Maximizing Performance Through Memory Hierarchy-Driven Data Layout Transformations

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COMPUTING SCIENCES RESEARCH
LAWRENCE BERKELEY NATIONAL LABORATORY

SCHOOL OF COMPUTING

The University of Texas at Austin
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ECP

DOE CSGF

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Outline

- Introduction: Bricks
- High-Dimensional Bricks
- GENE Microbenchmarks

Introduction: Bricks

Standard Array Layouts

- Standard array layouts can suffer from poor spatial locality
- Forced to recover locality by loop optimizations
  - Tiling
  - Polyhedral analysis
  - Scheduling languages
- Search for iteration order to support parallelization, locality, vectorization

0	1	2	⋯	99
100	101	102	⋯	199
200	201	202	⋯	⋮
⋮	⋮	⋮	⋱	899
900	901	902	⋯	999

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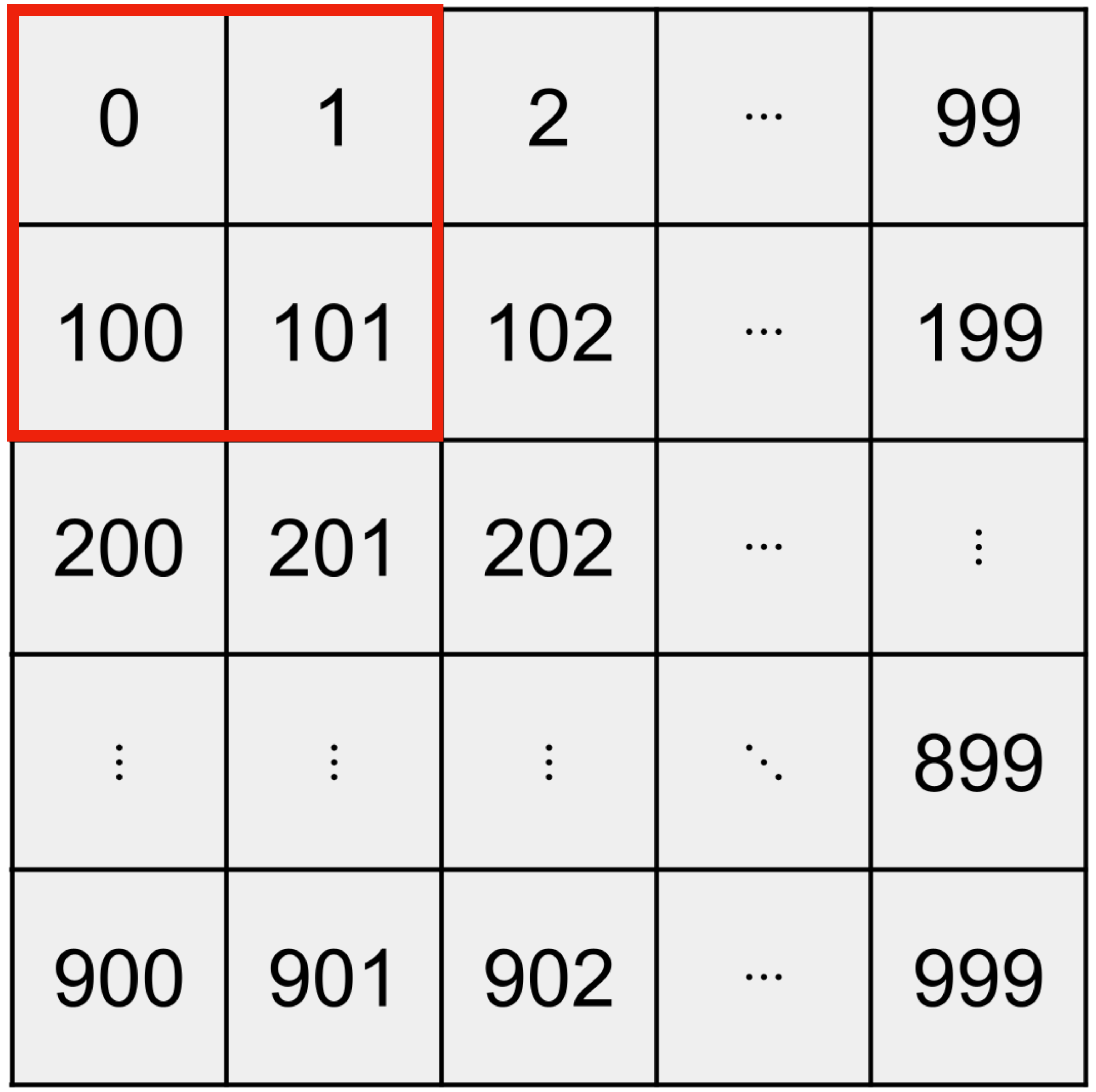

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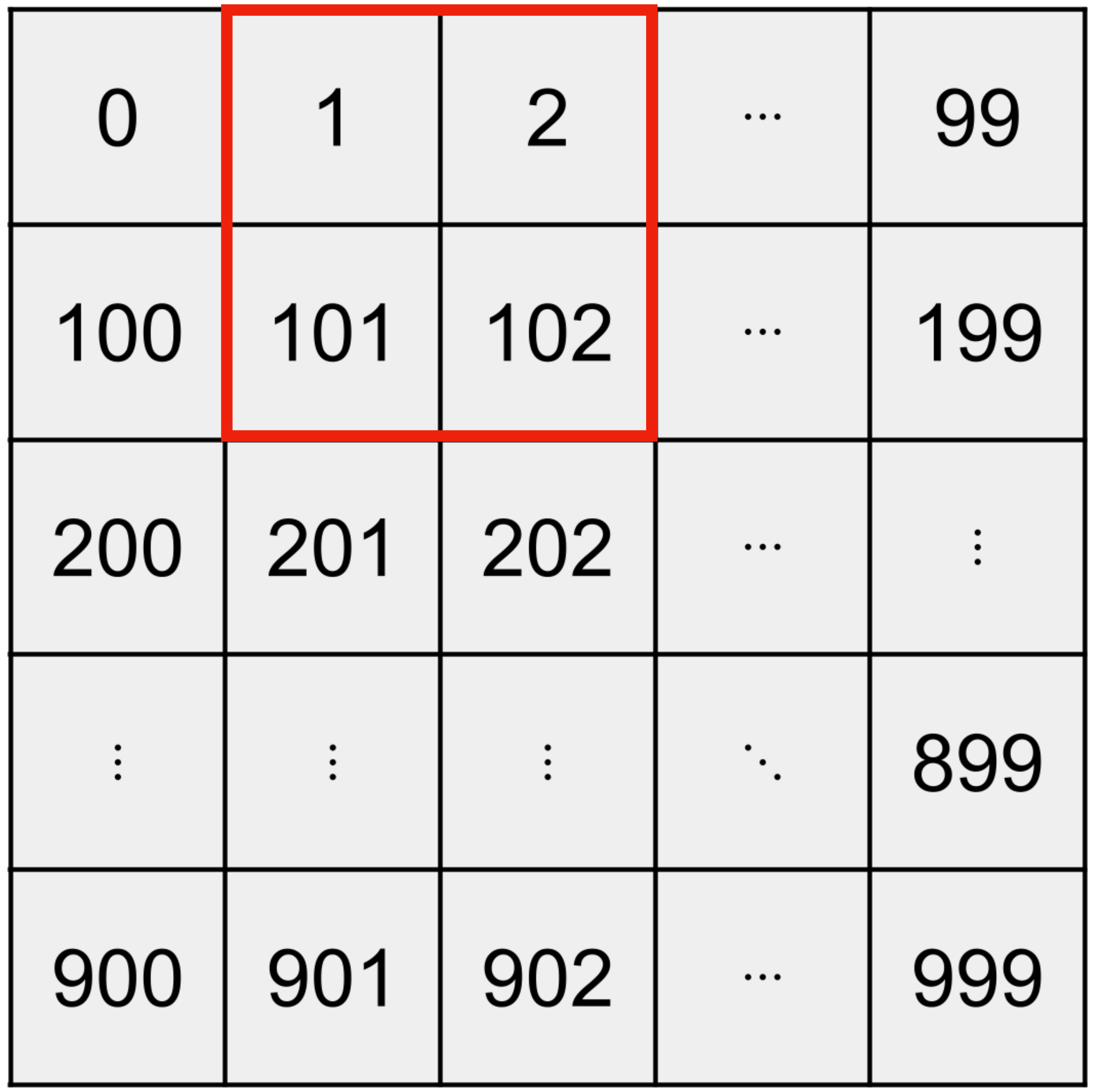

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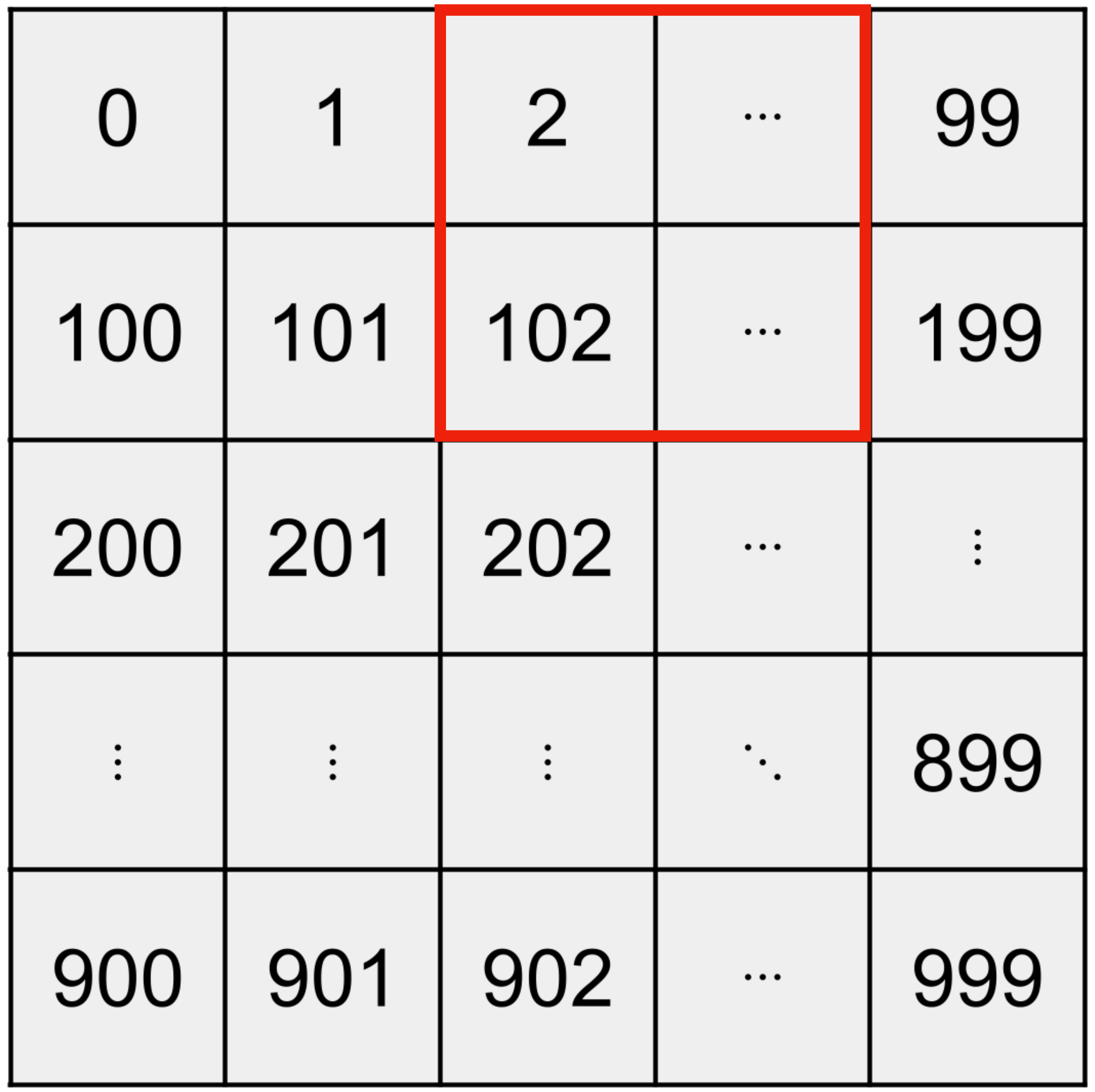

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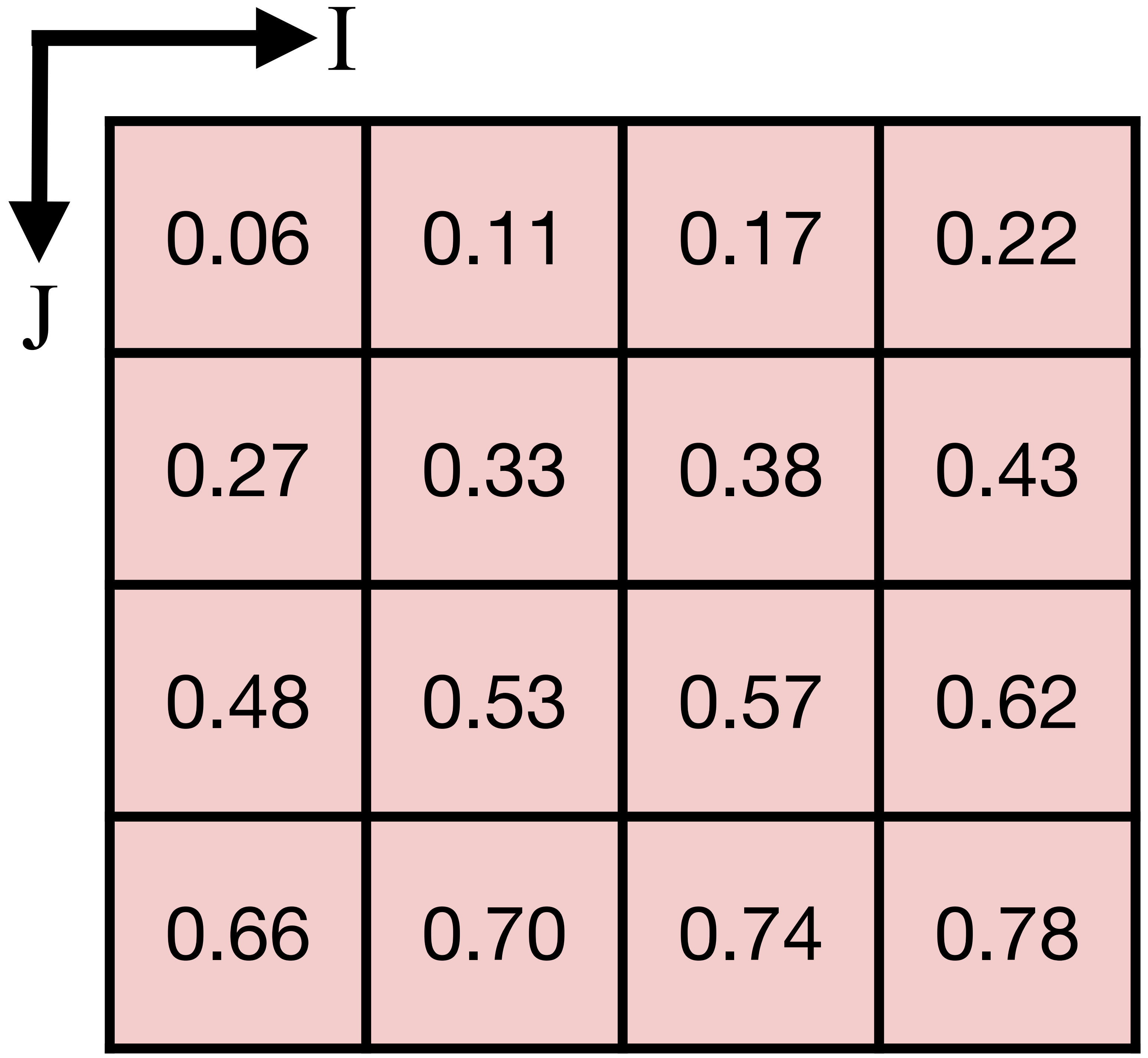
The Bricks Layout

What is a Brick?

- Each Brick is a small, **fixed-**size multidimensional array stored **contiguously** in memory
- Each Brick is a “unit” of locality
- Fine-grained parallelism occurs **inside** each Brick
- Coarse-grained parallelism occurs **across** Bricks



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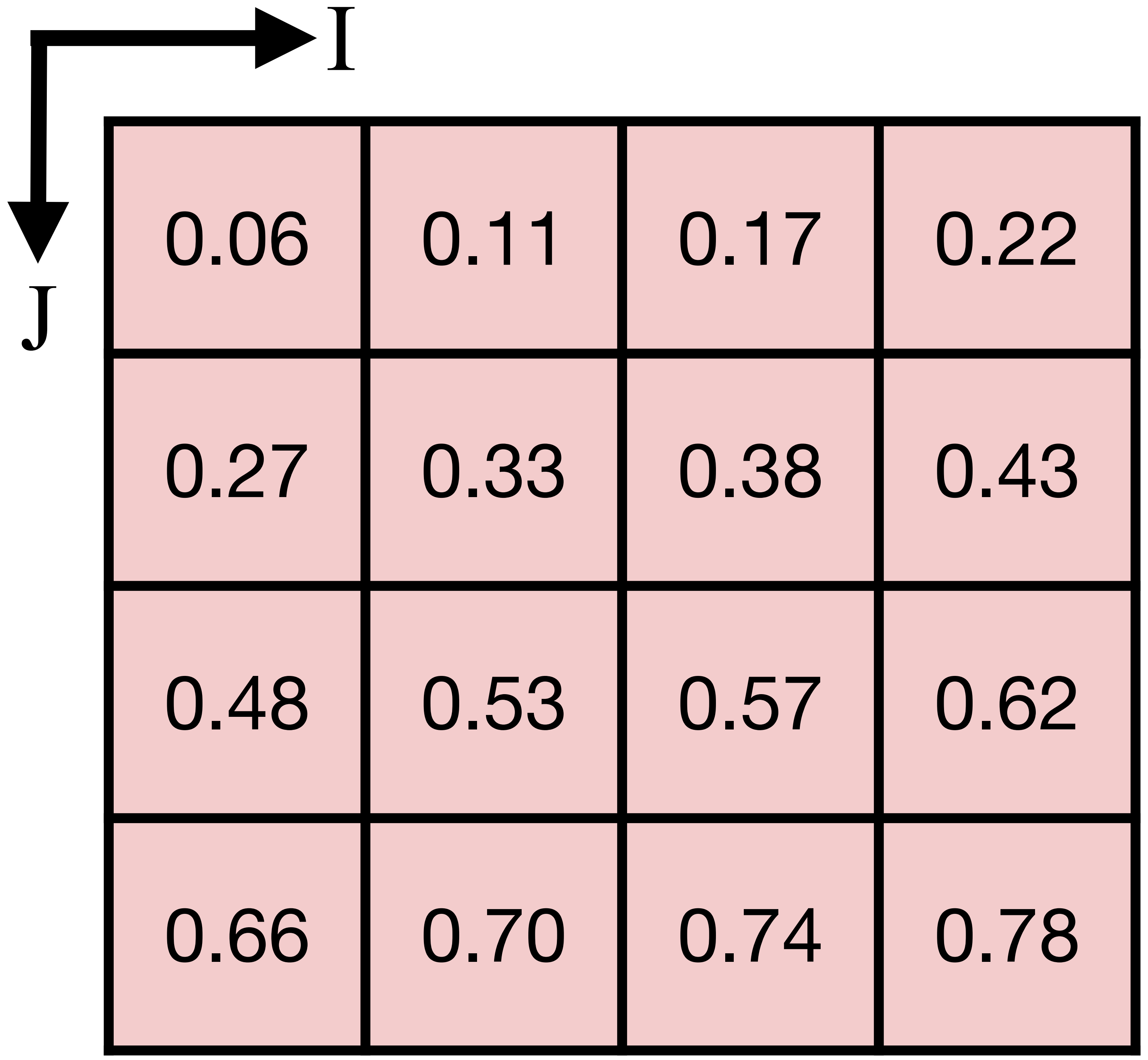
0.27	0.33	0.38	0.43
0.48	0.53	0.57	0.62
0.66	0.70	0.74	0.78

