Topology aware Cartesian grid mapping with MPI

Issue 120 Reading

Christoph Niethammer   Rolf Rabenseifner

niethammer@hlrs.de   **rabenseifner@hlrs.de**

High Performance Computing Center (HLRS), University of Stuttgart, Germany

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For further information, see also https://fs.hlrs.de/projects/par/mpi/EuroMPI2018-Cartesian/

The Problems of MPI_Dims_create + MPI_Cart_create

- The factorization of a given amount of MPI processes must be
  - Application topology aware [1]
  - Hardware topology aware
- Current definition of MPI_Dims_create is not prepared for this

  } Slides 2-3
- Extreme differences in latency and accumulated bandwidth between **inter**-node and **intra**-node communication

  } Slides 4-6
- The reordering by MPI_Cart_create:
  - Many implementations do nothing [2]

    } Slide 7-10
  - A perfect reordering may require complex domain decomposition algorithms (e.g. Metis) [3]

We propose a new interface together with a fast algorithm, which is application and hardware topology aware } Slides 11-22

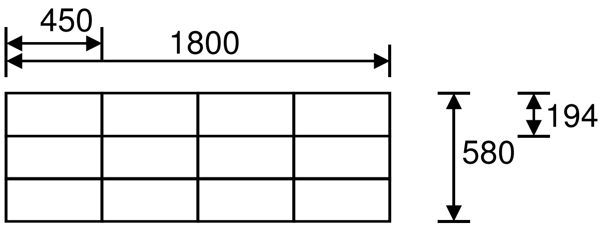
Implementation remarks } Slide 23-24

Benchmark + results } Slide 25-34

[1, 2, 3] see References on last slide } Slide 35

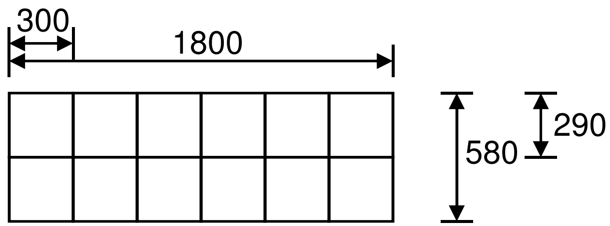
Examples

- Application topology awareness
  - 2-D example with 12 MPI processes and gridsize 1800x580
    - **MPI_Dims_create → 4x3**



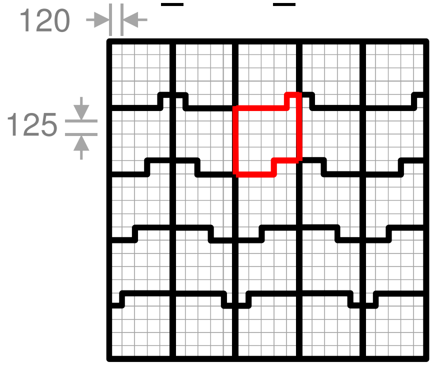
Boundary of a subdomain = 2(450+194) = **1288** ☹

    - **grid aware → 6x2 processes**



Boundary of a subdomain = 2(300+290) = **1180** ☺

- Hardware topology awareness
  - 2-D example with 25 nodes x 24 cores and gridsize 3000x3000
    - **MPI_Dims_create → 25 x 24**

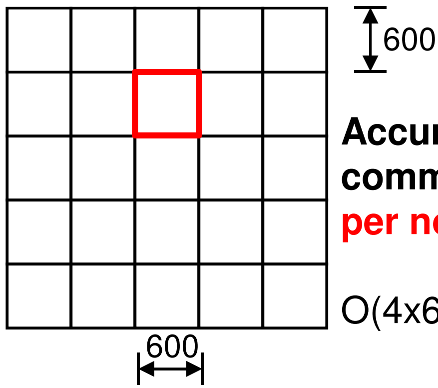


Accumulated communication per node

O(10x120+12x125)

= O(**2700**) ☹

    - **Hardware aware**
→ (5 nodes x 6 cores) X (5 nodes x 4 cores)



