A highly portable heterogeneous implementation of symmetry-preserving methods for magnetohydrodynamics

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Fusion HPC workshop 3
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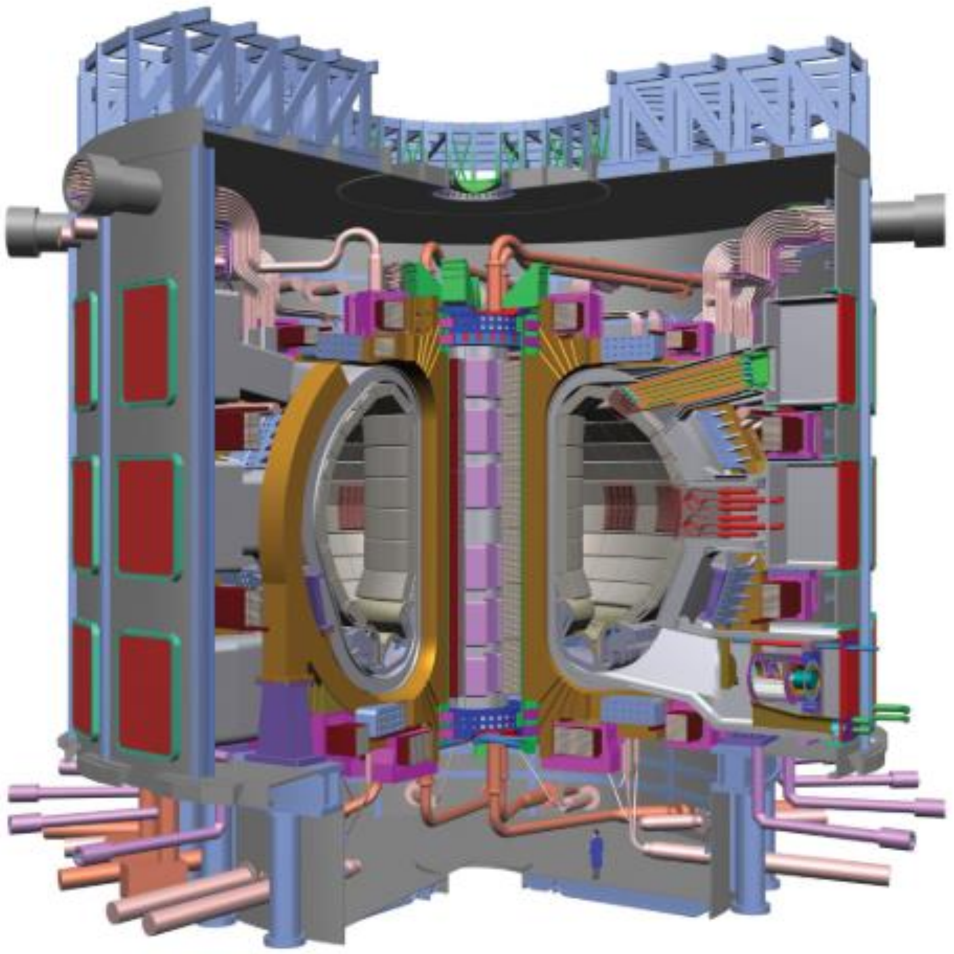
Outline

Symmetry preserving methods in MHD

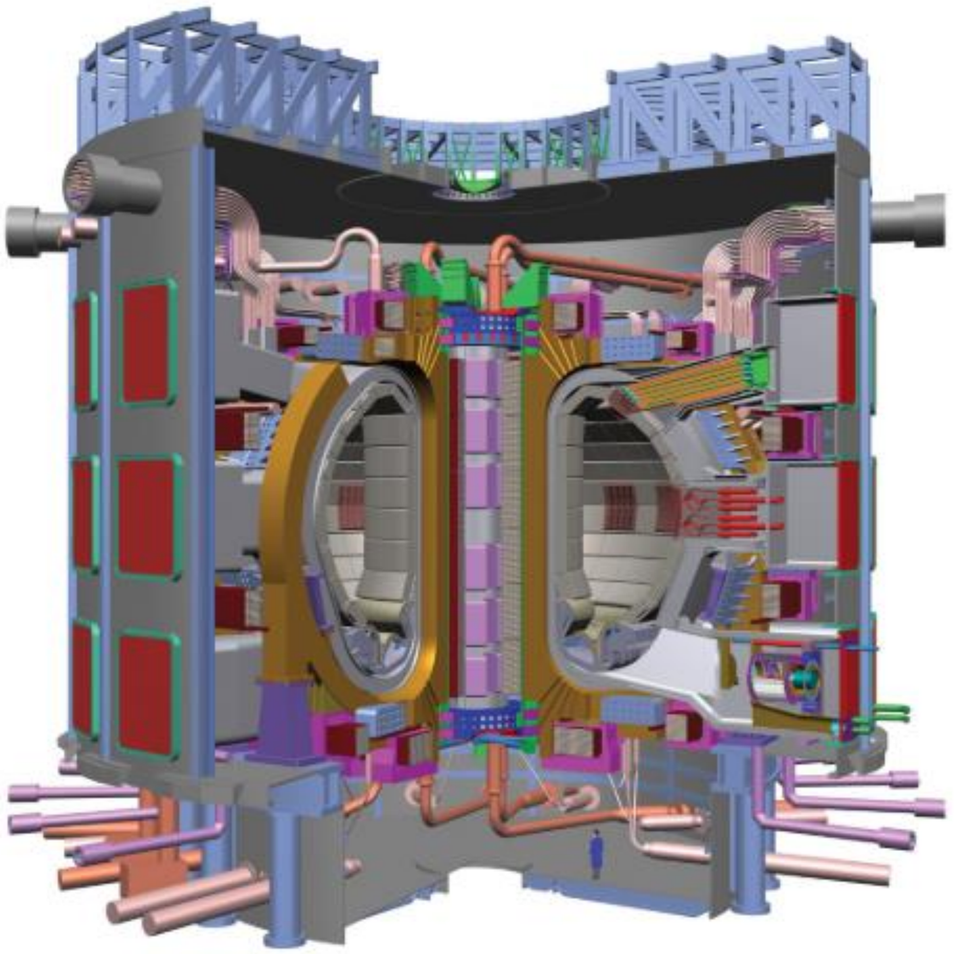
HPC^2 framework

Exploiting symmetries in geometry

MHD introduction

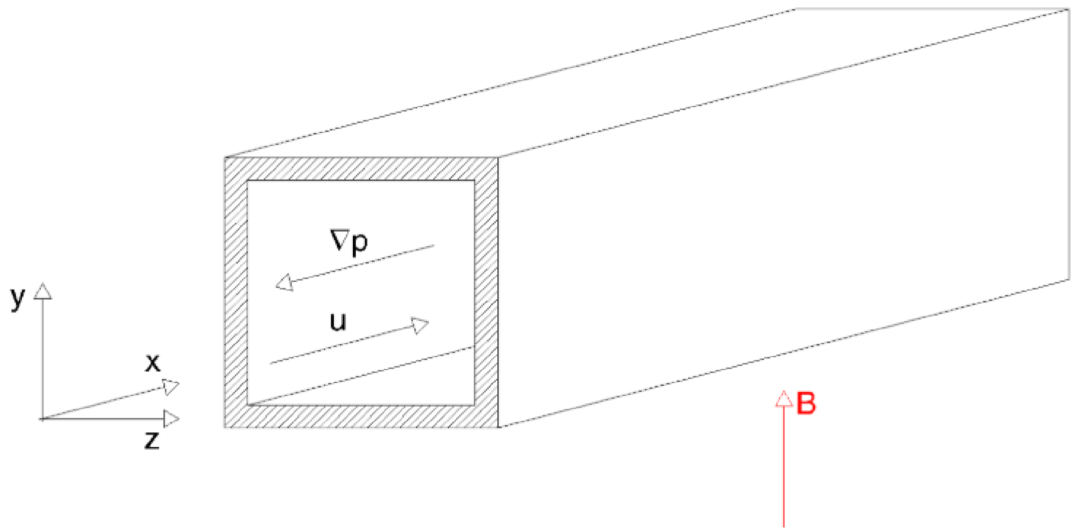


MHD introduction



Liquid metals in magnetic field

MHD introduction



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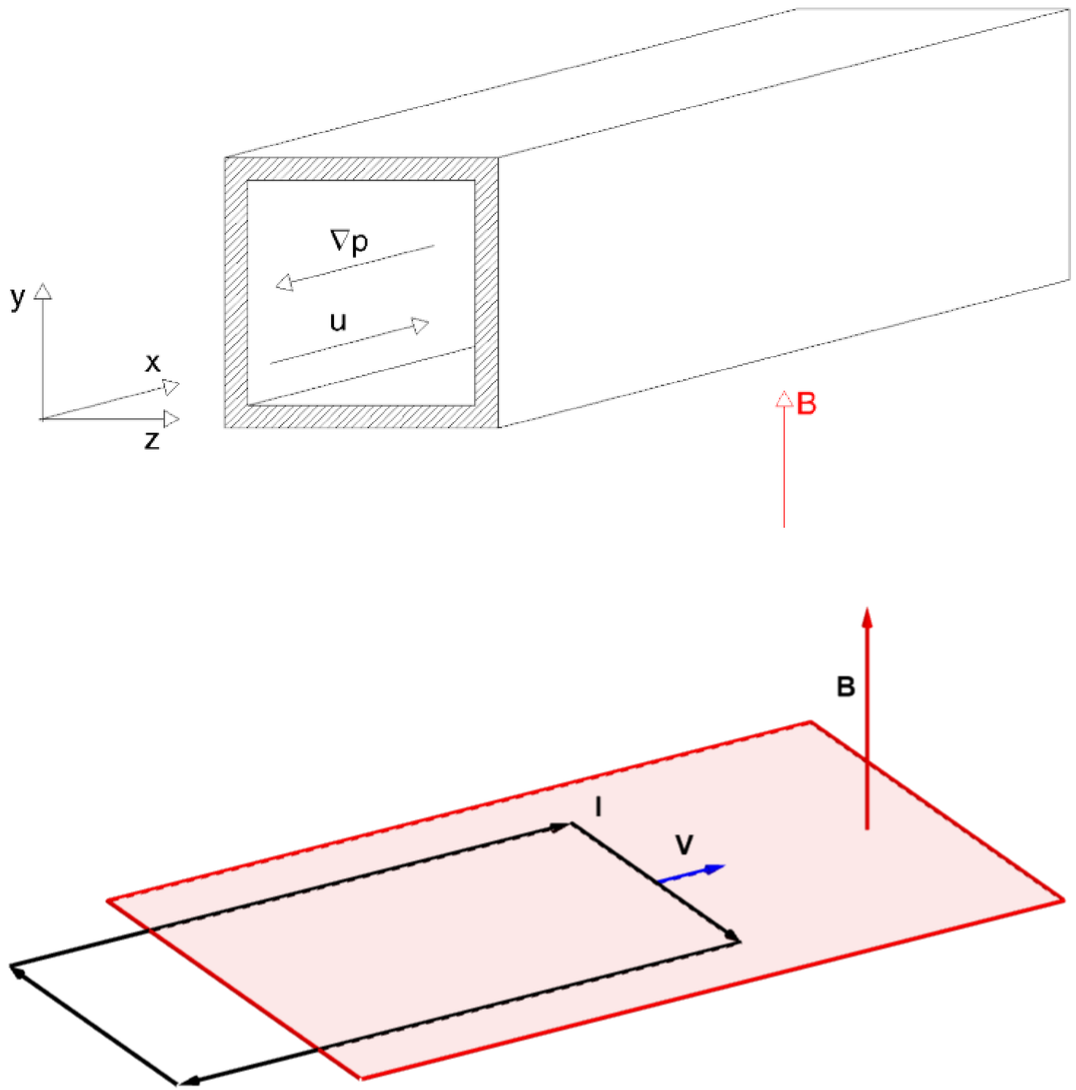

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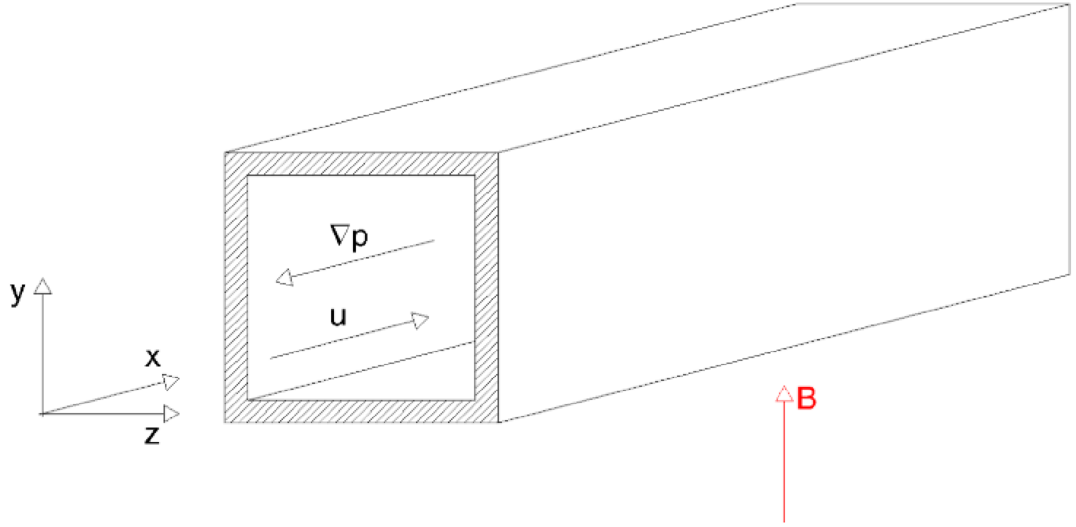

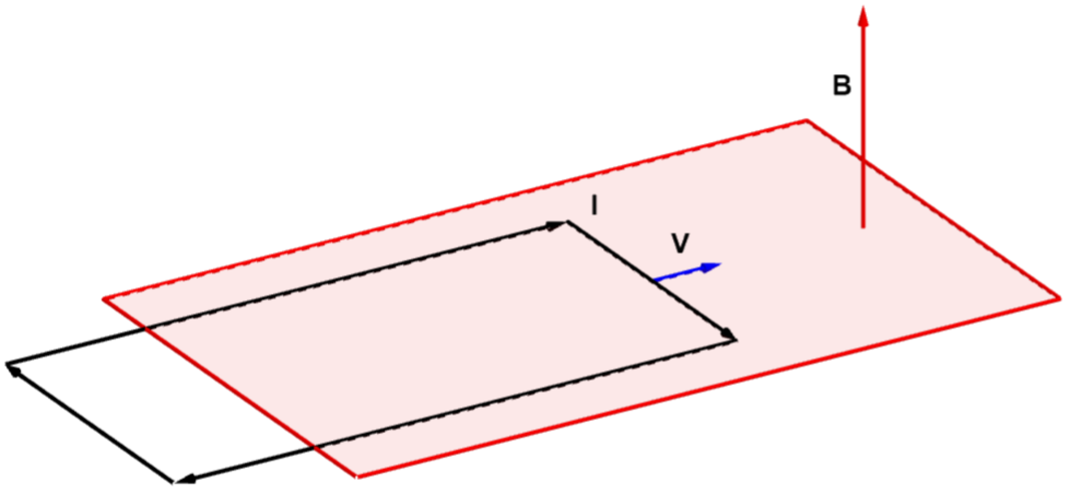

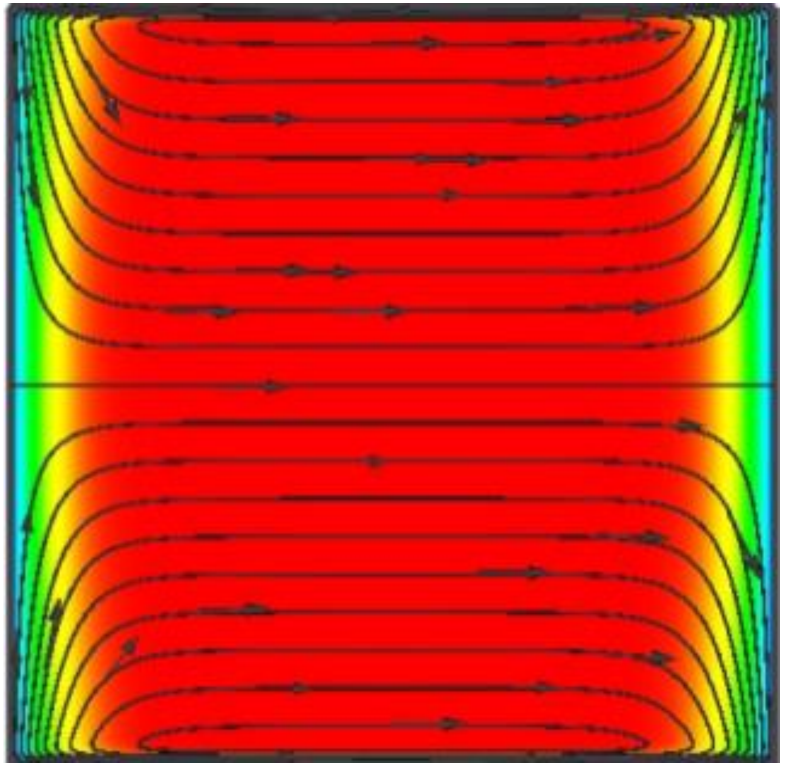

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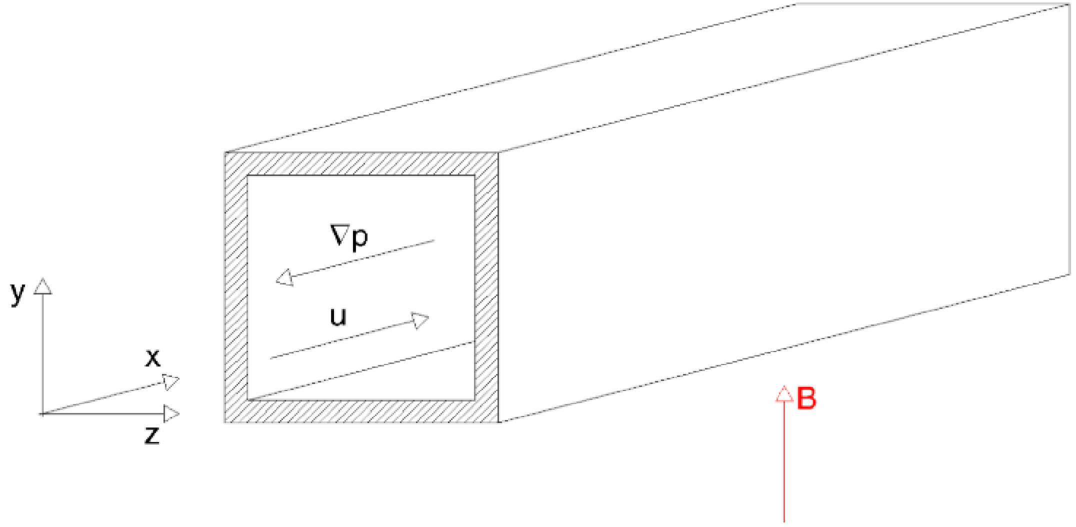