4x4 Brick storing a 4x4 block of user data

The Bricks Layout

Putting Bricks Together



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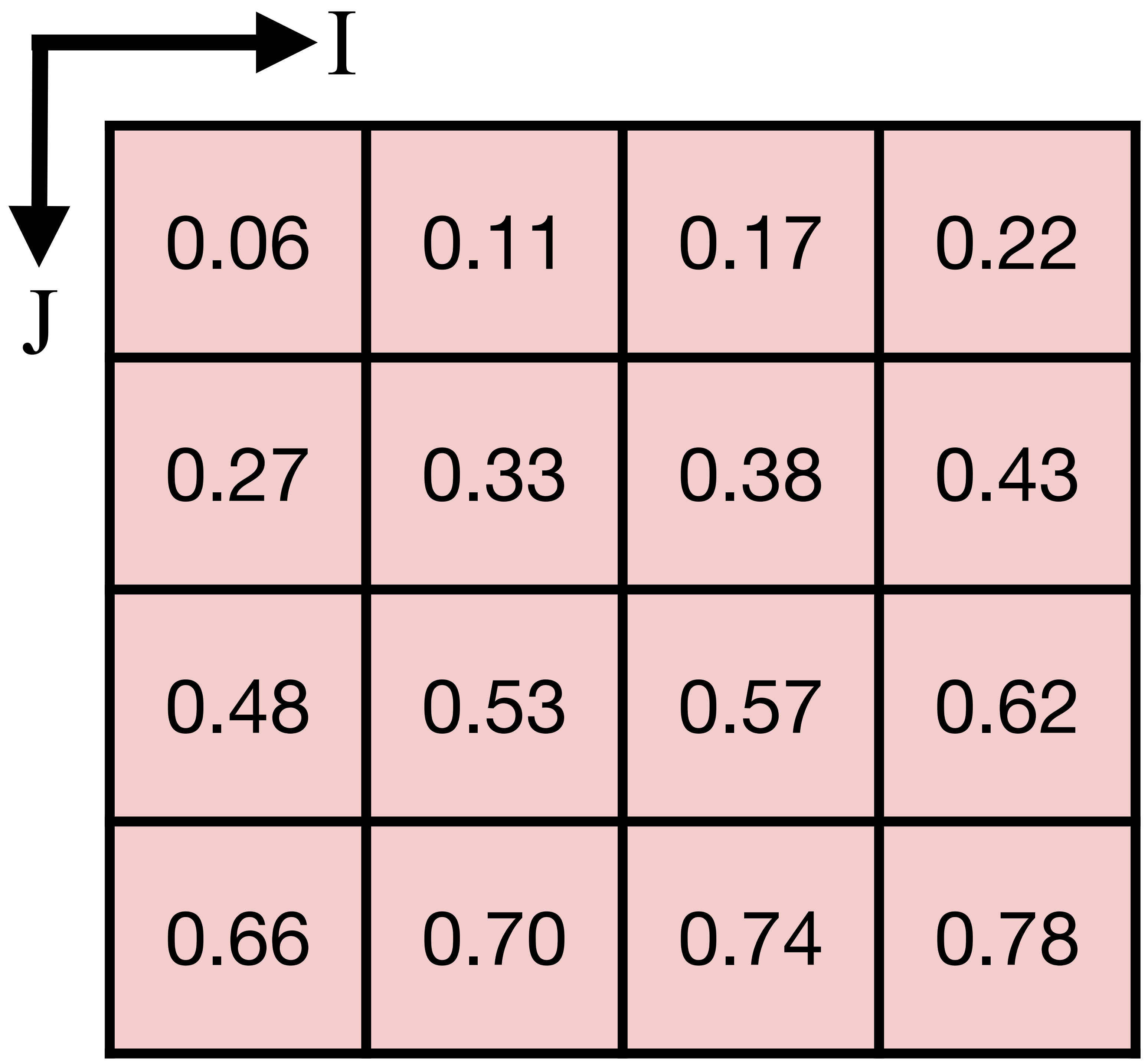
User data

The Bricks Layout

Putting Bricks Together

- Bricks are stored contiguously



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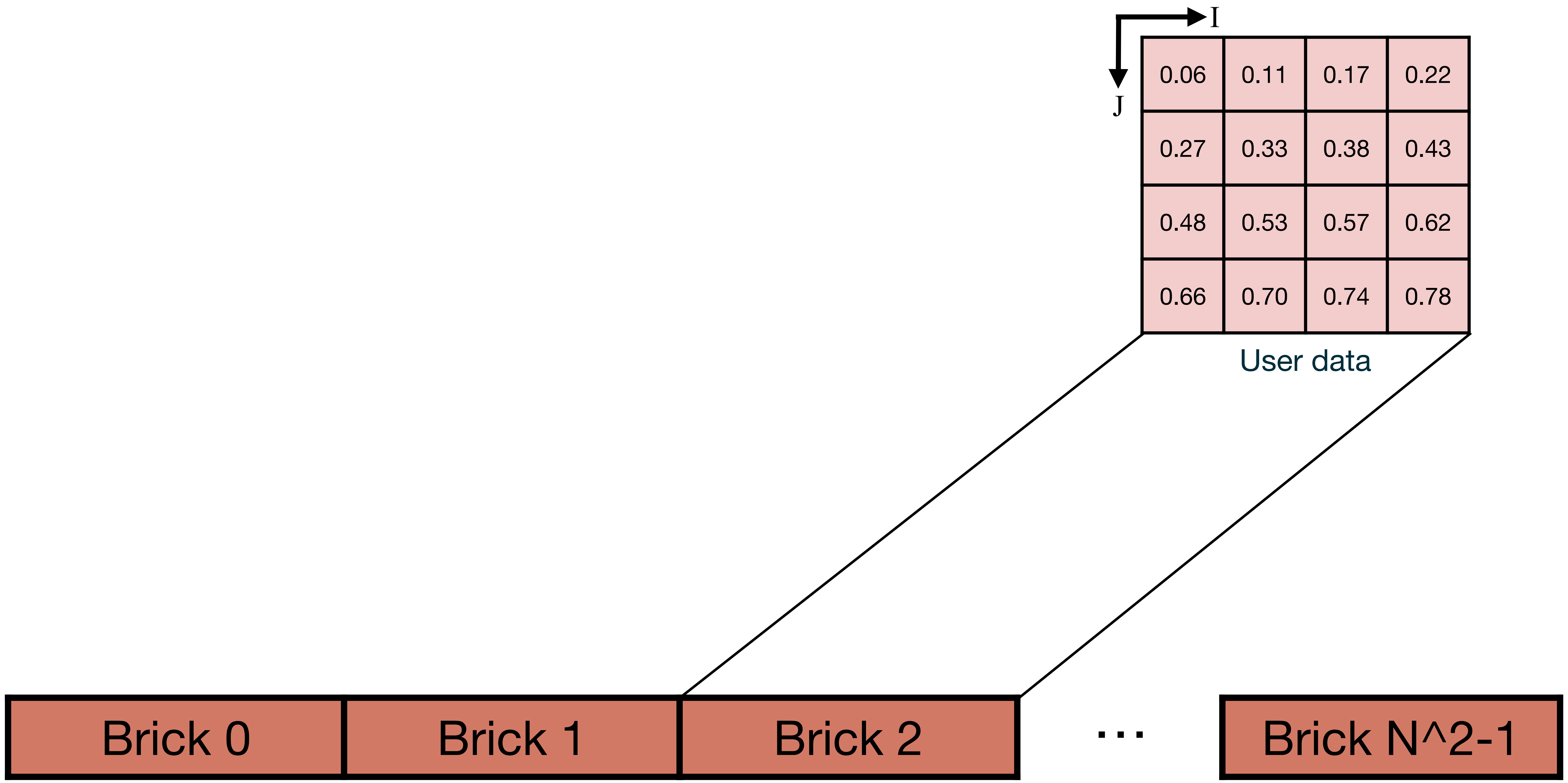

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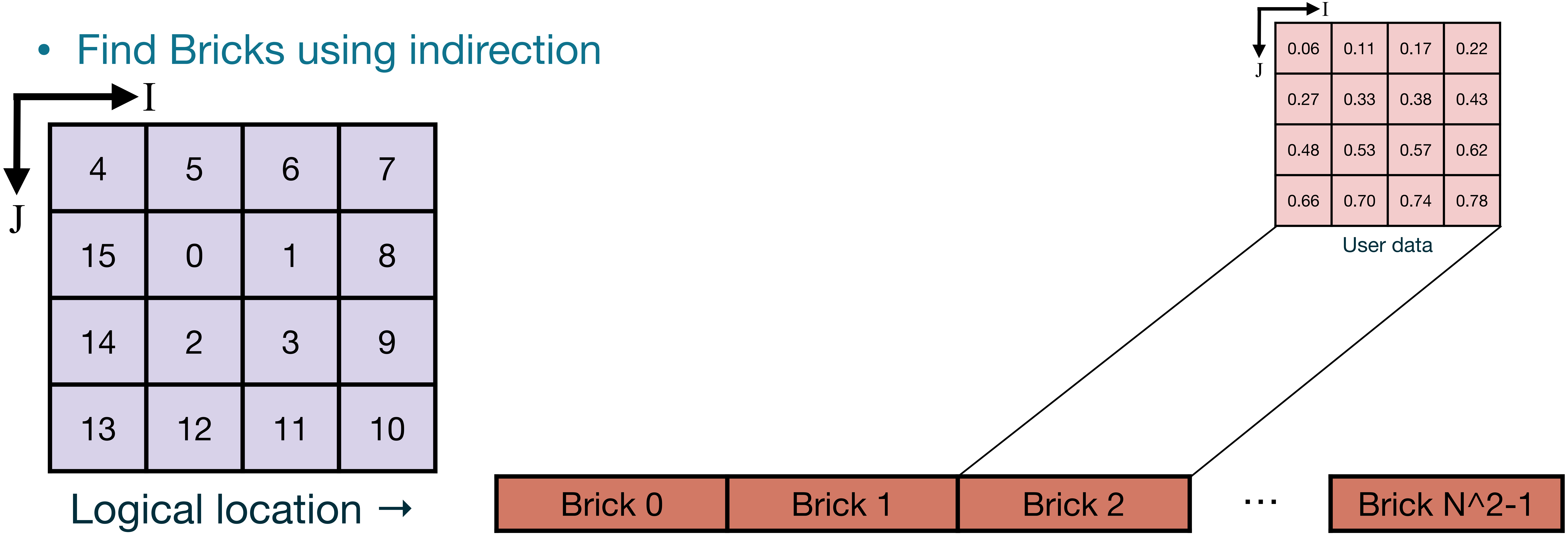
Putting Bricks Together

- Bricks are stored contiguously
- Find Bricks using indirection



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Logical location → physical location

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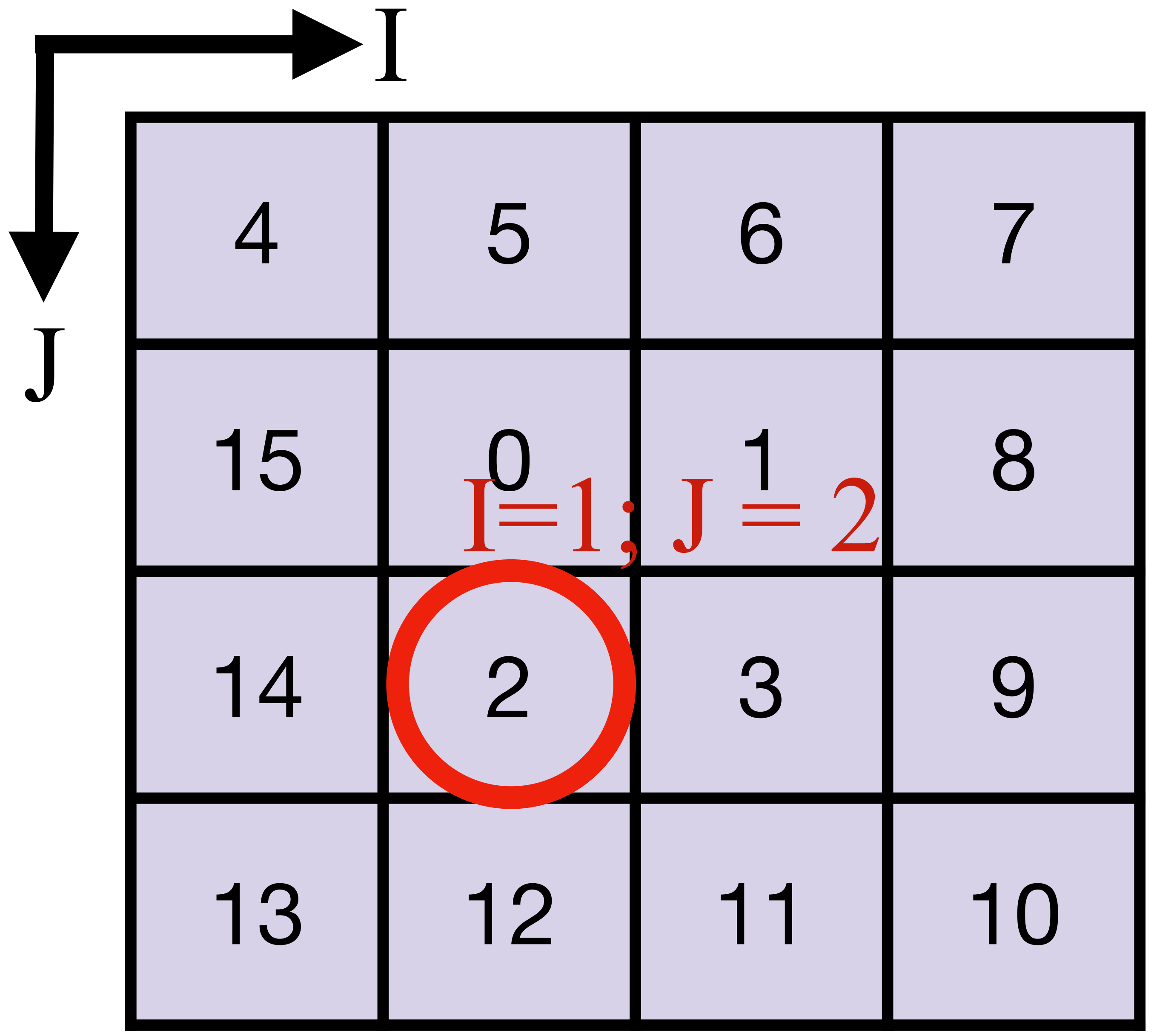

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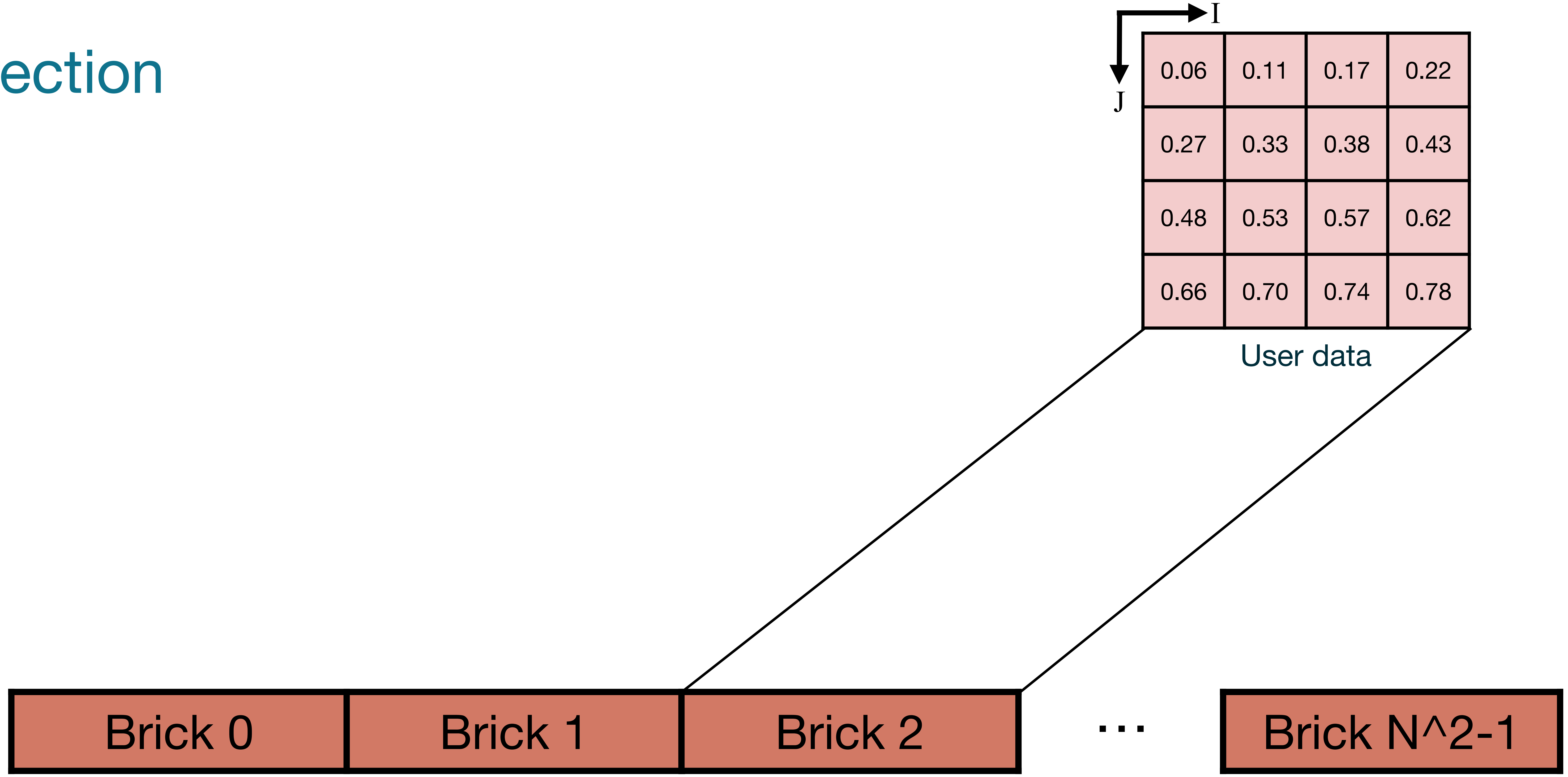

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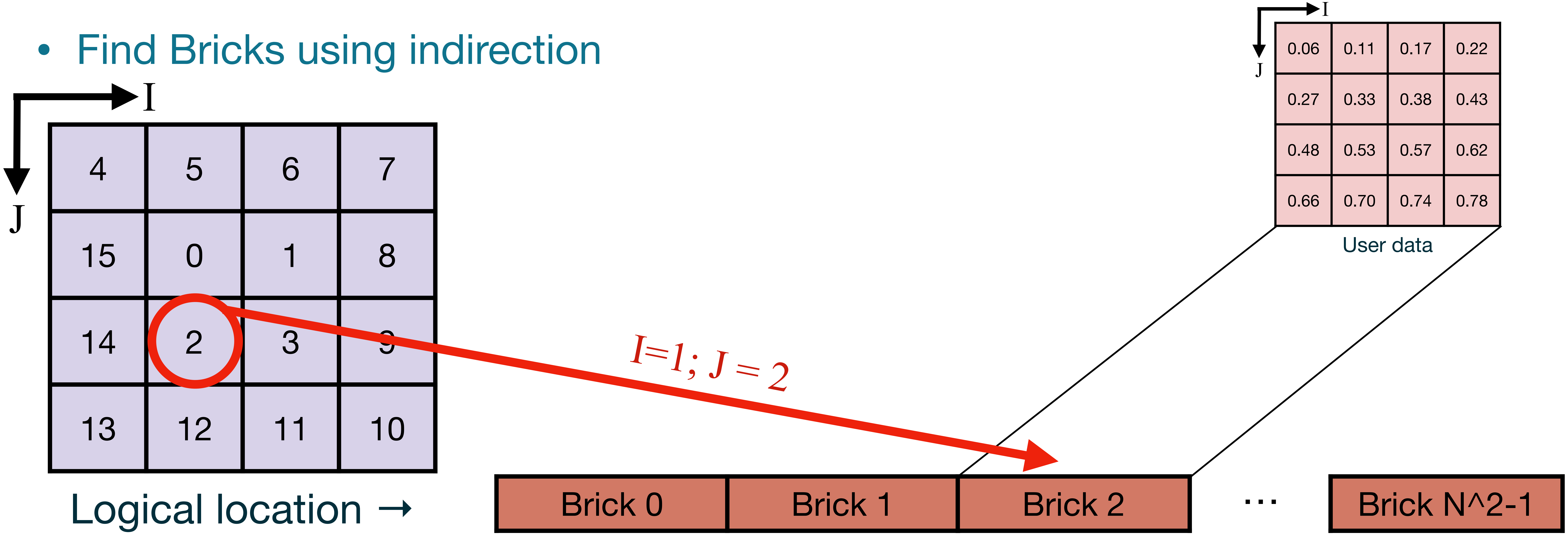