Accumulated communication per node

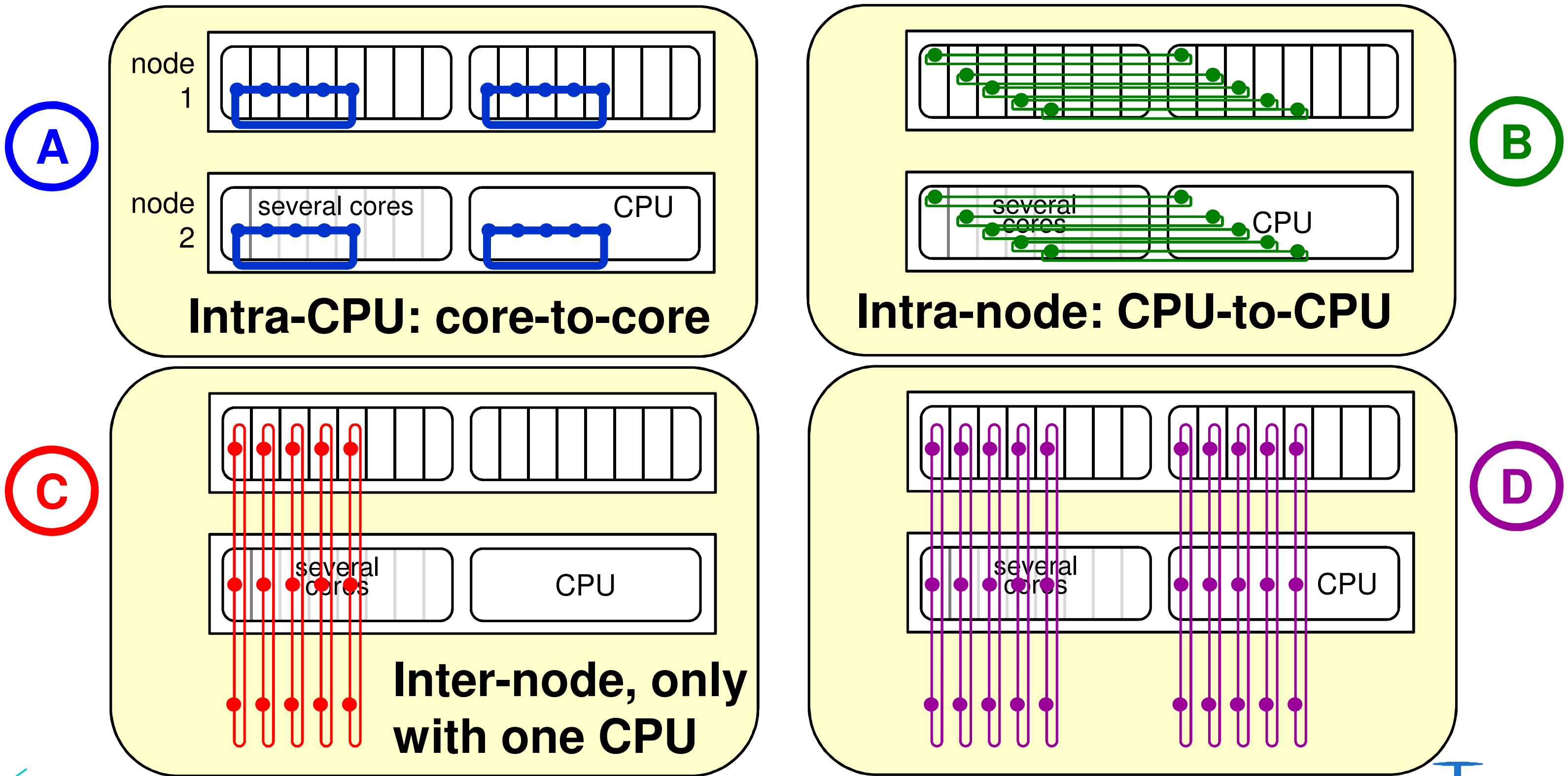
O(4x600) = O(**2400**) ☺

Ring Benchmarks for Inter- and Intra-node Communication

Benchmark halo_irecv_send_multiplelinks_toggle.c

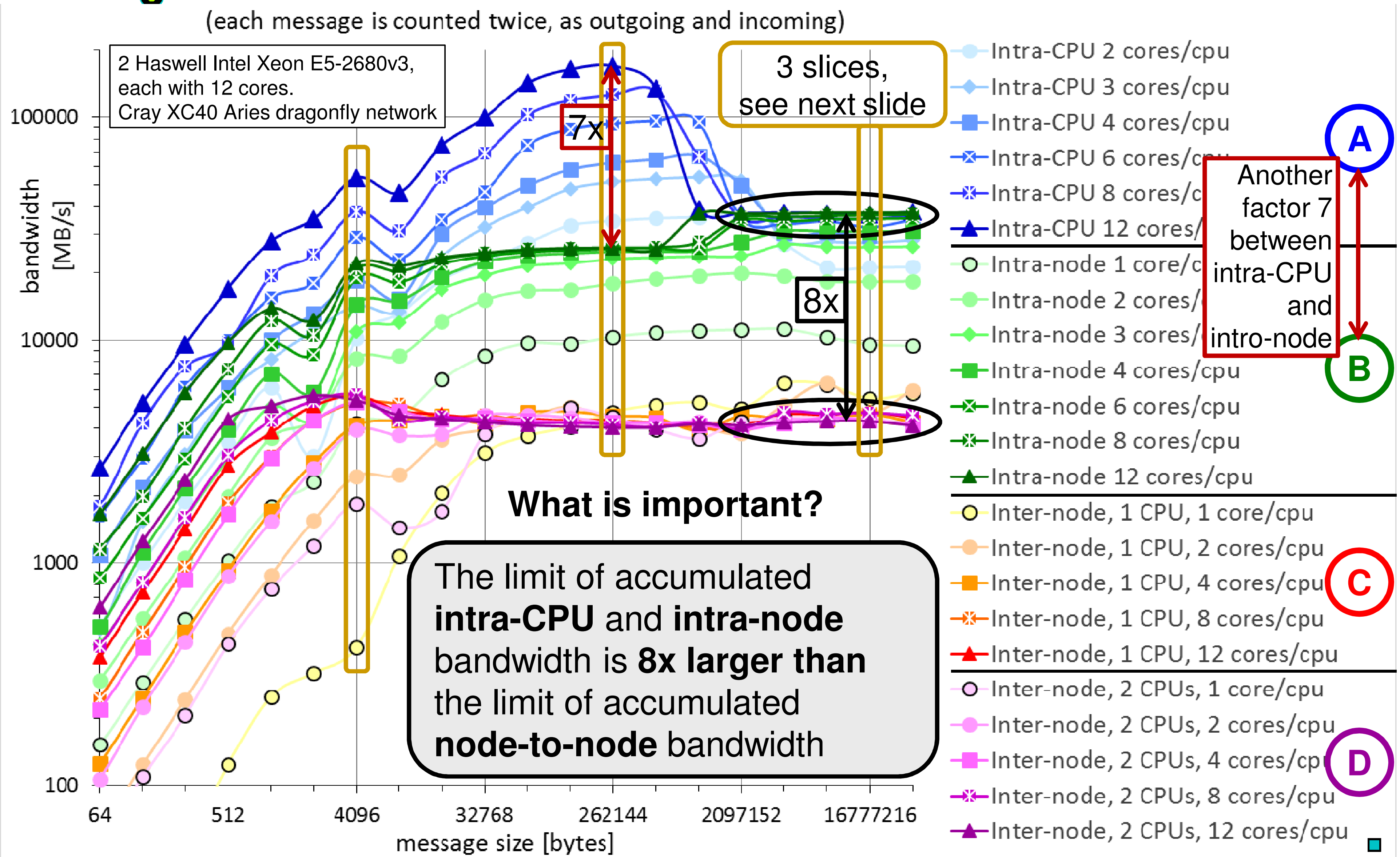
- Varying message size,
- number of ***communication cores per CPU***, and
- four communication schemes (example with 5 ***communicating cores per CPU***)

See HLRS online courses
http://www.hlrs.de/training/par-prog-ws/
→ Practical → MPI.tar.gz
→ subdirectory MPI/course/C/1sided/



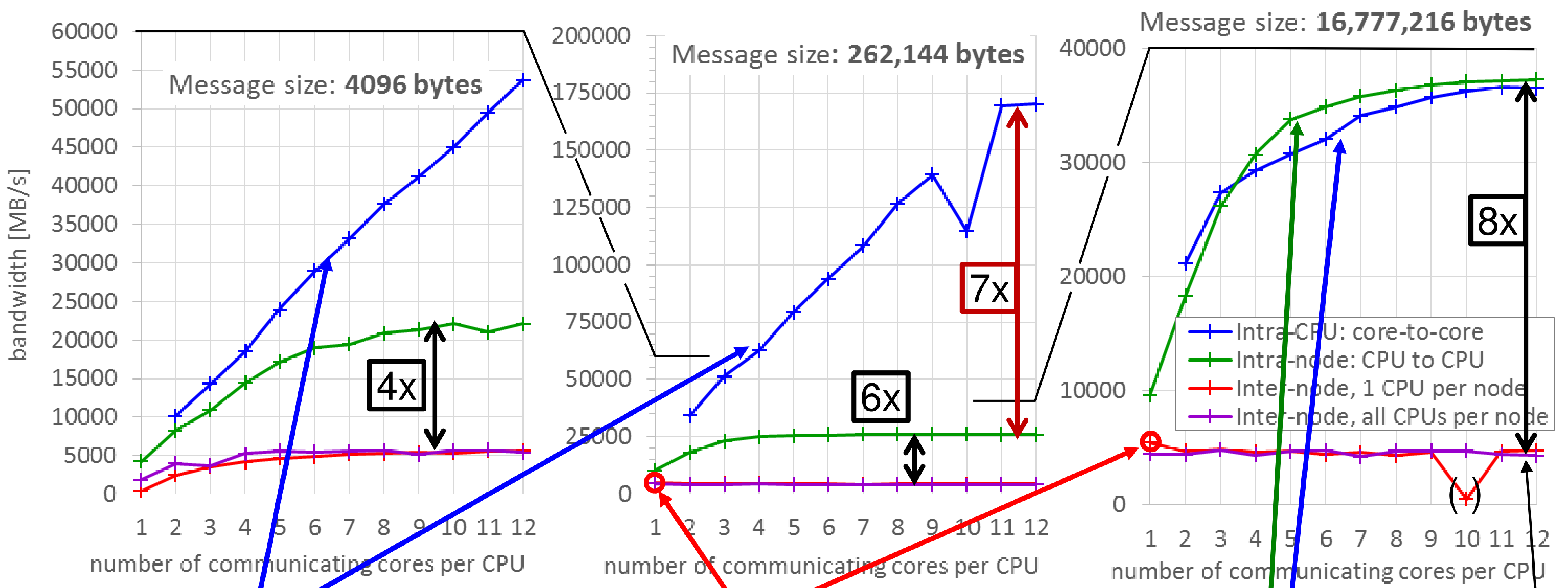
See HLRS online courses http://www.hlrs.de/training/par-prog-ws/
→ Practical → MPI.tar.gz → subdirectory MPI/course/C/1sided/

Duplex accumulated ring bandwidth per node



Measurement with halo_irecv_send_multiplelinks_toggle.c on 4 nodes of Cray XC40 hazelhen.hww.de, June 15, 2018, HLRS, by Rolf Rabenseifner (protocol 10)

Duplex accumulated ring bandwidth per node – scaling vs. asymptotic behavior



Core-to-core:
Linear scaling for small to medium size mes-sages due to caches

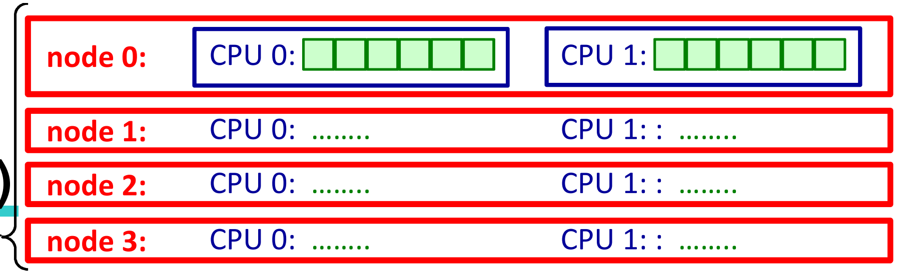
Node-to-node:
One duplex link by **one core** already fully saturates the network

Core-to-core & CPU-to-CPU:
Long messages:
Same asymptotic limit through **memory bandwidth**

Result: The limit of accumulated **intra-CPU** and **intra-node** bandwidth is **8x larger than** the limit of accumulated **node-to-node** bandwidth

Re-numbering on a cluster of SMPs (cores / CPUs / nodes)

- Example with 48 cores on:
  - **4 ccNUMA nodes**
  - **each node with 2 CPUs**
  - **each CPU with 6 cores**



- 2-dim application with 6000 x 8080 gridpoints
  - **Minimal communication with 2-dim domain composition with 1000 x 1010 gridpoints/core (shape as quadratic as possible**
    → minimal circumference
    → minimal halo communication)
  - **virtual 2-dim process grid: 6 x 8**

Process coordinate, direction 1 →

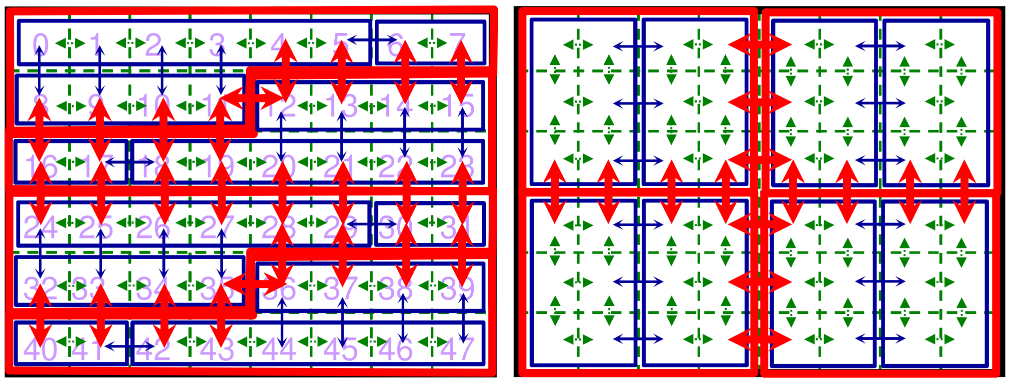
Process coordinate, direction 0 ↓

0	1	2	3	4	5	6	7
8	9	10	11	12	13	14	15
16	17	18	19	20	21	22	23
24	25	26	27	28	29	30	31
32	33	34	35	36	37	38	39
40	41	42	43	44	45	46	47

Order of the new ranks: Last coordinate is running contiguously
→ Perfect basis for MPI_Cart_create() without reorder, i.e. with reorder==0 / .FALSE.