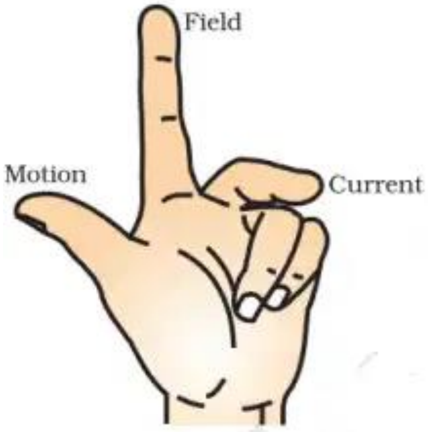

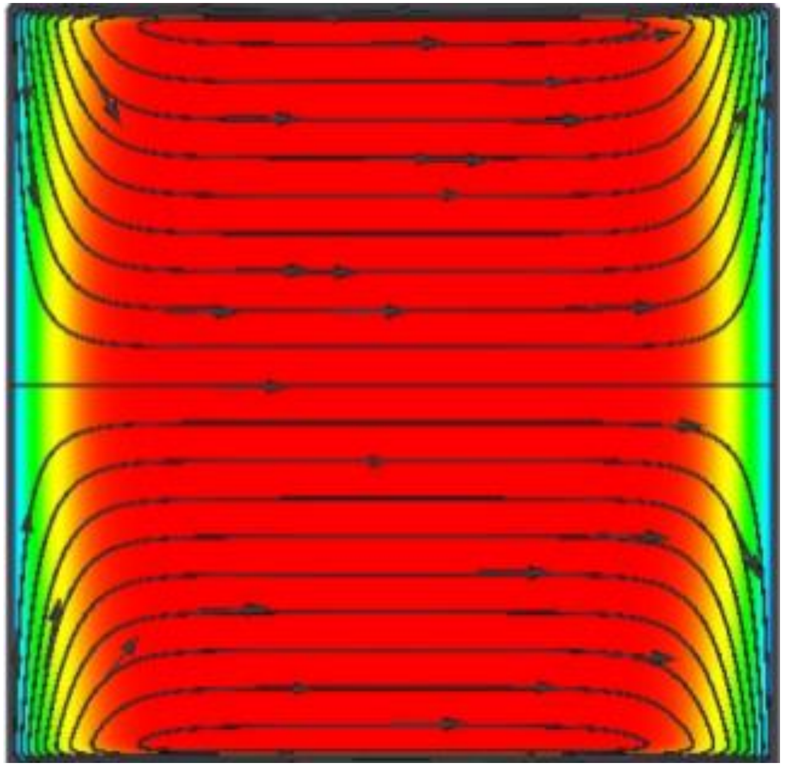

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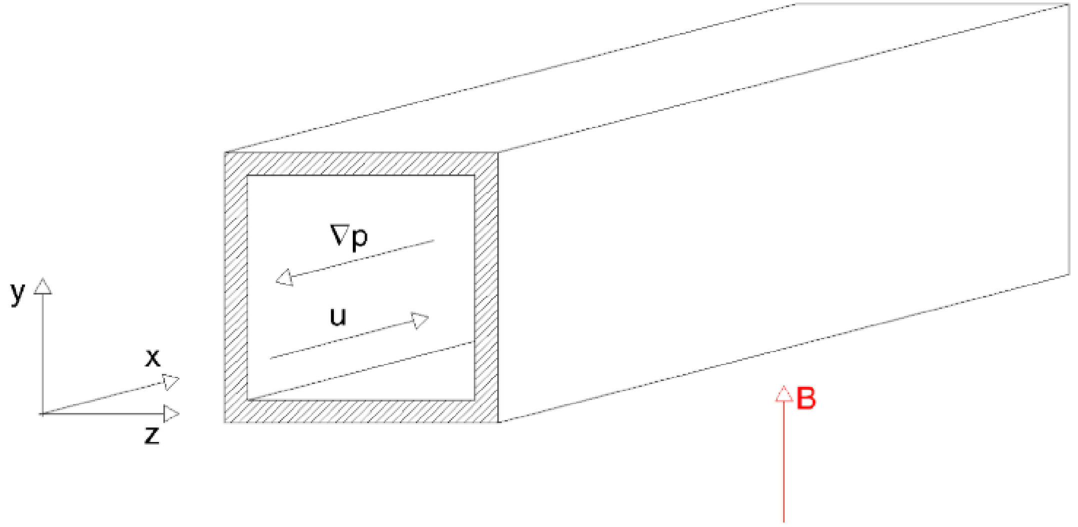

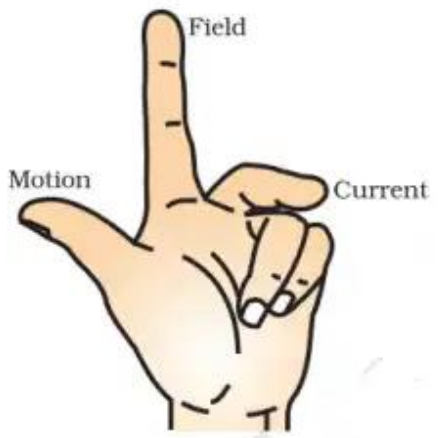

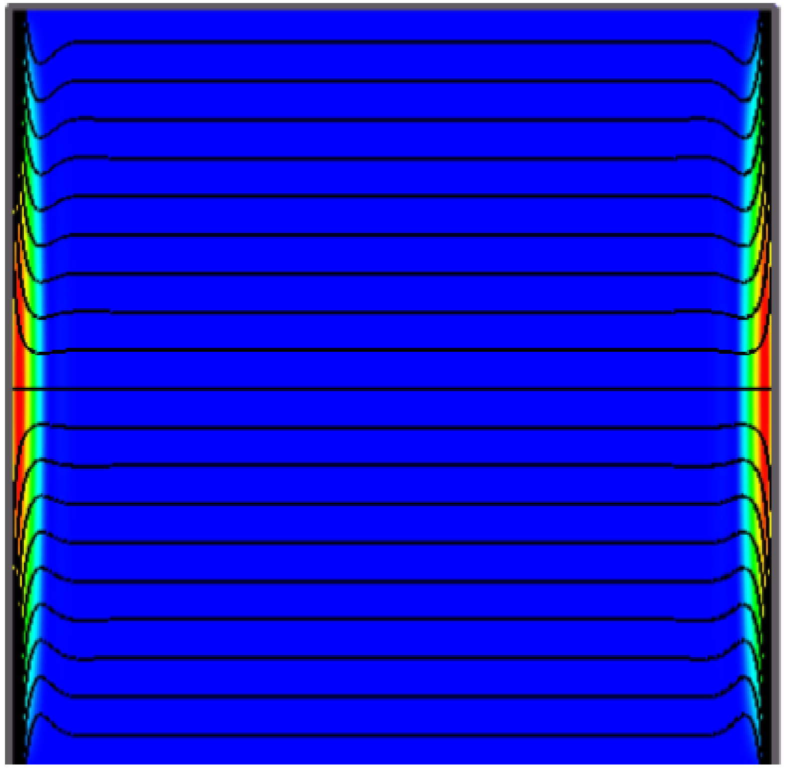

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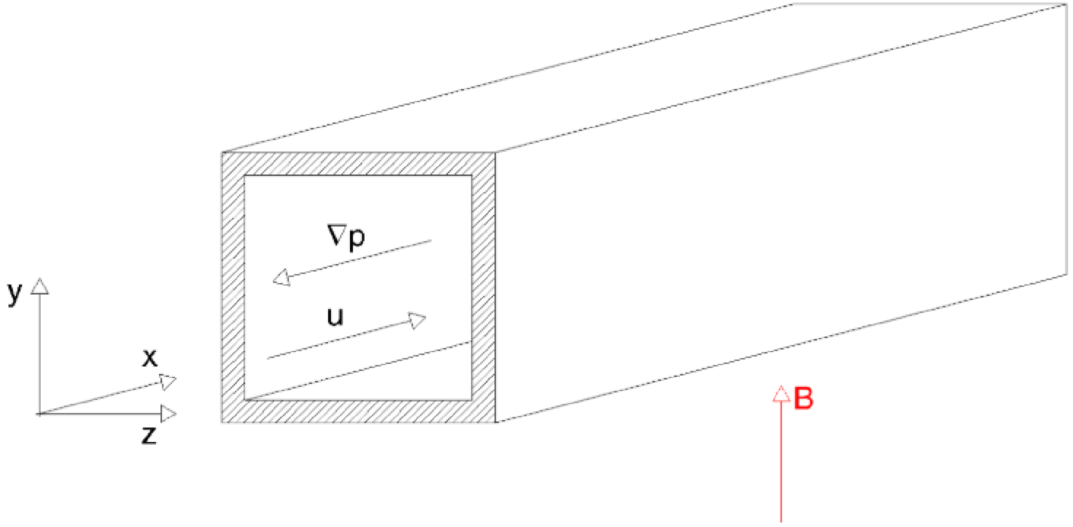
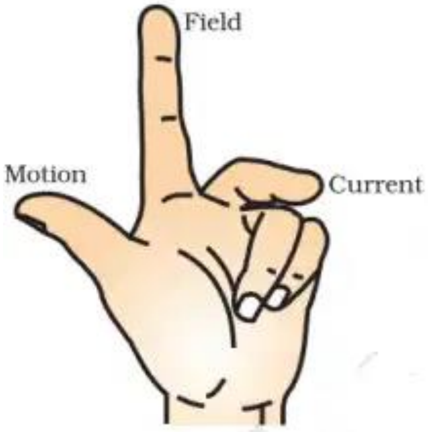
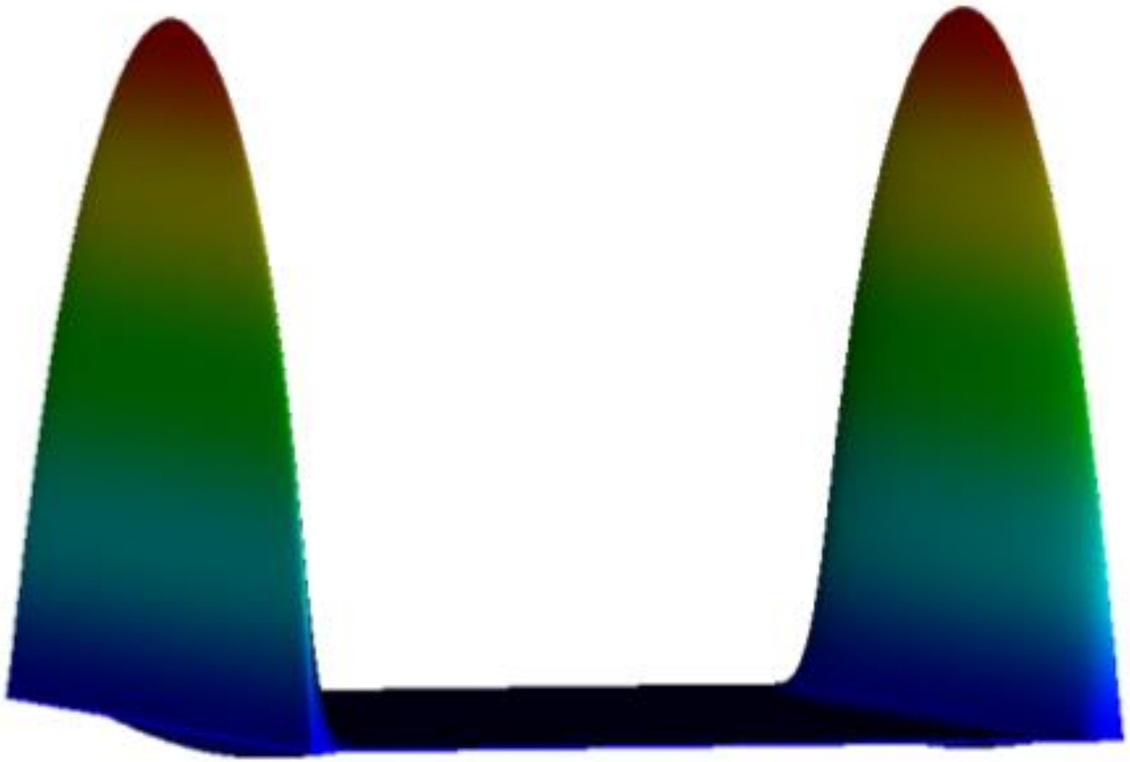






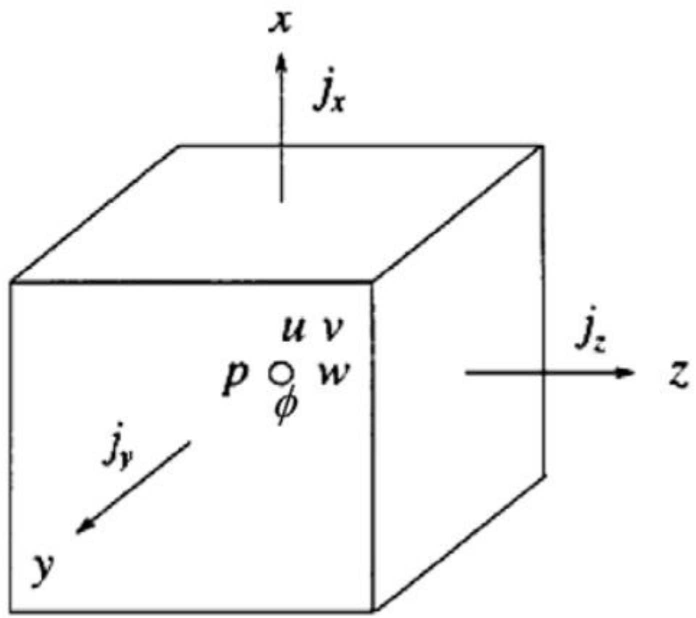
Lorentz force implementation

Following method of Ni et al.[1, 2]

Collocated + staggered current densities, *j*
Conserves current density

Scheme basics

Update U using projection method
Solve 2nd Poisson equation for φ: $\nabla \cdot (\nabla\varphi) = \nabla \cdot (\boldsymbol{u} \times \boldsymbol{B})$
Update *j*
Interpolate to cell center to calculate F_{Lor}



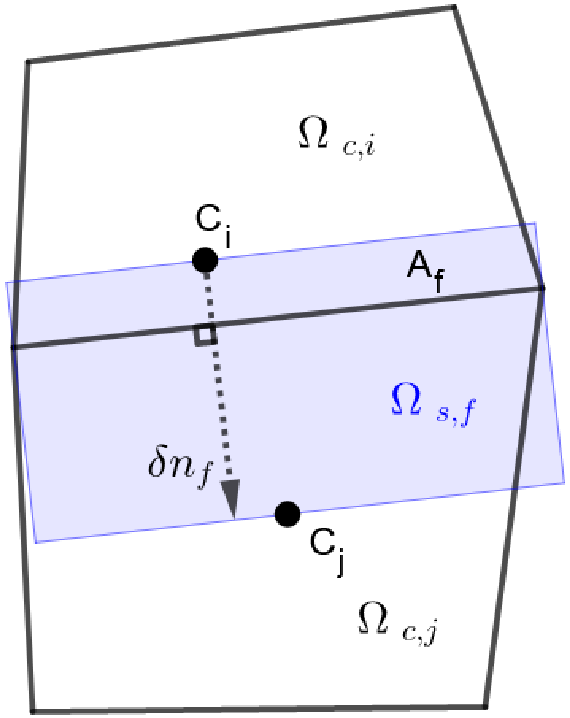
[1]Ni, M. J., Munipalli, R., Morley, N. B., Huang, P., & Abdou, M. A. (2007). “A current density conservative scheme for incompressible MHD flows at a low magnetic Reynolds number. Part I: On a rectangular collocated grid system”. *Journal of Computational Physics*, *227*(1), 174-204.
[2]Ni, M. J., Munipalli, R., Huang, P., Morley, N. B., & Abdou, M. A. (2007). “A current density conservative scheme for incompressible MHD flows at a low magnetic Reynolds number. Part II: On an arbitrary collocated mesh”. *Journal of Computational Physics*, *227*(1), 205-228.