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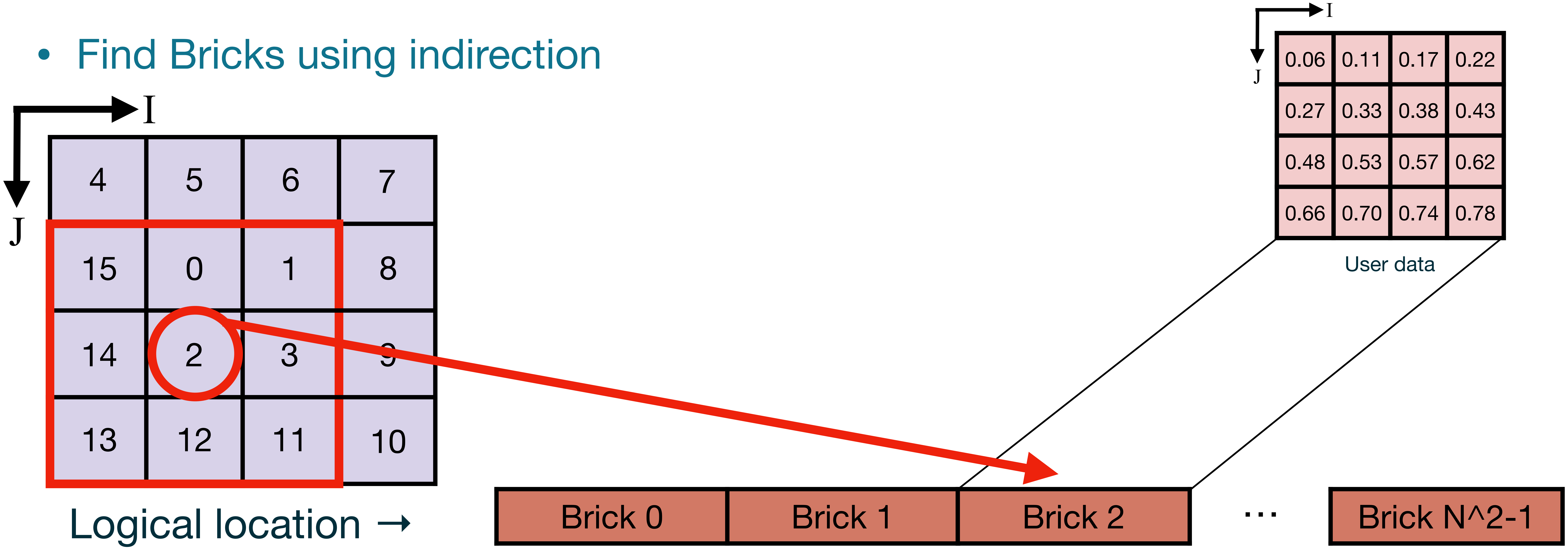

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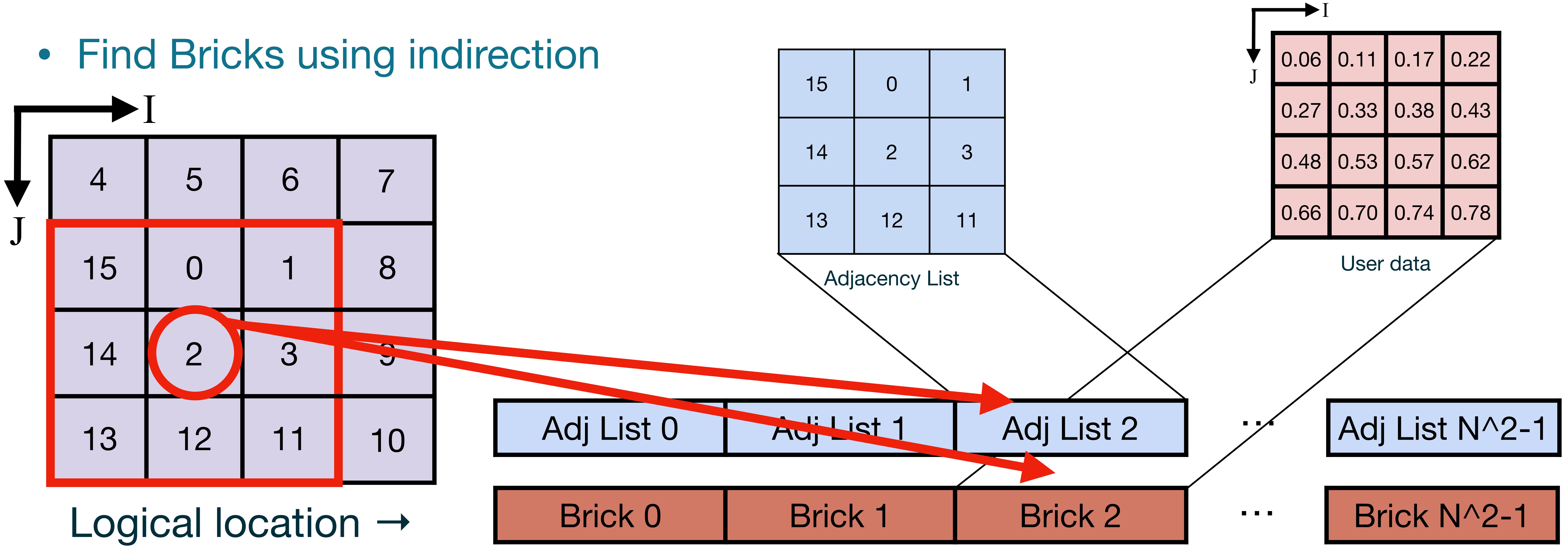

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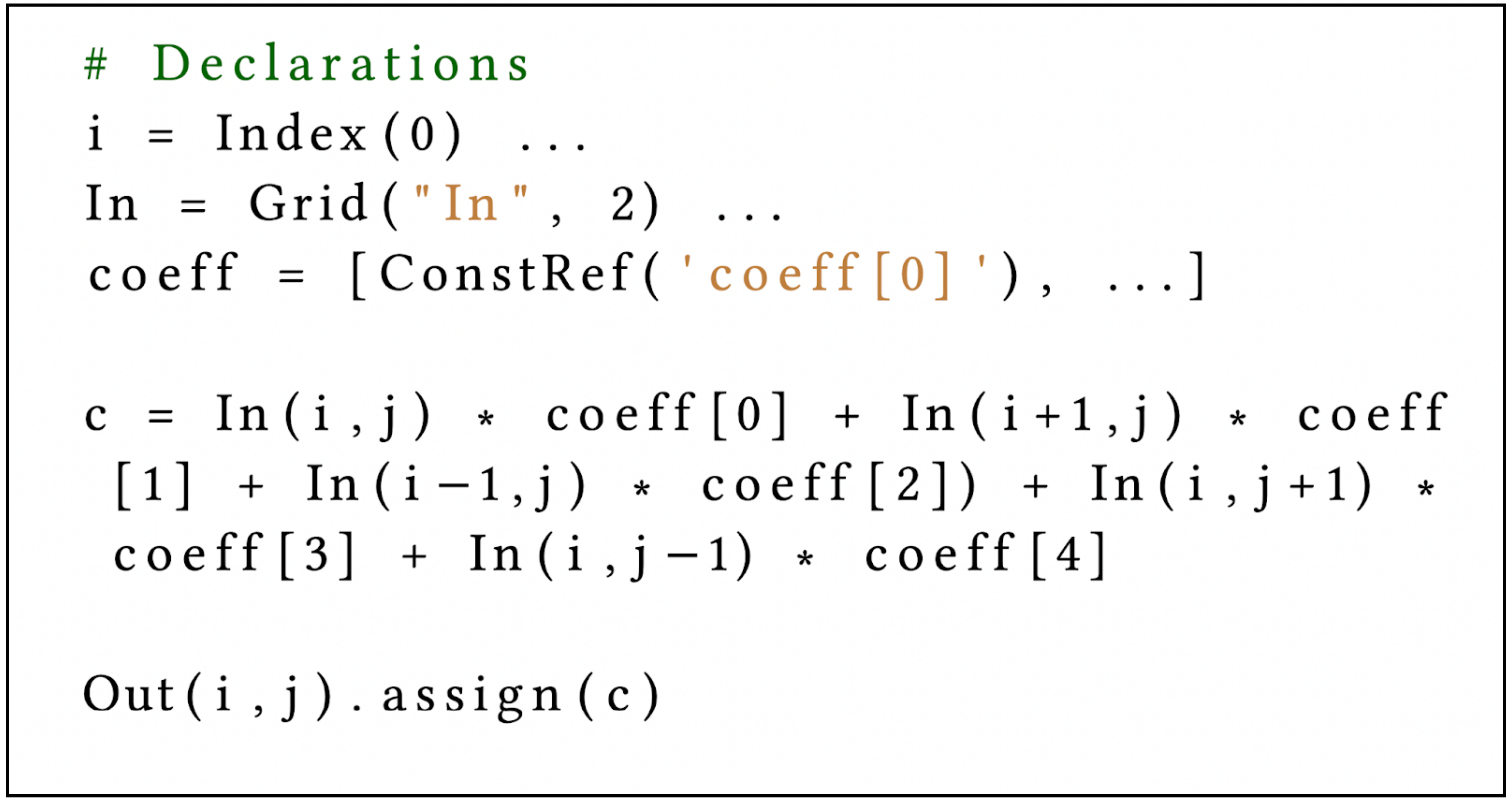
The Bricks Library

Performance-portable stencil computations

- Code generation for stencil computations[1]
  - Targets CPUs and GPUs (NVIDIA, AMD, Intel, SVE)
  - User only needs to specify Brick shape and computation



```
# Declarations
i = Index(0) ...
In = Grid("In", 2) ...
coeff = [ConstRef('coeff[0]'), ...]

c = In(i,j) * coeff[0] + In(i+1,j) * coeff
 [1] + In(i−1,j) * coeff[2]) + In(i,j+1) *
 coeff[3] + In(i,j−1) * coeff[4]

Out(i,j).assign(c)
```

Example specification of 2D, 5-point stencil[2]

[1] Delivering Performance-Portable Stencil Computations on CPUs and GPUs using Bricks

[2] Exploiting reuse and vectorization in blocked stencil computations on CPUs and GPUs

Bricks

Hardware-Aligned Layout

- N-D Grid → N-D Array of N-D Bricks

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[3] Improving Communication by Optimizing On-Node Data Movement with Data Layout

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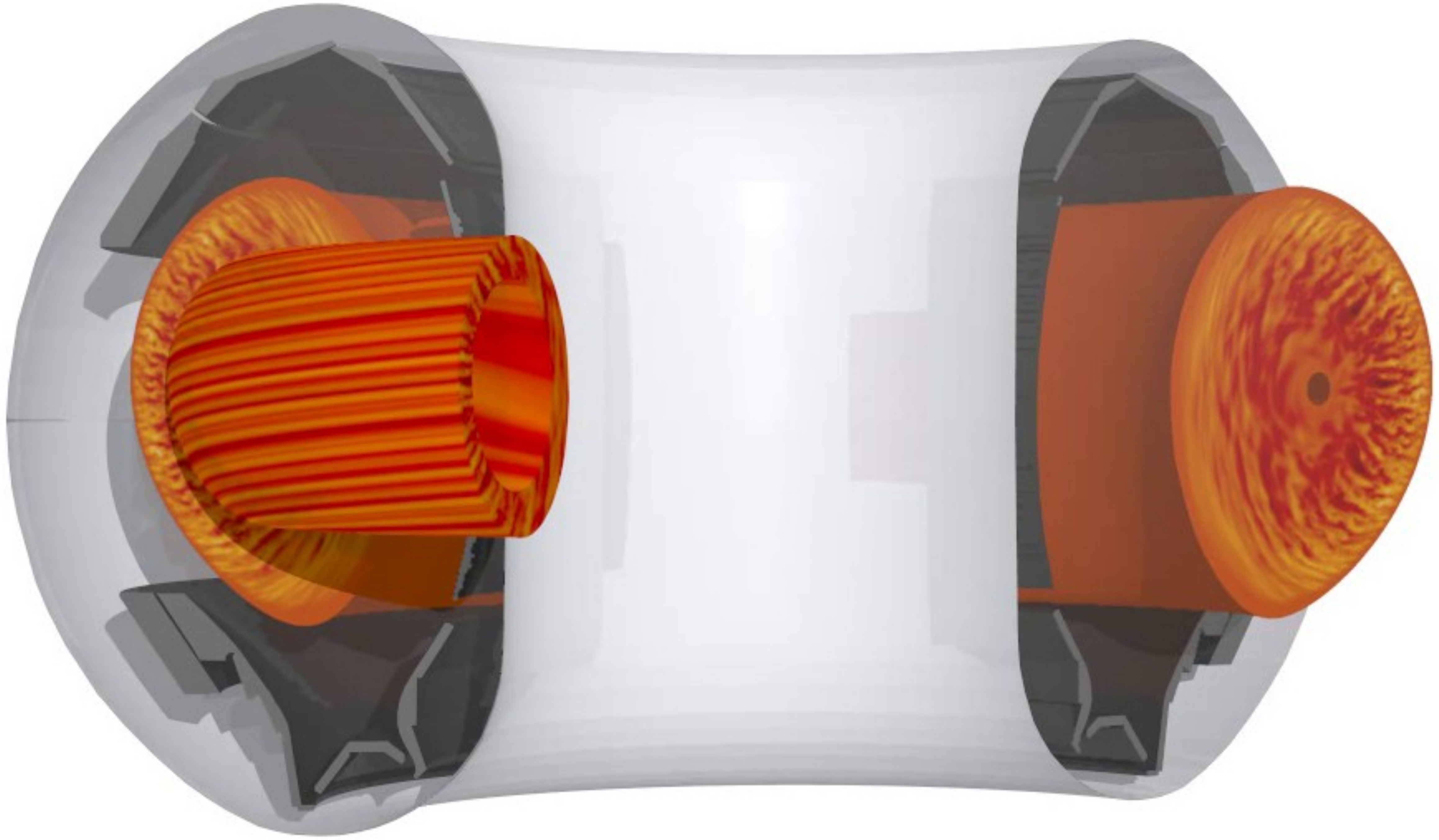
High-Dimensional Bricks: Example

Example: Bricks in Phase-Space Kernels

GENE

- GENE[4]: 6D physical+phase-space fusion code
  - IJK: space
    - J: in Fourier space
  - LM: phase space
  - N: species
  - GTensor: GPU implementation
- Core computations:
  - Stencils
  - FFT (along J-axis)
  - Gyroaveraging, linear solves…



[4] http://genecode.org

Bricks in Phase-Space Kernels

Challenges

- Extending Bricks library support
  - Complex types
  - Managing metadata in 6D
  - MPI layout optimization in a **subset** of the dimensions
  - Code generation for computations on arrays of mixed dimensionality

- Non-stencil computations with Bricks
  - FFT
  - Linear solves
  - Gyroaveraging

Bricks in Phase-Space Kernels

Challenges

- Extending Bricks library support
    - ✓ Complex types
    - ✓ Managing metadata in 6D
    - ✓ MPI layout optimization in a **subset** of the dimensions
    - – *Partially supported:* code generation for computations on arrays of mixed dimensionality

- Non-stencil computations with Bricks
    - ✓ FFT (for CUDA)
    - – Linear solves
    - – Gyroaveraging

Example

Star-shaped 2D Stencil along K and L axes of a 6D array

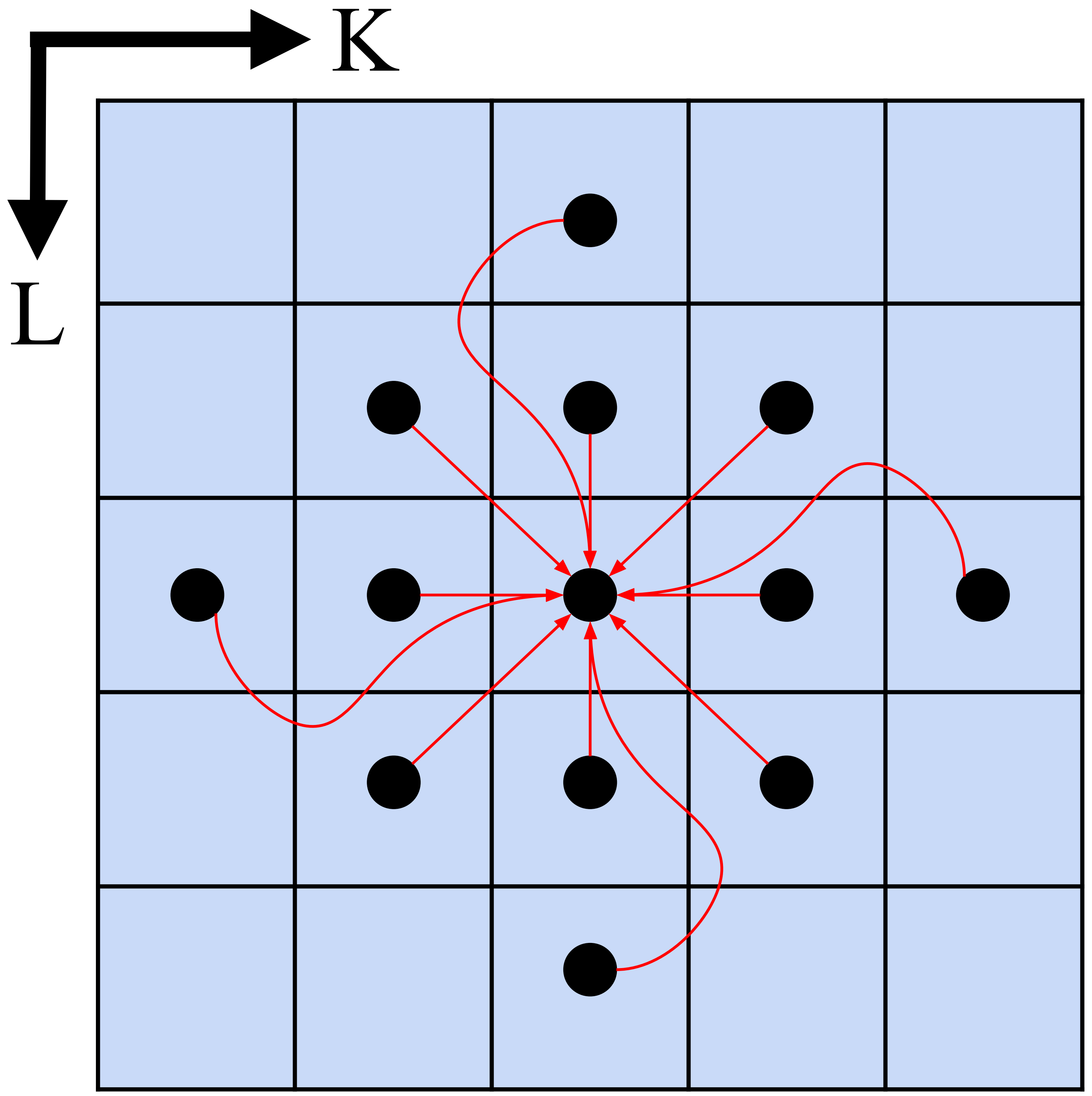
```
i, j, k, l, m, n = map(Index, range(6))

# Declare grid
input = Grid("bIn", 6, complex_valued=True)
output = Grid("bOut", 6, complex_valued=True)
coeffs = [ConstRef('coeff[0]'), ... ]

# Express computation
calc = coeffs[ 0] * input(i, j, k + 0, l - 2, m, n) + \
       coeffs[ 1] * input(i, j, k - 1, l - 1, m, n) + \
       coeffs[ 2] * input(i, j, k + 0, l - 1, m, n) + \
       ...
       coeffs[11] * input(i, j, k + 1, l + 1, m, n) + \
       coeffs[12] * input(i, j, k + 0, l + 2, m, n)

output(i, j, k, l, m, n).assign(calc)
```

