Implicitly Dealiased Convolutions on Shared-Memory and Distributed-Memory Parallel Processors

John C. Bowman — University of Alberta

Malcolm Roberts — Université de Strasbourg

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`www.math.ualberta.ca/∼bowman/talks`

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- The fast Fourier transform method exploits the properties that $\zeta_N^r = \zeta_{N/r}$ and $\zeta_N^N = 1$.

- However, the pseudospectral method requires a *linear convolution.*

- The unnormalized *backwards discrete Fourier transform* of $\{F_k : k = 0, \ldots, N\}$ is

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- The orthogonality of this transform pair follows from

$$\sum_{j=0}^{N-1} \zeta_N^{\ell j} = \begin{cases} N & \text{if } \ell = sN \text{ for } s \in \mathbb{Z}, \\ \dfrac{1 - \zeta_N^{\ell N}}{1 - \zeta_N^{\ell}} = 0 & \text{otherwise.} \end{cases}$$

Convolution Theorem

$$\sum_{j=0}^{N-1} f_j g_j \zeta_N^{-jk} = \sum_{j=0}^{N-1} \zeta_N^{-jk} \left(\sum_{p=0}^{N-1} \zeta_N^{jp} F_p \right) \left(\sum_{q=0}^{N-1} \zeta_N^{jq} G_q \right)$$

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- *Explicit zero padding* prevents mode $m-1$ from beating with itself and wrapping around to contaminate mode $N = 0 \bmod N$.

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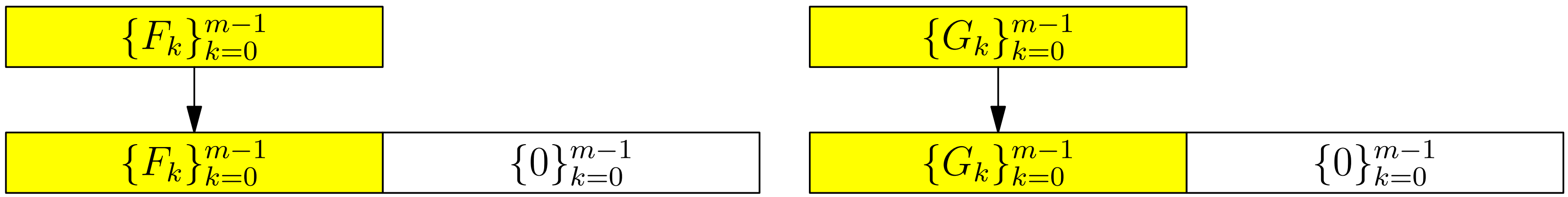

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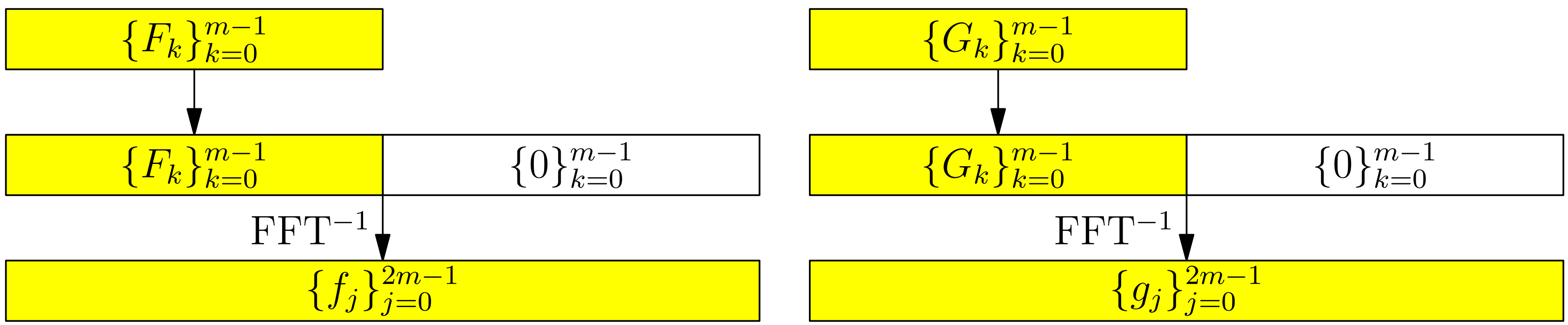

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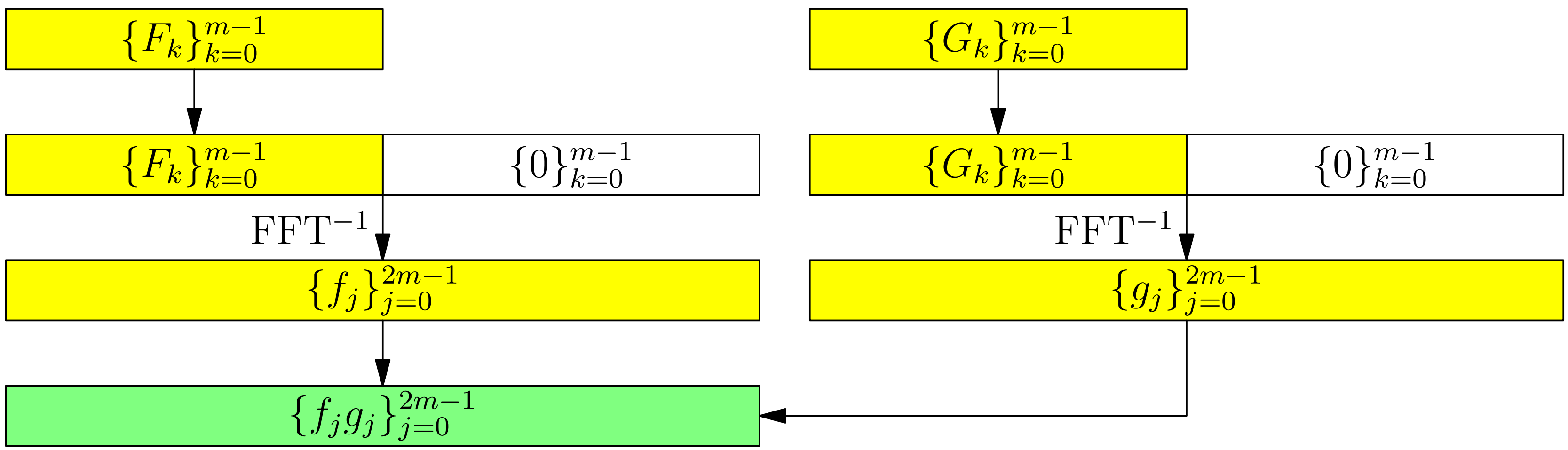

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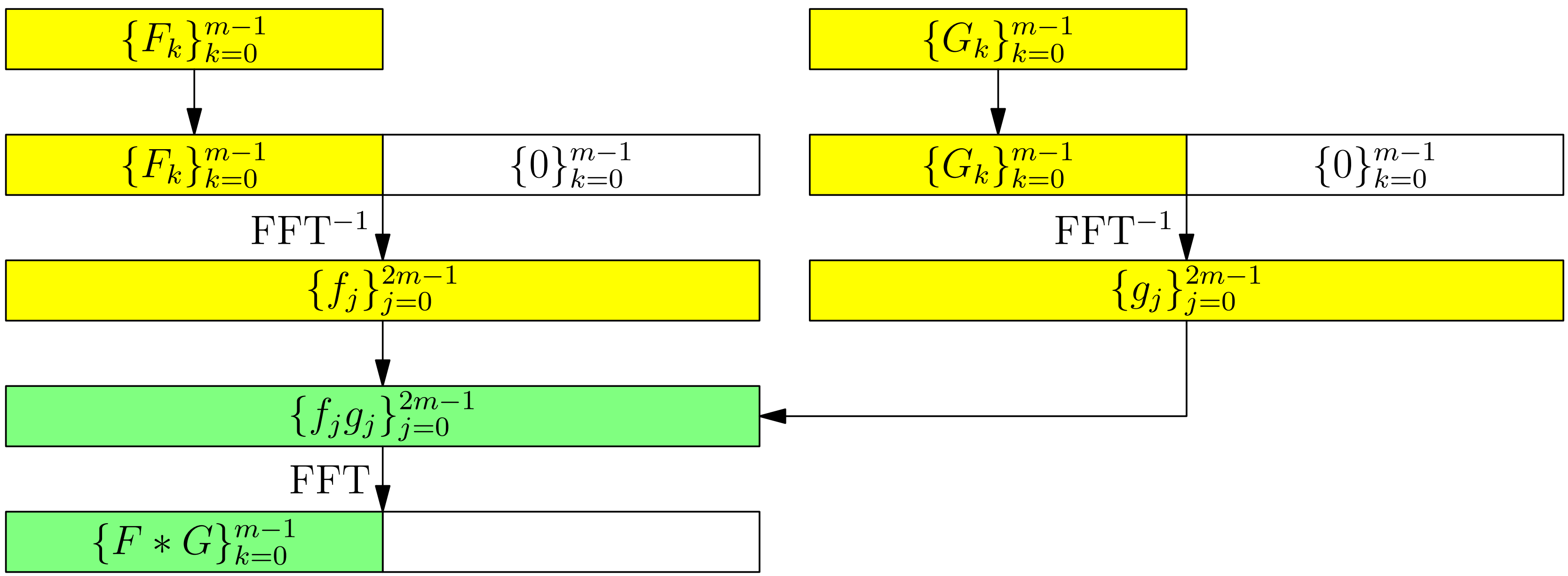

