Research Presentation for Computer Modelling Group Ltd.

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Outline

- Convolutions
  - Implicitly Dealiased FFT-based convolutions
  - Shared-memory implementation
  - Parallel `OpenMP`/`MPI` implementation
  - Pseudospectral simulations
- `GPU` programming
  - `OpenCL`
  - `schnaps`
  - Performance analysis.

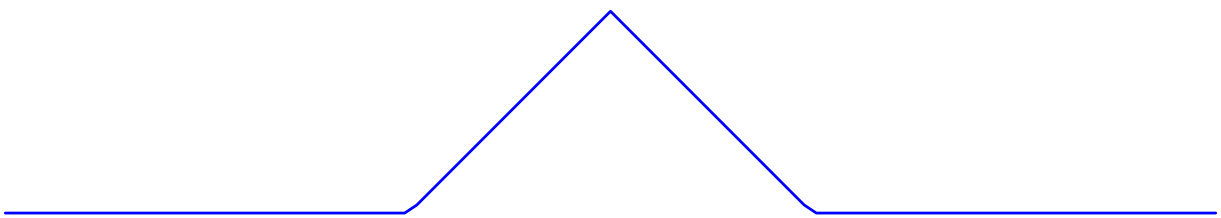
FFT-based convolutions

The convolution of $\{F_k\}_{k=0}^{m-1}$ and $\{G_k\}_{k=0}^{m-1}$ is

$$(F \star G)_k = \sum_{\ell=0}^{k} F_\ell G_{k-\ell}, \quad k=0, \ldots, m-1. \tag{1}$$

For example, if F and G are:

Then $F * G$ is:



FFT-based convolutions

Applications:

- Signal processing
- Machine learning: convolutional neural networks
- Image processing
- Particle-Image-Velocimitry
- Pseudospectral simulations of nonlinear PDEs

The convolution theorem:

$$\mathcal{F}\left[F * G\right] = \mathcal{F}\left[F\right] \odot \mathcal{F}\left[G\right]. \tag{2}$$

Using FFTs improves speed and accuracy.

FFT-based convolutions

Let $\zeta_m = \exp\left(\frac{2\pi i}{m}\right)$. Forward and backward Fourier transforms are given by:

$$f_j = \sum_{k=0}^{m-1} \zeta_m^{jk} F_k, \qquad F_k = \frac{1}{m} \sum_{j=0}^{m-1} \zeta_m^{-kj} f_k, \tag{3}$$

We will use the identity

$$\sum_{j=0}^{m-1} \zeta_m^{\ell j} = \begin{cases} m & \text{if } \ell = sm \text{ for } s \in \mathbb{Z}, \\ \frac{1-\zeta_m^{\ell m}}{1-\zeta_m^m} = 0 & \text{otherwise.} \end{cases} \tag{4}$$

FFT-based convolutions

The convolution theorem works because

$$\begin{aligned}\sum_{j=0}^{m-1} f_j g_j \zeta_m^{-jk} &= \sum_{j=0}^{m-1} \zeta_m^{-jk} \left(\sum_{p=0}^{m-1} \zeta_m^{jp} F_p\right) \left(\sum_{q=0}^{m-1} \zeta_m^{jq} G_q\right) \\ &= \sum_{p=0}^{m-1} F_p \sum_{q=0}^{m-1} G_q \sum_{j=0}^{m-1} \zeta_m^{j(-k+p+q)} \qquad (5) \\ &= m \sum_{s} \sum_{p=0}^{m-1} F_p G_{k-p+sm}.\end{aligned}$$

The terms $s \neq 0$ are aliases; they are bad.

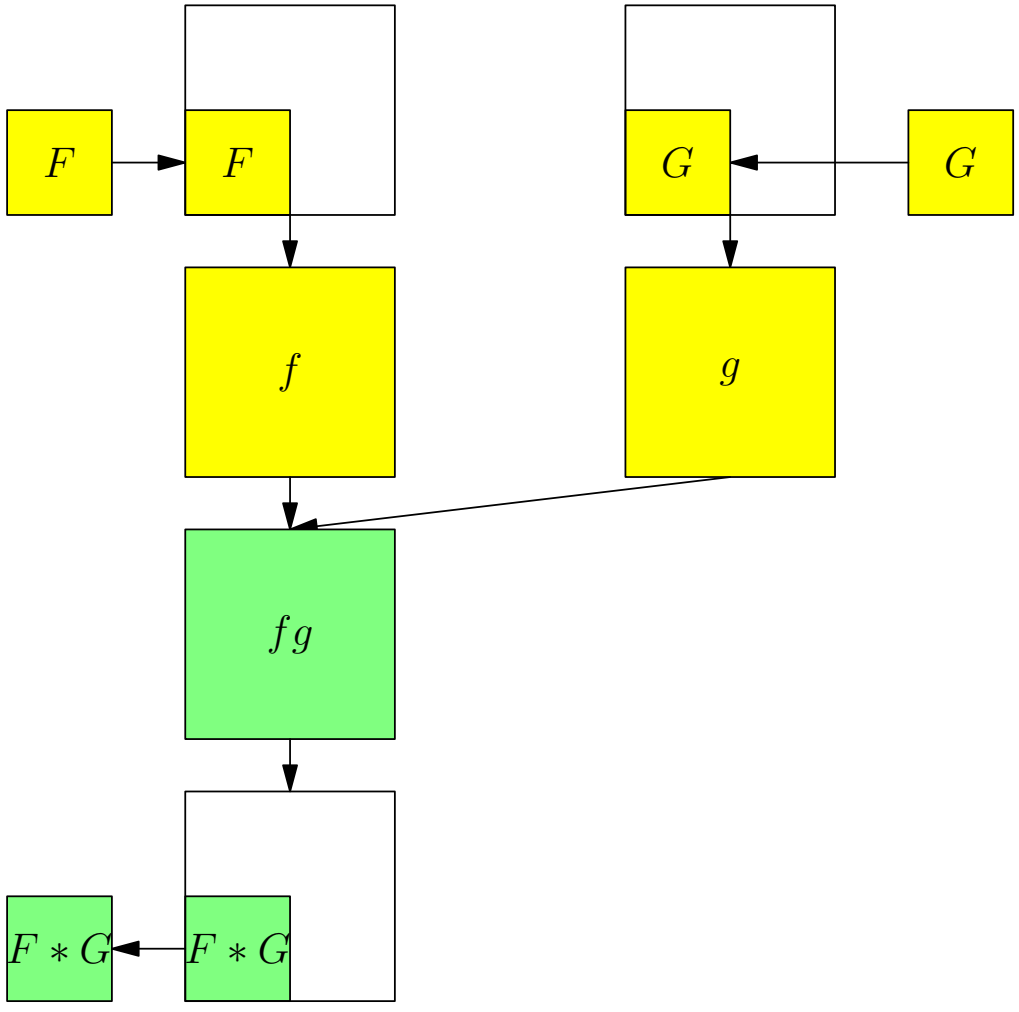
Conventional dealiasing: zero padding

Let $\widetilde{F} \doteq \{F_0, F_1, \ldots, F_{m-2}, F_{m-1}, \underbrace{0, \ldots, 0}_{m}\}$. Then,

$$\begin{aligned}
\left(\widetilde{F} *_{2m} \widetilde{G}\right)_k &= \sum_{\ell=0}^{2m-1} \widetilde{F}_{\ell \bmod (2m)} \widetilde{G}_{(k-\ell) \bmod (2m)} \\
&= \sum_{\ell=0}^{m-1} F_\ell \widetilde{G}_{(k-\ell) \bmod (2m)} \\
&= \sum_{\ell=0}^{k} F_\ell G_{k-\ell}.
\end{aligned} \tag{6}$$

There is also a "2/3" padded version for pseudospectral simulations, where the input $\{F_k\}_{k=-m}^{m-1}$ is padded to $3m$.

Dealiasing with conventional zero-padding



Dealiasing with implicit zero-padding

We modify the FFT to account for the zeros implicitly.

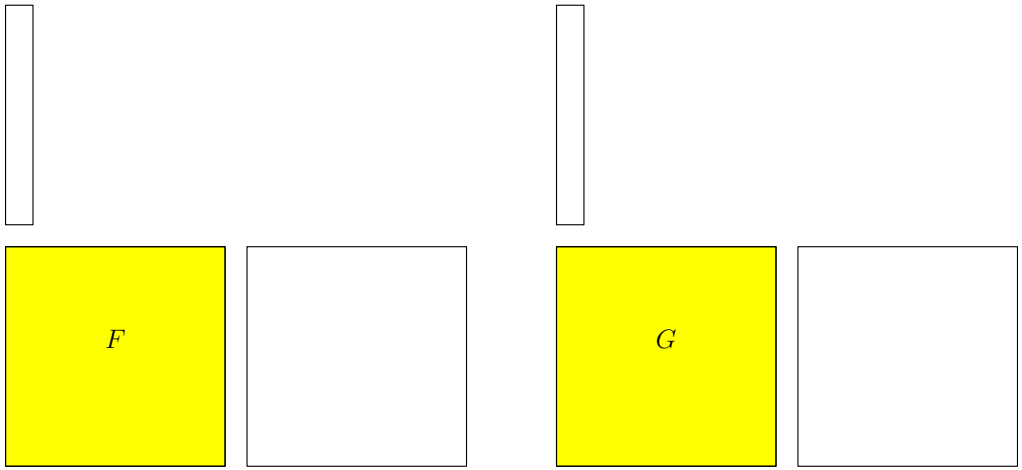
Let $\zeta_n = \exp(-i2\pi/n)$. The Fourier transform of $\widetilde{F}$ is

$$f_x = \sum_{k=0}^{2m-1} \zeta_{2m}^{xk} \widetilde{F}_k = \sum_{k=0}^{m-1} \zeta_{2m}^{xk} \widetilde{F}_k \tag{7}$$

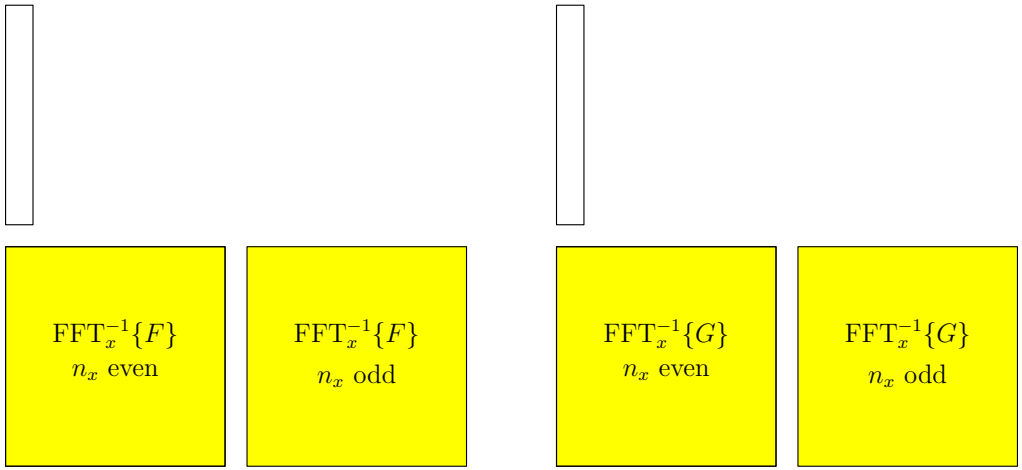
We can compute this using two discontiguous buffers:

$$f_{2x} = \sum_{k=0}^{m-1} \zeta_m^{xk} F_k \quad f_{2x+1} = \sum_{k=0}^{m-1} \zeta_m^{xk} \left(\zeta_{2m}^{k} F_k\right). \tag{8}$$