- How to locate the MPI processes on the hardware?
  - **Using sequential ranks in MPI_COMM_WORLD**
  - **Optimized placement**

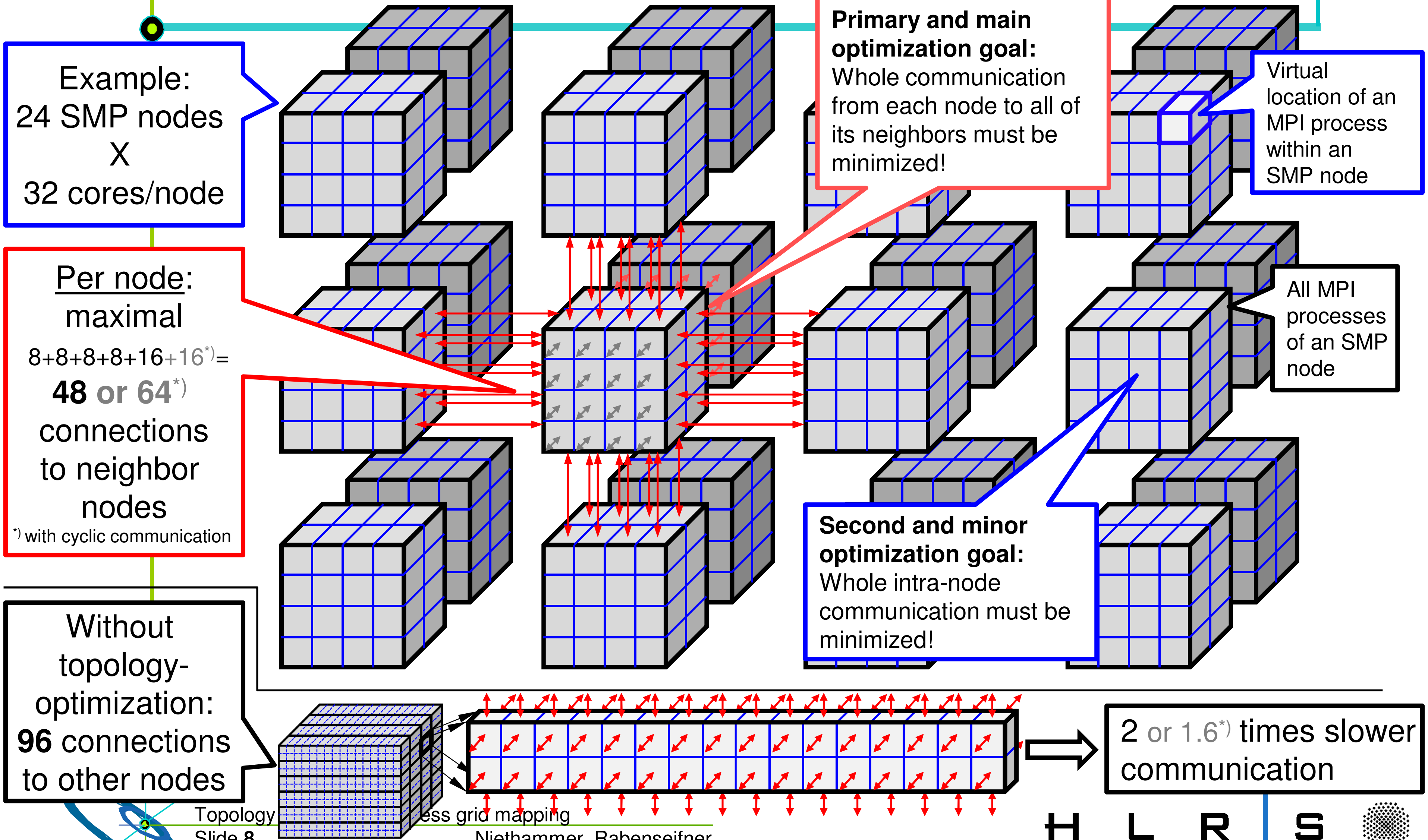
  → Proposed algorithm in slides 7-15



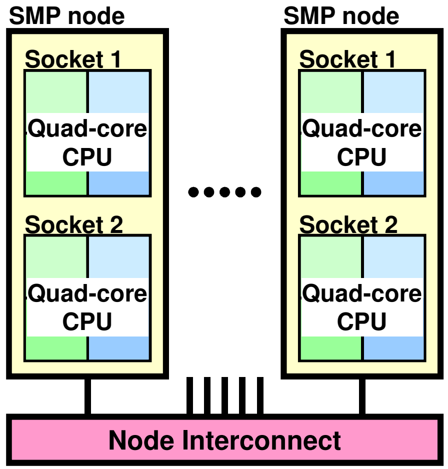
Non-optimal communications:
- **26** node-to-node (outer)
- **20** CPU-to-CPU (middle)
- 36 core-to-core (inner)

Optimized placement:
- **Only 14** node-to-node
- **Only 12** CPU-to-CPU
- 56 core-to-core

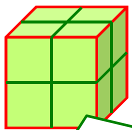
Hierarchical Cartesian Domain Decomposition



Levels of communication & data access



- Three levels:
  - Between the SMP nodes
  - Between the sockets inside of a ccNUMA SMP node
  - Between the cores of a socket
- On all levels, the communication should be minimized:
  - With 3-dimensional sub-domains:
    - **They should be as cubic as possible = minimal surface = minimal communication**



Outer surface corresponds to the data communicated to the neighbor nodes in all 6 directions → **Major optimization goal**

Inner surfaces correspond to the data communicated or accessed between the cores inside of a node → Least important

    - **“as cubic as possible” may be qualified** due to different communication bandwidth in each direction caused by sending (fast) non-strided or (slow) strided data

Back to the problems

1. All MPI libraries provide the necessary interfaces ☺ ☺ ☺,
   but **without** re-numbering in nearly all MPI-libraries ☹ ☹ ☹
   - **You may substitute MPI_Cart_create()**
     by the software solution of Bill Gropp (see Bill Gropp, EuroMPI 2018)

2. **The existing MPI-3.1 interfaces are not optimal**
   - **for cluster of ccNUMA node hardware,**
     - **We substitute MPI_Dims_create() + MPI_Cart_create()**
       by MPIX_Cart_weighted_create(… MPIX_WEIGHTS_EQUAL …)
   - **nor for application specific grid sizes**
     or direction-dependent bandwidth
     - **by MPIX_Cart_weighted_create(… weights ….)**

3. **Caution: The application must be prepared for rank re-numbering**
   - **All communication through the newly created**
     Cartesian communicator with re-numbered ranks!
   - **One must not load data based on MPI_COMM_WOLRD ranks!**

The new interfaces

Substitute for / enhancement to existing MPI-1

- MPI_Dims_create (size_of_comm_old, ndims, *dims[ndims]*);
- MPI_Cart_create (comm_old, ndims, dims[ndims], periods, reorder, **comm_cart*);

New:

- **MPI_Cart_weighted_create** (

```
    /*IN*/     MPI_Comm   comm_old,
    /*IN*/     int        ndims,
    /*IN*/     double     dim_weights[ndims], /*or MPIX_WEIGHTS_EQUAL*/
    /*IN*/     int        periods[ndims],
    /*IN*/     MPI_Info   info,      /* for future use, currently MPI_INFO_NULL */
    /*INOUT*/  int        dims[ndims],
    /*OUT*/    MPI_Comm   *comm_cart );
```

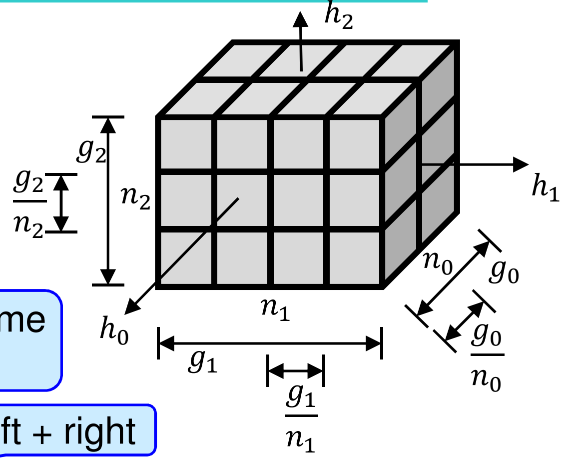
  - Arguments have same meaning as in MPI_Dims_create & MPI_Cart_create
  - See next slide for meaning of dim_weights[ndims]

