NUMA–aware strategies for the efficient execution of CFD simulations on CPU supercomputers

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Xavier Álvarez Farré[1], Andrey Gorobets[2], F. Xavier Trias[1] and Assensi Oliva[1]

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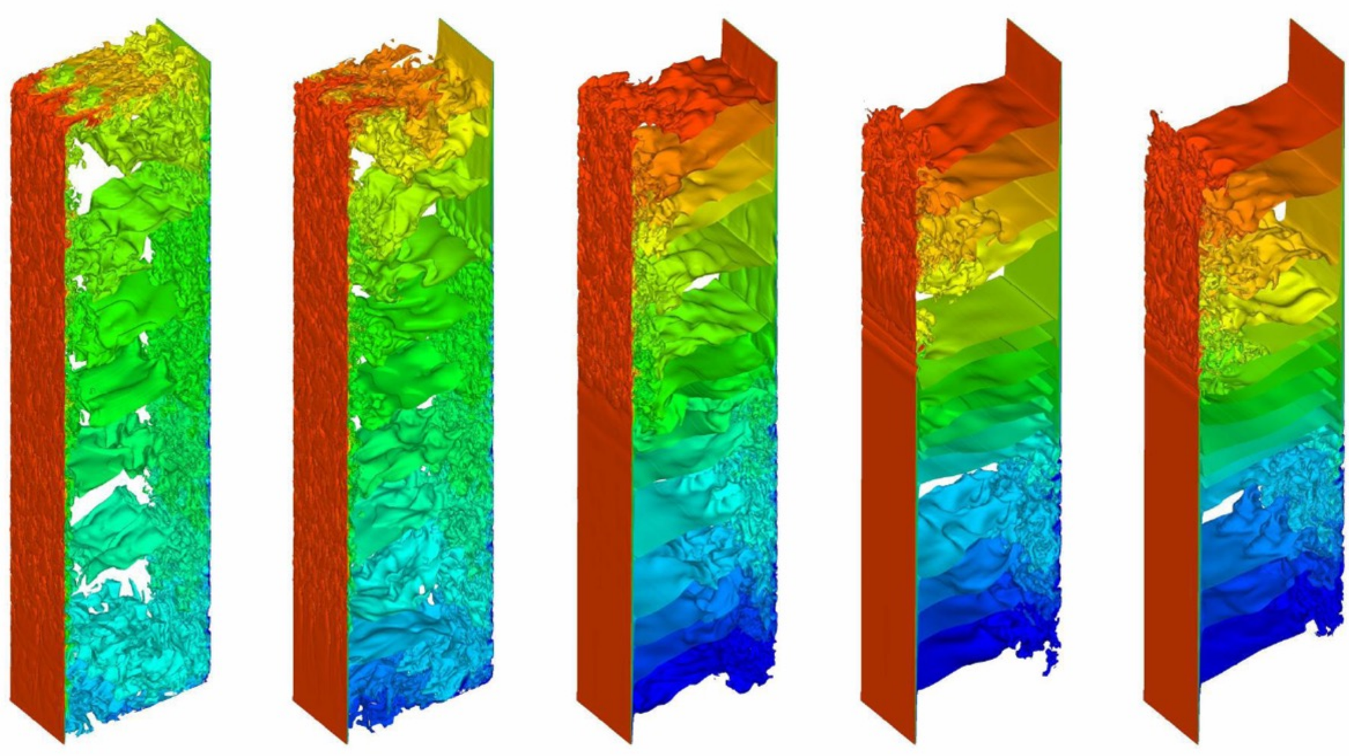
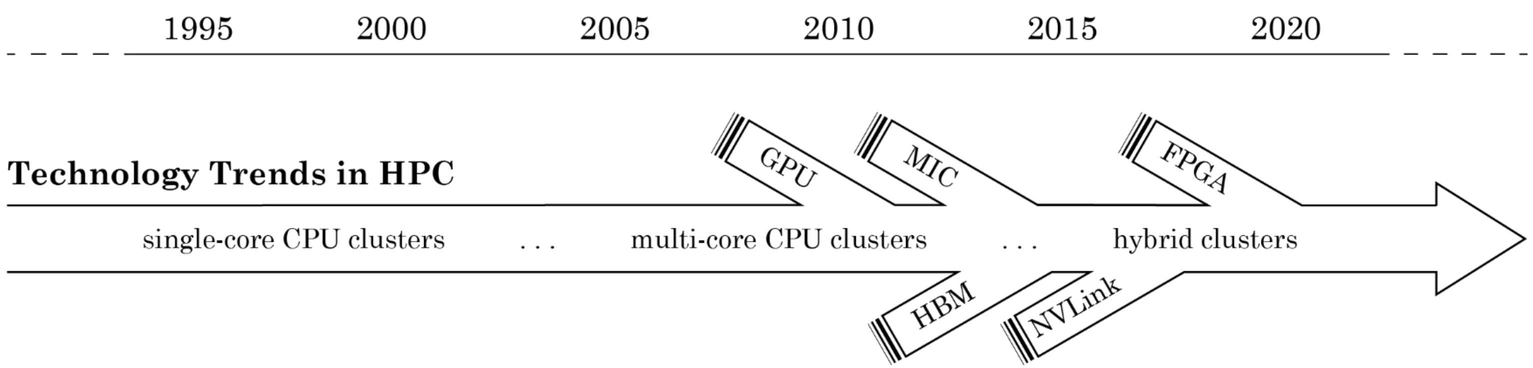
An algebraic approach for CFD simulations

BACKGROUND

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.




1995
2000
2005
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Technology Trends in HPC
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MIC
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multi-core CPU clusters
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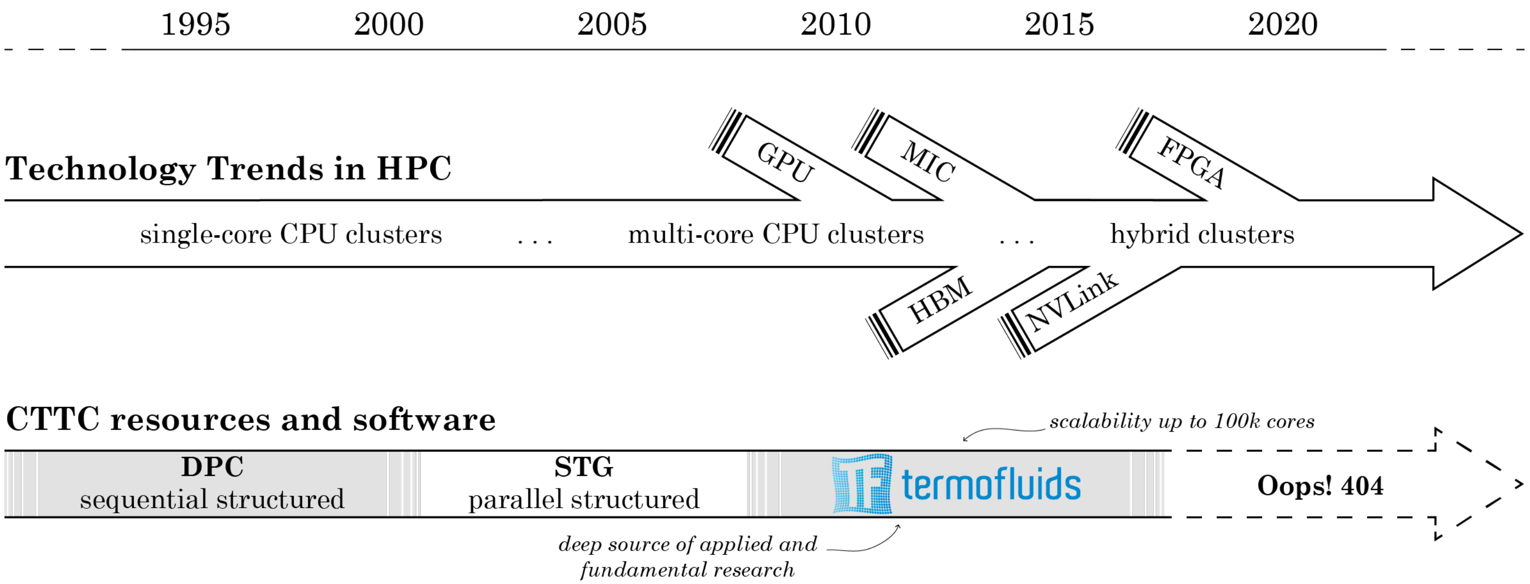
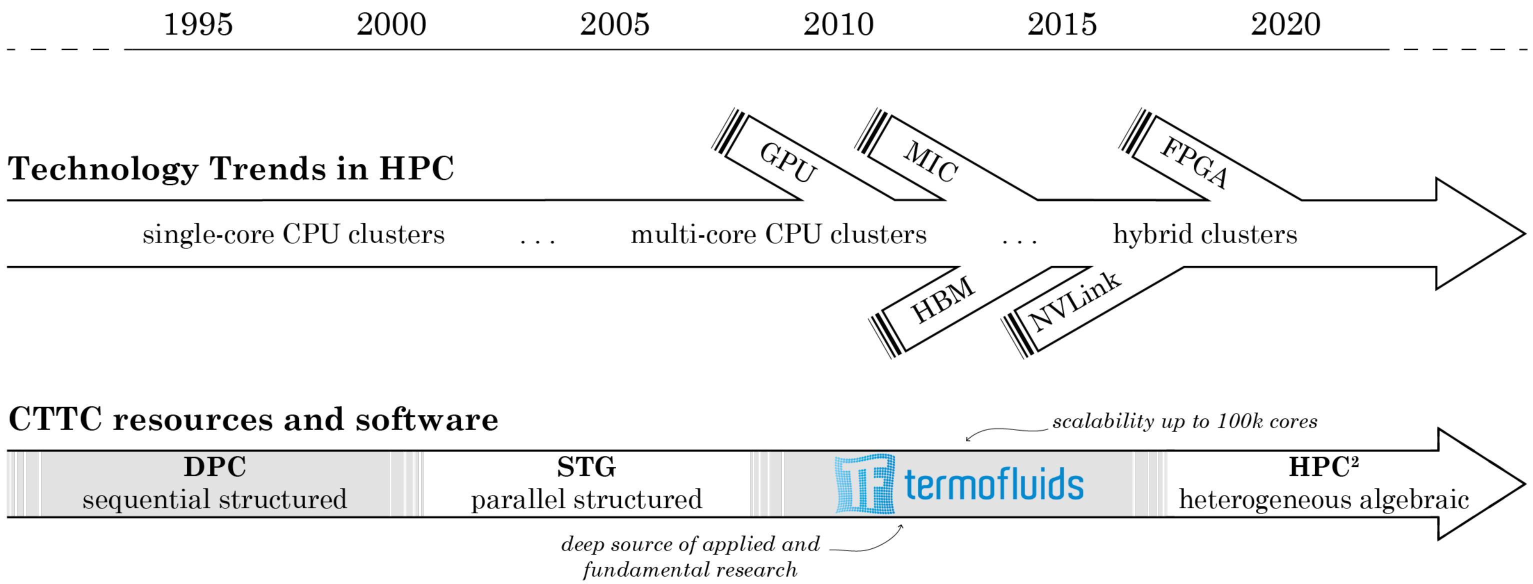
hybrid clusters
HBM
NVLink



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.

In an algebraic approach,
the traditional stencil data structures and sweeps are replaced by algebraic data structures and kernels[1].

$$\nabla \cdot u = 0, \qquad u + (u \cdot \nabla)u - \frac{1}{Re}\Delta u + \nabla p = 0$$

$$\mathbf{M}\mathbf{u_s} = \mathbf{0_c}, \qquad \mathbf{\Omega} d_t \mathbf{u_c} + \mathbf{M}\mathbf{U_s}\mathbf{u_c} - \mathbf{D}\mathbf{u_c} - \mathbf{M}^{\mathbf{T}}\mathbf{p_c} = \mathbf{0_c}$$

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- The discrete operators and mesh functions are stored as sparse matrices and vectors, respectively (i.e., the numerical method results fully integrated into the data).

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SpMV

axpy

- The discrete operators and mesh functions are stored as sparse matrices and vectors, respectively (i.e., the numerical method results fully integrated into the data).
- The algorithm for the DNS and LES of incompressible turbulent flows relies on a set of only three algebraic operations: **SpMV**, **axpy** and **dot**[2].

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Stencil-based method

Algebra-based method

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

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

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Multiple computing kernels
are required to implement different numerical methods.

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Multiple computing kernels
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Complex kernels
minimize intermediate calculations and help to increase the arithmetic intensity.

Algebra-based method

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

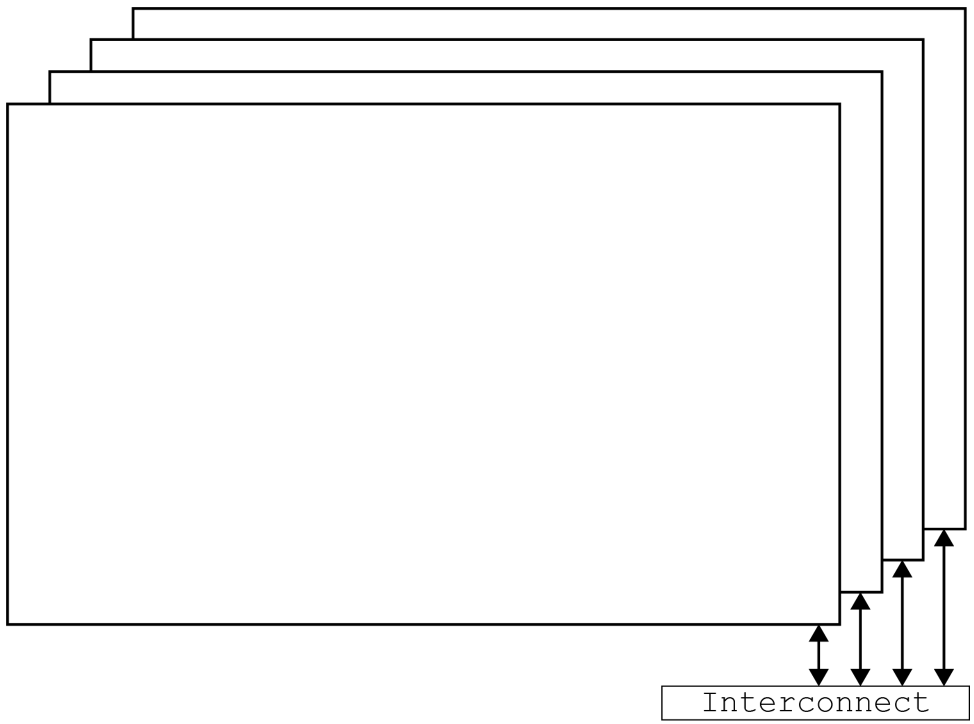
Unique computing kernels
are required to implement different numerical methods.

