NUMA–aware strategies for the heterogeneous execution of SpMV on modern supercomputers

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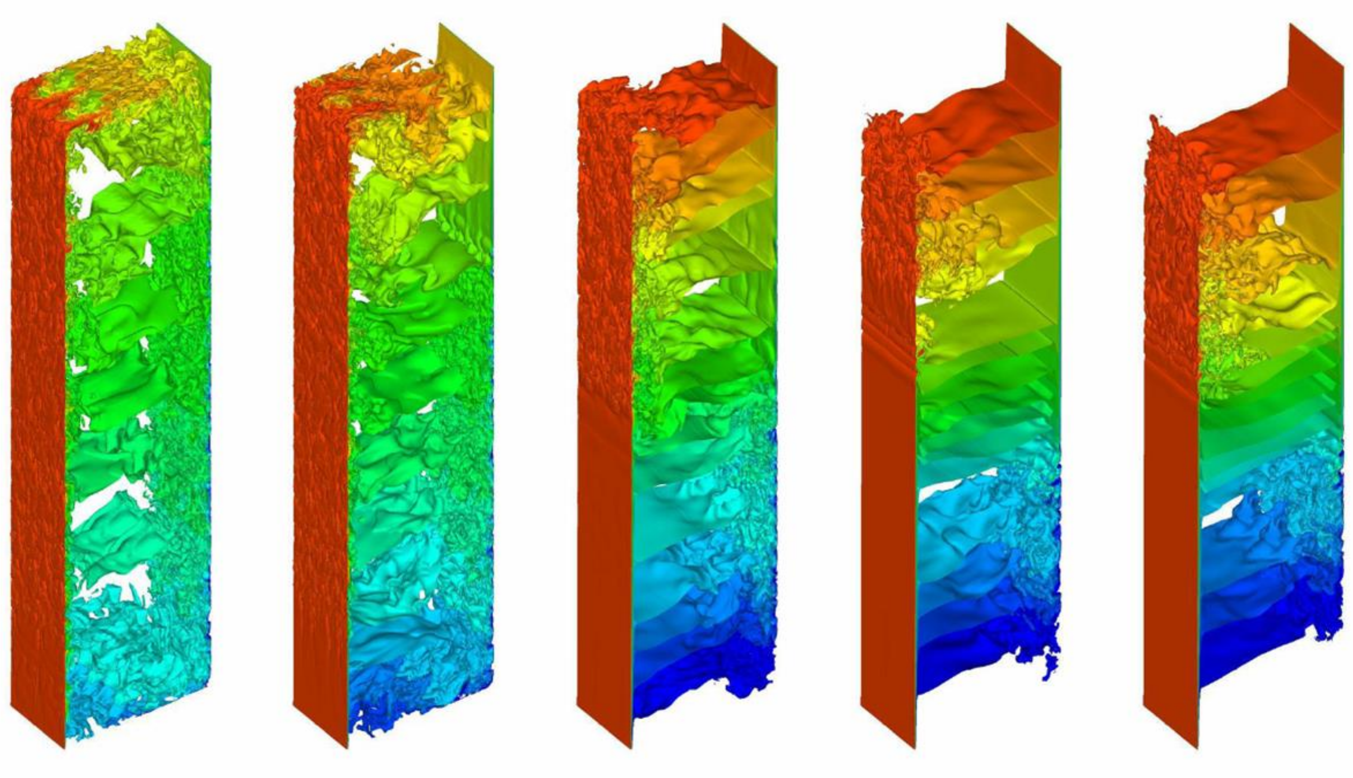
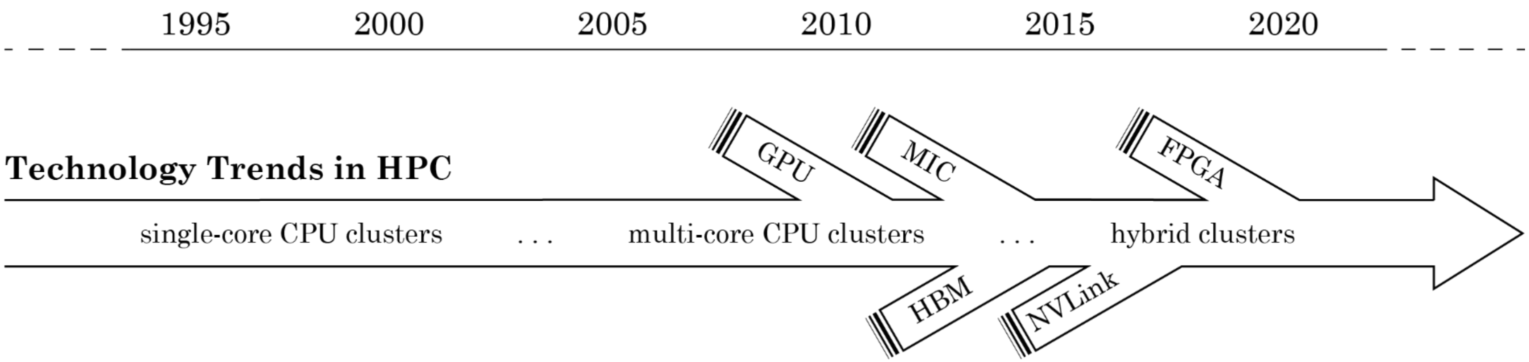
The role of SpMV in scientific computing software

INTRODUCTION

The Heat and Mass Transfer Technological Center

is a research group of the Technical University of Catalonia highly concerned about the environmental sustainability. Specifically, researchers at the CTTC have been enrolled in both fundamental and applied research, studying several phenomena: natural and forced convection, multi-phase flow, aerodynamics, among many others.

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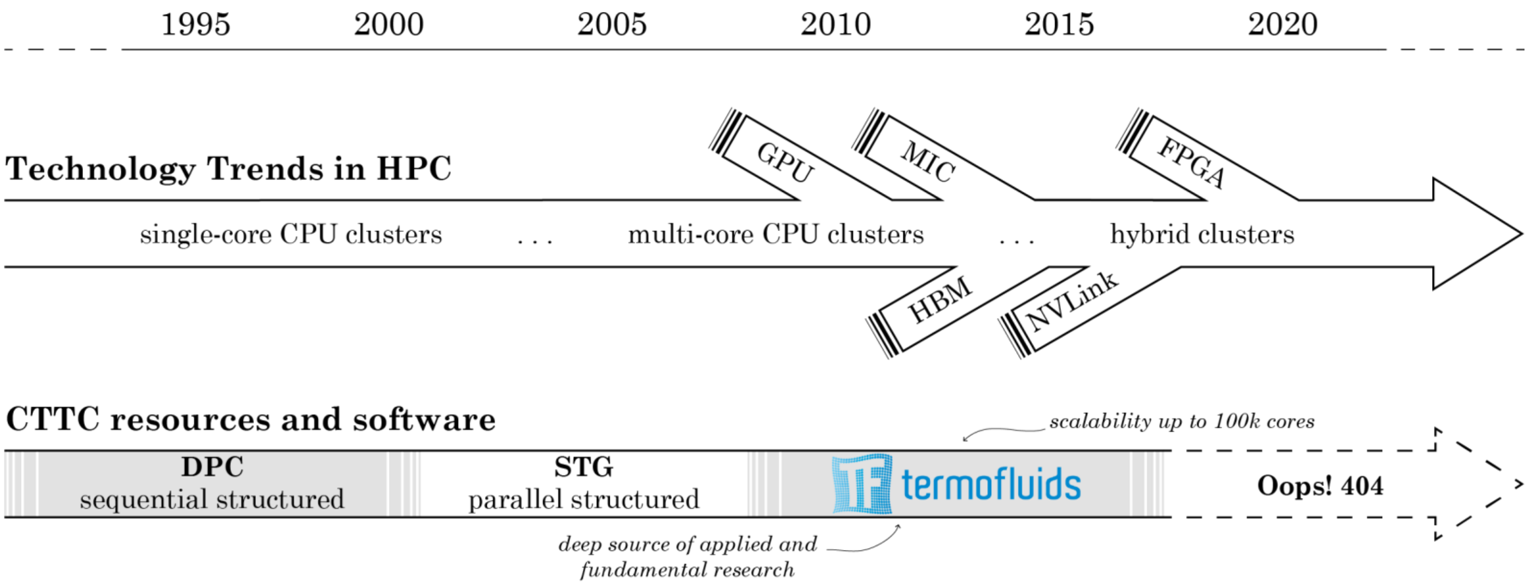
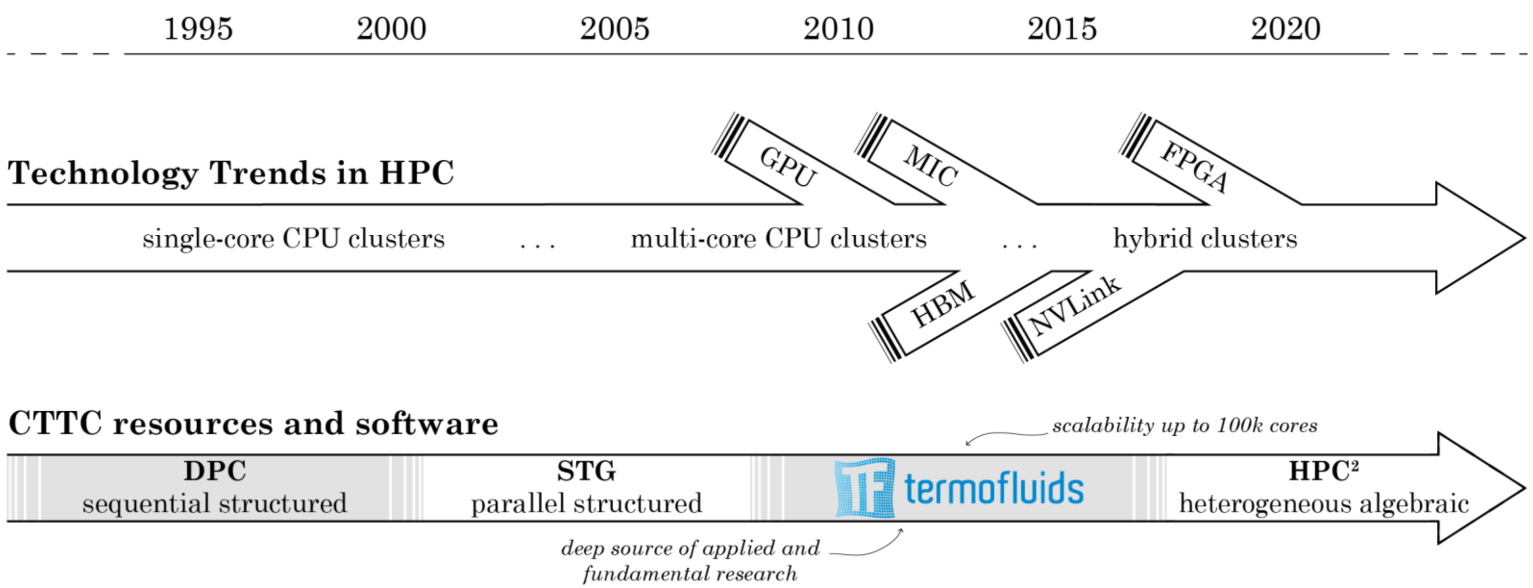


Since the beginning,
researchers of CTTC have developed and adapted CFD codes for the state-of-the art computer resources.



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Currently,
a fully-portable, algebra-based framework for heterogeneous computing is being developed. Namely, the traditional stencil data structures and sweeps are replaced by algebraic data structures and kernels, and the discrete operators and mesh functions are then stored as sparse matrices and vectors, respectively.

Stencil-based method

Algebra-based method

Stencil-based method

Given a mesh,
specific stencil loops or kernels are designed to compute quantities such as Gradient or Divergence.

Algebra-based method

Given a mesh,
specific sparse matrices are built to represent discrete operators such as Gradient or Divergence.

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Unique data-sets
are required to implement different numerical methods using different stencil kernels.

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Different data-sets
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Complex kernels
minimize intermediate calculations and data usage, and maximize the arithmetic intensity.

Algebra-based method

Given a mesh,
specific sparse matrices are built to represent discrete operators such as Gradient or Divergence.

Different data-sets
are required to implement different numerical methods using the same algebraic kernels.

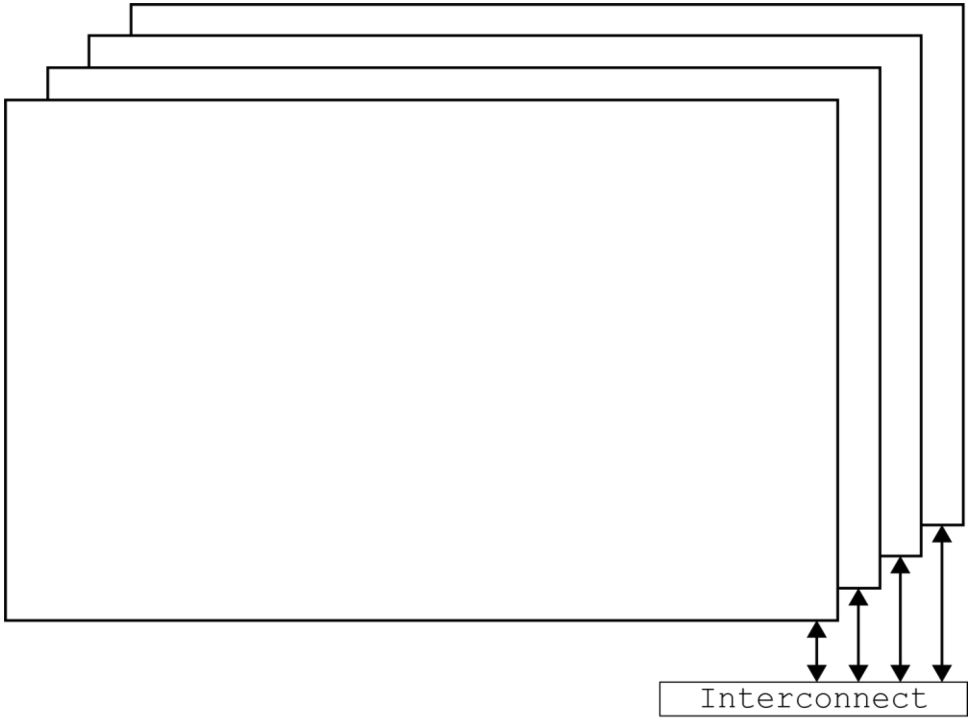
Simple kernels
are reusable and exist in many optimized libraries. Thus, an algebra-based framework is naturally portable.