The weights w_i

- **Given:**
  - d-dimensional Cartesian grid with a total grid size of $G = \prod_{i=0}^{d-1} g_i$ elements
  - The communication cost in each direction $i = 0, d\text{-}1$ is multiplied
    - with a halo width h_i,
    - and a communication cost factor c_i,

communication time per grid point

2 = left + right



- → total communication cost is $2g_1g_2h_0c_0 + 2g_0g_2h_1c_1 + 2g_0g_1h_2c_2$
- The weight w_i is defined as total cost for the communication in one direction:
  - $w_i = 2\frac{G}{g_i}h_ic_i$

common factors, like $2G$ or absolute values of c_i, are not relevant

User level

- With a domain decomposition (i.e., factorization) to $N = \prod_{i=0}^{d-1} n_i$ nodes, the total communication costs per node is

$$2\frac{g_1g_2}{n_1n_2}h_0c_0 + 2\frac{g_0g_2}{n_0n_2}h_1c_1 + 2\frac{g_0g_1}{n_0n_1}h_2c_2 = \sum_{i=0}^{d-1}\frac{n_i}{N}w_i$$

Primarily for the node decomposition and secondarily on core level

➔ The topology functions have to find a factorization with minimal $\sum_{i=0}^{d-1} n_i w_i$

→ common factors $2G$ and $\frac{1}{N}$ are not relevant →

MPI library level

MPIX routines, courtesy of Christoph Niethammer, HLRS

The weights w_i

Note that

- The proposal for the MPI standard does not discuss the implementation.
- It uses the same figure, but n_i expresses number of processes, i.e. dims[i], and not number of nodes in one direction, as on previous slide.
- Can be implemented with **MPI_Cart_ml_create_from_types()** → next slide

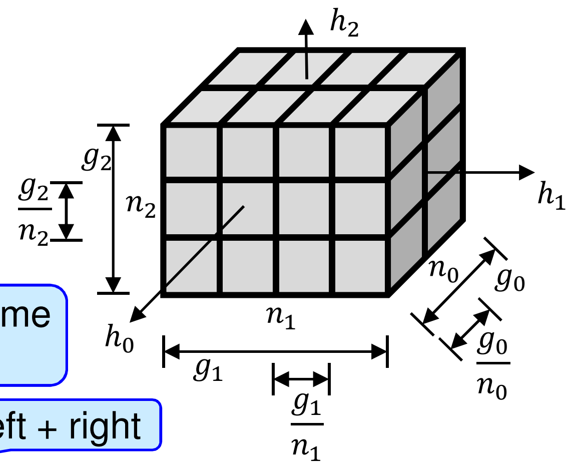
---

User level

- **Given:**
  - d-dimensional Cartesian grid with a total grid size of $G = \prod_{i=0}^{d-1} g_i$ elements
  - The communication cost in each direction $i = 0, d$-1 is multiplied
    - with a halo width h_i,
    - and a communication cost factor c_i,

communication time per grid point

2 = left + right



- → total communication cost is $2g_1g_2h_0c_0 + 2g_0g_2h_1c_1 + 2g_0g_1h_2c_2$
- The weight w_i is defined as total cost for the communication in one direction:
  - $w_i = 2\frac{G}{g_i}h_ic_i$

common factors, like $2G$ or absolute values of c_i, are not relevant

H L R S

MPIX routines, courtesy of Christoph Niethammer, HLRS

Further Interfaces (1)

If the application wants to choose the hardware levels,
then the most simple interface is to choose a split type for each level
(except for the last one):

e.g., with
25*25*24 = **15000 processes**
on **625 ccNUMA nodes** with
2 CPUs/node and **12 cores/CPU**

e.g., nsplit_types=2, split_types=
{ MPI_COMM_TYPE_SHARED,
OMPI_COMM_TYPE_NUMA
within OpenMPI, or for further
splitting: MPIX_COMM_TYPE_
HW_TOPOLOGY}

Substitute for / enhancement to existing MPI-1
MPI_Dims_create (size_of_comm_old, ndims, *dims*);
MPI_Cart_create (comm_old, ndims, dims, periods,
reorder, **comm_cart*);

```
MPI_Cart_ml_create_from_types(MPI_Comm comm_old,
              int nsplit_types,      int split_types[nsplit_types],
              int ndims,             double dim_weights[ndims],
              int periods[ndims],    MPI_Info info,
/*OUT*/       int dims[ndims],   MPI_Comm *comm_cart );
```

e.g., 3 dimensions with a data
grid with 1000 x 1100 x 950
elements ➔ dim_weights[] =
{ 1.0/1000, 1.0/1100, 1.0/950 }

Rank mapping is based on:

- Node level: 625 = 5 x 25 x 5
- CPU level: 2 = 2 x 1 x 1
- Core level: 12 = 3 x 1 x 4

Result (product): **30 x 25 x 20**

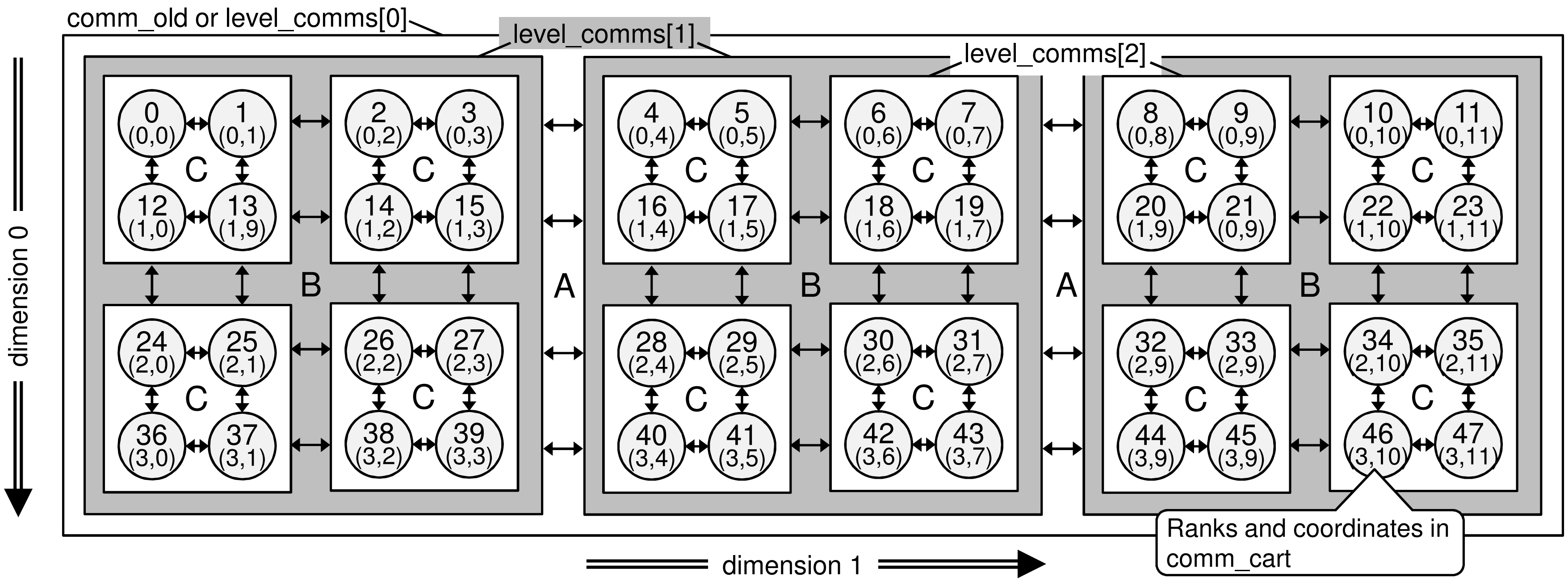
The Cartesian communicator reflects this result: **30 x 25 x 20**

Note that MPI_Dims_create() would produce
25 x 25 x 24
which would never fit to the needed node-level distribution
5 x 25 x 5

Next steps for the application:
MPI_Comm_rank (comm_cart, &my_rank);
MPI_Cart_coords (comm_cart, my_rank, ndims, *coords*)

2-D Cartesian Example (proposed for the MPI standard)

with
- 48 processes and ndims=2,
- dim_weights=$({}^{1.0}/_{4},\ {}^{1.0}/_{12})$, and
- nsplit_types=2 (e.g. splitting into ccNUMA nodes and those into CPUs)
- or appropriate level_comms[0] .. [2]



The optimization chooses an appropriate re-ordering of the ranks of comm_cart that
1st communication A (e.g., node to node) is minimized,
2nd B (e.g., CPU to CPU) is minimized, and 3rd C (e.g., core to core) is minimized

Further Interfaces (2)

If the application wants to choose the hardware levels,
but appropriate split types (as for MPI_COMM_SPLIT_TYPE() do not exist,
then the splitting can be done by the application
and an array with the hierarchical set of communicators is the input:

Substitute for / enhancement to existing MPI-1
MPI_Dims_create (size_of_comm_old, ndims, *dims*);
MPI_Cart_create (comm_old, ndims, dims, periods, reorder, **comm_cart*);

e.g., nlevels=3, and
level_comms[0] is comm_old,
level_comms[1 and 2] are the result
recursively called MPI_ Comm_split_type
with the type_levels from previous slide.

```
MPI_Cart_ml_create_from_comms(int nlevels,
              MPI_Comm level_comms[nlevels],
              int ndims,   double dim_weights[ndims],   int periods[ndims],  MPI_Info info,
/*OUT*/       int dims[ndims],   MPI_Comm *comm_cart );
```

Same as above

Same as above

Further Interfaces (3) – the basis

MPI_Cart_ml_create_from_comms(… level_comms, …)
can be implemented based on **MPI_Dims_ml_create(),**
which can be implemented through **MPI_Dims_weighted_create**()
provided that the **level_comms** have same size on each level

MPI_Dims_weighted_create (int nnodes, int ndims, double dim_weights[ndims],
int periods[ndims], MPI_Info info, /***INOUT***/ *int dims[ndims]*);

MPI_Dims_ml_create (int nnodes, int ndims, double dim_weights[ndims],
int nlevels, int sizes[nlevels], int periods[ndims], MPI_Info info,
/***OUT***/ *int dims_ml[ndims][nlevels]*); ← Multi-level info

Further Interfaces (3) – the basis (a)

MPI_Dims_weighted_create (int nnodes, int ndims, double dim_weights[ndims],
int periods[ndims], MPI_Info info, /***INOUT***/ *int dims[ndims]*);

The factorization of nnodes into the array dims is chosen in a way to minimize the communication according to the given weights. Note that this means that this function looks for a factorization with minimal sum $\sum_i$ *dims[i]* · *dims_weight[i]*.