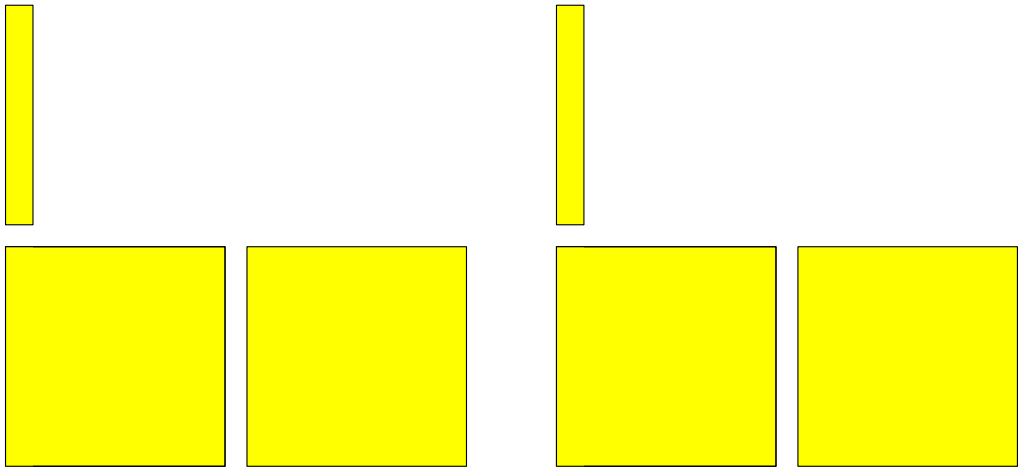
Dealiasing with implicit zero-padding



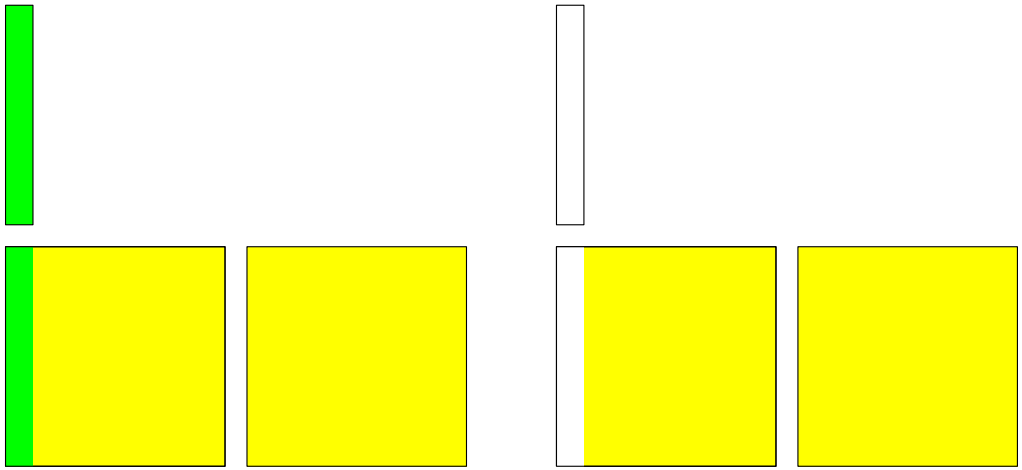
Dealiasing with implicit zero-padding



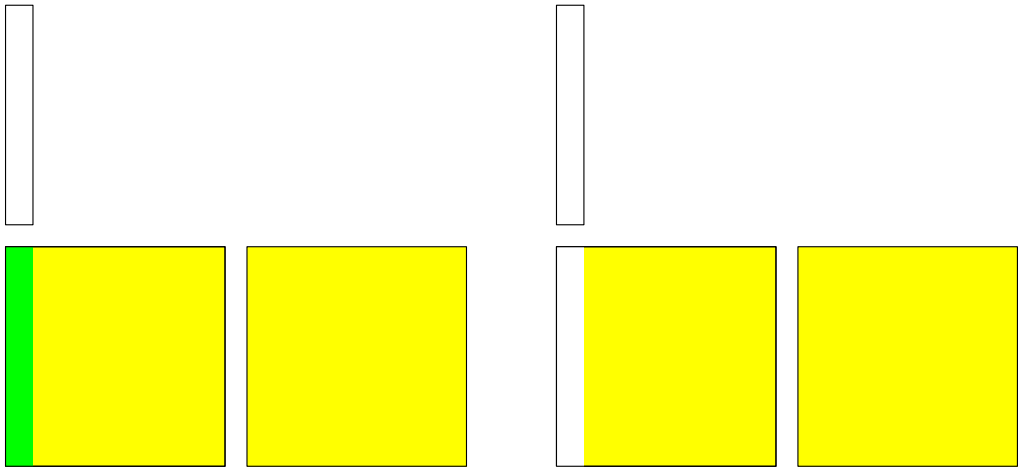
Dealiasing with implicit zero-padding



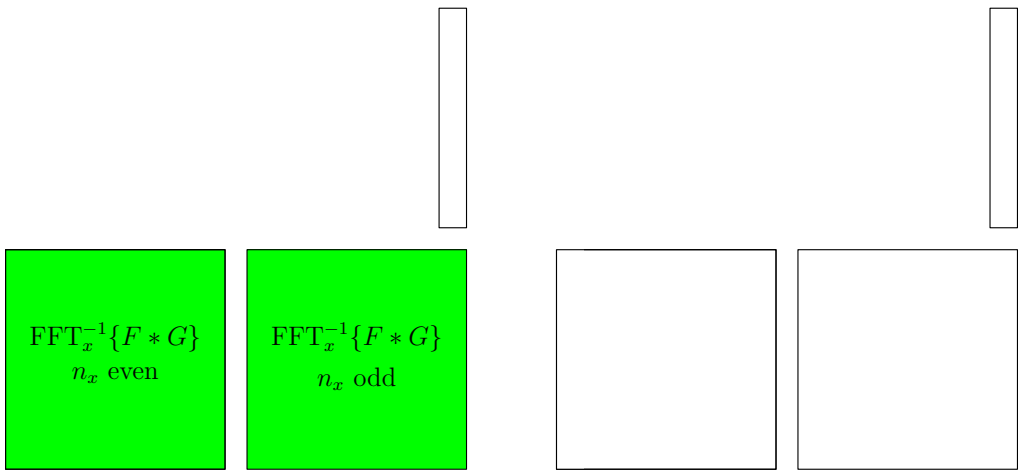
Dealiasing with implicit zero-padding



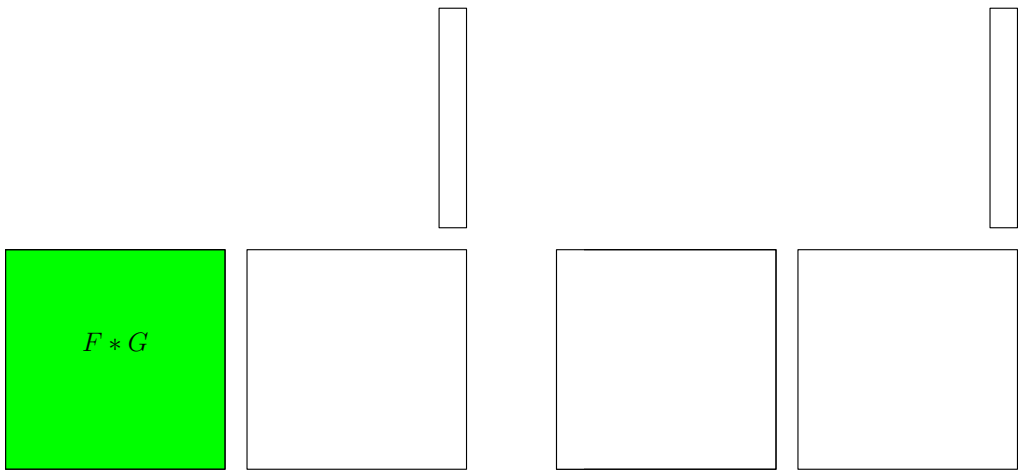
Dealiasing with implicit zero-padding



Dealiasing with implicit zero-padding



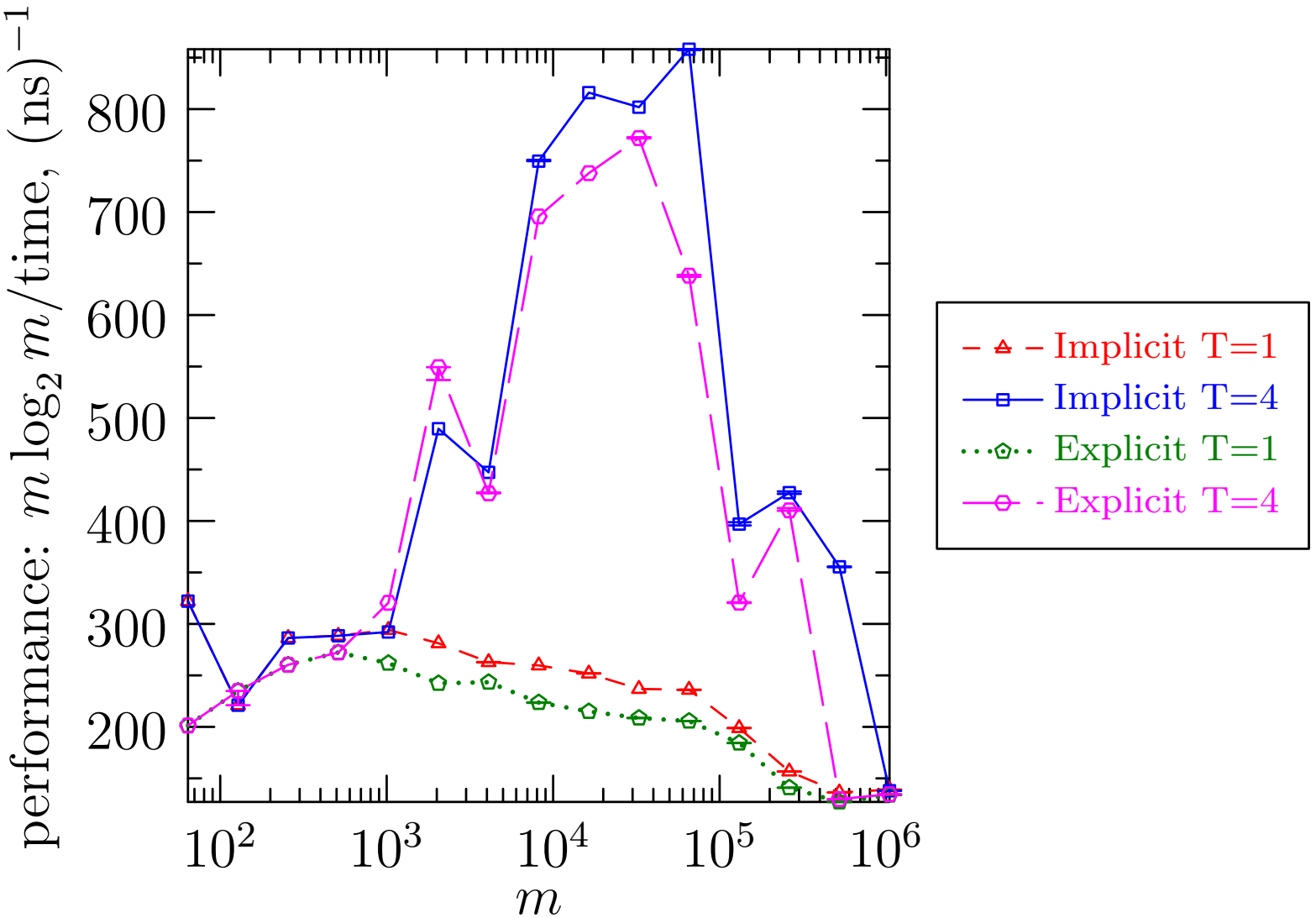
Dealiasing with implicit zero-padding



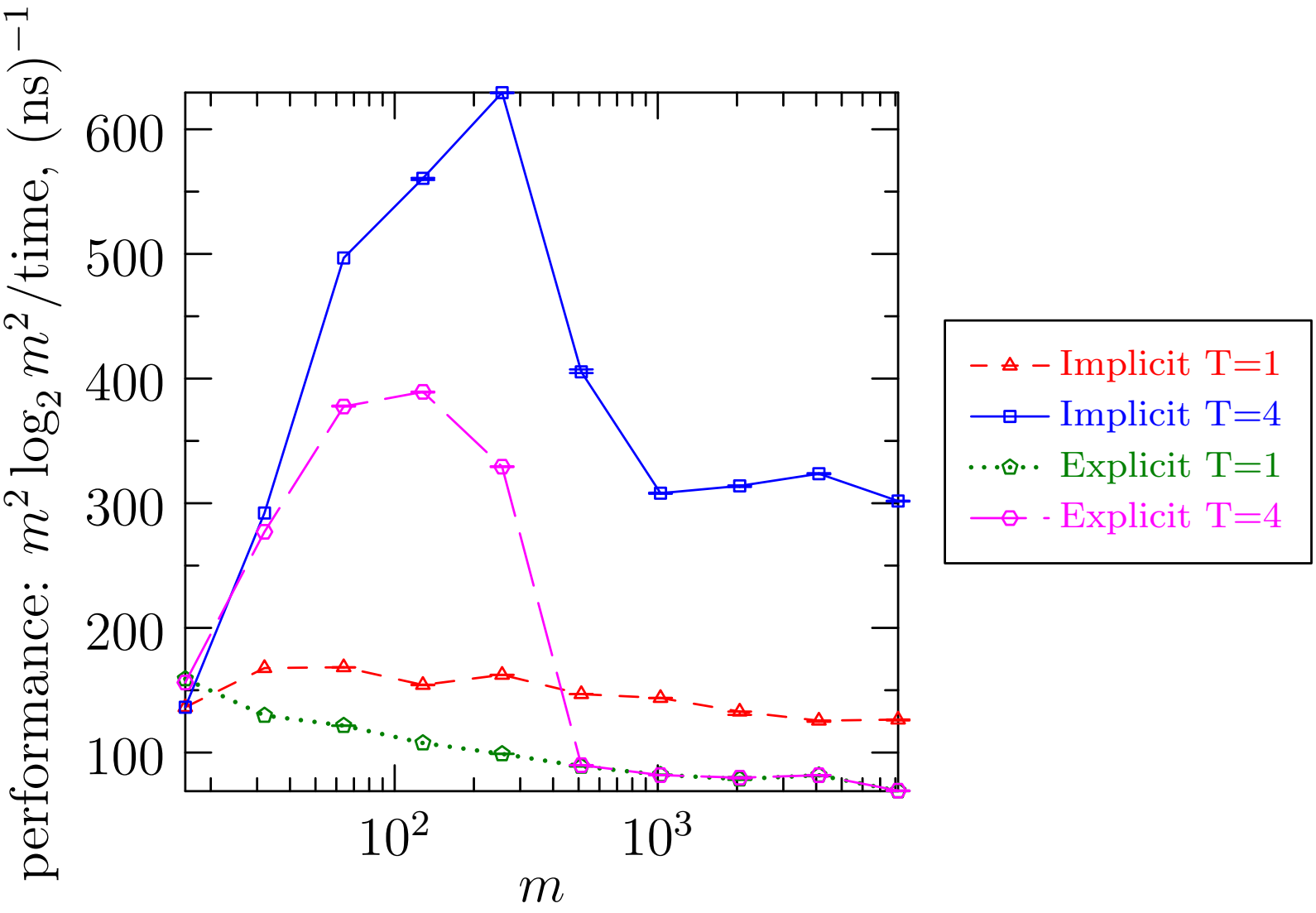
Shared-memory implementation

- Implicit dealiasing requires less memory.
- We avoid FFTs on zero-data.
- By using discontiguous buffers, we can use multiple NUMA nodes.
- SSE2 vectorization instructions.
- Additional threads requires additional sub-dimensional work buffers.
- We use strides instead of transposes because we need to multi-thread.

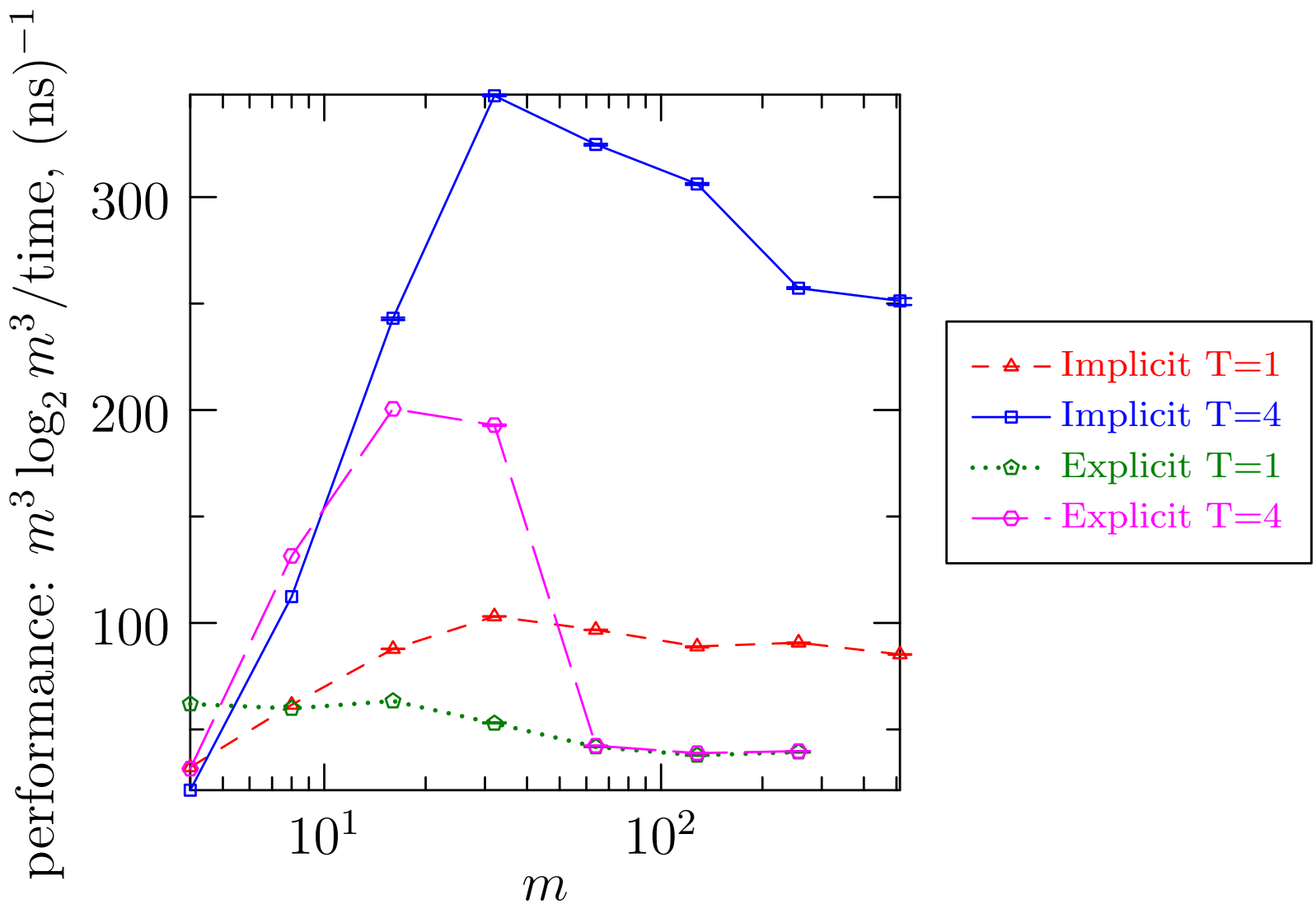
Multi-threaded performance: 1D



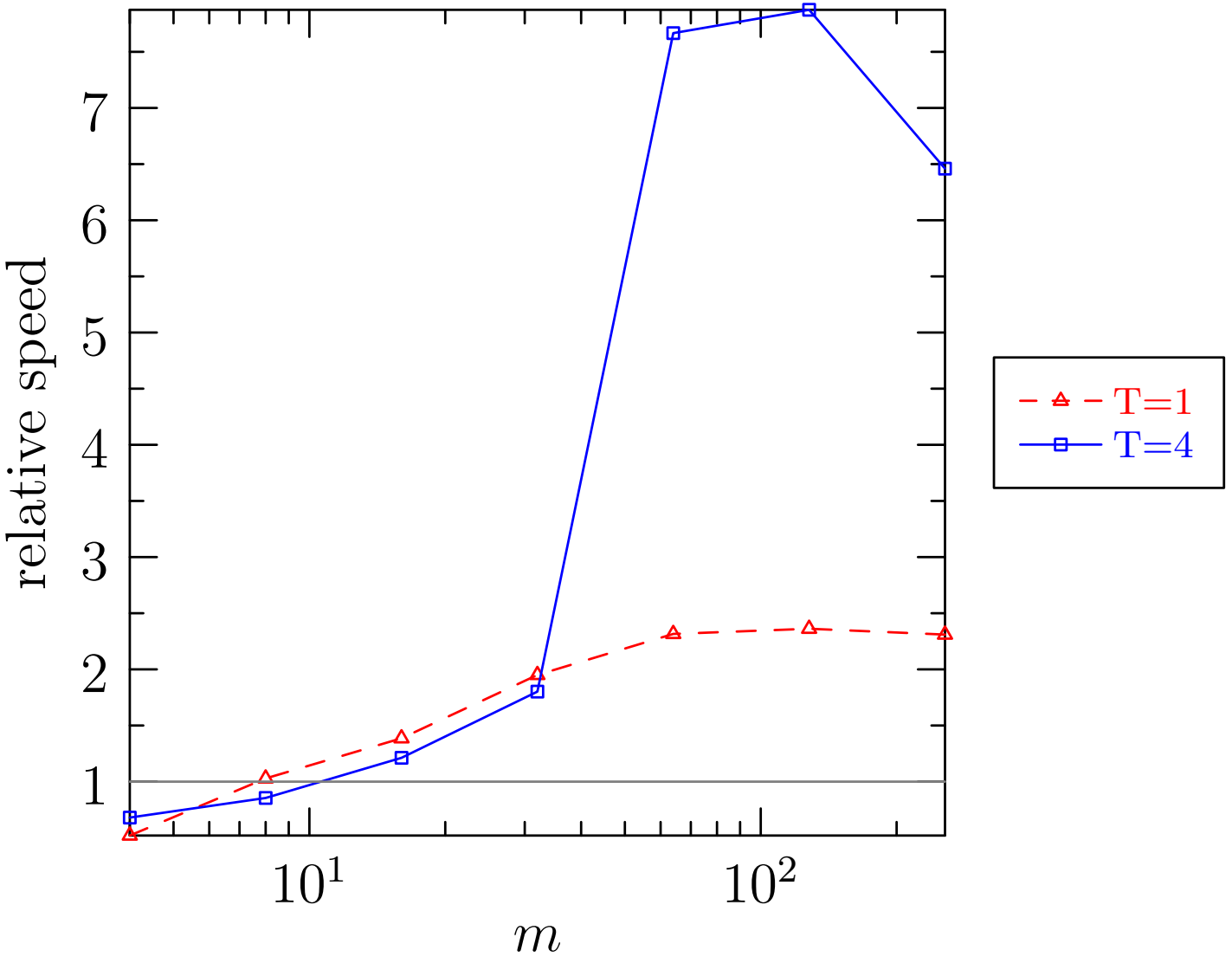
Multi-threaded performance: 2D



Multi-threaded performance: 3D



Multi-threaded speedup: 3D



Distributed-memory implementation

- Implicit dealiasing requires less communication.
- By using discontiguous buffers, we can overlap communication and computation.
- We use a hybrid `OpenMP`/`MPI` parallelization for clusters of multi-core machines.
- 2D `MPI` data decomposition.
- We make use of the *hybrid transpose* algorithm.