Example specification of a 2D stencil along K and L axes of a 6D array



Data access pattern of a star-shaped 2D stencil

Example

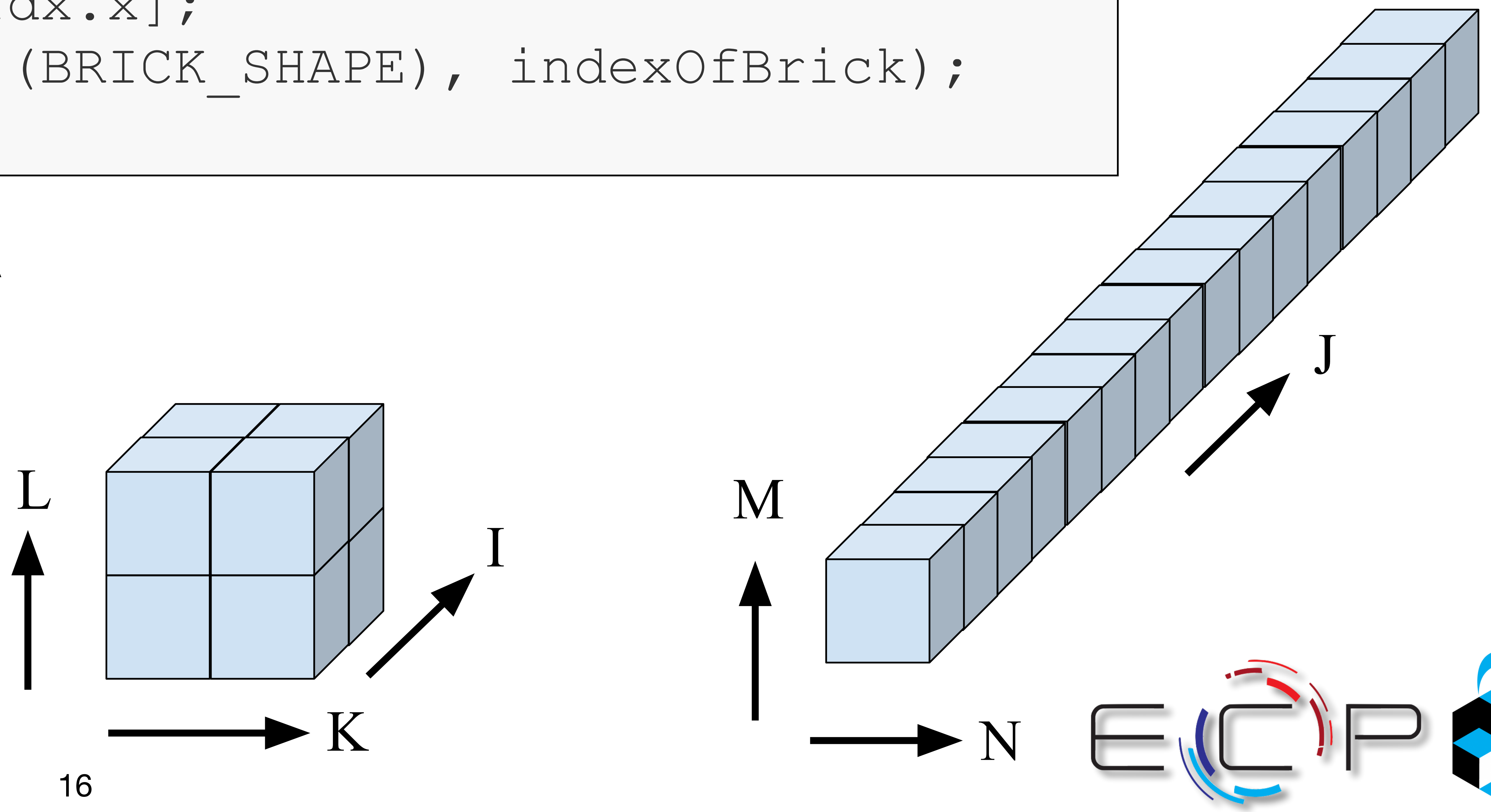
Using Generated Code

```
#define BRICK_SHAPE 1,1,2,2,16,2
//                  N,M,L,K, J,I

__global__ void
starShaped2DStencil(unsigned *brickIndices, // logical -> physical location
                    brick::Brick<BRICK_SHAPE> bIn, // input data
                    brick::Brick<BRICK_SHAPE> bOut, // output data
                    const double coeff[13]) // stencil coefficients
{
  unsigned indexOfBrick = brickIndices[blockIdx.x];
  brick("star_shaped_2d_stencil.py", "CUDA", (BRICK_SHAPE), indexOfBrick);
}
```

Including generated code in C++/CUDA

1 x 1 x 2 x 2 x 16 x 2 6D Brick
with good data reuse properties



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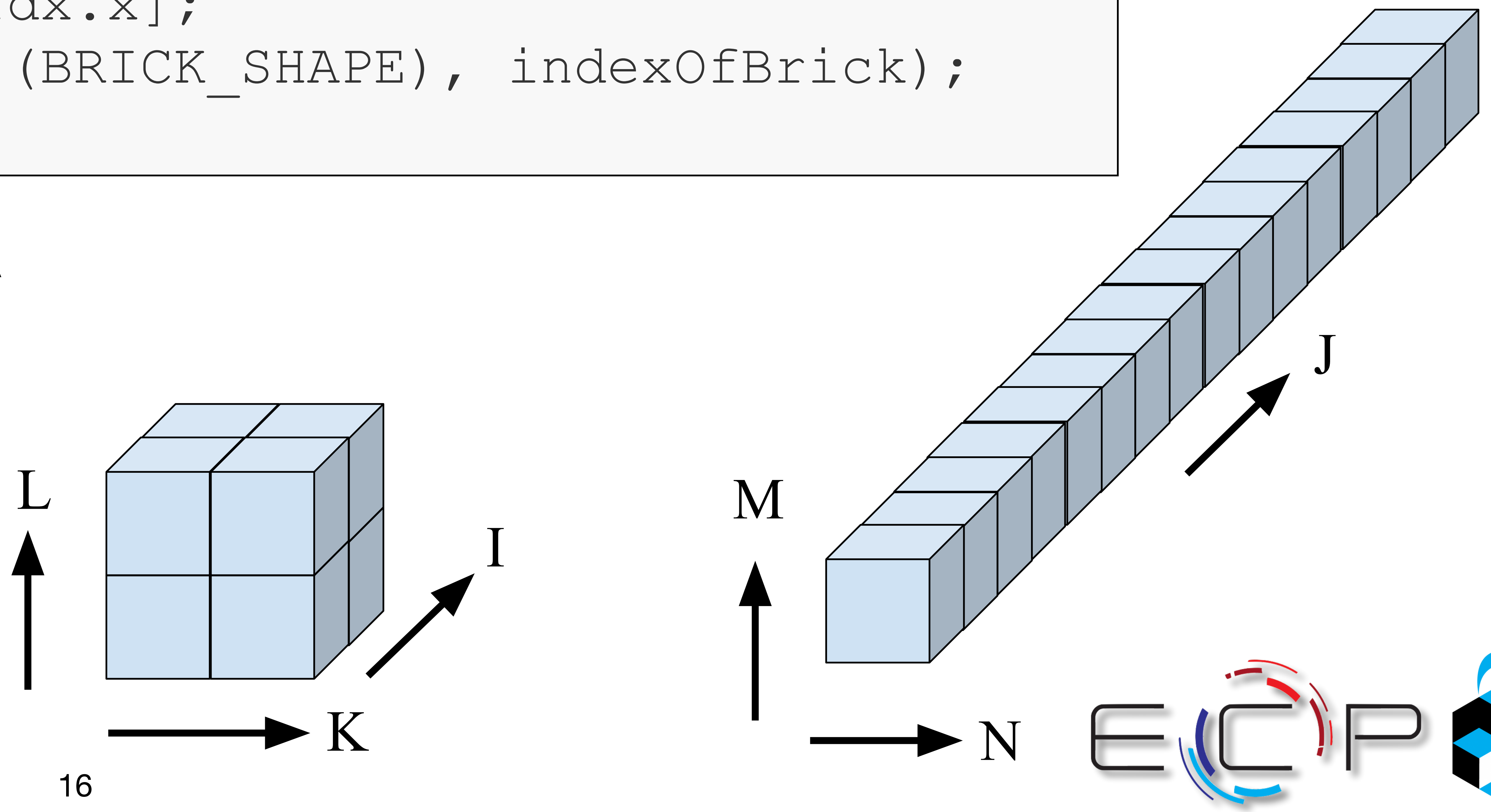

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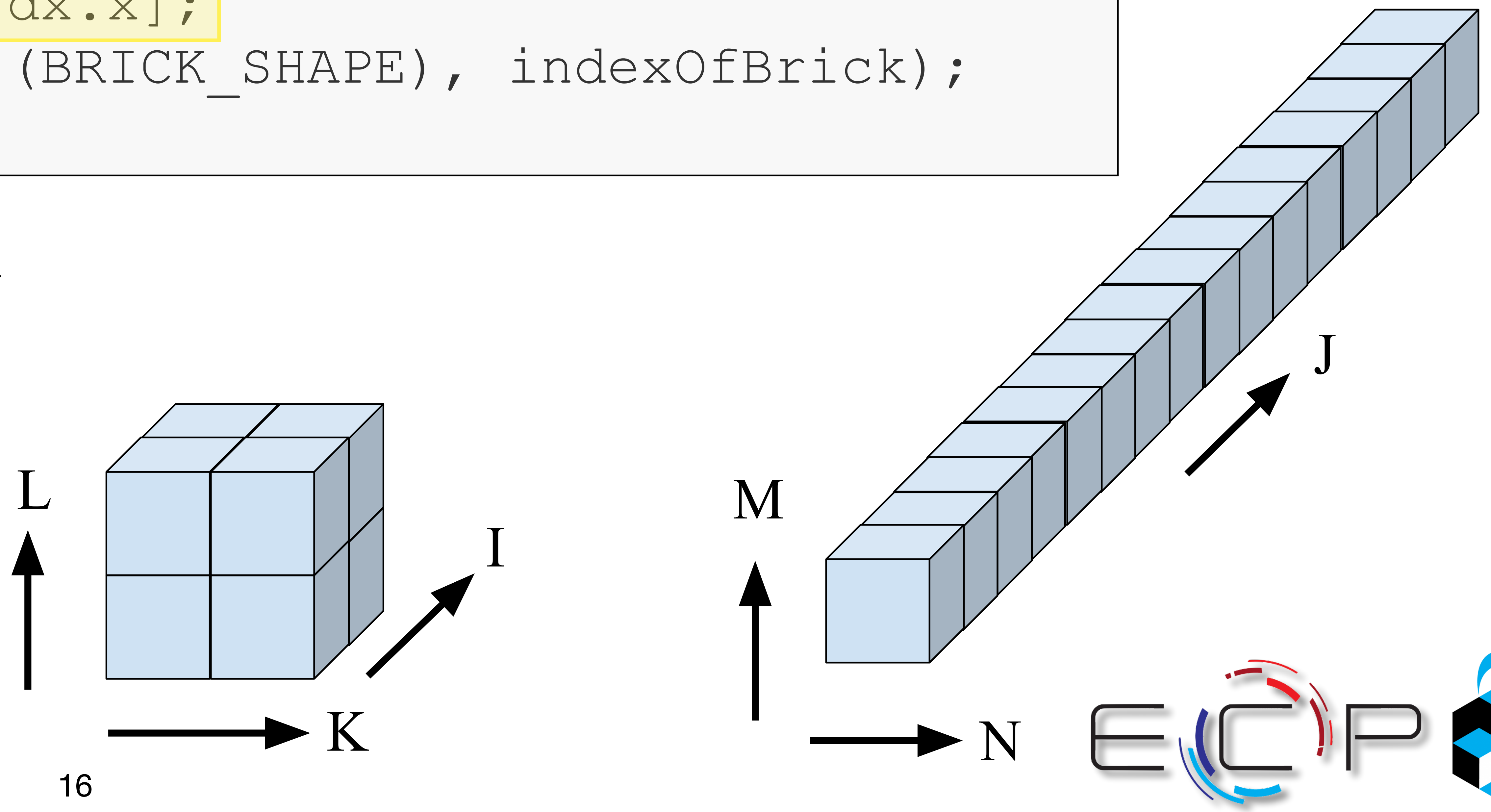

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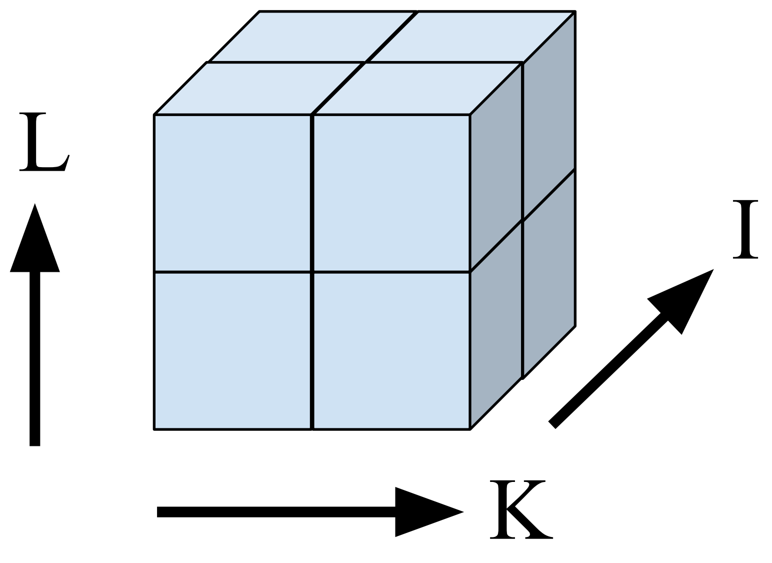
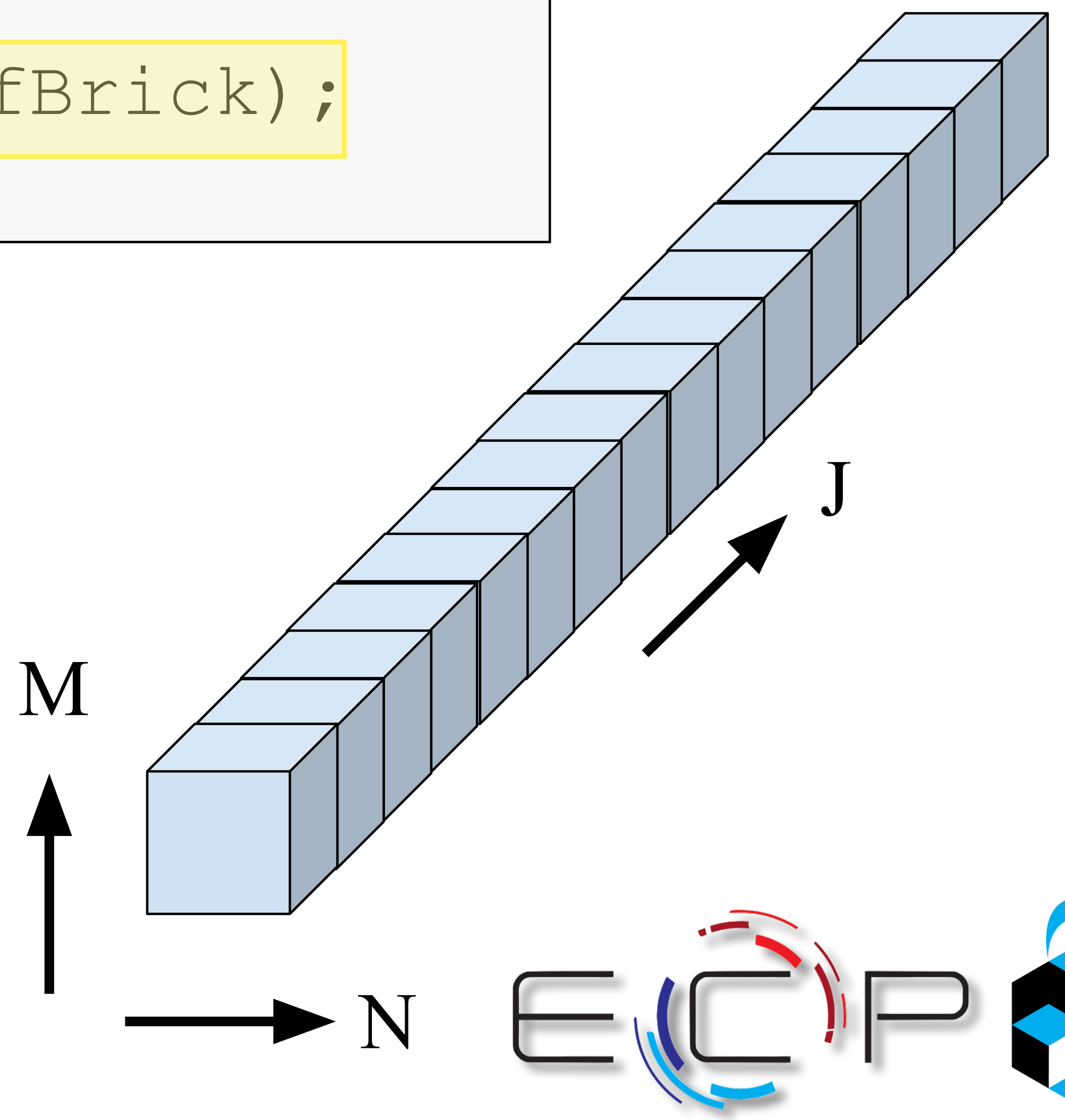


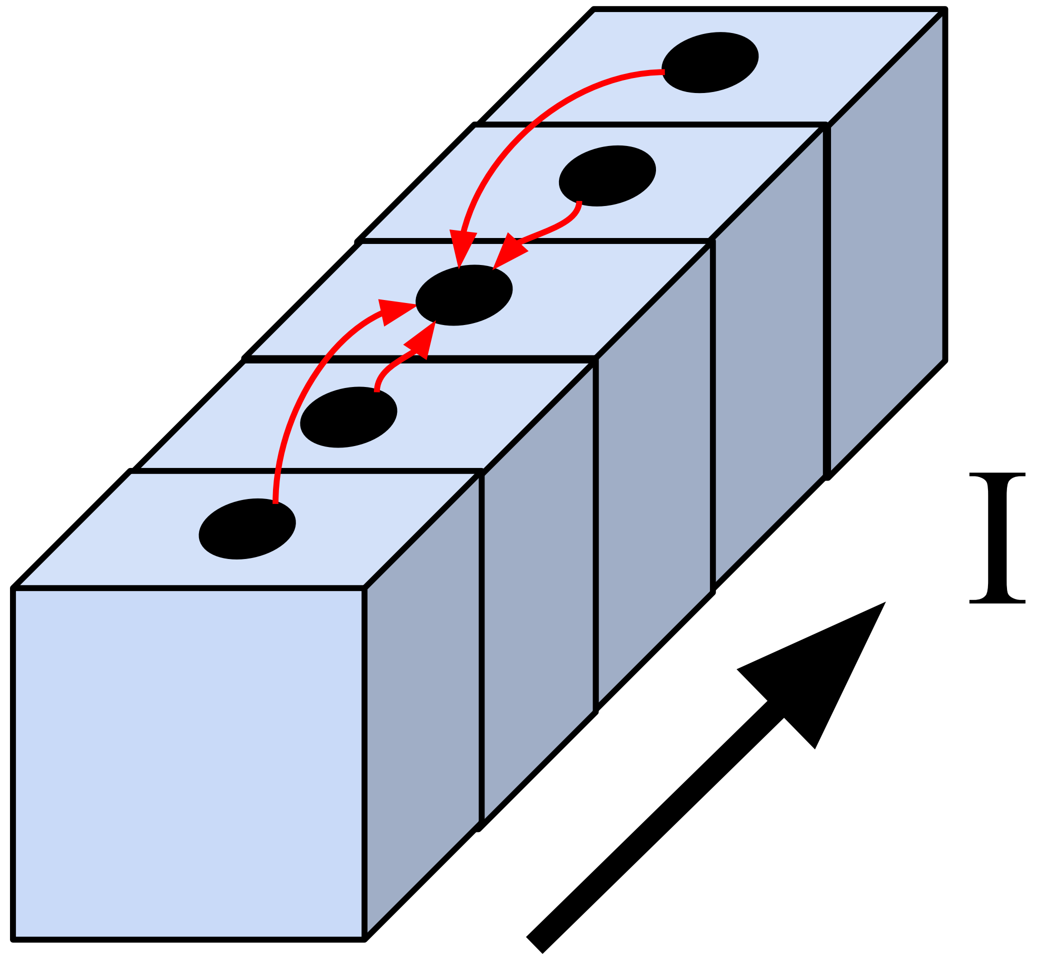


GENE Microbenchmarks

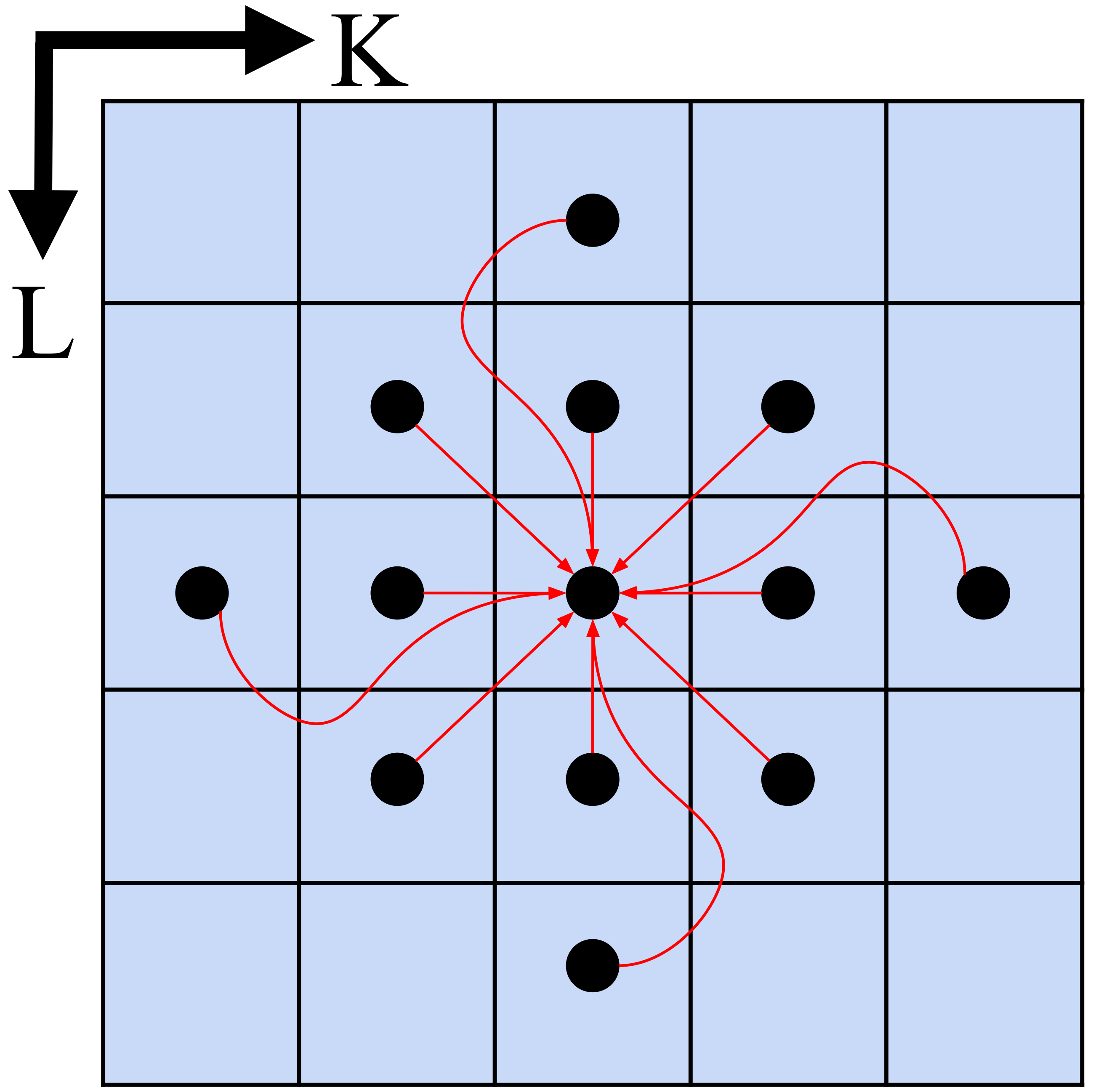
Stencils

GENE Microbenchmarks[4]