Preserving symmetries

Following method of Trias et al.[1]

Conserve physical properties by mimicking continuous operators

- Use projected distances in gradients
- Use midpoint interpolation
- Use face-volume weighted interpolation

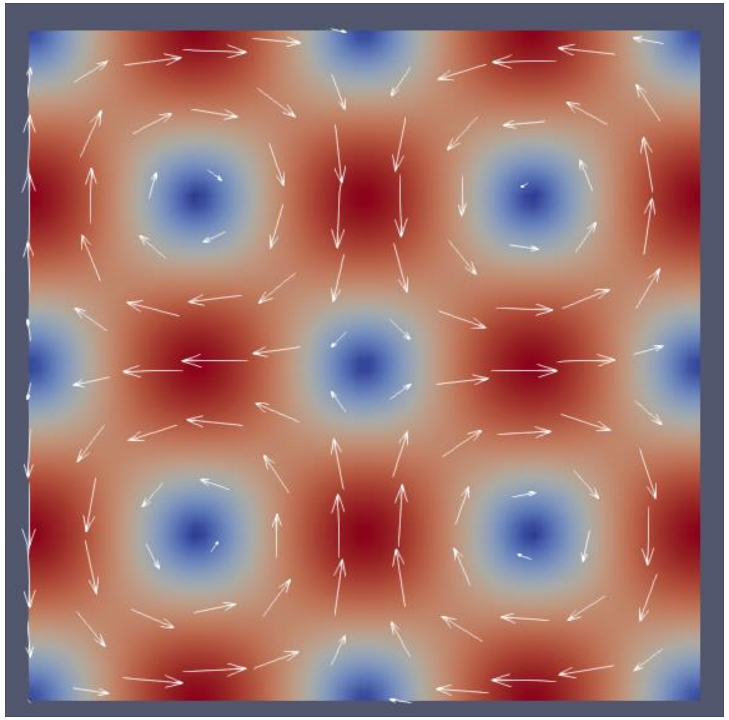


Consequences for MHD

Avoid iterative correction schemes
Conserve total momentum from Lorentz force: $\int_\Omega \nabla \cdot (\boldsymbol{J}(\boldsymbol{B} \times \boldsymbol{r}))\mathrm{d}\Omega$

[1]Trias, F. X., Lehmkuhl, O., Oliva, A., Pérez-Segarra, C. D., & Verstappen, R. W. C. P. (2014). "Symmetry-preserving discretization of Navier–Stokes equations on collocated unstructured grids". *Journal of Computational Physics*, *258*, 246-267.

Case 1: 2D Taylor-Green vortex in transverse magnetic field



HydroDynamic TGV

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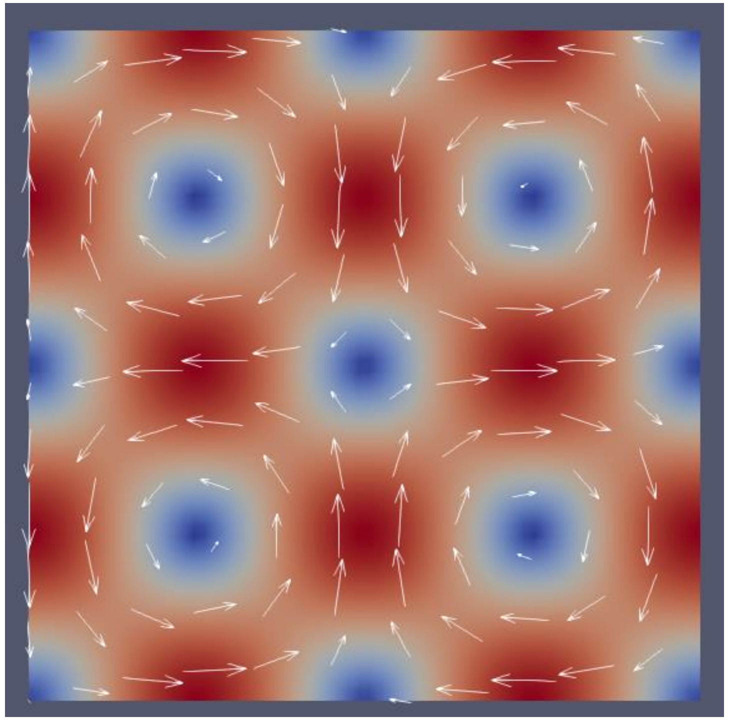

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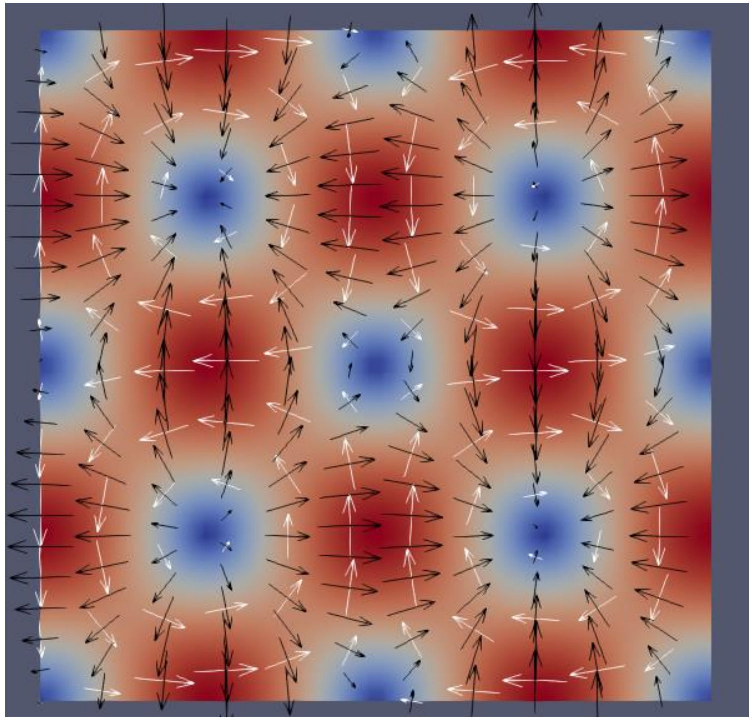

Transverse *B*-field

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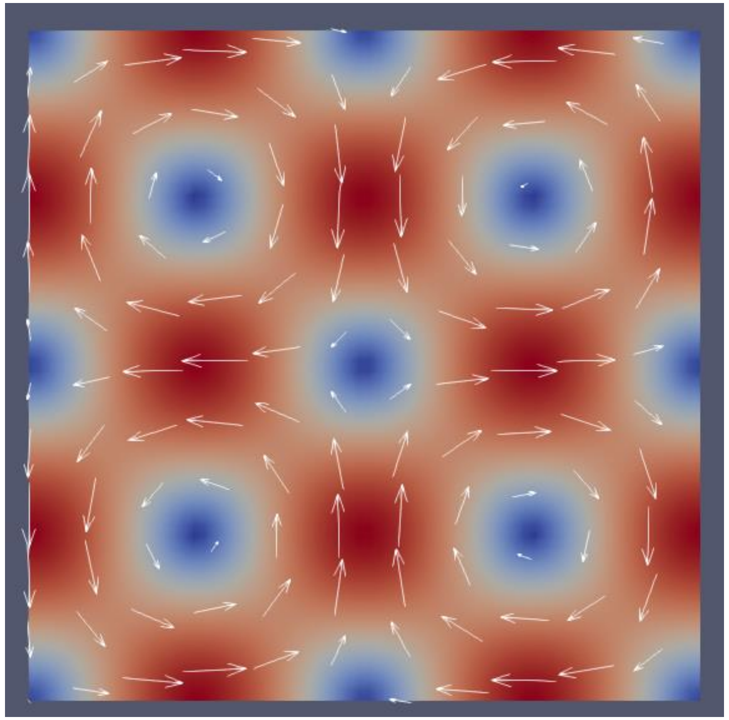

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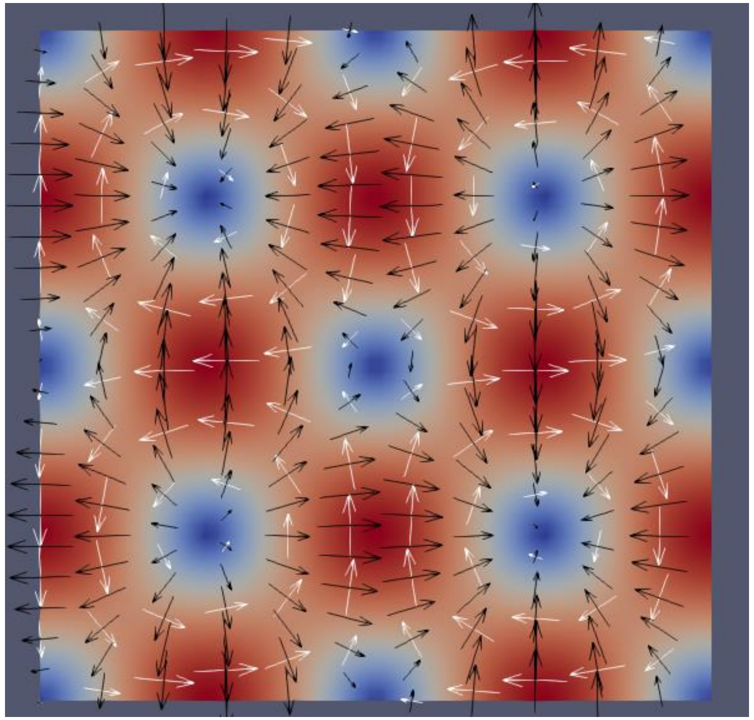

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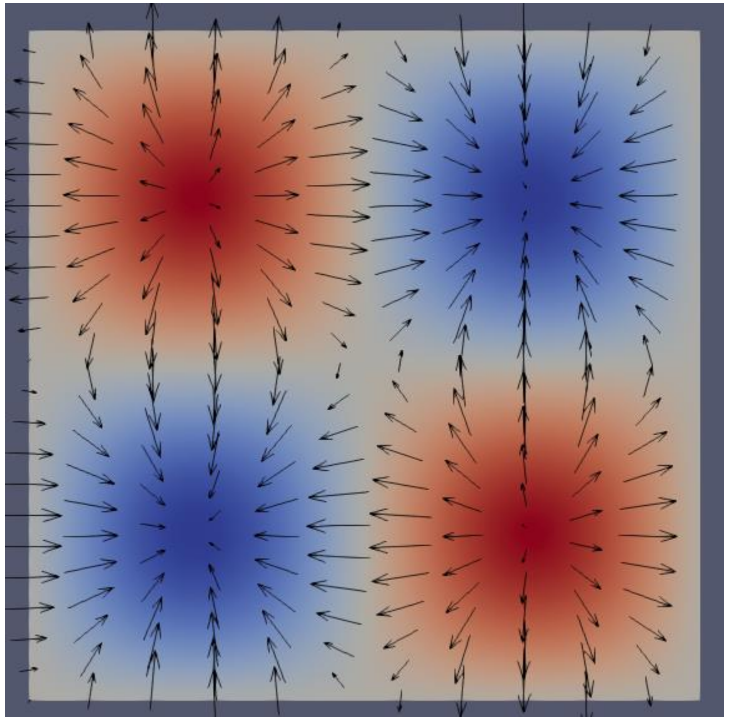

Imposed φ-field

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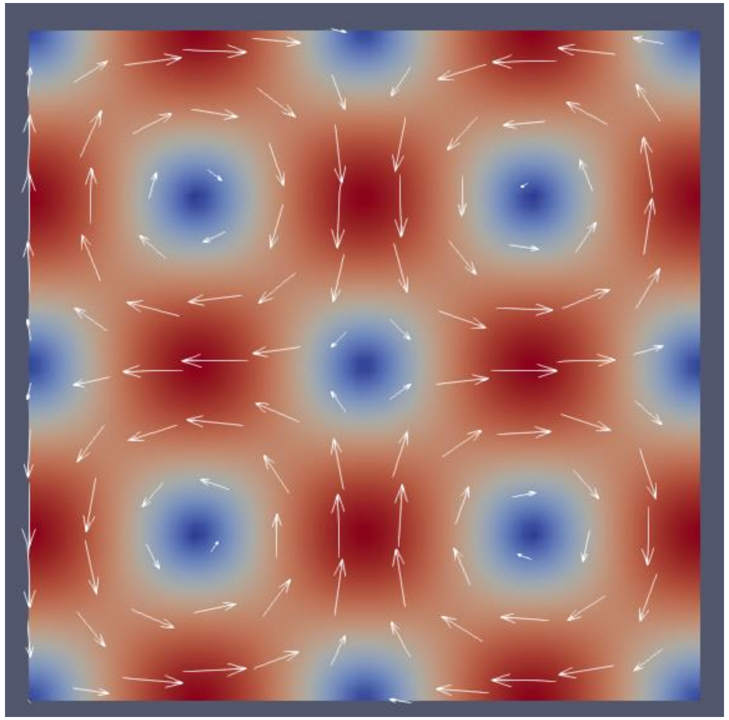

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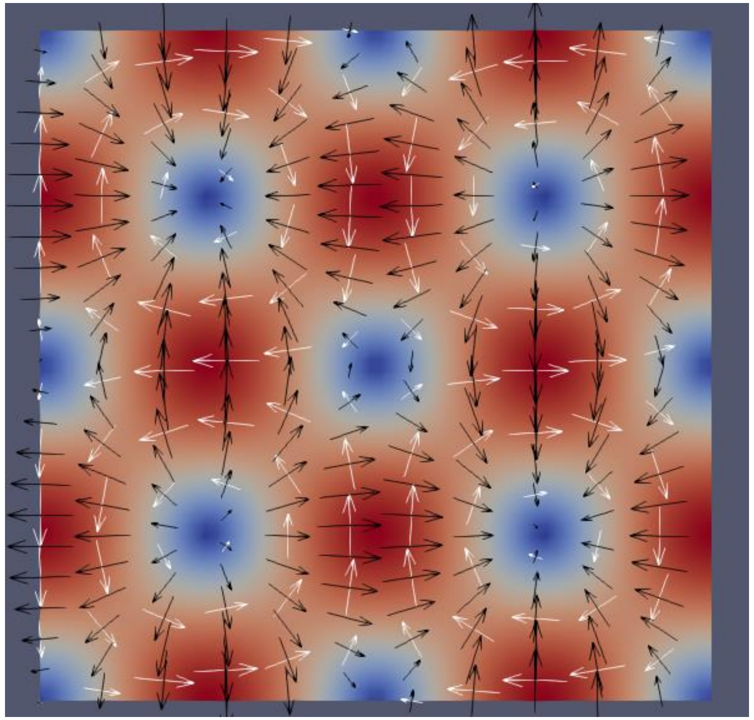

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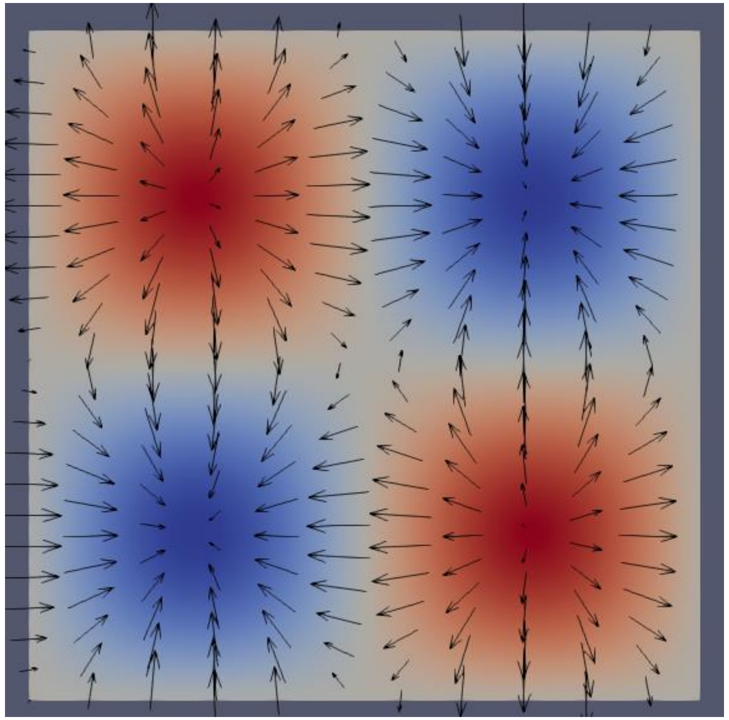
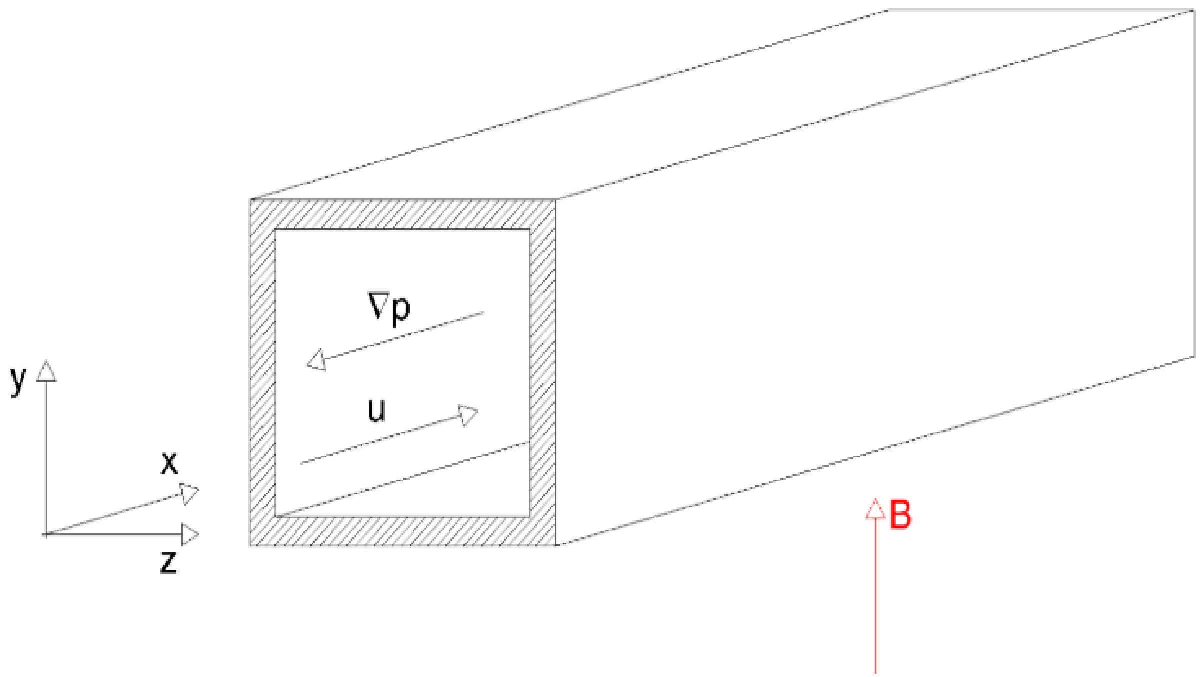