Hybrid MPI Transpose

Matrix transpose is an essential primitive of high-performance computing.

They allow one to localize data on one process so that shared-memory algorithms can be applied.

I will discuss two algorithms for transposes:

- Direct Transpose.
- Recursive Transpose.

We combine these into a *hybrid transpose*.

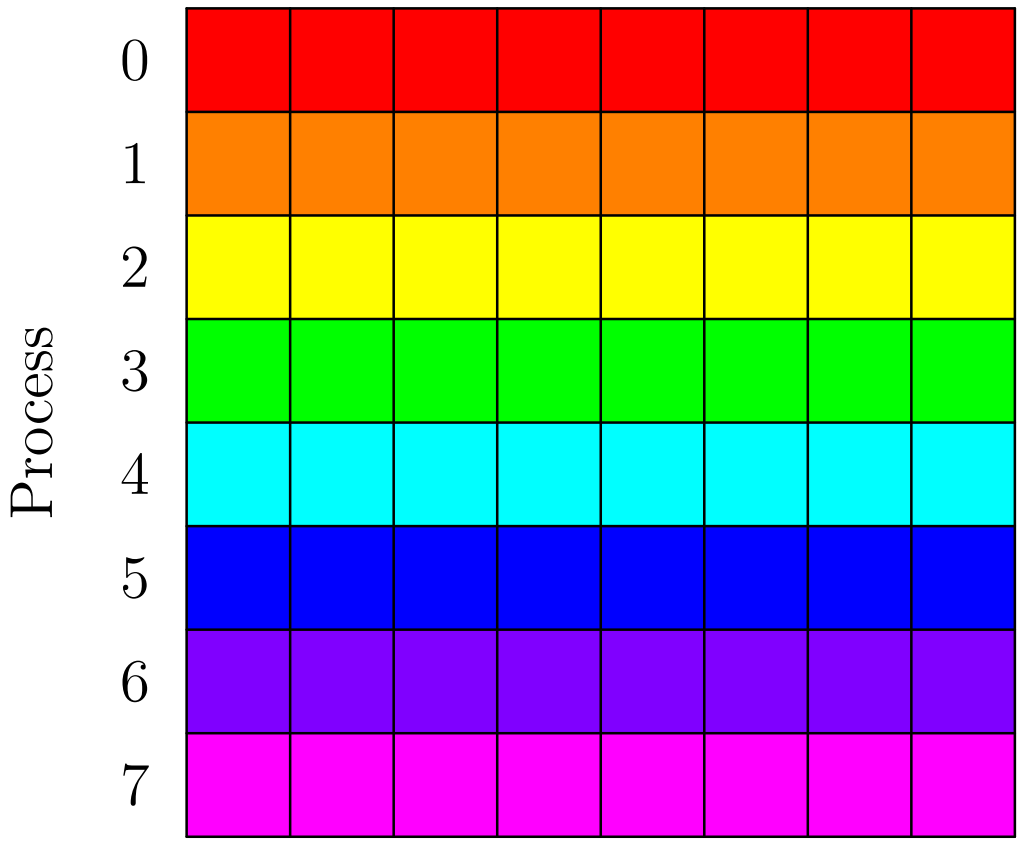
Direct (AlltoAll) Transpose

- Efficient for $P \gg m$ (large messages).
- Most direct method.
- Many small messages when $P \approx m$.

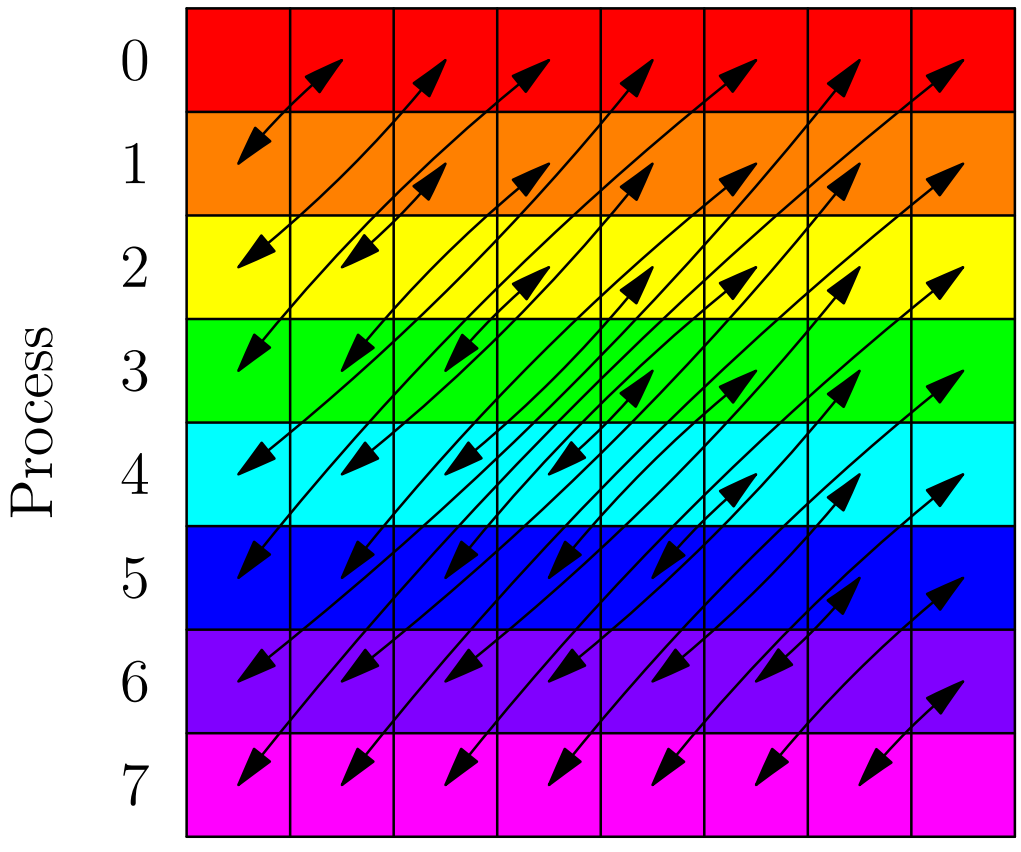
Implementations:

- `MPI_Alltoall`
- `MPI_Send`, `MPI_Recv`

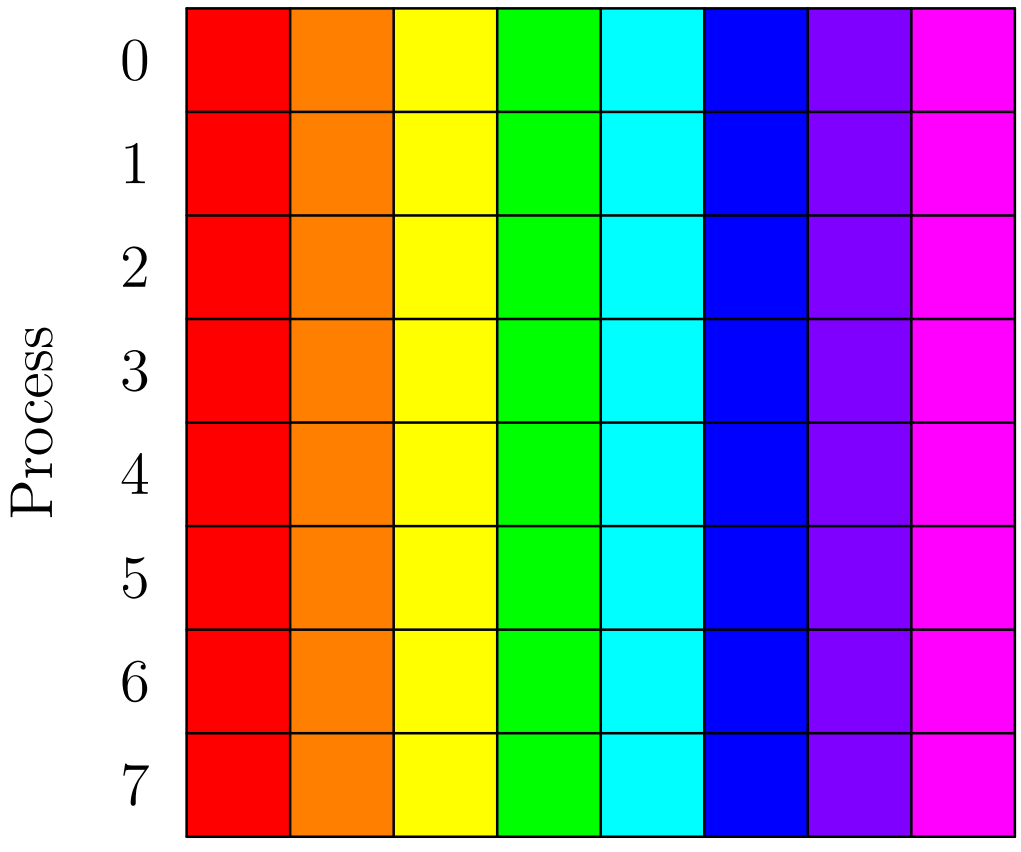
Direct (AlltoAll) Transpose



Direct (AlltoAll) Transpose



Direct (AlltoAll) Transpose



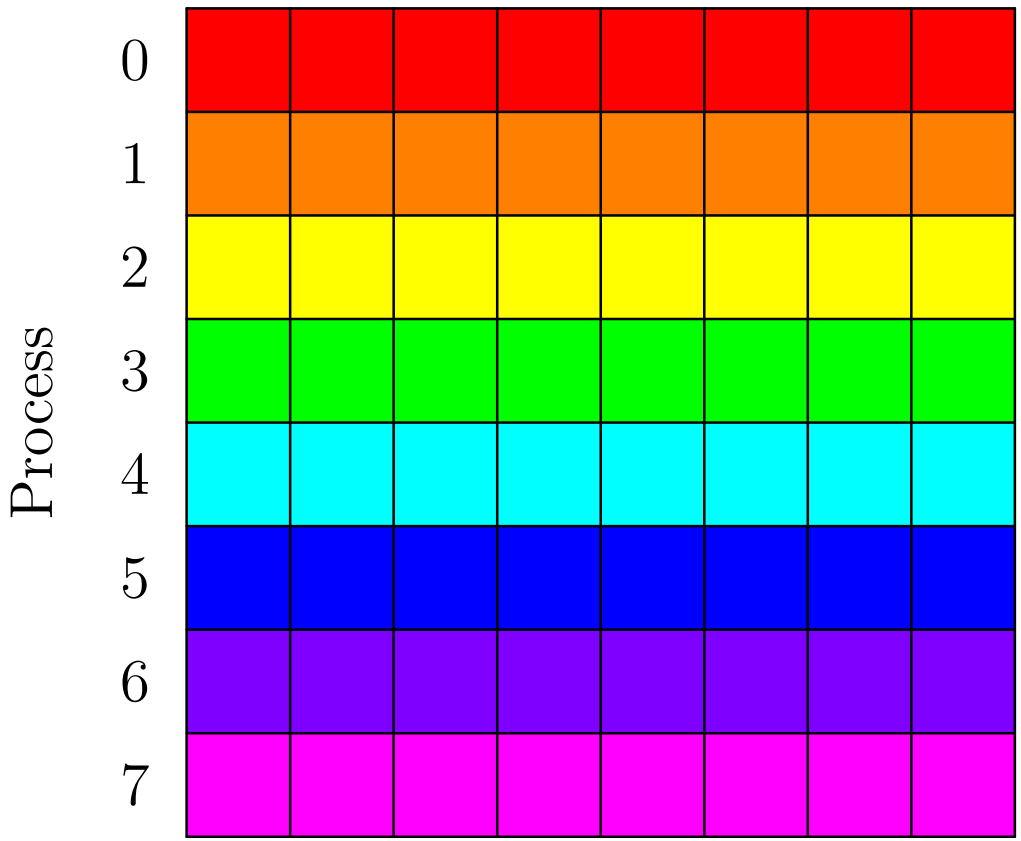
Recursive Transpose

- Efficient for $P \ll m$ (large messages).
- Recursively subdivides transpose into smaller block transposes.
- $\log m$ phases.
- Communications are grouped to reduce latency.
- Requires intermediate communication.

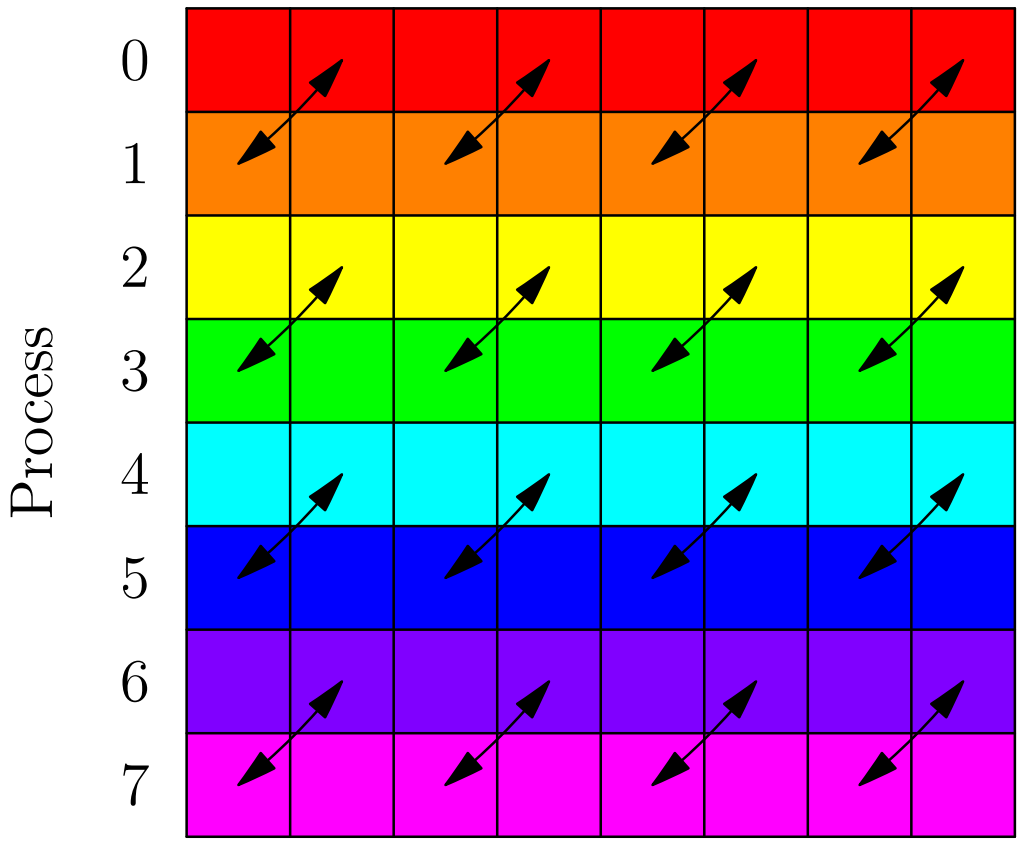
Implementations:

- `FFTW`

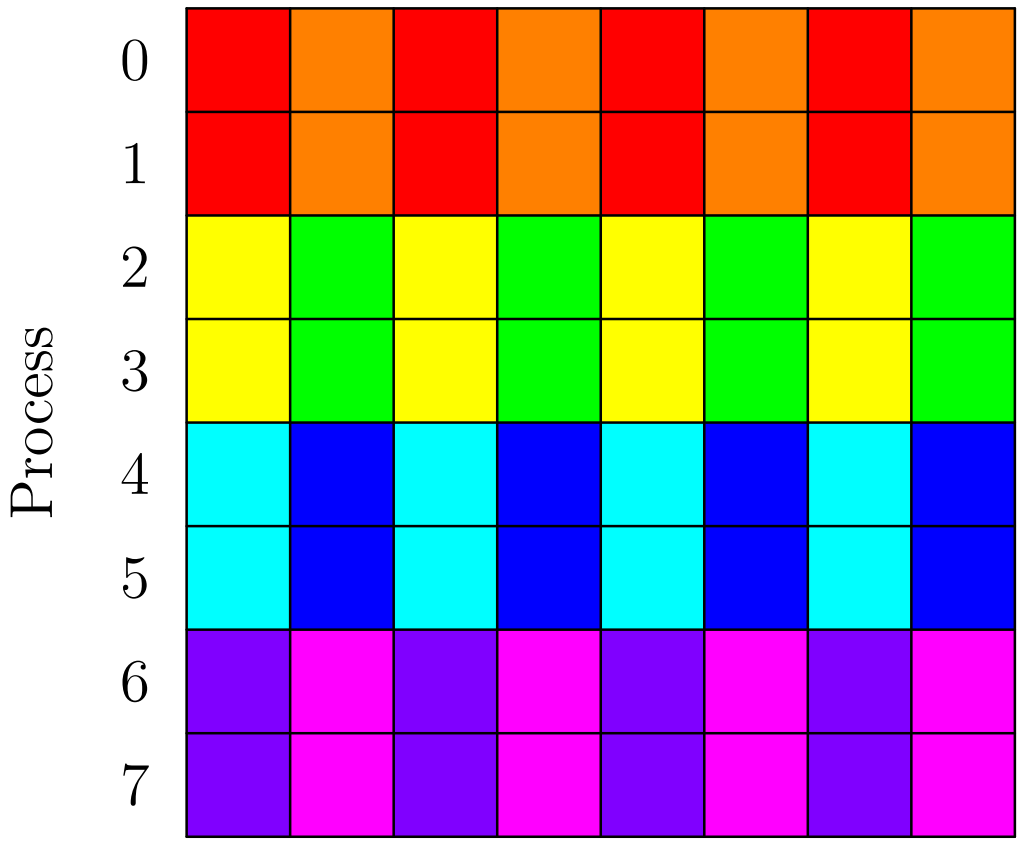
Recursive Transpose



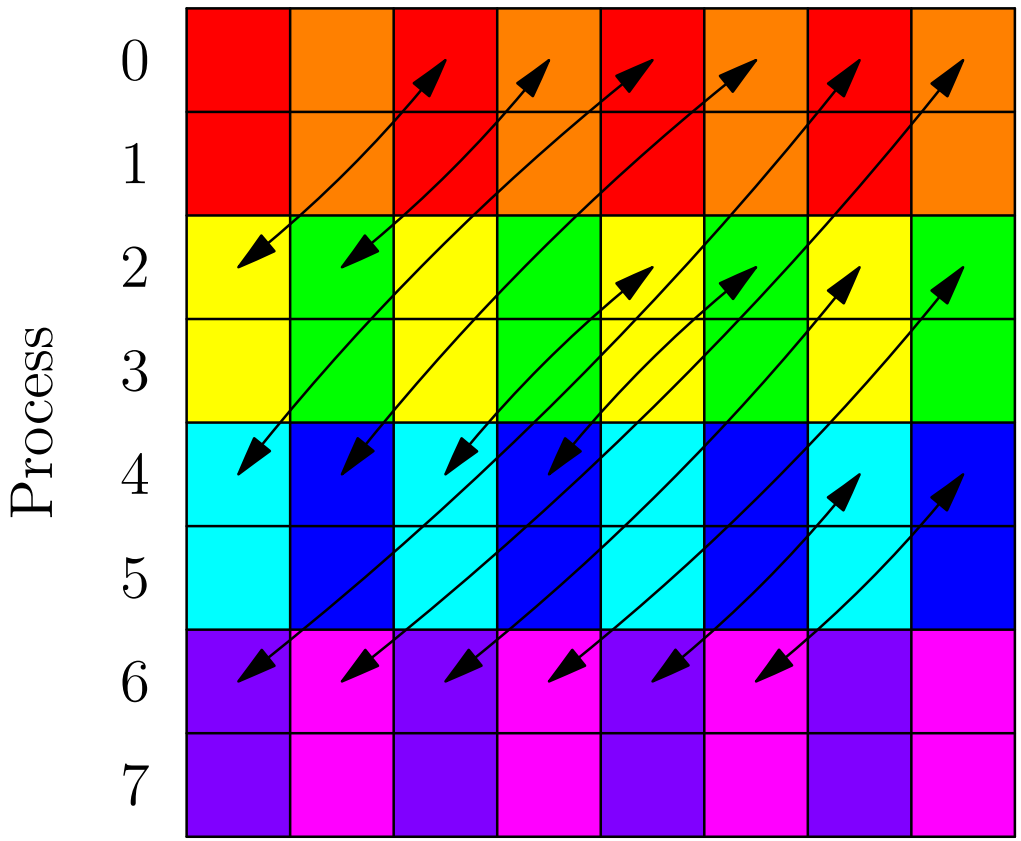
Recursive Transpose



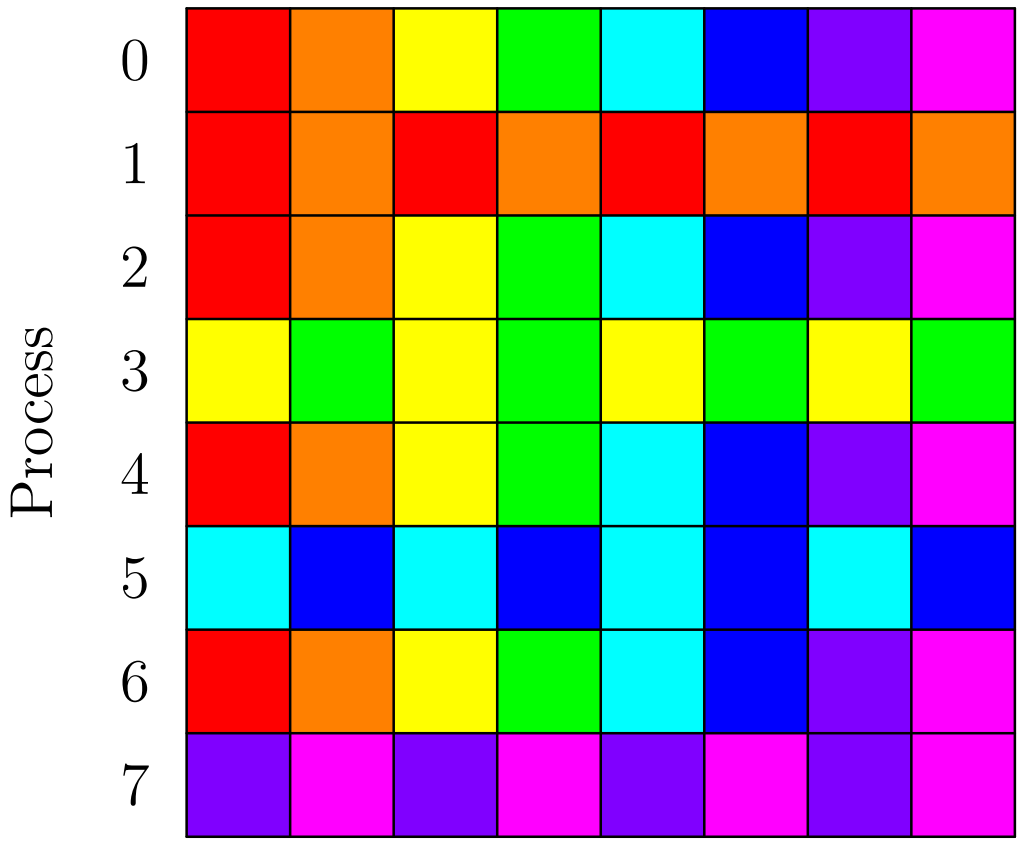
Recursive Transpose



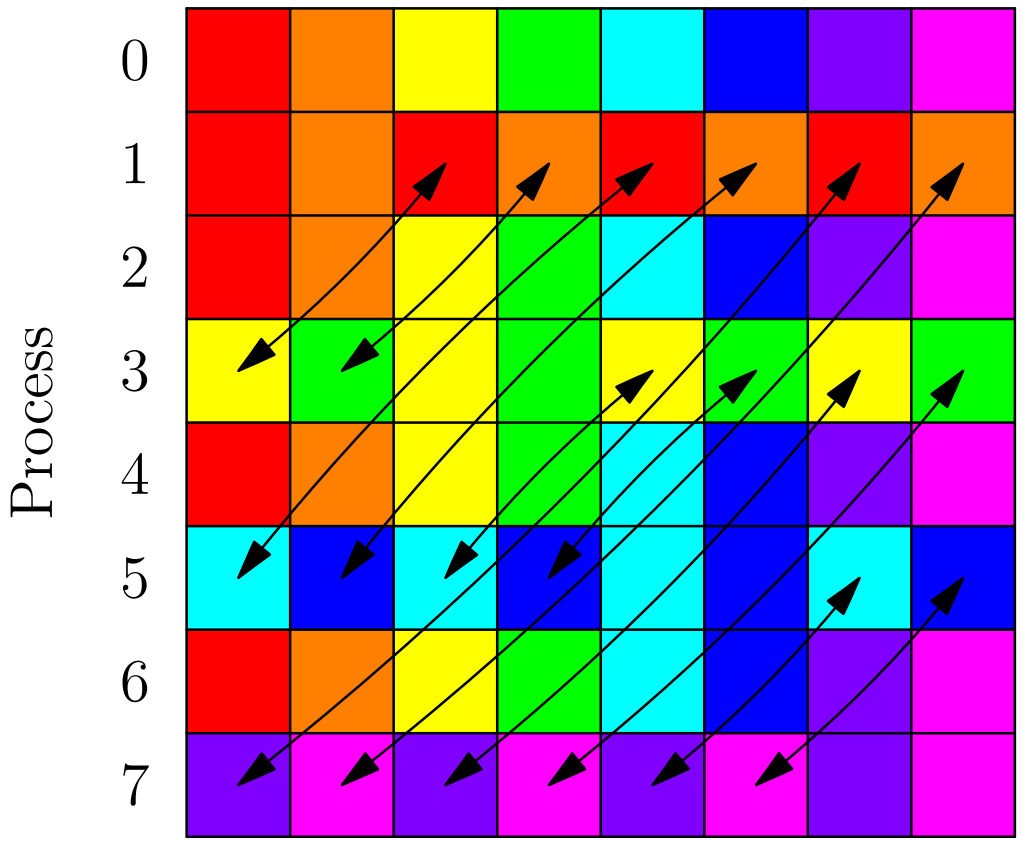
Recursive Transpose



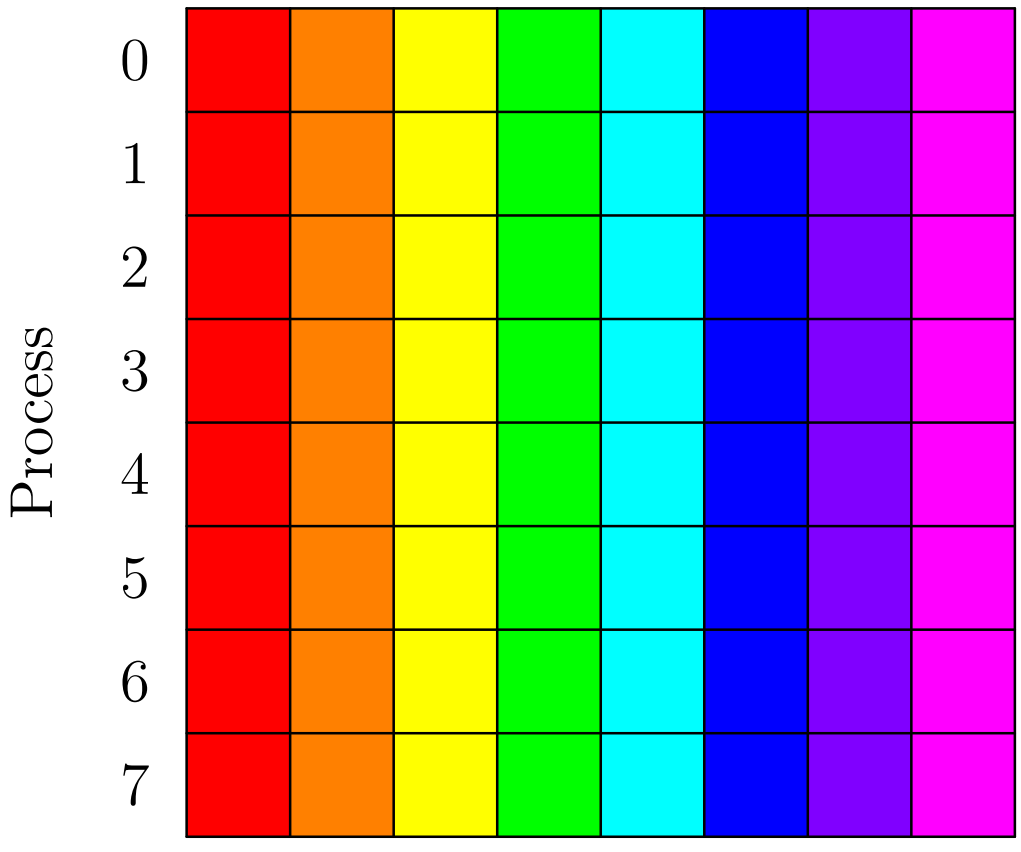
Recursive Transpose



Recursive Transpose



Recursive Transpose



Hybrid Transpose

- Recursive, but just one level.
- Use the empirical properties of the cluster to determine best parameters.
- *Optionally* group messages to reduce latency.

Implementation:

- `FFTW++`

Direct transpose communication cost: $\frac{P-1}{P^2}m^2$, P messages.

Hybrid cost with $P = ab$: $\frac{(a-1)bm^2}{P^2} + \frac{(b-1)am^2}{P^2}$, $a + b$ messages.