Workload distribution and parallel execution of SpMV kernel on hybrid systems

IMPLEMENTATION

High-performance computing systems

High-performance computing systems

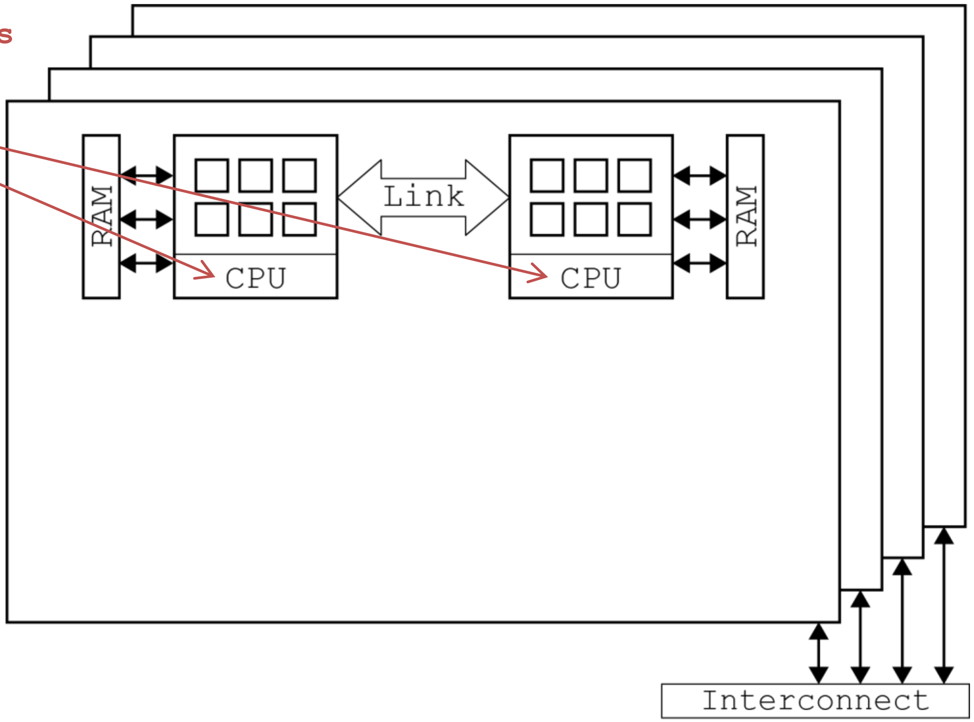


multiple nodes interconnected via high-bandwidth network

we use MPI at this level

High-performance computing systems

multiple multi-core CPU per node
we use OpenMP at this level



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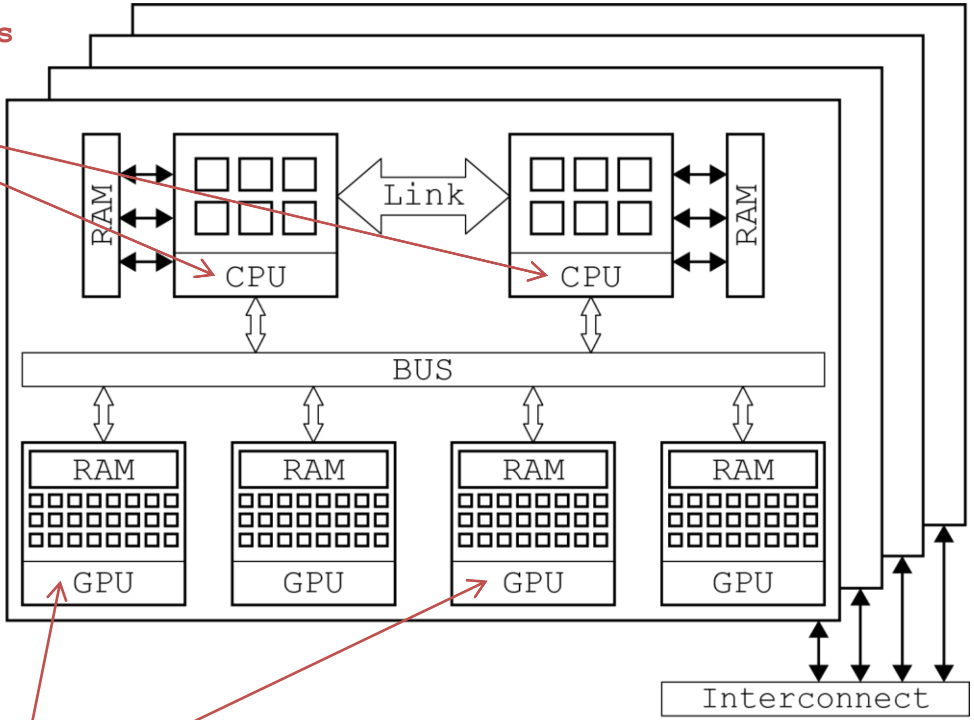
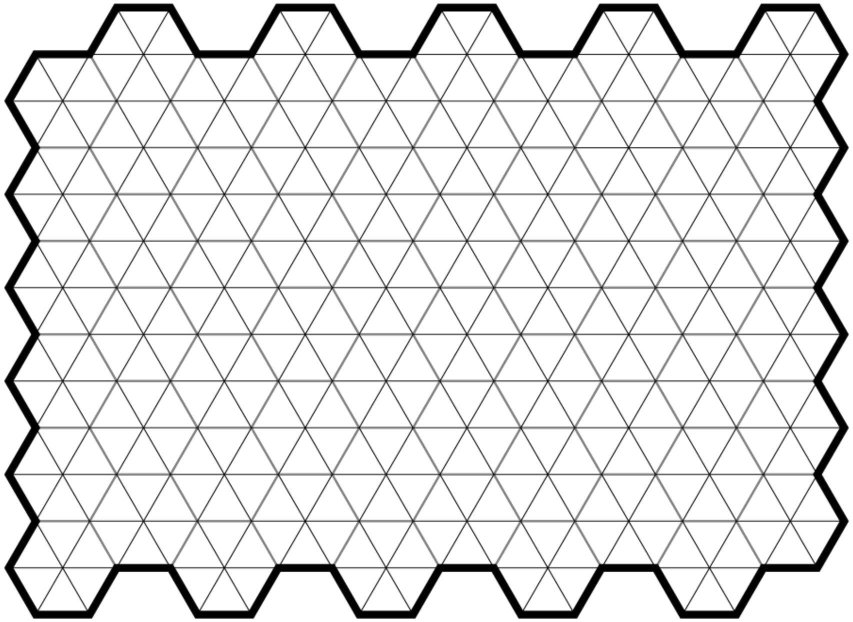


multiple accelerators per node
we use OpenCL/CUDA at this level

multiple nodes interconnected via high-bandwidth network
we use MPI at this level

Multilevel workload distribution

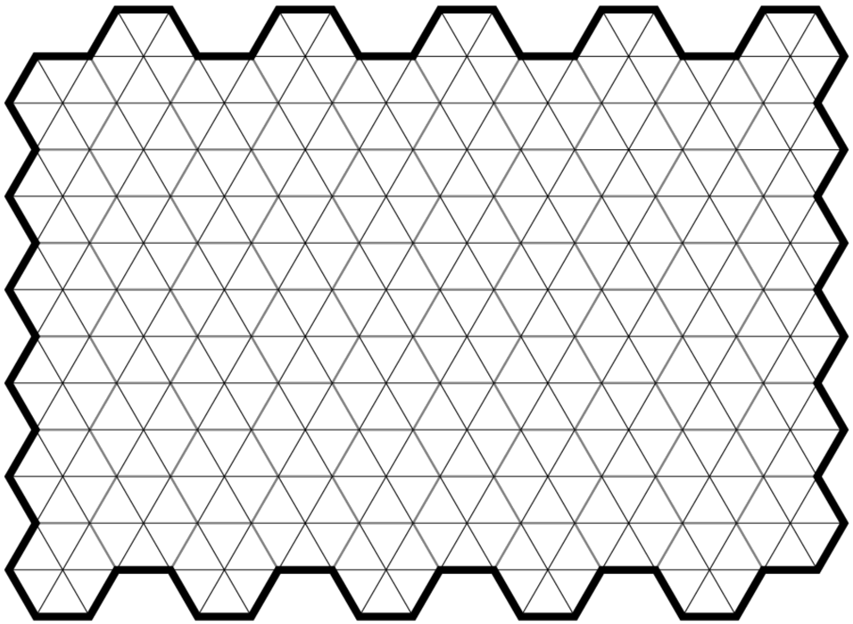


Multilevel workload distribution consists of dividing the computational domain (mesh) into subsets recursively to distribute it among the hardware of a computing system.

First-level

Second-level

Third-level



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First-level decomposition divides the workload among the computing nodes, that is, the MPI processes.

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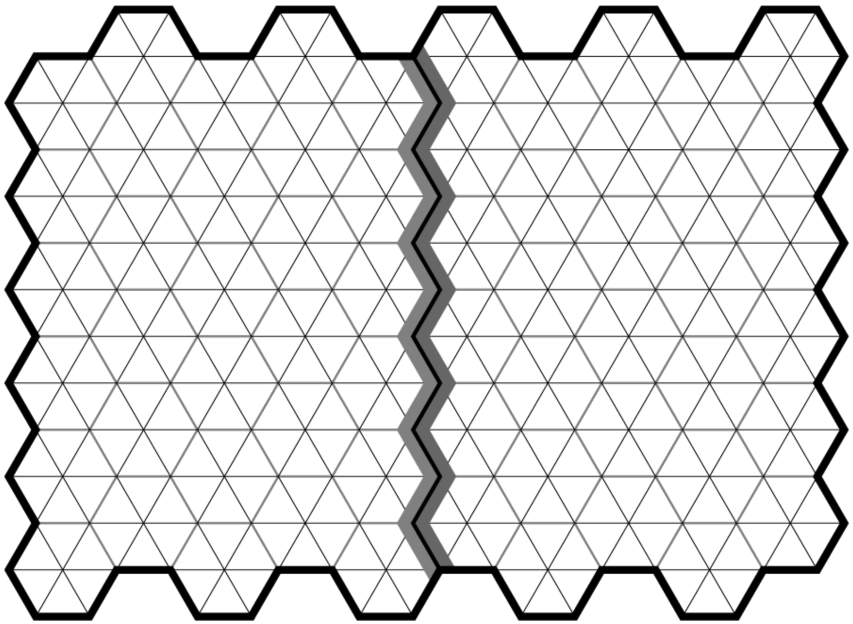
Third-level

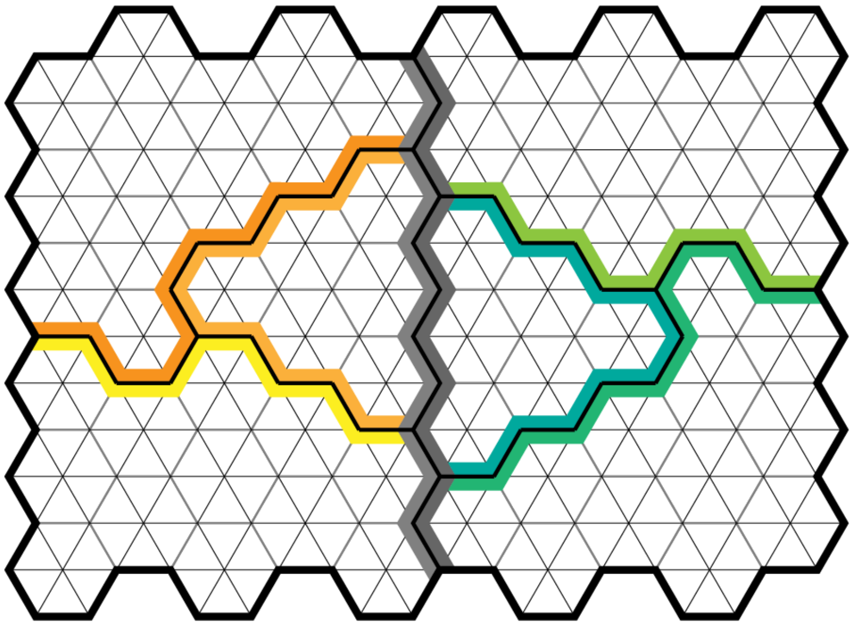


Multilevel workload distribution consists of dividing the computational domain (mesh) into subsets recursively to distribute it among the hardware of a computing system.

First-level decomposition divides the workload among the computing nodes, that is, the MPI processes.

Second-level decomposition divides the first-level partitions to share each MPI's workload among its available hardware, that is, the host and co-processors.

Third-level



Multilevel workload distribution

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First-level

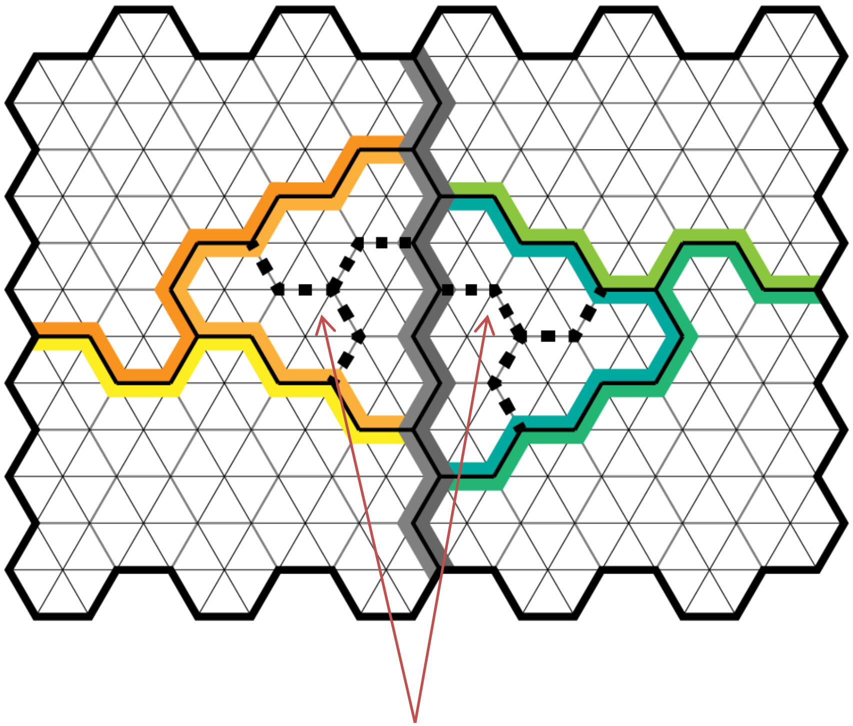
decomposition divides the workload among the computing nodes, that is, the MPI processes.

Second-level

decomposition divides the first-level partitions to share each MPI's workload among its available hardware, that is, the host and co-processors.

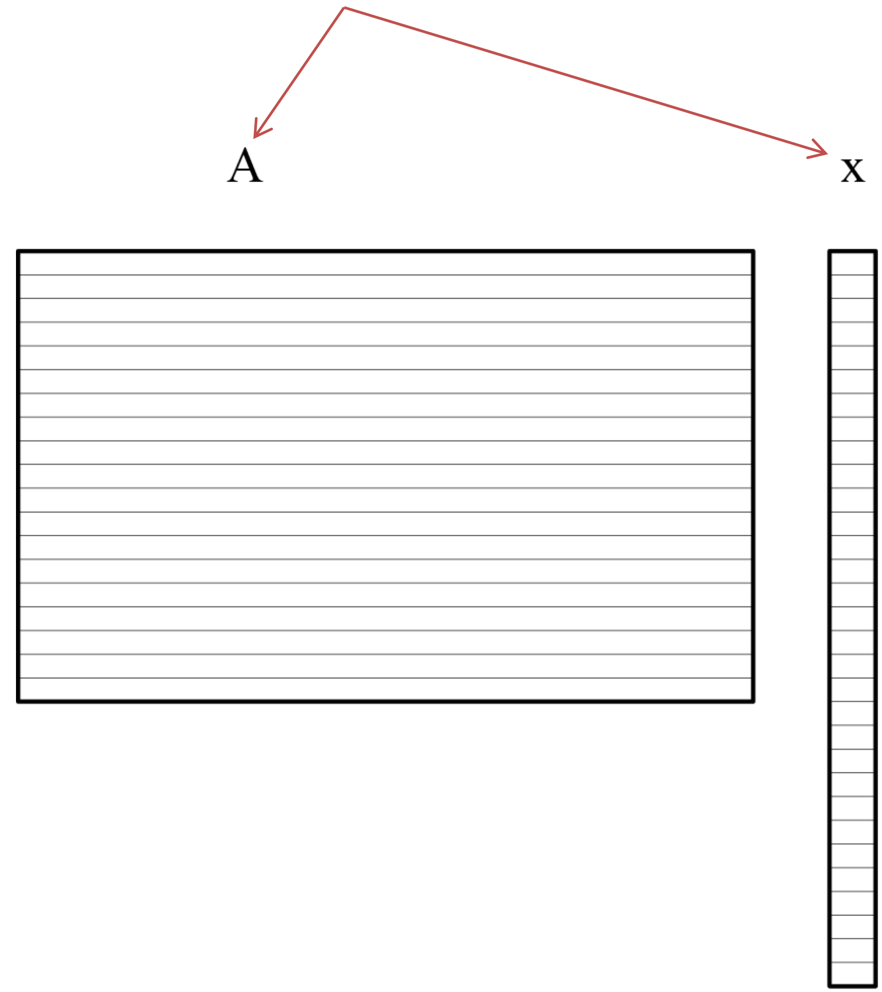
Third-level

decomposition divides the second-level partitions to distribute the workload of a device whose shared-memory space introduces a significant NUMA factor, that is, multiple NUMA nodes in a manycore CPU.



Sparse matrices and vectors

blocks represent the second-level partition of sparse matrix and vector instances assigned to each device.



Sparse matrices and vectors represent discrete operators and mesh functions in our algebra-based framework, respectively. Thus, sparse matrix rows and vector elements are distributed among subdomains, and classified into three subsets:

Inner

Interface

Halo

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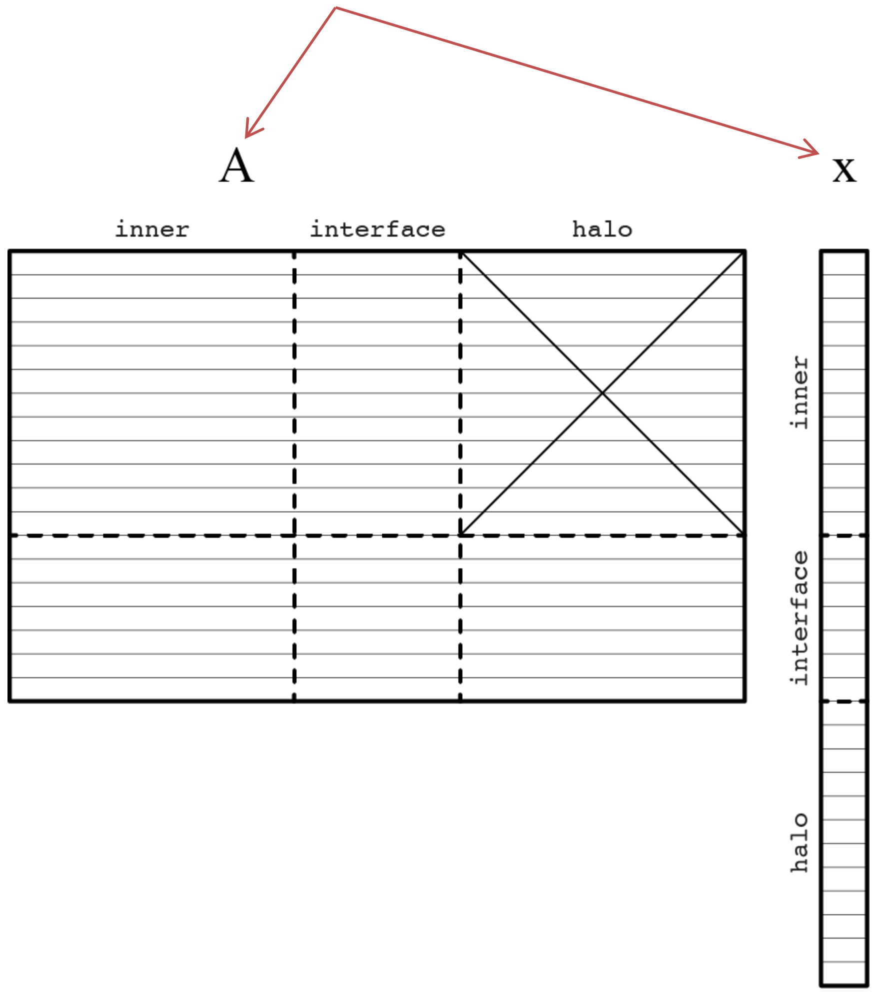

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subset is composed of local elements which are coupled with local elements only.