- 1D / 2D stencils along 6D arrays
- (1D) 5-point stencil
  - Fused with operations on 5D coefficients (no J-dependence)
- (2D) Arakawa *K-L* stencil
  - 5D coefficients: no J-dependence



Data access pattern of 1D stencil



Data access pattern of 2D stencil

[4][6] Toward exascale whole-device modeling of fusion devices: Porting the GENE gyrokinetic microturbulence code to GPU

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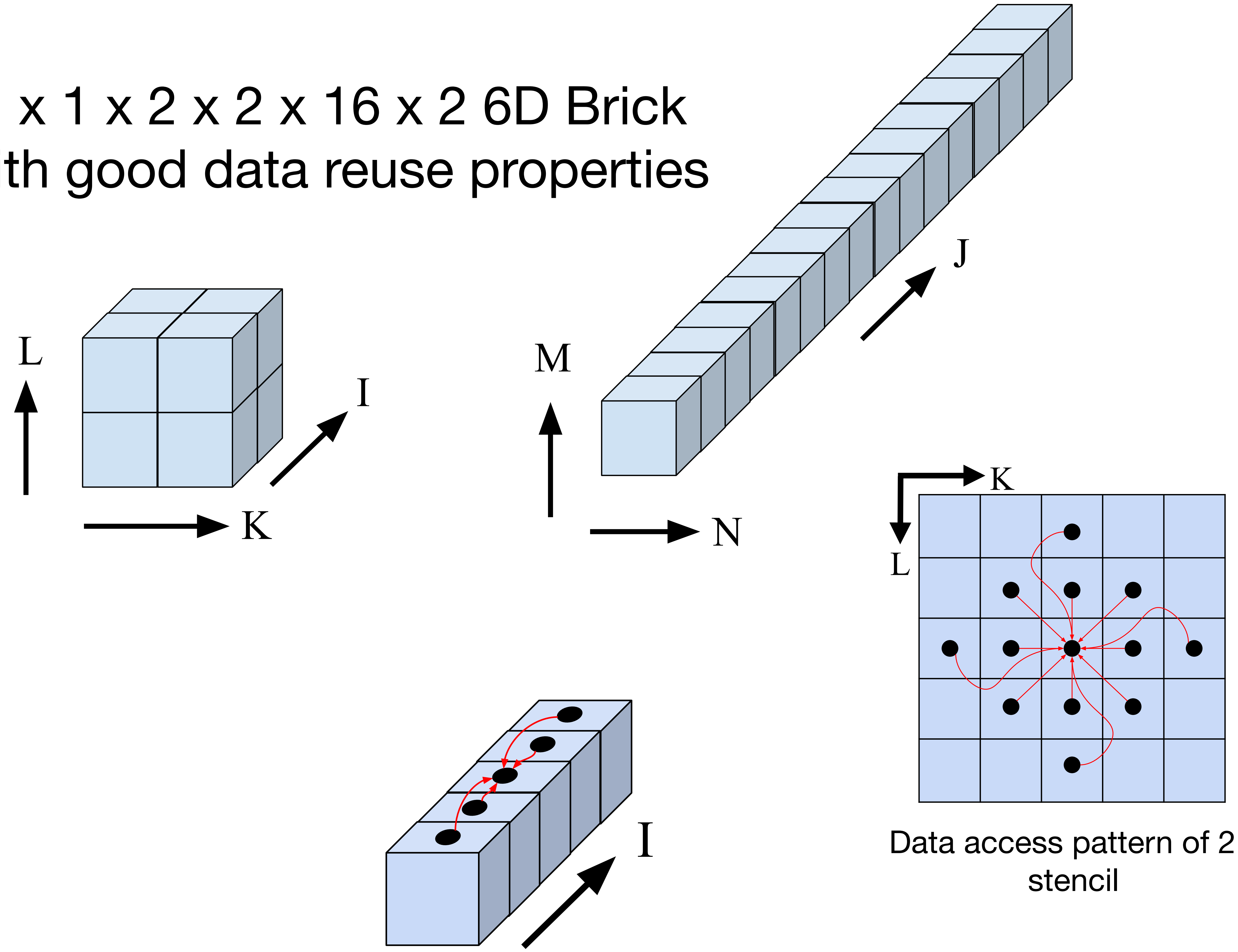

1 x 1 x 2 x 2 x 16 x 2 6D Brick with good data reuse properties

Data access pattern of 2D stencil

Data access pattern of 1D stencil

[4] [Toward exascale whole-device modeling of fusion devices: Porting the GENE gyrokinetic microturbulence code to GPU]

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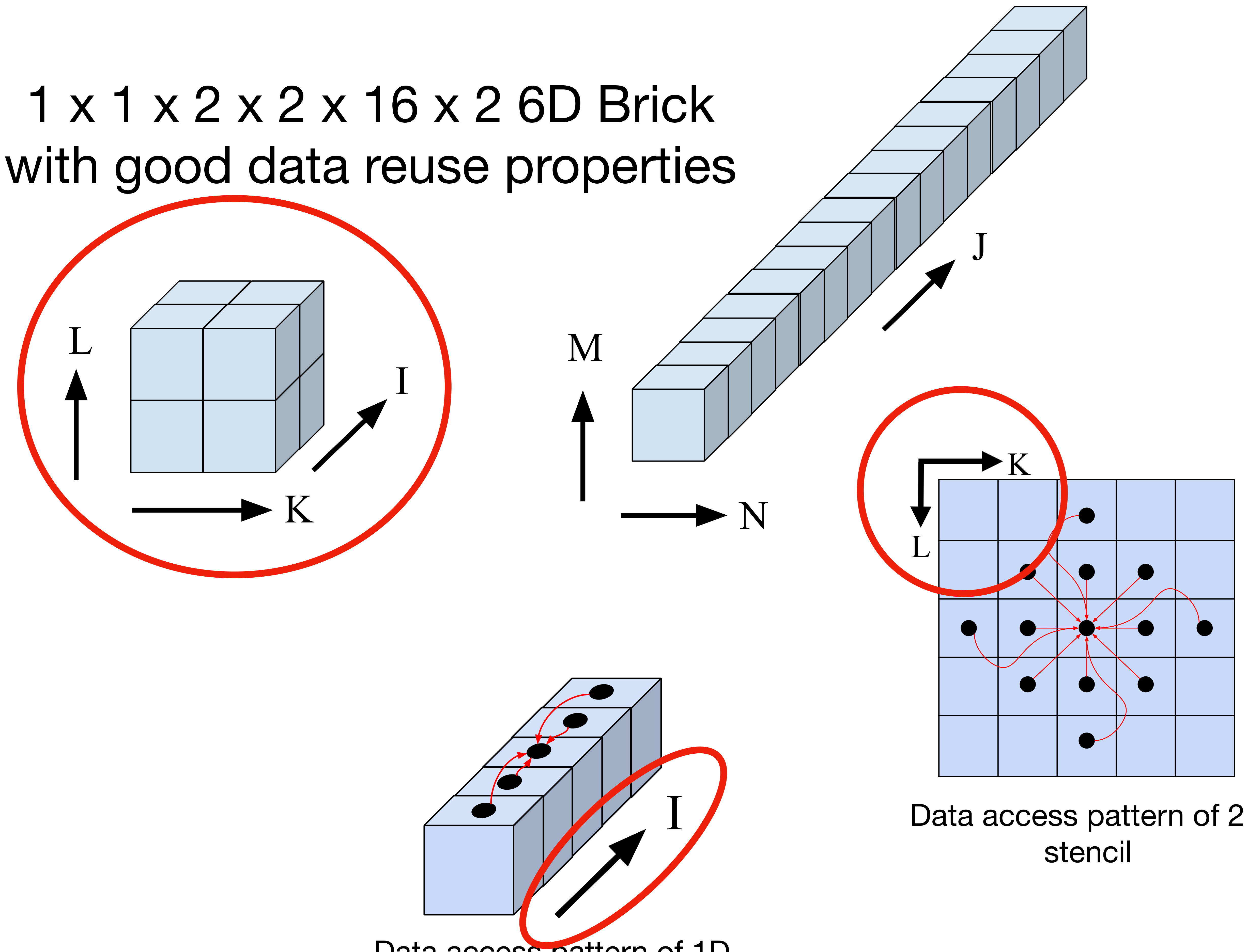

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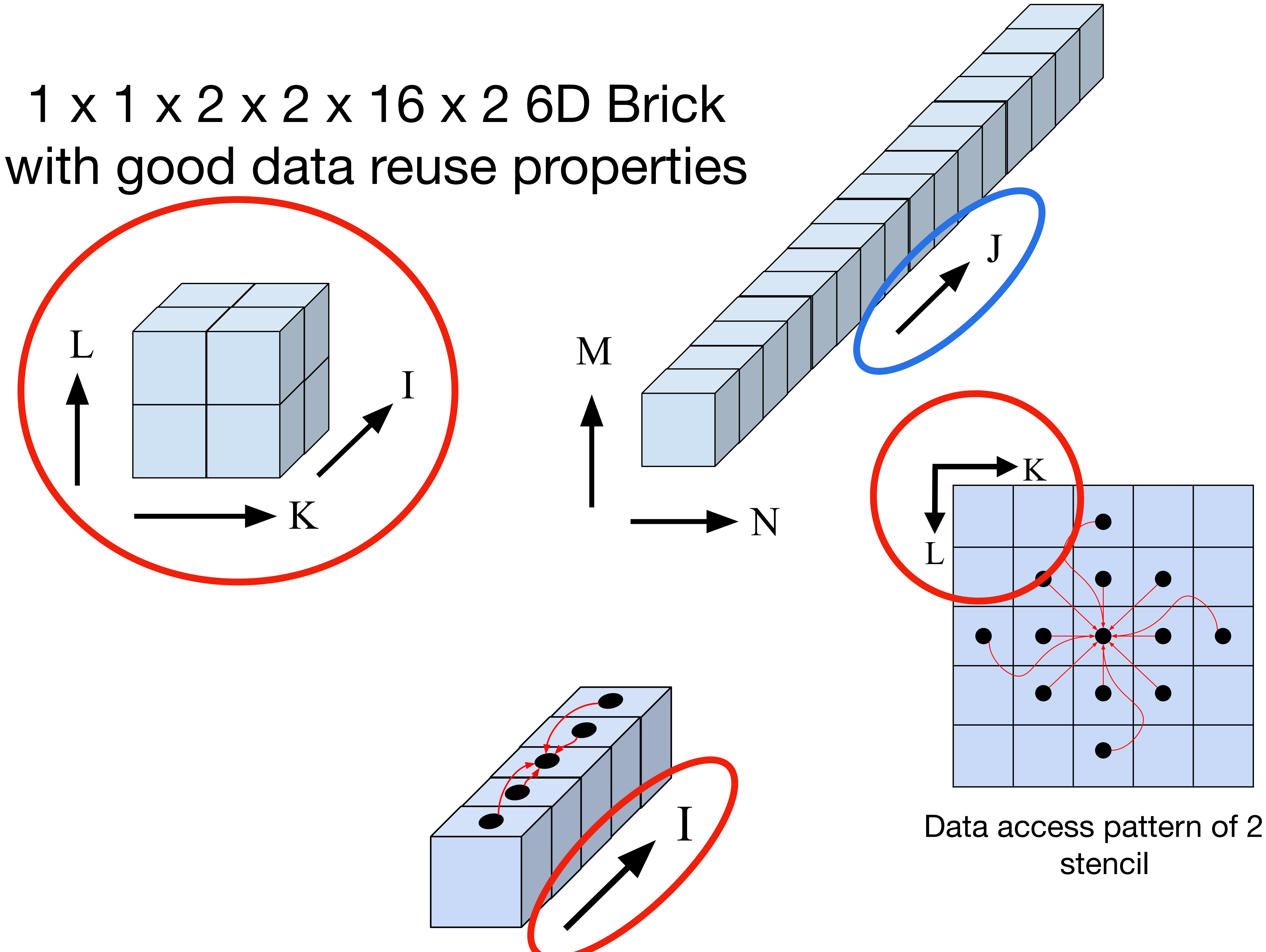

Data access pattern of 2D stencil

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[4]6Toward exascale whole-device modeling of fusion devices: Porting the GENE gyrokinetic microturbulence code to GPU

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Managing Adjacency Lists

- Full adjacency list includes 3^D elements (Δ = -1, 0, or 1 on each axis)

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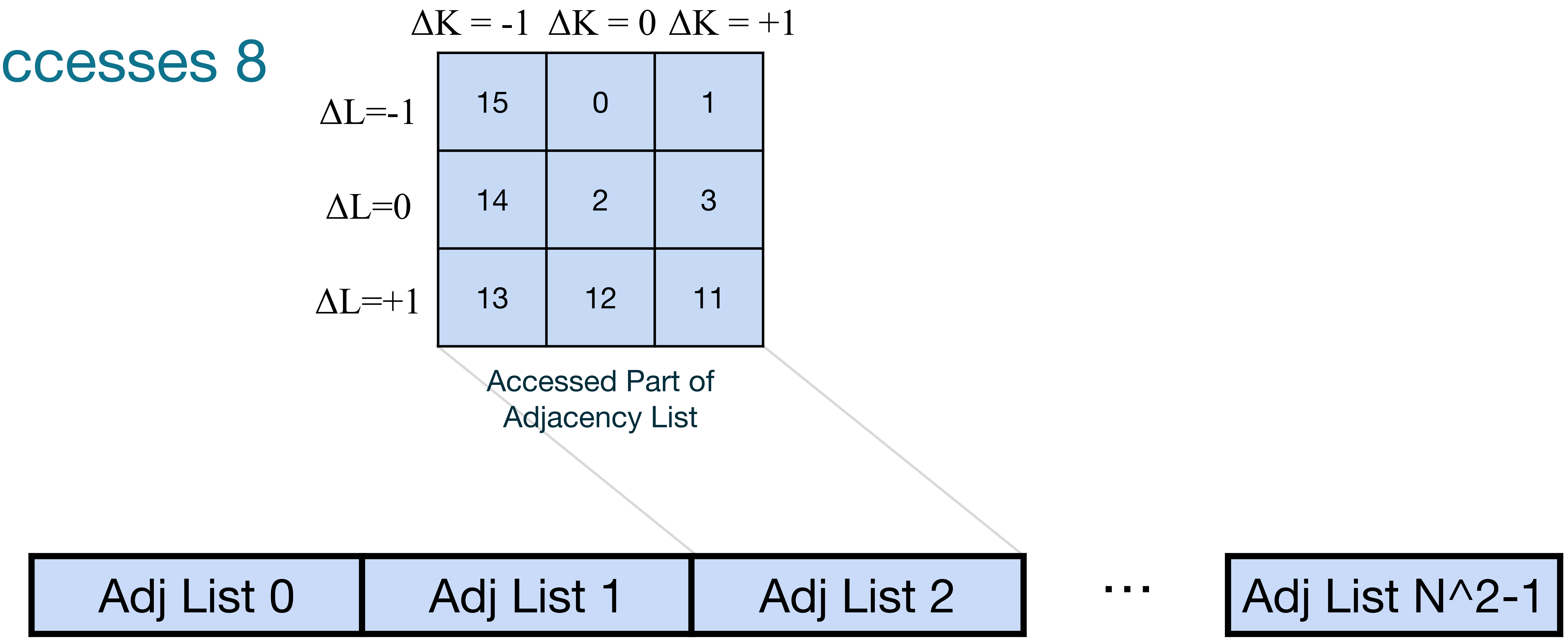


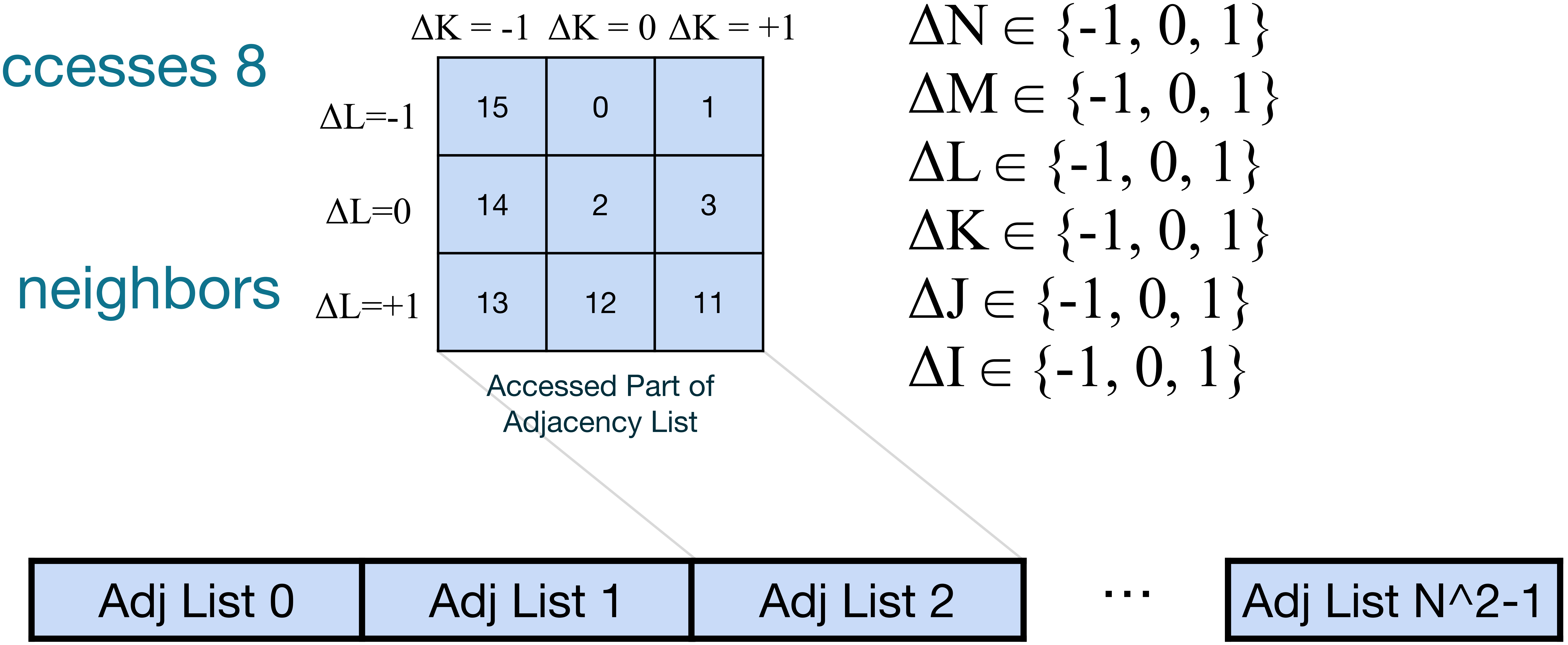
	ΔK = -1	ΔK = 0	ΔK = +1
ΔL=-1	15	0	1
ΔL=0	14	2	3
ΔL=+1	13	12	11