Hybrid Transpose

Let τ_ℓ be the message latency, and τ_d the time to send one element. The time to send n elements is

$$\tau_\ell + n\tau_d. \tag{9}$$

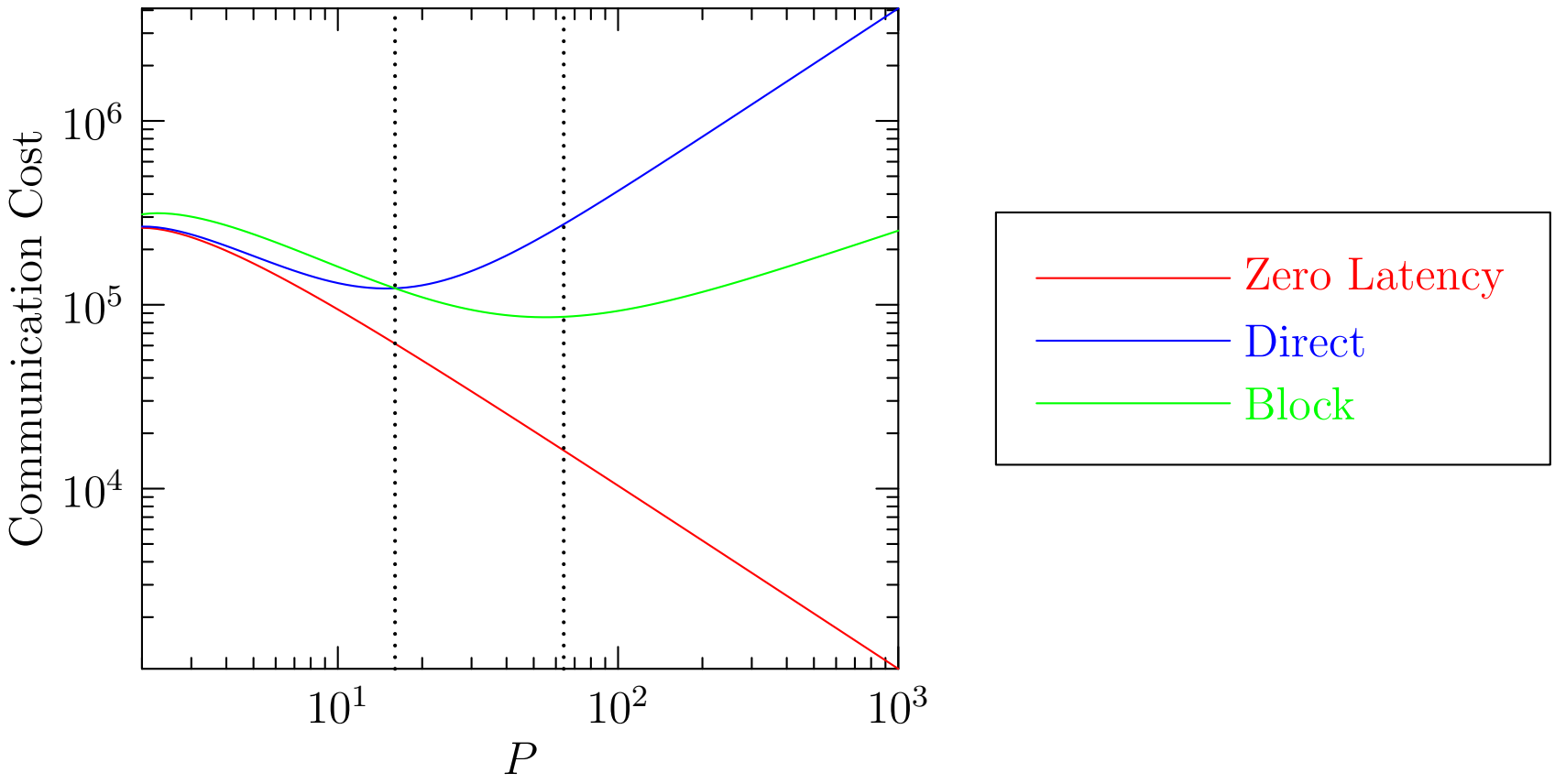
The time required to do a direct transpose is

$$T_D = \tau_\ell (P-1) + \tau_d \frac{P-1}{P^2} m^2 = (P-1)\left(\tau_\ell + \tau_d \frac{m^2}{P^2}\right) \tag{10}$$

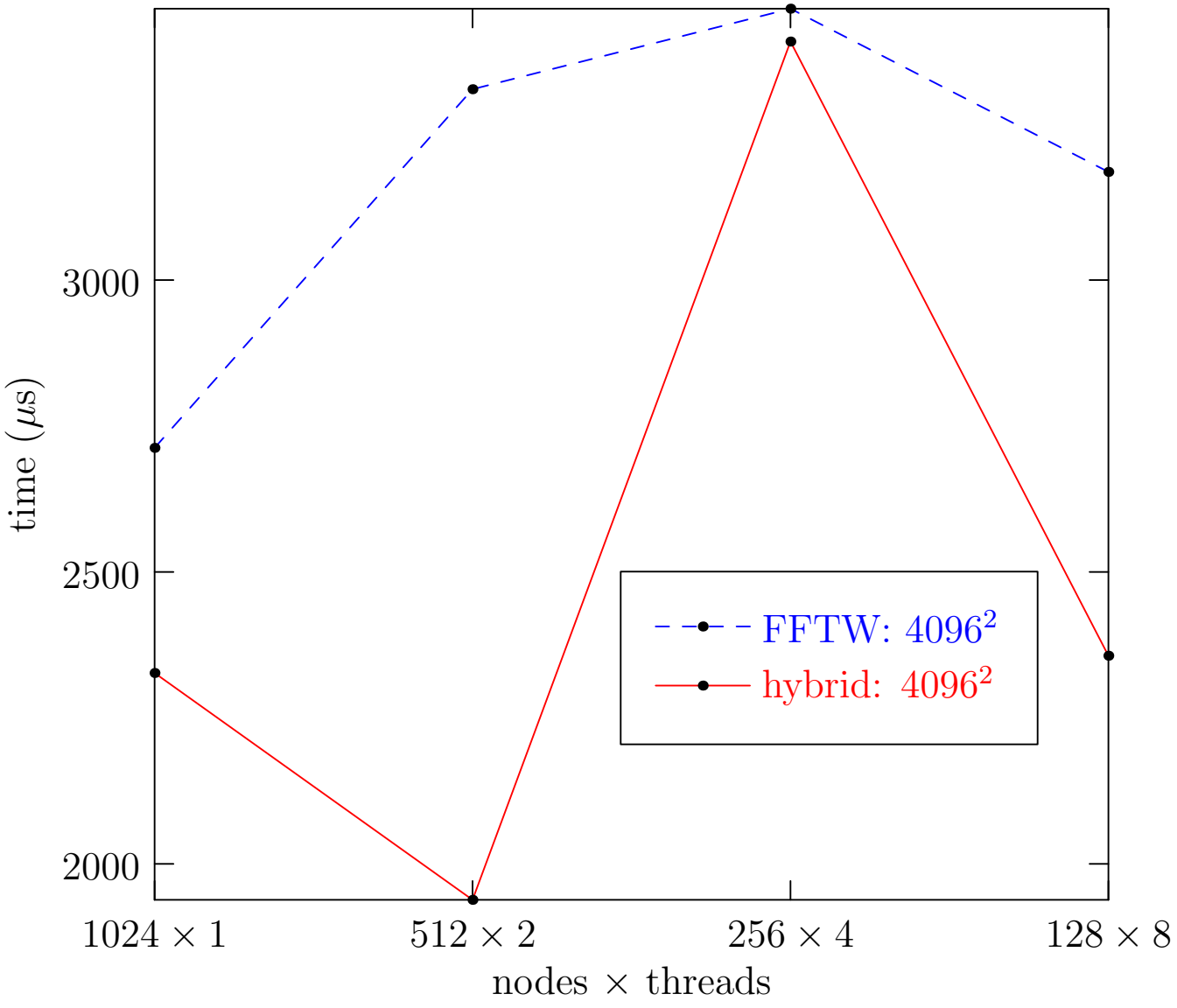
The time for a block transpose is

$$T_B(a) = \tau_\ell \left(a + \frac{P}{a} - 2\right) + \tau_d \left(2P - a - \frac{P}{a}\right) \frac{m^2}{P^2}. \tag{11}$$

Hybrid Transpose



Hybrid Transpose



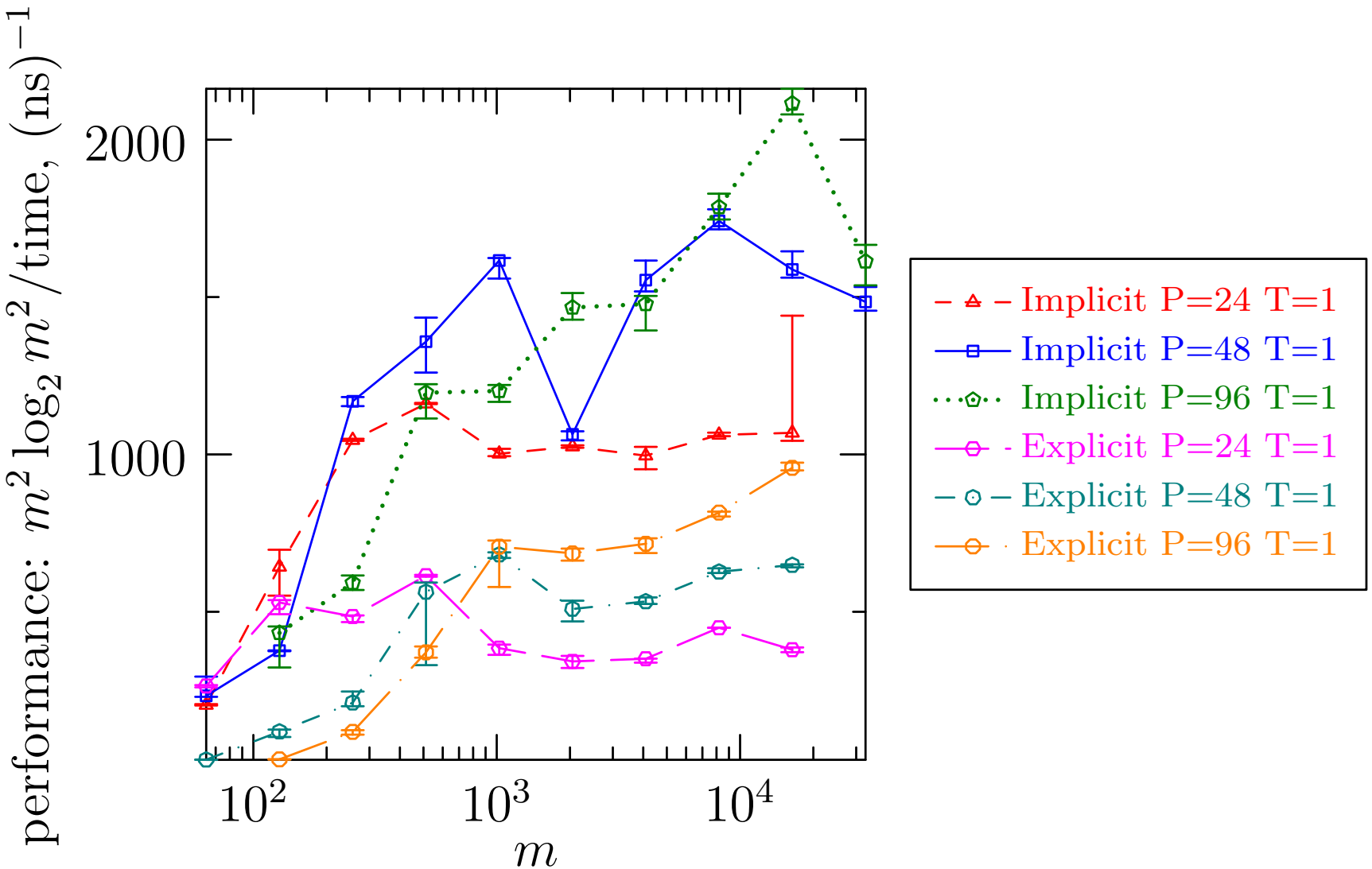
Hybrid Transpose

The hybrid transpose

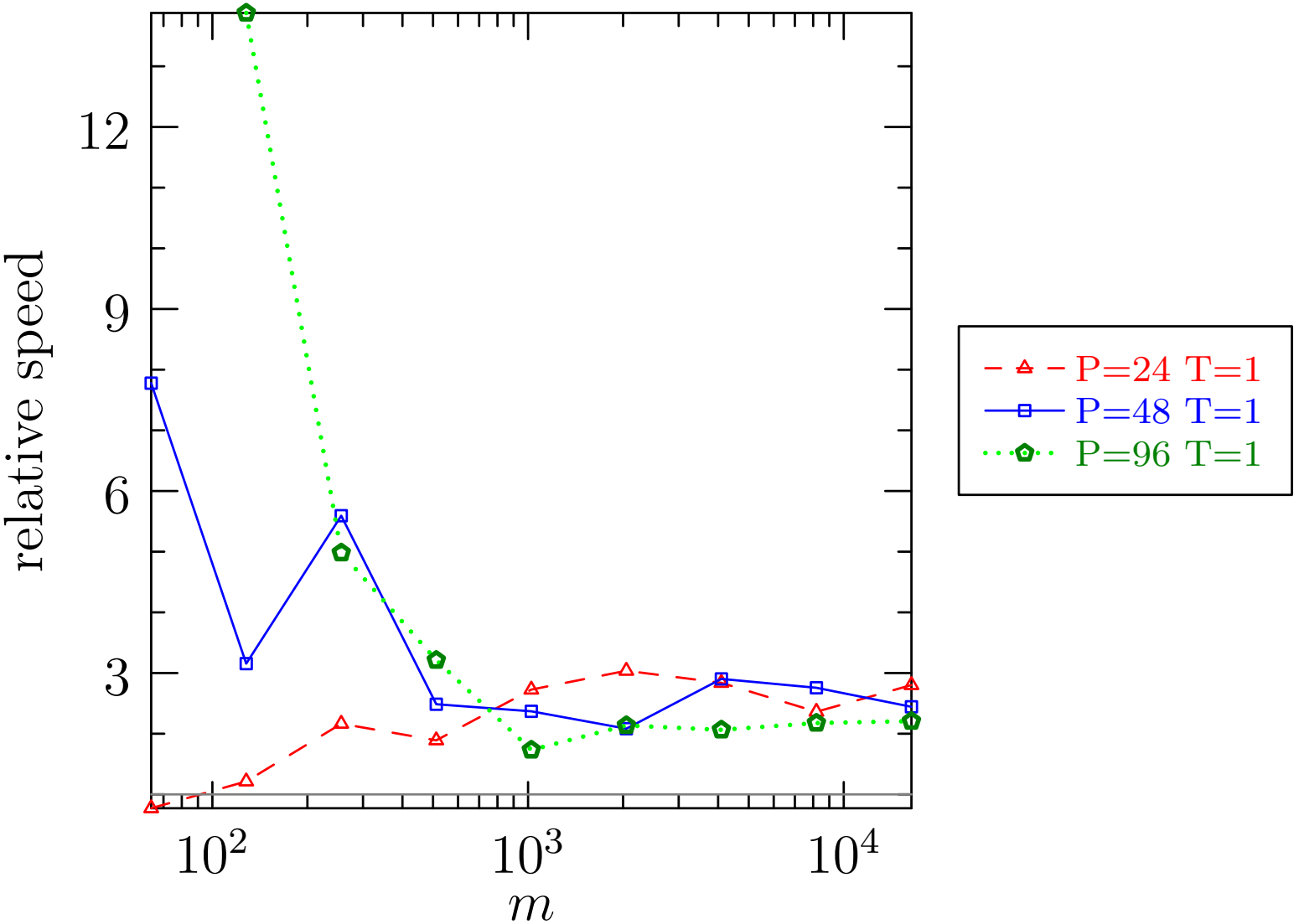
- Uses a direct transpose for large message sizes.
- Uses a block transpose for small message sizes.
- Offers a performance advantage when $P \approx m$.
- Can be tuned based upon the values of τ_ℓ and τ_d for the cluster.

We use the hybrid transpose in computing convolutions using implicit dealiasing on clusters.