Rationale. As shown in Figure 7.3, the total communication cost per node (left and right, in all dimensions) would be $C = 2\sum_i w_i / \prod_{j,j\neq i} d_j$ and with nnodes=$N = \prod_j d_j$, the cost is $C = \frac{2}{N}\sum_i w_i d_i$ (End of rationale.)

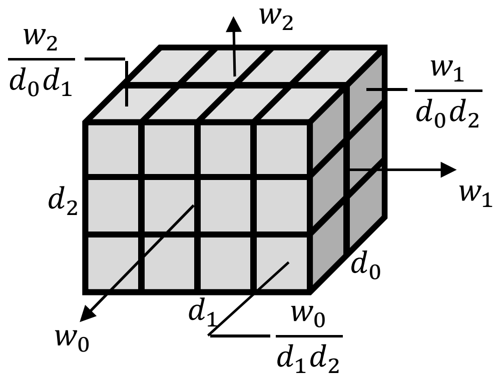


Figure 7.3: Communication model:
The dim_weights[i]=w_i express the total communication cost in the direction of dimension i. The communication cost of one process in direction i is therefore $w_i / \prod_{j,j\neq i} d_j$ with dims[i]=d_i.

Further Interfaces (3) – the basis (b)

MPI_Dims_ml_create (int nnodes, int ndims, double dim_weights[ndims],
int nlevels, int sizes[nlevels], int periods[ndims], MPI_Info info,
/***OUT***/ *int *dims_ml[ndims][nlevels]*);

It uses internally MPI_Dims_weighted_create() for each level → next slide

int *dims_ml

- represents in C an C++ a contigous two dimensional array *dims_ml[ndims][nlevels]*
- and *dims_ml(ndims,nlevels)* in Fortran

Further Interfaces Summary of (1-3)

Substitute for / enhancement to existing MPI-1
MPI_Dims_create (size_of_comm_old, ndims, *dims*);
MPI_Cart_create (comm_old, ndims, dims, periods, reorder, **comm_cart*);

e.g., with 25*25*24 = **15000 processes** on **625 ccNUMA nodes** with **2 CPUs/node** and **12 cores/CPU**

e.g., { MPI_COMM_TYPE_SHARED, OMPI_COMM_TYPE_NUMA within OpenMPI, or for further splitting: MPIX_COMM_TYPE_HW_TOPOLOGY}

```
MPI_Cart_ml_create_from_types(MPI_Comm comm_old,
            int nsplit_types,       int split_types[nsplit_types],
            int ndims,              double dim_weights[ndims],
            int periods[ndims],     MPI_Info info,
/*OUT*/     int dims[ndims],   MPI_Comm *comm_cart );
```

e.g., 3 dimensions with a data grid with 1000 x 1100 x 950 elements ➔ dim_weights[] = { 1.0/1000, 1.0/1100, 1.0/950 }

Rank mapping is based on:

- Node level: 625 = 5 x 25 x 5
- CPU level: 2 = 2 x 1 x 1
- Core level: 12 = 3 x 1 x 4

Result (product): **30 x 25 x 20**

The Cartesian communicator reflects this result: **30 x 25 x 20**

Next steps:
MPI_Comm_rank (comm_cart, &my_rank);
MPI_Cart_coords (comm_cart, my_rank, ndims, *coords*)

```
MPI_Cart_ml_create_from_comms(int nlevels,
            MPI_Comm level_comms[nlevels],
            int ndims,   double dim_weights[ndims],   int periods[ndims],  MPI_Info info,
/*OUT*/     int dims[ndims],   MPI_Comm *comm_cart );
```

e.g., level_comms[0] is comm_old, level_comms[1 and 2] are the result recursively called MPI_Comm_split_type with the type_levels from above.

Same as above

Same as above

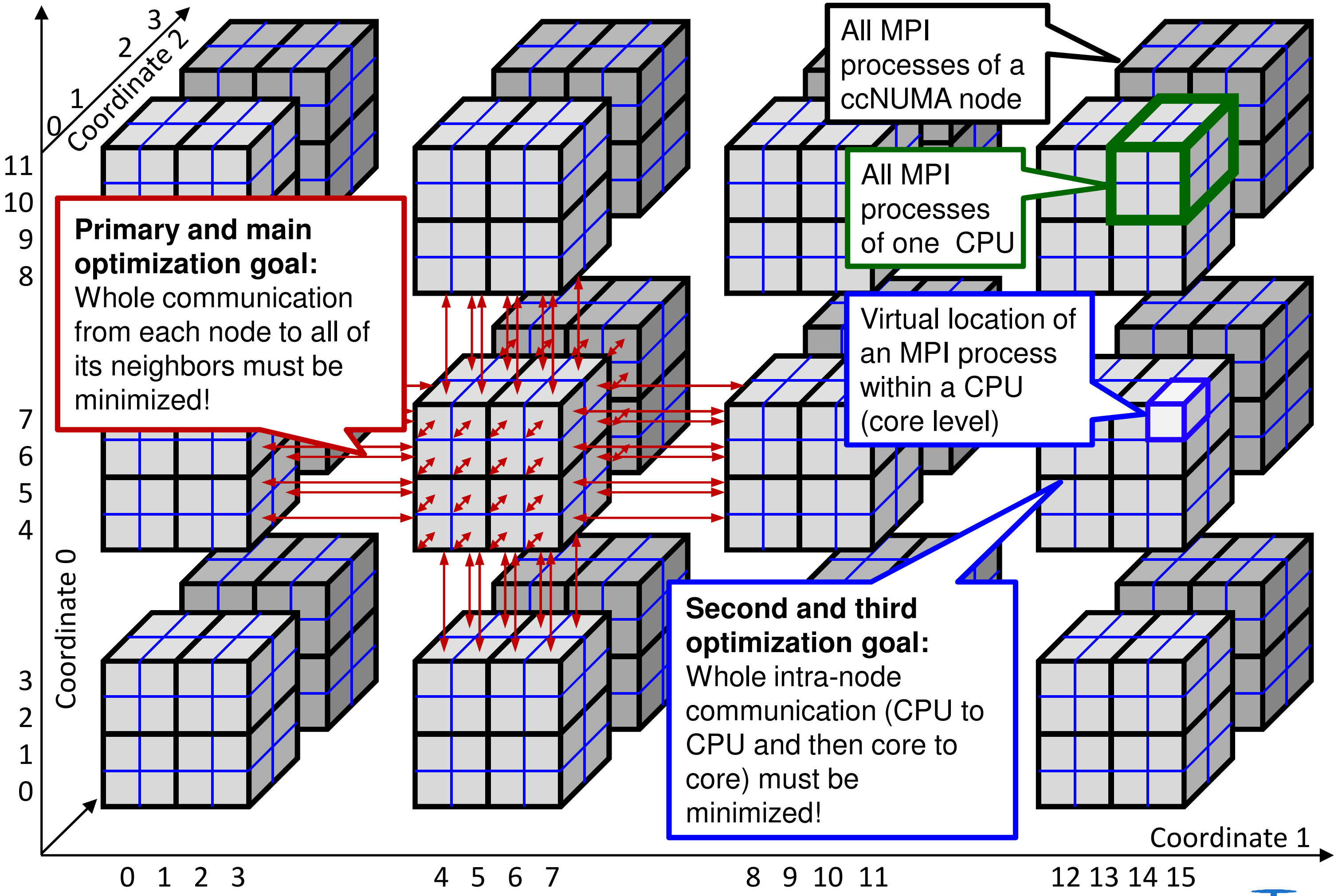
```
MPI_Dims_weighted_create ( int nnodes, int ndims, double dim_weights[ndims],
            int periods[ndims], MPI_Info info,  /*INOUT*/ int dims[ndims]);
```

```
MPI_Dims_ml_create ( int nnodes, int ndims, double dim_weights[ndims],
            int nlevels,  int sizes[nlevels], int periods[ndims],  MPI_Info info,
            /*OUT*/  int dims_ml[ndims][nlevels] );
```

Multi-level info

Hierarchical Cartesian Domain Decomposition

(figure used in the proposal for the MPI standard)



Further Interfaces (4)

Substitute for / enhancement to existing MPI-1
MPI_Dims_create (size_of_comm_old, ndims, *dims*);
MPI_Cart_create (comm_old, ndims, dims, periods, reorder, **comm_cart*);