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

Hierarchical implementation of the HPC² framework

IMPLEMENTATION

High-performance computing systems



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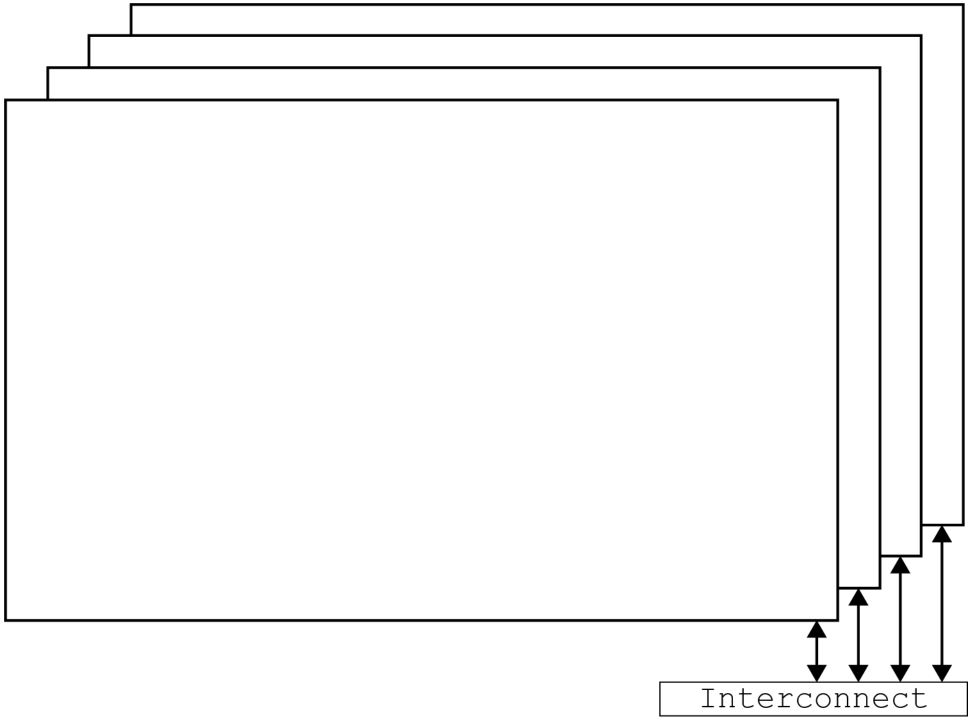
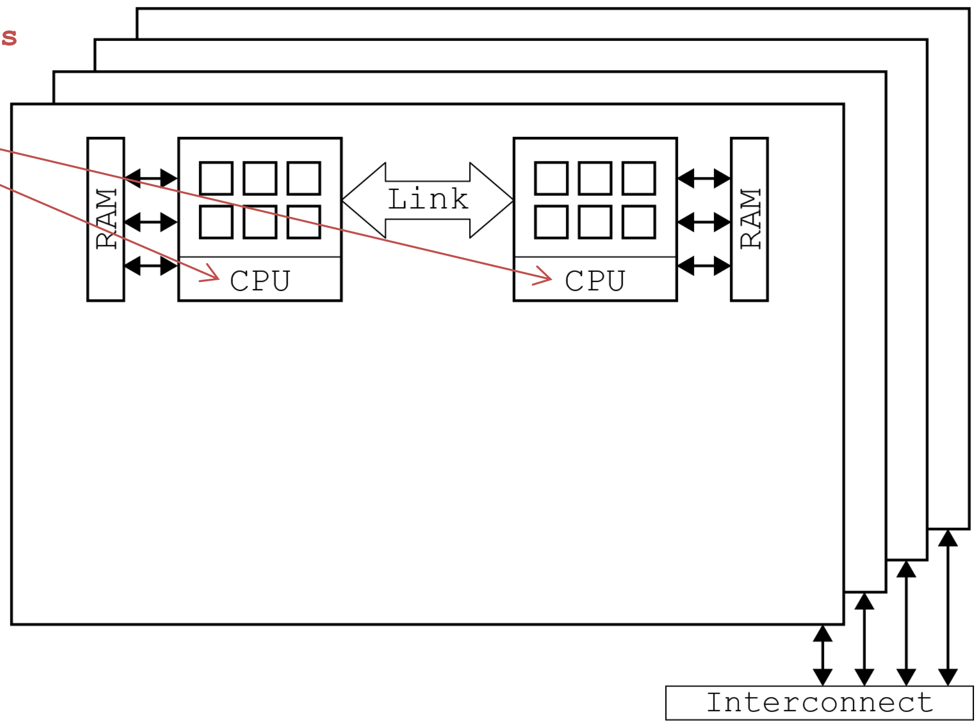


multiple nodes interconnected via
high-bandwidth network
we use MPI at this level

High-performance computing systems

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



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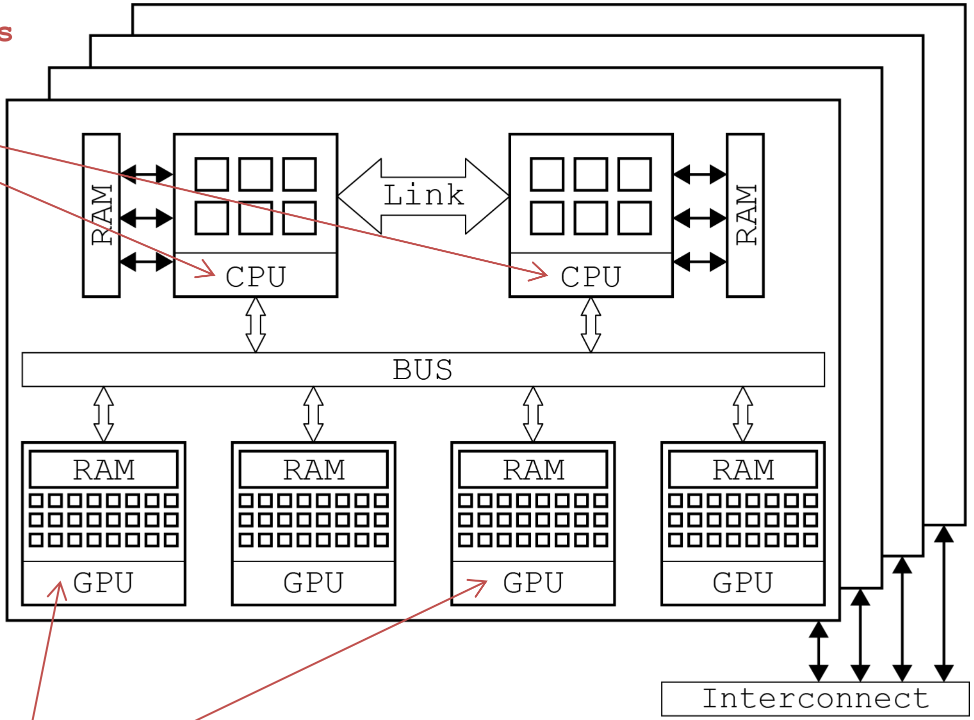


multiple accelerators per node
we use OpenCL/CUDA at this level

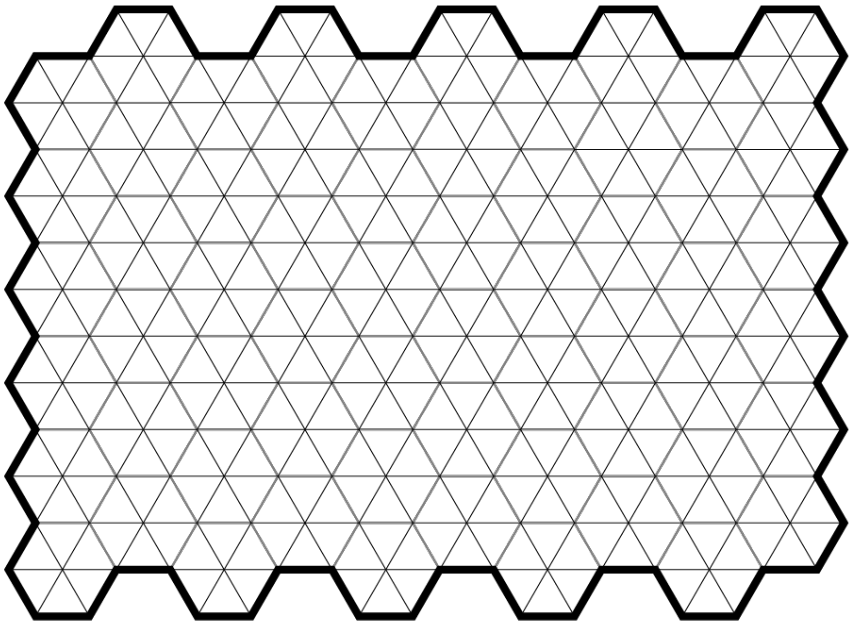
multiple nodes interconnected via high-bandwidth network
we use MPI at this level

Multilevel workload distribution 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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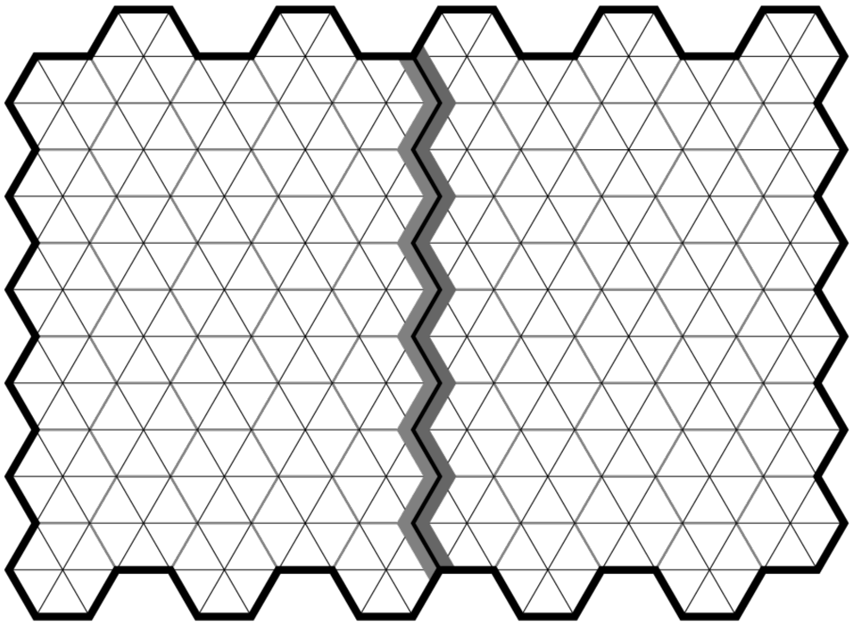

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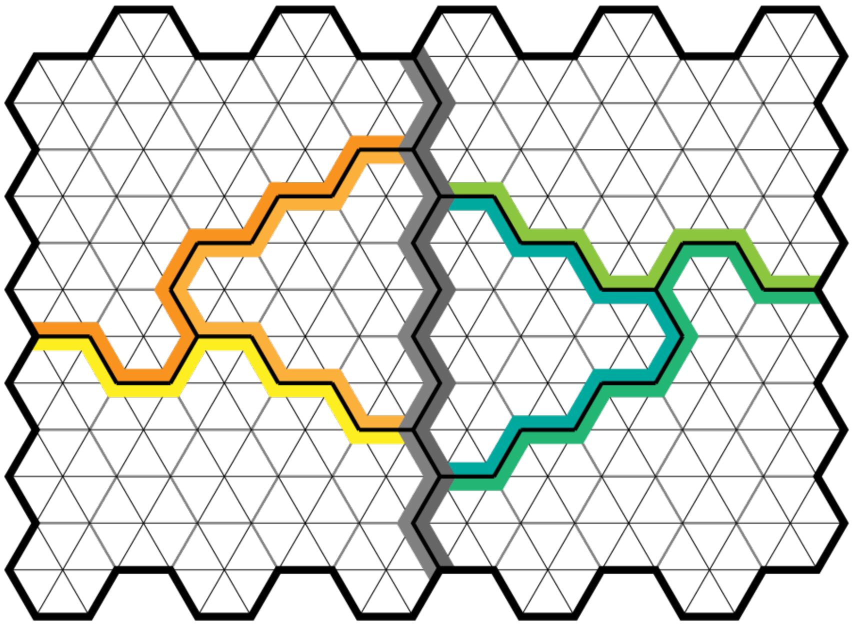
First-level decomposition divides the workload among the computing nodes, that is, the MPI processes.

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



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

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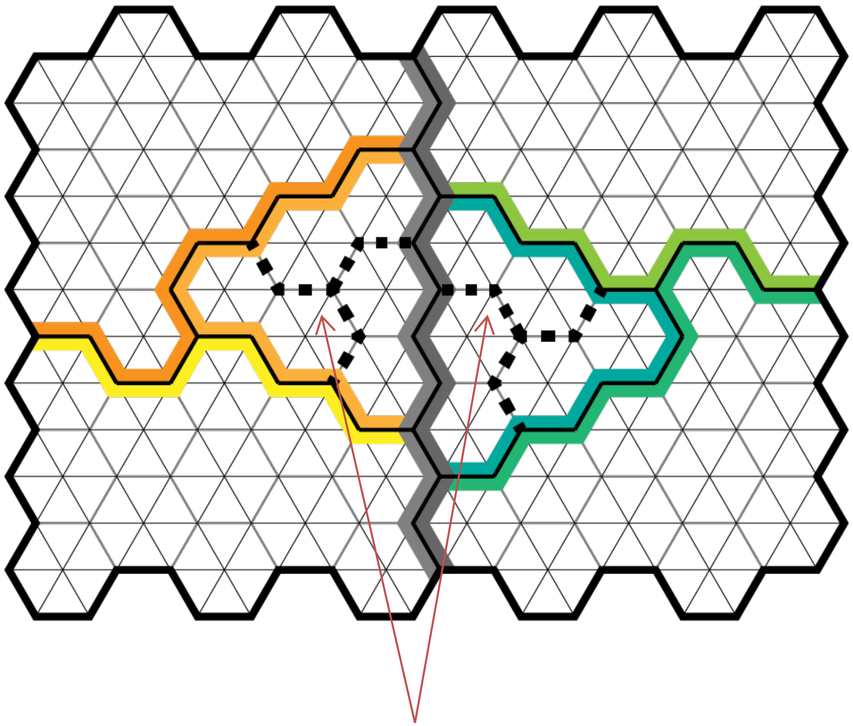
Second-level decomposition divides the first-level partitions to share each MPI's workload among its available hardware, that is, the host and co-processors.