Accessed Part of Adjacency List

Metadata Reduction

Managing Adjacency Lists

- Full adjacency list includes 3^D elements (Δ = -1, 0, or 1 on each axis)
- A 2D stencil in 6D only accesses 8 neighbors (32B)
- Adjacency list holds 729 neighbors (2.9KB)



	$\Delta K = -1$	$\Delta K = 0$	$\Delta K = +1$
$\Delta L = -1$	15	0	1
$\Delta L = 0$	14	2	3
$\Delta L = +1$	13	12	11

Accessed Part of Adjacency List

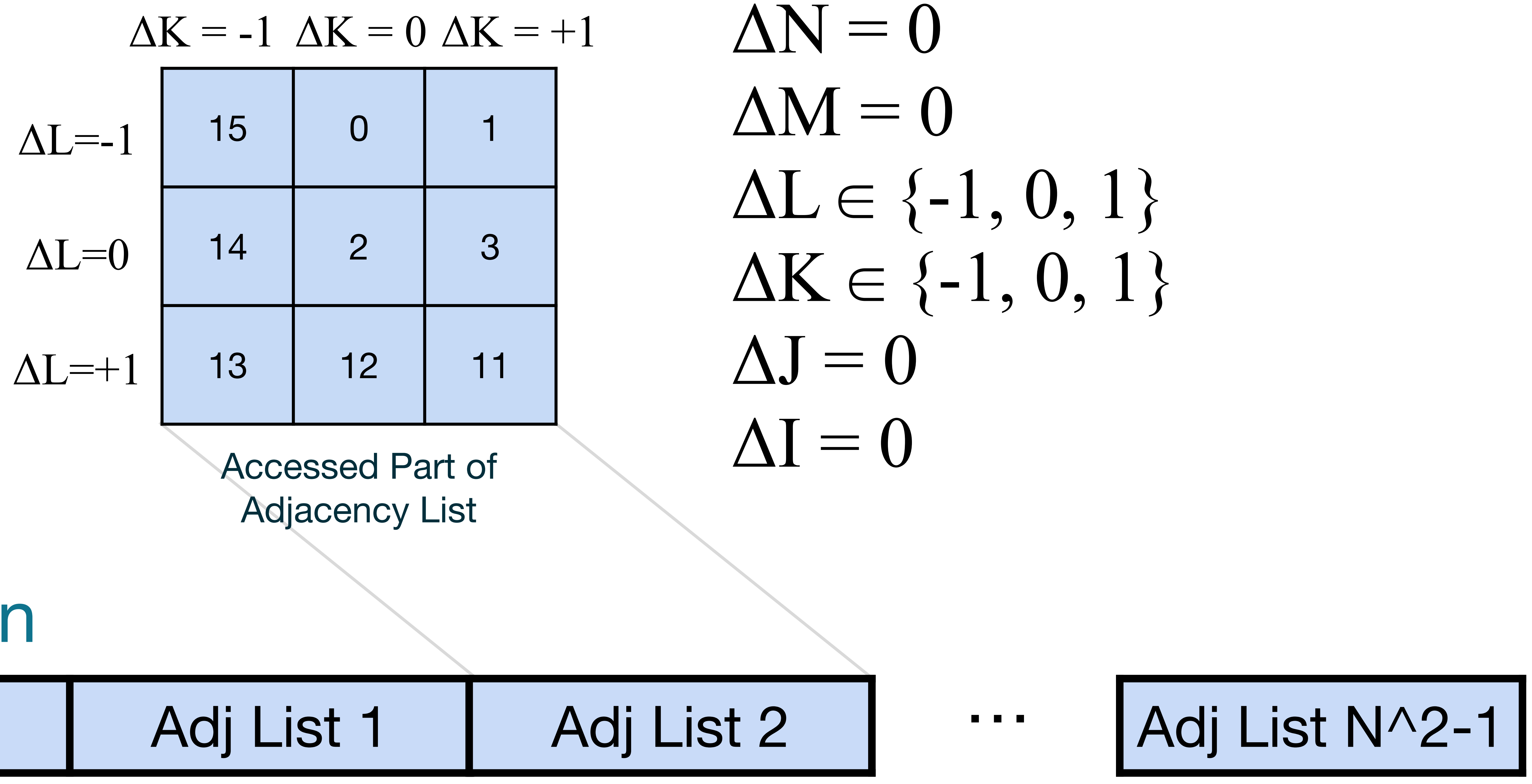
Adj List 0 | Adj List 1 | Adj List 2 | … | Adj List N^2-1

$$\Delta N \in \{-1, 0, 1\}$$
$$\Delta M \in \{-1, 0, 1\}$$
$$\Delta L \in \{-1, 0, 1\}$$
$$\Delta K \in \{-1, 0, 1\}$$
$$\Delta J \in \{-1, 0, 1\}$$
$$\Delta I \in \{-1, 0, 1\}$$

Metadata Reduction

Managing Adjacency Lists

- Full adjacency list includes 3^D elements (Δ = -1, 0, or 1 on each axis)
- A 2D stencil in 6D only accesses 8 neighbors (32B)
- Adjacency list holds 729 neighbors (2.9KB)
- Now users can exclude axes from an adjacency list



	ΔK = -1	ΔK = 0	ΔK = +1
ΔL=-1	15	0	1
ΔL=0	14	2	3
ΔL=+1	13	12	11

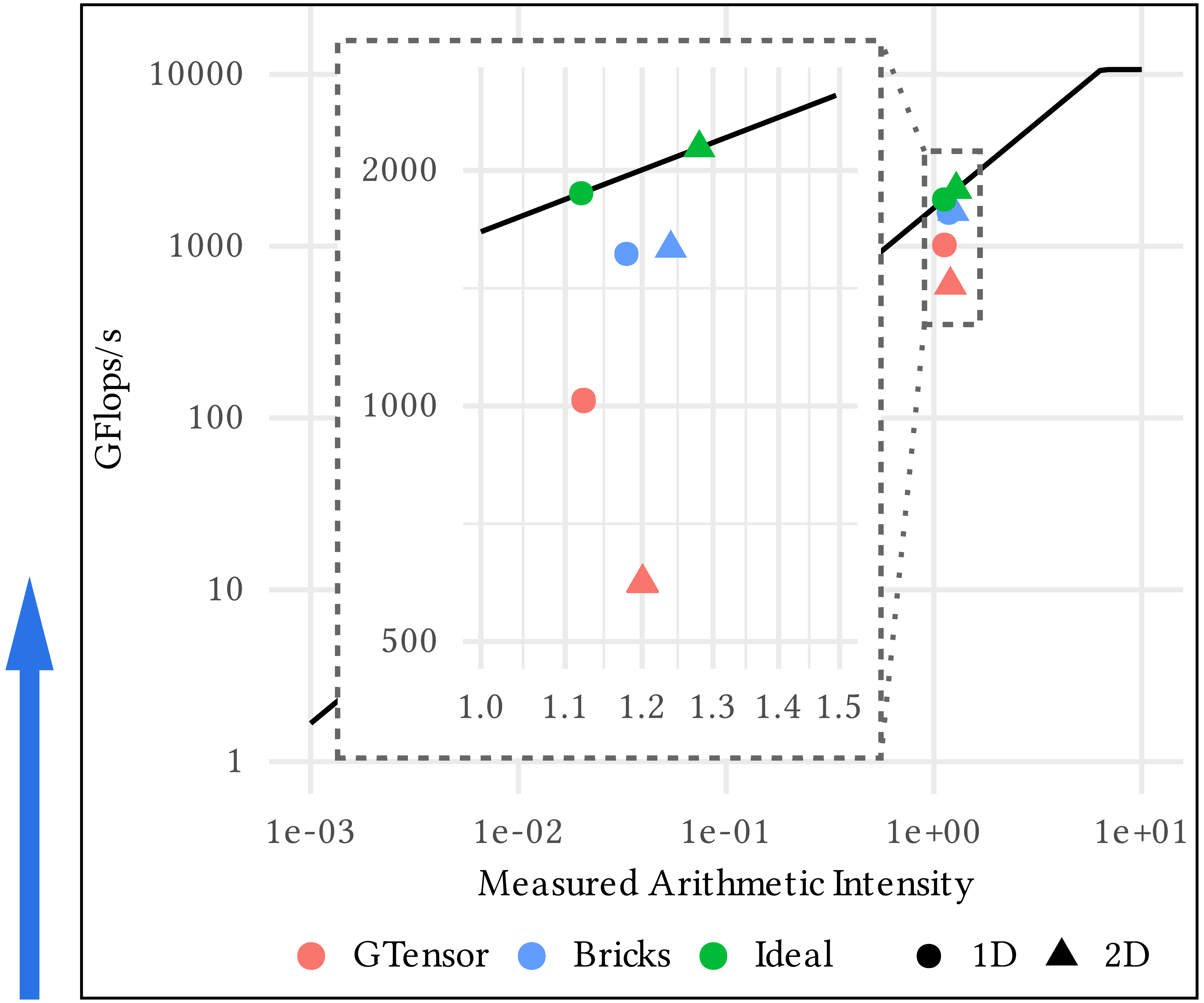
Accessed Part of Adjacency List

$$\Delta N = 0$$
$$\Delta M = 0$$
$$\Delta L \in \{-1, 0, 1\}$$
$$\Delta K \in \{-1, 0, 1\}$$
$$\Delta J = 0$$
$$\Delta I = 0$$

Stencils

Results

- NVIDIA A100 GPUs on Perlmutter
- 3.2% (2D) / 4.9% (1D) increase in arithmetic intensity
- 2.67x (2D) / 1.54x (1D) increase in GStencil/s
- Lower occupancy → increased L1 efficiency

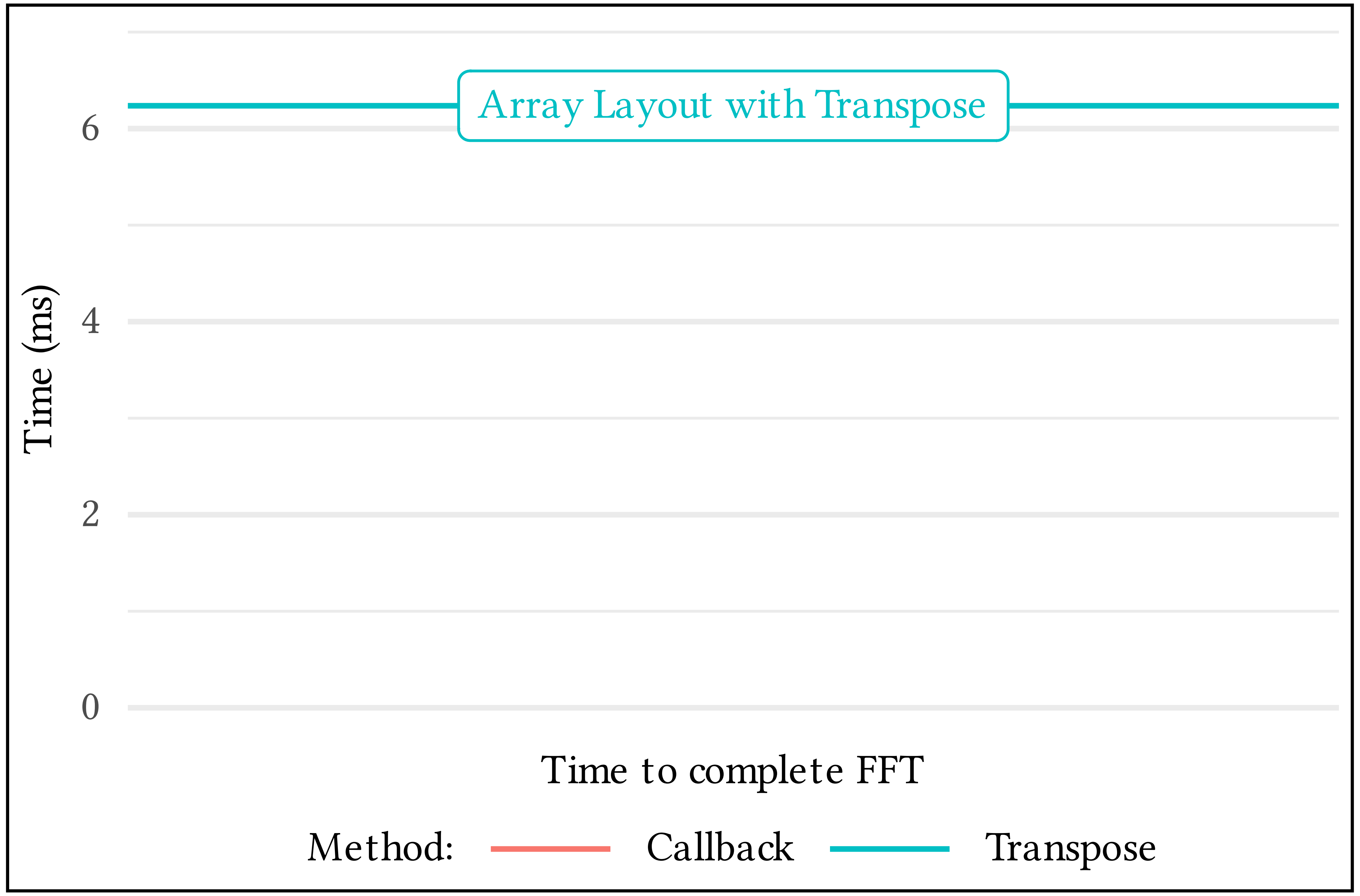


Higher is better

FFT

cuFFT for Bricks

- cuFFT along J-axis requires either:
  - Transpose I-J



Lower is better

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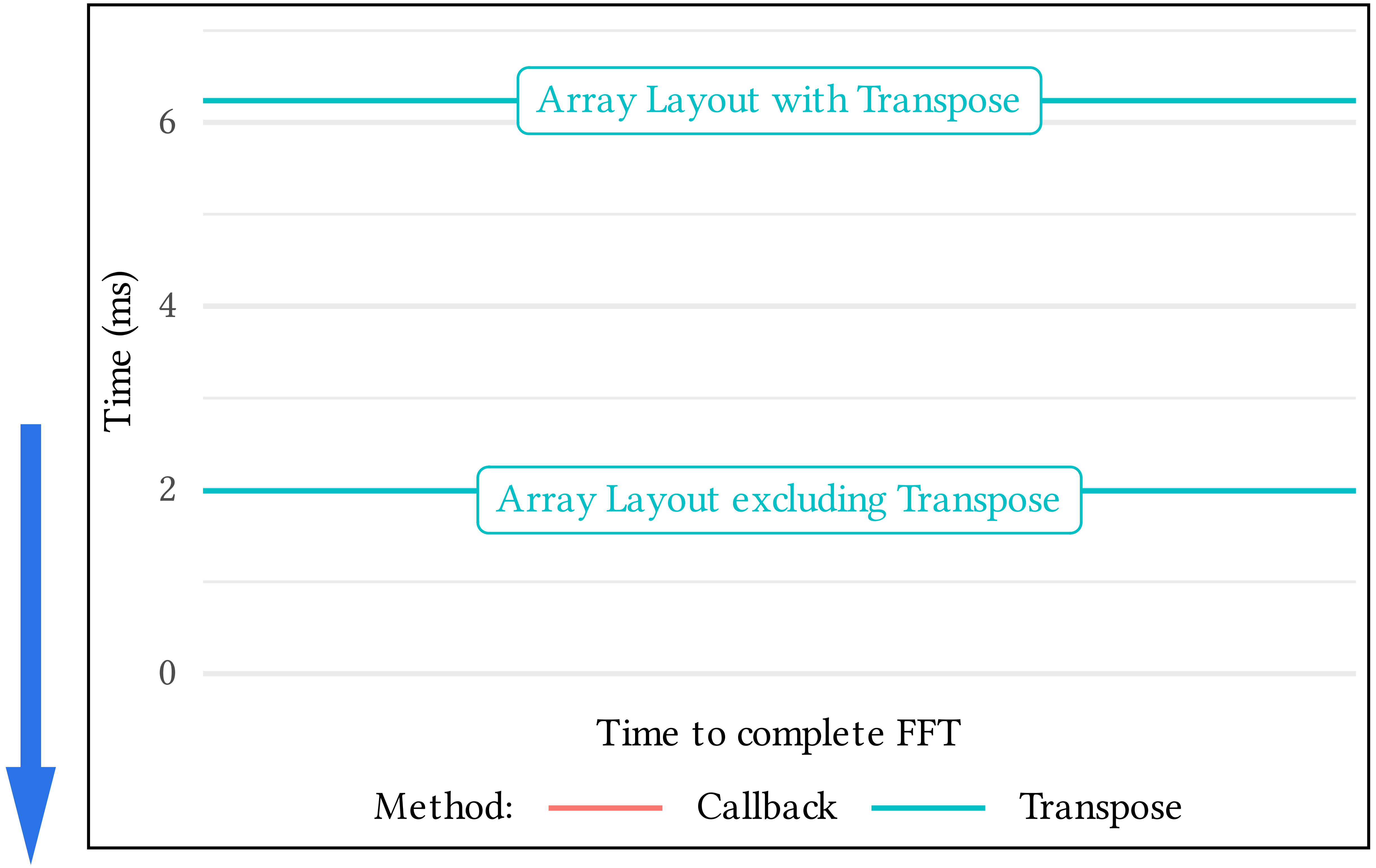
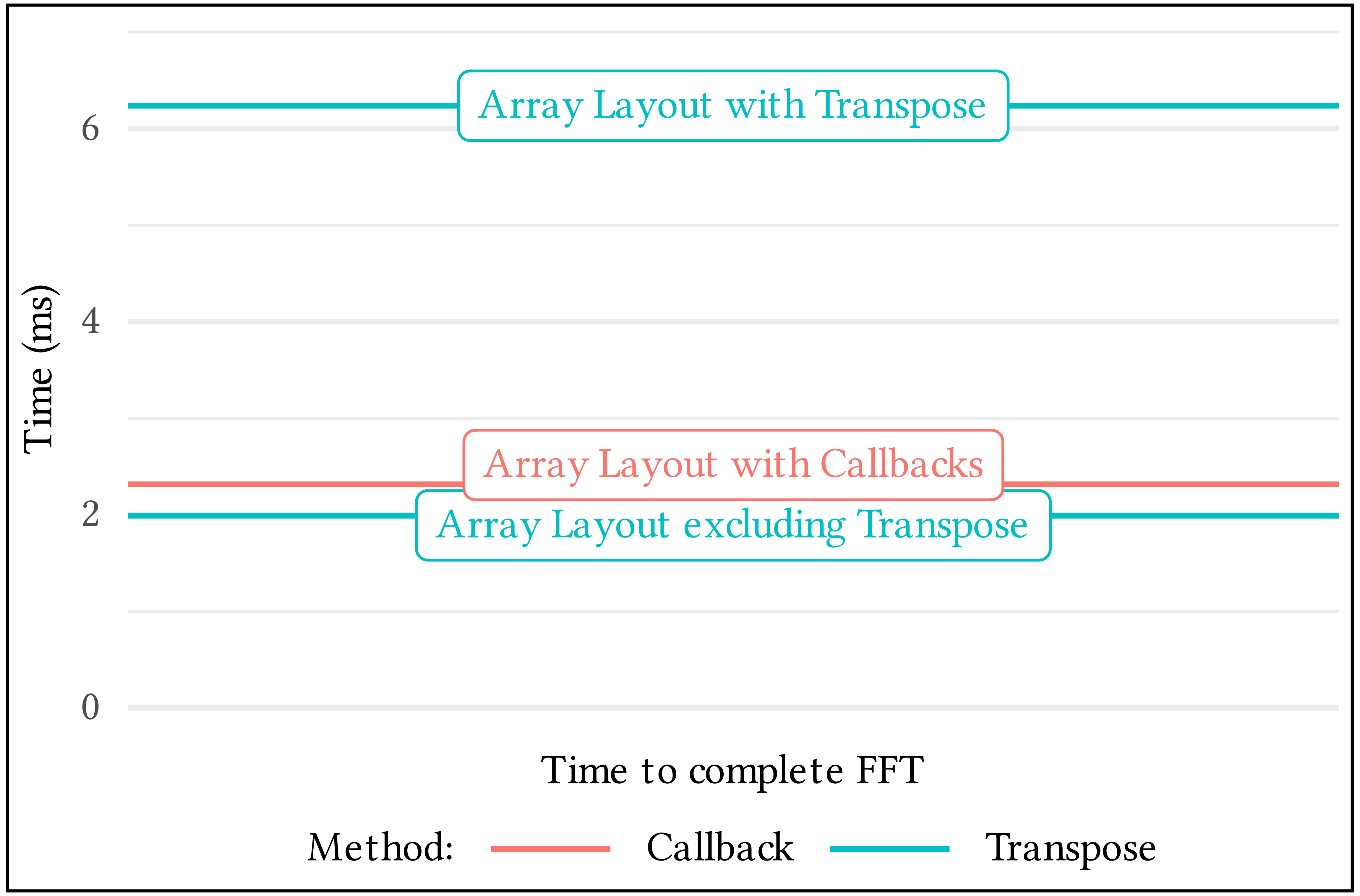