From previous slides

MPI_Dims_ml_create (int nnodes, int ndims, double dim_weights[ndims],
int nlevels, int sizes[nlevels], int periods[ndims], MPI_Info info,
/***OUT***/ *int dims_ml[ndims][nlevels]*);

MPI_Cart_ml_create (MPI_Comm comm_old, int ndims, int *periods,
int nlevels, int dims_ml[ndims][nlevels], MPI_Info info,
/***OUT***/ *int *dims, MPI_Comm *comm_cart*);

This interface requires that comm_old is **ranked sequentially in the hardware**

We proposed the algorithm in

- Christoph Niethammer and Rolf Rabenseifner. 2018. Topology aware Cartesian grid mapping with MPI. EuroMPI 2018. https://eurompi2018.bsc.es/
→ Program → Poster Session → Abstract+Poster
- https://fs.hlrs.de/projects/par/mpi/EuroMPI2018-Cartesian/
→ All info + slides + software
- http://www.hlrs.de/training/par-prog-ws/
→ Practical → MPI.tar.gz → MPI/course/C/eurompi18/

Here, you get the new optimized interface + implementation + documentation

MPIX_Dims_weighted_create() is based on the ideas in:

- Jesper Larsson Träff and Felix Donatus Lübbe. 2015. Specification Guideline Violations by MPI Dims Create. In *Proceedings of the 22nd European MPI Users' Group Meeting (EuroMPI '15)*. ACM, New York, NY, USA, Article 19, 2 pages.

Implementation Remarks

- The portable MPIX routines internally use MPI_Comm_split_type(…, **MPI_COMM_TYPE_SHARED**, …) to split comm_old into ccNUMA nodes,
- plus (may be) additional splitting into NUMA domains.
- With using hyperthreads, it ***may be helpful*** to apply <u>**sequential** ranking</u> to the hyperthreads,
  – i.e., in MPI_COMM_WORLD, ranks 0+1 should be
    - **the first two hyperthreads**
    - of the first core
    - of the first CPU
    - of the first ccNUMA node
- Especially with weights w_i based on $\frac{G}{g_i}$, it is important
  – that the data of the grid points is **not** read in based on (**old**) ranks in MPI_COMM_WORLD,
  – because the domain decomposition must be done based on **comm_cart** and its dimensions and (**new**) ranks

Internal implementation plan

- **MPIX_Cart_weighted_create(...)**
  - chooses available and useful types for splitting, e.g., {MPI_COMM_TYPE_SHARED, OMPI_COMM_TYPE_NUMA or MPIX_COMM_TYPE_HALFNODE}

  → **MPIX_Cart_ml_create_from_types(...)**
- **MPIX_Cart_ml_create_from_types(...)**
  - loop over MPIX_Comm_split_type

  → **MPIX_Cart_ml_create_from_comms(...)**
- **MPIX_Cart_ml_create_from_comms(...)**
  - must calculate level_sizes[nlevels] and wether they are equally sized within the same level
  - if (equally-sized) then

    → **MPIX_Dims_ml_create(...)**
    - Appropriate renumbering based on dims_ml and the level_comms
    - Calculation of dims[] & creation of comm_cart → **MPI_Cart_create(…)** without reorder
  - else, e.g., algorithm of Thorsten Hoefler
- **MPIX_Cart_ml_create(...)** → Usable only for sequentially ranked comm_old
    - Appropriate renumbering based on dims_ml and the sequential comm_old
    - Calculation of dims[] & creation of comm_cart → **MPI_Cart_create(…)** without reorder
- **MPIX_Dims_ml_create(...)**

  → **MPIX_Dims_weighted_create(...)** on each level
- **MPIX_Dims_weighted_create(...)**
  - This is the important new base routine with a new fast brute force algorithm

Benchmark: halo_irecv_send_toggle_3dim_grid_solution.c

- Input per measurement, e.g.on 8 nodes x 2 CPUs x 12 cores: — Example
  - cart_method: — 2
    - **0=end, 1=Dims_create+Cart_create,**
    - **2=Cart_weighted_create(MPIX_WEIGHTS_EQUAL),**
    - **3=dito(weights), 4=dito manually, 5=Cart_ml_create(dims_ml)**
  - start grid sizes integer start values — 1 2 4
  - Using MPI_Type_vector, **for each dimension a pair of blocklength&stride** — 0 0 0 0 0 0 (0 0 = contiguous)
  - weights (double values) **(only with cart_method==4)** — 1.00 0.50 0.25
  - number of hardware levels **(only with cart_method==5)** — 3

    dims_ml: for each of the 3 Cartesian dimensions a list of 3 dimensions from outer to inner hardware level, e.g., 8 nodes x 2 CPUs x 12 cores are split into 1x2x4 nodes x 2x1x1 CPUs x 2x3x2 cores
    - **dims_ml[d=0] =** 1 2 2
    - **dims_ml[d=1] =** 2 1 3
    - **dims_ml[d=2] =** 4 1 2
- Input can be concatenated to one line per experiment:
  - 1 1 2 4 0 0 0 0 0 0
  - 2 1 2 4 0 0 0 0 0 0
  - 3 1 2 4 0 0 0 0 0 0
  - 4 1 2 4 0 0 0 0 0 0 4. 2. 1.
  - 5 1 2 4 0 0 0 0 0 0 3 1 2 2 2 1 3 4 1 2
  - 3 2 2 2 256 1024 4 32 0 0
  - 0

Start a 16-node batch-job with your own input file: **Report your acceleration factors to the course group**

examples for strided data in direction 0 & 1

Additional Remarks

- Caution with stdout and stdin when switching I/O from process world_rank==0 to cart_rank==0:
  - **Before** establishing the new comm_cart, all I/O on stdout/stdin is done by world_rank==0 (in **MPI_COMM_WORLD)**
  - **After** establishing the new comm_cart, all I/O on stdout/stdin is done by cart_rank==0 (in comm_cart)
  - In between, we recommended (although it is not guaranteed that an *output on comm_cart* may overtake an *output on MPI_COMM_WORLD*):
    - **MPI_Barrier(MPI_COMM_WORLD);**
    - **sleep(1);** // costs nearly nothing, e.g., 30 Mio € TCO/year / (365 days/year * 24 hours/day * 3600 sec/hour) * 1 sec = 1€
    - **MPI_Barrier(comm_cart);**
- The following slide shows the win through the re-ranking by the new routines:
  - Less % is better – the communication time reduction factors are:
    - **1.1-1.2**
    - **1.75**
    - **2.75**
    - **4.5-5.0**

Base grid sizes	Nodes x CPUs x cores	MPI_Dims_create + MPI_Cart_create Communicat. time [ms]	dims_ml[d=0] dims_ml[d=1] dims_ml[d=2]	MPIX_Cart_weighted_create(MPIX_WEIGHTS_EQUAL) Communication time [ms]	dims_ml[d=0] dims_ml[d=1] dims_ml[d=2]	MPIX_Cart_weighted_create(...weights...) Communicat. time [ms]	dims_ml[d=0] dims_ml[d=1] dims_ml[d=2]
2 x 2 x 2	8x2x12	84.545 = baseline	8 = 8 x 1 x 1 6 = 1 x 2 x 3 4 = 1 x 1 x 4	52.666 = 62%	8 = 2 x 2 x 2 6 = 2 x 1 x 3 4 = 2 x 1 x 2	48.556 = 57%	8 = 2 x 2 x 2 6 = 2 x 1 x 3 4 = 2 x 1 x 2
	64x2x12	194.856 = baseline	16=16 x 1 x 1 12= 4 x 1 x 3 8= 1 x 2 x 4	73.756 = 38%	16= 4 x 2 x 2 12= 4 x 1 x 3 8= 4 x 1 x 2	72.051 = 37%	16= 4 x 2 x 2 12= 4 x 1 x 3 8= 4 x 1 x 2
	512x2x12	247.631 = baseline	32=32 x 1 x 1 24=16 x 1x1.5 16= 1 x 2 x 8	85.530 = 35%	32= 8 x 2 x 2 24= 8 x 1 x 3 16= 8 x 1 x 2	85.491 = 35%	32= 8 x 2 x 2 24= 8 x 1 x 3 16= 8 x 1 x 2
1 x 2 x 4	8x2x12	172.850 = baseline	8 = 8 x 1 x 1 6 = 1 x 2 x 3 4 = 1 x 1 x 4	63.796 = 37%	8 = 2 x 2 x 2 6 = 2 x 1 x 3 4 = 2 x 1 x 2	37.953 = 22%	4 = 1 x 2 x 2 6 = 2 x 1 x 3 8 = 4 x 1 x 2
	64x2x12	360.364 = baseline	16=16 x 1 x 1 12= 4 x 1 x 3 8= 1 x 2 x 4	91.524 = 25%	16= 4 x 2 x 2 12= 4 x 1 x 3 8 = 4 x 1 x 2	74.199 = 21%	8 = 2 x 2 x 2 12= 4 x 1 x 3 16= 8 x 1 x 2
	512x2x12	457.858 = baseline	32=32 x 1 x 1 24=16 x 1x1.5 16= 1 x 2 x 8	125.468 = 27%	32= 8 x 2 x 2 24= 8 x 1 x 3 16= 8 x 1 x 2	93.615 = 20%	16= 4 x 2 x 2 24= 8 x 1 x 3 32=16 x 1 x 2
4 x 2 x 1	8x2x12	40.050 = baseline	8 = 8 x 1 x 1 6 = 1 x 2 x 3 4 = 1 x 1 x 4	59.421 =148%	8 = 2 x 2 x 2 6 = 2 x 1 x 3 4 = 2 x 1 x 2	36.778 =92%	16 = 4 x 2 x 2 6 = 2 x 1 x 3 2 = 1 x 1 x 2
	64x2x12	78.503 = baseline	16=16 x 1 x 1 12= 4 x 1 x 3 8= 1 x 2 x 4	100.203 =128%	16= 4 x 2 x 2 12= 4 x 1 x 3 8 = 4 x 1 x 2	69.802 =89%	32= 8 x 2 x 2 12= 4 x 1 x 3 4 = 2 x 1 x 2
	512x2x12	103.002 = baseline	32=32 x 1 x 1 24=16 x 1x1.5 16= 1 x 2 x 8	93.189 = 90%	32= 8 x 2 x 2 24= 8 x 1 x 3 16= 8 x 1 x 2	85.044 =83%	64=16 x 2 x 2 24= 8 x 1 x 3 8= 4 x 1 x 2