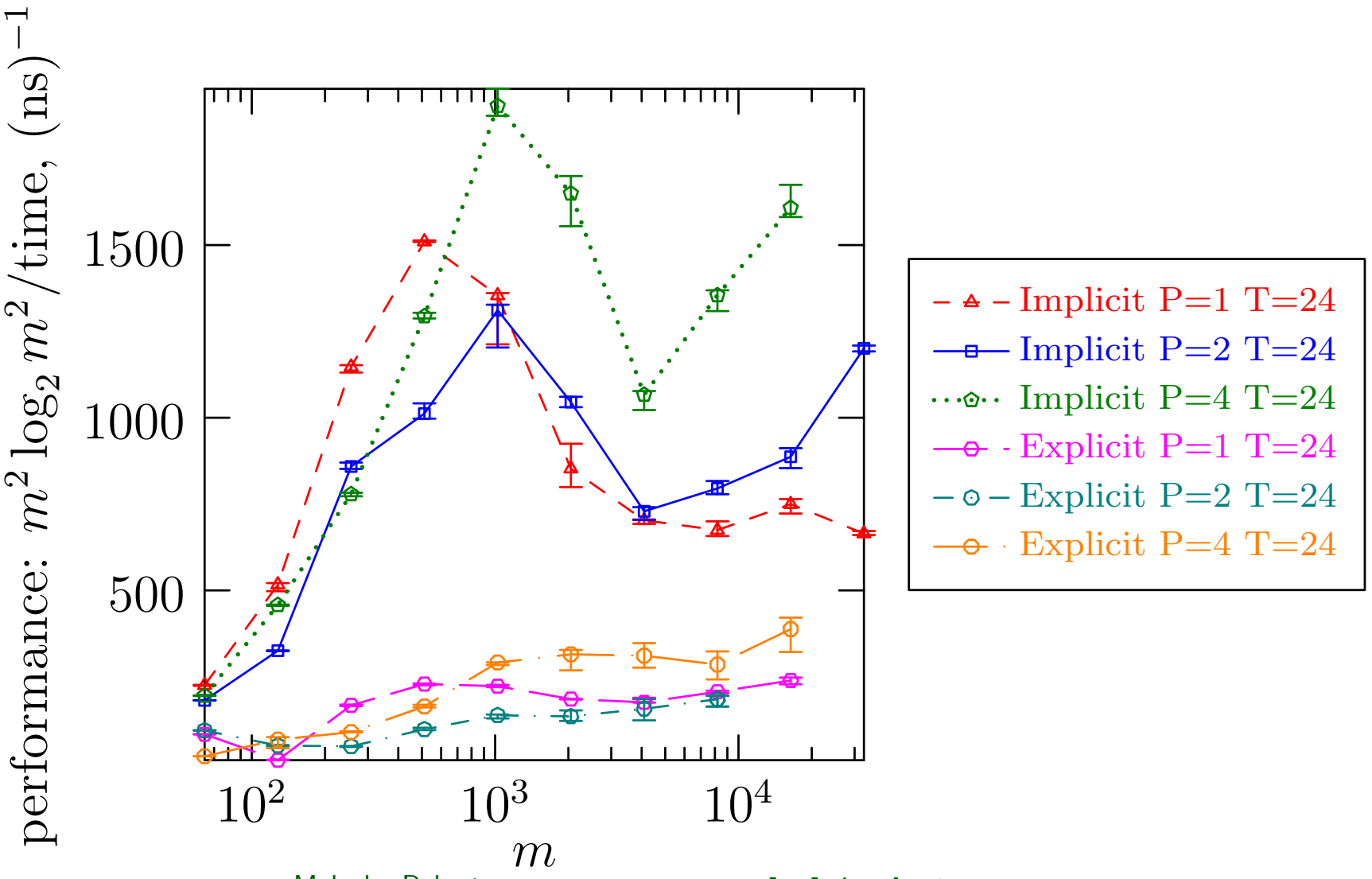
MPI Convolution: 2D performance



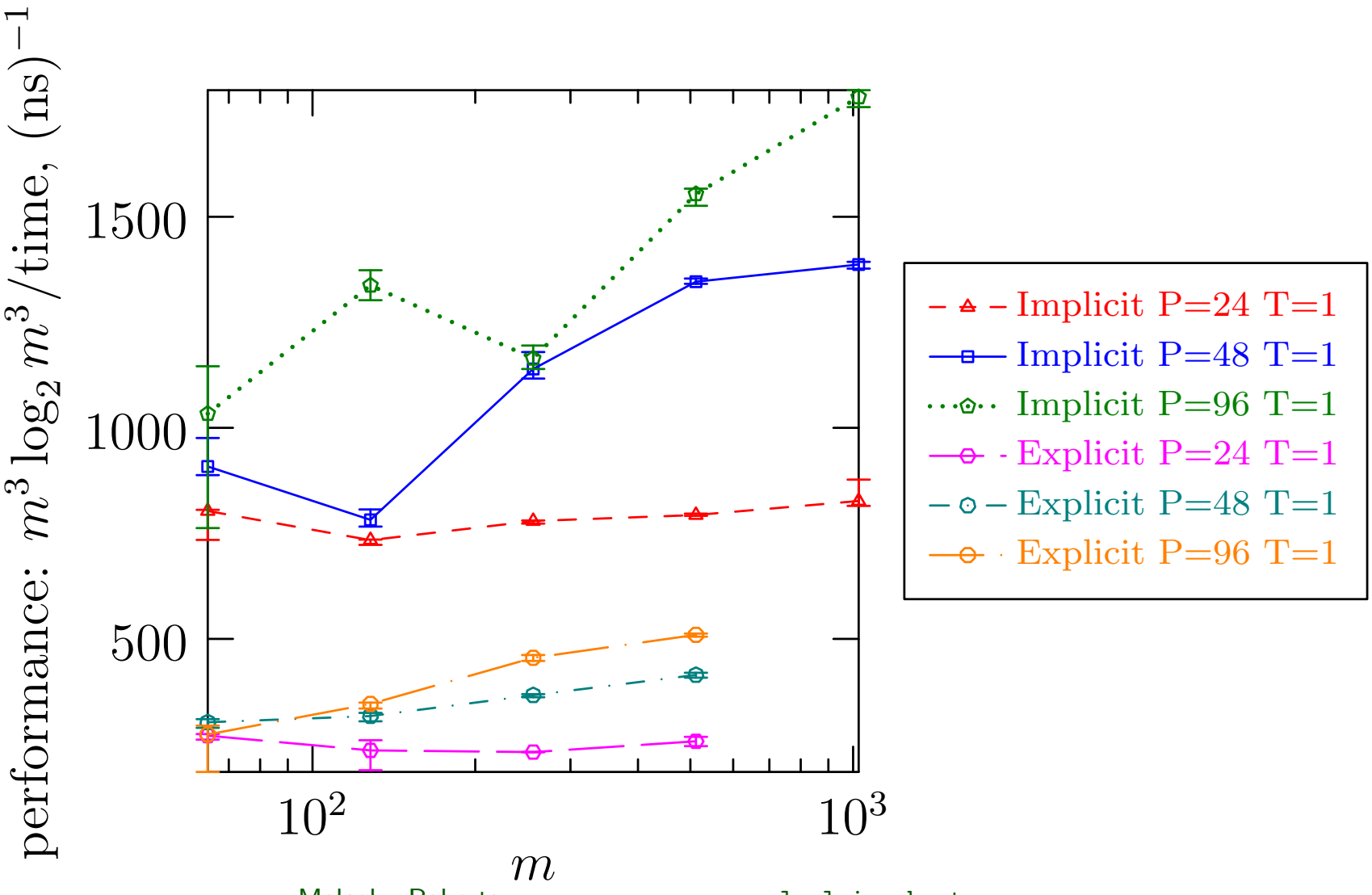
MPI Convolution: 2D performance



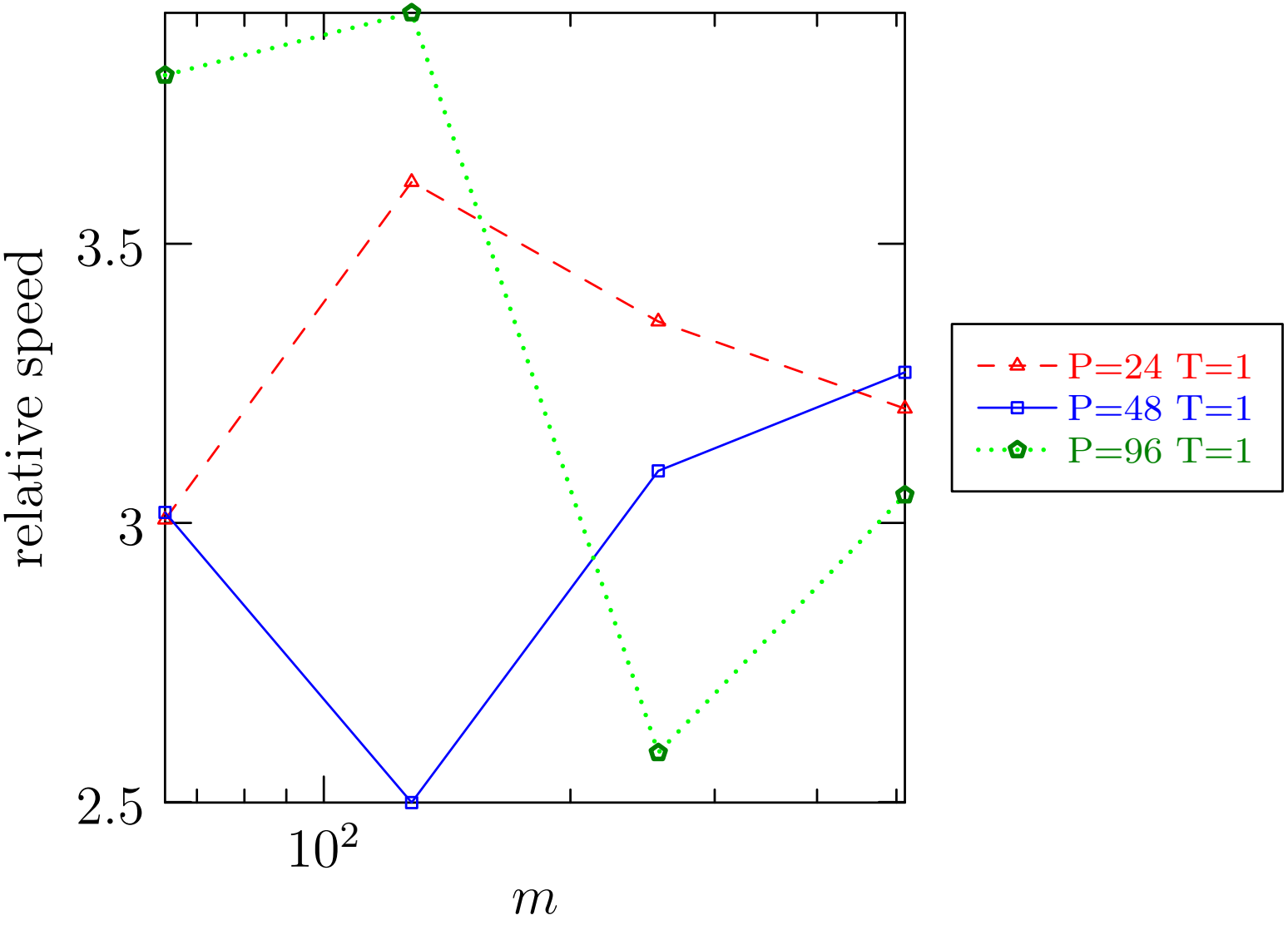
MPI Convolution: multithreaded 2D performance