Lower is better

FFT

cuFFT for Bricks

- cuFFT along J-axis requires either:
  - Transpose I-J
  - User-defined callbacks

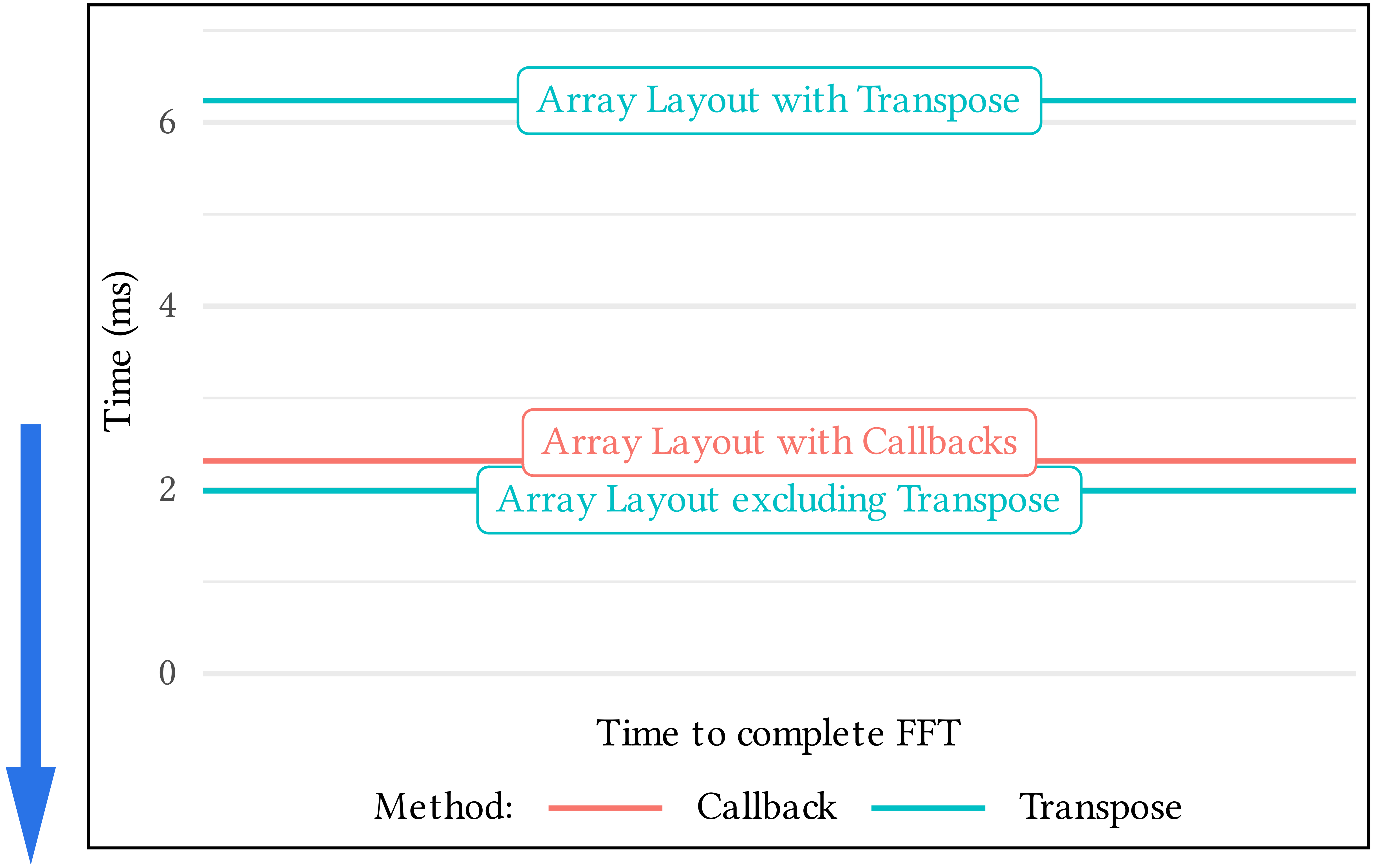


Lower is better

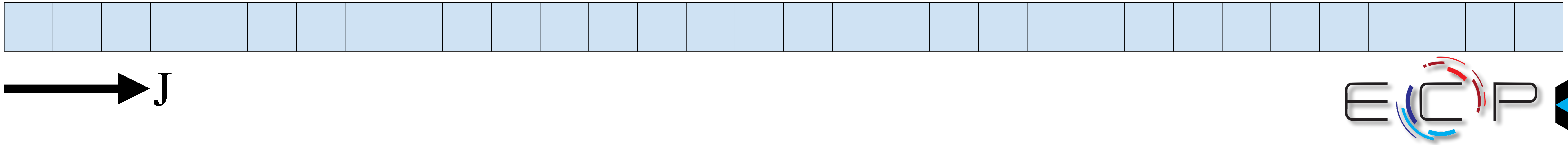
FFT

cuFFT for Bricks

- cuFFT along J-axis requires either:
  - Transpose I-J
  - User-defined callbacks
- Bricks implementation creates callbacks using C++ templates



Lower is better



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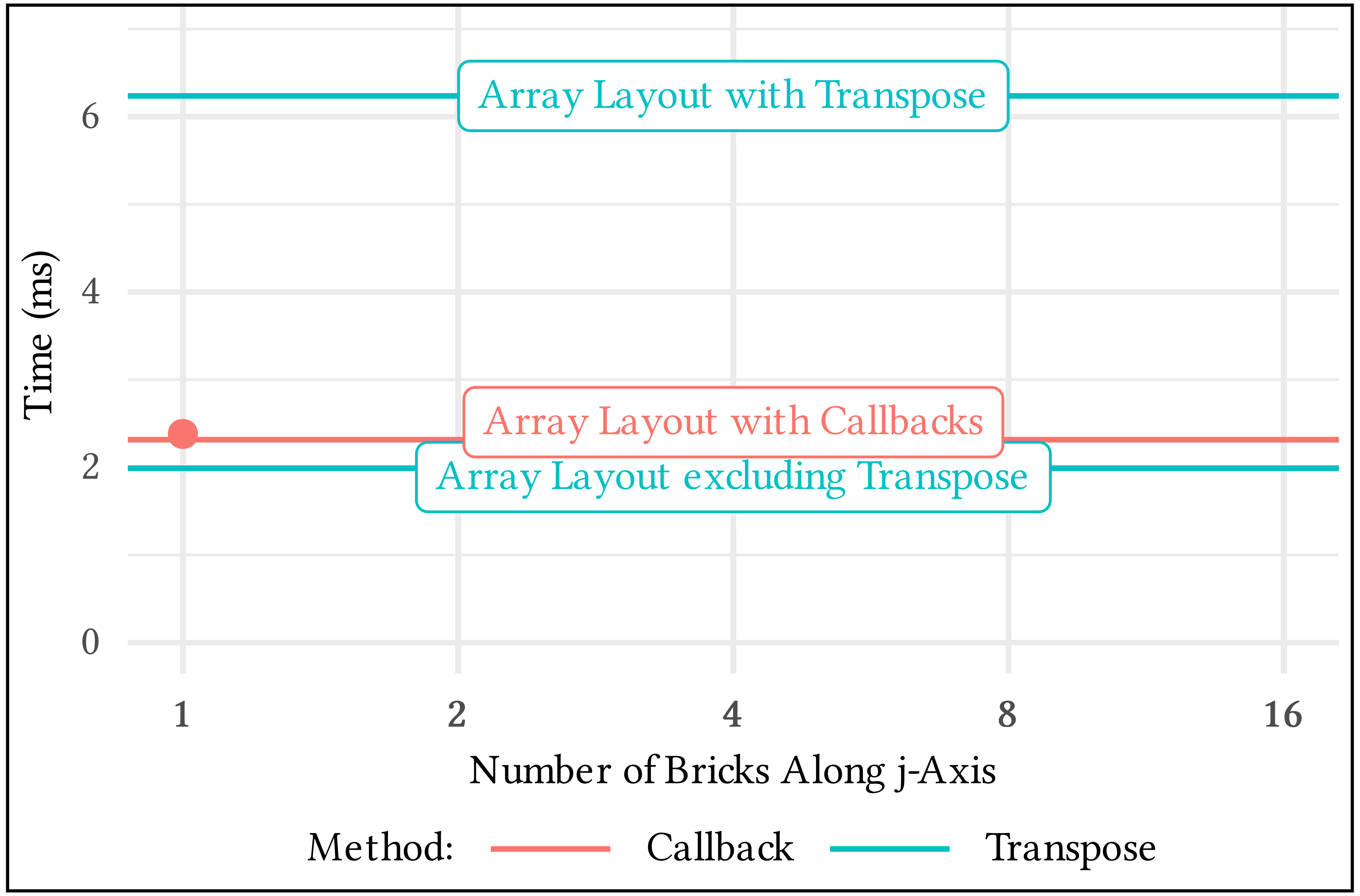
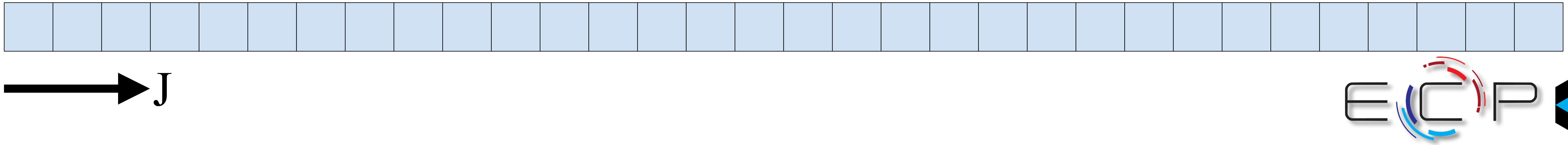


Lower is better



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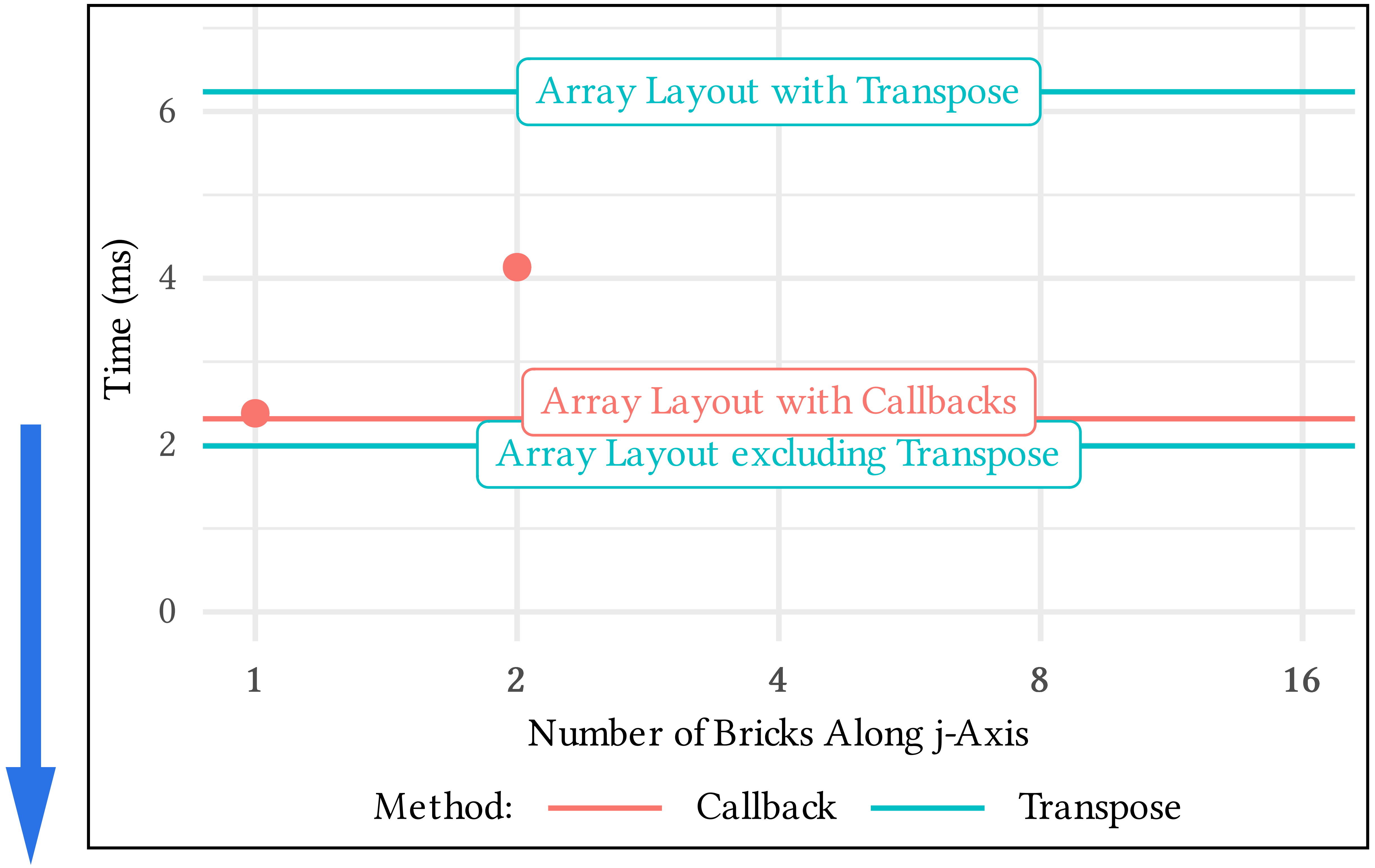
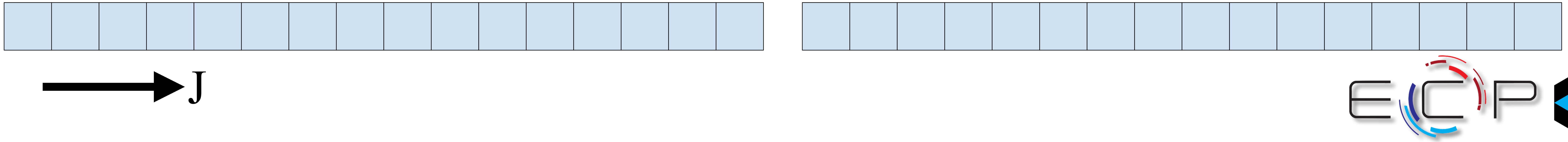


Lower is better



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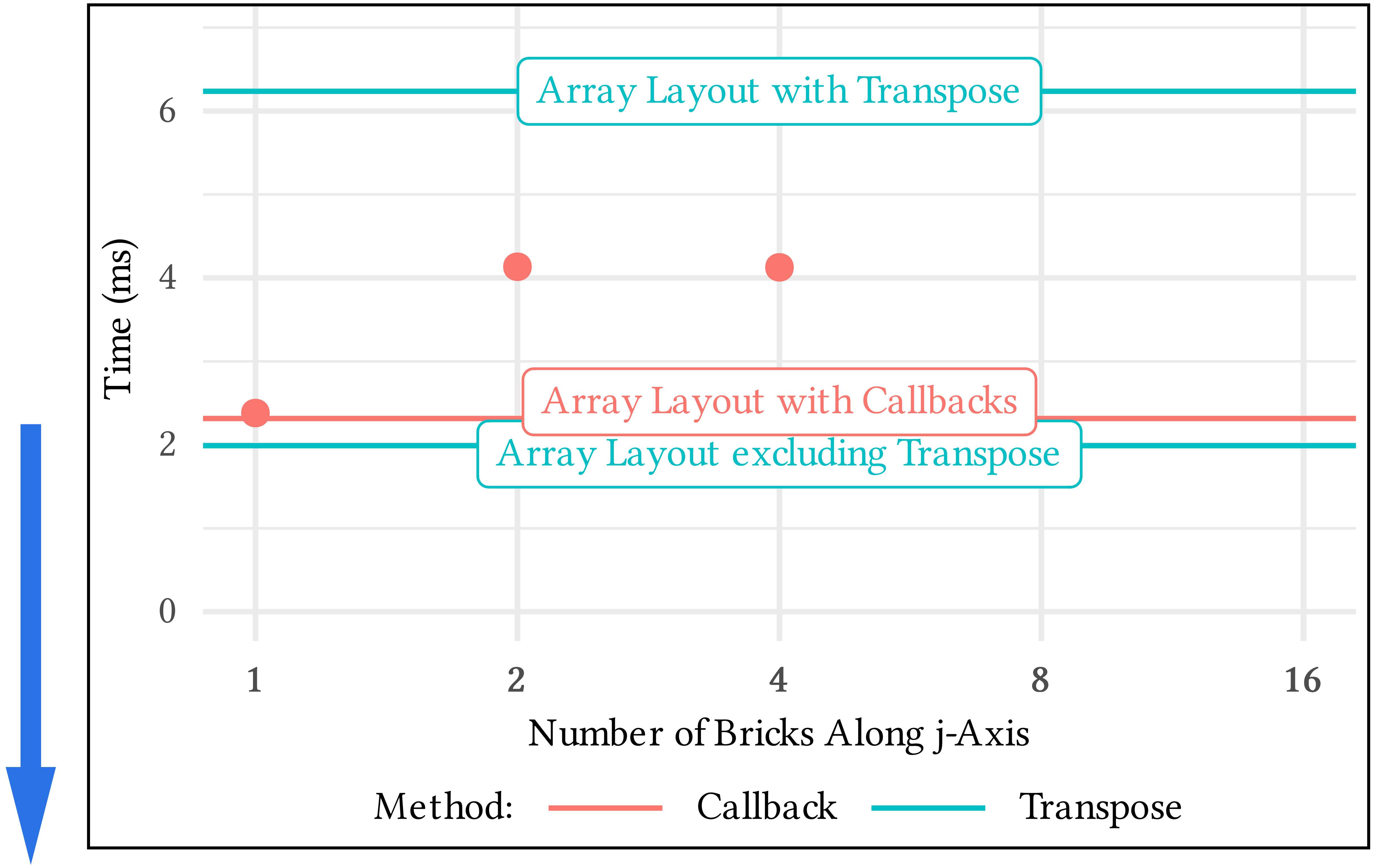
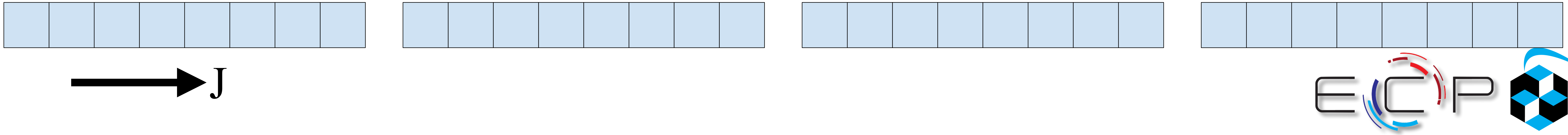