Halosize/process ~= 26 MB — Depend on chosen dims

Used process dimensions

Internally applied dimen-sions on each hardware level

Base factors, not absolute values

By default, communica-tion time strongly depends on cuboid's direction

Optimized communi-cation times are nearly indepen-dent of cubid's form

On Cray XC40 Hazel hen at HLRS Stuttgart, Jan 2019

As Exercise: To do (1)

- **cp ~/MPI/course/C/Ch9/MPIX_*/* .**
  - You get the benchmark skeleton halo_irecv_send_toggle_3dim_grid_skel.c
  - And all MPIX_*.c files and the header MPIX_interface_proposal.h
- **mpicc –o halo_skel.exe halo_irecv_send_toggle_3dim_grid_skel.c MPIX_*.c**
- First test with non-optimized cart_method==1**, i.e., MPI_Dims_create + MPICart_create**
  - Choose your batch job: **halo_skel_[LRZ|VSC|HLRS].sh** which contains
    - **Number of nodes and cores/node**
    - **and, e.g.,**
      mpirun –np 192 ./halo_skel.exe < input-skel.txt

      1 2 2 2 000000
      1 1 2 4 000000
      0
  - Start your batchjob
  - Try to understand the output:
    - **It contains two experiments: a grid with cubic and one with non-cubic ratio**
    - **The number of MPI processes, e.g. 192, is factorized**
      → domain decomposition into, e.g., 8 x 6 x 4 processes
    - **The measurements are done for 10 global gridsizes**
    - **The domain decomposition implies the local gridsizes**
    - **The local gridsizes imply the size of the halos in each direction**
    - **→ the sum of the time for the communication into the 3 dimensions x 2 directions (left+right)**

See **next slide**

Exercise: To do (2)

```
cart_method = 1
start grid sizes integer start values for 3 dimensions = 2 2 2
blocklength & sgtride pairs for each of the 3 dimensions = 1 0   1 0   1 0
Creating the Cartesian communicator and further input arguments:
cart_method == 1: MPI_Dims_create + MPI_Cart_create
[MPI_Barrier and switching to output via stdout through rank==0 in comm_cart]
ndims=3 dims= 8 6 4
  message size     transfertime  duplex bandwidth per process and neighbor (grid&halo in #floats)
                                                  gridsizes total=  per process=  halosizes=
       128 bytes     34.537 usec   3.706 MB/s    16    12    12     2   2    3        16=     6 +     6 +      4
       432 bytes     39.840 usec  10.843 MB/s    24    24    24     3   4    6        54=    24 +    18 +     12
      1728 bytes     41.122 usec  42.021 MB/s    48    48    48     6   8   12       216=    96 +    72 +     48
      6688 bytes     23.961 use                  96    96    92    12  16   23       836=   368 +   276 +    192
     25576 bytes     93.703 use                 184   186   184    23  31   46      3197=  1426 +  1058 +    713
    104408 bytes    271.721 use                 376   372   372    47  62   93     13051=  5766 +  4371 +   2914
    411192 bytes   1033.001 usec    .056 MB/s   744   738   740    93 123  185     51399= 22755+17205 +  11439
   1636392 bytes   4398.680 use    72.019 MB/s 1480  1476  1476   185 246  369    204549= 90774+68265 +  45510
   6561336 bytes  18173.518 usec  361.038 MB/s 2960  2958  2956   370 493  739    820167=364327+273430+182410
  26194104 bytes  76132.216 usec  344.061 MB/s 5912  5910  5908   739 985 1477   3274263=1454845+1091503+727915

cart_method = 1
start grid sizes integer start values for 3 dimensions = 1 2 4
blocklength & sgtride pairs for each of the 3 dimensions = 0 0   0 0   0 0
cart_method == 1: MPI_Dims_create + MPI_Cart_create
ndims=3 dims= 8 6 4
  message size     transfertime  duplex bandwidth per process and neighbor (grid&halo in #floats)
       160 byte      14.720 usec  10.870 MB/s     8    12    24     1   2    6        20=    12 +     6 +      2
       ...
  34936960        156869.278 usec 222.714 MB/s 2960  5910 11816   370 985 2954   4367120=2909690+1092980+364450
```

192 processes: Input for `MPI_Dims_create()`

These base values (per process) are multiplied with $\sqrt[3]{\#processes}$ and then with 1, 2, 4, 8, … 512, e.g., $2 \cdot \sqrt[3]{192} \cdot 512 =$ **5912** (rounded to a multiple the dimension)

divide by dims[i]

First value for our table

* 2 directions * 4 byte

multiply for 2-d halo array size

Same values, because MPI_Dims_create() factorizes the #processes independent from the user's gridsizes.

Second value for our table

Exercise: To do (3)

- **Fill in the table**

Given from MPI_Dims_create()

	Nodes	CPUs	cores
d=0: **8** =	**8**	x 1	x 1
d=1: **6** =	**1**	x 2	x 3
d=2: **4** =	**1**	x 1	x 4
Total 192 =	**8**	**x 2**	**x12**

Given by batchjob and hardware

Please, calculated by hand:
Fill in maximal factors.
Factorize first the cores and start with d=2.
Then the CPUs & then the nodes.
(All based on sequential ranking of MPI_COMM_WORLD)

Defined in batch job + hardware knowledge

Execution time of **largest** grid and halo size of both measurements

Halosize/process ~= 26 MB		**MPI_Dims_create + MPI_Cart_create**		**MPIX_Cart_ml_create(MPIX_WEIGHTS_EQUAL)**		**MPIX_Cart_weighted_create(...weights...)**	
Base grid sizes	Nodes x CPUs x cores	Communicat. time [ms]	dims_ml[d=0] dims_ml[d=1] dims_ml[d=2]	Communication time [ms]	dims_ml[d=0] dims_ml[d=1] dims_ml[d=2]	Communicat. time [ms]	dims_ml[d=0] dims_ml[d=1] dims_ml[d=2]
2 x 2 x 2	__x__x__	______ = baseline	__ = _ x _ x _ __ = _ x _ x _ __ = _ x _ x _				
1 x 2 x 4	Same as above	______ = baseline	Same as above				

Exercise: To do (4)

- **cp halo_irecv_send_toggle_3dim_grid_skel.c halo_optim.c**
- **Edit halo_optim.c**
  - On lines 160, 165, 171, and 184, substitute the /* **TODO: …** */ by correct code

```
153  if (cart_method == 1) {
154    if (my_world_rank==0) printf("cart_method == 1: MPI_Dims_create + MPI_Cart_create\n");
155    MPI_Dims_create(size, ndims, dims);
156    MPI_Cart_create(MPI_COMM_WORLD, ndims, dims, periods, 0, &comm_cart);
157  } else if (cart_method == 2) {
158    if (my_world_rank==0) printf("cart_method == 2: MPIX_Cart_weighted_create( MPIX_WEIGHTS_EQUAL )\n");

160    /* TODO: Appropriate call to MPIX_Cart_weighted_create(...) with MPIX_WEIGHTS_EQUAL
161            instead of calling MPI_Dims_create() and MPI_Cart_create() as in method 1 */

163  } else if (cart_method == 3) {

165    /* TODO: Appropriate calculation of weights[ ] based on gridsize_avg_per_proc_startval[ ] */

167    if (my_world_rank==0) { printf("cart_method == 3: MPIX_Cart_weighted_create( weights := ____________TODO____________)\n");
168      printf("weights= "); for (d=0; d<ndims; d++) printf(" %lf",weights[d]); printf("\n");
169    }

171    /* TODO: Appropriate call to MPIX_Cart_weighted_create(...) with weights
172            instead of MPIX_WEIGHTS_EQUAL as in method 2 */

174  } else if (cart_method == 4) {
175    for (d=0; d<ndims; d++) weights[d] = 4.0 / gridsize_avg_per_proc_startval[d];
176    if (my_world_rank==0) { printf("cart_method == 4: MPIX_Cart_weighted_create( manual weights )\n");
177      printf("weights (double values) for %d dimensions (e.g., ", ndims);
178      for (d=0; d<ndims; d++) printf(" %lf",weights[d]); printf(") ?\n");
179      for (d=0; d<ndims; d++) scanf("%lf",&weights[d]);
180      printf("weights= "); for (d=0; d<ndims; d++) printf(" %lf",weights[d]); printf("\n");
181    }
182    MPI_Bcast(weights, ndims, MPI_DOUBLE, 0, MPI_COMM_WORLD);

184    /* TODO: Appropriate call to MPIX_Cart_weighted_create(...)
185            same as in method 3, but without the calculation of the weights */

187  } else { …
```