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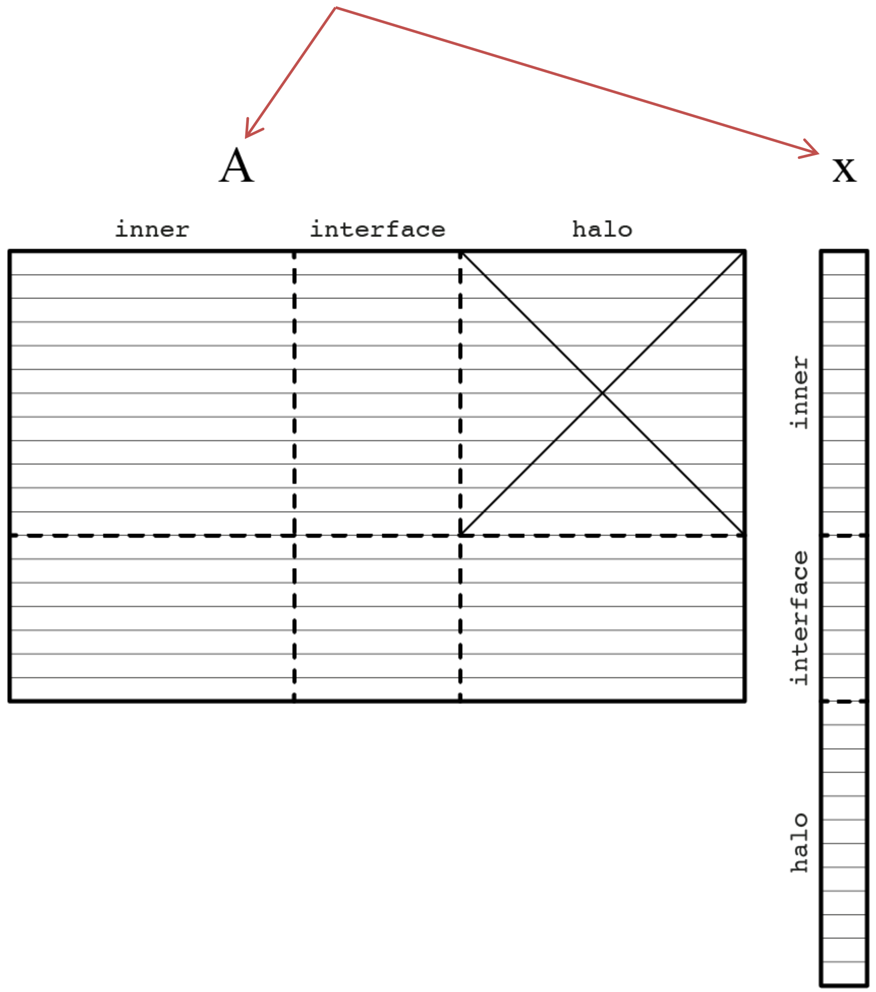

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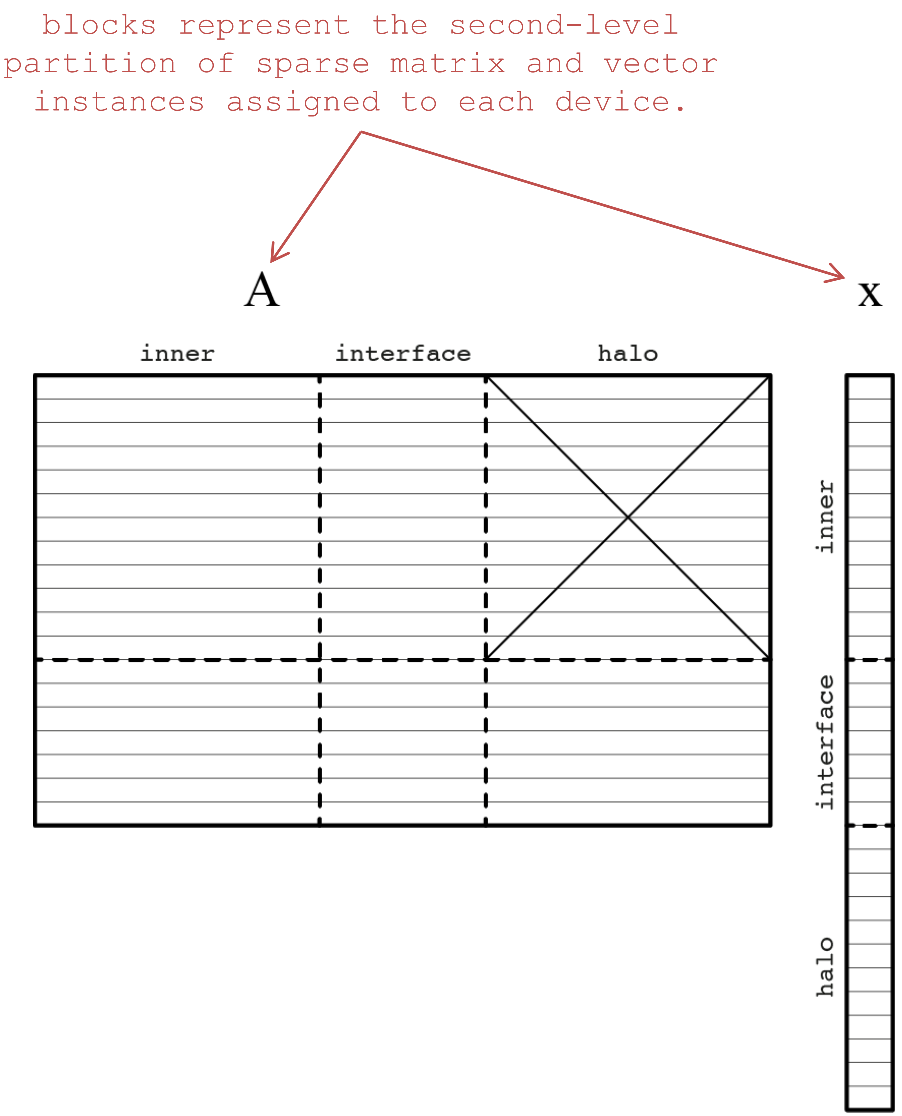
subset is composed of local elements which are coupled with local elements only.

Interface

subset is composed of local elements which are coupled with an element from other subdomain.

Halo



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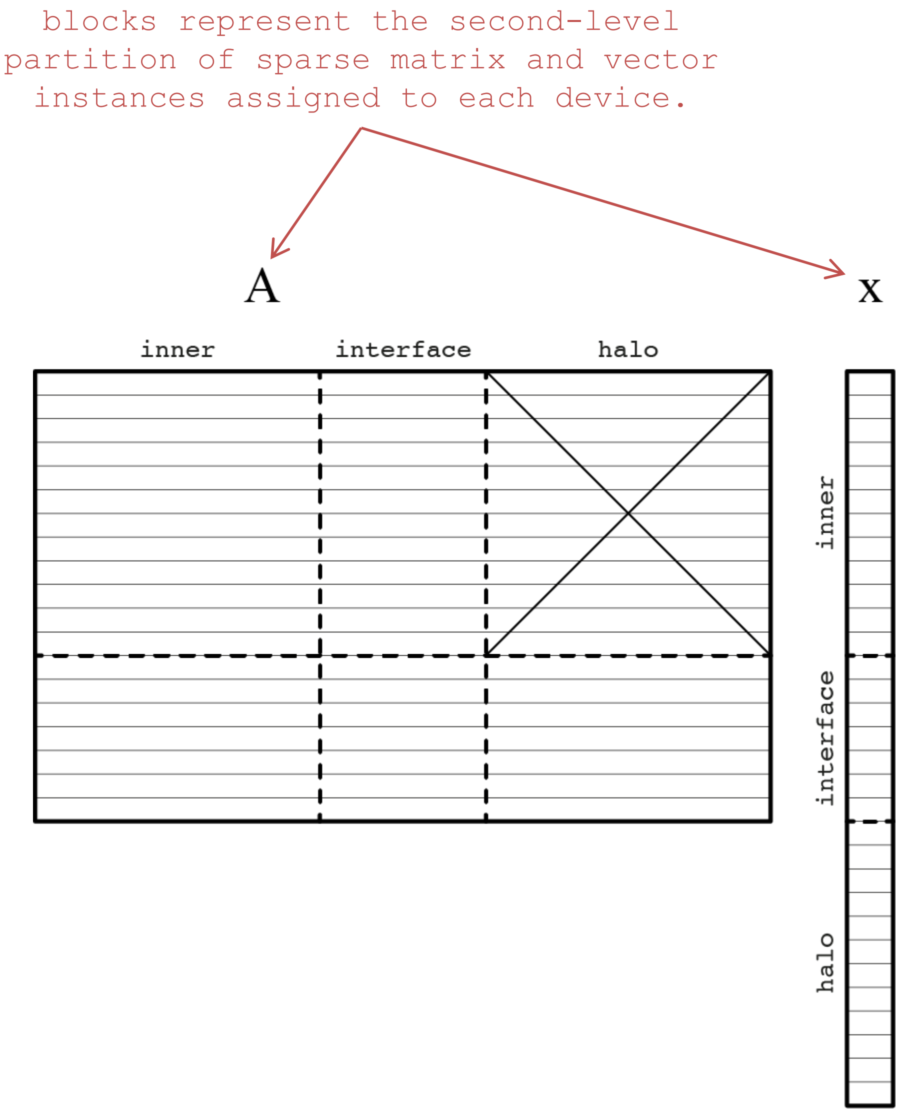
Halo

subset is composed of elements from other subdomains which are coupled with local elements.



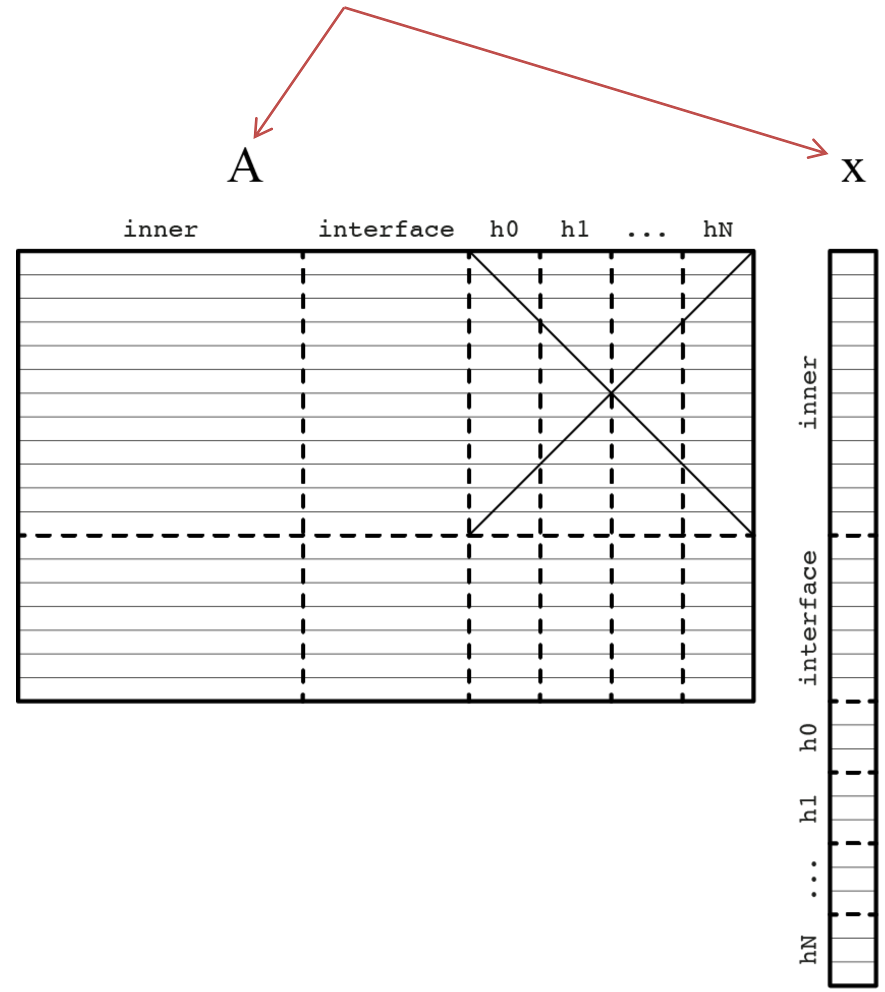
Sparse matrices and vectors represent discrete operators and mesh functions in our algebra-based framework, respectively. Thus, sparse matrix rows and vector elements are distributed among subdomains, and classified into three subsets:

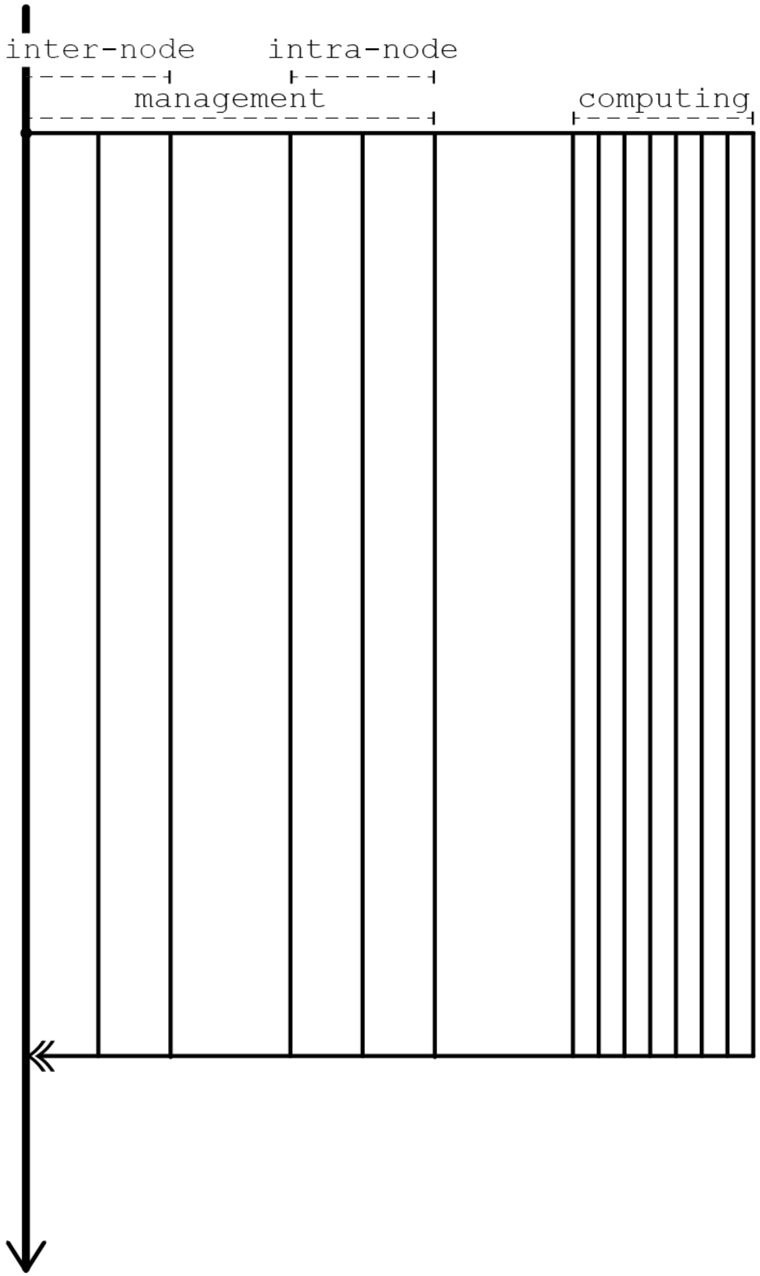
Inner subset is composed of local elements which are coupled with local elements only.

Interface subset is composed of local elements which are coupled with an element from other subdomain.

Halo subset is composed of elements from other subdomains which are coupled with local elements.

blocks represent the second-level partition of sparse matrix and vector instances assigned to each device.