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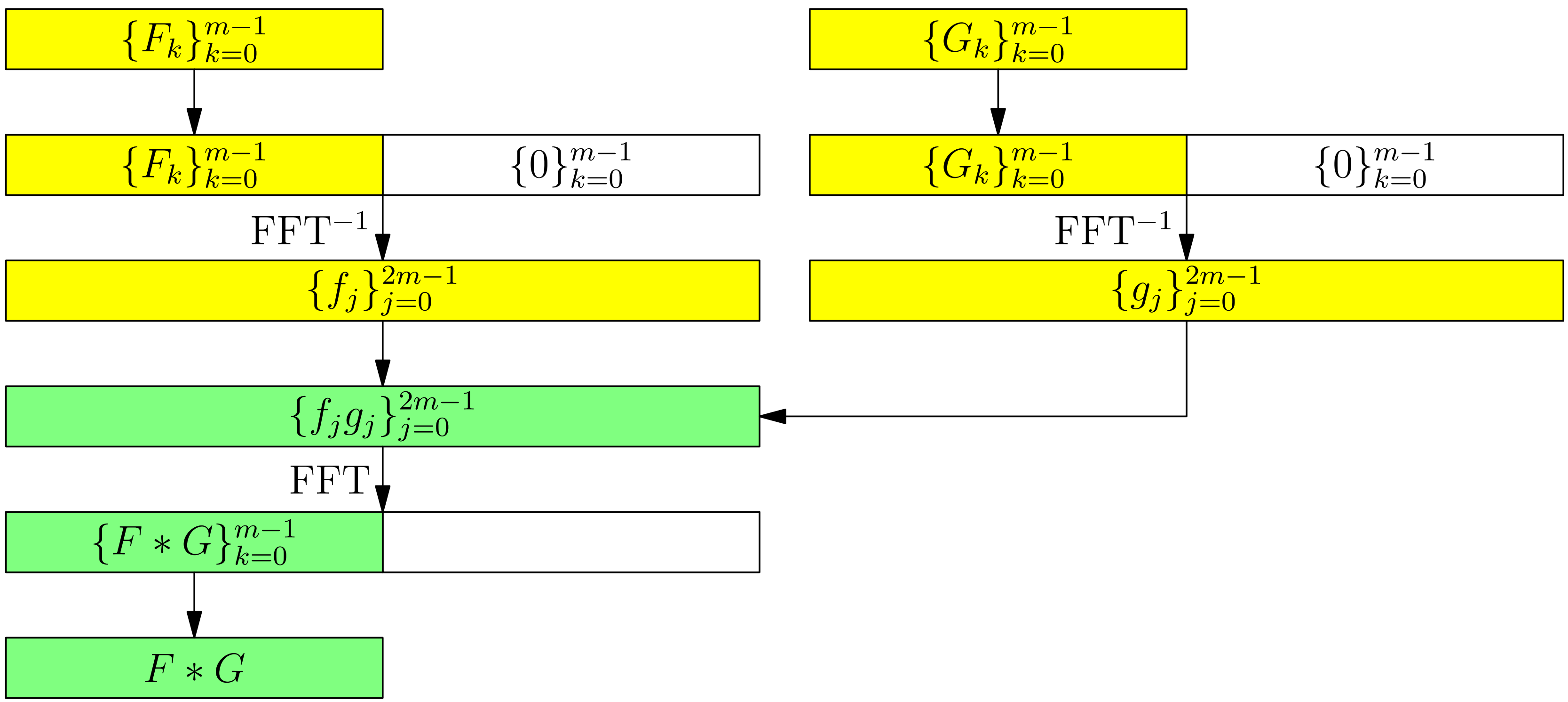

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- This requires computing two subtransforms, each of size m, for an overall computational scaling of order $2m \log_2 m = N \log_2 m$.

- Odd and even terms of the convolution can then be computed separately, multiplied term-by-term, and transformed again to Fourier space:

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\begin{aligned}
2mF_k &= \sum_{j=0}^{2m-1} \zeta_{2m}^{-kj} f_j \\
&= \sum_{\ell=0}^{m-1} \zeta_{2m}^{-k2\ell} f_{2\ell} + \sum_{\ell=0}^{m-1} \zeta_{2m}^{-k(2\ell+1)} f_{2\ell+1} \\
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- No bit reversal is required at the highest level.
- A 1D implicitly padded convolution is implemented in our `FFTW++` library.
- This in-place convolution was written to use six out-of-place transforms, thereby avoiding bit reversal at all levels.

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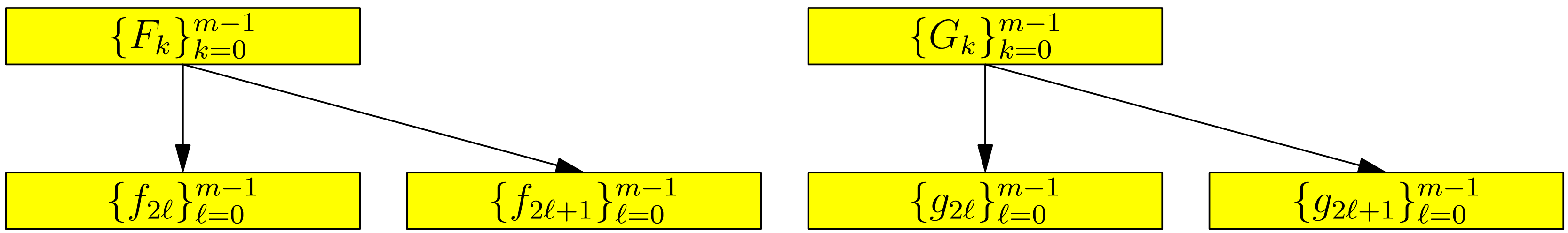

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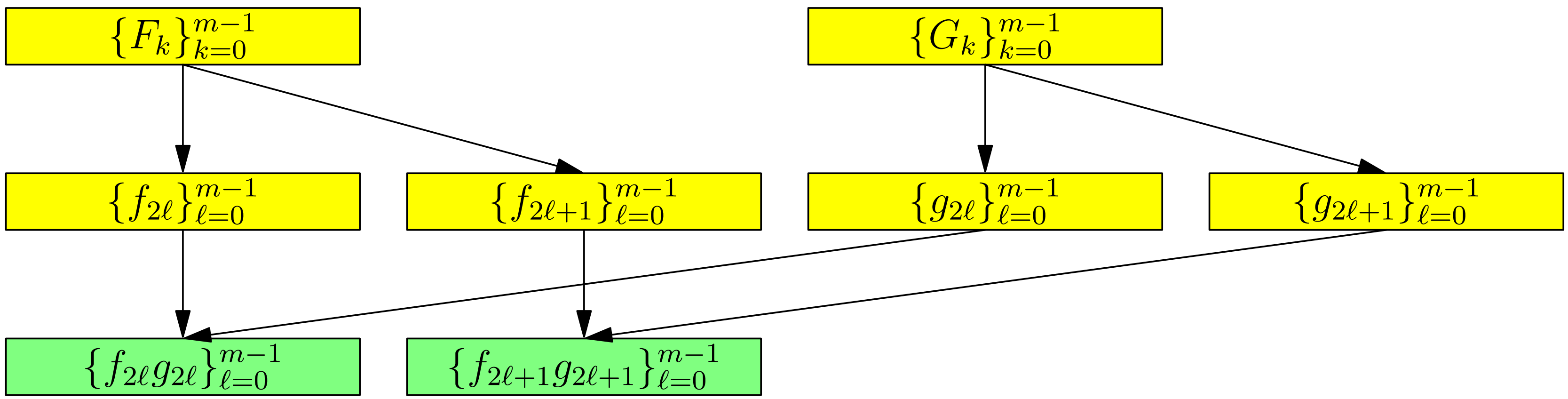

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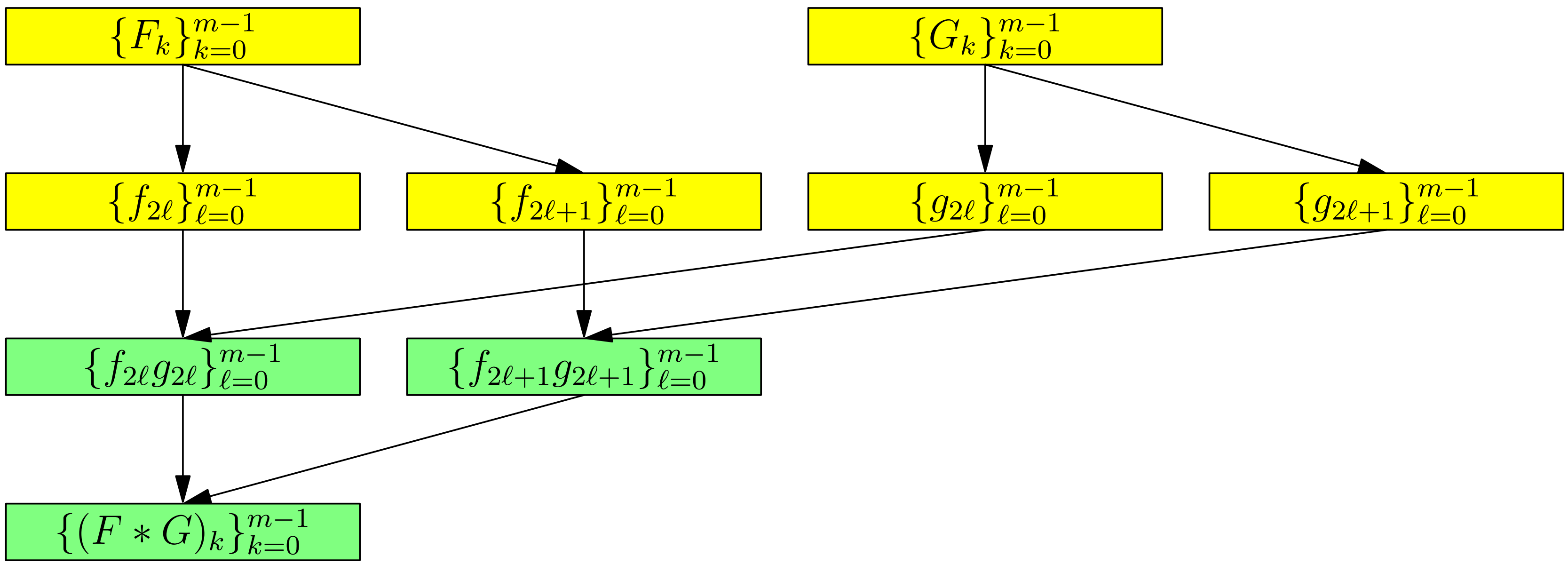