Lower is better



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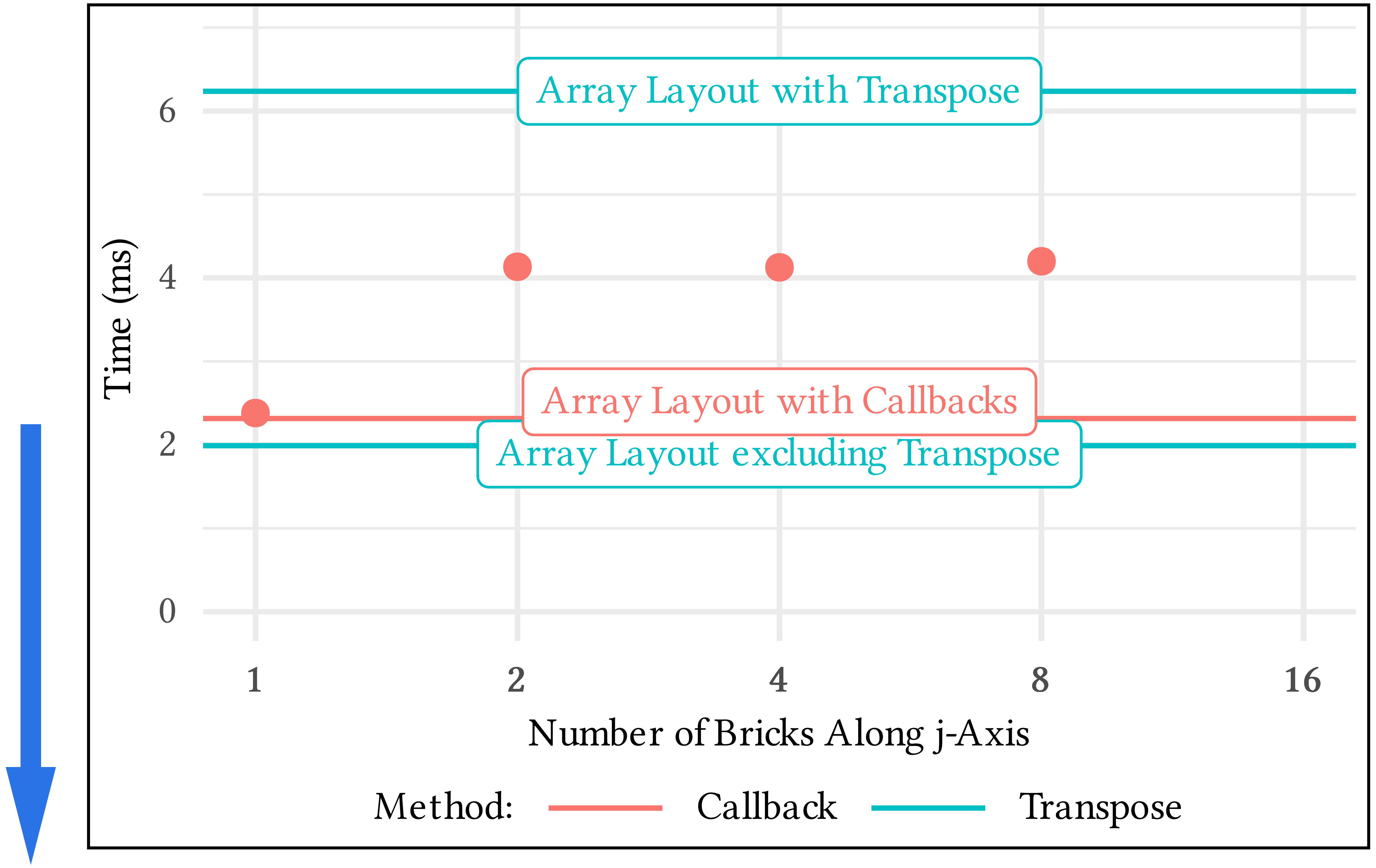
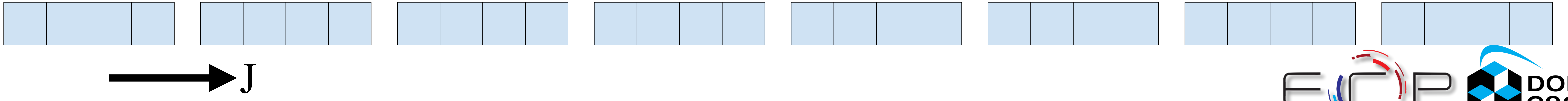


Lower is better



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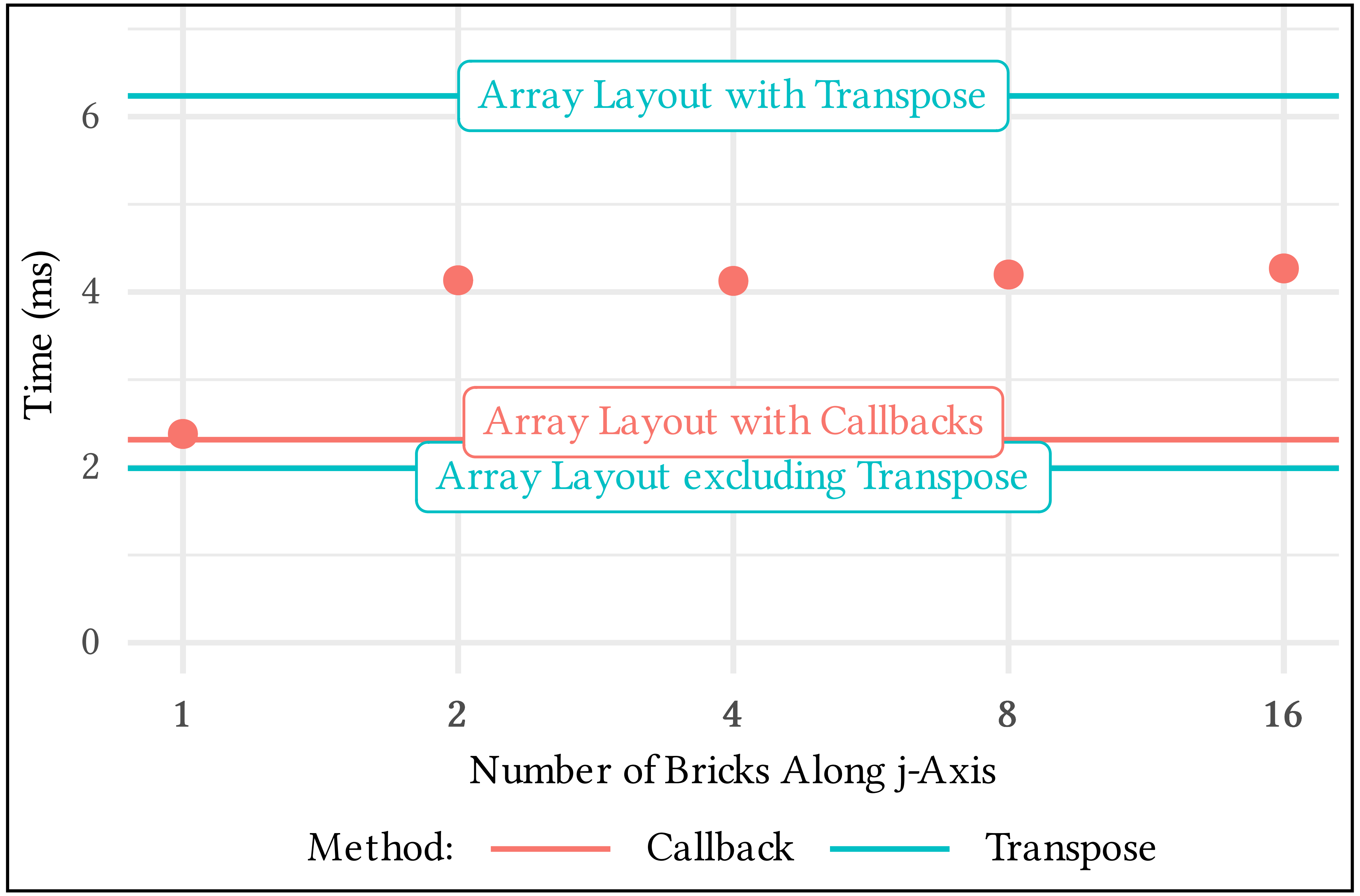
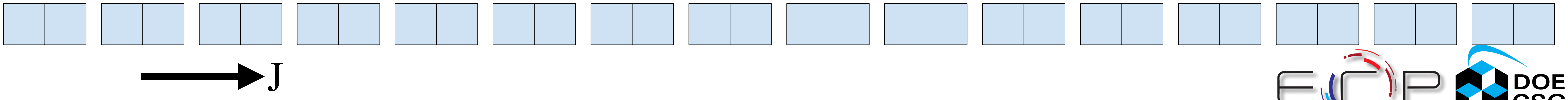


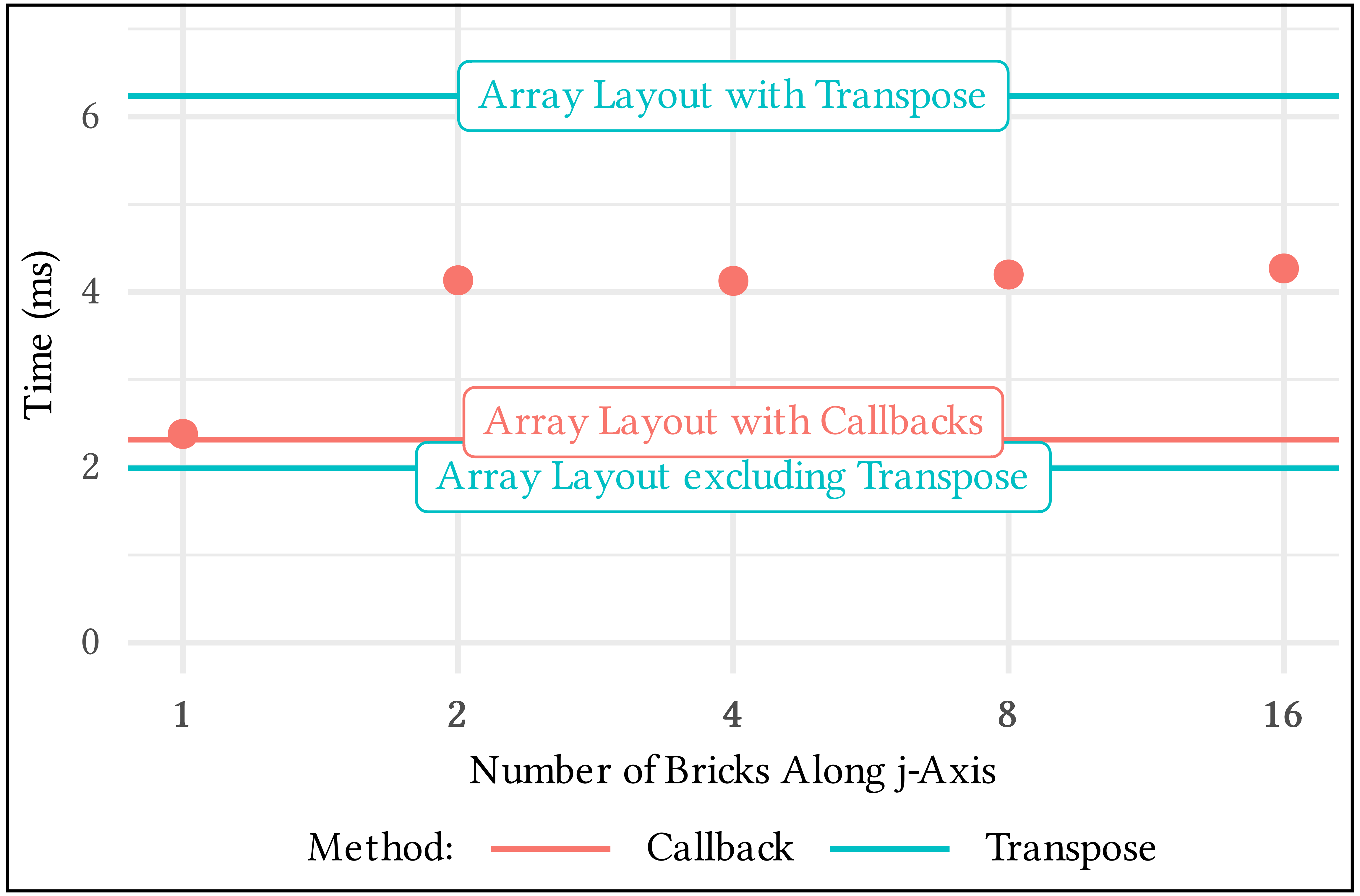
Lower is better



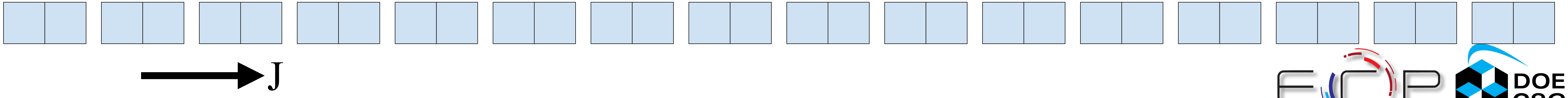
FFT

cuFFT for Bricks

- cuFFT along J-axis requires either:
  - Transpose I-J
  - User-defined callbacks
- Bricks implementation creates callbacks using C++ templates
- Slowdown 1.83x-1.93x moving from 1 Brick/FFT → 16 Bricks/FFT



Lower is better



Summary

- We extended the Bricks layout/library to efficiently handle high-dimensional layouts, complex types, and FFT computations on GPUs

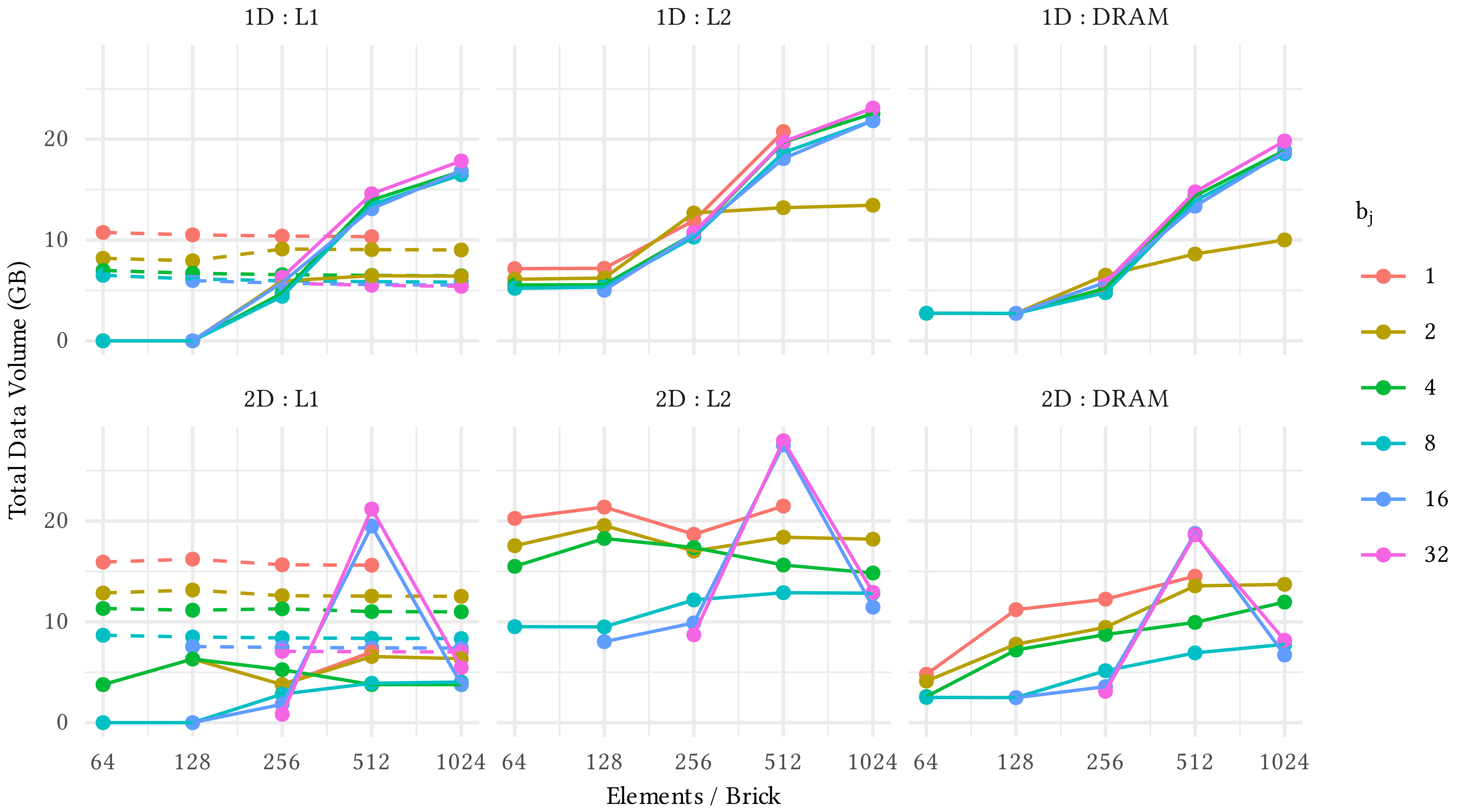
- Bricks can navigate trade-offs in high-dimensional settings by tuning Brick shape

- **Moving Forward:** Other high-dimensional applications such as QCD, custom Bricks solutions to FFTs and other non-stencil operations

Backup Slides

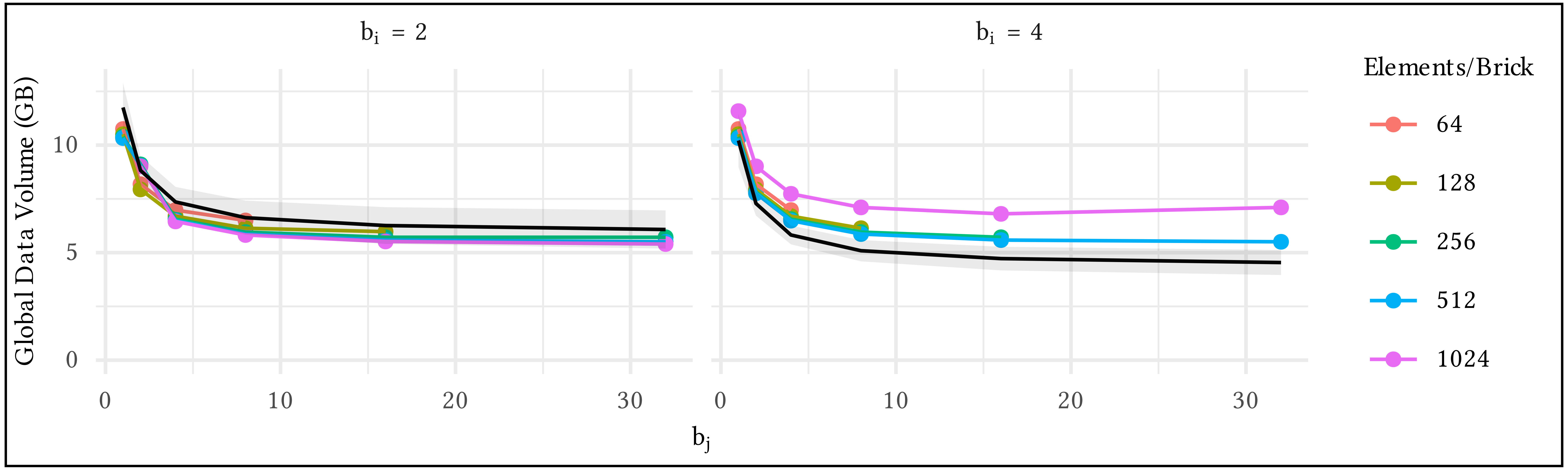
Tuning Bricks

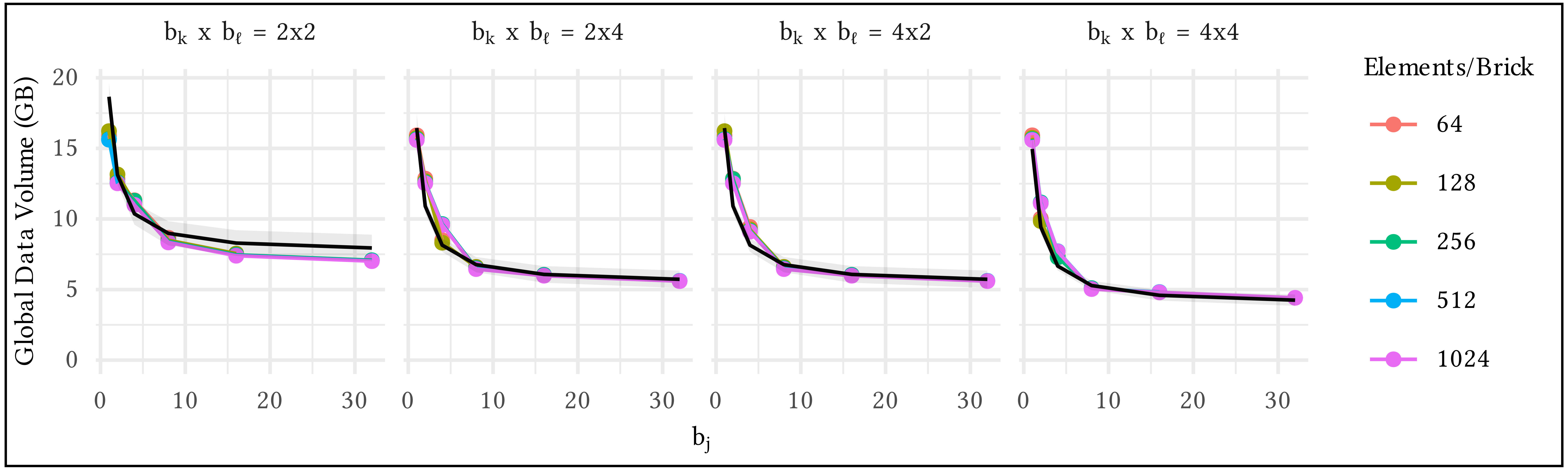
Hardware Resource Usage



Tuning Bricks

Bricks Shape


b_i = 2
b_i = 4
Global Data Volume (GB)
b_j
Elements/Brick


b_k x b_ℓ = 2x2
b_k x b_ℓ = 2x4
b_k x b_ℓ = 4x2
b_k x b_ℓ = 4x4
Global Data Volume (GB)
b_j
Elements/Brick