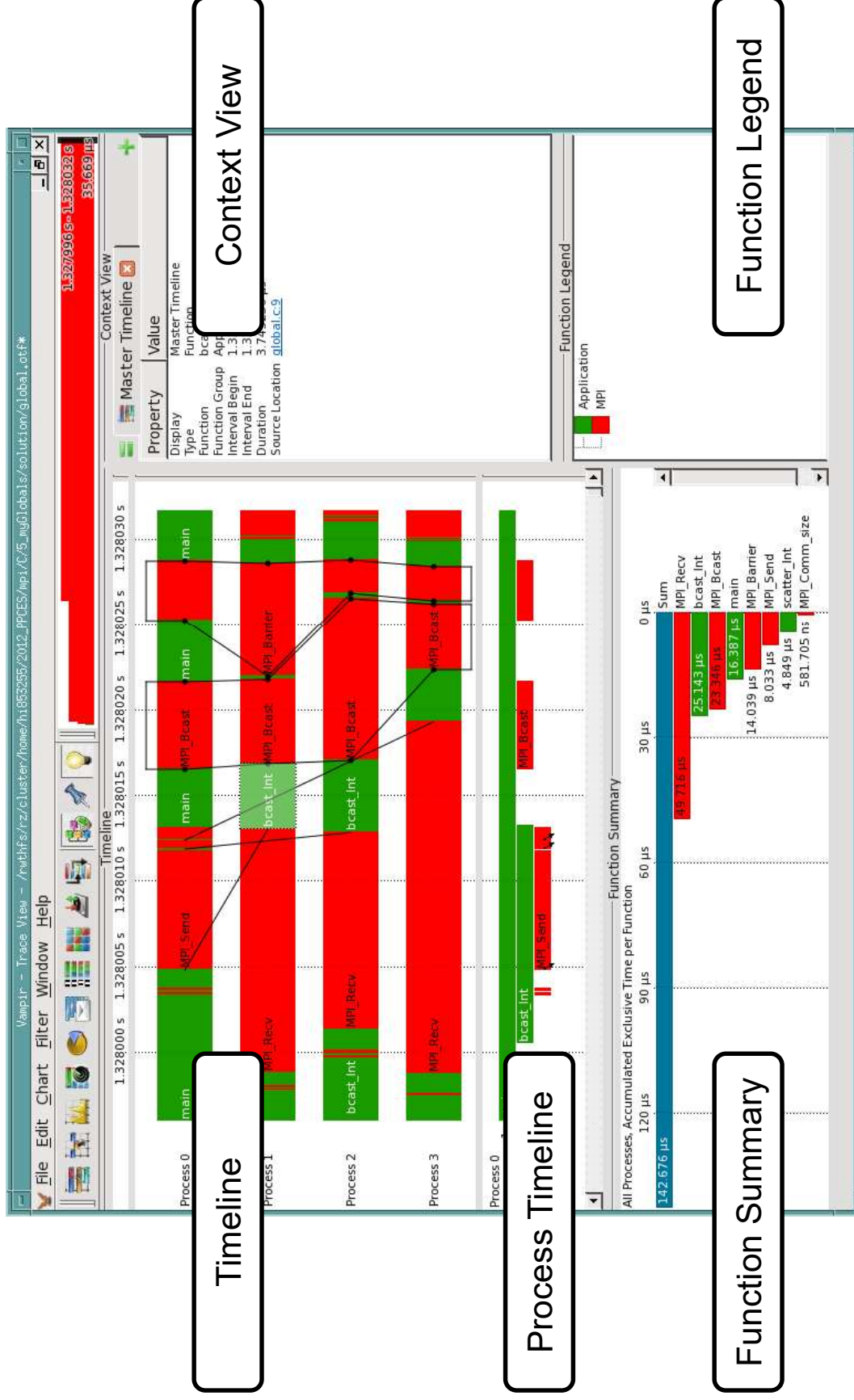
■ Intel MPI

```
module load UNITE vampirtrace
export VT_BUFFER_SIZE=128M
$MPIEXEC -genvlist VT_BUFFER_SIZE,LD_LIBRARY_PATH \
    <program> <args>
```