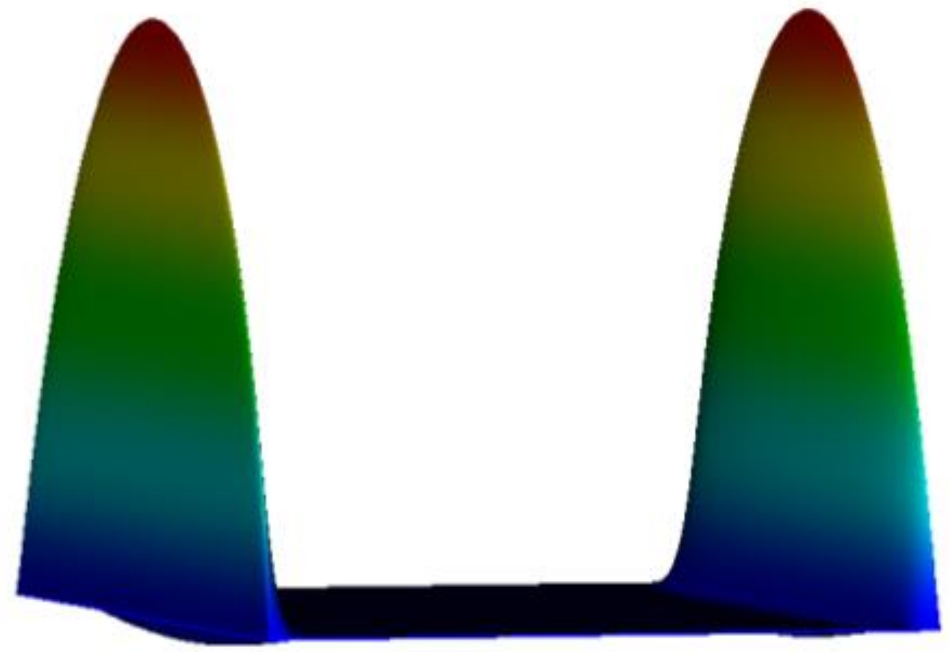
Magneto-HydroDynamic TGV

Transverse *B*-field

Imposed *φ*-field

Case 2: MHD duct flow

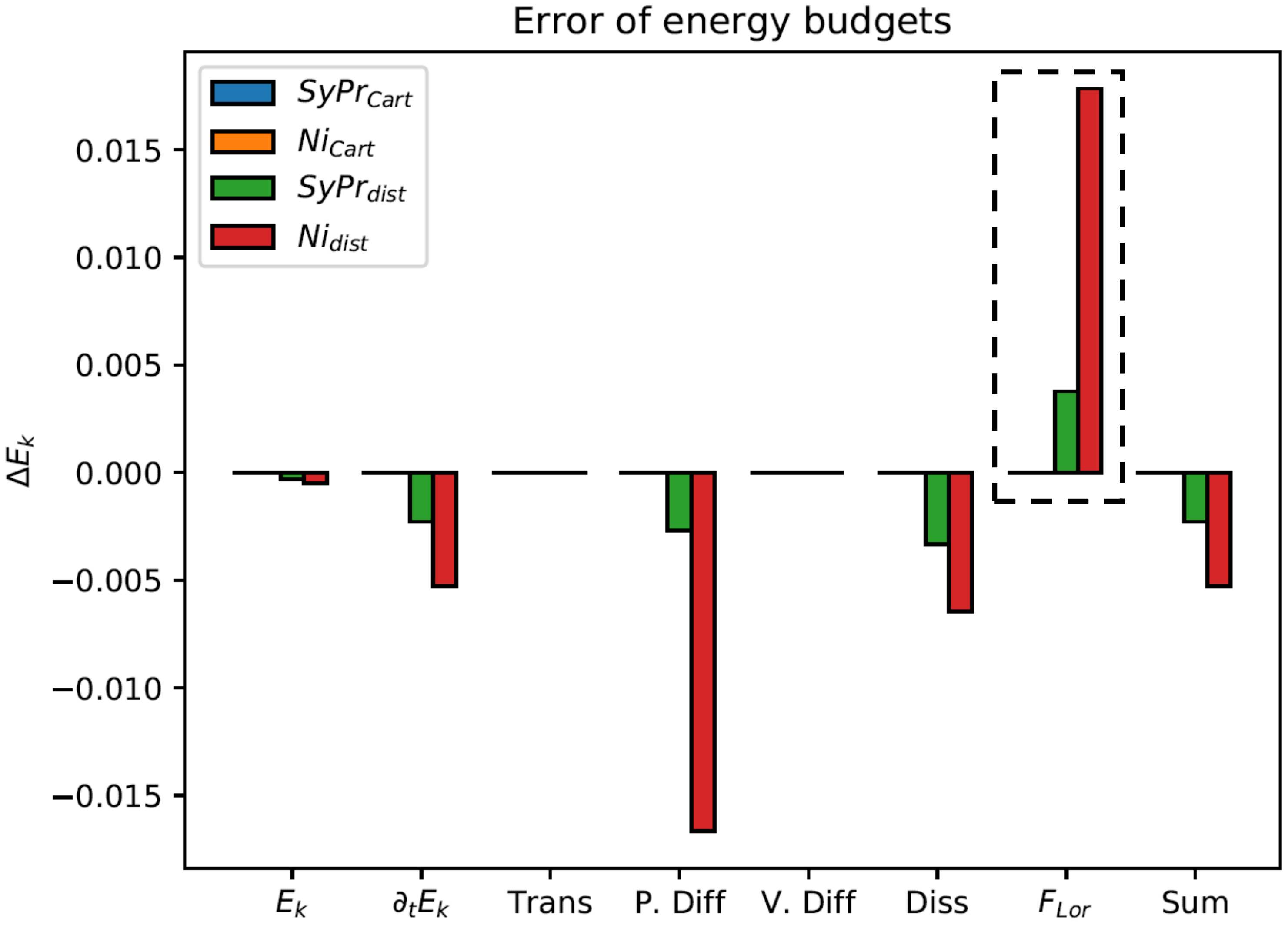




Accuracy results

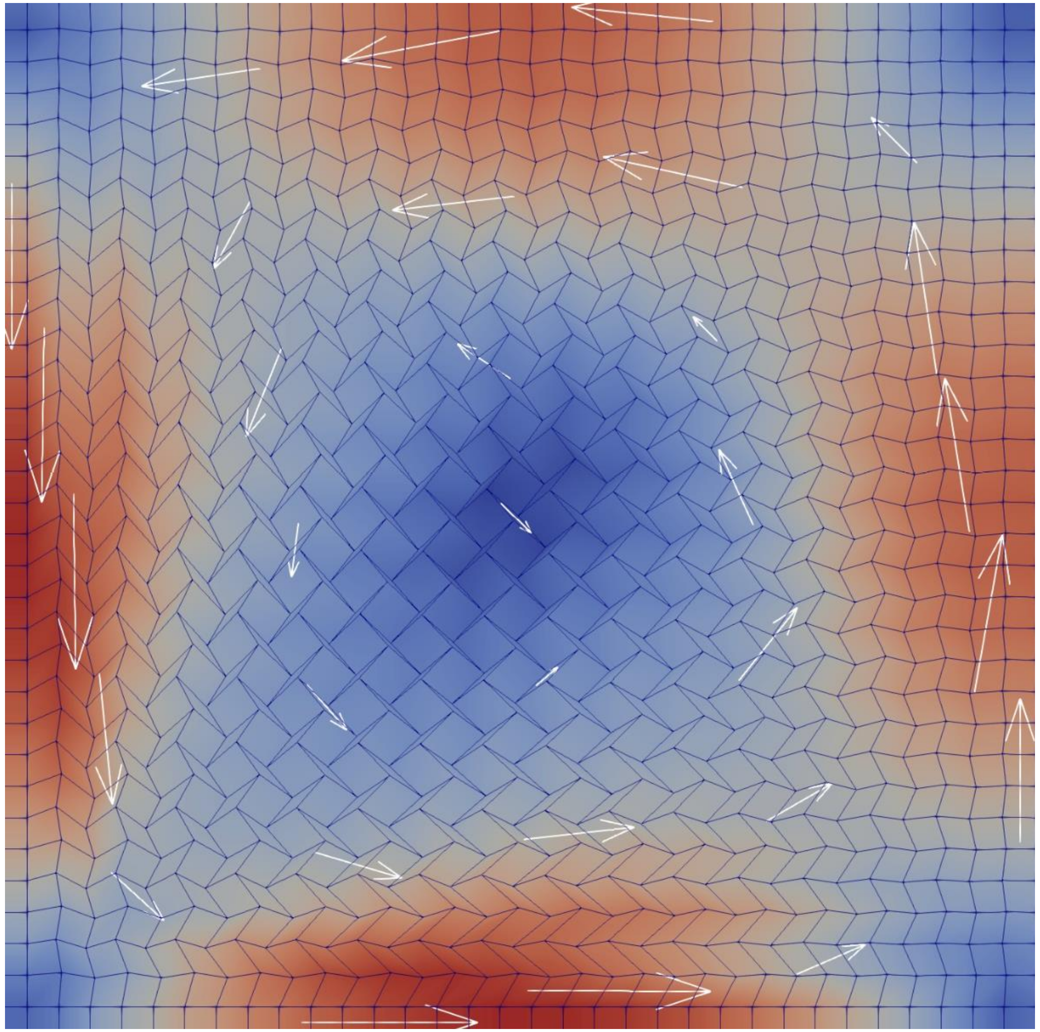
2D Taylor-Green vortex
Should not generate Lorentz Force
Should not dissipate energy

Results
Symmetry Preserving method outperforms Ni method
Especially on distorted grids

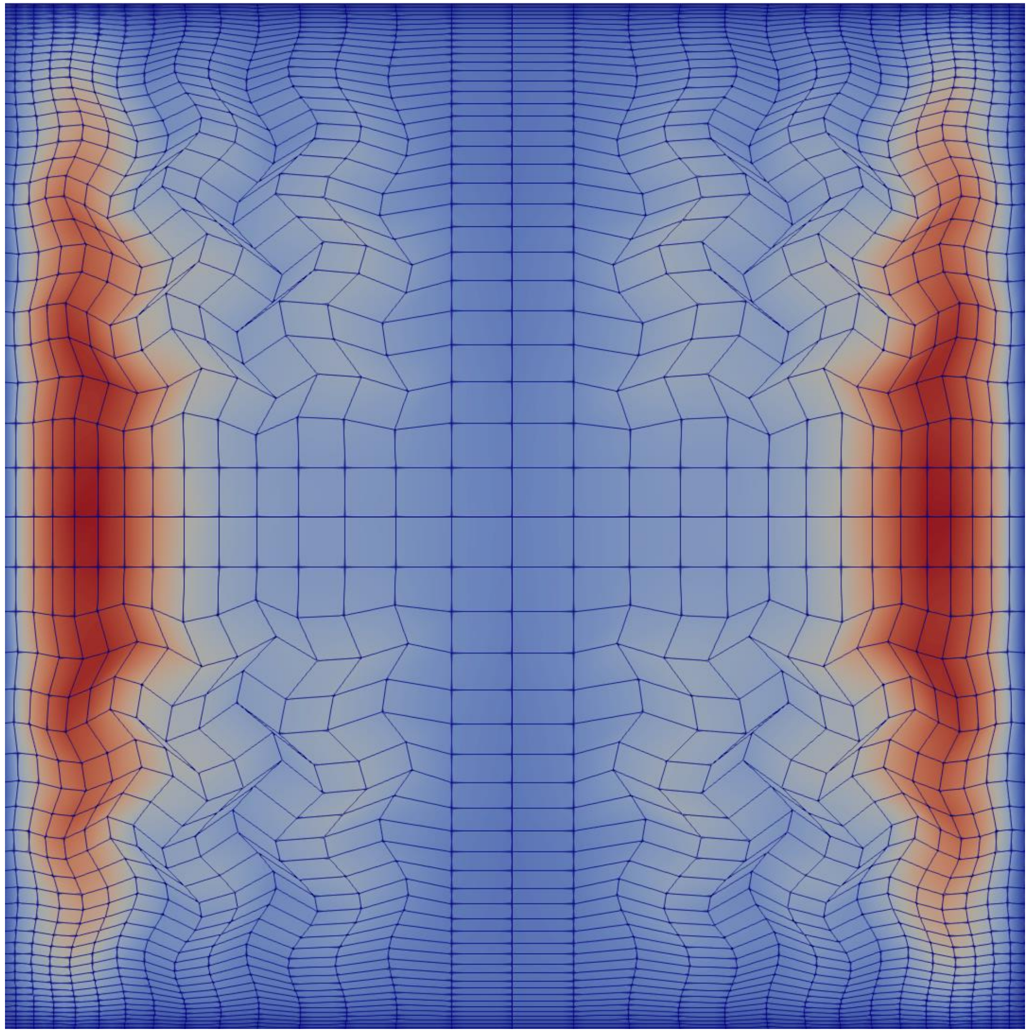


Stability for highly distorted meshes

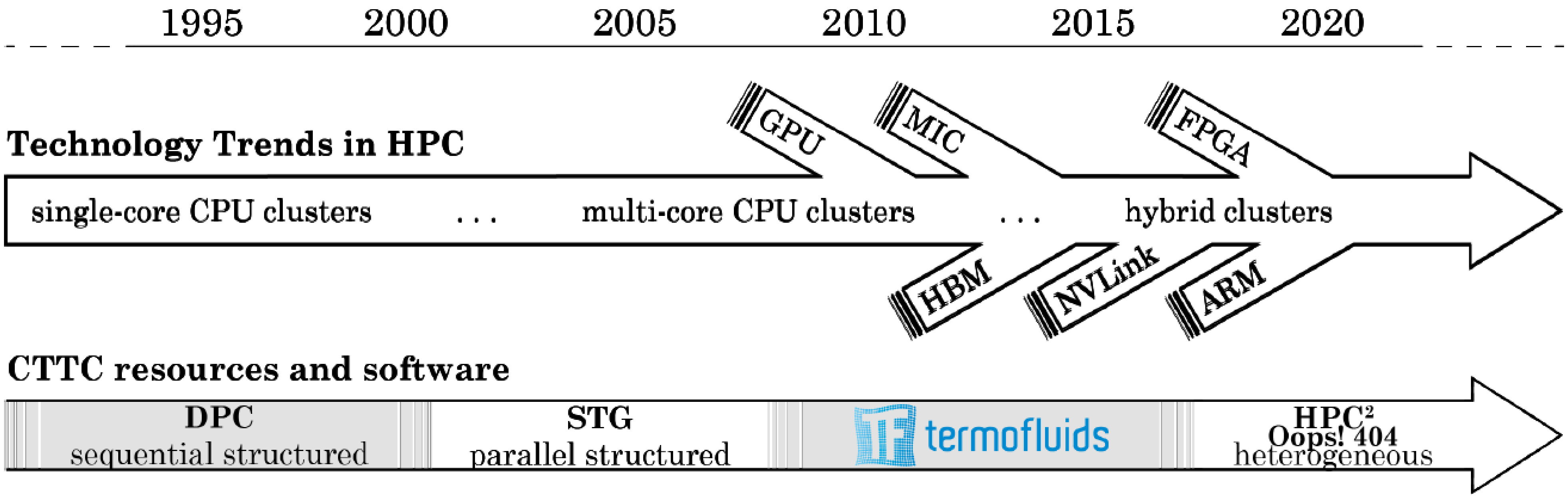
Taylor green vortex



M-profile in duct



HPC^2



Highly-portable code for HPC

Stencil based → Algebra based

Only a few algebraic kernels are needed

Algebraic kernels

From continuous NS equations:

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

To discrete algebraic equations:

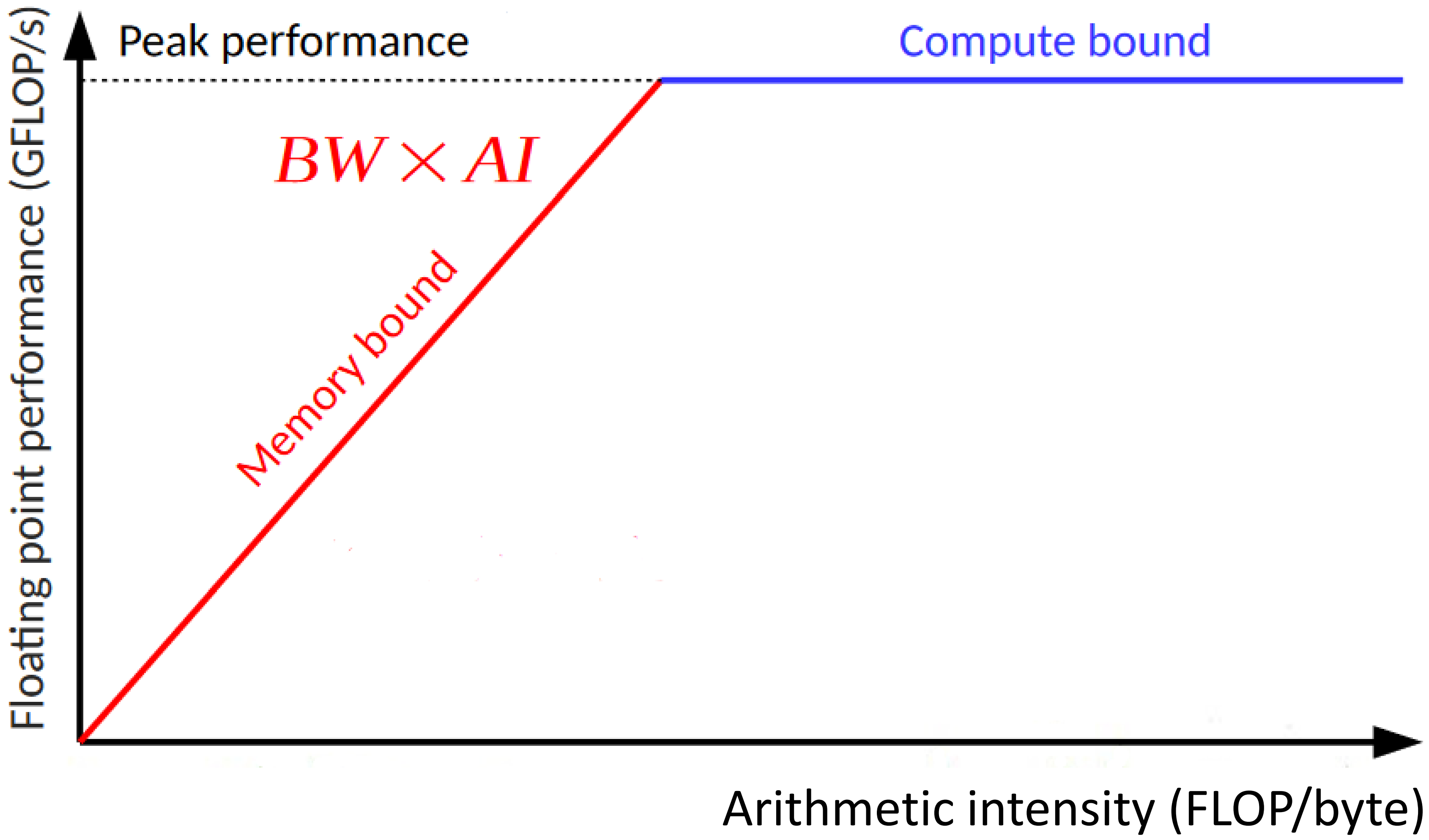
$$M \mathbf{u}_s = \mathbf{0}_c, \qquad \Omega \partial_t \mathbf{u}_c + C(\mathbf{u}_s)\, \mathbf{u}_c + D \mathbf{u}_c + \Omega G p_c = \mathbf{0}_c$$

Using three kernels only:

$$\boldsymbol{y} \leftarrow A\boldsymbol{x}, \qquad \boldsymbol{z} \leftarrow a\boldsymbol{x} + b\boldsymbol{y}, \qquad r \leftarrow \boldsymbol{x} \cdot \boldsymbol{y}$$

SpMV axpy dot

Memory boundedness



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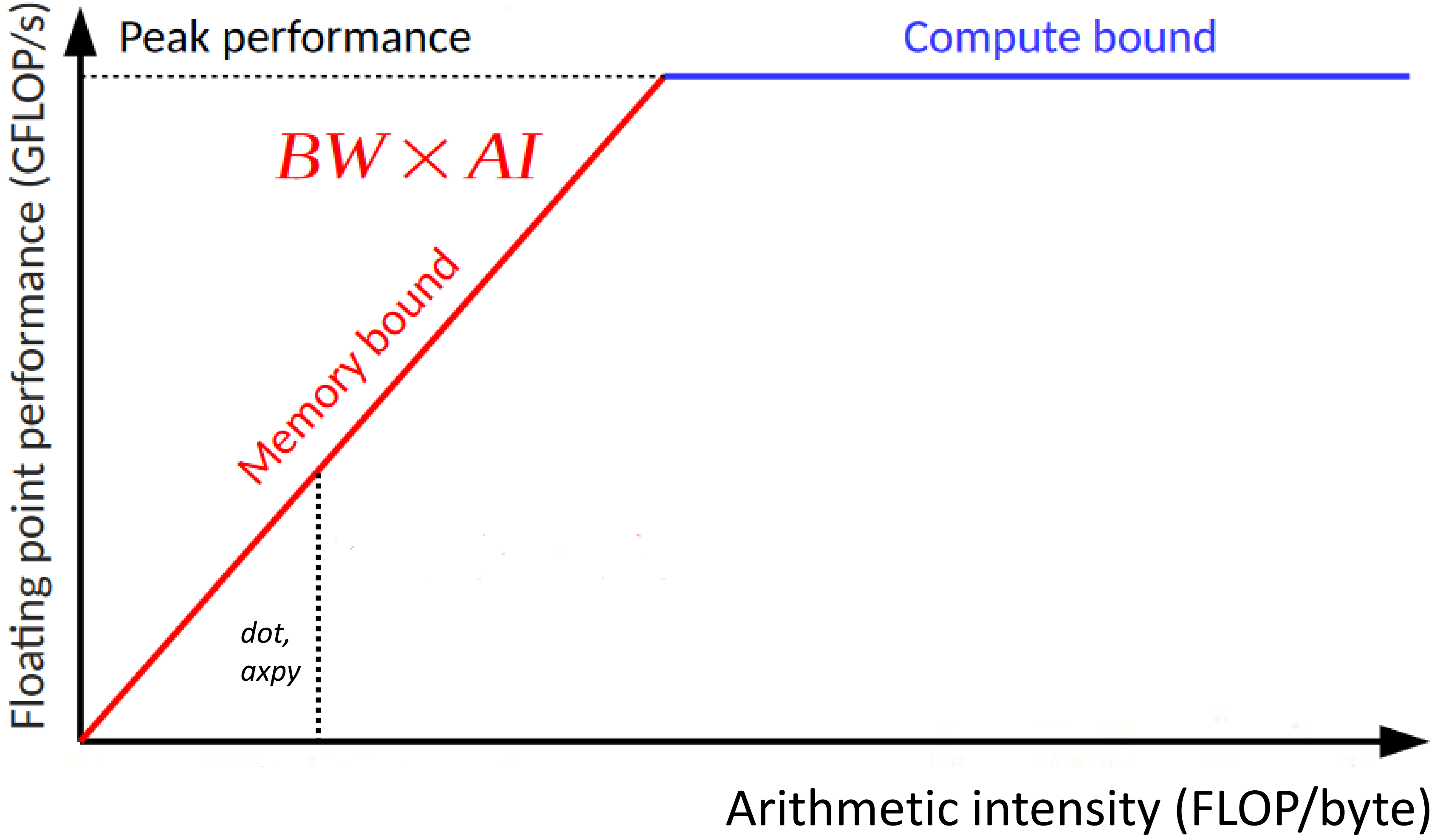

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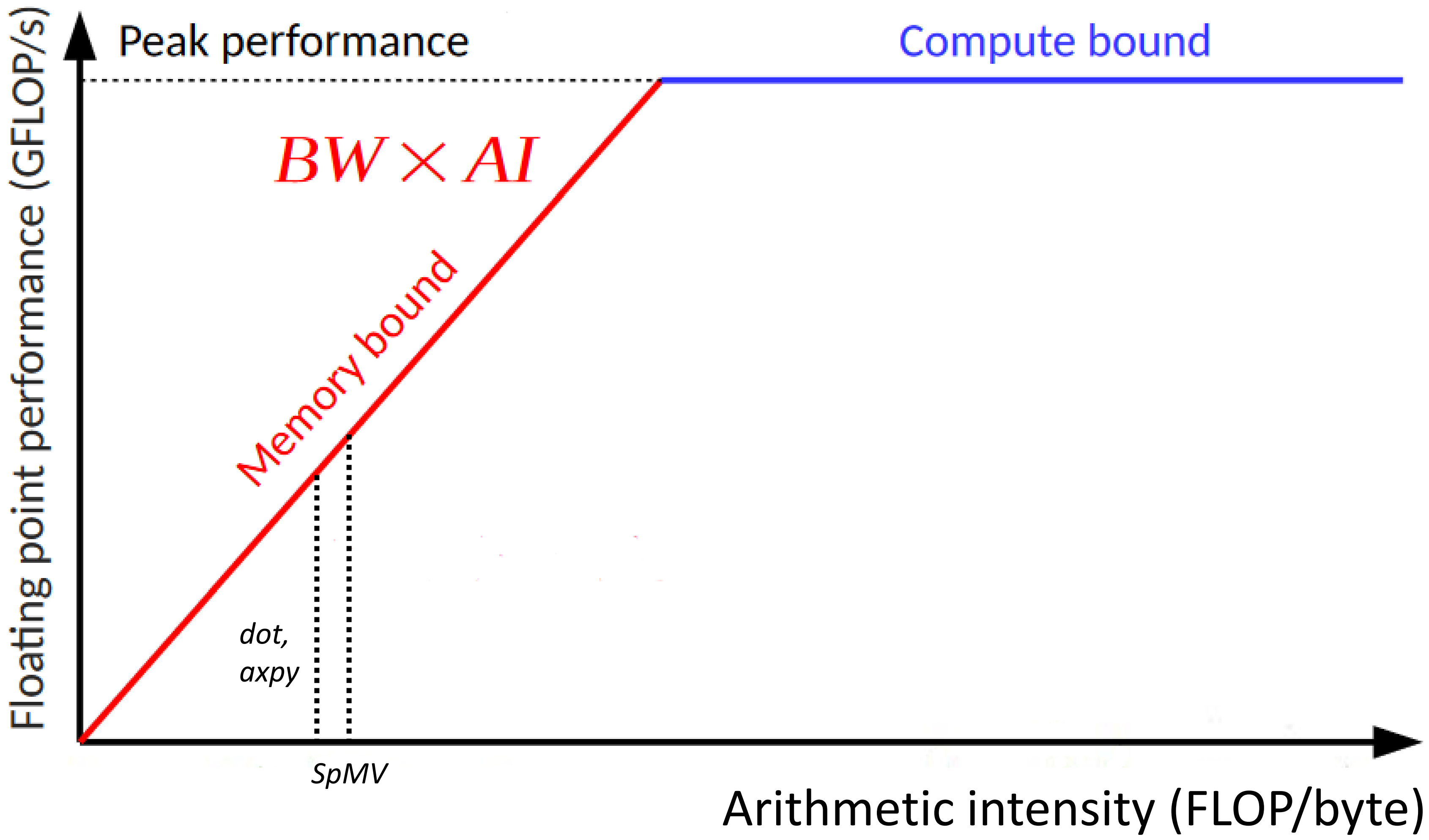
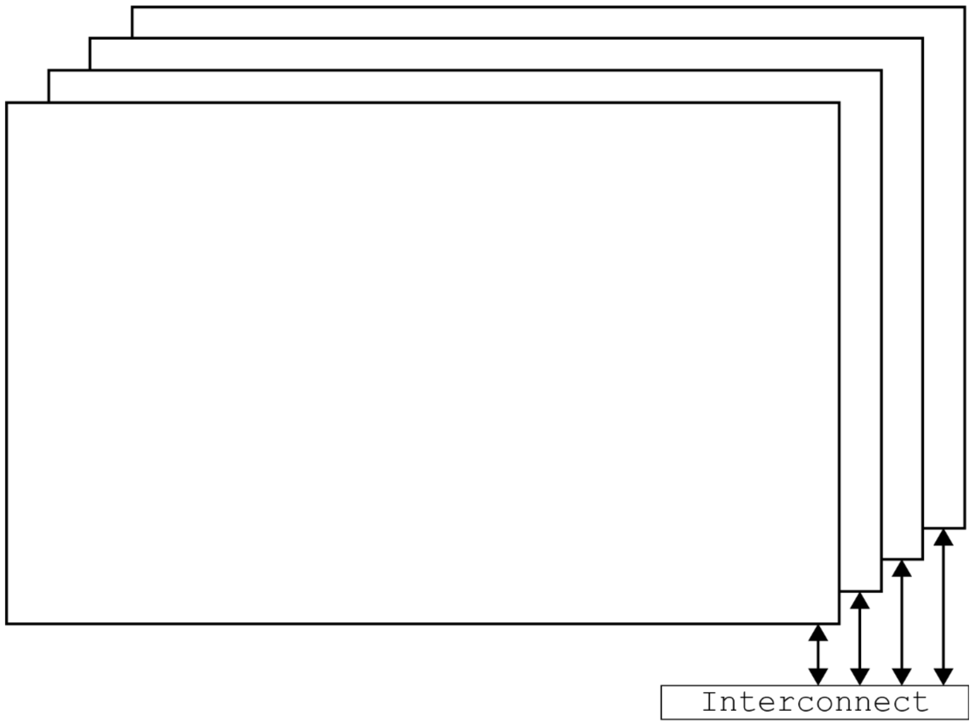


HPC²: hierarchy

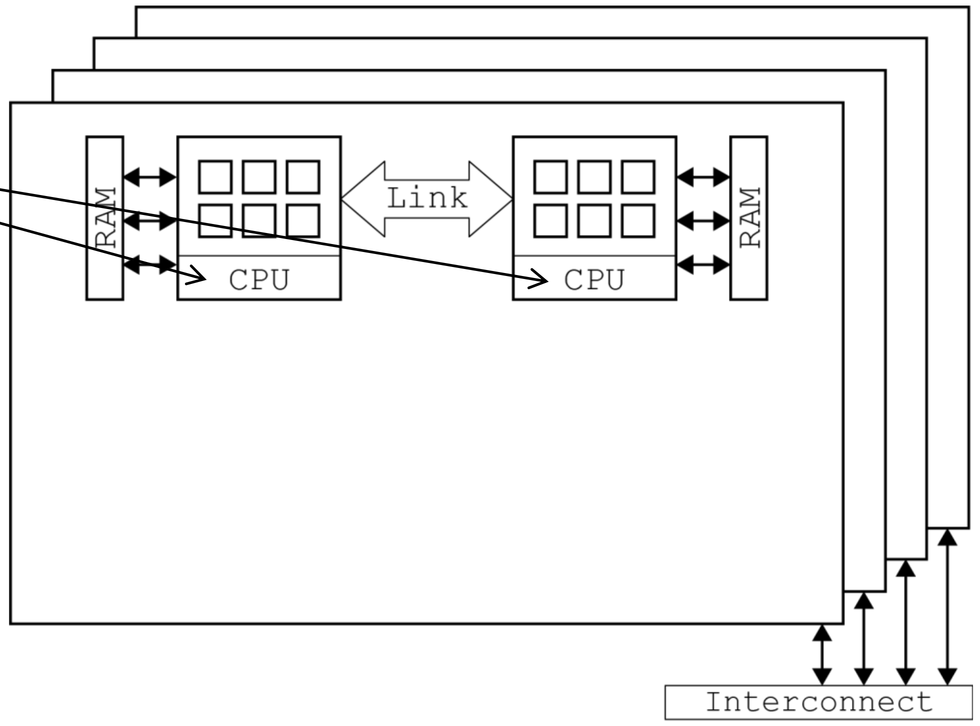


multiple nodes interconnected via high-bandwidth network
MPI is used at this level

X.Álvarez, A.Gorobets, and F.X.Trias. "A hierarchical parallel implementation for heterogeneous computing. Application to algebra-based CFD simulations on hybrid supercomputers". *Computers & Fluids, 214:104768, 2021.*