Input: vector f, vector g
Output: vector f

```
u ← fft^{-1}(f);
v ← fft^{-1}(g);
u ← u * v;
for k = 0 to m − 1 do
    f[k] ← ζ_{2m}^k f[k];
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v ← v * f;
f ← fft(u);
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for k = 0 to m − 1 do
    f[k] ← f[k] + ζ_{2m}^{-k} u[k];
end
return f/(2m);
```
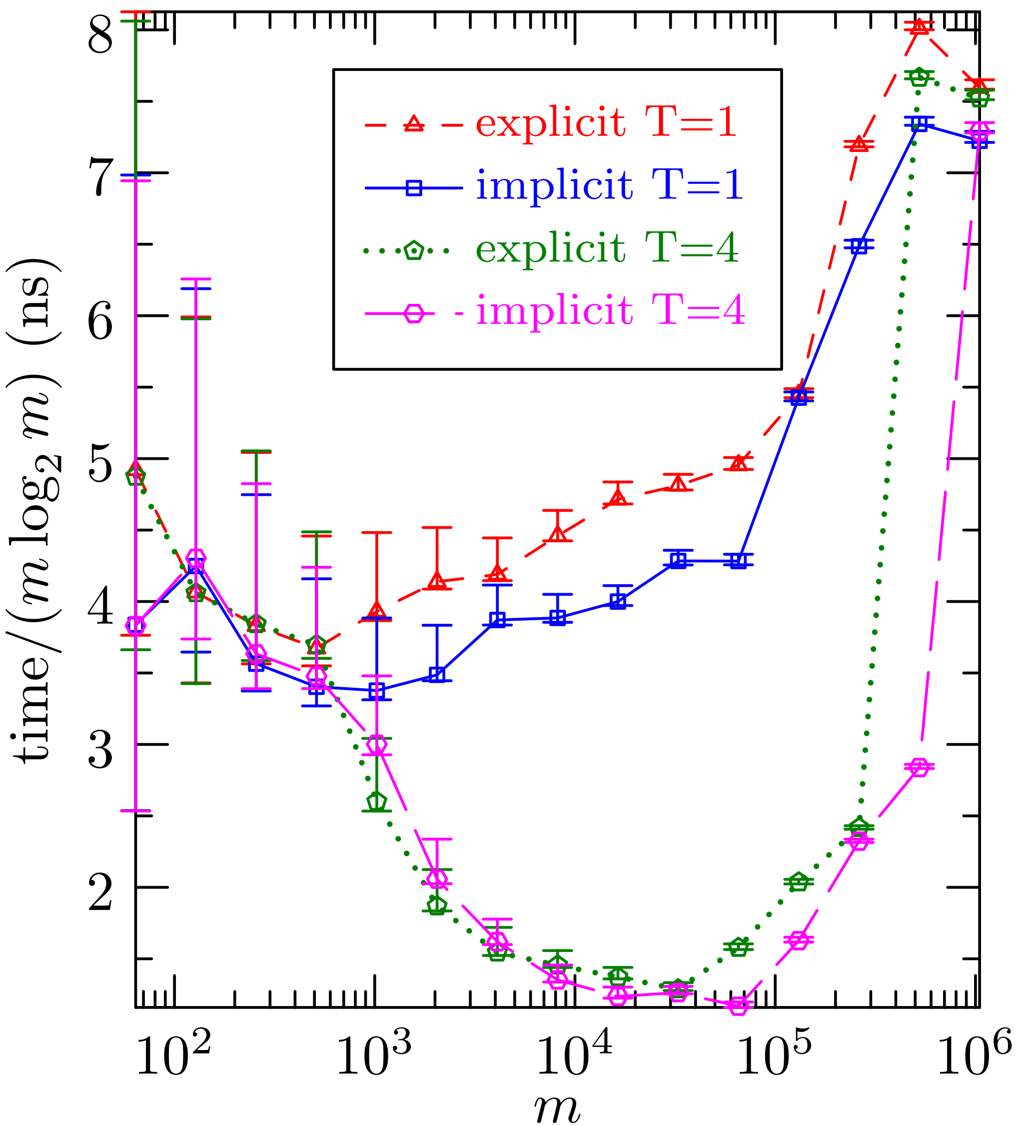

Implicit Padding in 1D



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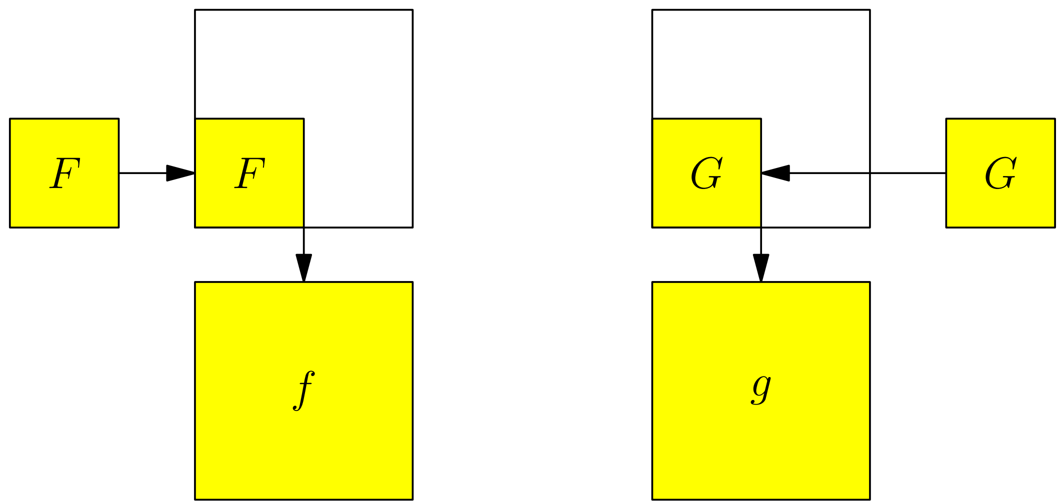

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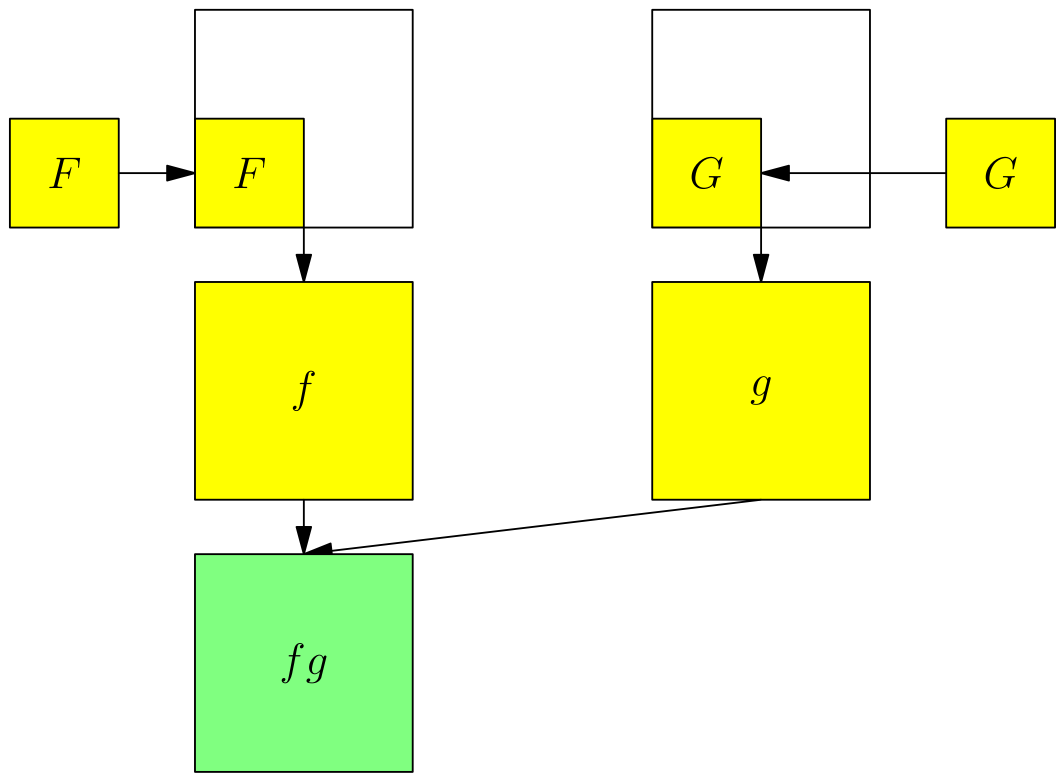

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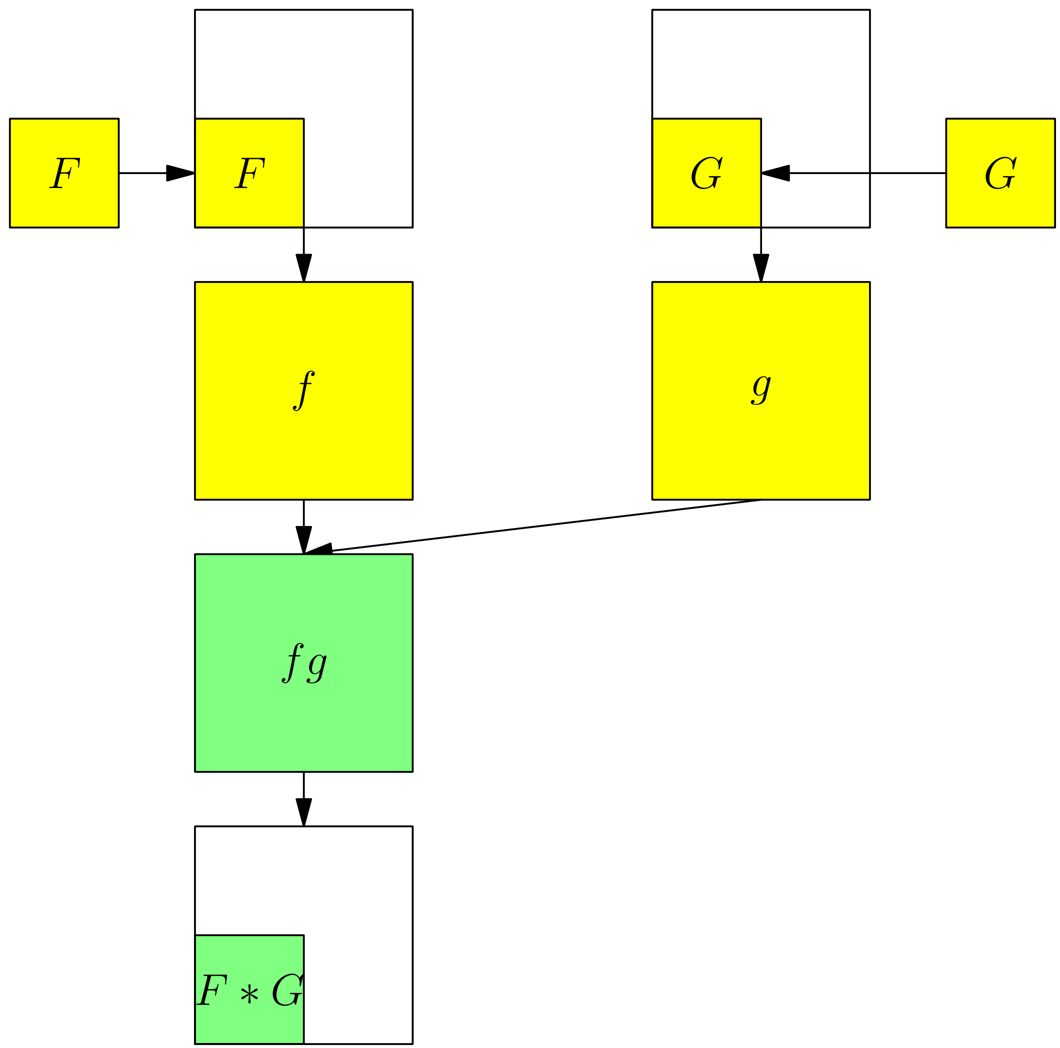