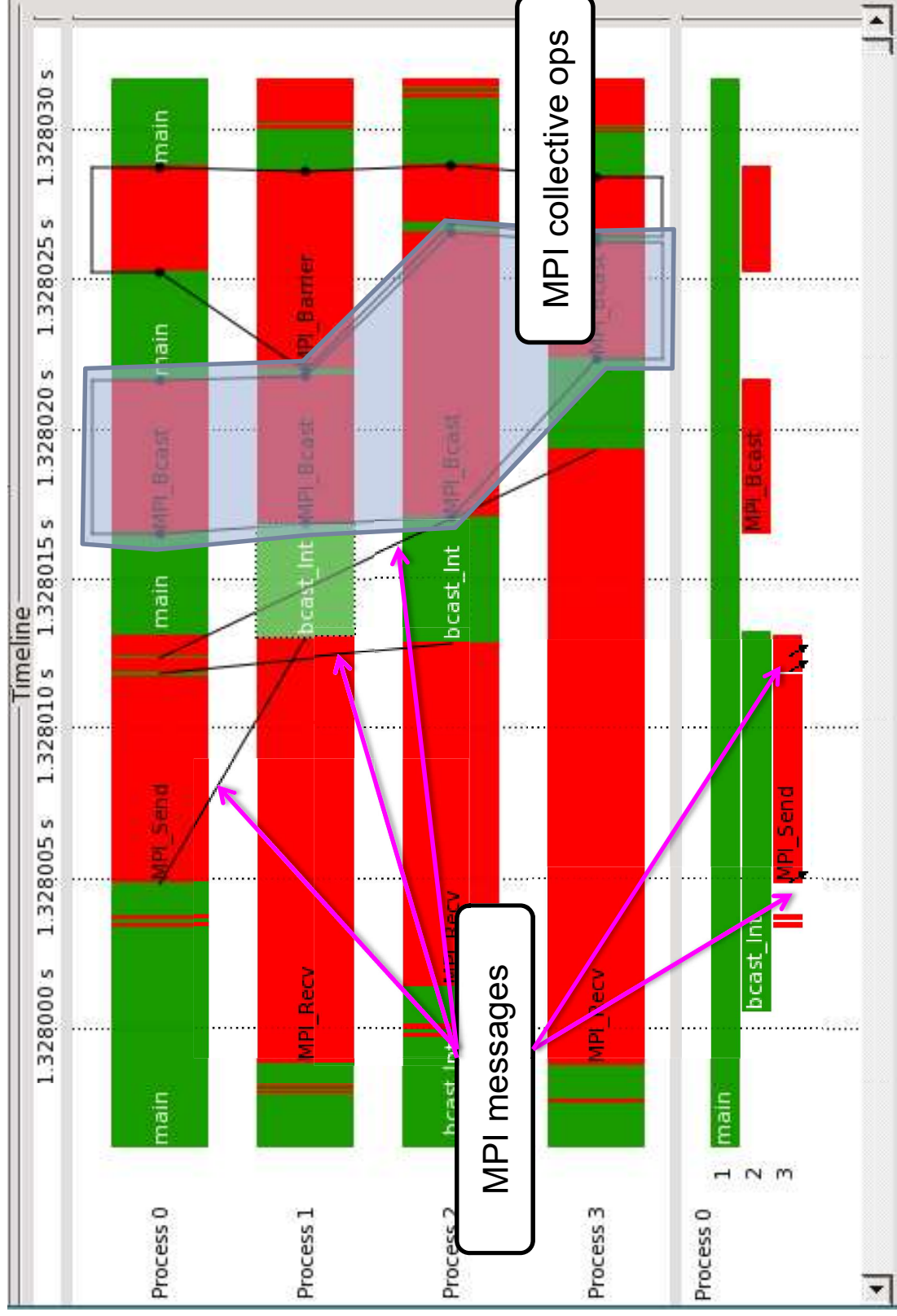



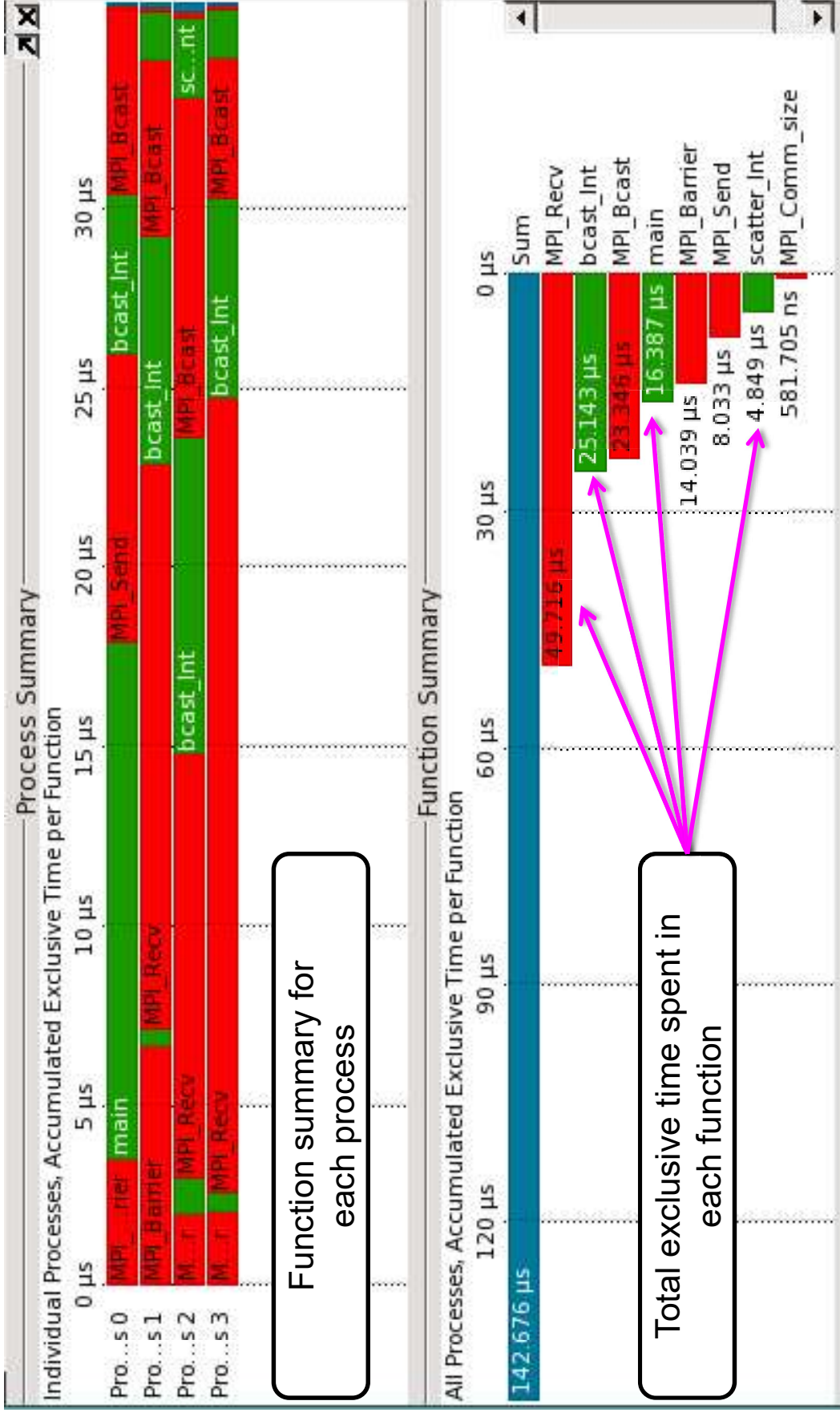
- **Commercial performance analysis tool, developed at TU Dresden**
- **Reads traces in OTF format, written by VampirTrace or any other tracing framework that supports OTF**
 - MPI events
 - IO events
 - Hardware performance counters
- **Could be used simply as a timeline browser**
- **Vampir Server**
 - Distributed trace analysis
 - Better scalability – can handle much larger traces