Exercise: To do (5)

- **mpicc –o halo_optim.exe halo_optim.c MPIX_*.c**
- Check: **diff halo_optim.c halo_irecv_send_toggle_3dim_grid_solution.c**
- Now, use all three cart_method==1, 2, 3
  - Choose your batch job:
    - **halo_optim_[LRZ|VSC|HLRS].sh** which contains:
    - **mpirun –np 192 ./halo_optim.exe < input-optim.txt**
  - Start your batchjob → output file **output_optim.txt**
  - Fill in the table

Cart_method | Base gridsizes | Block length + stride for each dimension

```
1  2 2 2  0 0 0 0 0 0
2  2 2 2  0 0 0 0 0 0
1  1 2 4  0 0 0 0 0 0
2  1 2 4  0 0 0 0 0 0
3  1 2 4  0 0 0 0 0 0
0
```

0 = end

Note, that the optimization changes the dims-array → modified halo sizes!

Although halos may be larger, the optimized communication time should be shorter!

Halosize/process ~= 26 MB		cart_method==1 MPI_Dims_create + MPI_Cart_create		cart_method==2 MPIX_Cart_weighted_create(MPIX_WEIGHTS_EQUAL)		cart_method==3 MPIX_Cart_weighted_create(...weights...)	
Base grid sizes	Nodes x CPUs x cores	Communicat. time [ms]	dims_ml[d=0] dims_ml[d=1] dims_ml[d=2]	Communication time [ms]	dims_ml[d=0] dims_ml[d=1] dims_ml[d=2]	Communicat. time [ms]	dims_ml[d=0] [d=1] [d=2]
2 x 2 x 2	__x__x__	______ = baseline	__ = _ x _ x _ __ = _ x _ x _ __ = _ x _ x _	______ = _____% of baseline	__ = _ x _ x _ __ = _ x _ x _ __ = _ x _ x _	Same as with MPIX_WEIGHTS_EQUAL	
1 x 2 x 4	__x__x__	______ = baseline	Same as above	______ = _____% of baseline	__ = _ x _ x _ __ = _ x _ x _ __ = _ x _ x _	______ = _____% of baseline	__ = _ x _ x _ __ = _ x _ x _ __ = _ x _ x _

Reported by MPI_Cart_weighted_create()

Exercise: Results – HLRS, Stuttgart, hazelhen

Halosize/process ~= 26 MB		MPI_Dims_create + MPI_Cart_create		MPIX_Cart_weighted_create(MPIX_WEIGHTS_EQUAL)		MPIX_Cart_weighted_create(...weights...)	
Base grid sizes	Nodes x CPUs x cores	Communicat. time [ms]	dims_ml[d=0] dims_ml[d=1] dims_ml[d=2]	Communication time [ms]	dims_ml[d=0] dims_ml[d=1] dims_ml[d=2]	Communicat. time [ms]	dims_ml[d=0] dims_ml[d=1] dims_ml[d=2]
2 x 2 x 2	8 x 2 x 12	78.748 = baseline	8 = 8 x 1 x 1 6 = 1 x 2 x 3 4 = 1 x 1 x 4	50.971 = 65% of baseline	8 = 2 x 2 x 2 6 = 2 x 1 x 3 4 = 2 x 1 x 2	Same as with MPIX_WEIGHTS_EQUAL	
1 x 2 x 4	8 x 2 x 12	168.891 = baseline	Same as above	64.691 = 38% of baseline	8 = 2 x 2 x 2 6 = 2 x 1 x 3 4 = 2 x 1 x 2	38.406 = 23% of baseline	4 = 1 x 2 x 2 6 = 2 x 1 x 3 8 = 4 x 1 x 2

Exercise: Results – LRZ, Garching, ivyMUC

Halosize/process ~= 26 MB		MPI_Dims_create + MPI_Cart_create		MPIX_Cart_weighted_create(MPIX_WEIGHTS_EQUAL)		MPIX_Cart_weighted_create(...weights...)	
Base grid sizes	Nodes x CPUs x cores	Communicat. time [ms]	dims_ml[d=0] dims_ml[d=1] dims_ml[d=2]	Communication time [ms]	dims_ml[d=0] dims_ml[d=1] dims_ml[d=2]	Communicat. time [ms]	dims_ml[d=0] dims_ml[d=1] dims_ml[d=2]
2 x 2 x 2	12 x 2 x 8	34.814 = baseline	8 = 6 x 1.3 x 1 6 = 1 x 1.5 x 2 4 = 1 x 1 x 4	26.675 = 77% of baseline	6 = 3 x 1 x 2 8 = 2 x 2 x 2 4 = 2 x 1 x 2	Same as with MPIX_WEIGHTS_EQUAL	
1 x 2 x 4	12 x 2 x 8	54.344 = baseline	Same as above	35.665 = 66% of baseline	6 = 3 x 1 x 2 8 = 2 x 2 x 2 4 = 2 x 1 x 2	22.933 = 42% of baseline	4 = 1 x 2 x 2 6 = 3 x 1 x 2 8 = 4 x 1 x 2

Exercise: Results – VSC, Vienna, ___(not yet done)___

Halosize/process ~= 26 MB		MPI_Dims_create + MPI_Cart_create		MPIX_Cart_weighted_create(MPIX_WEIGHTS_EQUAL)		MPIX_Cart_weighted_create(...weights...)	
Base grid sizes	Nodes x CPUs x cores	Communicat. time [ms]	dims_ml[d=0] dims_ml[d=1] dims_ml[d=2]	Communication time [ms]	dims_ml[d=0] dims_ml[d=1] dims_ml[d=2]	Communicat. time [ms]	dims_ml[d=0] dims_ml[d=1] dims_ml[d=2]
2 x 2 x 2	12 x 2 x 8	______ = baseline	8 = 6 x 1.3 x 1 6 = 1 x 1.5 x 2 4 = 1 x 1 x 4	______ = _____% of baseline	__ = _ x _ x _ __ = _ x _ x _ __ = _ x _ x _	Same as with MPIX_WEIGHTS_EQUAL	
1 x 2 x 4	12 x 2 x 8	______ = baseline	Same as above	______ = _____% of baseline	__ = _ x _ x _ __ = _ x _ x _ __ = _ x _ x _	______ = _____% of baseline	__ = _ x _ x _ __ = _ x _ x _ __ = _ x _ x _

Exercise: Your result: ______________________

Halosize/process ~= 26 MB		MPI_Dims_create + MPI_Cart_create		MPIX_Cart_weighted_create(MPIX_WEIGHTS_EQUAL)		MPIX_Cart_weighted_create(...weights...)	
Base grid sizes	Nodes x CPUs x cores	Communicat. time [ms]	dims_ml[d=0] dims_ml[d=1] dims_ml[d=2]	Communication time [ms]	dims_ml[d=0] dims_ml[d=1] dims_ml[d=2]	Communicat. time [ms]	dims_ml[d=0] dims_ml[d=1] dims_ml[d=2]
2 x 2 x 2	__x__x__	______ = baseline	__ = _ x _ x _ __ = _ x _ x _ __ = _ x _ x _	______ = _____% of baseline	__ = _ x _ x _ __ = _ x _ x _ __ = _ x _ x _	Same as with MPIX_WEIGHTS_EQUAL	
1 x 2 x 4	__x__x__	______ = baseline	Same as above	______ = _____% of baseline	__ = _ x _ x _ __ = _ x _ x _ __ = _ x _ x _	______ = _____% of baseline	__ = _ x _ x _ __ = _ x _ x _ __ = _ x _ x _

References

[1] Pavan Balaji et al. 2009-2012. Topology awareness in MPI Dims create. https://github.com/mpi-forum/mpi-forumhistoric/issues/195 Accessed 2018-07-19.

Another approach using the existing MPI_Cart_create() interface:

[2] William D. Gropp, Using Node [and Socket] Information to Implement MPI Cartesian Topologies, Parallel Computing, 2019, and in: Proceedings of the 25th European MPI User' Group Meeting, EuroMPI'18, ACM, New York, NY, USA, 2018, pp. 18:1-18:9. doi:10.1145/3236367.3236377.
Slides: http://wgropp.cs.illinois.edu/bib/talks/tdata/2018/nodecart-final.pdf.

And for unstructured grids:

[3] T. Hoefler and M. Snir. 2011. Generic Topology Mapping Strategies for Large-scale Parallel Architectures. In *Proceedings of the 2011 ACM International Conference on Supercomputing (ICS'11)*. ACM, 75–85.

Used as theoretical basis for implementing MPI_Dims_weighted_create():

[4] Jesper Larsson Träff and Felix Donatus Lübbe. 2015. Specification Guideline Violations by MPI Dims Create. In *Proceedings of the 22nd European MPI Users' Group Meeting (EuroMPI '15)*. ACM, New York, NY, USA, Article 19, 2 pages.