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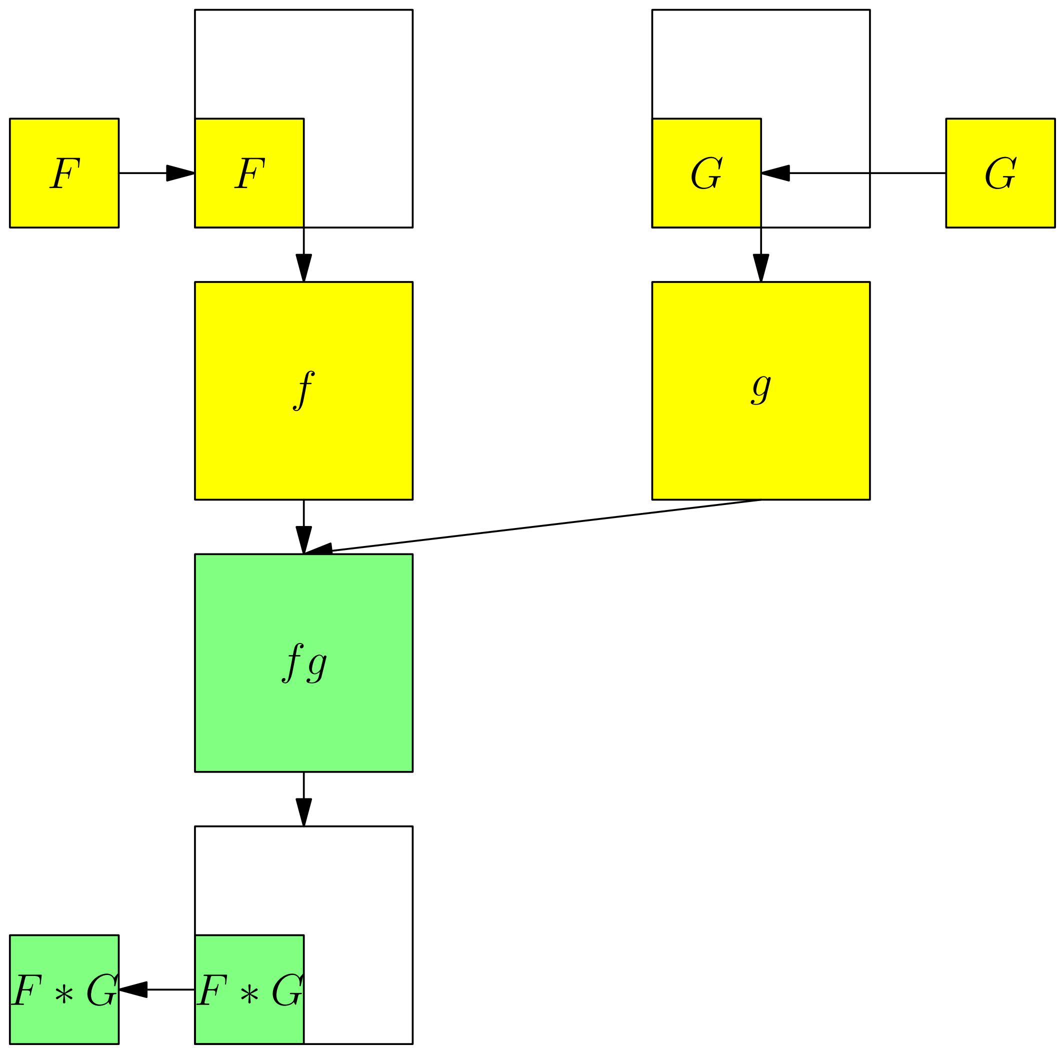
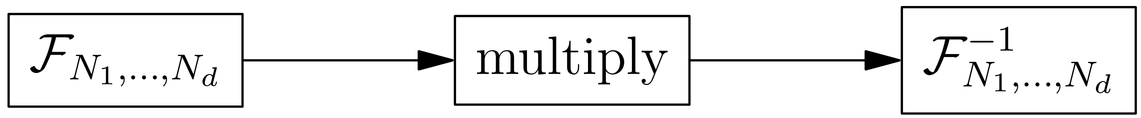


Recursive Convolution

- Naive way to compute a multiple-dimensional convolution:



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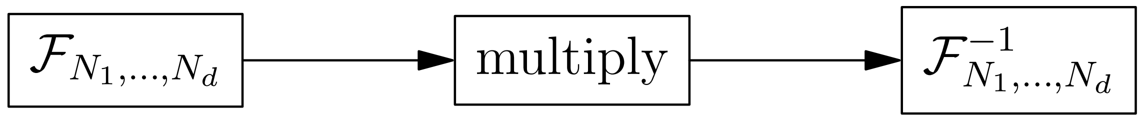
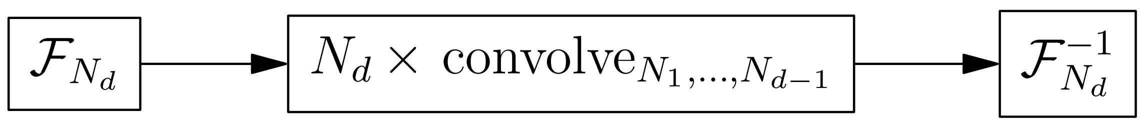


- The technique of *recursive convolution* allows one to avoid computing and storing the entire Fourier image of the data:



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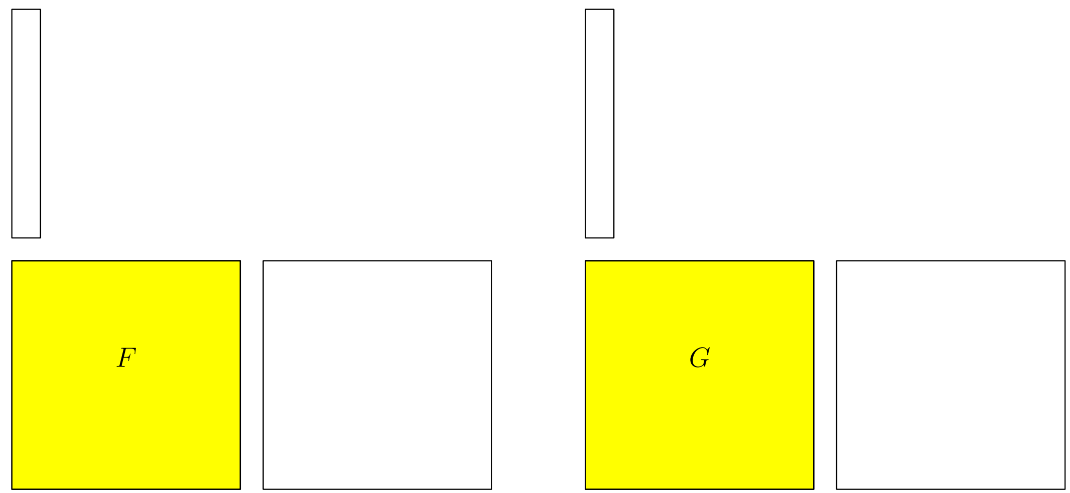

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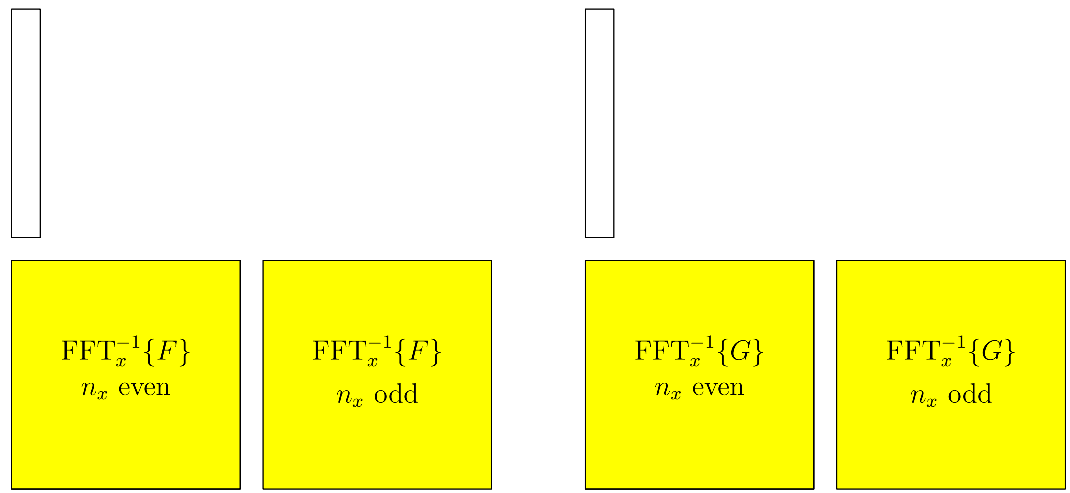