Vampir – trace view

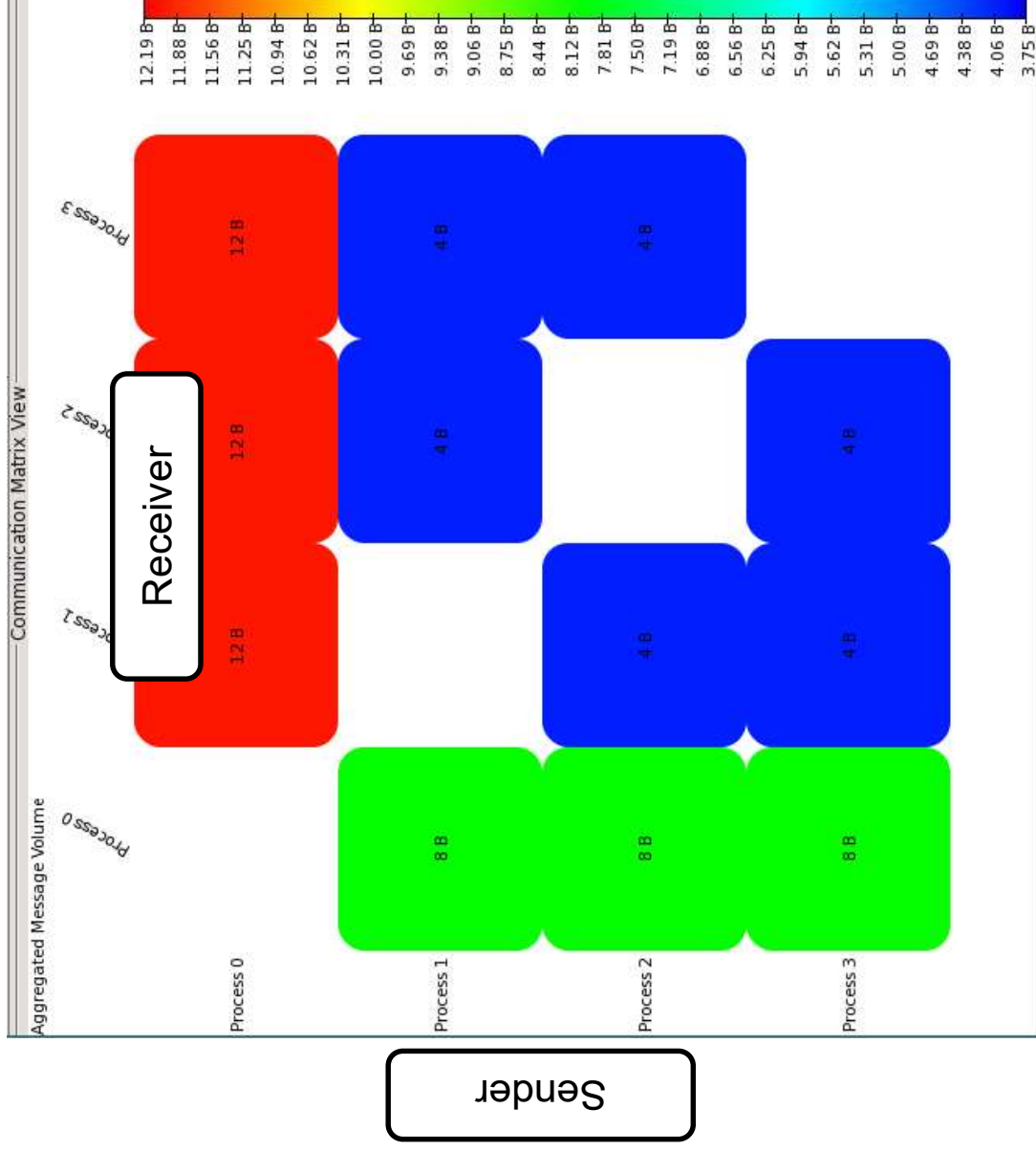


Vampir – timeline and process timeline





Vampir – communication matrix



Vampir demonstration

Debugging of MPI applications

TotalView

Parallel debugging

- **Parallel applications are hard to debug**
 - Multiple processes running concurrently on different nodes
 - Communication schemes could be very sophisticated
 - `print(f)` debugging doesn't scale
- **Parallel debuggers**
 - Client/server model
 - Can debug multiple processes over the network
 - Built-in mechanisms to deal with multiple code/data instances