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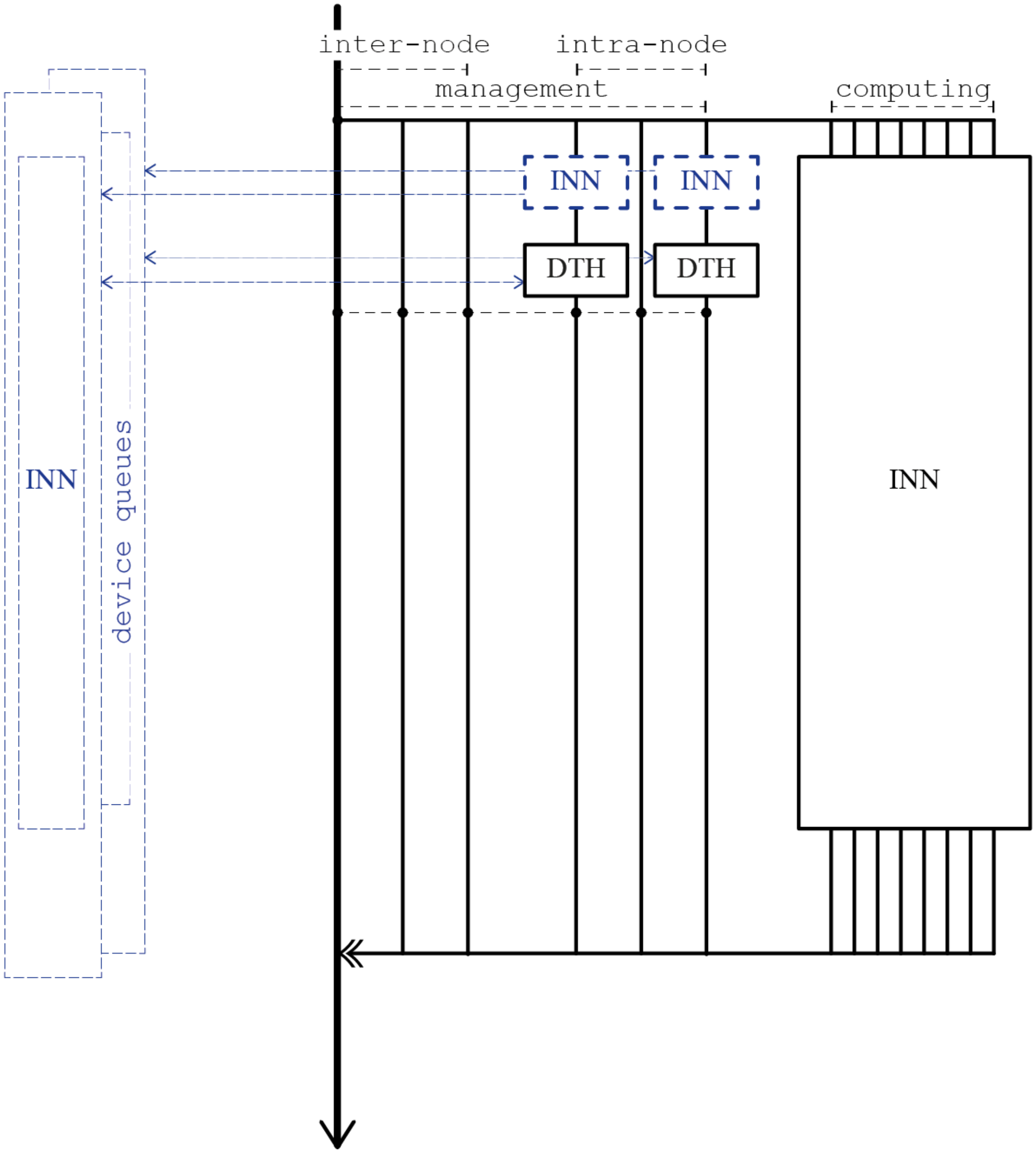
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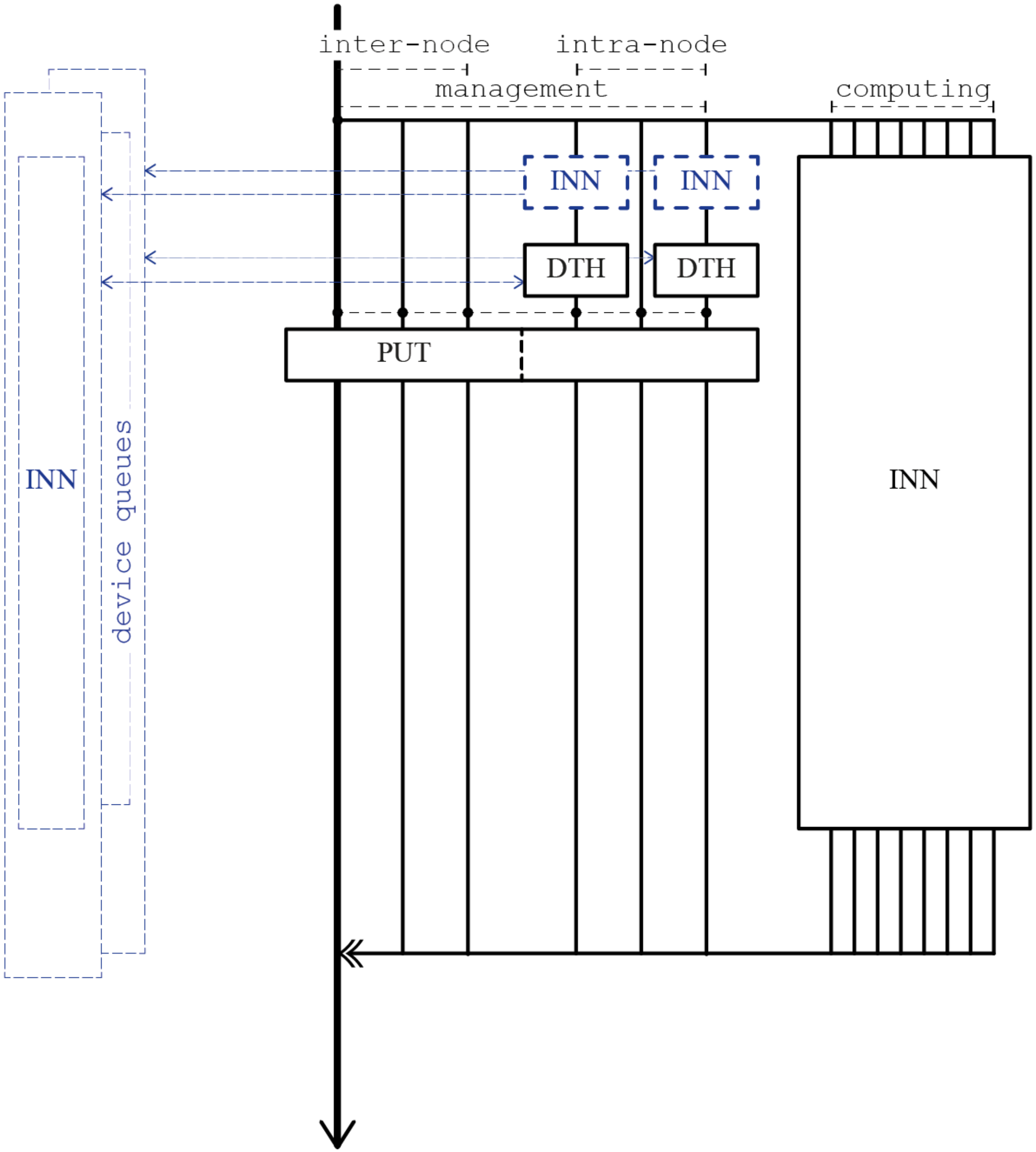
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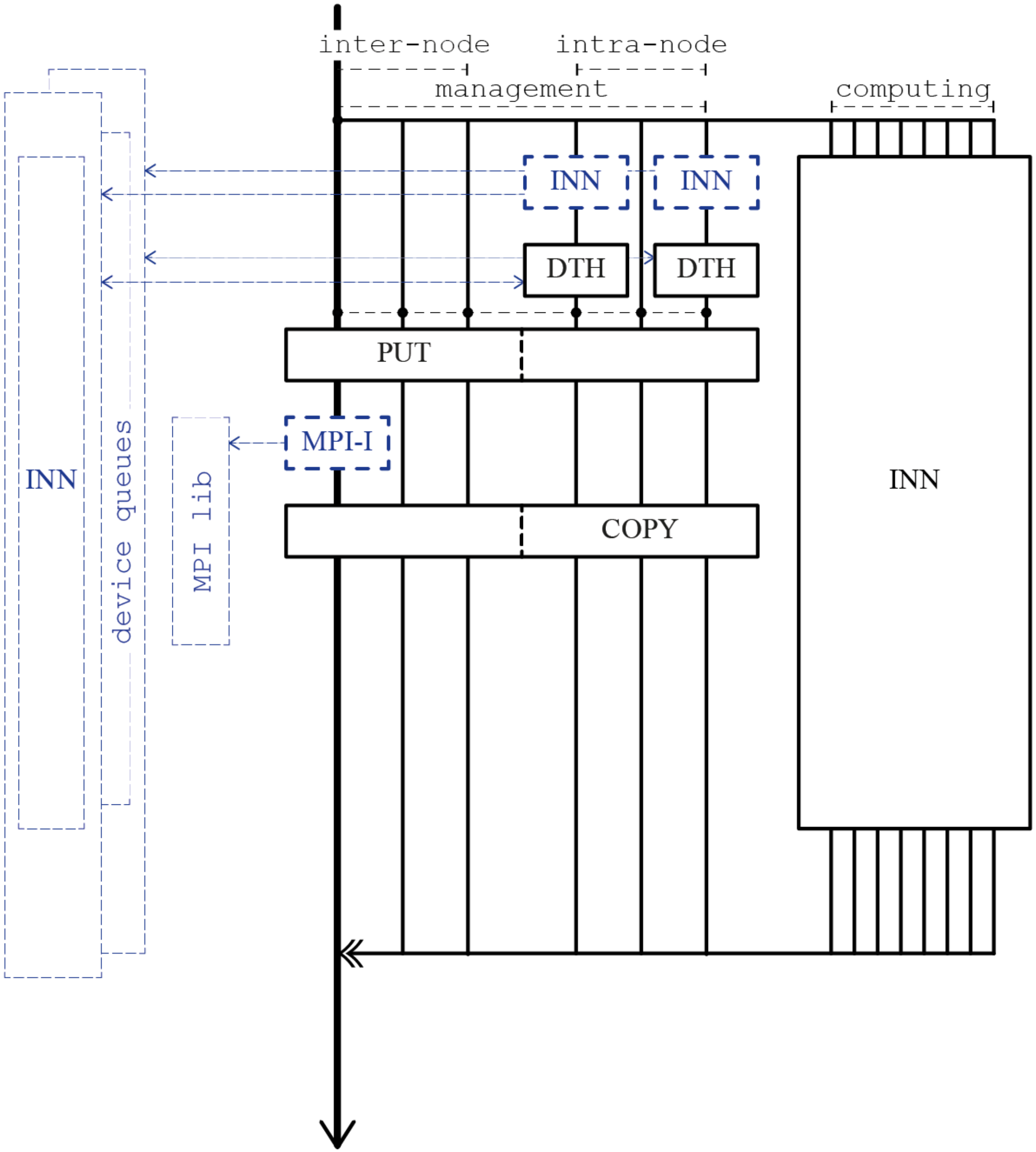
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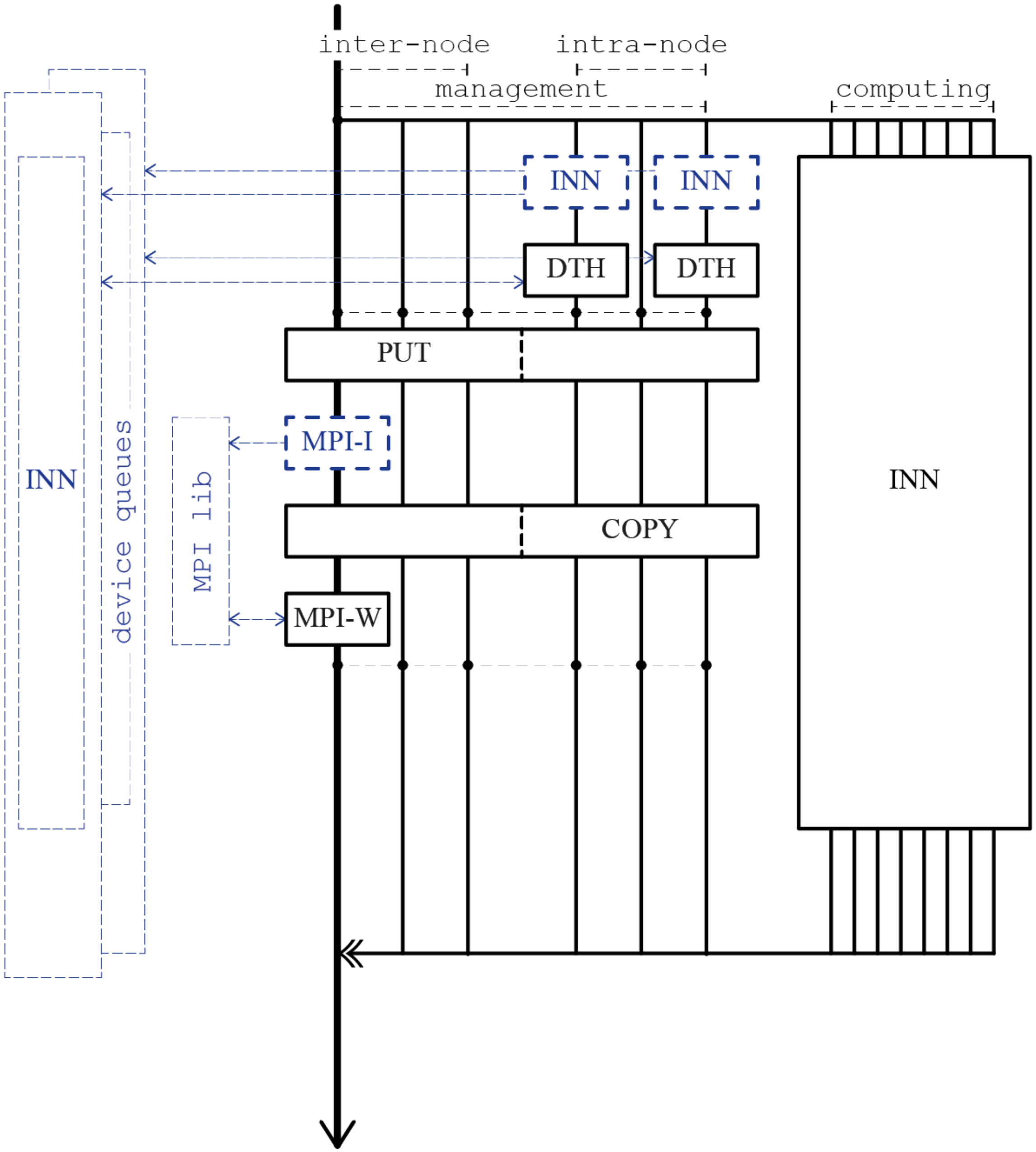
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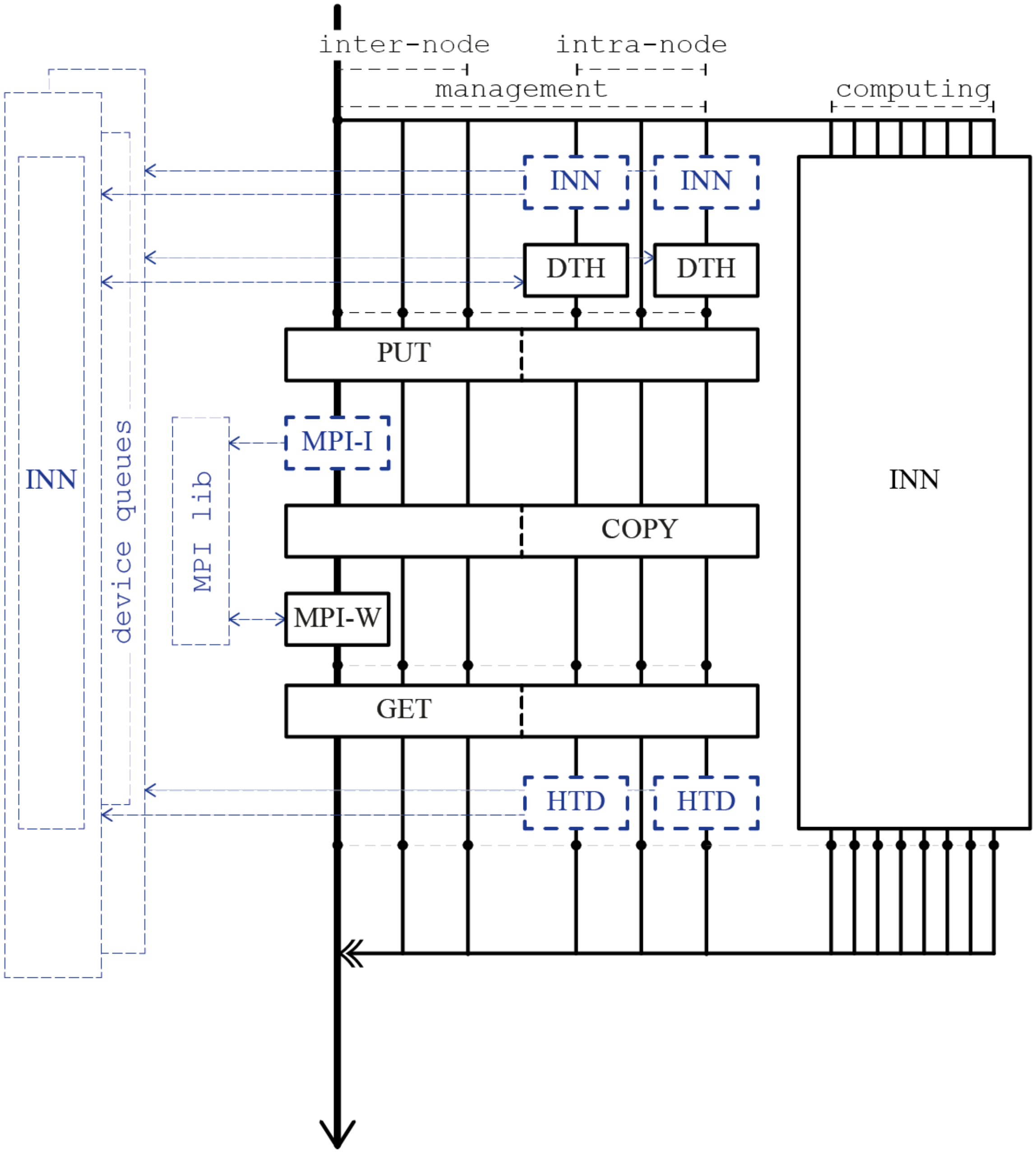
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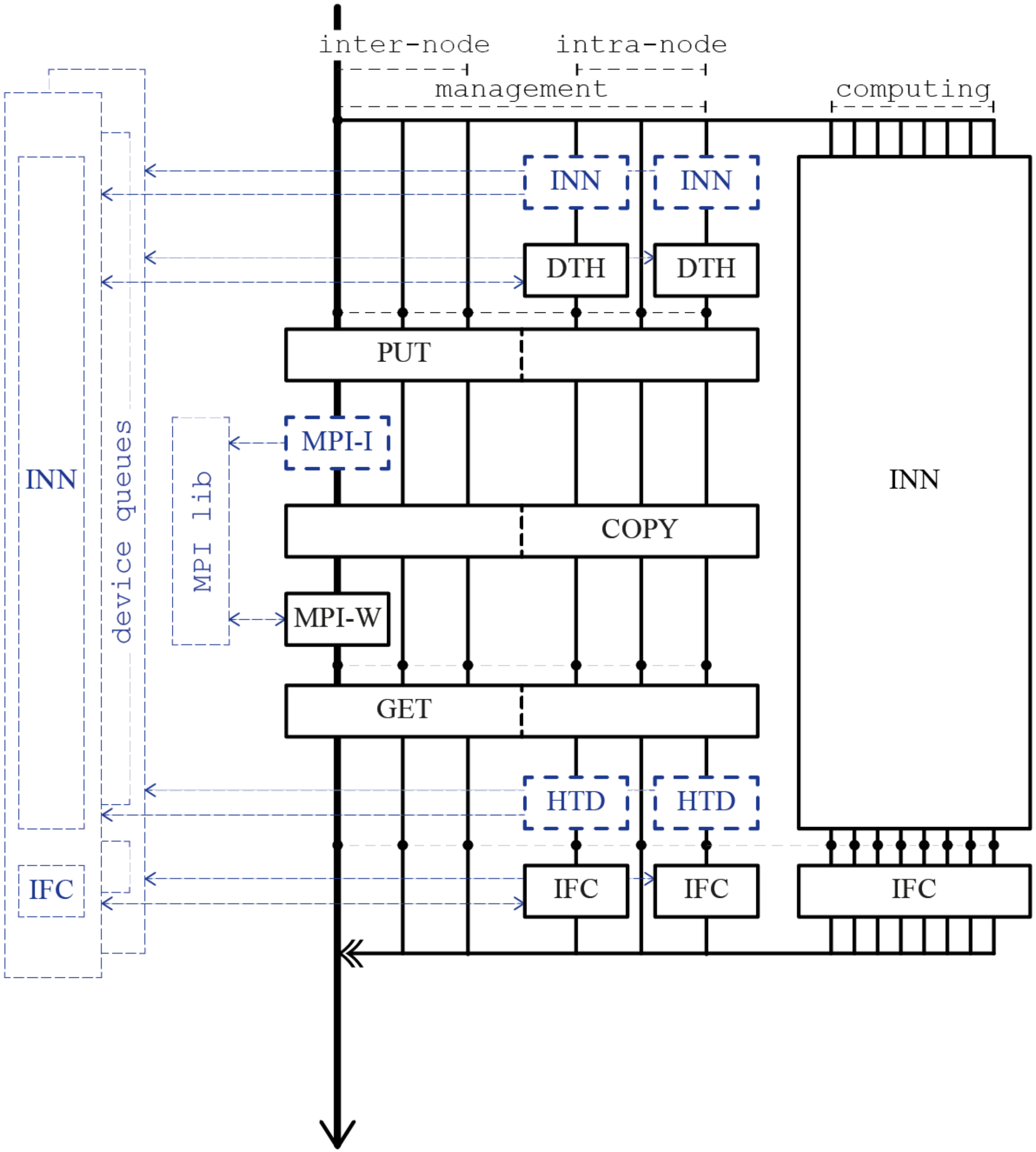
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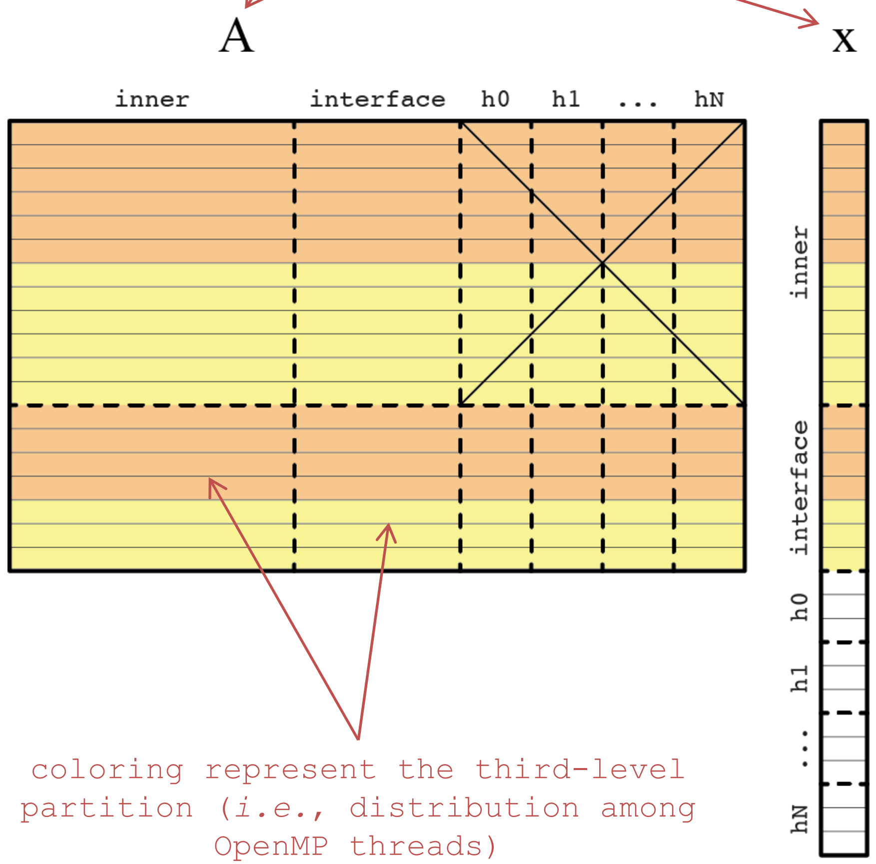
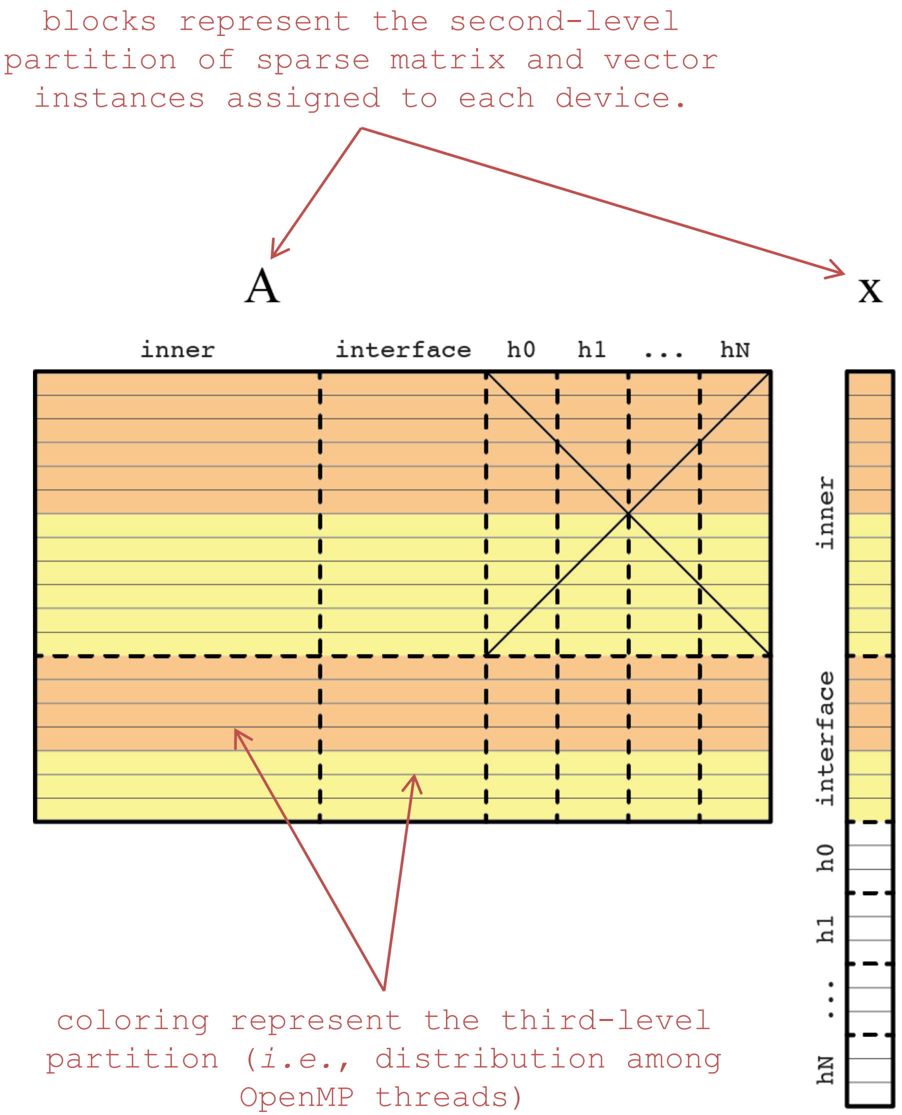
Third-level partition