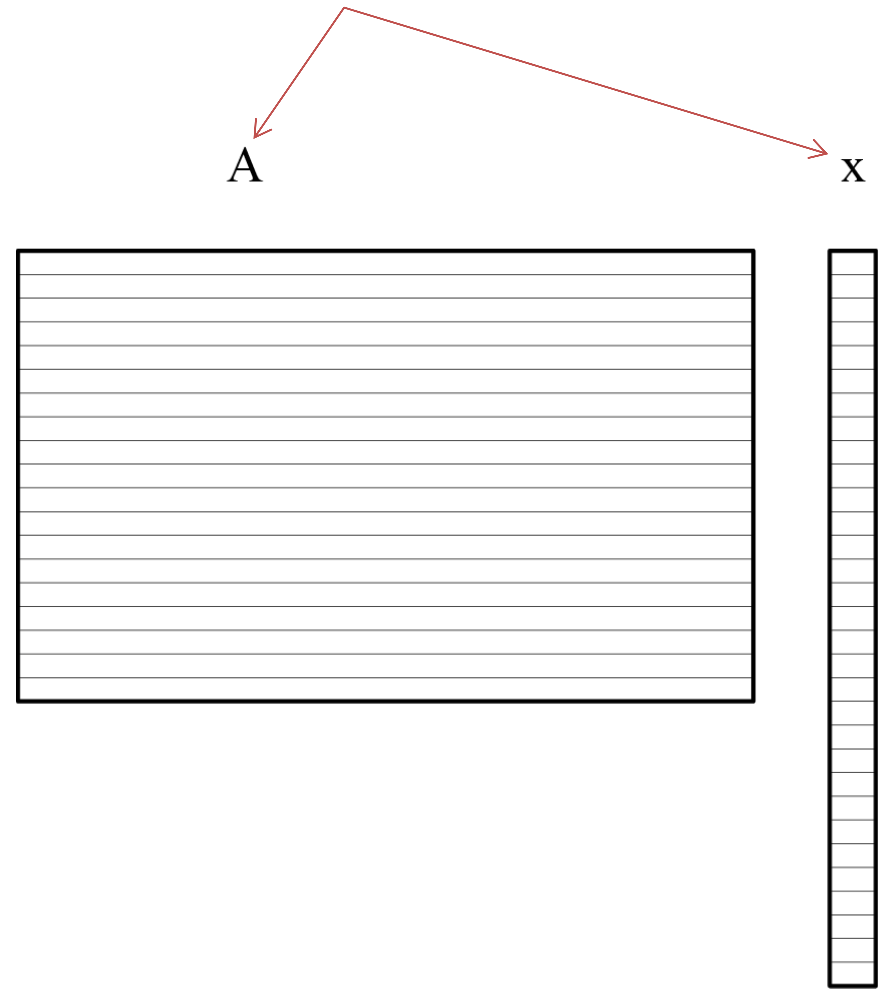
Third-level decomposition divides the second-level partitions to distribute the workload of a device whose shared-memory space introduces a significant NUMA factor, that is, multiple NUMA nodes in a manycore CPU.



can be done with implicit dynamic scheduling or explicit static limits

Sparse matrices and vectors

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

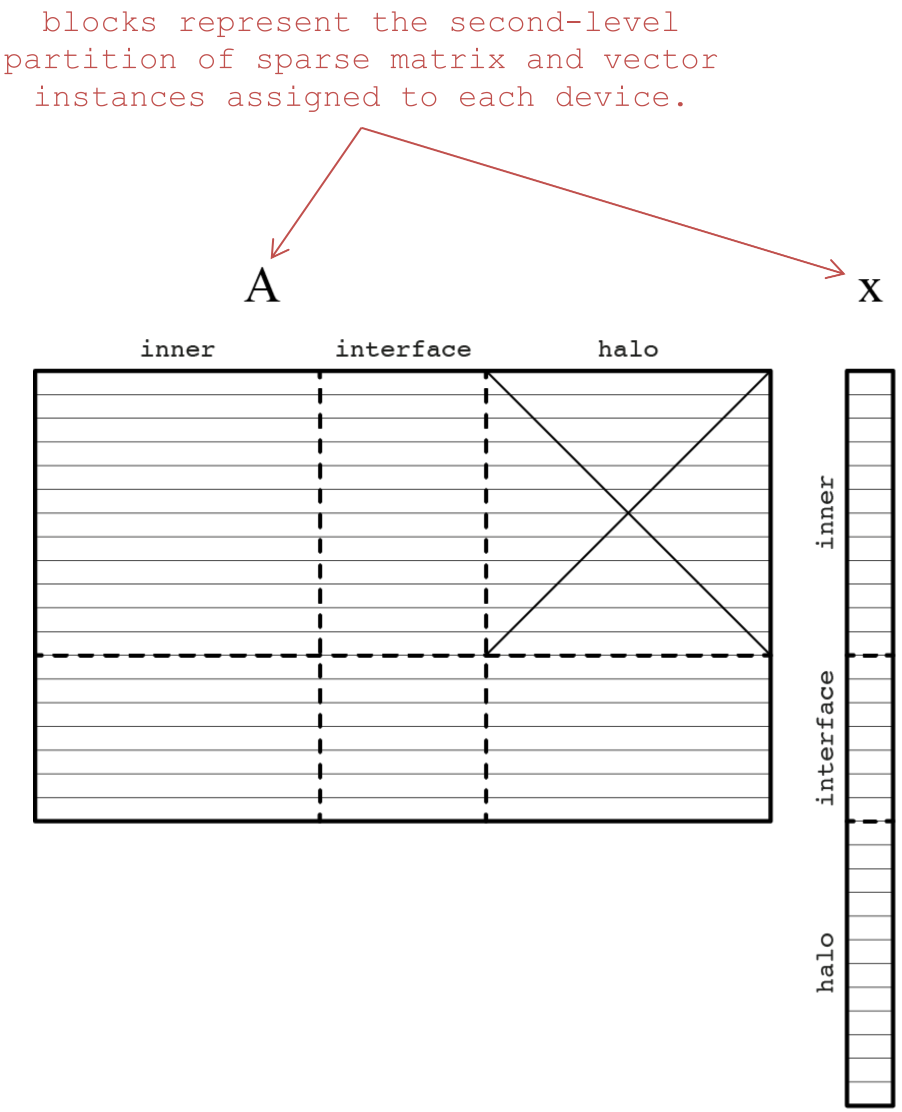


Sparse matrices and vectors represent discrete operators and mesh functions in our algebra-based framework, respectively. Thus, sparse matrix rows and vector elements are distributed among subdomains, and classified into three subsets:

Inner

Interface

Halo



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

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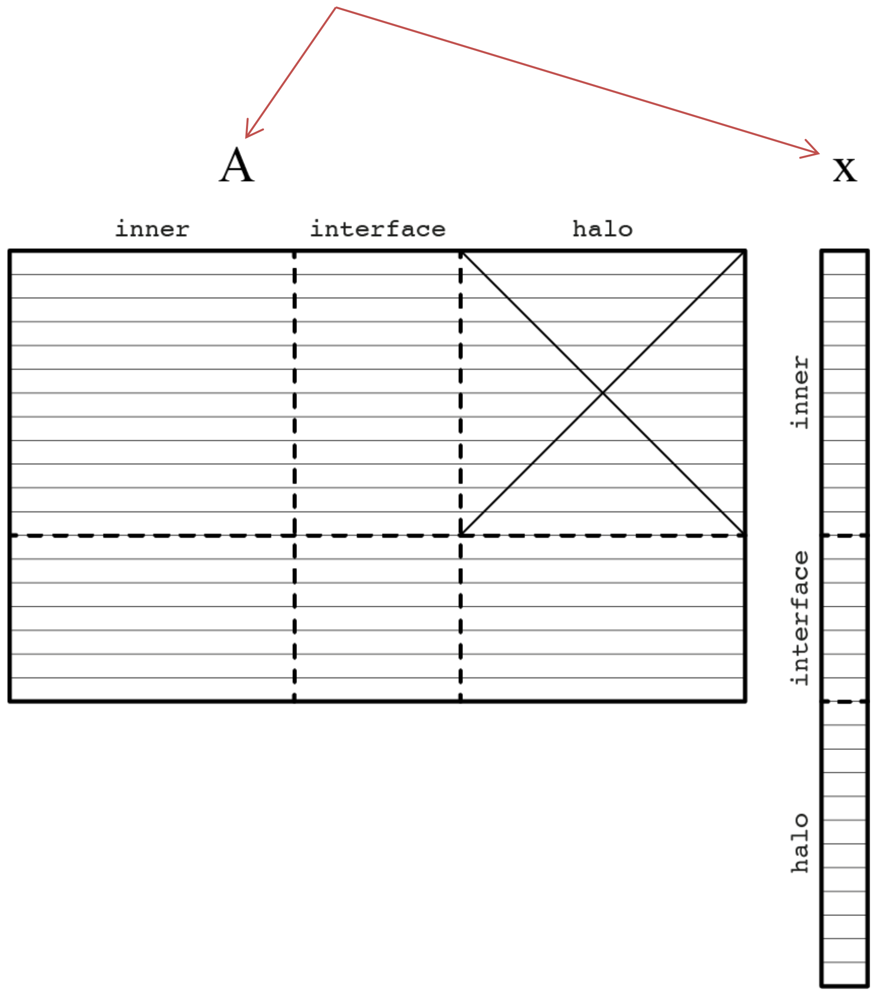

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Inner subset is composed of local elements which are coupled with local elements only.

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

Halo

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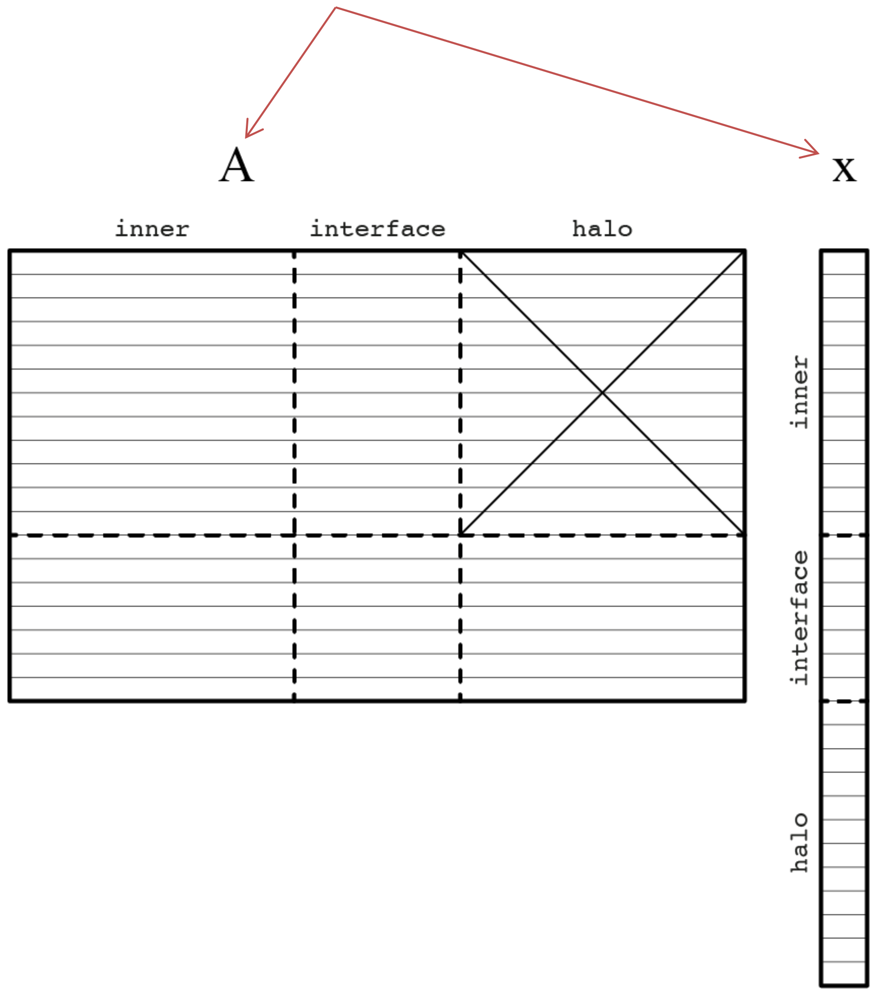