HPC^2: hierarchy

multiple multi-core CPU per node
OpenMP is used at this level



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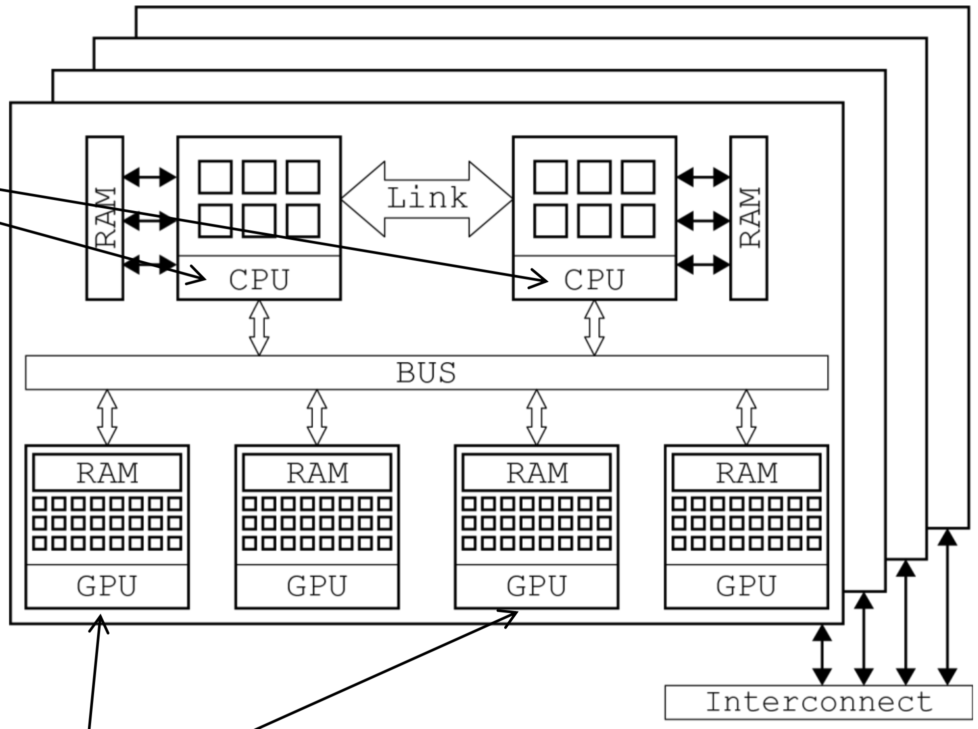

multiple accelerators per node
OpenCL/CUDA is used at this level

multiple nodes interconnected
via high-bandwidth network
MPI is used at this level

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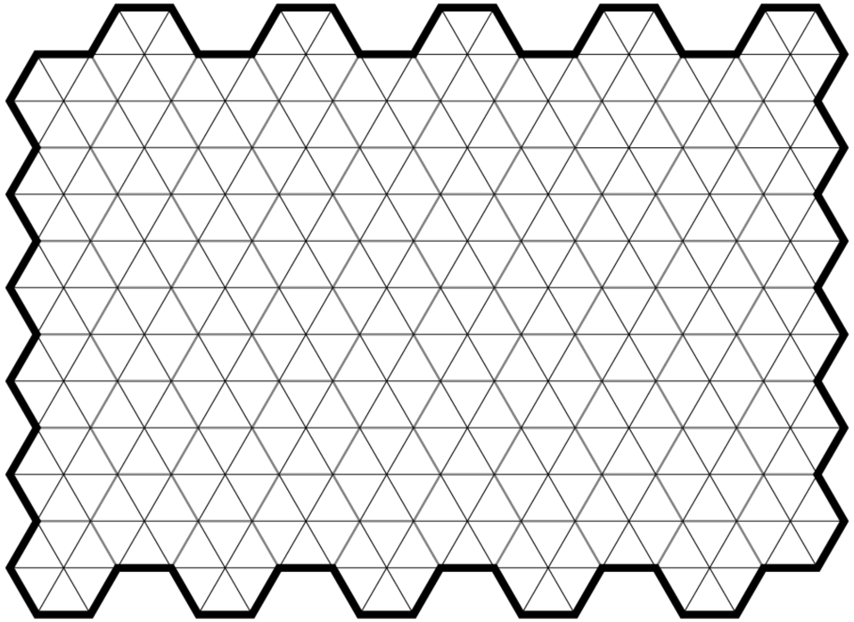
HPC^2: hierarchy



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HPC²: hierarchy

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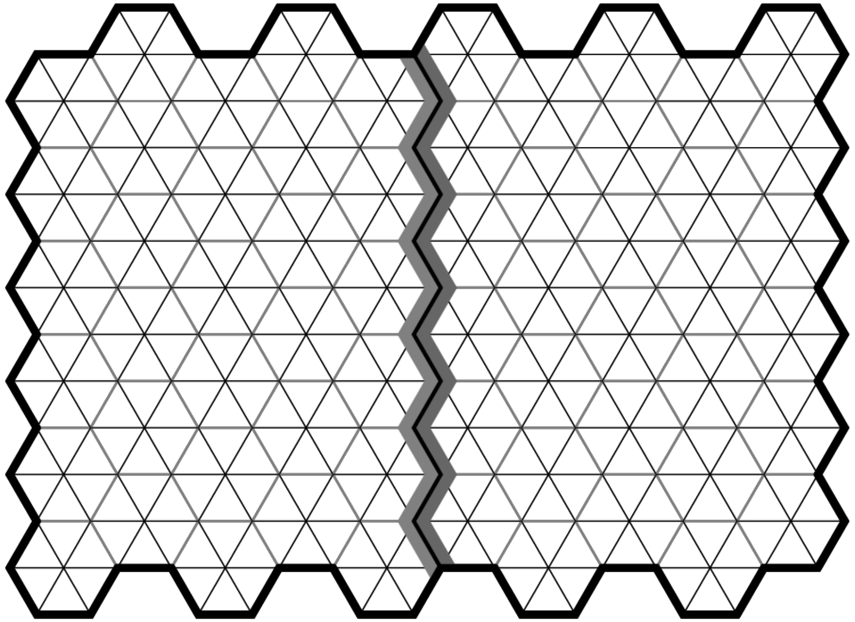

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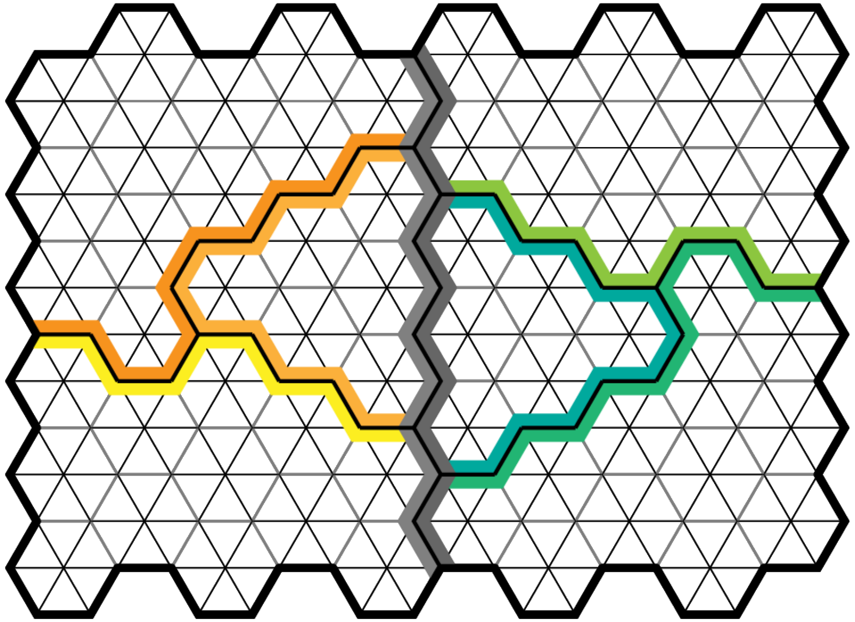
HPC²: hierarchy

1. The MPI process
2. The host and co-processors



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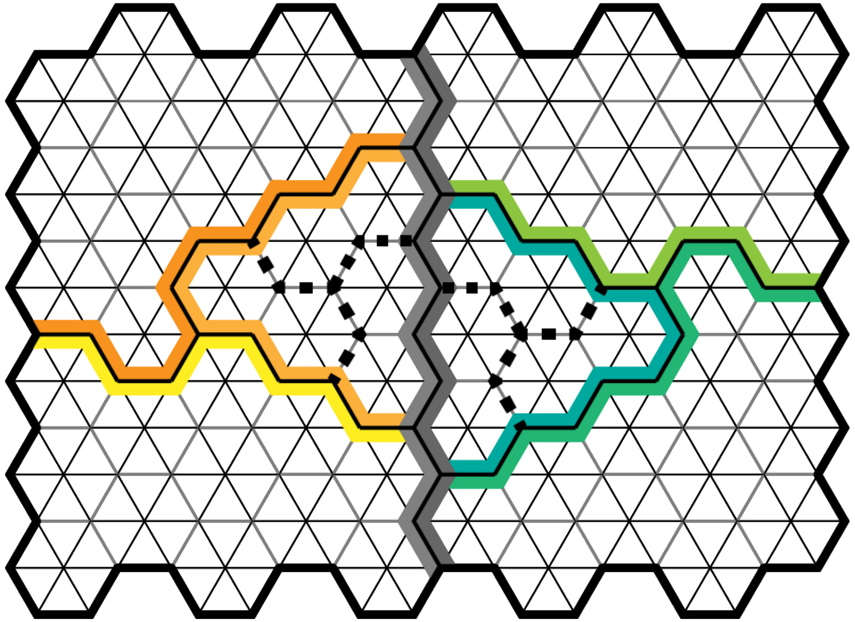
HPC^2: hierarchy

1. The MPI process
2. The host and co-processors
3. Multiple NUMA nodes in a manycore CPU



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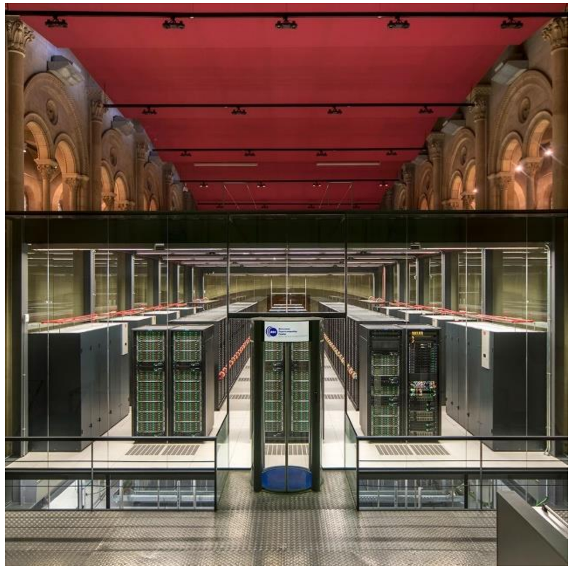
HPC^2: tested architectures

MareNostrum 4	Lomonosov-2	TSUBAME3.0
		
rank #42 3456 nodes with: 2× Intel Xeon 8160 1× Intel Omni-Path	rank #156 1696 nodes with: 2× Intel Xeon E5-2697 v3 1× NVIDIA Tesla K40M 1× InfiniBand FDR	rank #31 540 nodes with: 2× Intel Xeon E5-2680 v4 4× NVIDIA Tesla P100 4× Intel Omni-Path

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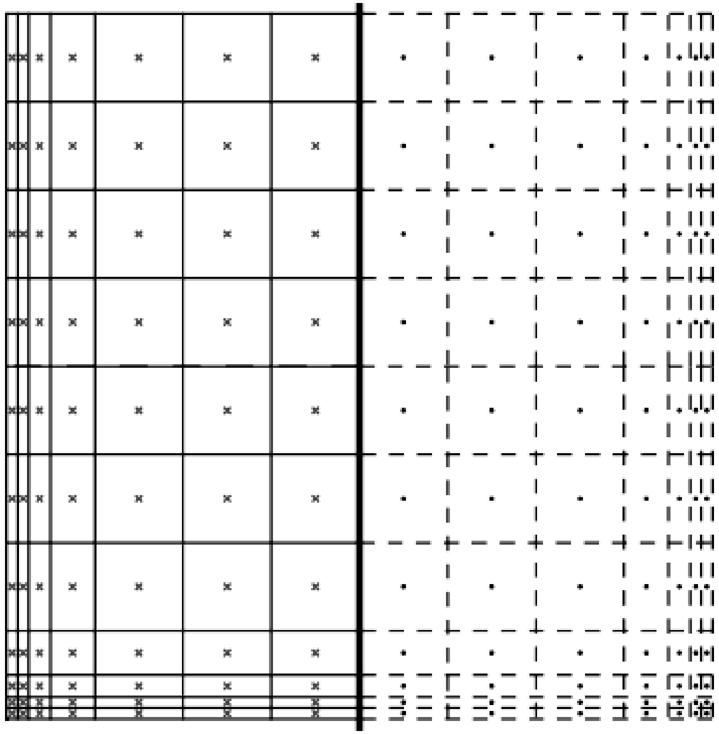
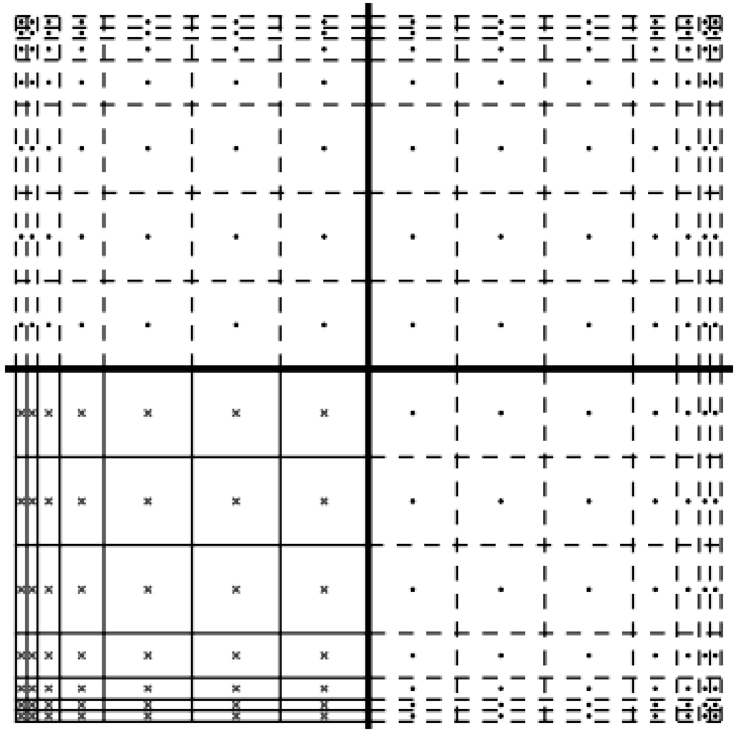
Exploiting symmetries



1 Symmetry

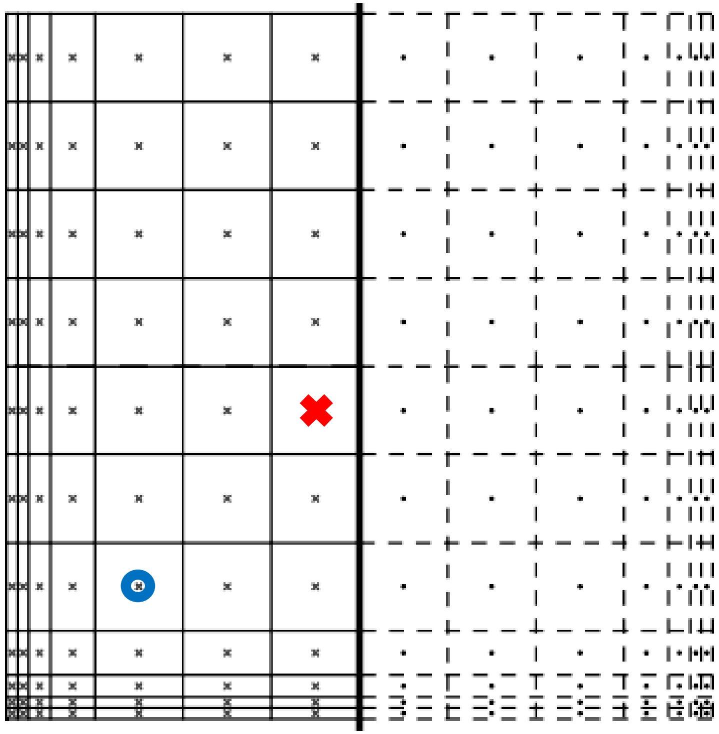


2 Symmetries

Symmetry-aware ordering

À.Alsalti-Baldellou, X.Álvarez-Farré, F.X.Trias, and A.Oliva. "Exploiting spatial symmetries for solving Poisson's equation", (submitted).