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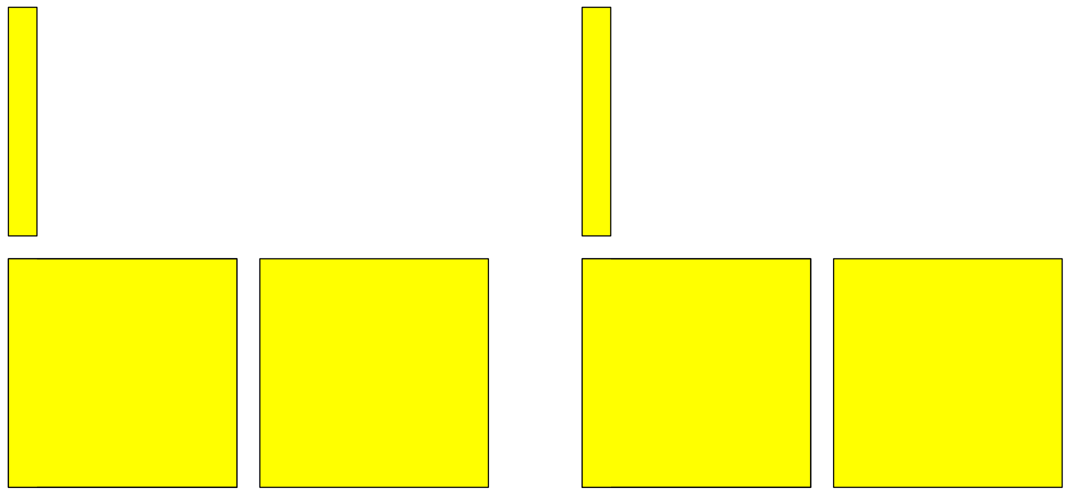

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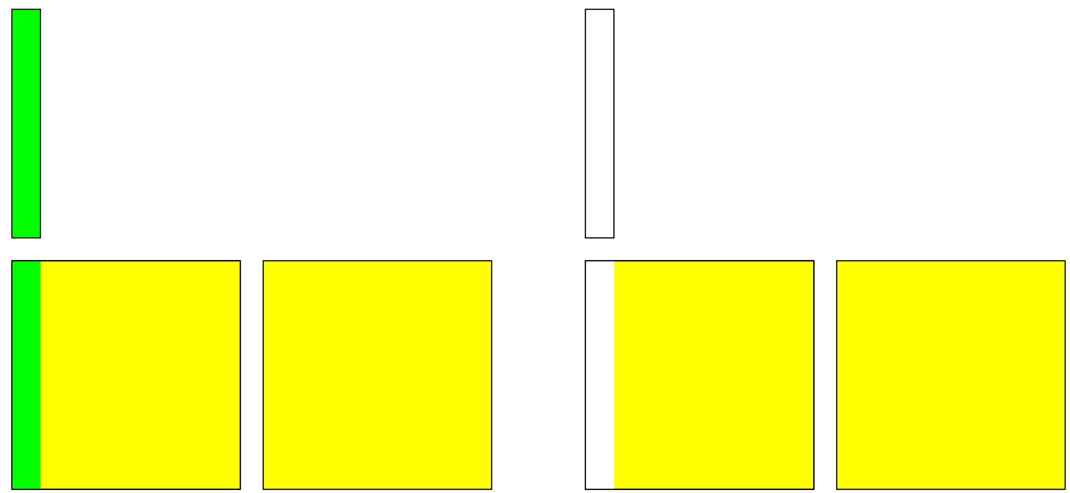

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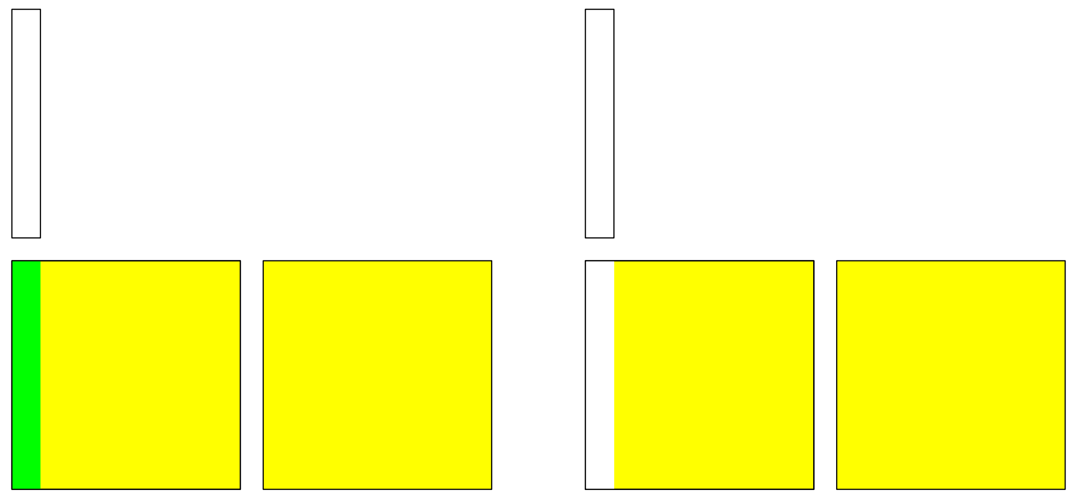

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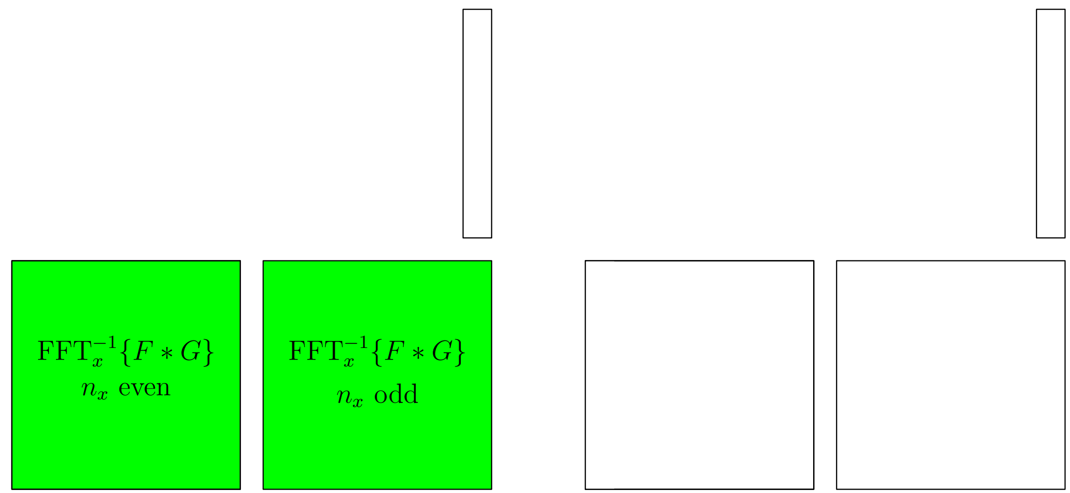

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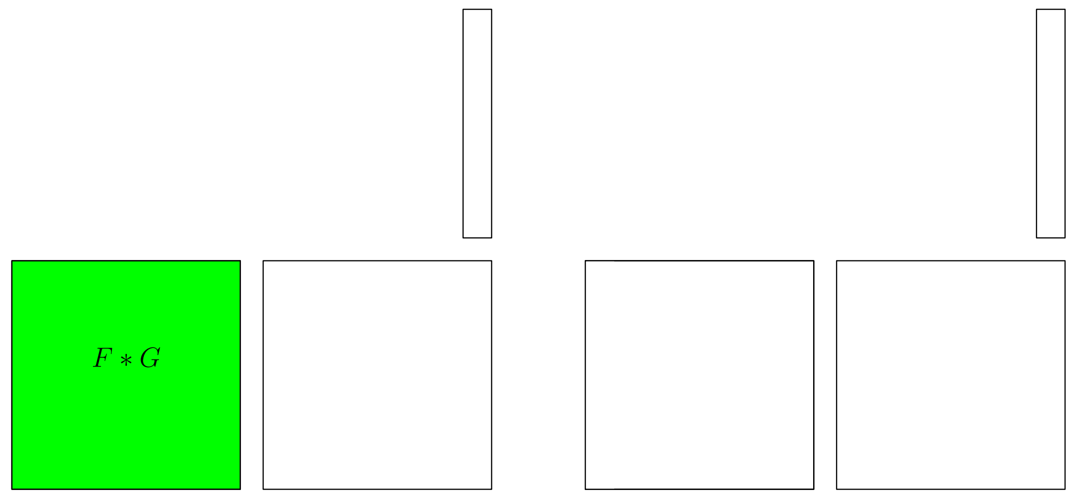