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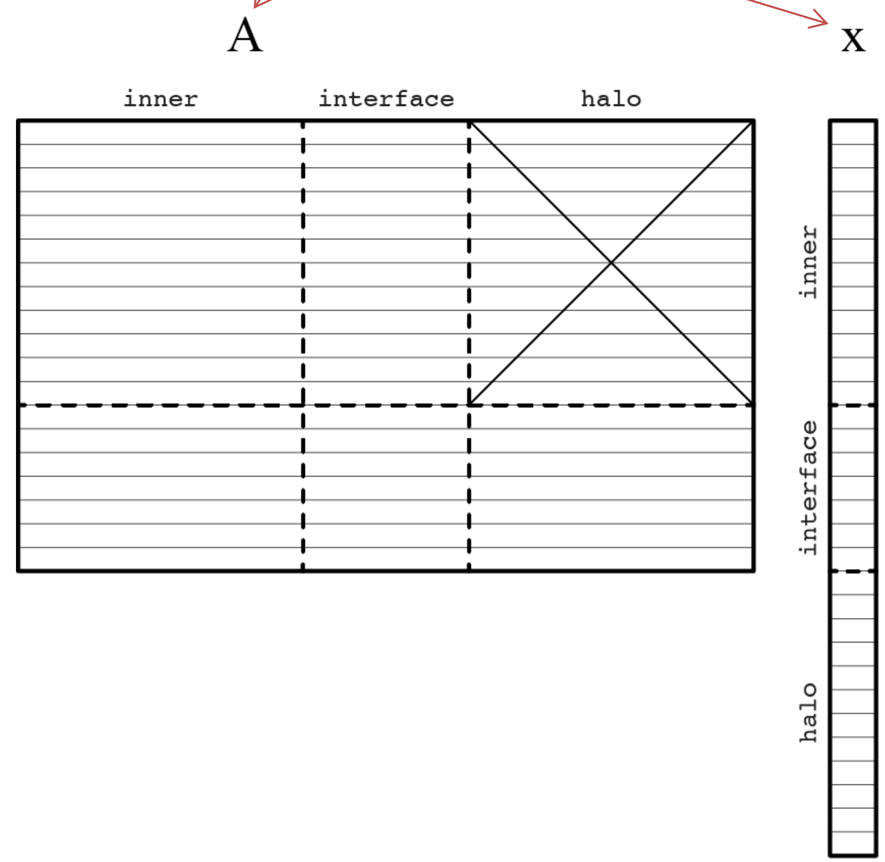
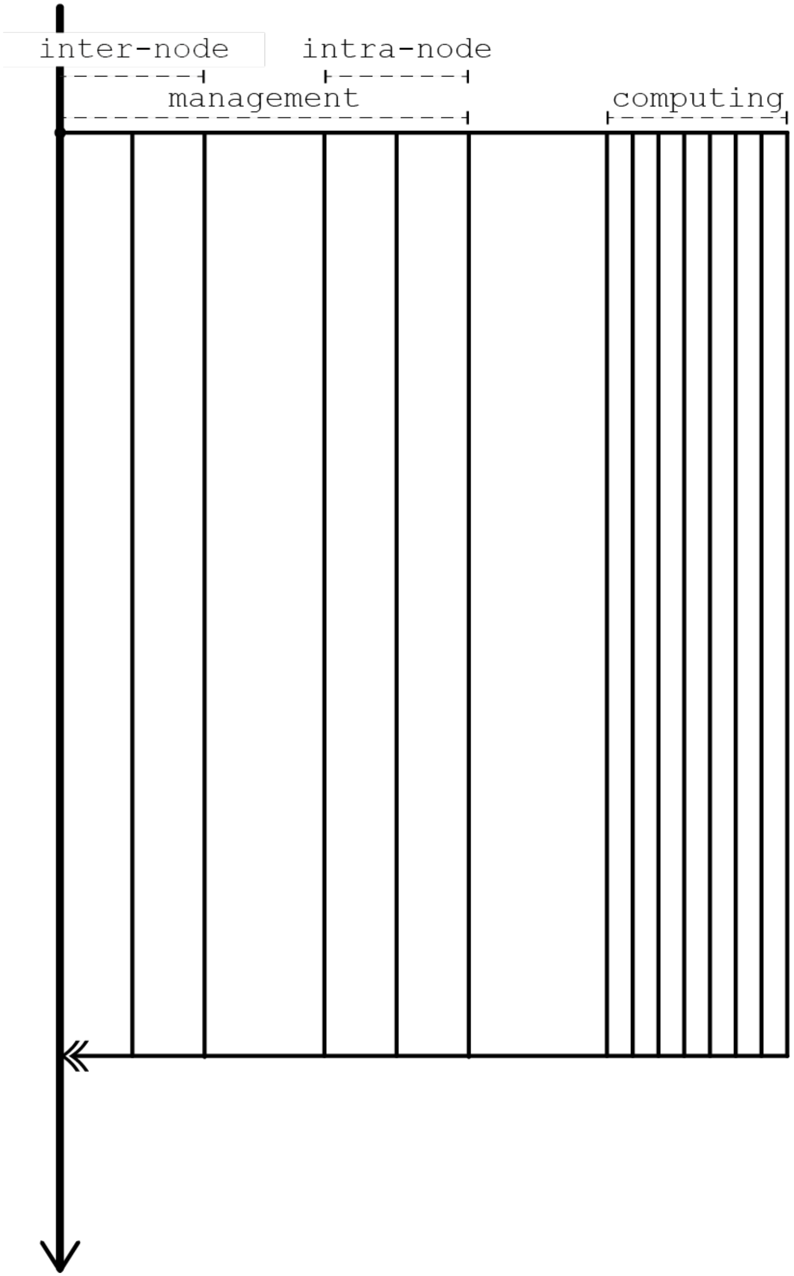
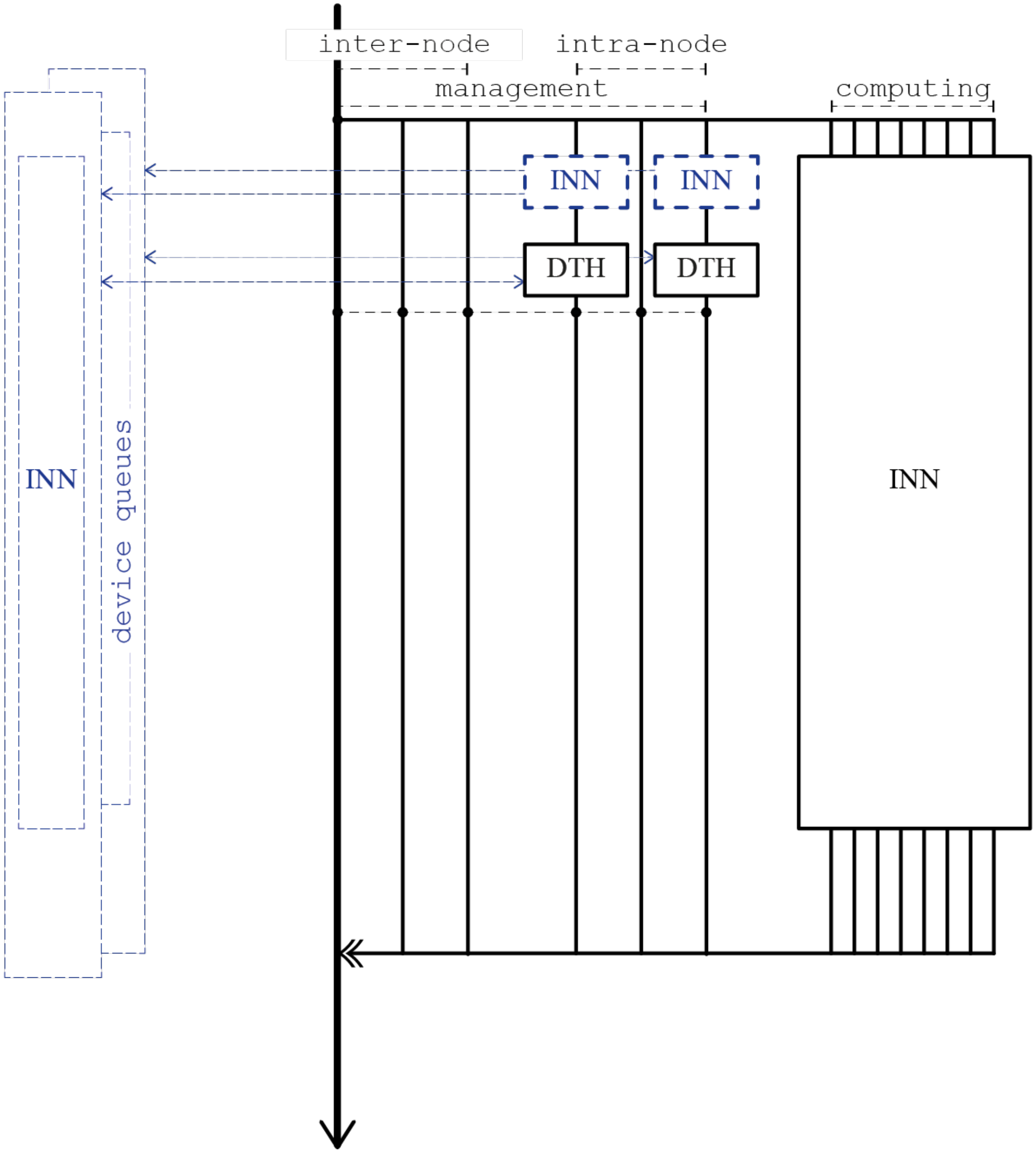