Exploiting symmetries



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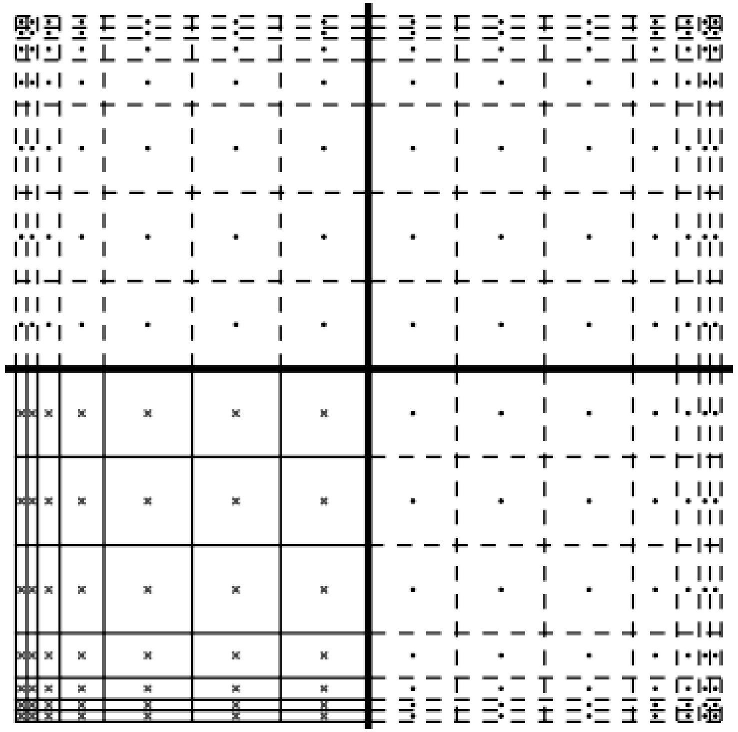

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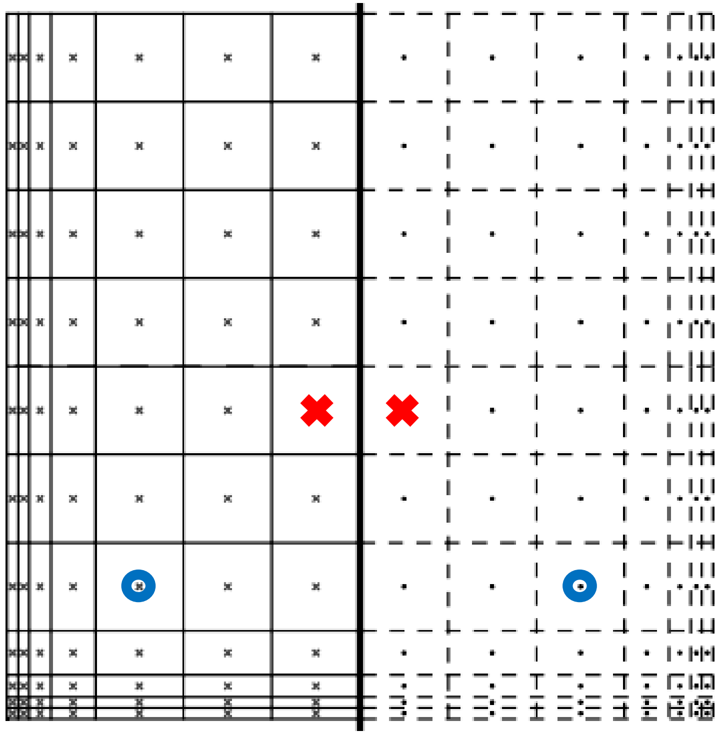

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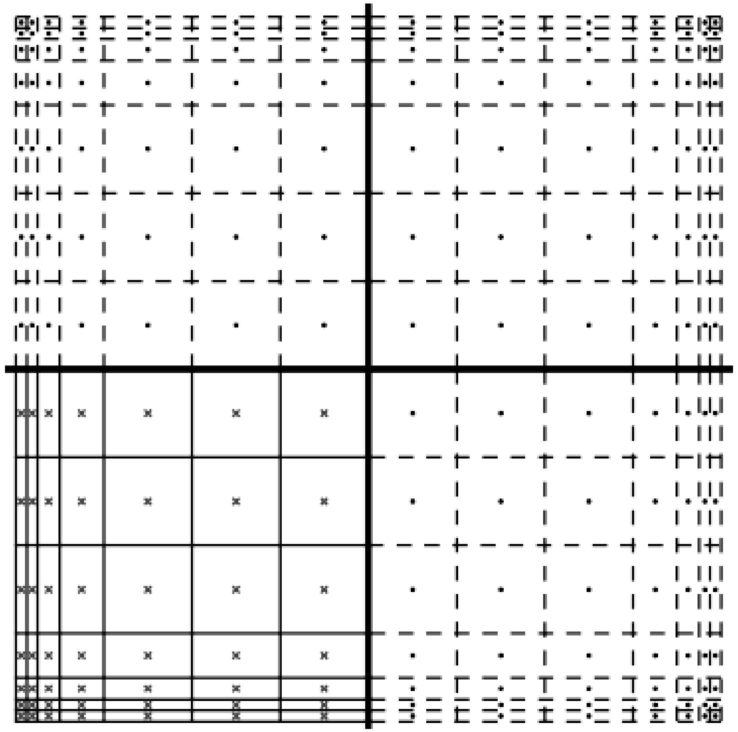

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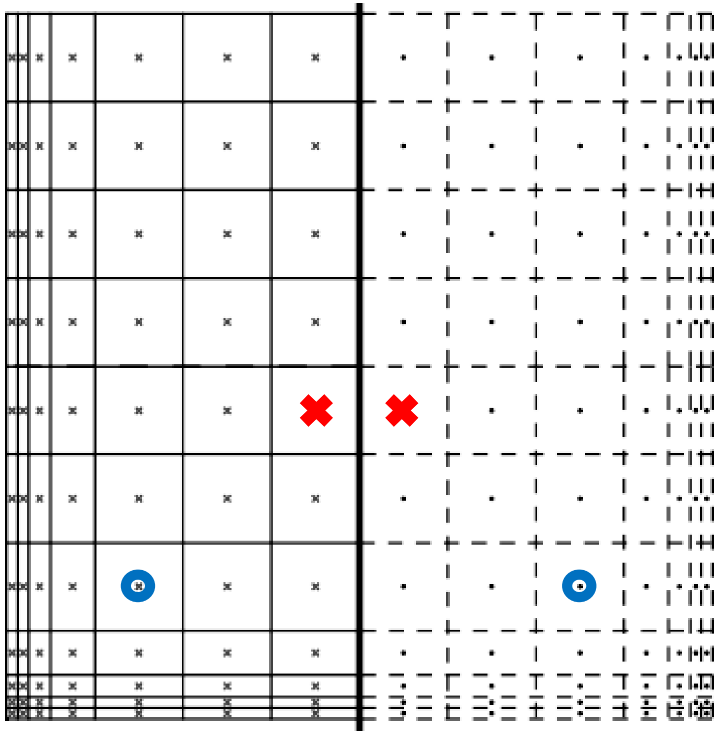

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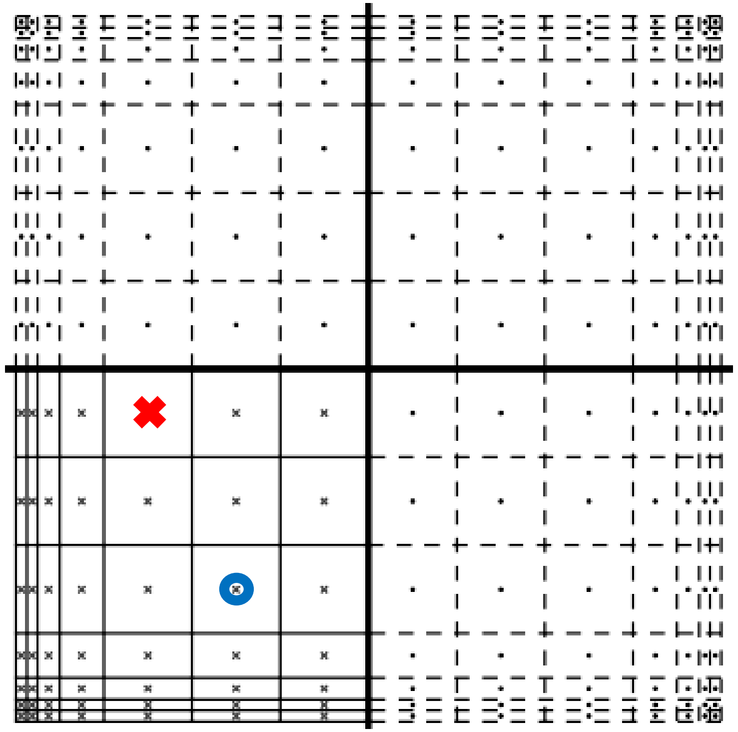

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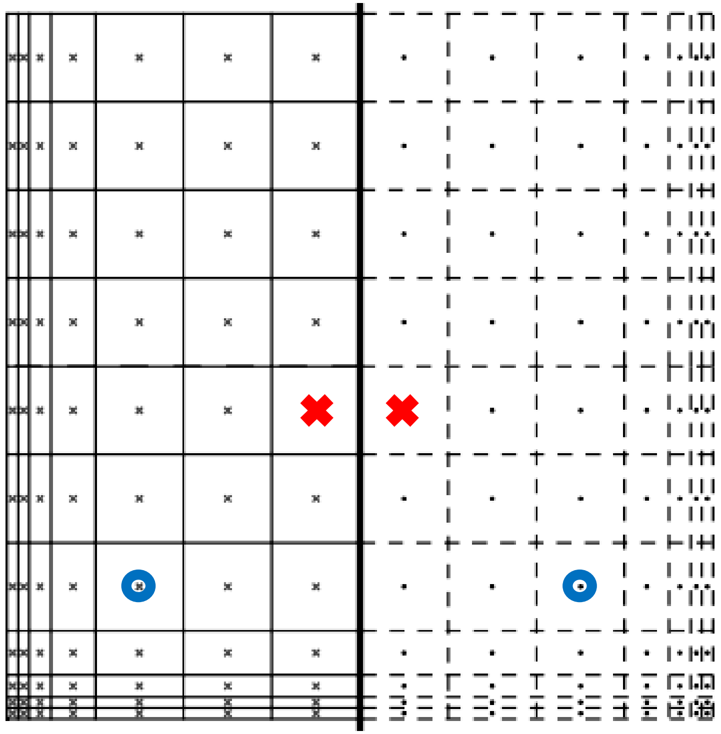

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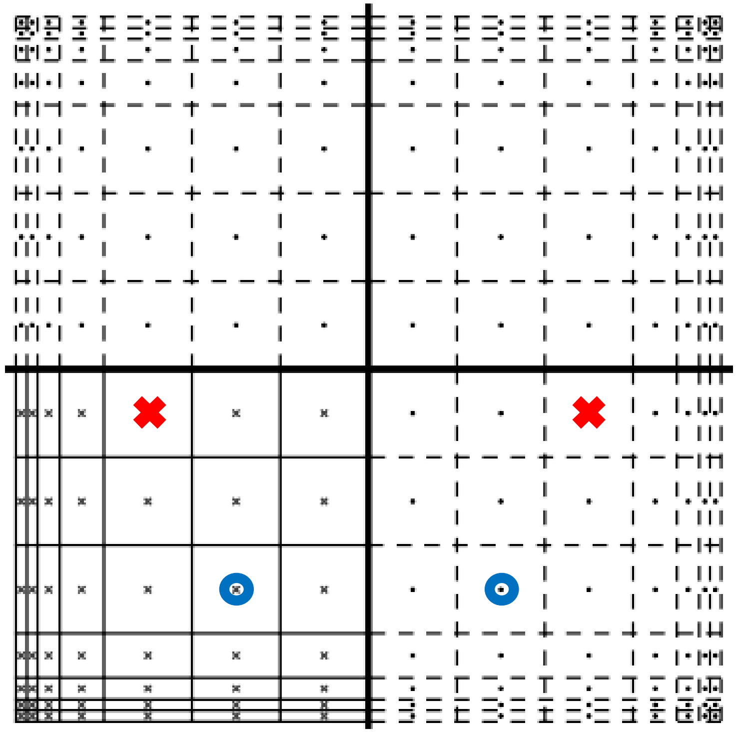

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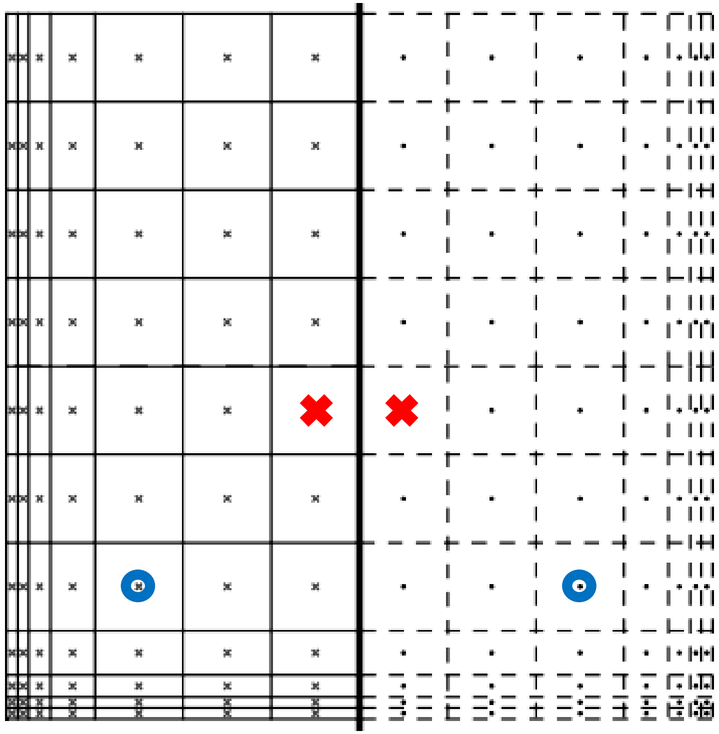
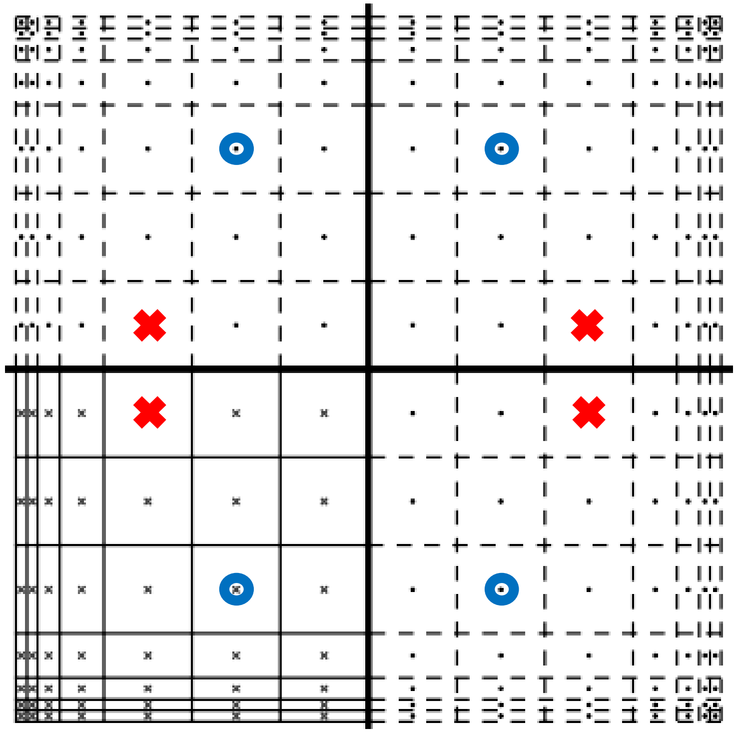


1 Symmetry



2 Symmetries

Symmetry-aware ordering

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Block-diagonalising L

$$L = \begin{array}{c|c} L_{inn} & L_{out} \\ \hline L_{out} & L_{inn} \end{array} \in R^{N \times N}$$

$$S = \sqrt{\frac{1}{2}} \begin{array}{c|c} I_{N/2} & I_{N/2} \\ \hline I_{N/2} & -I_{N/2} \end{array} \in R^{N \times N}$$

$$\hat{L} = SLS^{-1} = \begin{array}{c|c} L_{inn} + L_{out} & 0 \\ \hline 0 & L_{inn} - L_{out} \end{array}$$

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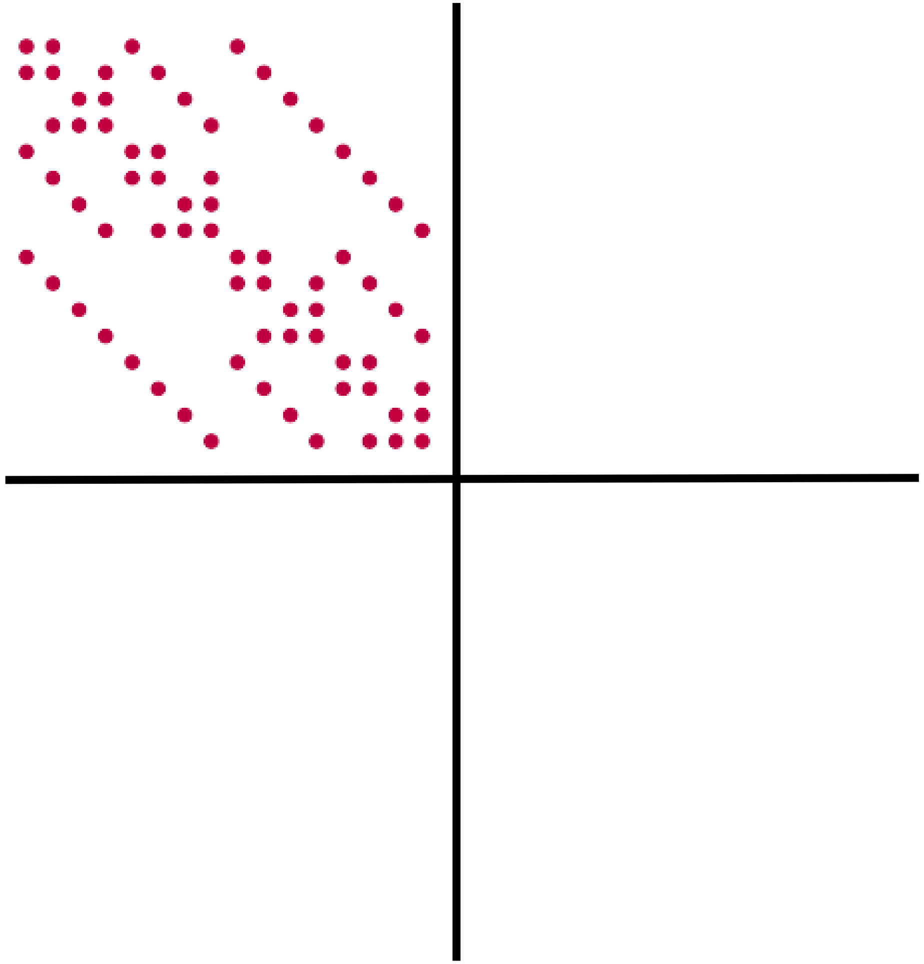