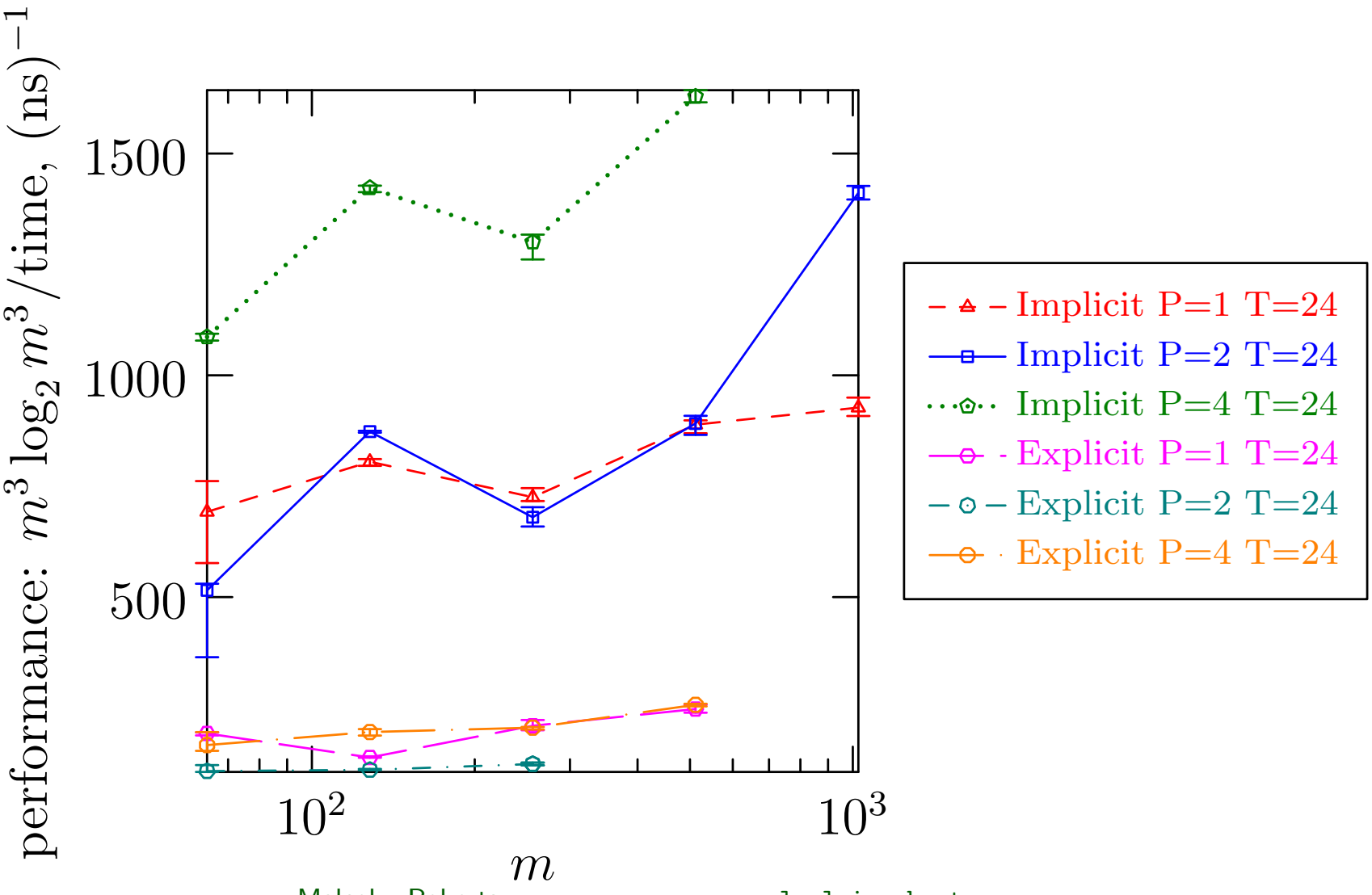
MPI Convolution: 3D performance



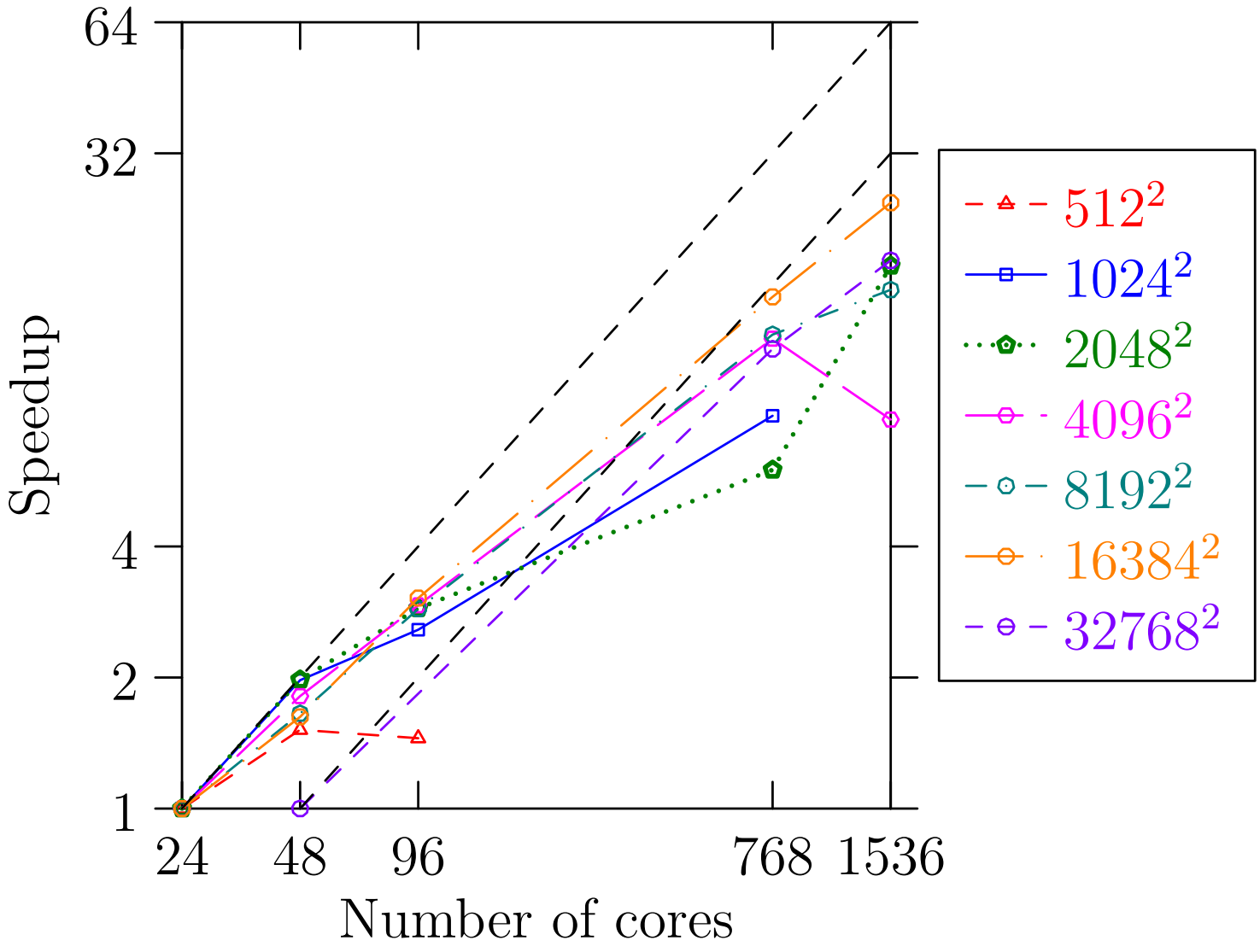
MPI Convolution: 3D performance



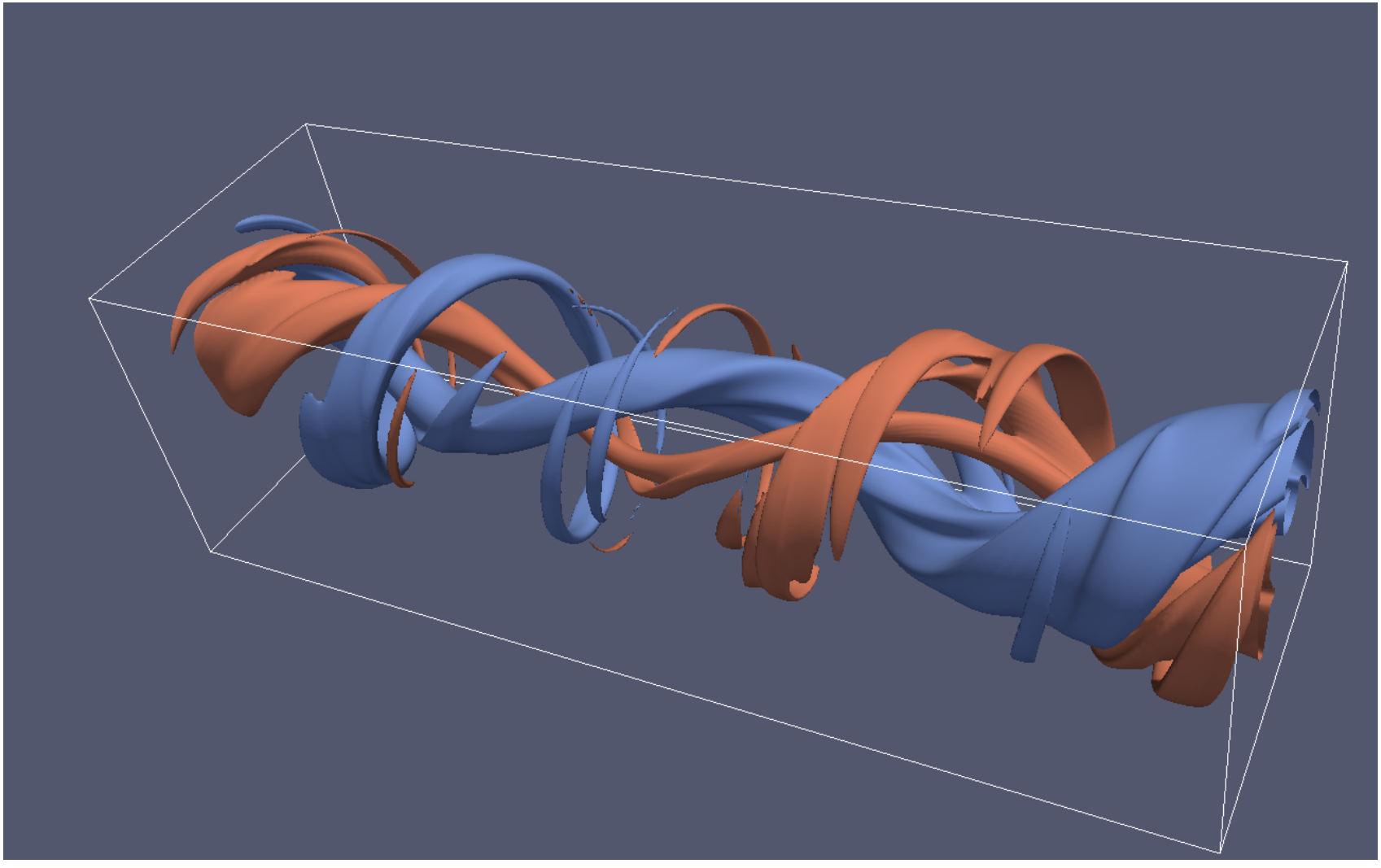
MPI Convolution: multithreaded 3D performance



MPI Convolution: 3D scaling



Application: Pseudospectral simulation



Application: Pseudospectral simulation

Convolutions Summary

Implicitly dealiased convolutions:

- use less memory
- have less communication costs,
- and are faster than conventional zero-padding techniques.

The hybrid transpose is faster for small message size.

Collaboration with John Bowman, University of Alberta.

Implementation in the open-source project `FFTW++`:

`fftwpp.sf.net`

We have around 13 000 downloads (plus clones).

Running on GPUs

Computing on general-purpose GPU has two advantages:

- High performance
- Low energy consumption

There are a variety of options for running on GPU:

- CUDA: Libraries available, tools available. Nvidia-only.
- OpenMP 4.0: pragma-based, high-level.
- OpenACC: Being rolled into OpenMP
- OpenCL: Similar to CUDA, but released later.
  - Works on all vendors, very flexible.
  - Runs on GPUs, CPUs, mics (Xeon Phi).

OpenCL

One writes a normal program, in which the code for the GPU is contained in a string.

At run-time, the program:

1. Selects the OpenCL platform(s) and device(s).
2. Creates an OpenCL context and queue.
3. Compiles the programs into kernels.
4. Allocates buffers on the device.
5. Launches kernels in the queue: managed with events.

OpenCL

Kernels are the code from the interior of loops.

Example: the C code

```
void myfunc(double* a, double* b, int n) {
for(int i = 0; i < n; ++i) {
  a[i] *= b[i];
}
```

becomes:

```
kernel void mykernel(__global double* a,
                     __global double* b) {
  int i = get_local_id(0);
  a[i] *= b[i];
}
```

OpenCL

Since the kernel has no loop dependencies, everything is vectorized: even RAM buffers are aligned to the vector width.

The `__global` keyword specifies that one uses the global device memory.

One has access to the cache with `__local`; if one wants to have data in the cache, then one writes a loop to put it there.

Coalescent memory access is crucial.

So, one has a lot of control, but there's a bit more work.

But the performance is good!

OpenCL

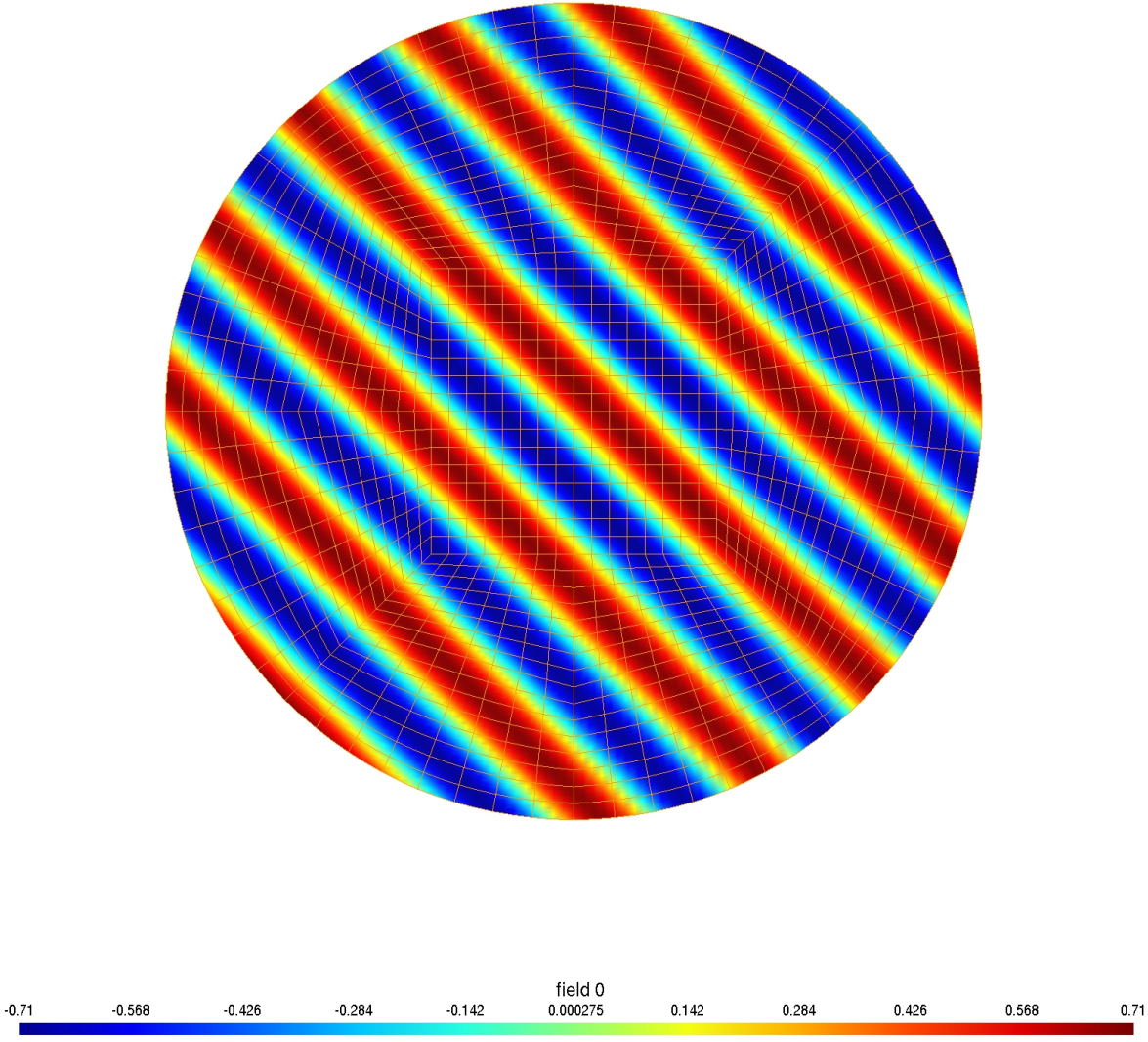
We developed a discontinuous-Galerkin code for solving hyperbolic conservation laws:

schnaps

Solver for **C**onservative **H**ypebolic **N**on-linear systems **A**pplied to **P**lasma**S**

$$\frac{\partial w}{\partial t} + \sum_{k=1}^{k=d} \frac{\partial}{\partial k} F^k(w) = S \tag{12}$$

schnaps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-0.71
-0.568
-0.426
-0.284
-0.142
0.000275
0.142
0.284
0.426
0.568
0.71

schnaps

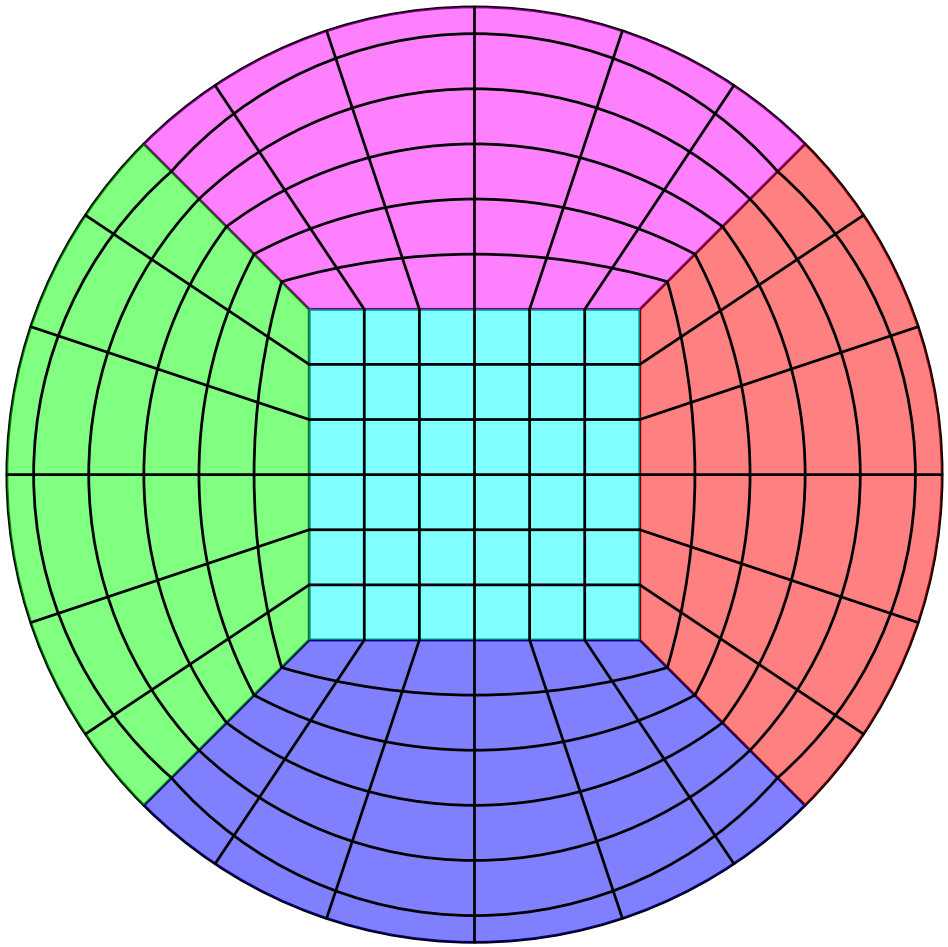
Discontinuous Galerkin method:

- Deals well with complex geometries.
- Local refinement: non-uniform grid.

OpenCL implementation:

- Hexahedral elements for coalescent memory access.
- Macrocell / subcell formulation.
- Array of structs of arrays: yet more coalescence.