inter-node
intra-node
management
computing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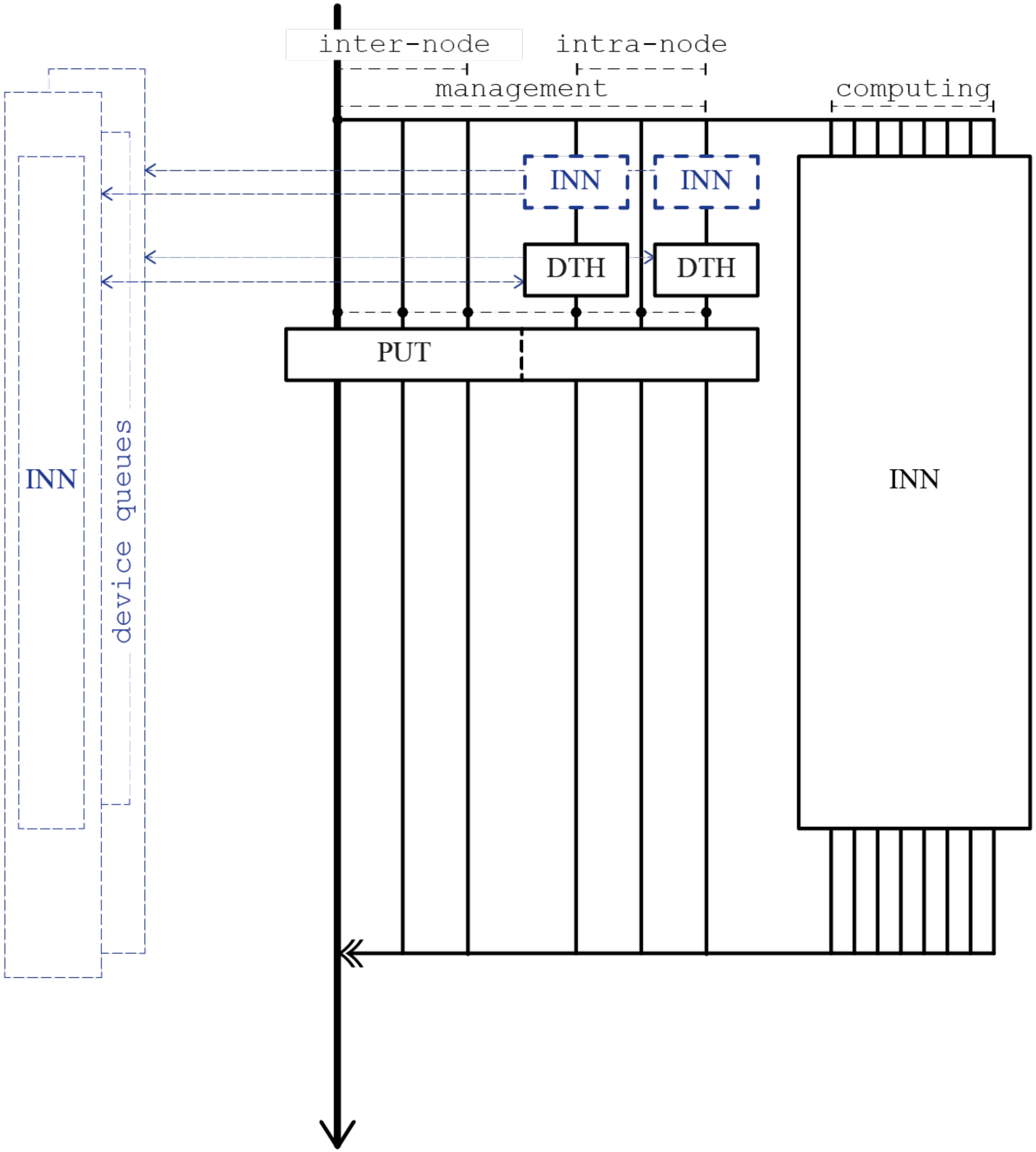
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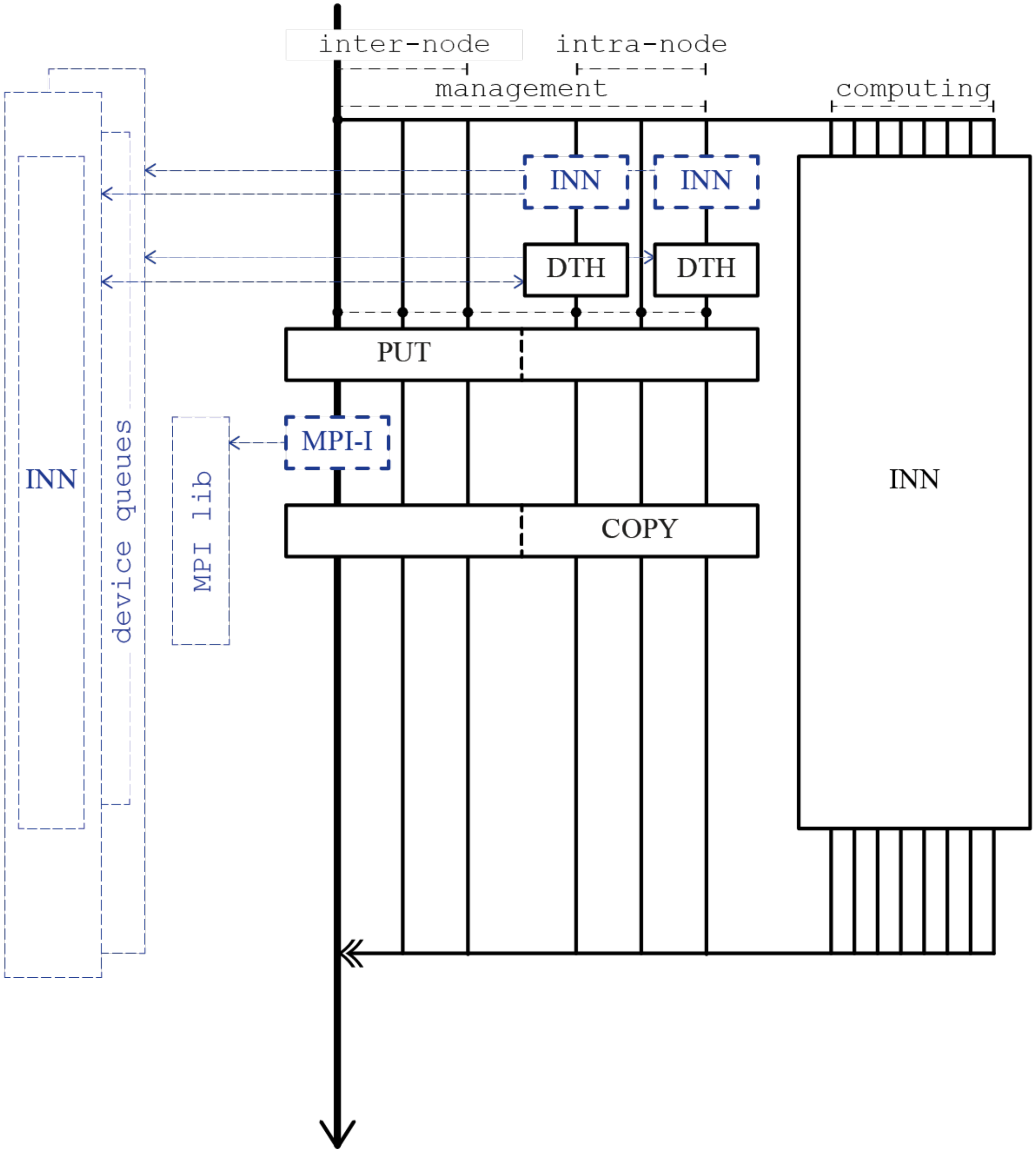
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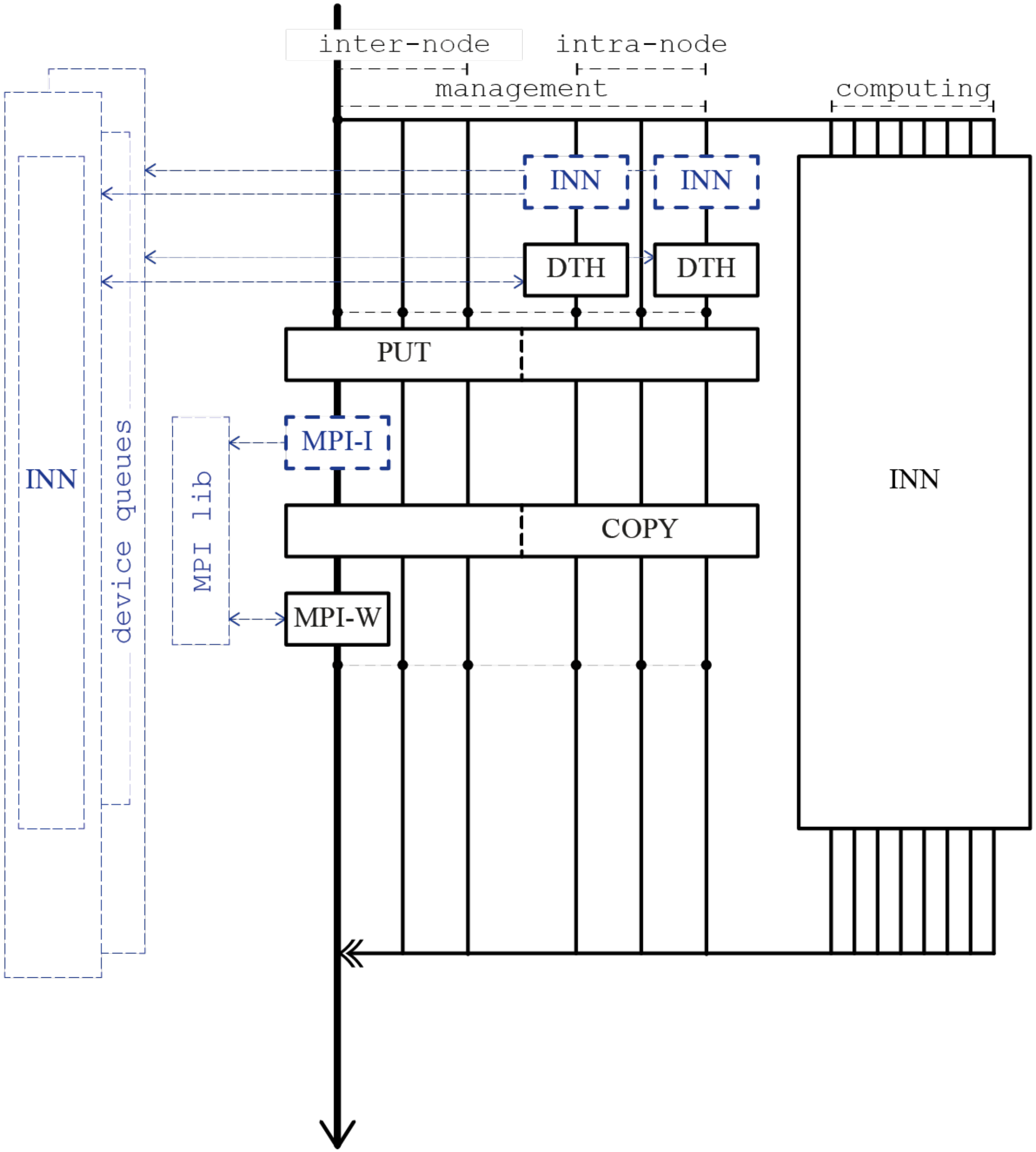
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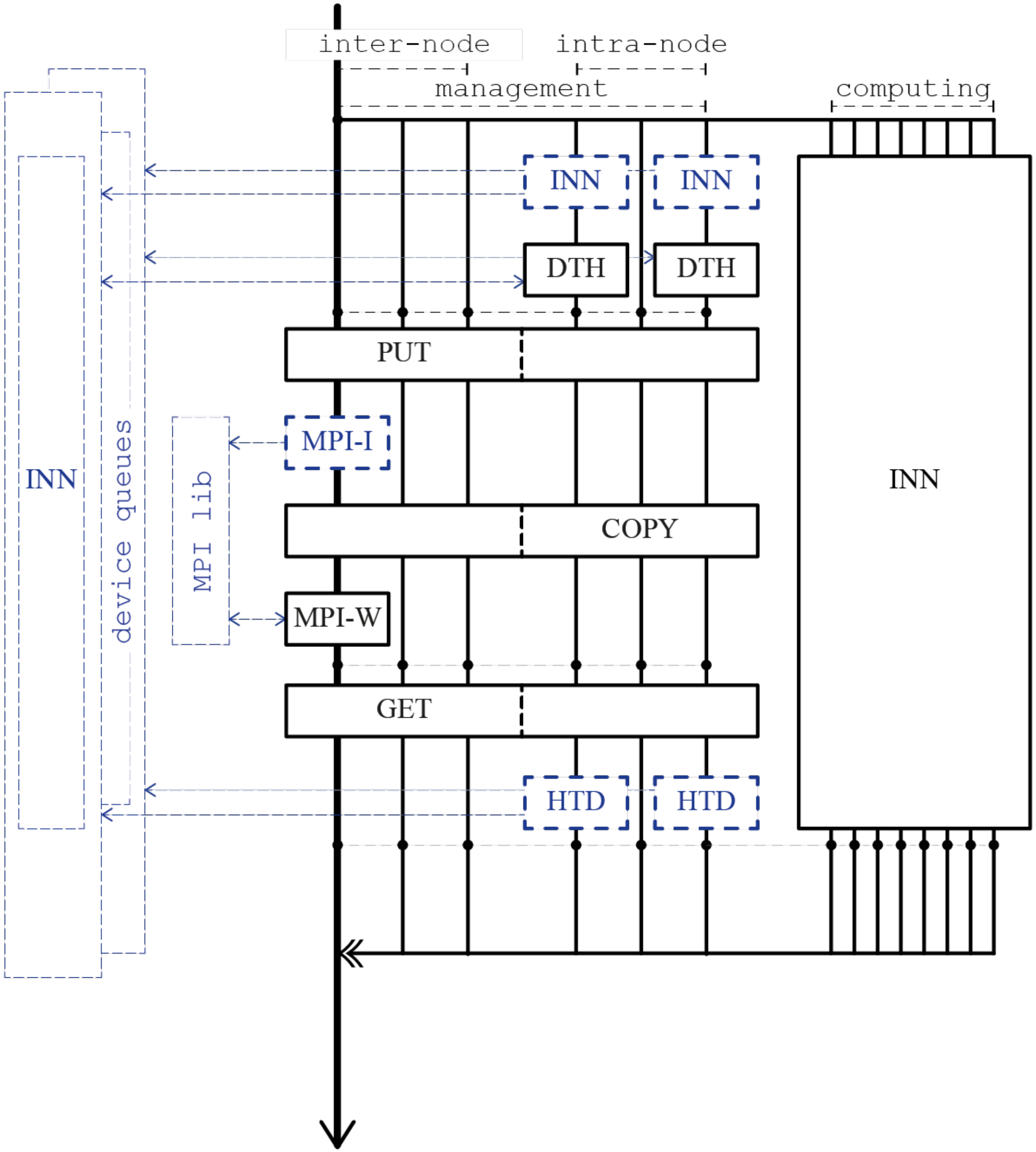
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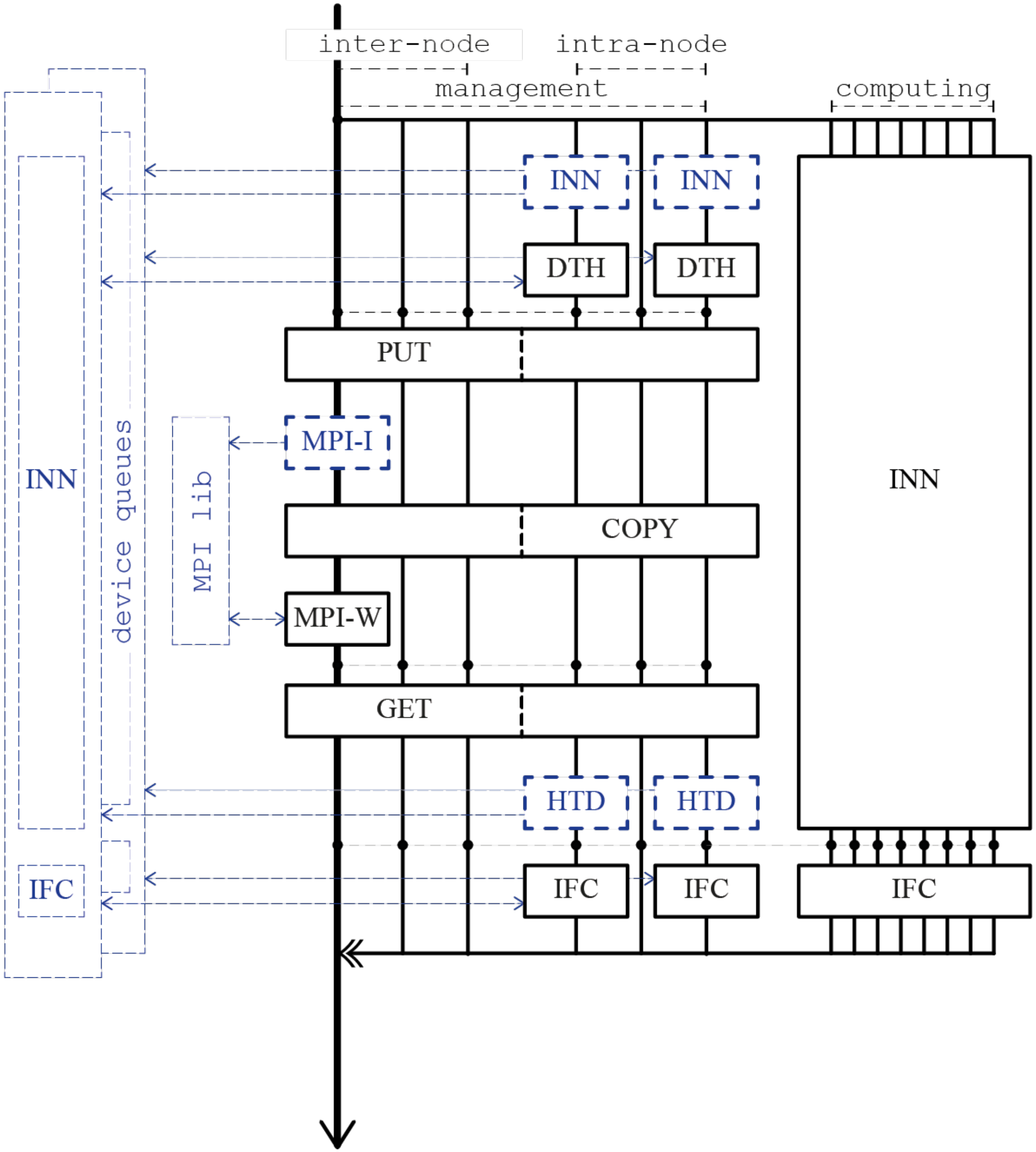
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MPI lib

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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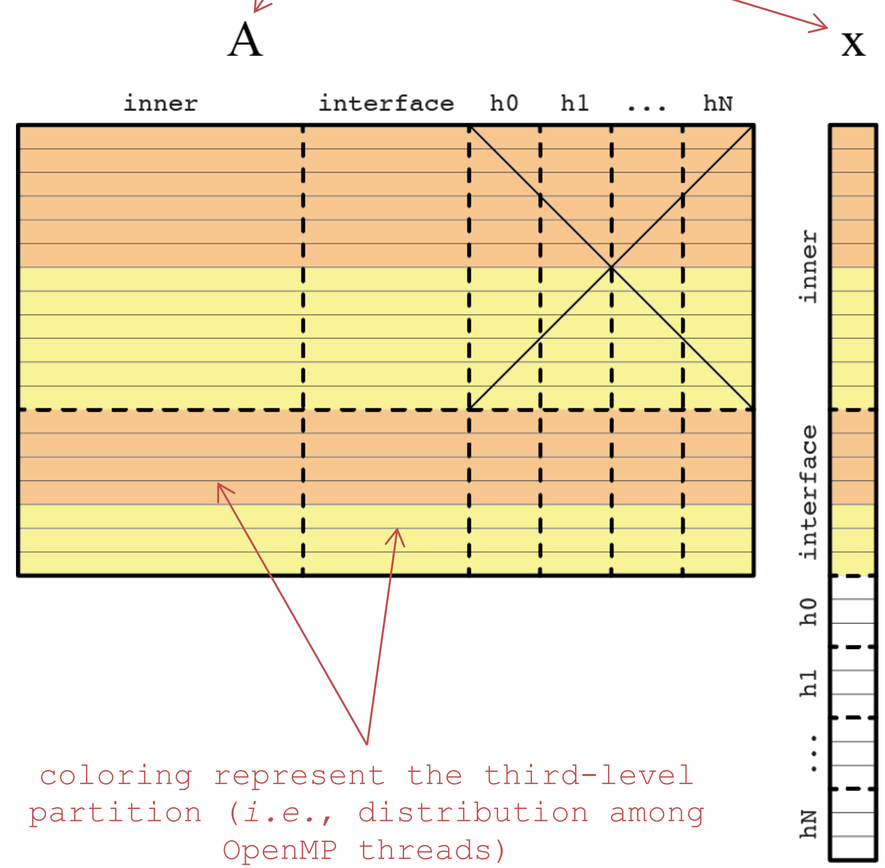

coloring represent the third-level partition (*i.e.*, distribution among OpenMP threads)

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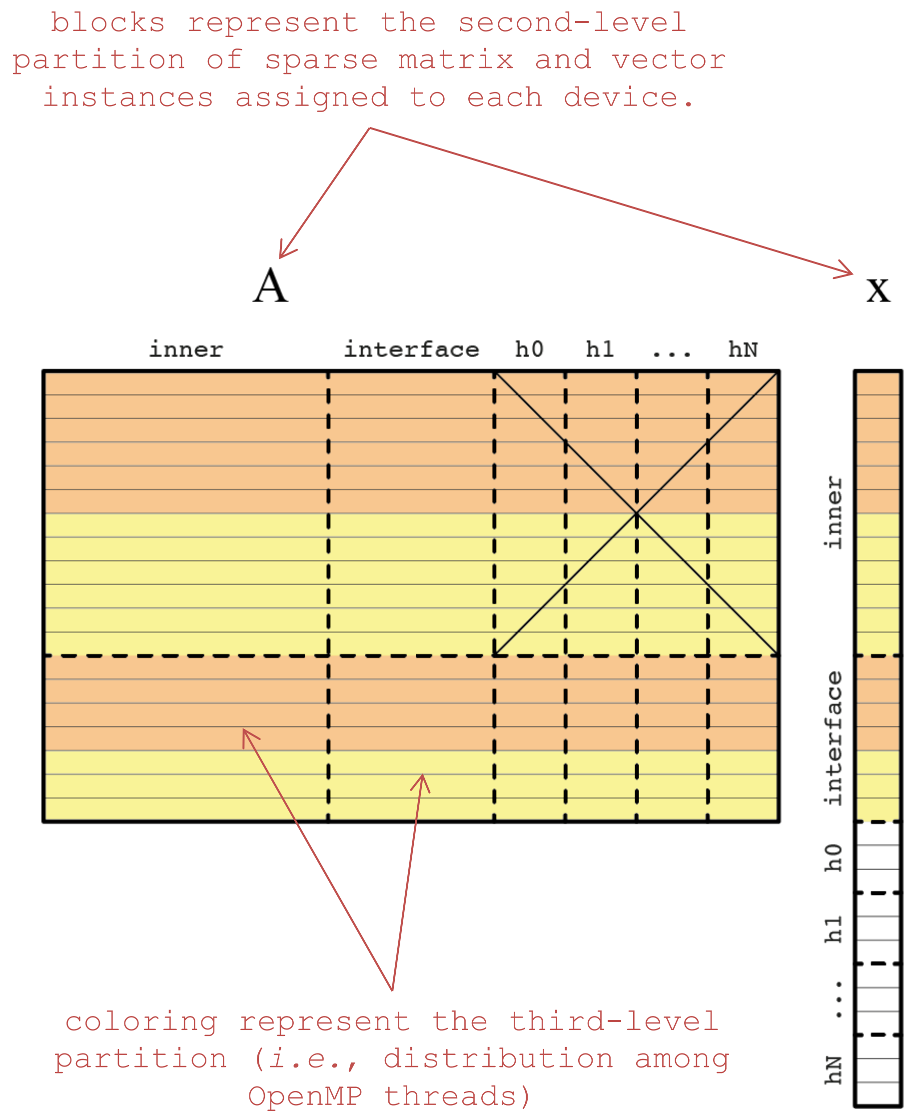
However, in NUMA configurations, a thread accessing to the memory allocated by another memory controller goes through a much slower bus.