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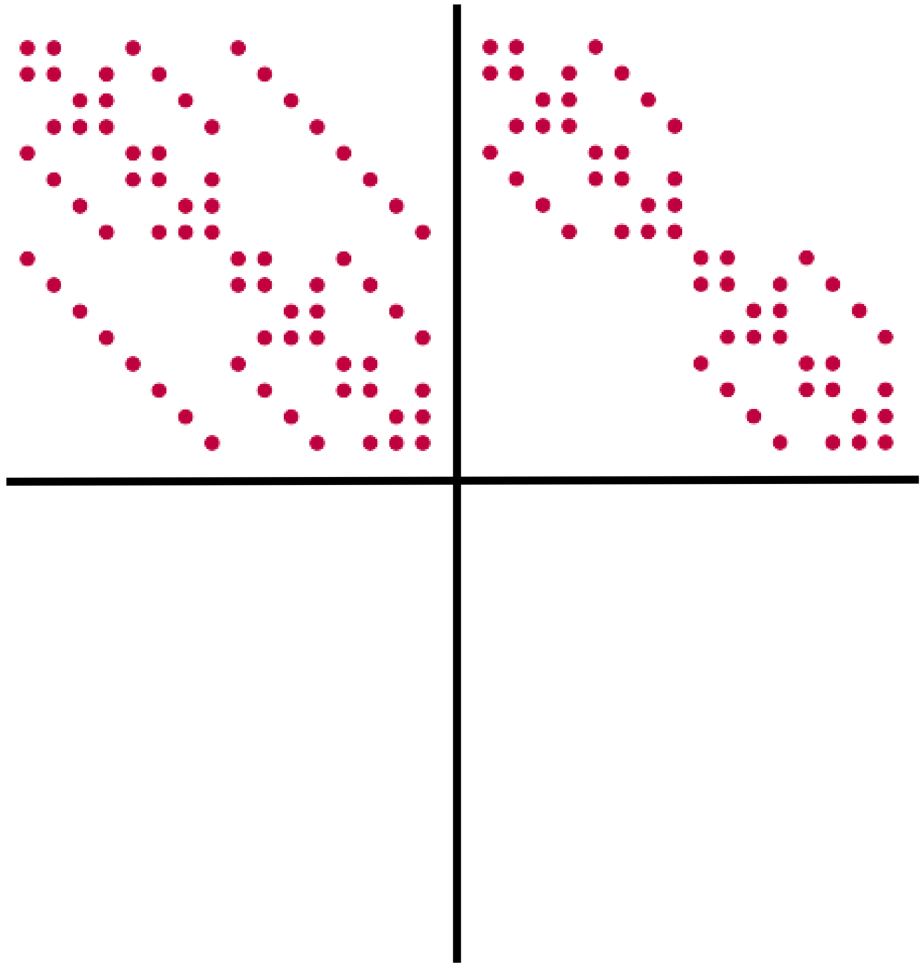

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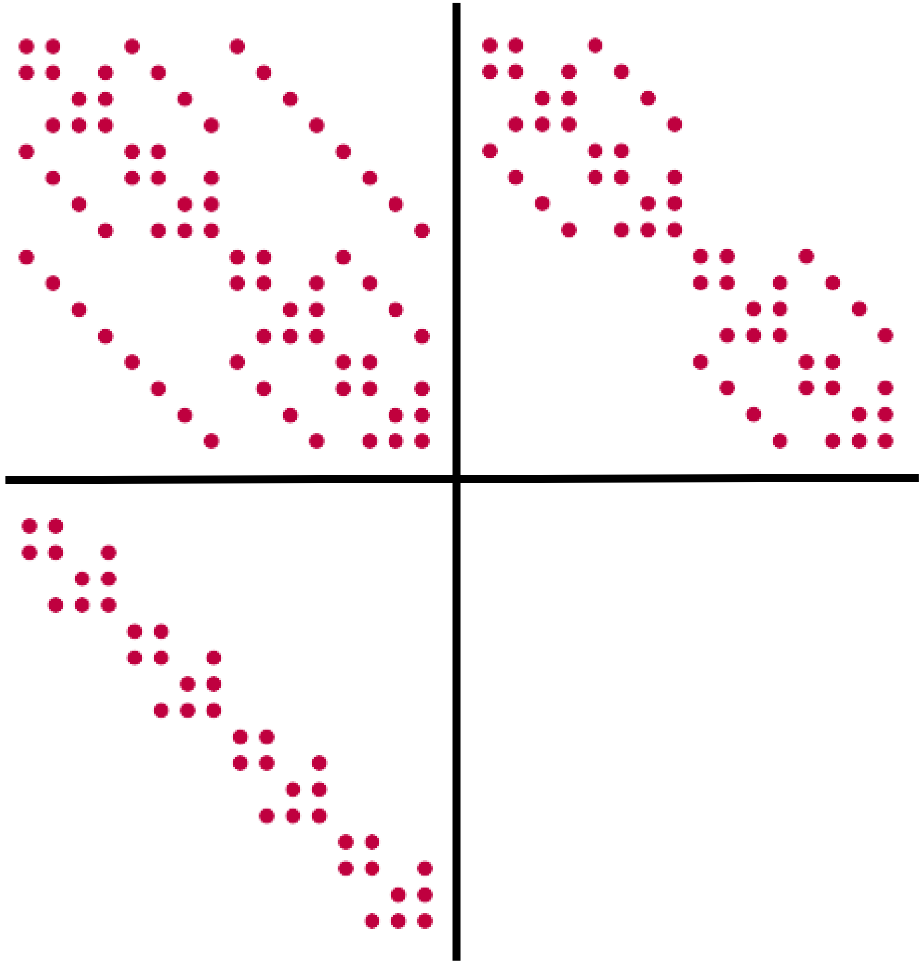

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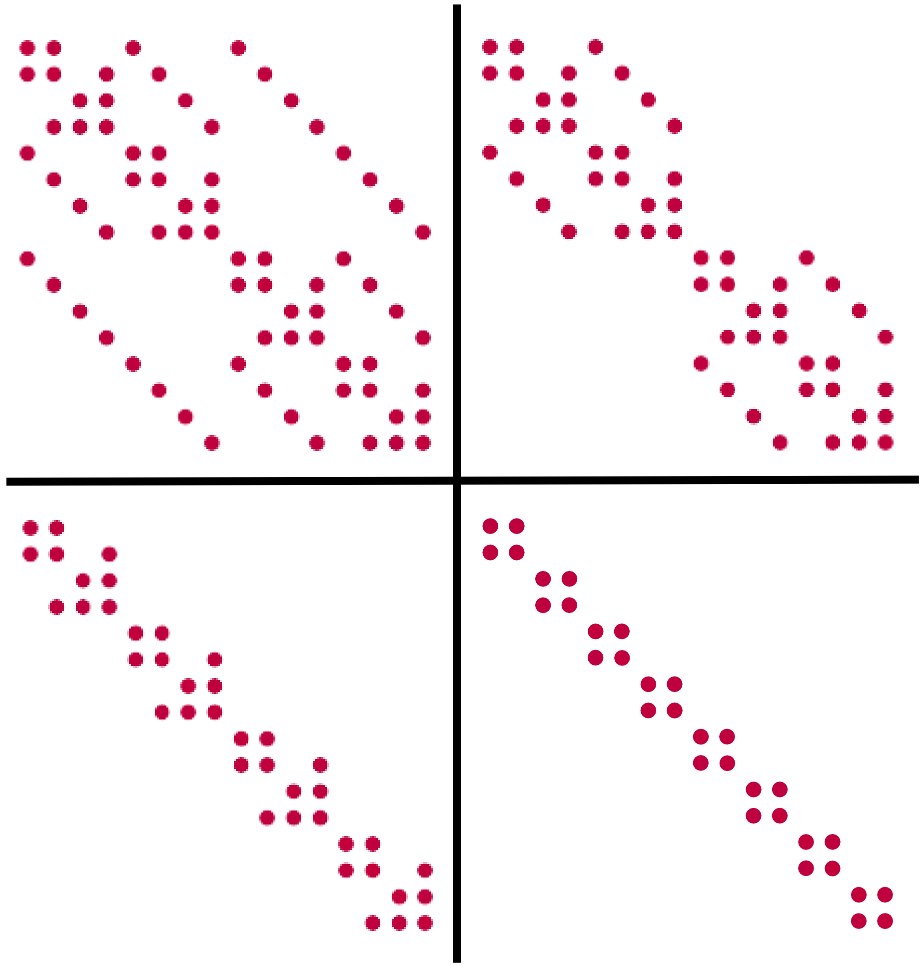

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Sparse matrix-matrix product

Rewriting the SpMV product:

$$\hat{L}\mathbf{v} = \underbrace{\begin{pmatrix} L_{inn}^{0} & & 0 \\ & \ddots & \\ 0 & & L_{inn}^{p} \end{pmatrix} \begin{pmatrix} \mathbf{v}^{0} \\ \hline \vdots \\ \hline \mathbf{v}^{p} \end{pmatrix}}_{L_{inn}\left(\mathbf{v}^{0} \;\middle|\; \dots \;\middle|\; \mathbf{v}^{p}\right)} + L_{out}\mathbf{v}$$

into an SpMM product

A reduction in time complexity

A reduction in memory footprint

An increase in arithmetic intensity

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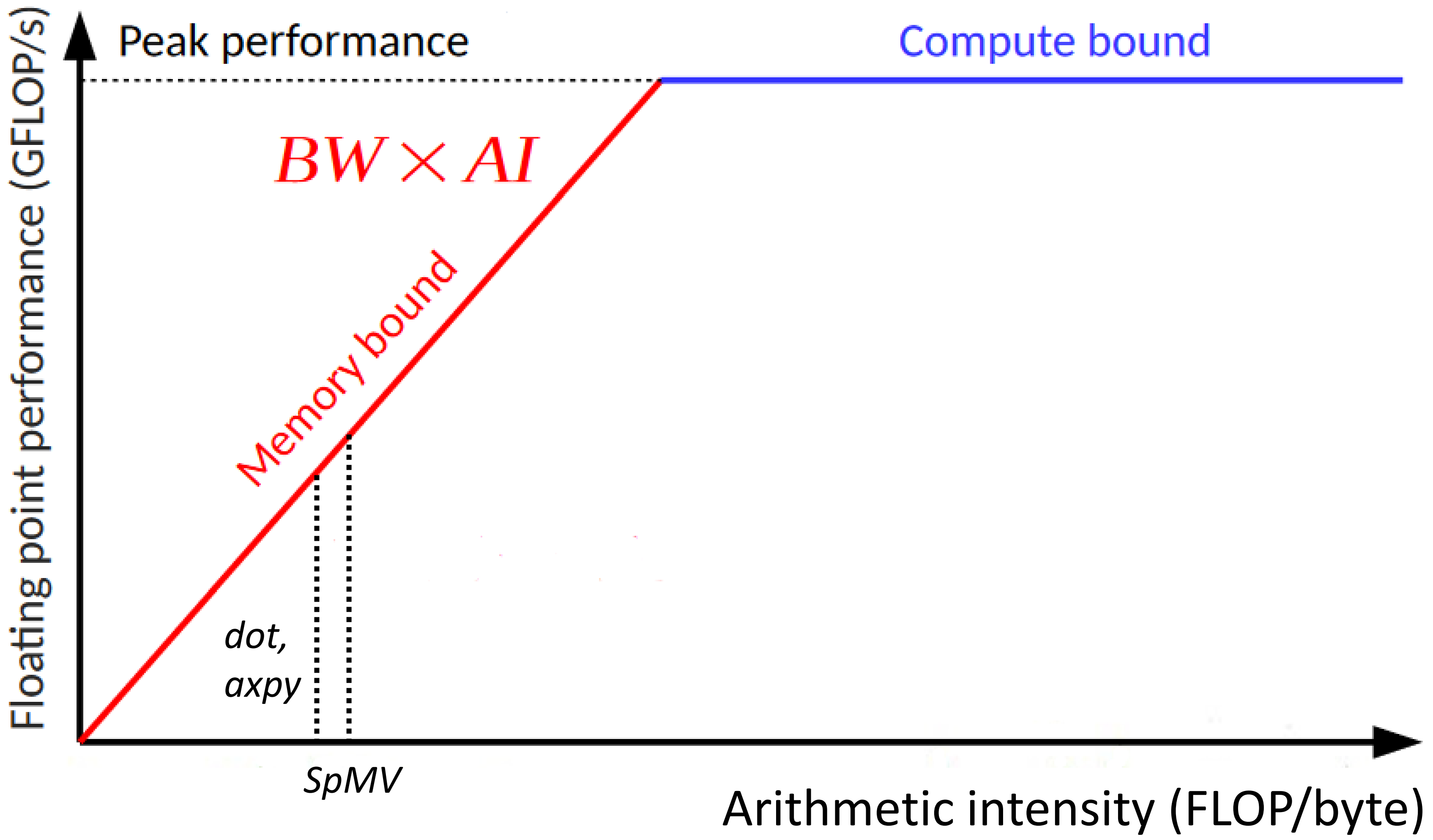
Increasing arithmetic intensity



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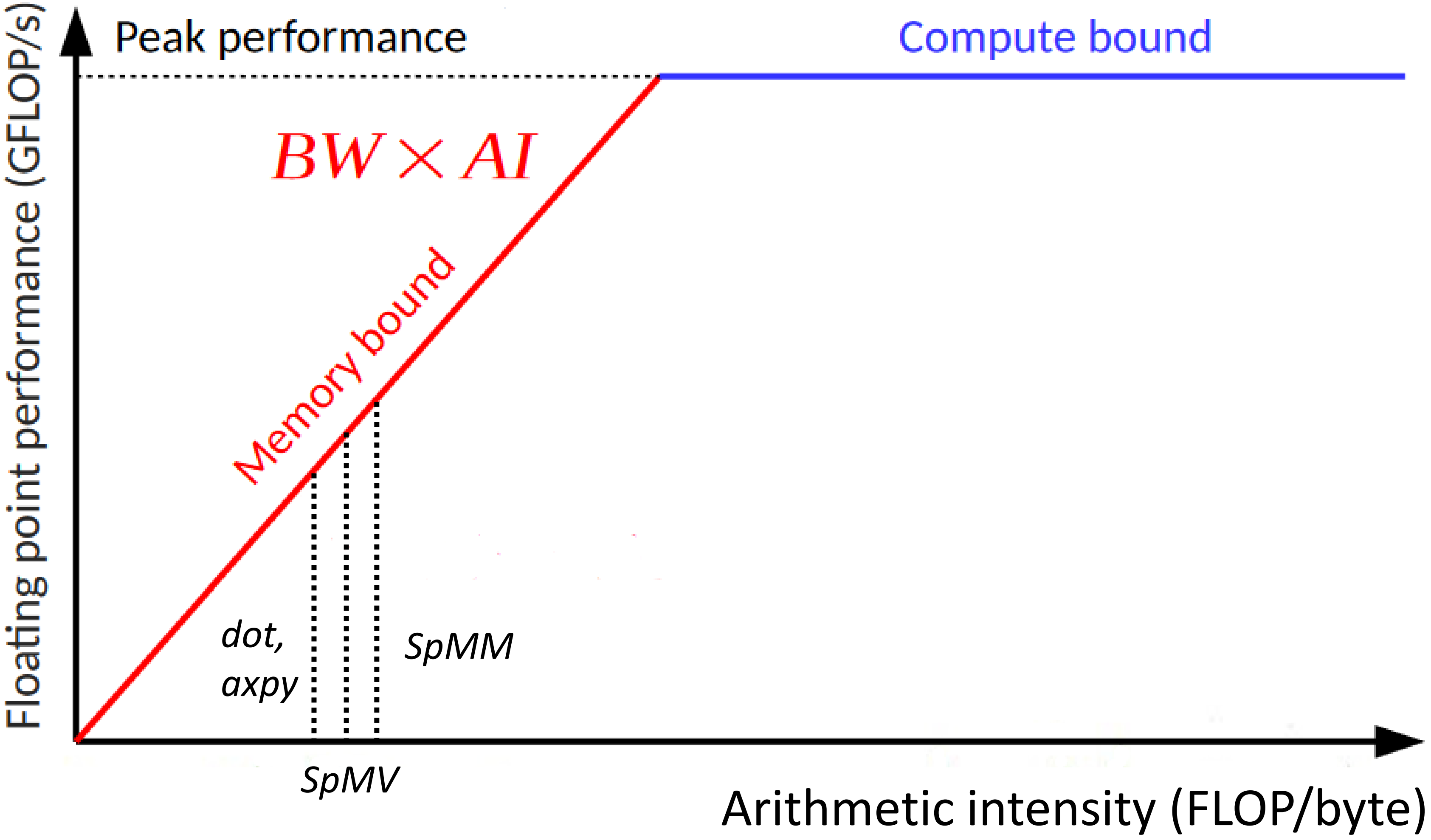
Increasing arithmetic intensity



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Summarising

Symmetry preserving methods in MHD

HPC^2 framework

Exploiting symmetries in geometry

Thank you for attending!