- **TotalView**

- **Allinea DDT**

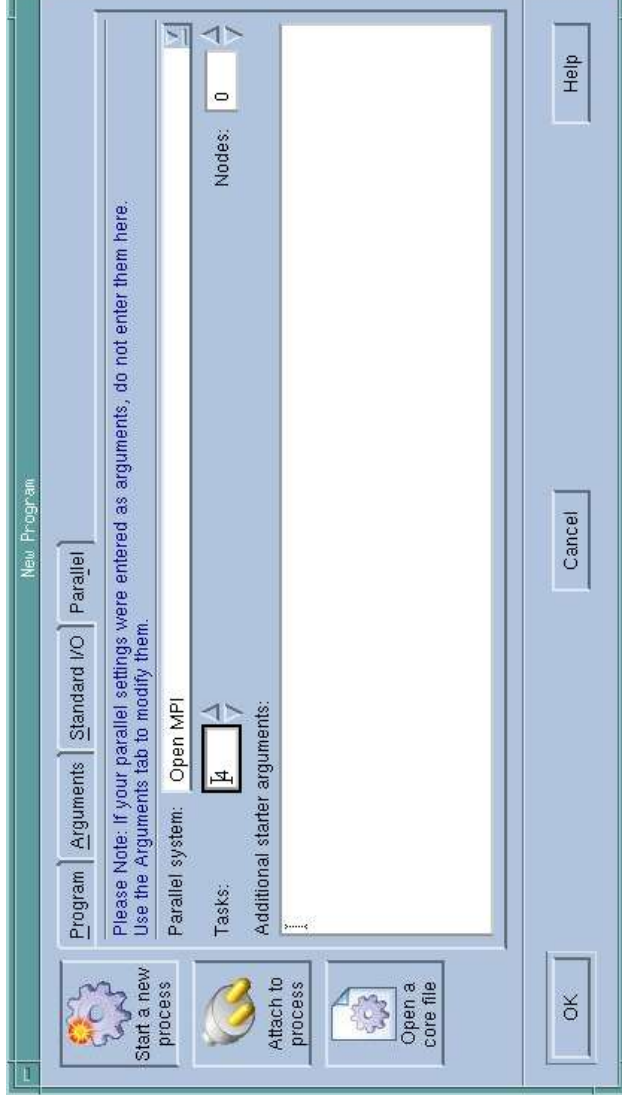
- **Versatile mixed-mode debugger**
 - MPI
 - OpenMP / general threading libraries
 - CUDA
- **Commercial, developed by Rogue Wave Software**
- **All MPI libraries on the RWTH BULL cluster have built-in support to launch programs under TotalView**
 - Open MPI
 - Intel MPI
 - TotalView can break automatically inside the `MPI_INIT` call