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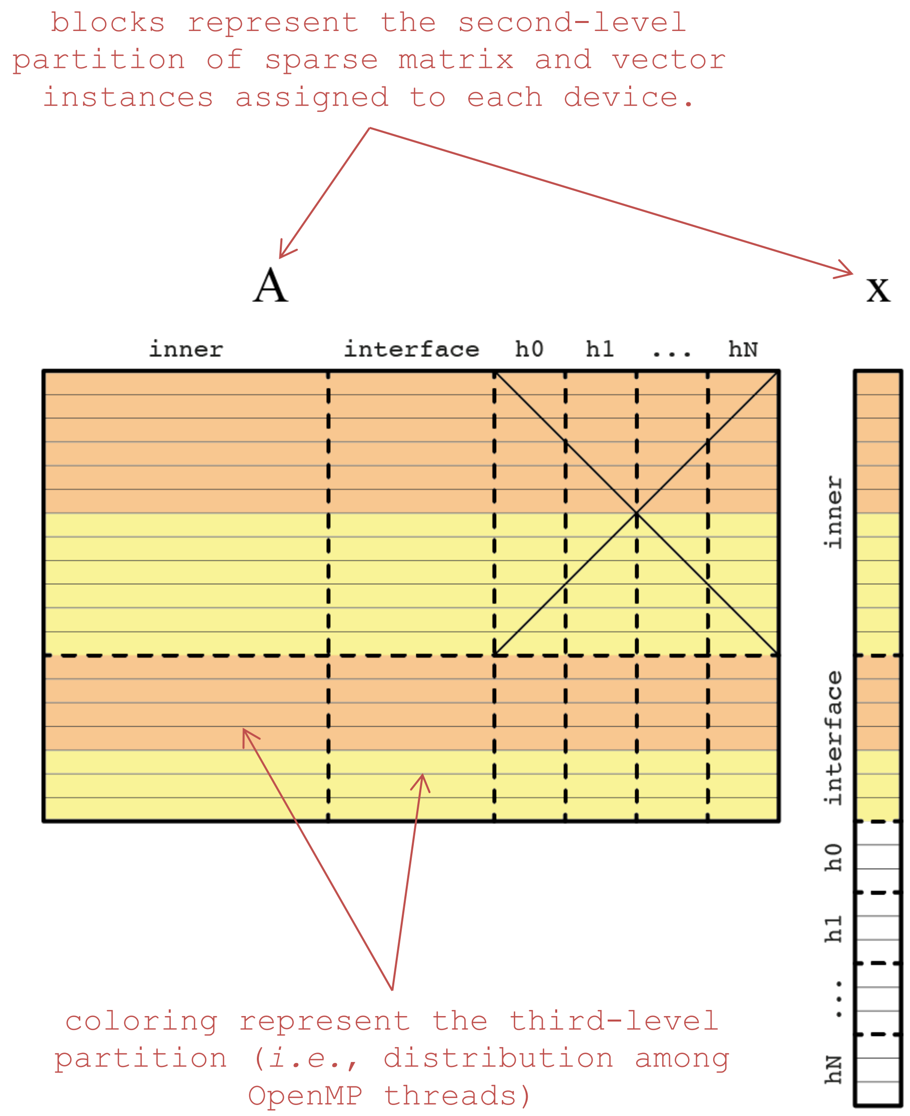

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Thread migration must be avoided to ensure an efficient memory access!

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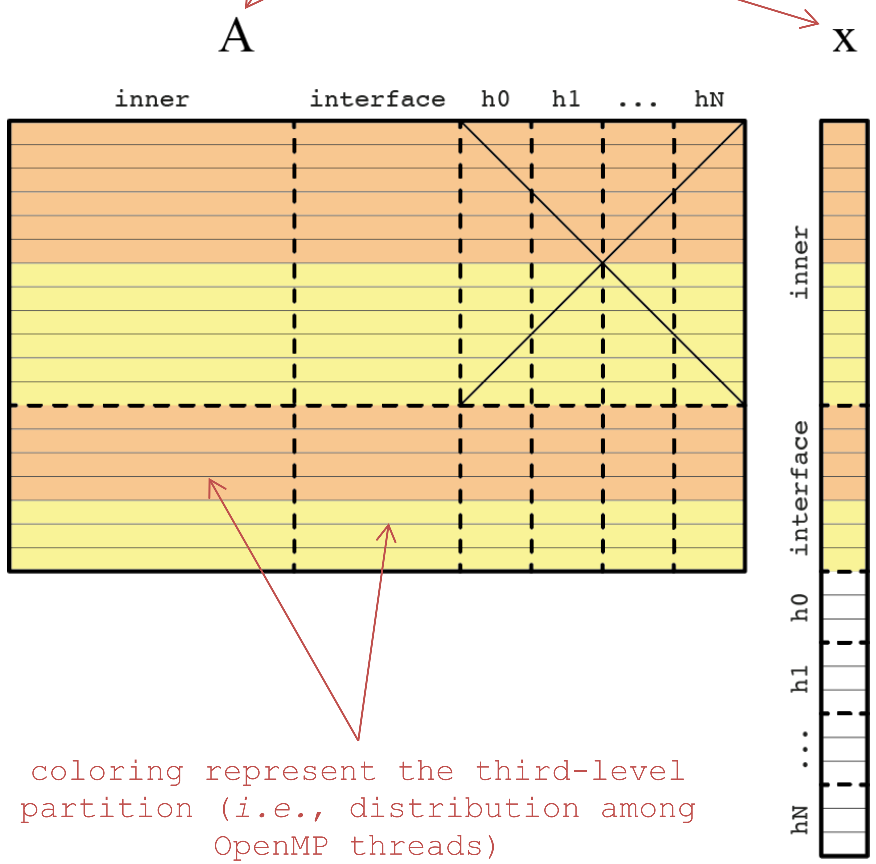

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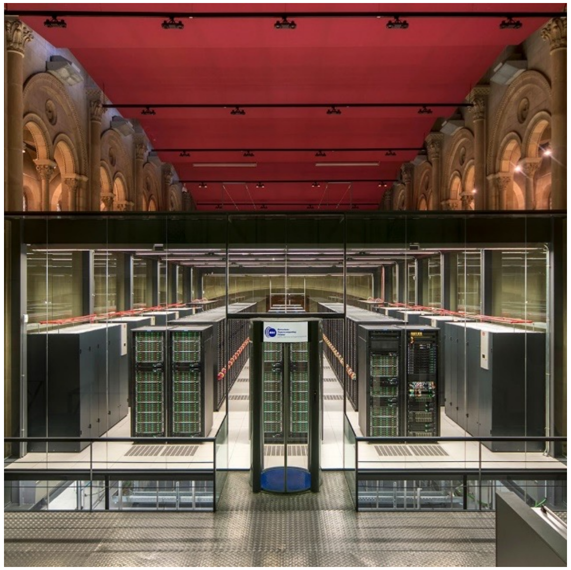
Execution of SpMV on different modern supercomputers

PERFORMANCE STUDY

Testing setup

MareNostrum 4



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

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].

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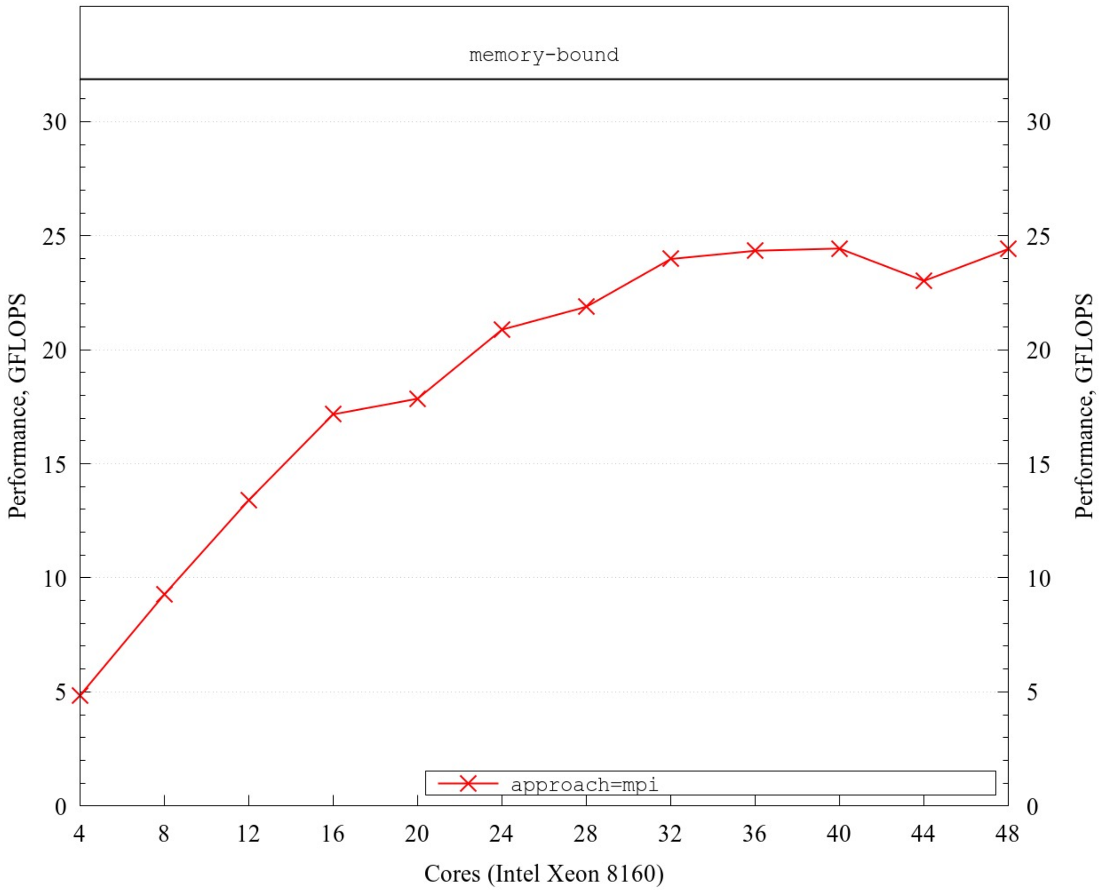

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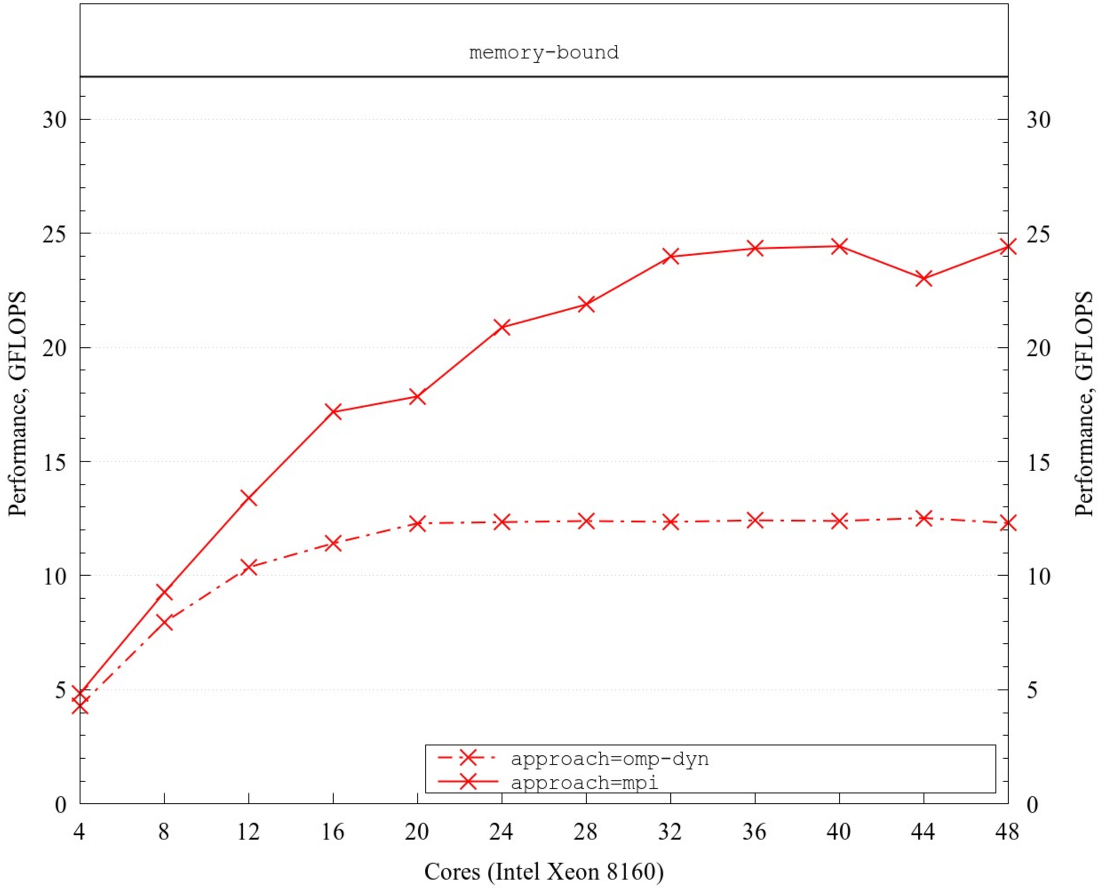