blocks represent the second-level partition of sparse matrix and vector instances assigned to each device.



coloring represent the third-level partition (*i.e.*, distribution among OpenMP threads)

Third-level partition
consists of sharing the device's workload in a shared-memory space. This can be implicitly achieved with the OpenMP scheduler.



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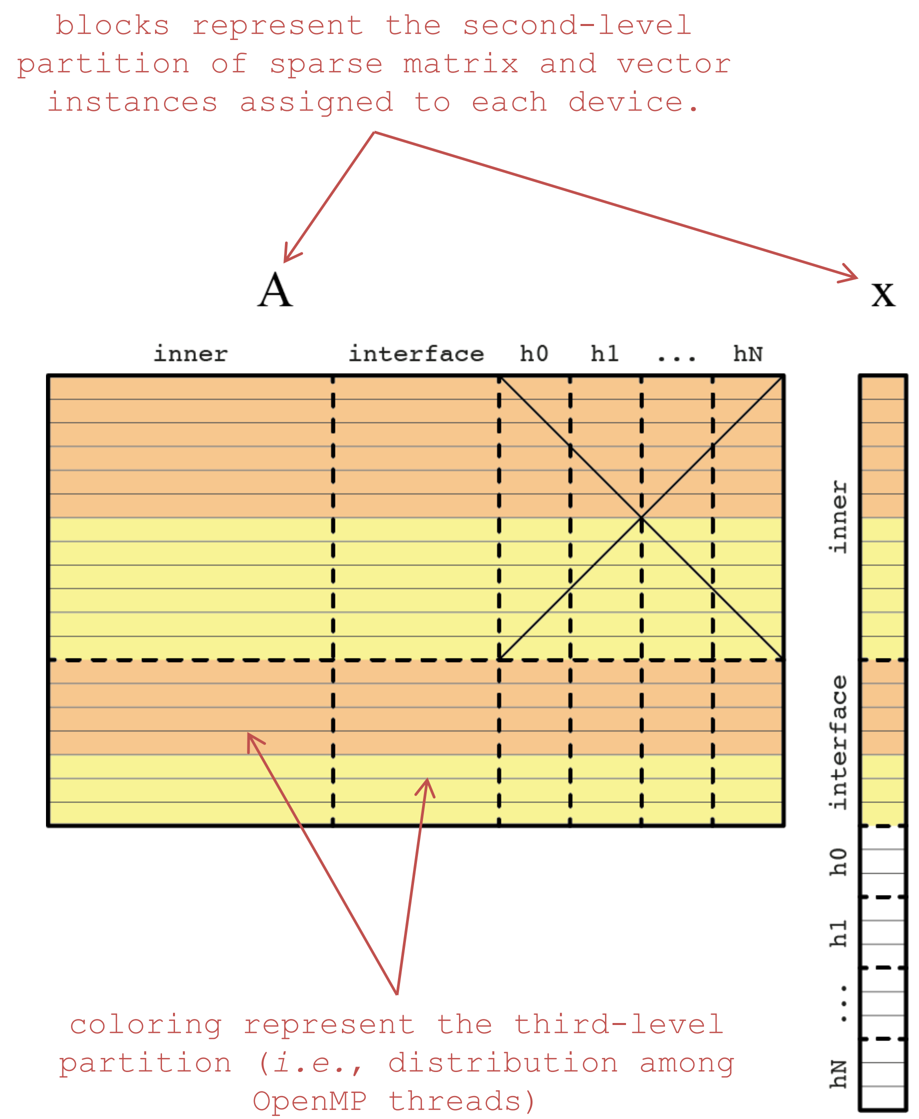
However, in NUMA configurations, a thread accessing to the memory allocated by another memory controller goes through a much slower bus.



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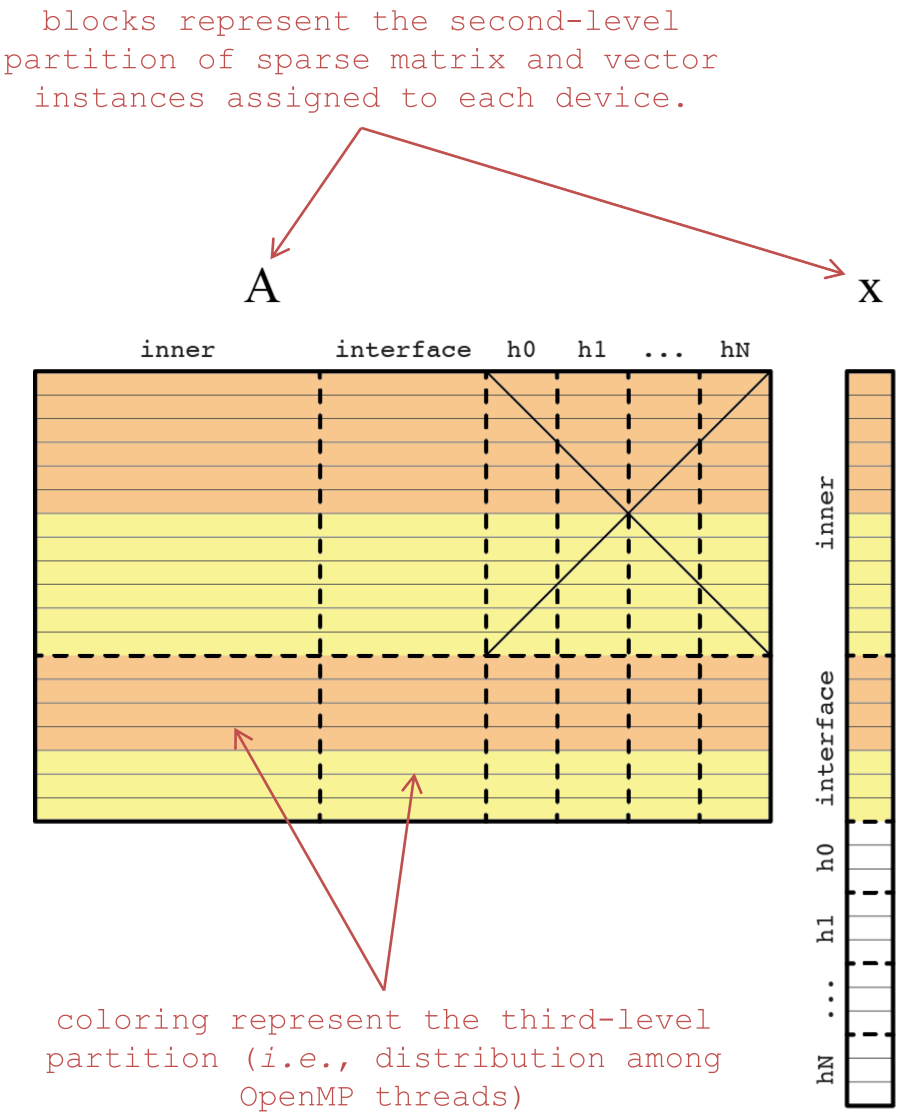
Since SpMV is executed separately for inner and interface, our third-level partitioning distributes the inner and interface subsets among threads separately too. In other words, each OpenMP thread is assigned a chunk of inner and a chunk of interface.