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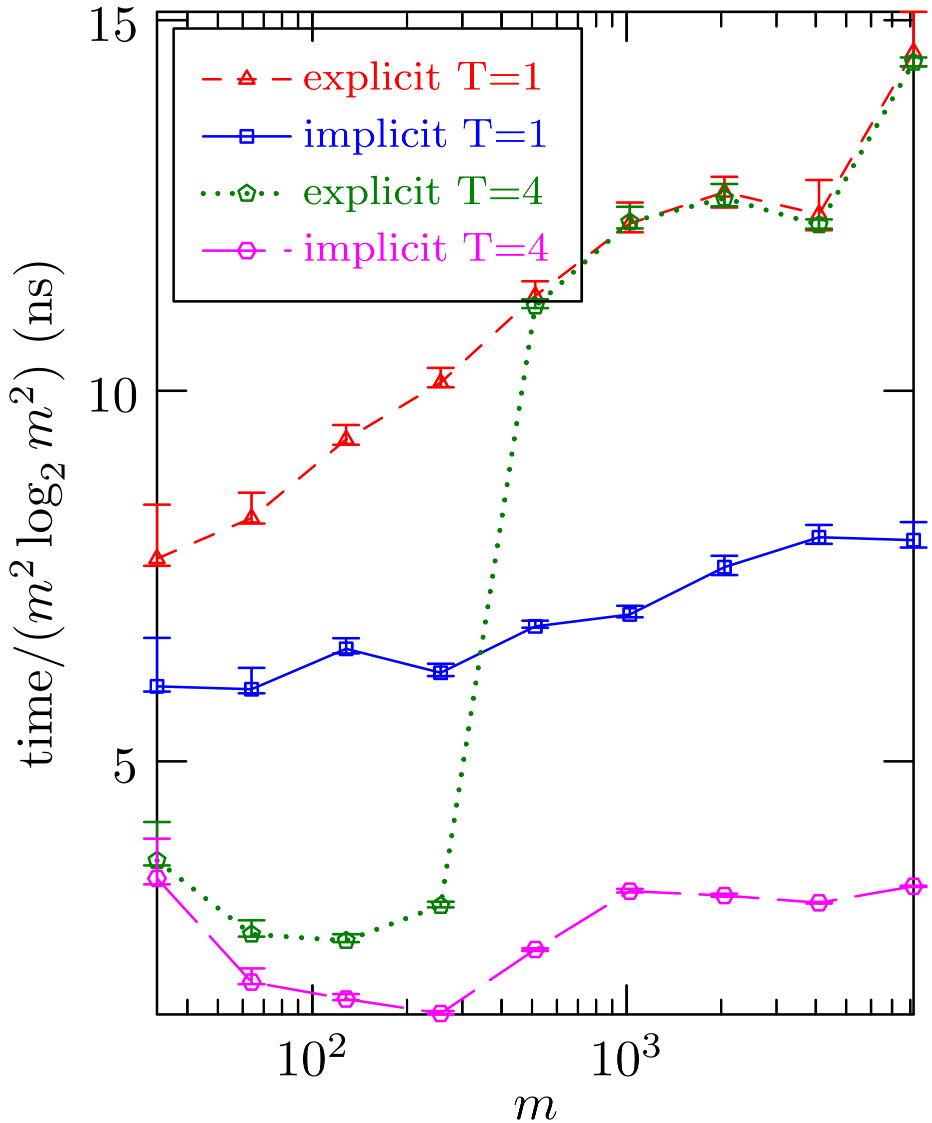
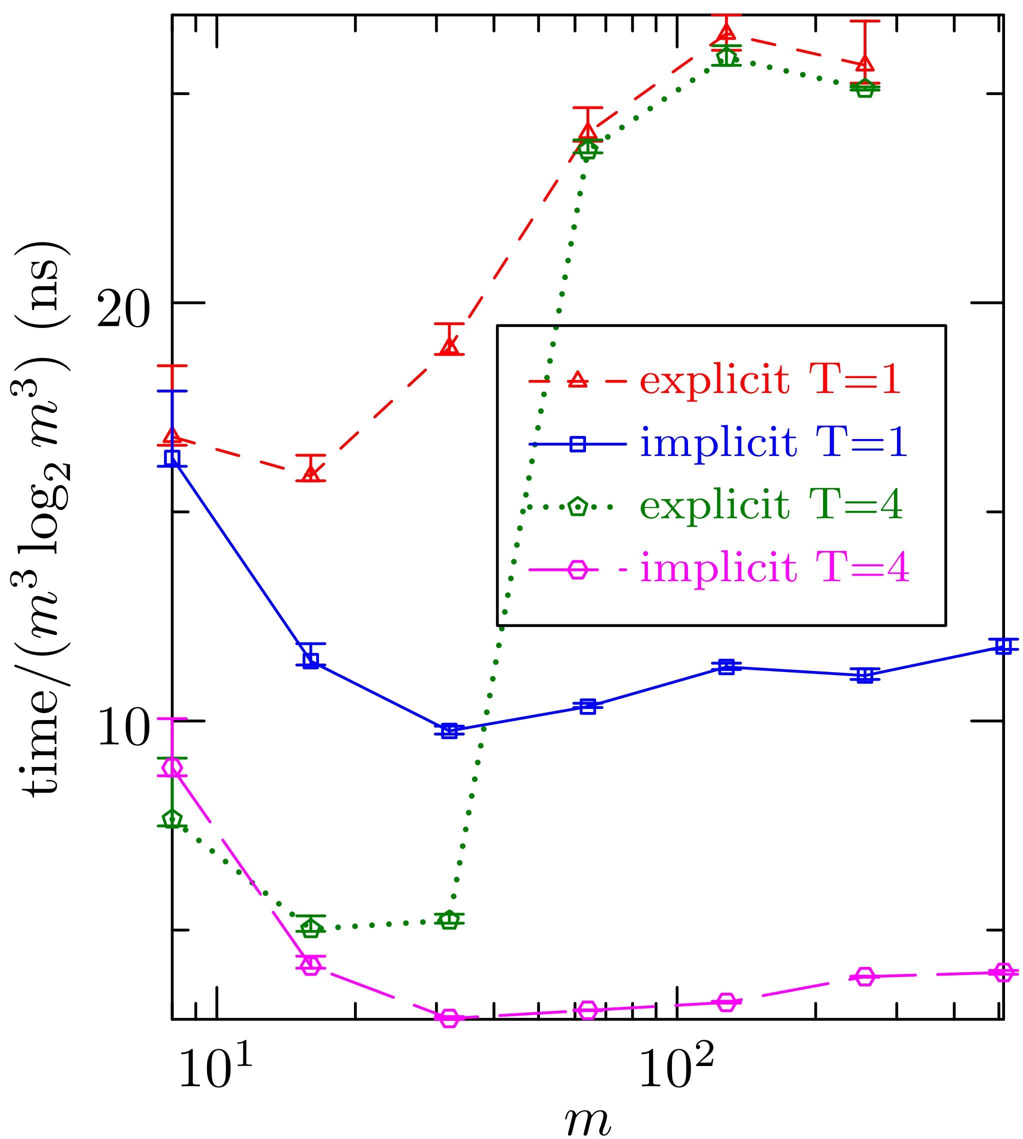


Implicit Padding in 3D



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- A *Hermitian convolution* arises since the input vectors are real:

$$f_{-k} = \overline{f_k}.$$

Hermitian Convolution

- The backwards implicitly padded centered Hermitian transform appears as

$$u_{3\ell+r} = \sum_{k=0}^{m-1} \zeta_m^{\ell k} w_{k,r},$$

where

$$w_{k,r} \doteq \begin{cases} U_0 + \operatorname{Re} \zeta_3^{-r} U_{-m} & \text{if } k = 0, \\ \zeta_{3m}^{rk}\left(U_k + \zeta_3^{-r} \overline{U_{m-k}}\right) & \text{if } 1 \leq k \leq m-1. \end{cases}$$

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- We exploit the Hermitian symmetry $w_{k,r} = \overline{w_{m-k,r}}$ to reduce the problem to three complex-to-real Fourier transforms of the first $c+1$ components of $w_{k,r}$ (one for each $r = -1, 0, 1$), where $c \doteq \lfloor m/2 \rfloor$ zeros.

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- However, loop dependencies in the resulting algorithm prevented the top level of the 1D transforms from being multithreaded.
- Unrolling the loop to process four inputs and outputs simultaneously allows loop independence to be achieved, significantly improving performance in both the serial and parallel contexts.

Shared-Memory Parallelization

- To facilitate an in-place implementation, in our original paper [SIAM J. Sci. Comput. 33, 386 (2011)], we stored the transformed values for $r = 1$ in reverse order in the upper half of the input vector.

- However, loop dependencies in the resulting algorithm prevented the top level of the 1D transforms from being multithreaded.

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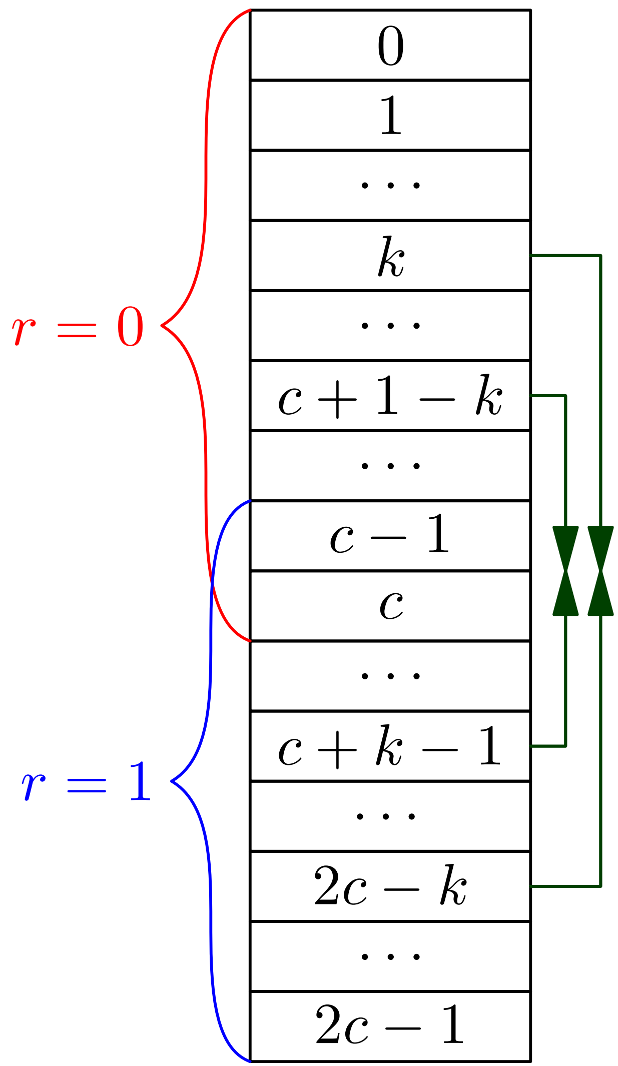
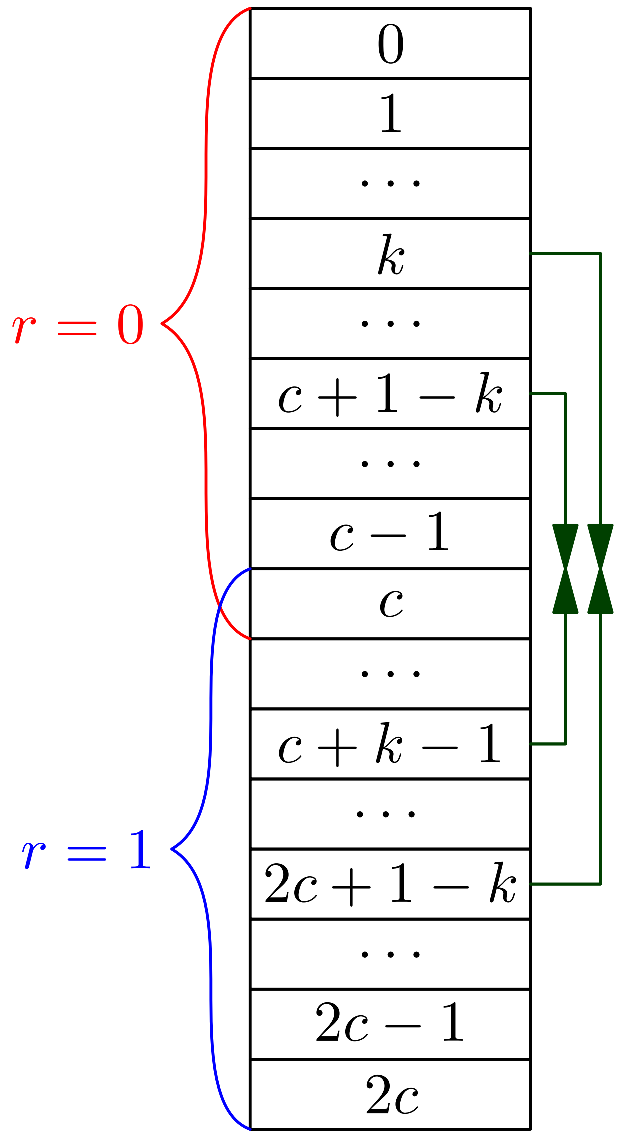
- As a result, even in 1D, implicit dealiasing of pseudospectral convolutions is now significantly faster than explicit zero padding [Roberts & Bowman 2016].