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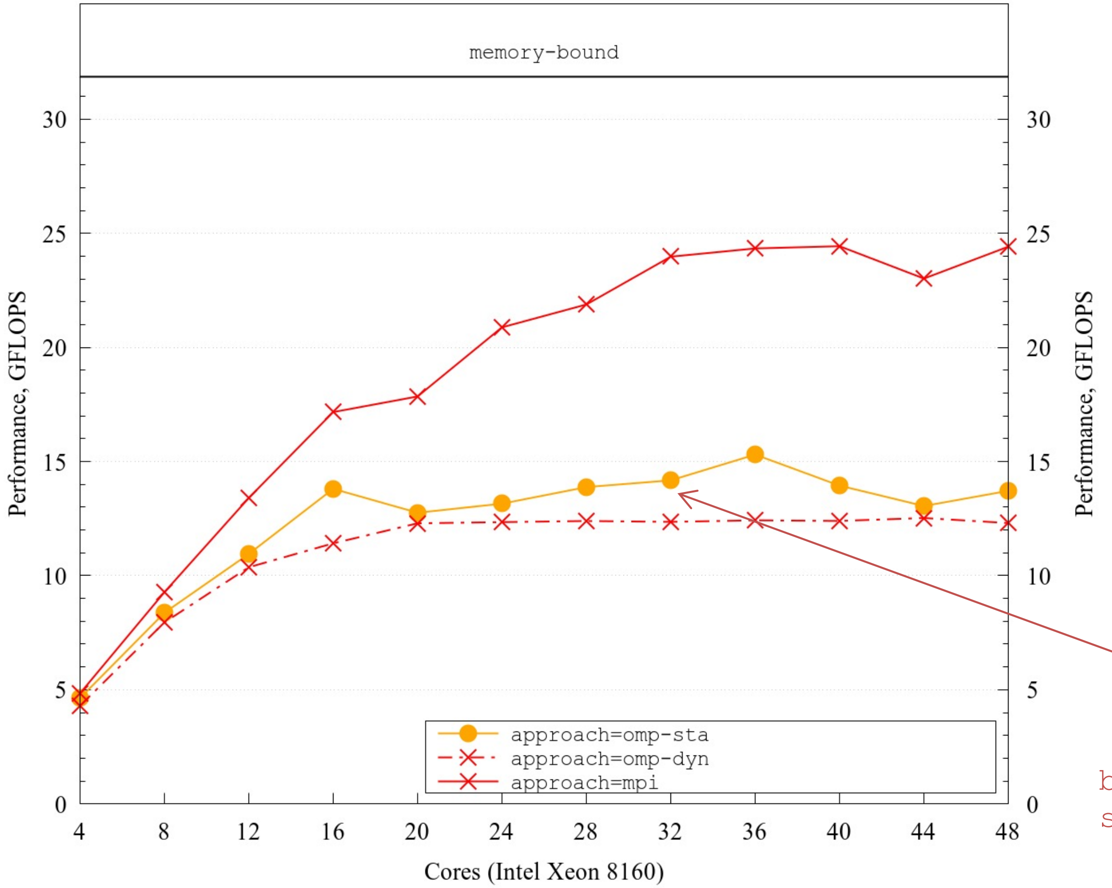

without thread binding, the static scheduling is still in troubles

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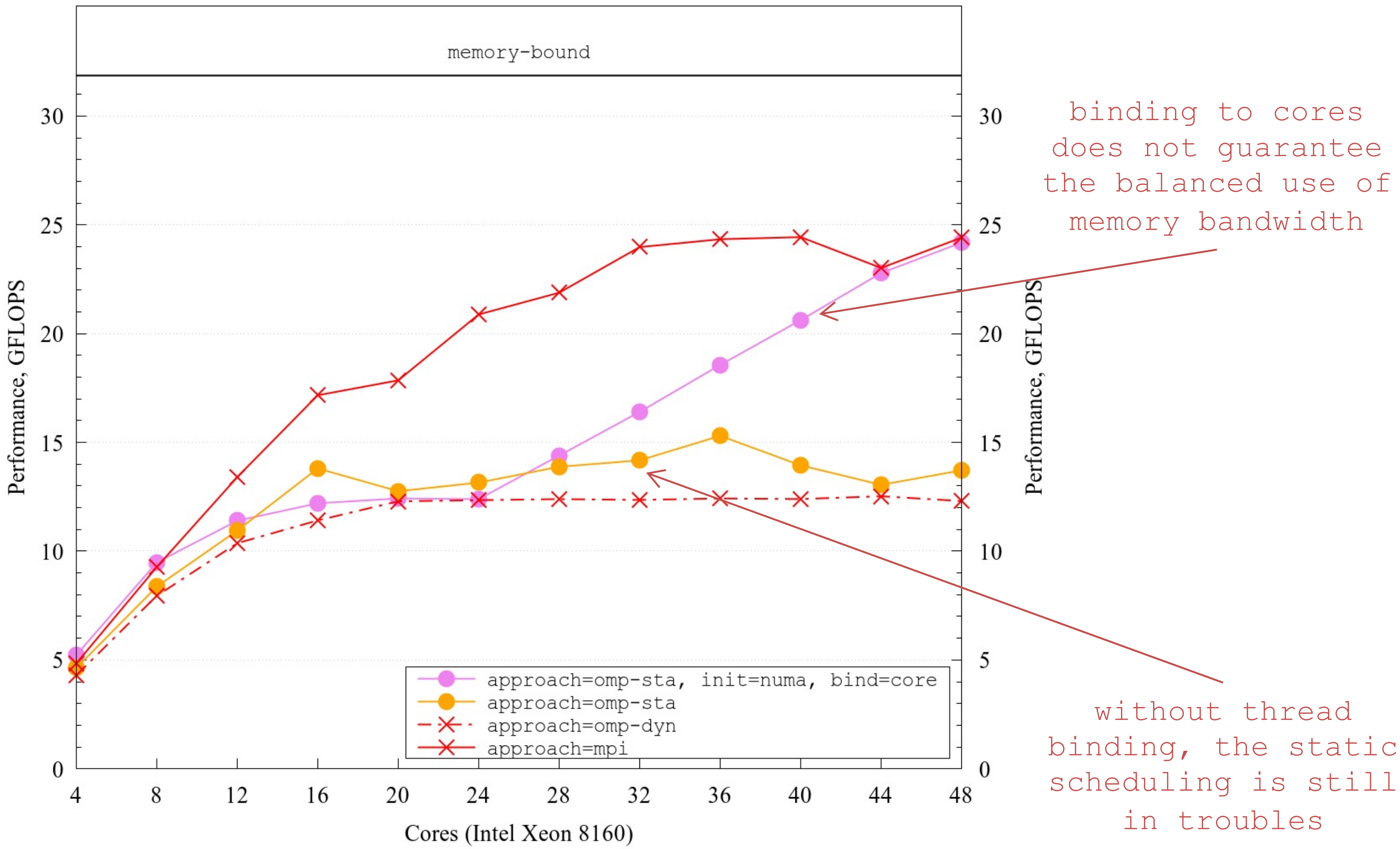

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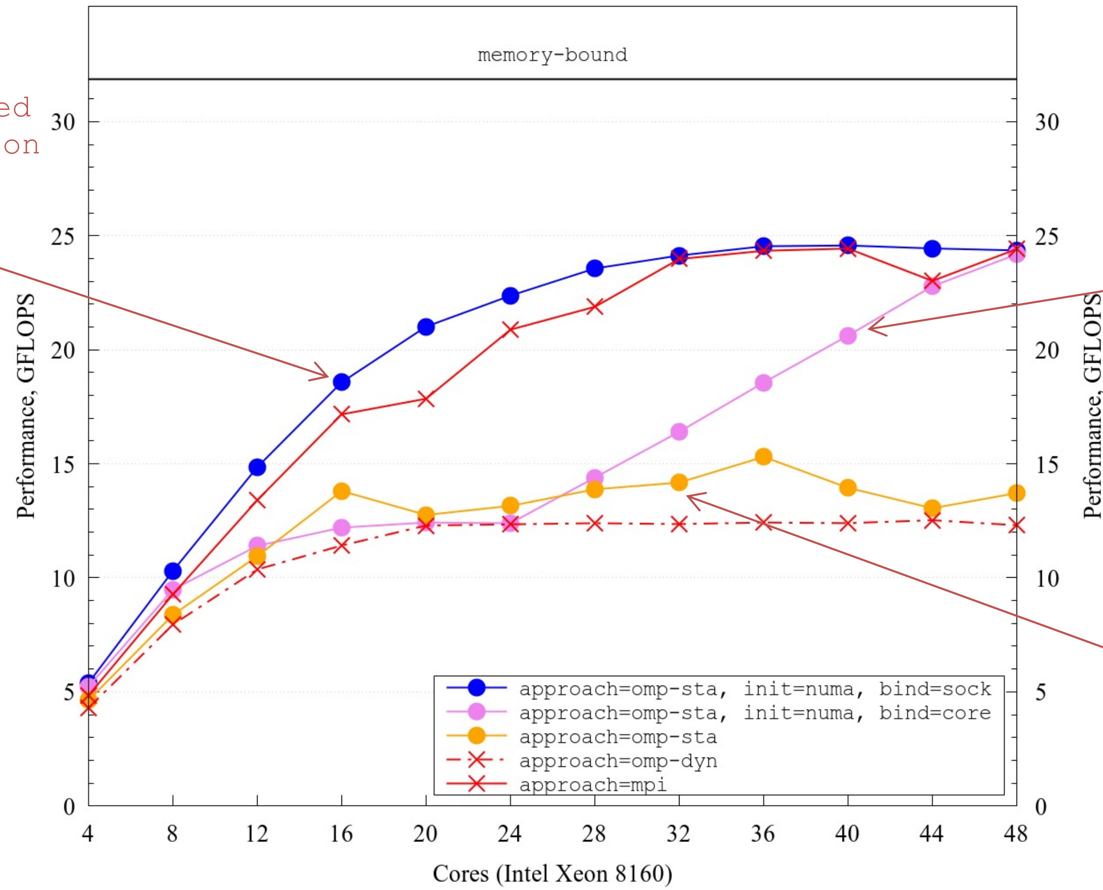
thread binding to sockets and threaded memory initialization is our choice



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

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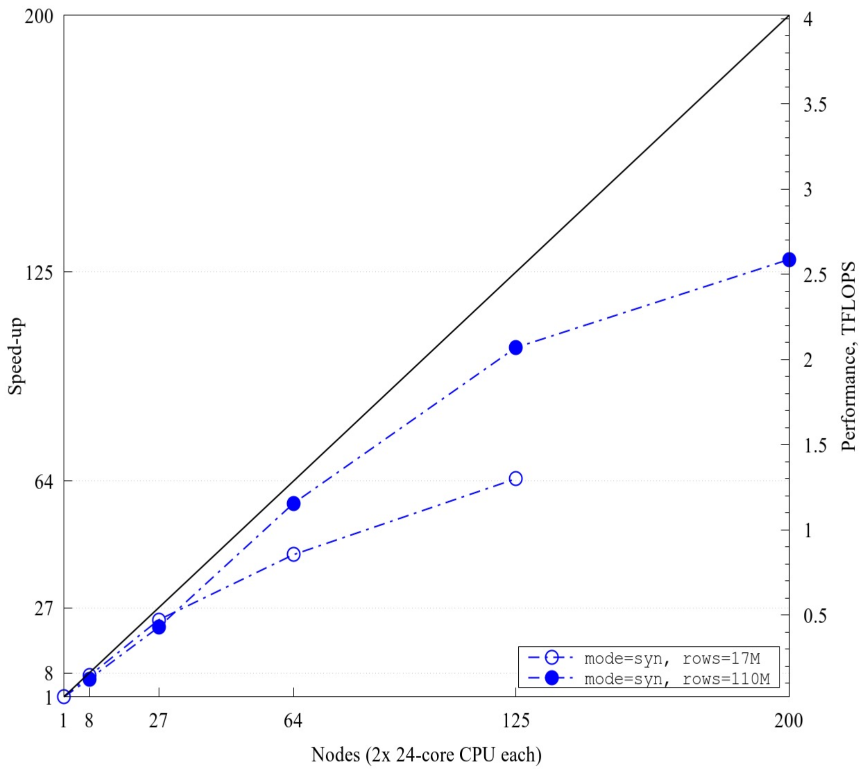
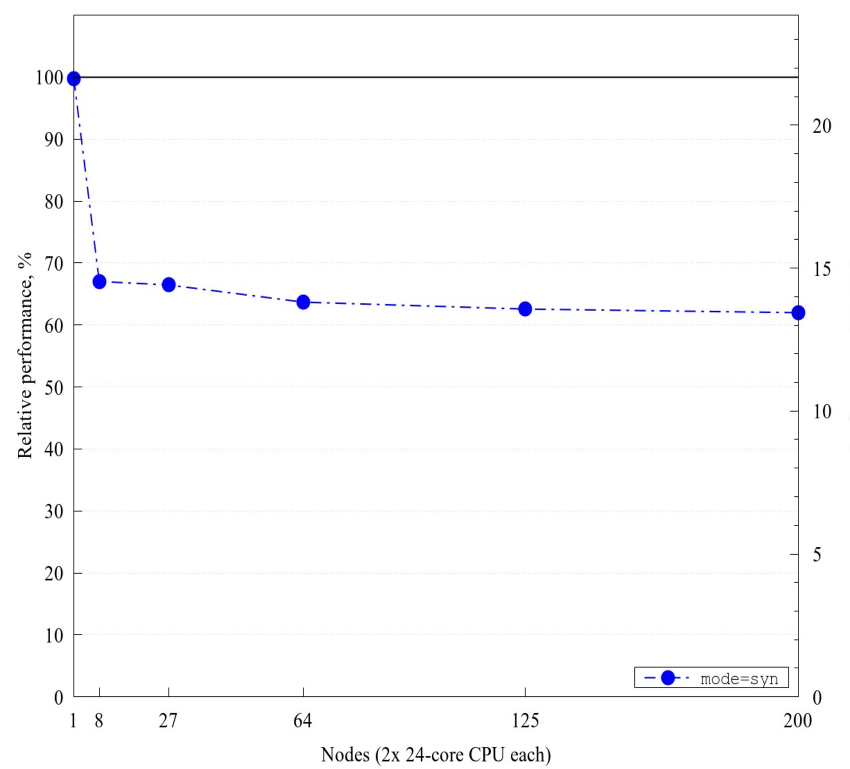
Test case 2:

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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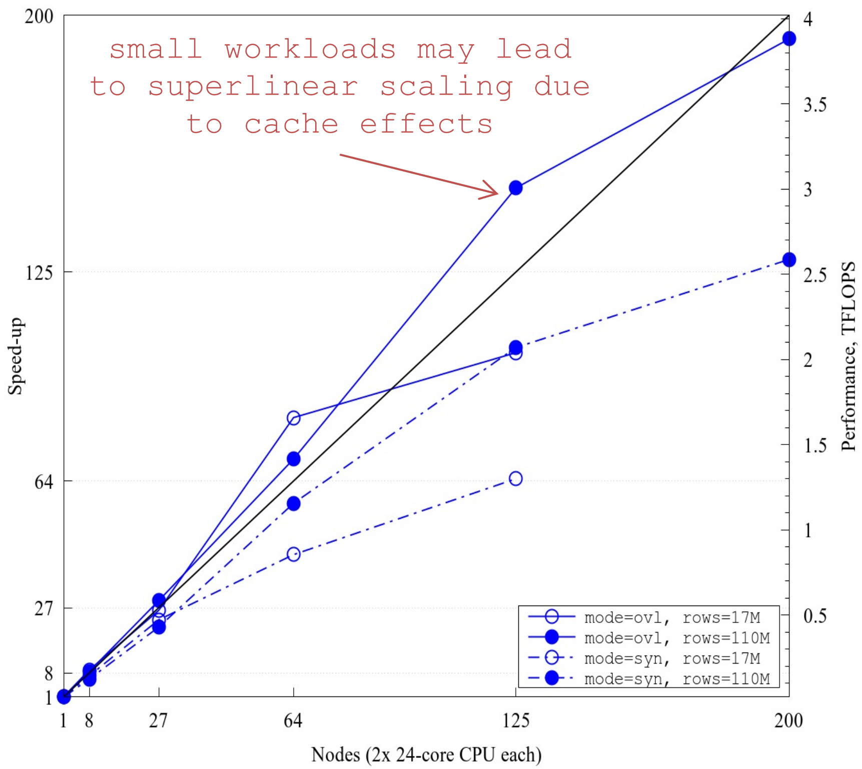