Using TotalView

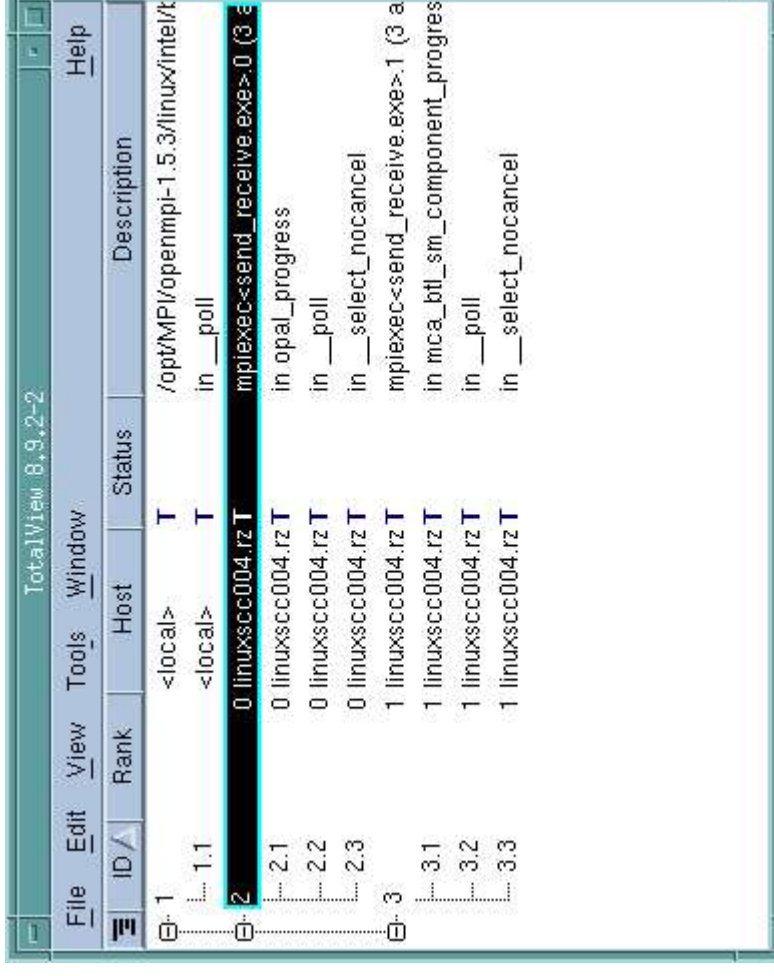
- TotalView is in the UNITE module category
- Launch via the MPI program launcher

```
cluster$ module load UNITE totalview  
cluster$ $MPIEXEC -np 4 -tv <program> <args>
```

- Use the built-in parallel launcher



- Summary of processes, ranks and top of thread stacks



The screenshot shows the TotalView Root Window with a table of processes. The table has columns for ID, Rank, Host, Status, and Description. The first three rows are expanded to show thread stacks. The second row, ID 2, Rank 0, is highlighted with a red box.

ID	Rank	Host	Status	Description
1	<local>	<local>	T	/opt/MPI/openmpi-1.5.3/linux/intel/t
1.1	<local>	<local>	T	in __poll
2	0	linuxscc004.rz	T	mpirexec<send_receive.exe> 0 (3 a
2.1	0	linuxscc004.rz	T	in opal_progress
2.2	0	linuxscc004.rz	T	in __poll
2.3	0	linuxscc004.rz	T	in __select_nocancel
3	1	linuxscc004.rz	T	mpirexec<send_receive.exe> 1 (3 a
3.1	1	linuxscc004.rz	T	in mca_btl_sm_component_progres
3.2	1	linuxscc004.rz	T	in __poll
3.3	1	linuxscc004.rz	T	in __select_nocancel

- Also used to quickly switch focus from one process to another

TotalView – Process Window

Group (Control)

Go Halt Kill Restart Next Step Out Run To GoBack Prev UnStep Caller BackTo Live

File Edit View Group Process Thread Action Point Debug Tools Window Help

mpirexec<colls.exe>.0

Rank 0: mpirexec<colls.exe>.0 (At Breakpoint 1)

Thread 1 (139986187368192): colls.exe (At Breakpoint 1)