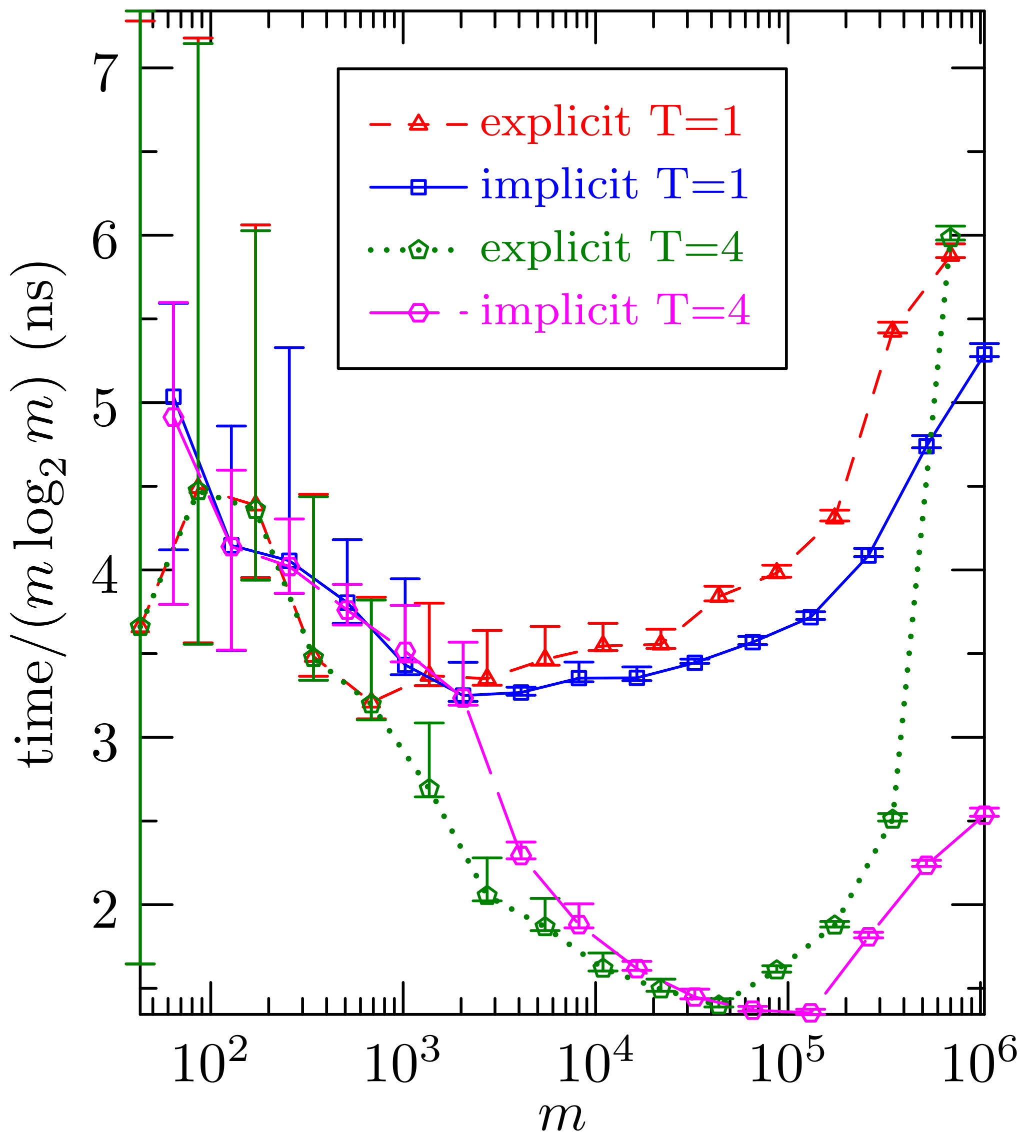
Hermitian Convolution for $m = 2c$



Hermitian Convolution for $m = 2c + 1$



1D Implicit Hermitian Convolution



Distributed-Memory Parallelization

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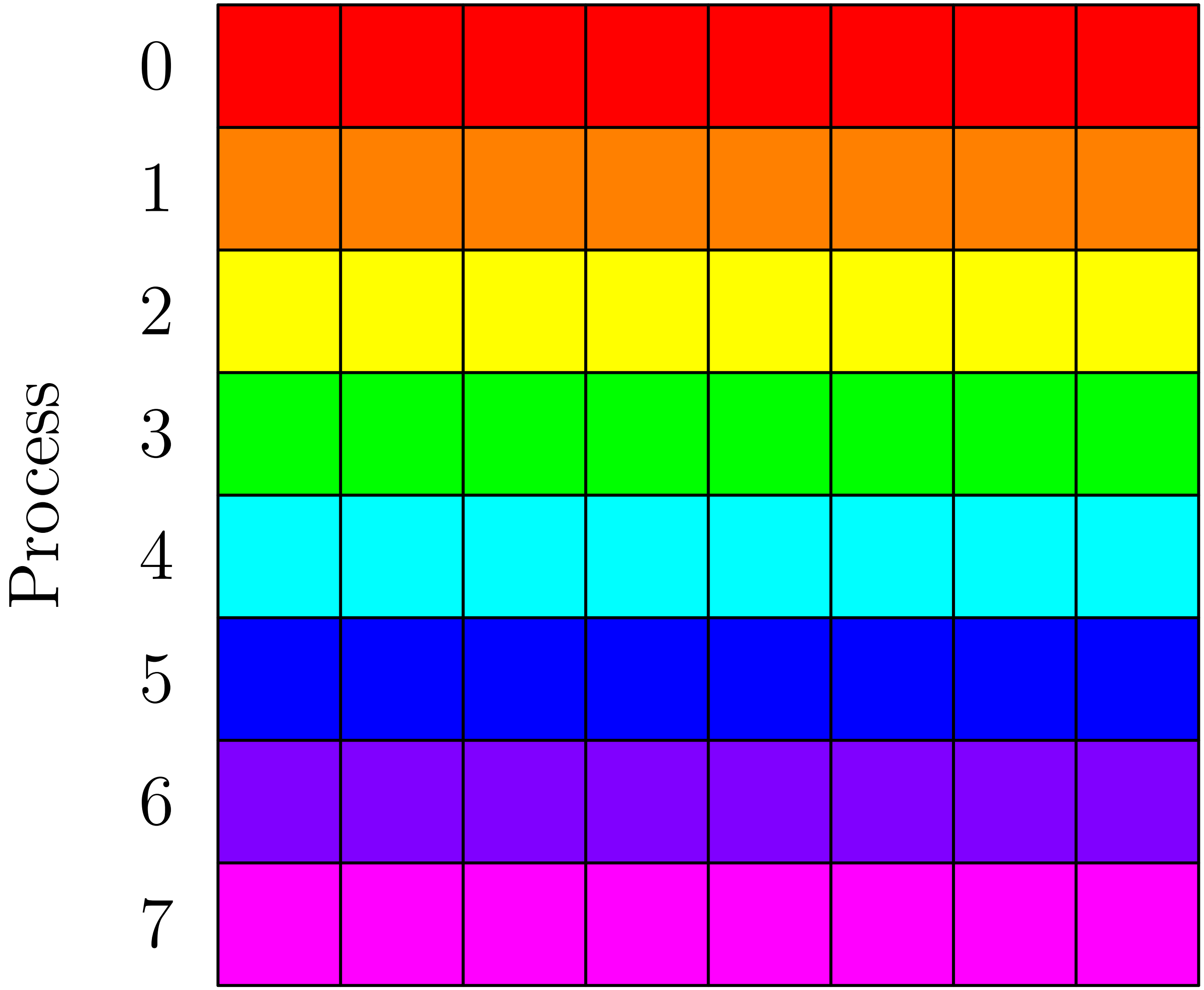
- Local transposition is not required within a single MPI node.
- We have developed an adaptive algorithm, dynamically tuned to choose the optimal block size.