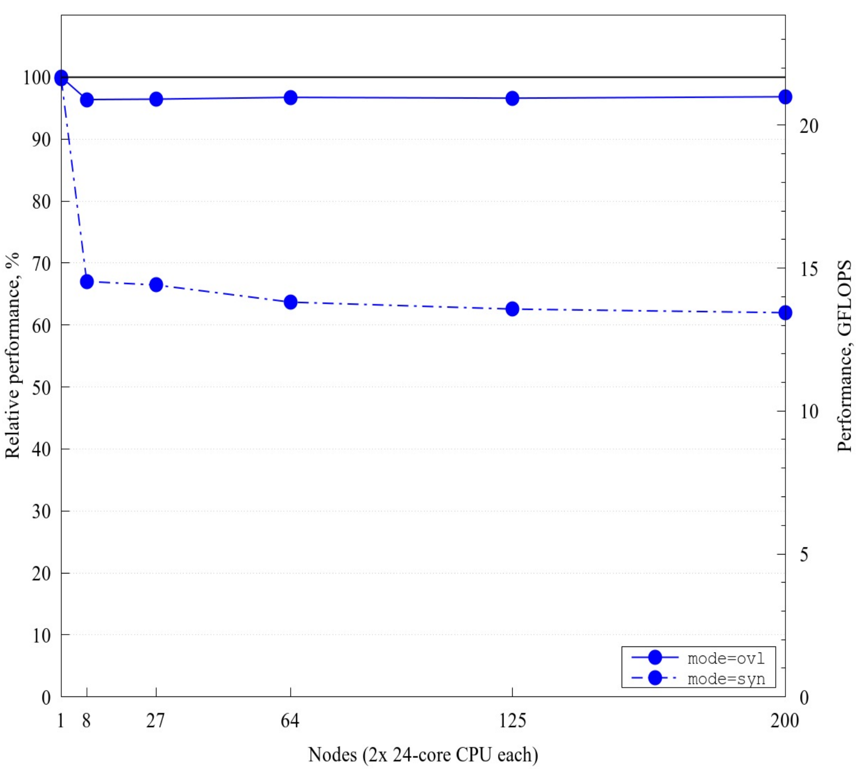

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Single-node performance of SpMV kernel vs number of cores on TSUBAME3.0 for both sequential and parallel management of communications. The sparse matrix used arise from the symmetry-preserving discretization[1] of the Laplacian operator on unstructured hex-dominant mesh of 17 million cells. The sparse matrix storage format used is block-transposed ELLPACK[2].

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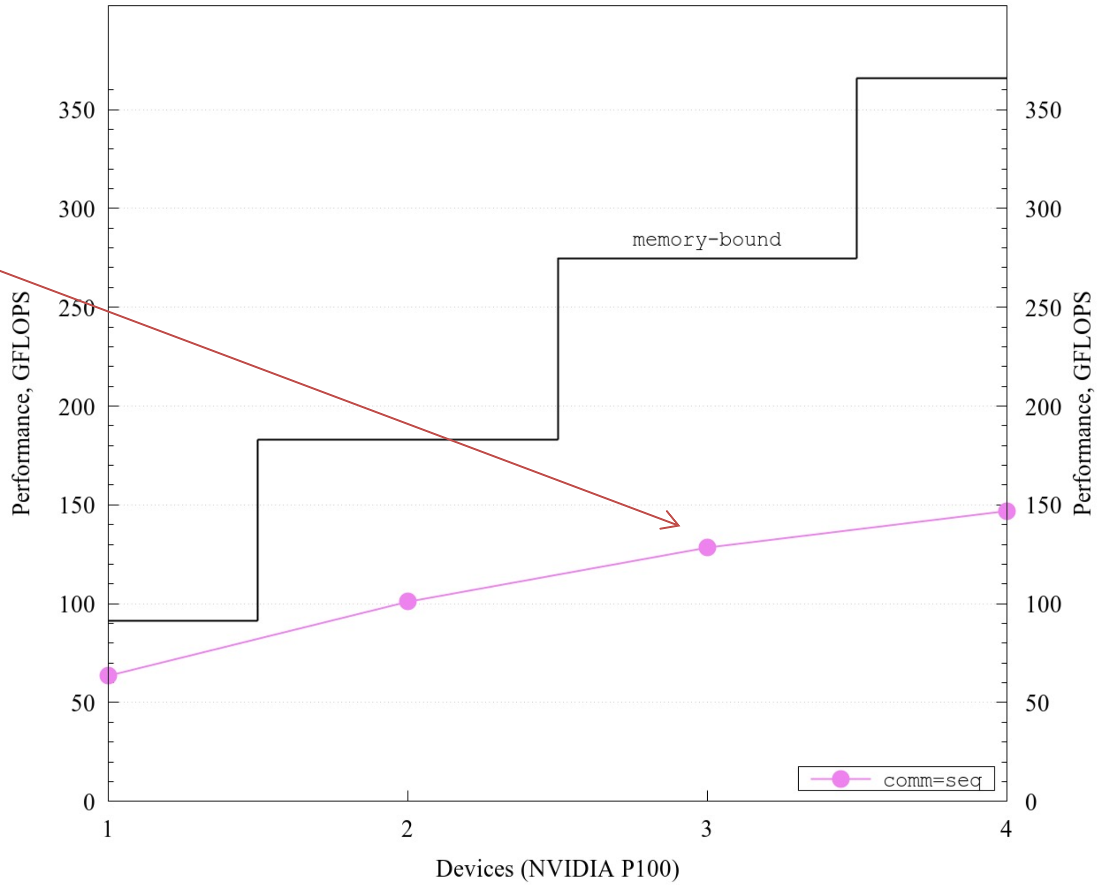

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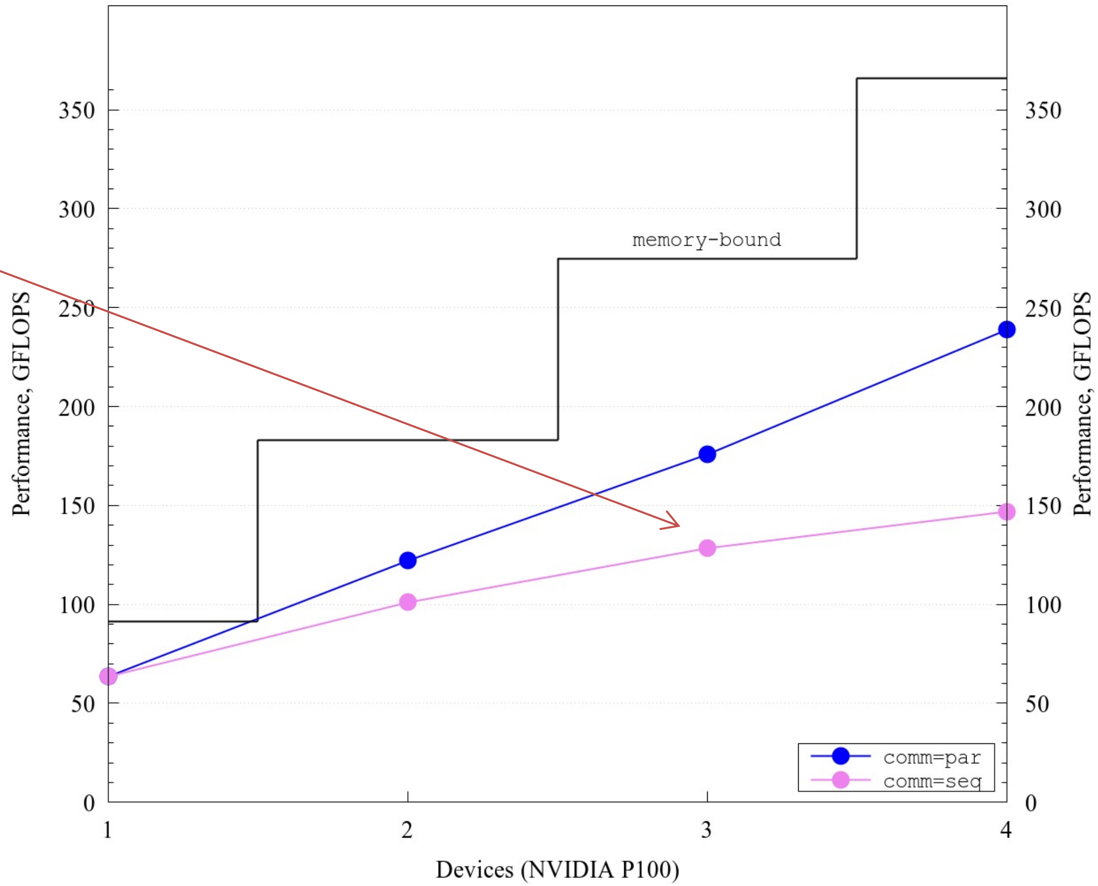

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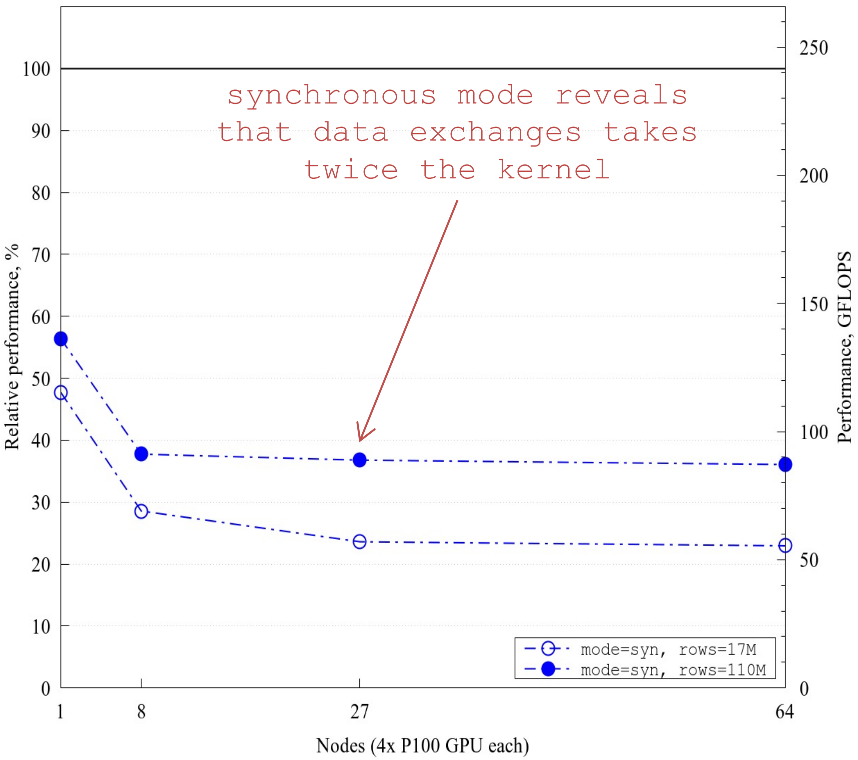

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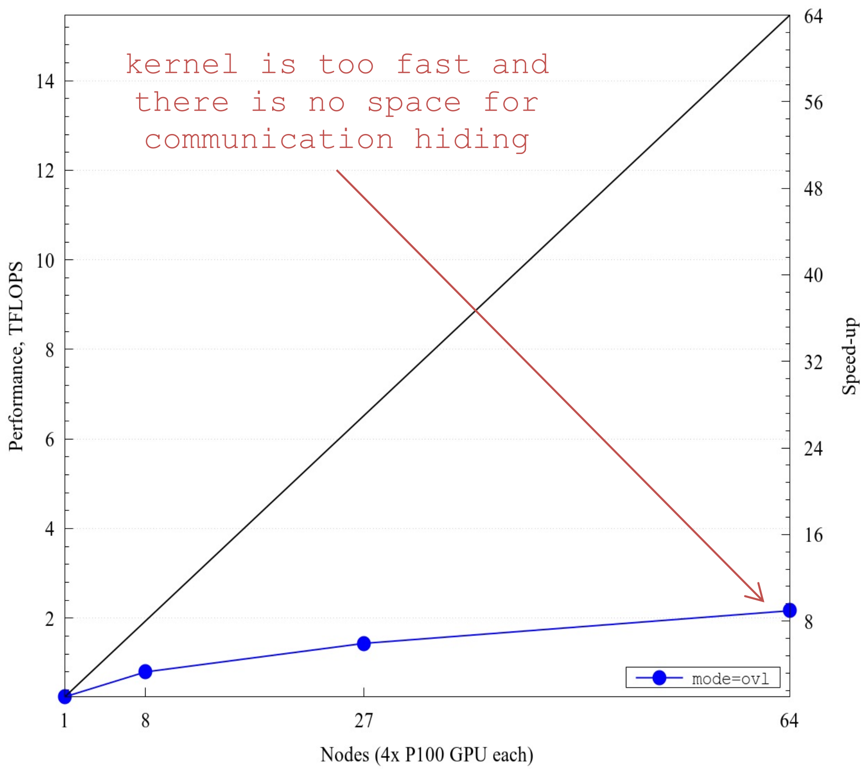

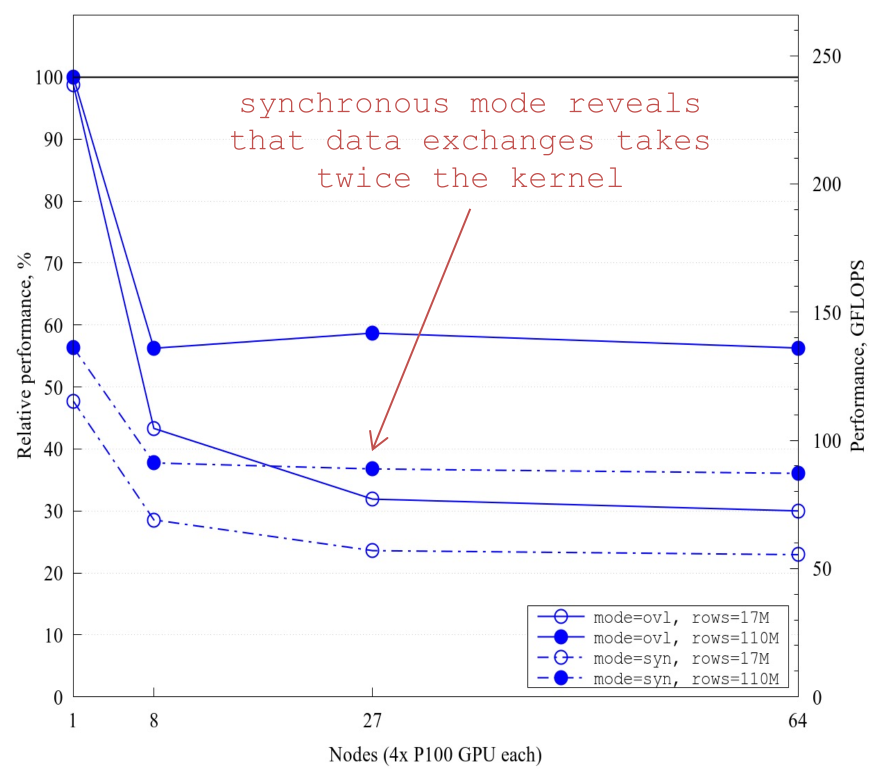

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Future work

- 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