Stack Trace

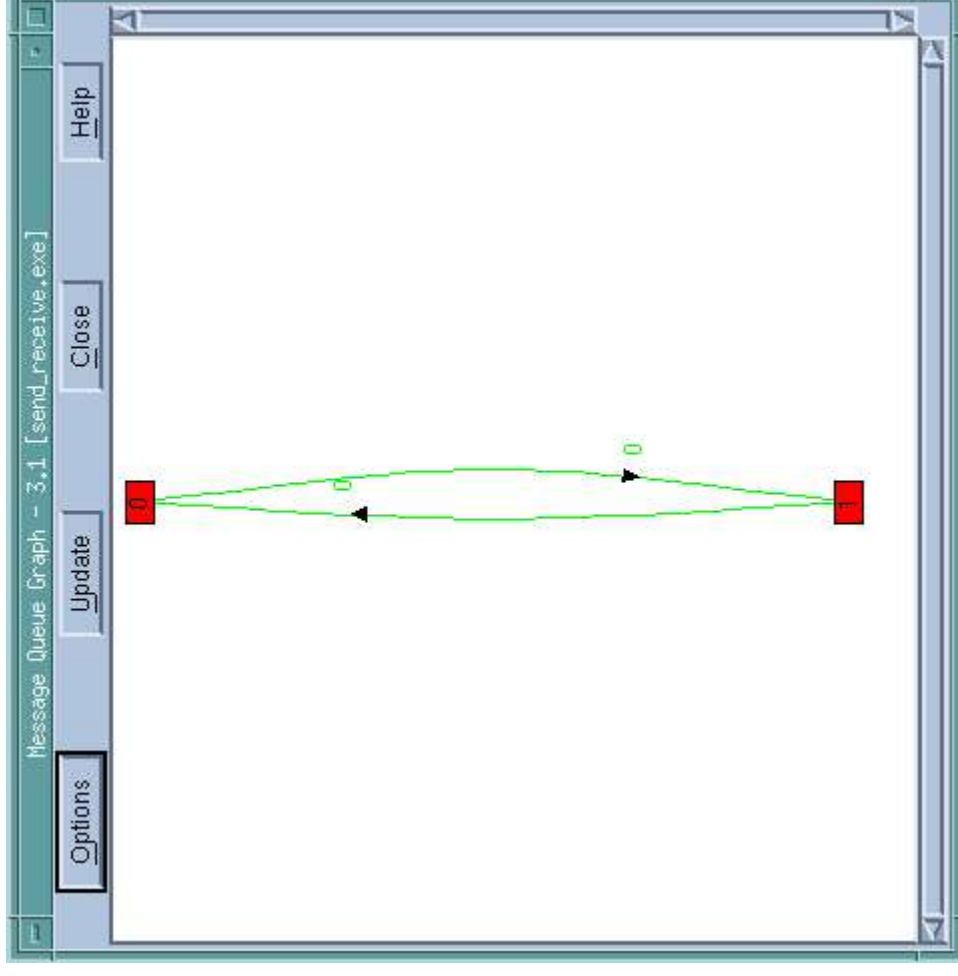
C main, FP=7ffdf602230
_libc_start_main, FP=7ffdf6022f0
_start, FP=7ffdf602300

Function "main":
argc: 0x00000001 (1)
argv: 0x7ffdf602318 -> 0x7ffdf6041bb -> "colls.exe"
Local variables:
myRank: 0x00000000 (0)
numProcs: 0x00000002 (2)
i: 0x00000033 (51)
myRandomNumber: 0x0000002b (43)
inspectRank: 0x00000000 (0)
mySendBuffer: 0x0072a240 -> 0x13feda48 (335469128)