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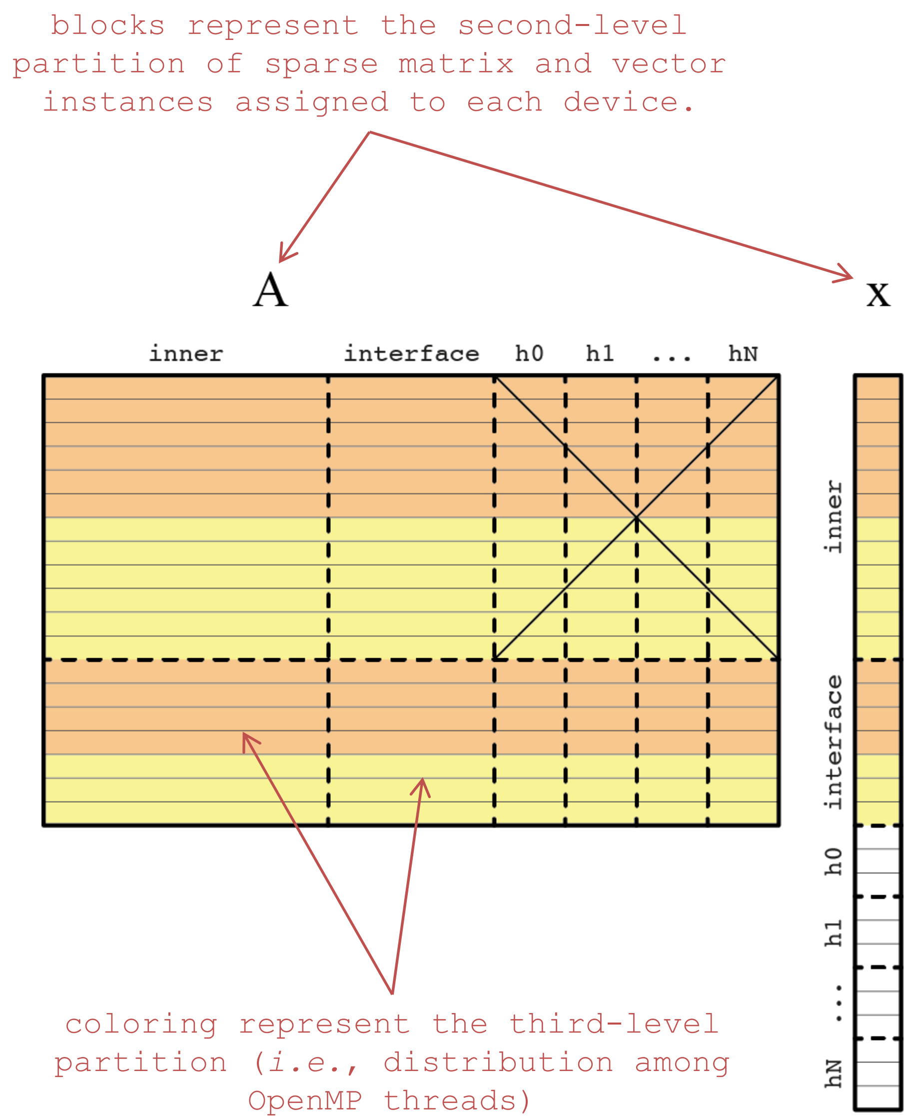
Thread migration must be avoided to ensure an efficient memory access!

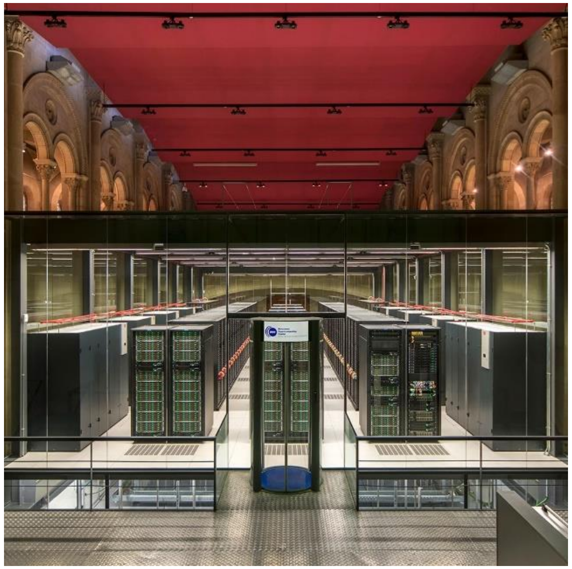


Execution of SpMV on different modern supercomputers

PERFORMANCE STUDY

Testing setup

MareNostrum 4



rank #42
3456 nodes with:
- 2× Intel Xeon 8160
- 1× Intel Omni-Path

Lomonosov-2

rank #156
1696 nodes with:
- 1× Intel Xeon E5-2697 v3
- 1× NVIDIA Tesla K40M
- 1× InfiniBand FDR

TSUBAME3.0

rank #31
540 nodes with:
- 2× Intel Xeon E5-2680 v4
- 4× NVIDIA Tesla P100
- 4× Intel Omni-Path

Test case 1:

Single-node performance of SpMV kernel vs number of cores on MareNostrum 4. The sparse matrix used arise from the symmetry-preserving discretization[1] of the Laplacian operator on unstructured hex-dominant mesh of 17 million cells. The sparse matrix storage format used is ELLPACK[2].

[1] F. Xavier Trias et al. "Symmetry-preserving discretization of Navier–Stokes equations on collocated unstructured grids", JCP 258 (2014), 246–267.
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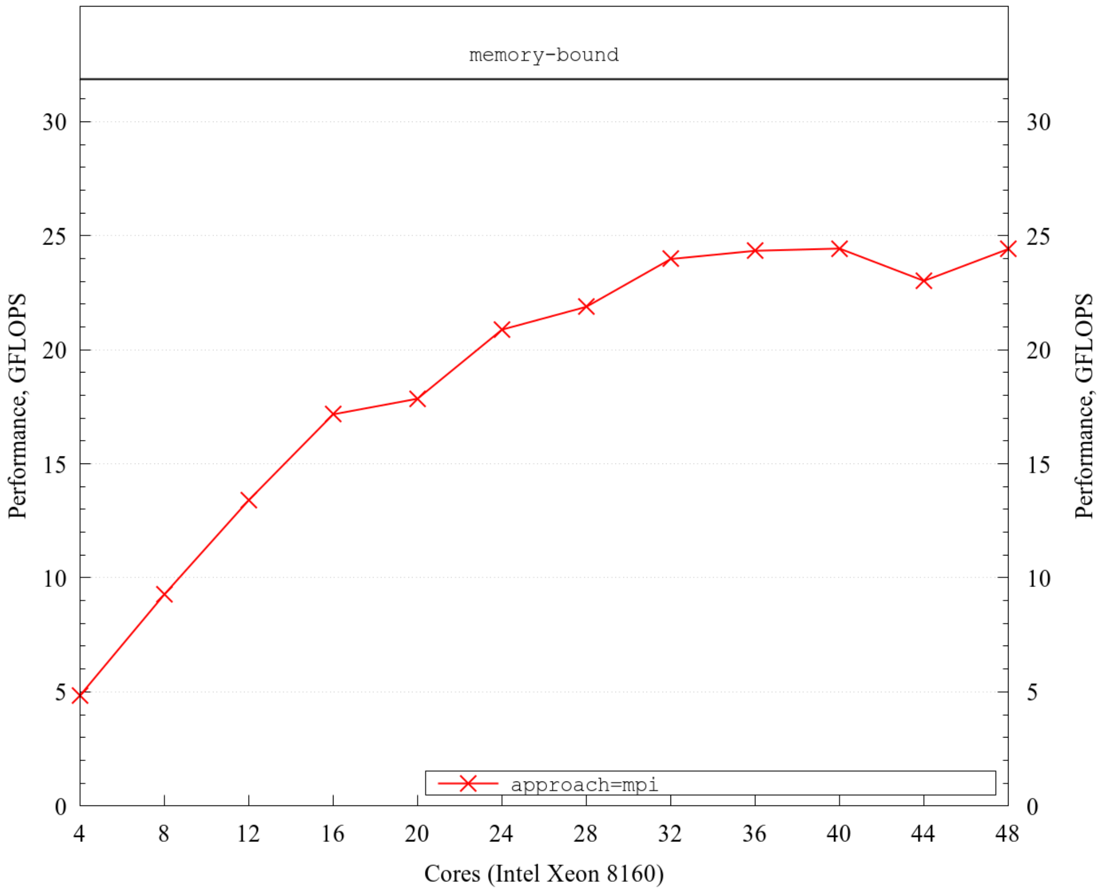

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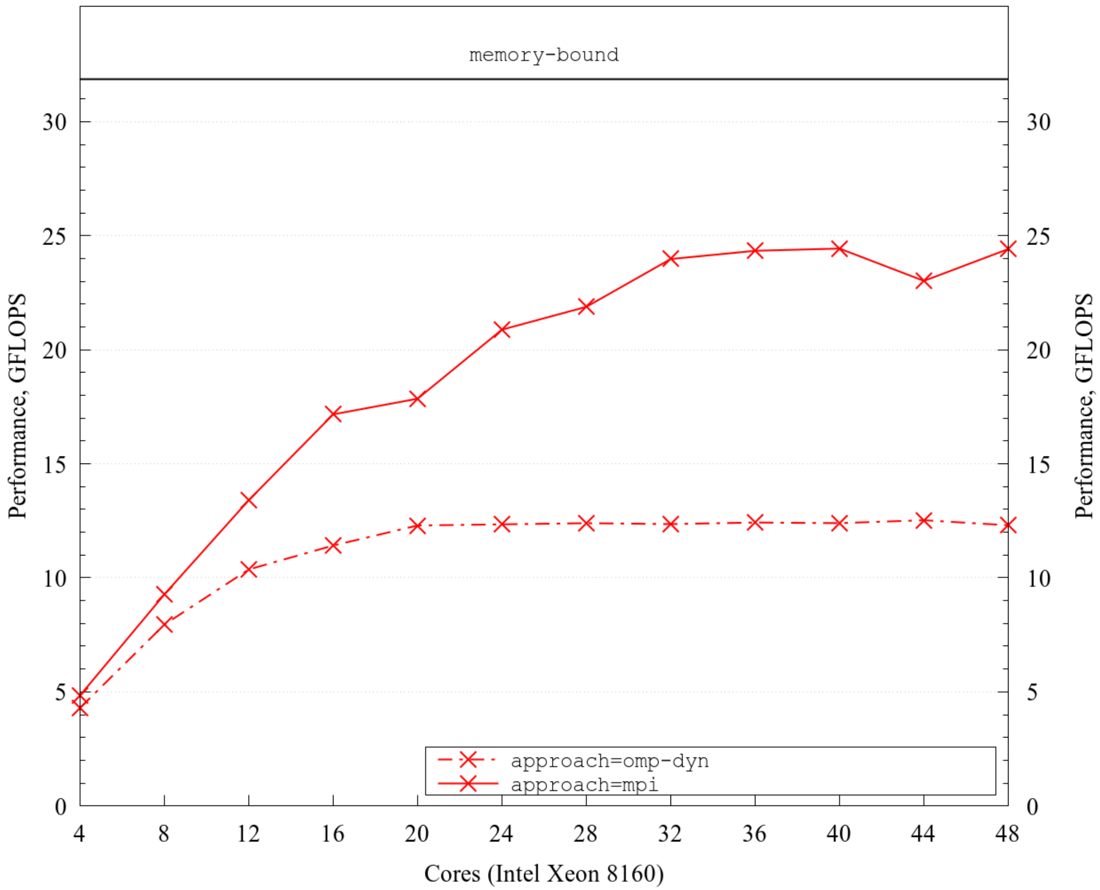

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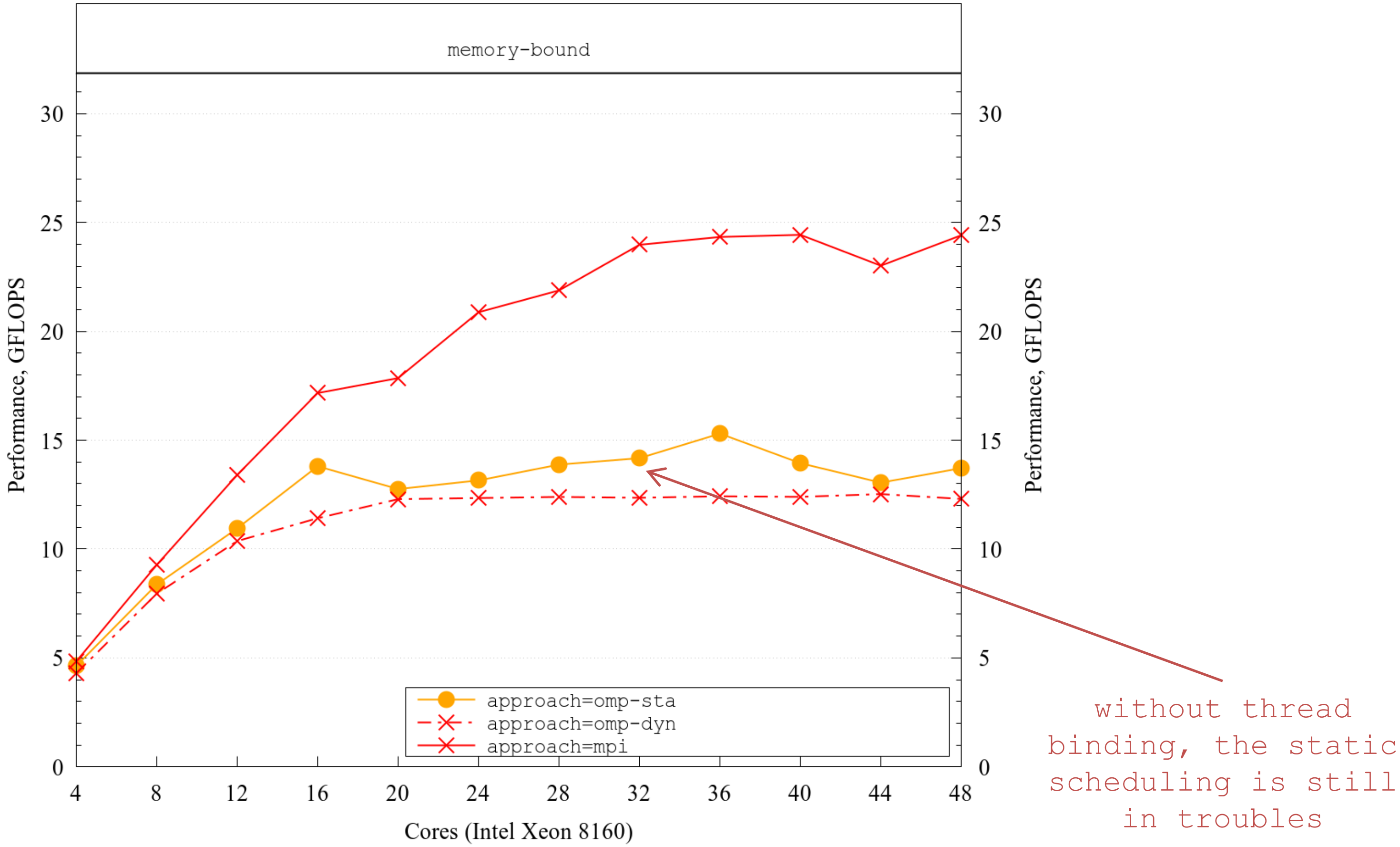

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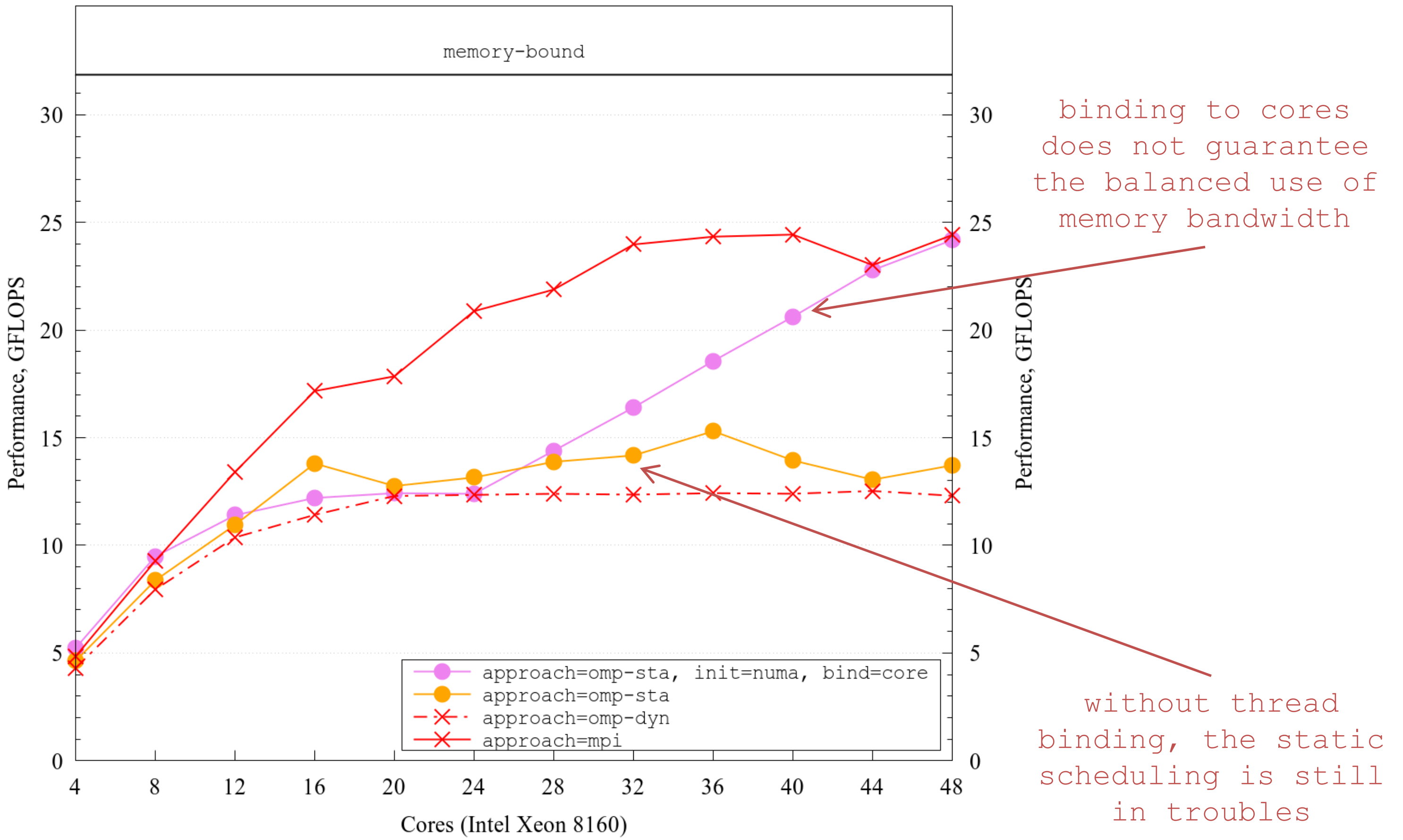