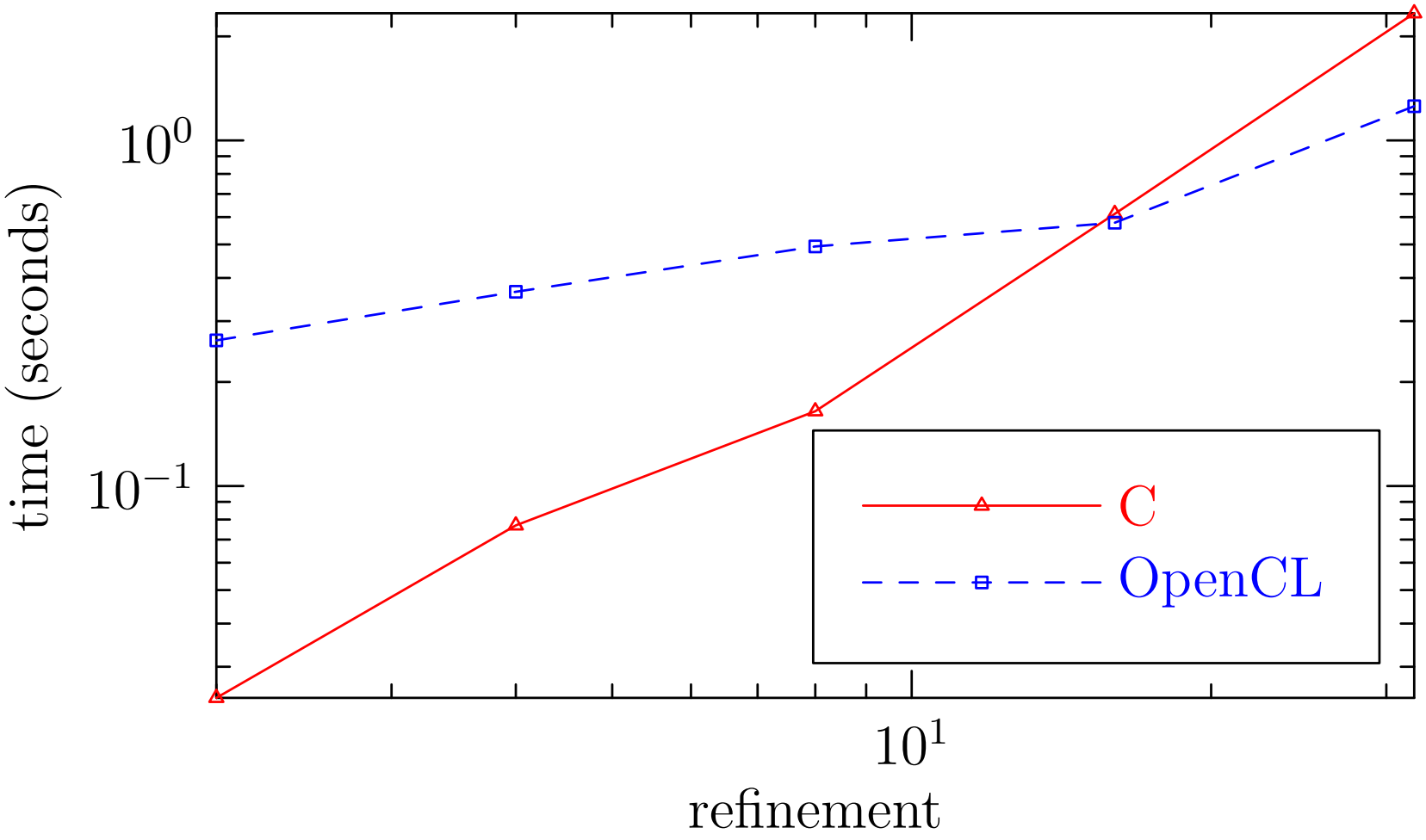
schnaps



schnaps

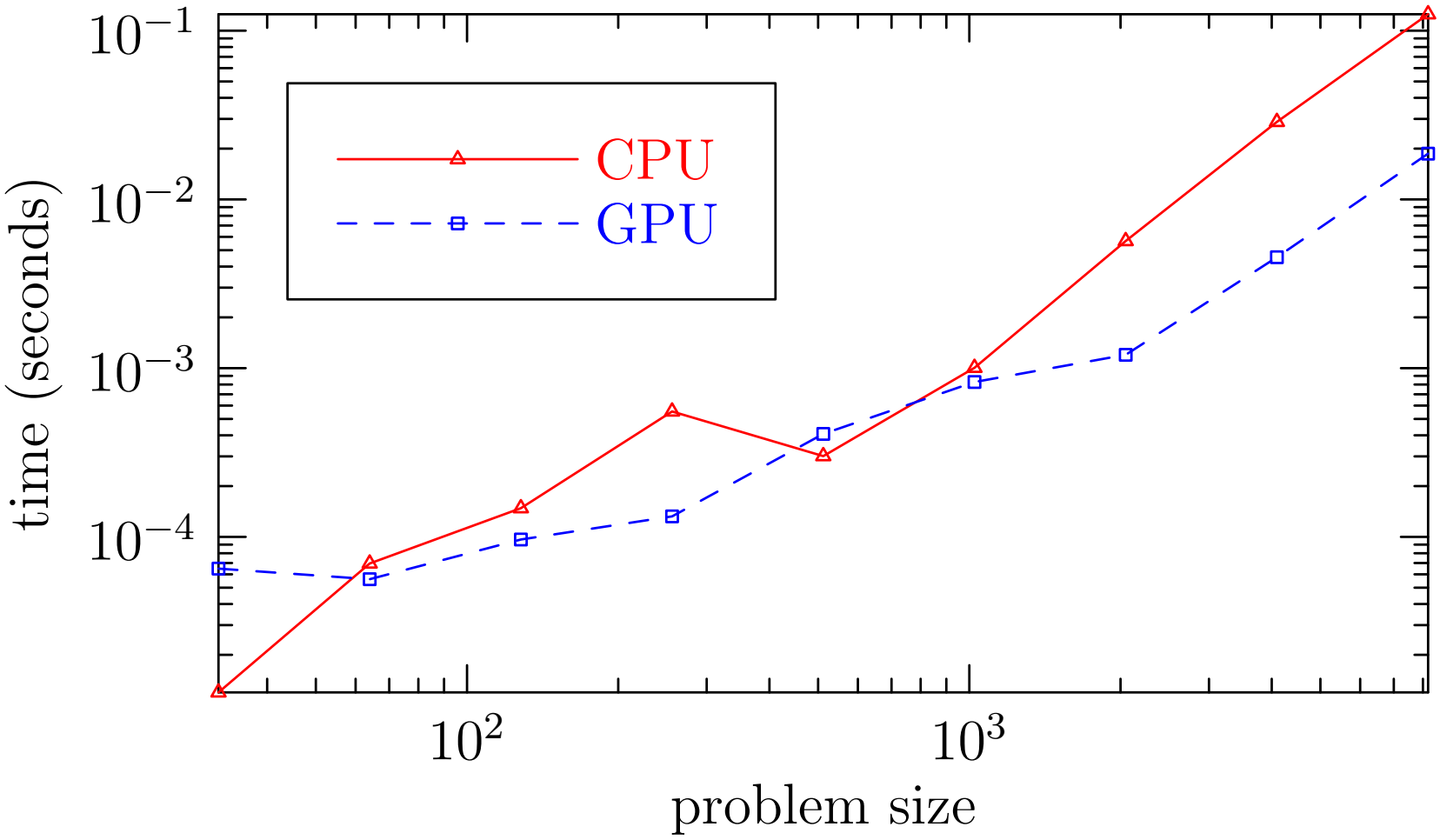
But, is it **fast**?

Performance analysis of schnaps

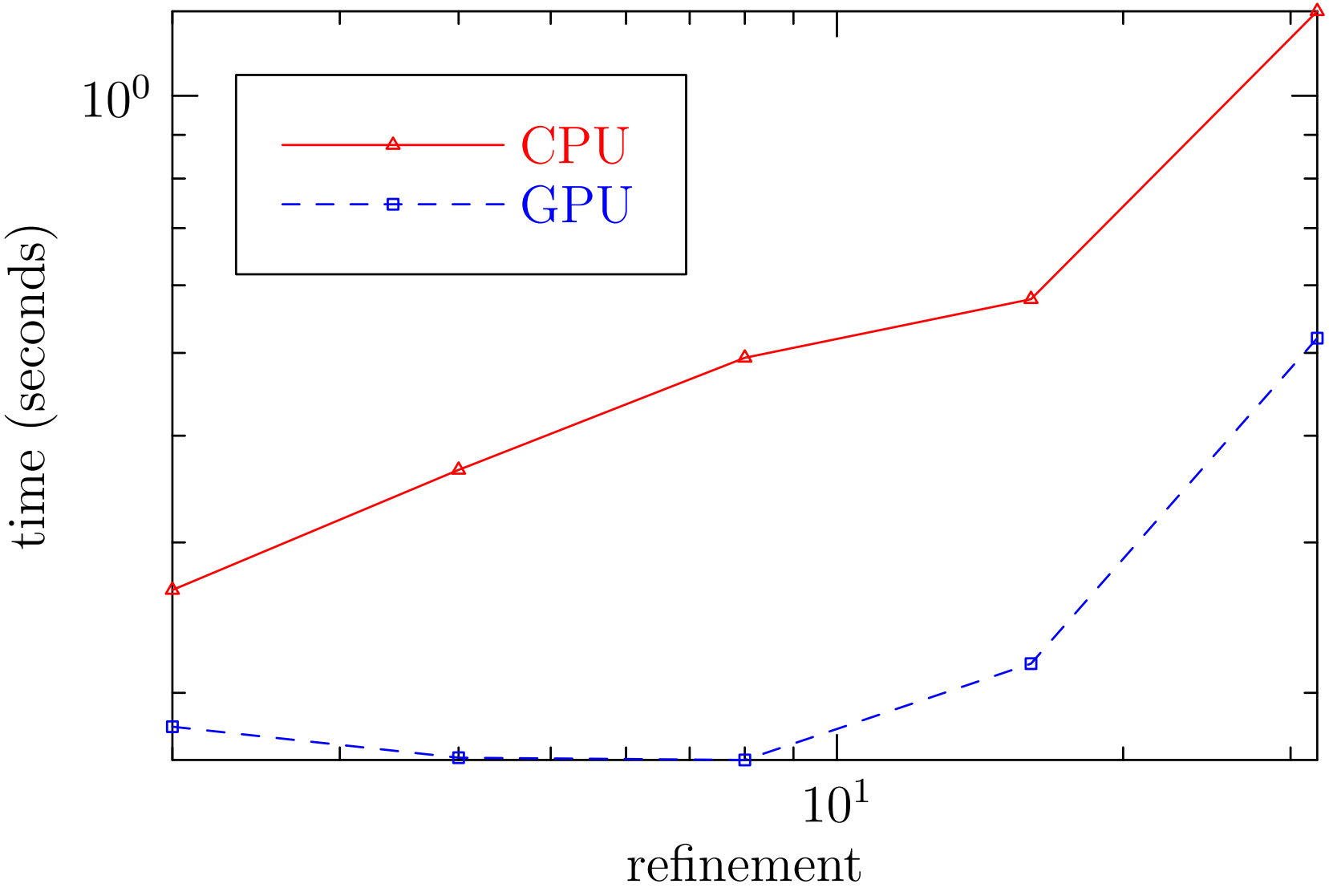


Performance analysis schnaps

clFFT, an FFT library written in OpenCL by AMD.

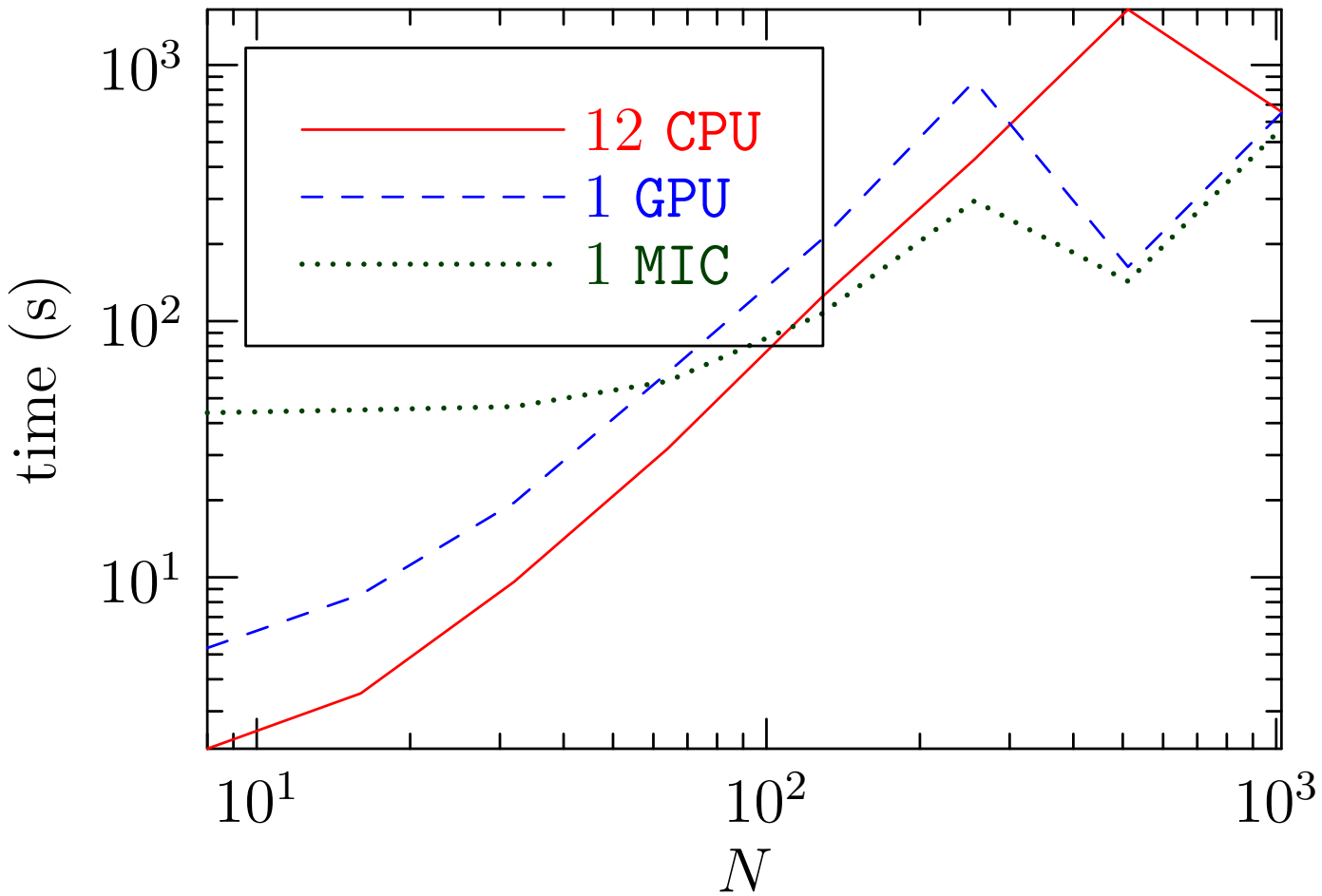


Performance analysis of schnaps



Performance analysis of schnaps

schnaps works well on the Xeon Phi.



schnaps summary

We observe that:

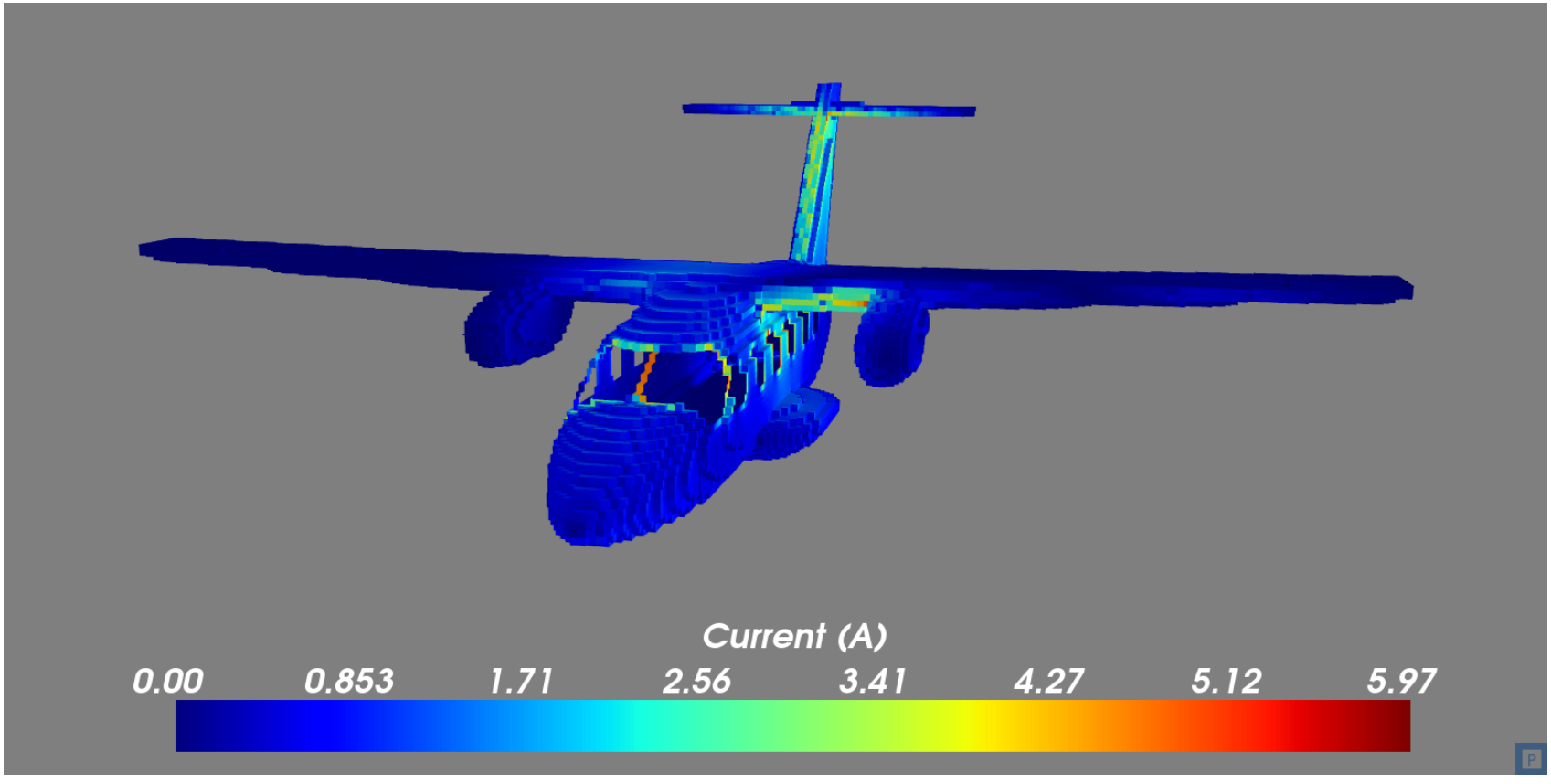
1. The C code makes use of all the cores.
2. The C and OpenCL code speeds on the CPU are close for large problem sizes.
3. The performance difference of schnaps between the CPU and GPU is near what we should expect.

Thus, we claim that our code makes effective use of the GPU.

We can further improve the code by profiling.

Collaboration with Philippe Helluy and TONUS, University of Strasbourg.

Example simulation: Maxwell's equations



Conclusion

I presented two projects:

- `FFTW++`
  - Implicitly Dealiased Convolutions: faster, less memory.
  - `OpenMP` and/or `MPI` implementation.
  - Hybrid `MPI` transpose.
  - Application to a wide variety of situations.
- `schnaps`
  - `OpenCL` implementation of the discontinuous Galerkin method.
  - Good performance on the `CPU`, `GPU`, and `mic`.

Thank you for your attention!

Timing statistics