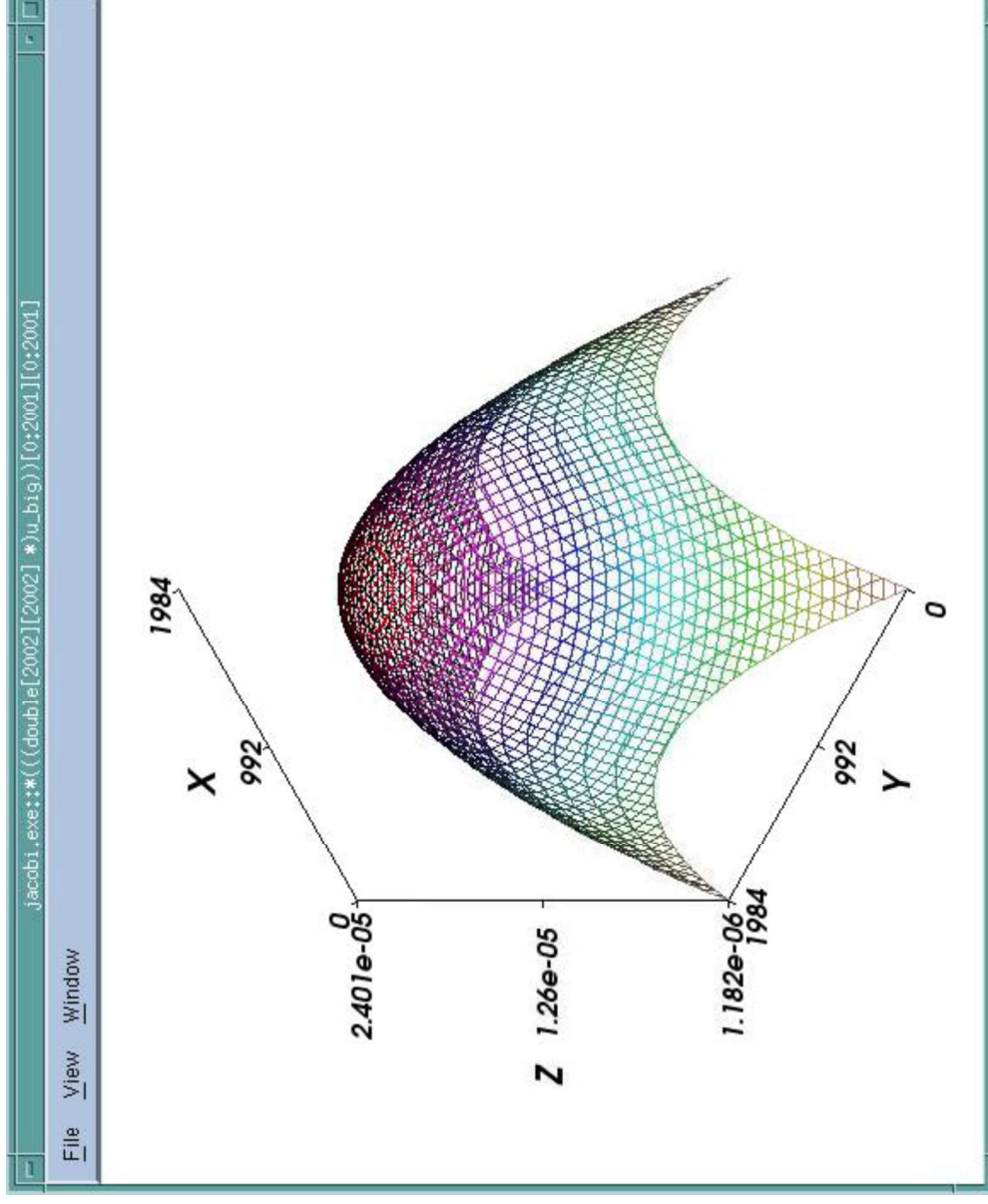
Stack frame

Function main in colls.c
159 int *myRecvBuffer = (int *)malloc(sizeof(int)*numProcs);
160
161 // Seed the random number generator with a rank-specific value
162 srand(MPI_Wtime()+123*myRank);
163 myRandomNumber = random() % 100;
164
165 if (argc > 1)
166 {
167 inspectRank = atoi(argv[1]);
168 if (inspectRank < 0 || inspectRank >= numProcs)
169 MPI_Abort(MPI_COMM_WORLD, 1);
170 }
171 printf("Rank %2.i has the random number %i\n", myRank, myRandomNumber);
172
173 int myData = -1;
174
175 // Use MPI barrier to synchronize the output
176 MPI_Barrier(MPI_COMM_WORLD);
177
178 // ---- Broadcast operation ----
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■ Cycle (deadlock) detected



- Built-in multidimensional data visualizer



TotalView demonstration

More on the tools

- **More in-depth introduction to TotalView and other correctness tools:**
 - 05.09.2012 – Correctness Tools tutorial
- **More in-depth introduction to Vampir and other performance tools:**
 - 12.09.2012 – Performance Tools tutorial

Q & A session

Lab session of your choice

- **Continue working on exercises from the basic MPI tutorial**

- Hand-outs are available over there to your right

- **Parallelise from scratch a PDE solver**

- Hand-outs are available on your desk

- **Practice tracing with VampireTrace and Vampire**

- `make vampir`

- **Practice TotalView debugging**

- `make totalview`