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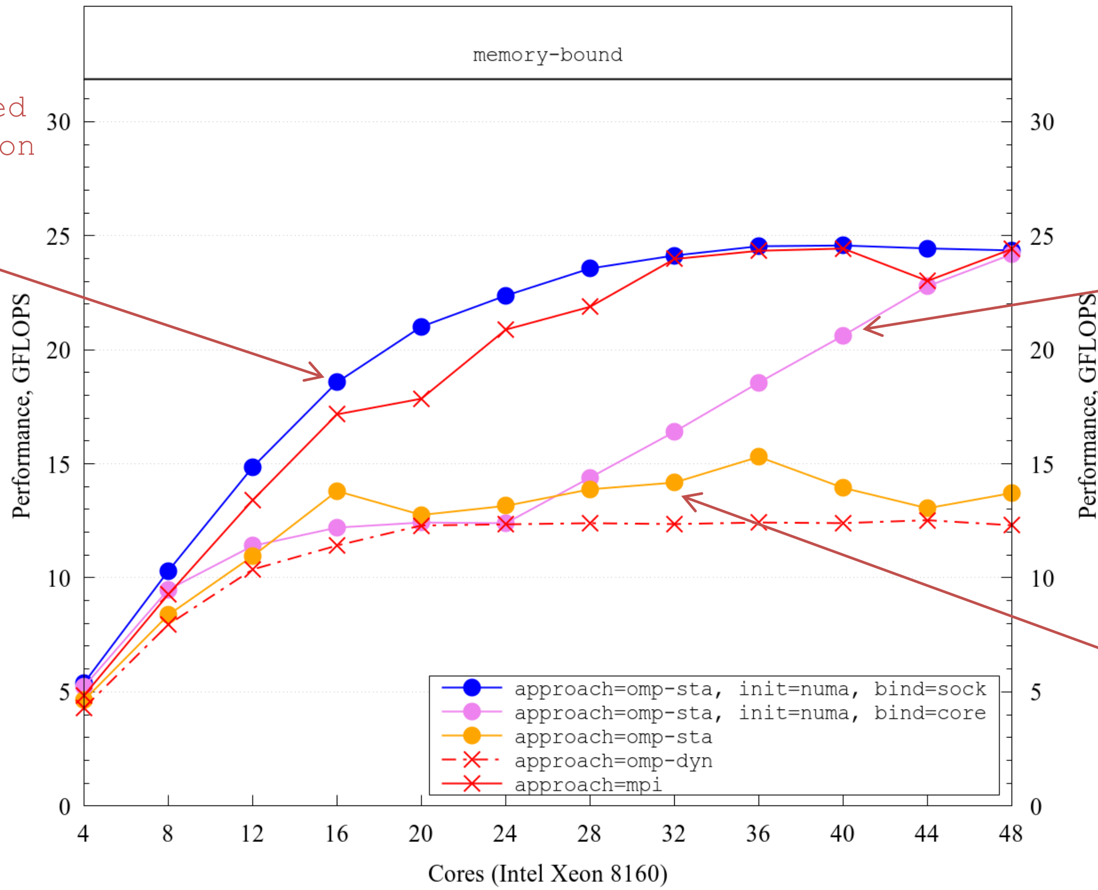
thread binding to sockets and threaded memory initialization is our choice



binding to cores does not guarantee the balanced use of memory bandwidth

without thread binding, the static scheduling is still in troubles

[1] F. Xavier Trias et al. "Symmetry-preserving discretization of Navier–Stokes equations on collocated unstructured grids", JCP 258 (2014), 246–267.
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Test case 2:

Multi-node strong (left) and weak (right) scaling of SpMV kernel on MareNostrum 4. The sparse matrix used arise from the symmetry-preserving discretization[1] of the Laplacian operator on unstructured hex-dominant mesh of 17 million cells (results for 110 million cells are also reported in strong scaling). The sparse matrix storage format used is ELLPACK[2].

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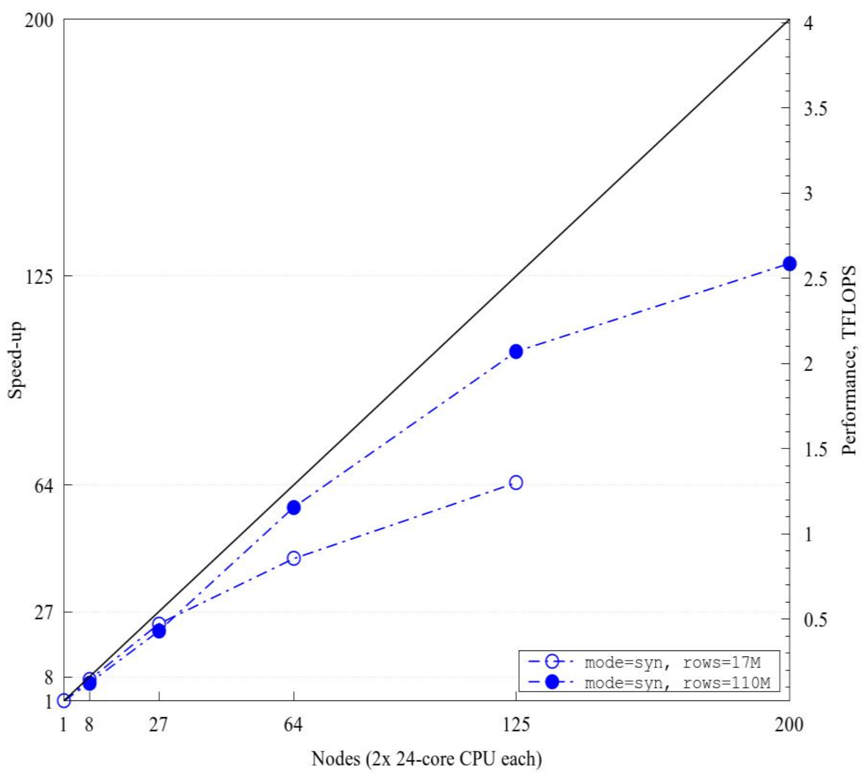

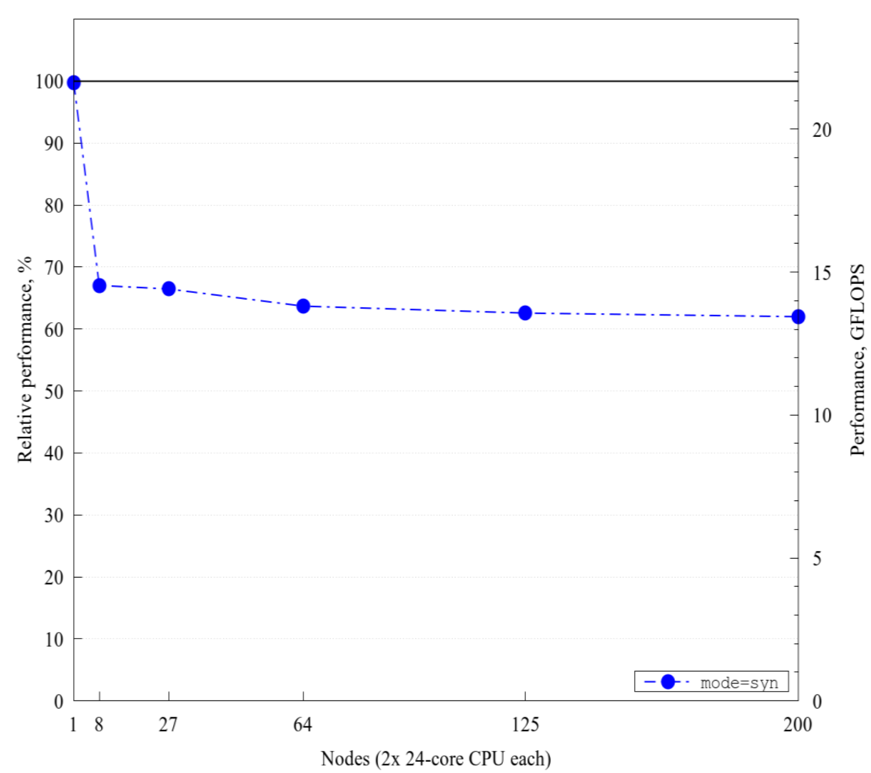

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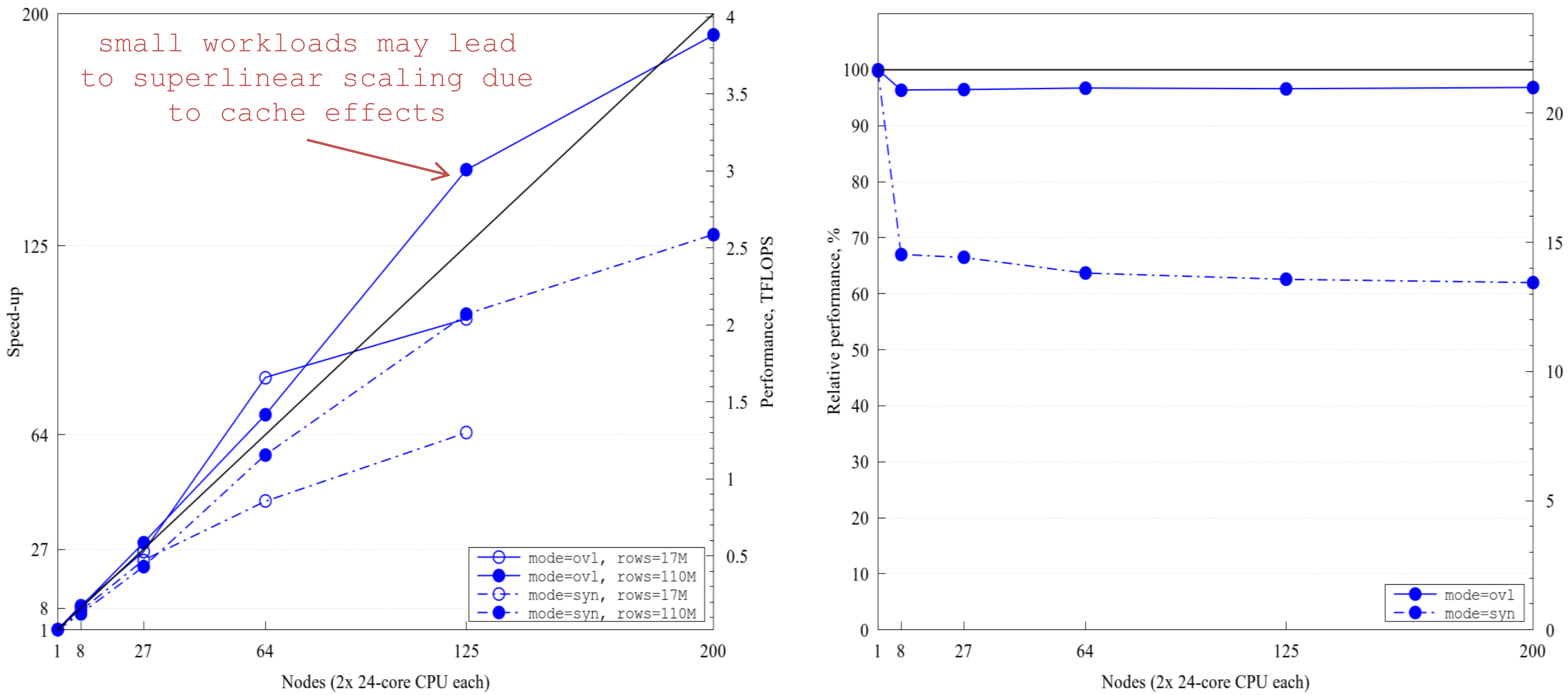

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Test case 3:

Multi-node strong (left) and weak (right) scaling of SpMV kernel on Lomonosov-2 for CPU-only, GPU-only and heterogeneous execution. The sparse matrix used arise from the symmetry-preserving discretization[1] of the Laplacian operator on unstructured hex-dominant mesh of 1 million cells. The sparse matrix storage format used is ELLPACK[2] and its block-transposed variant for CPU and GPU, respectively.

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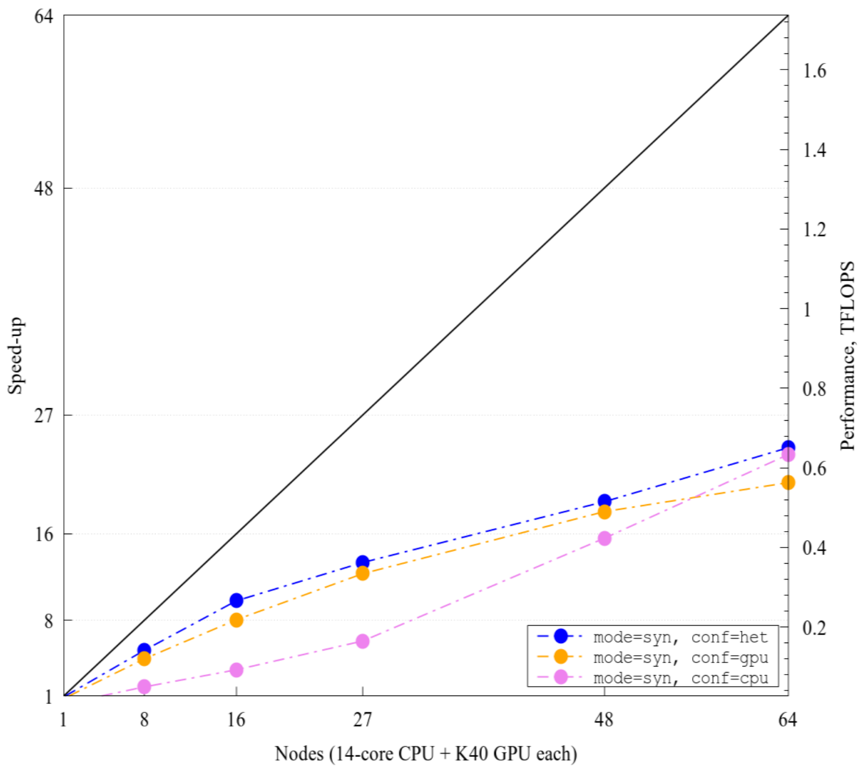

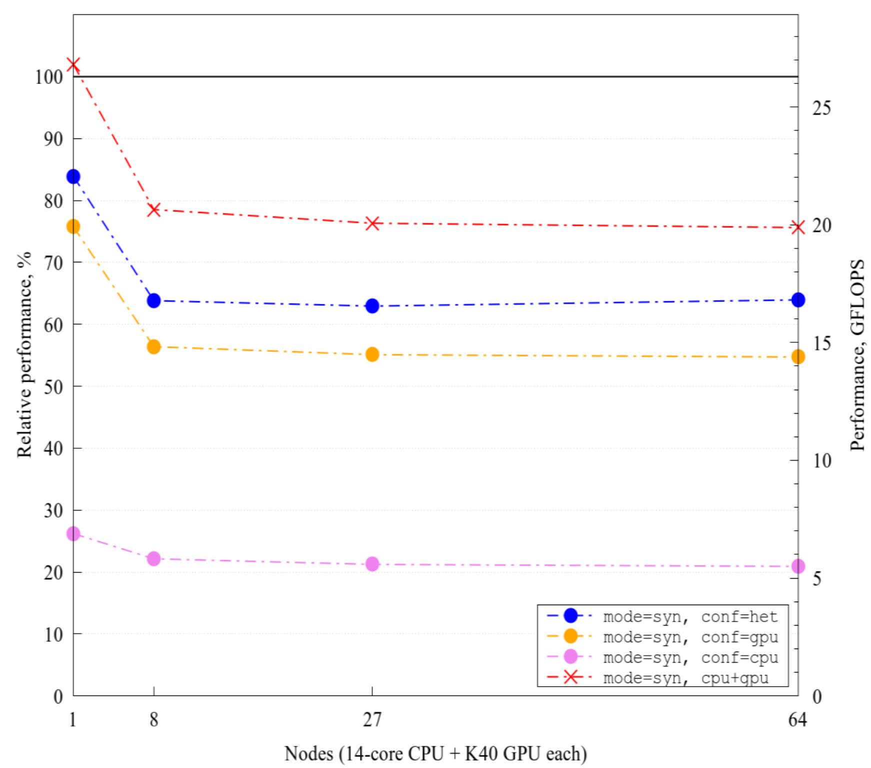

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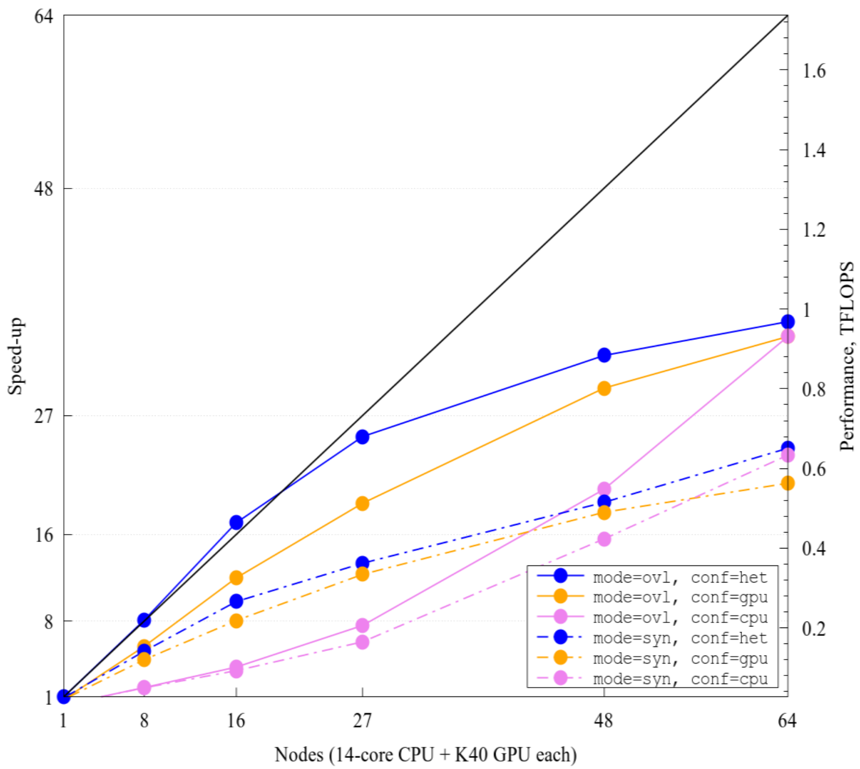

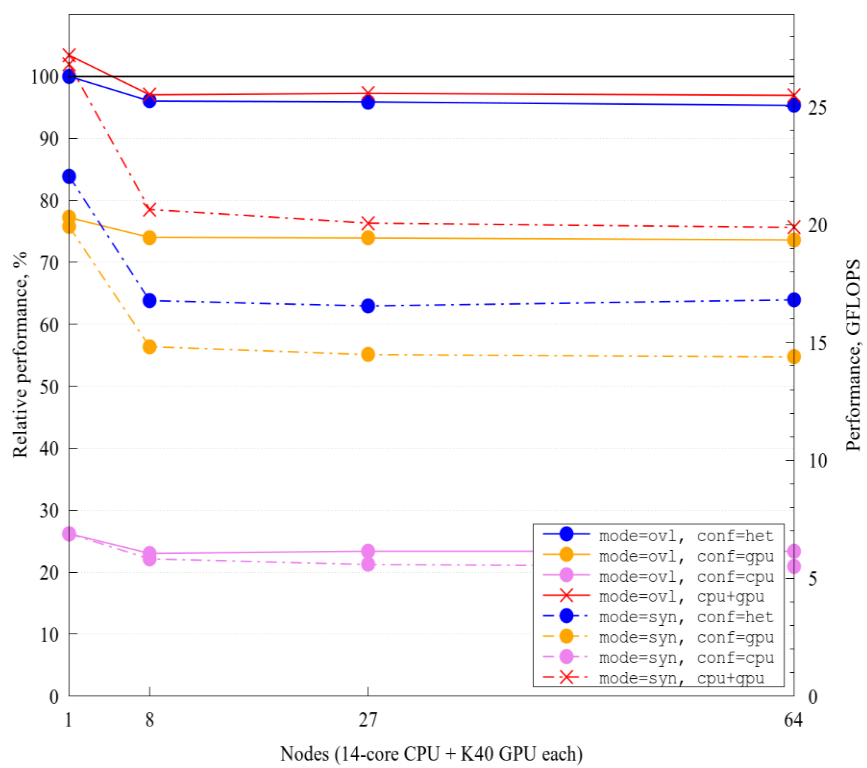

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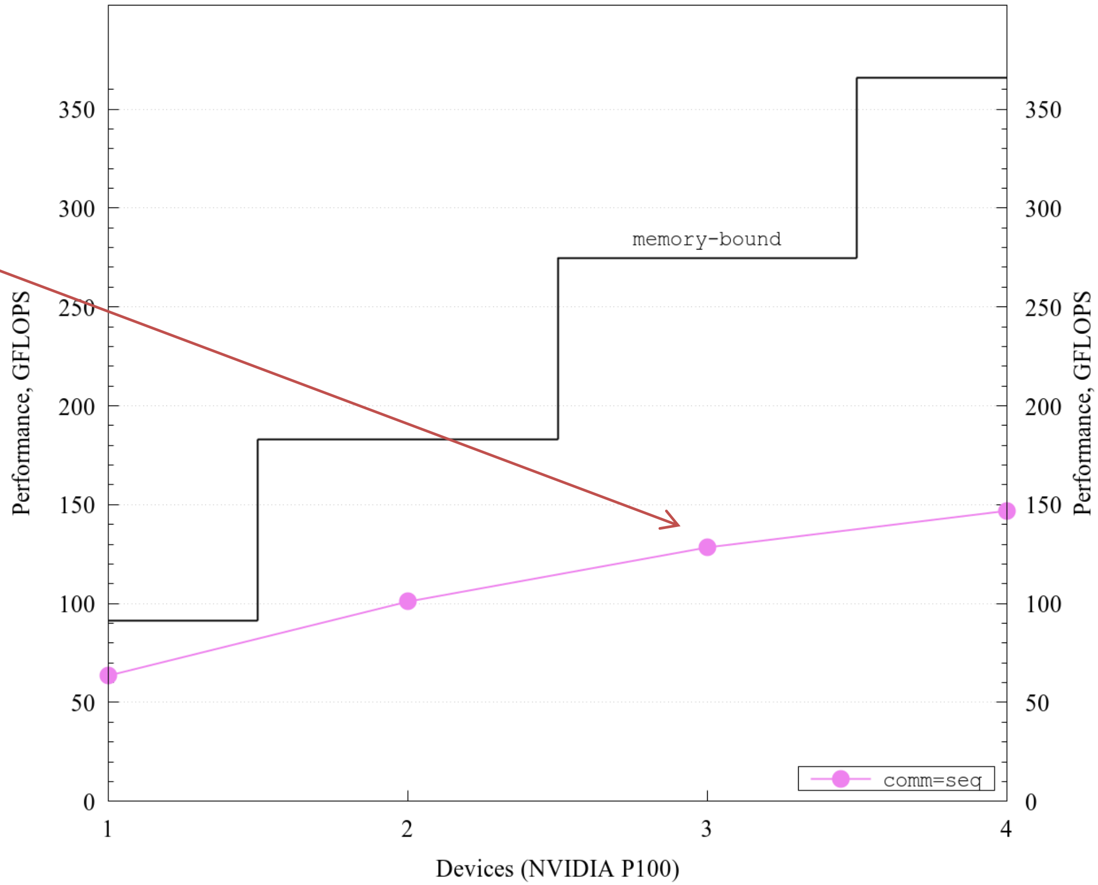

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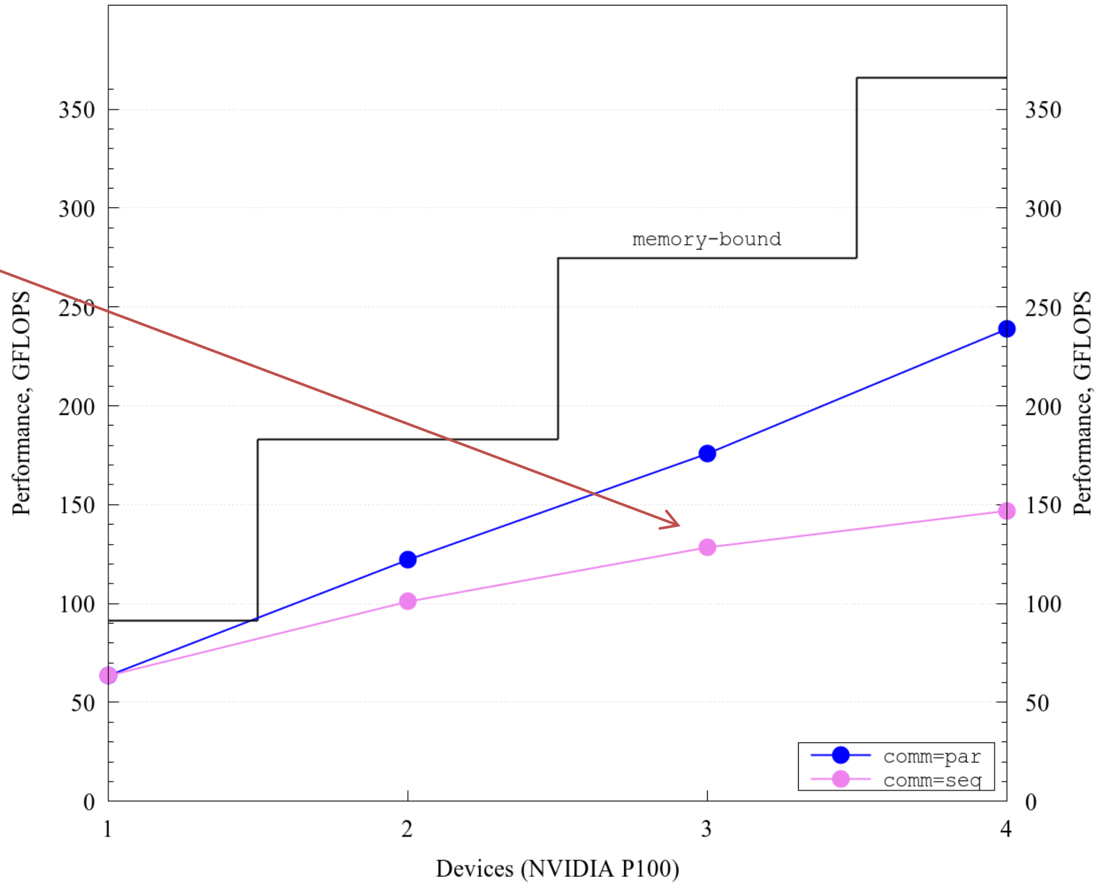

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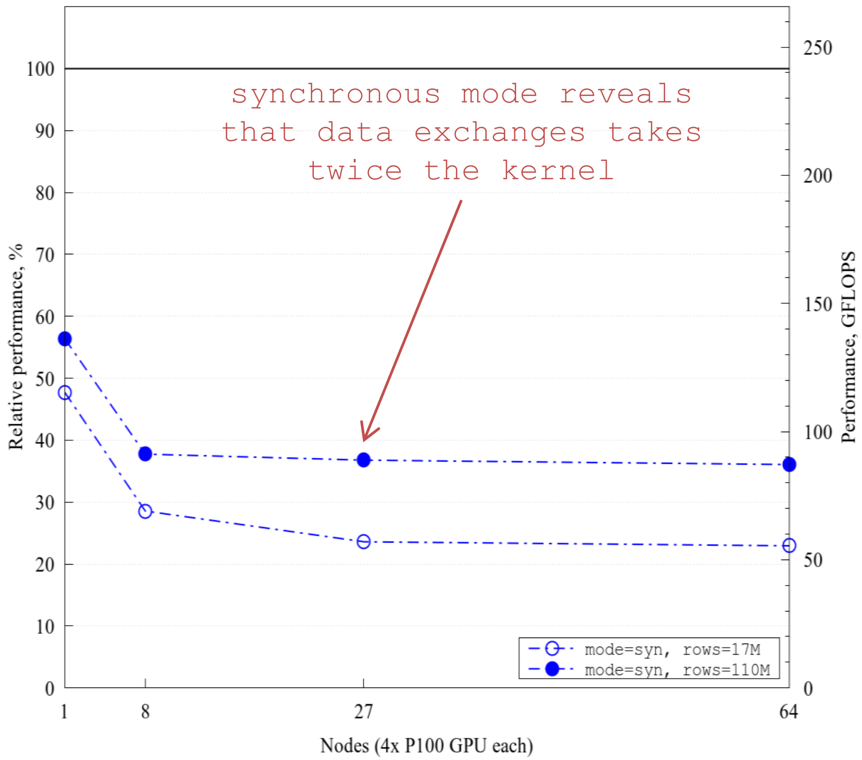

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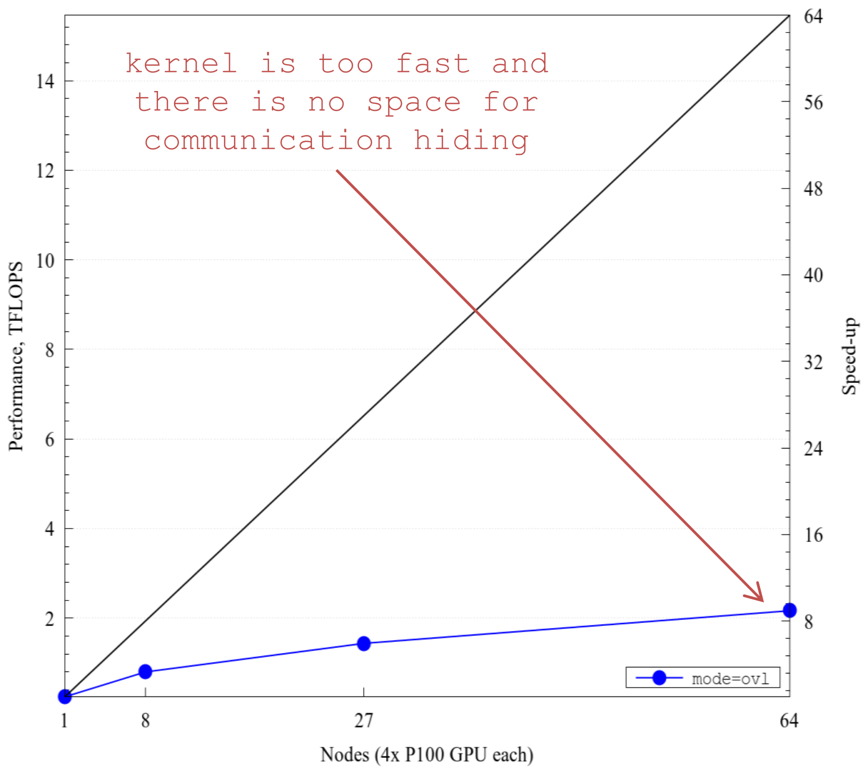

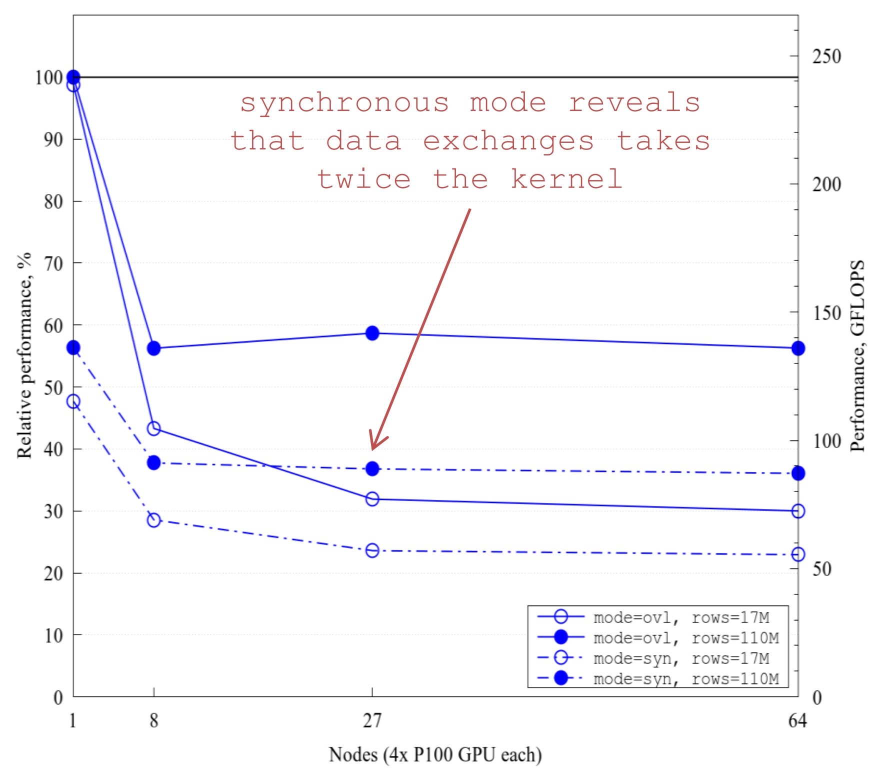

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Future work

- To design a new update mechanism to accelerate the data exchanges, for instance, taking into account NUMA factor in inter- and intra-node exchanges.

Thank you for attending