8×8 Block Transpose over 8 processors



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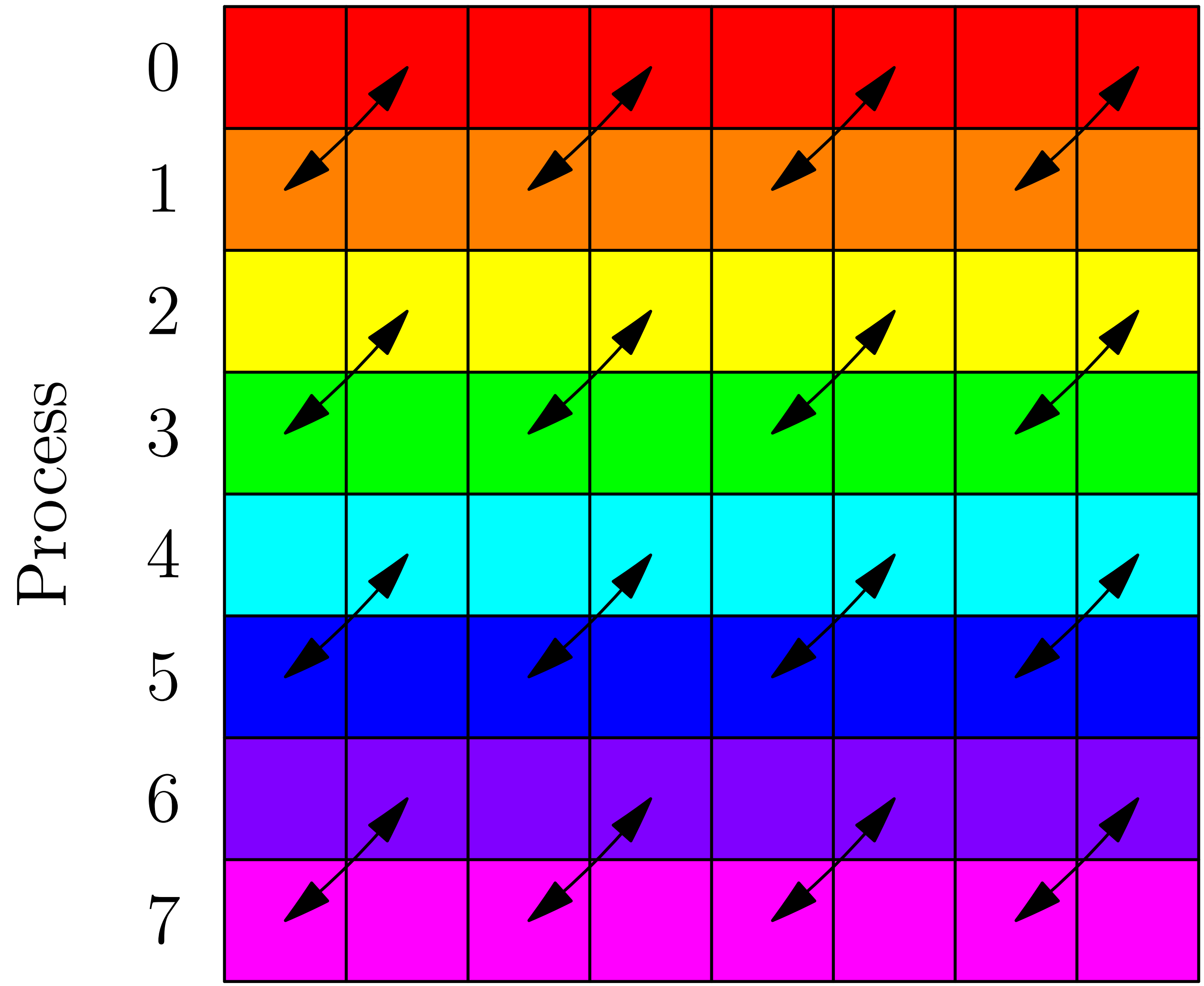

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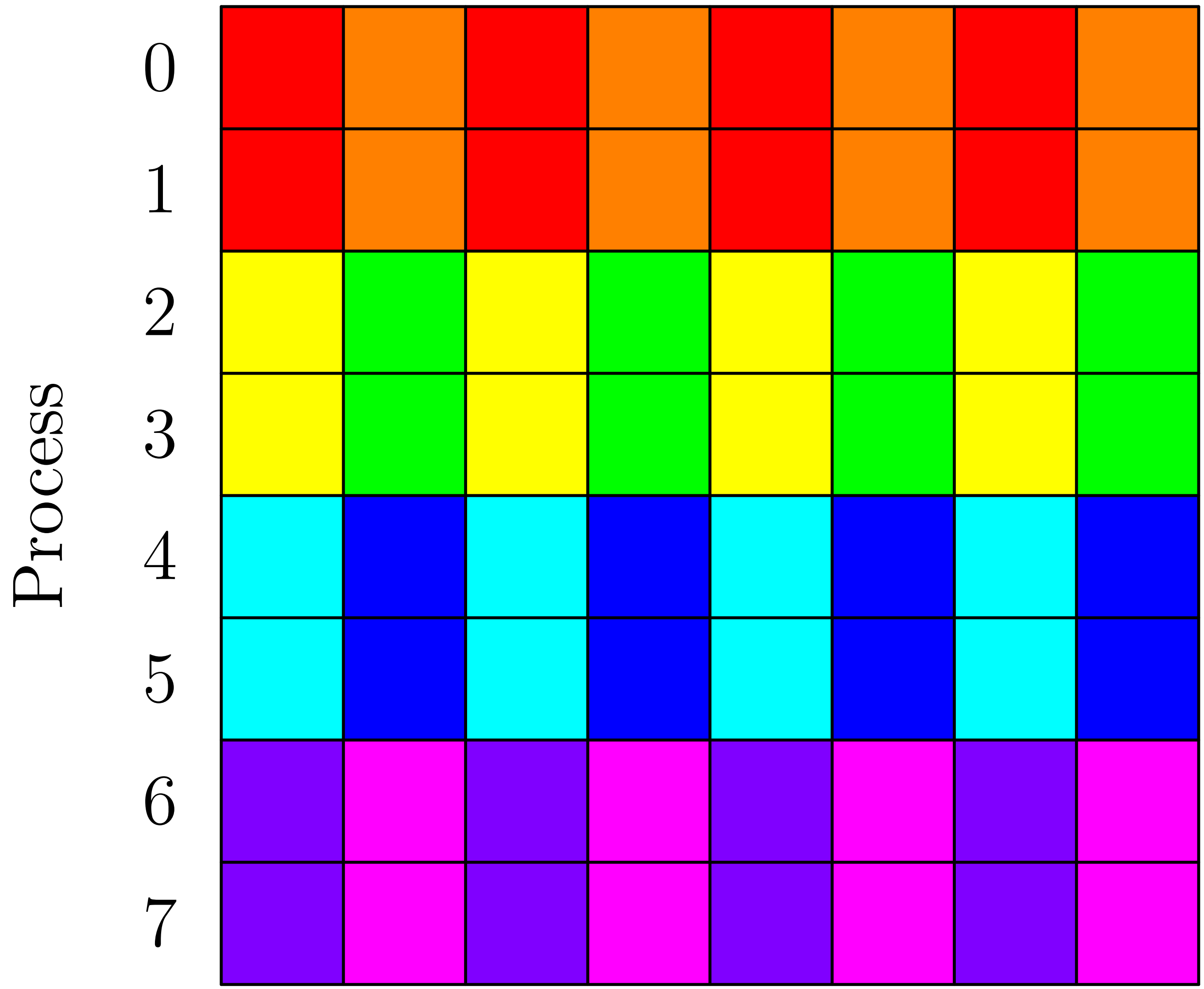

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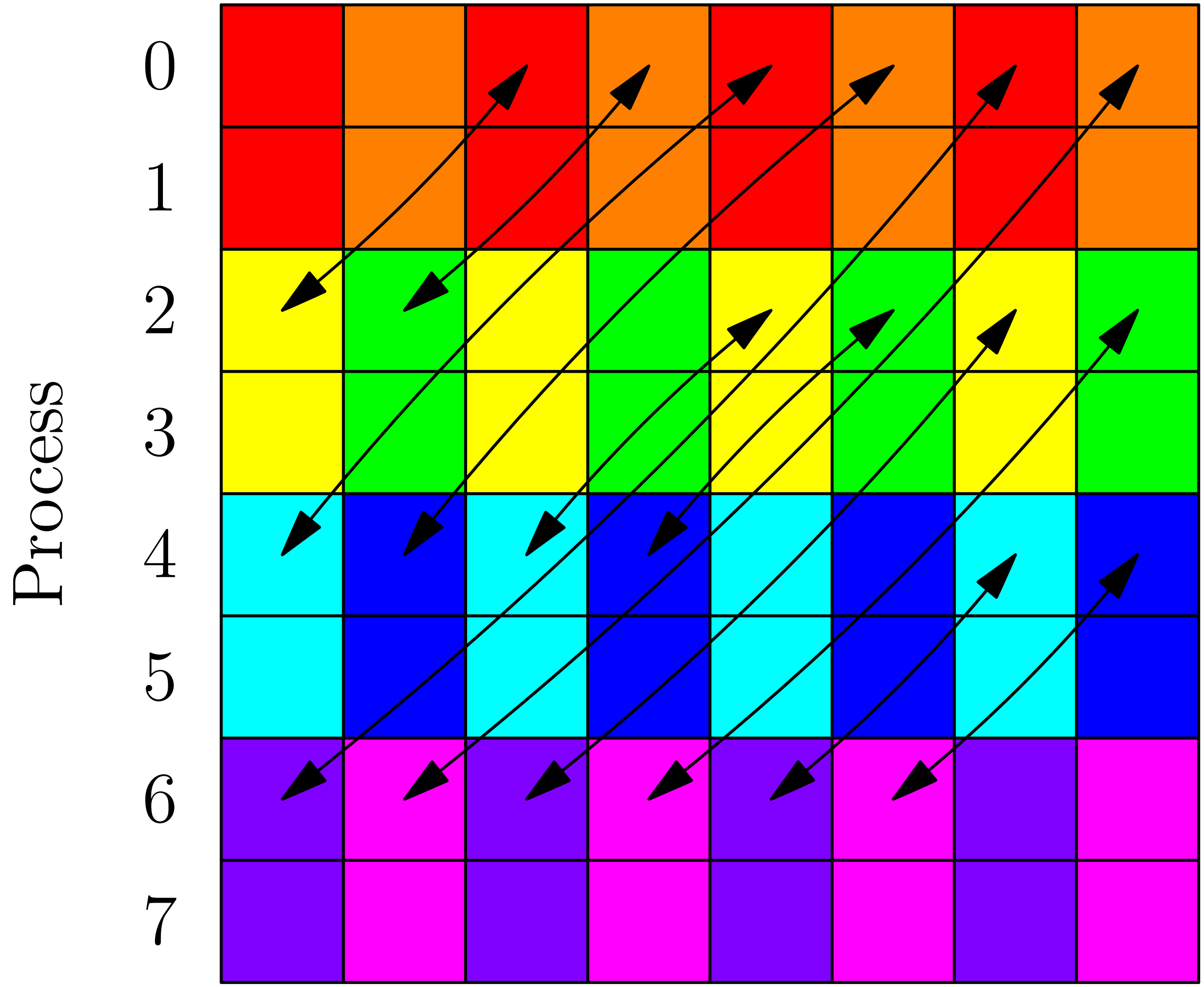

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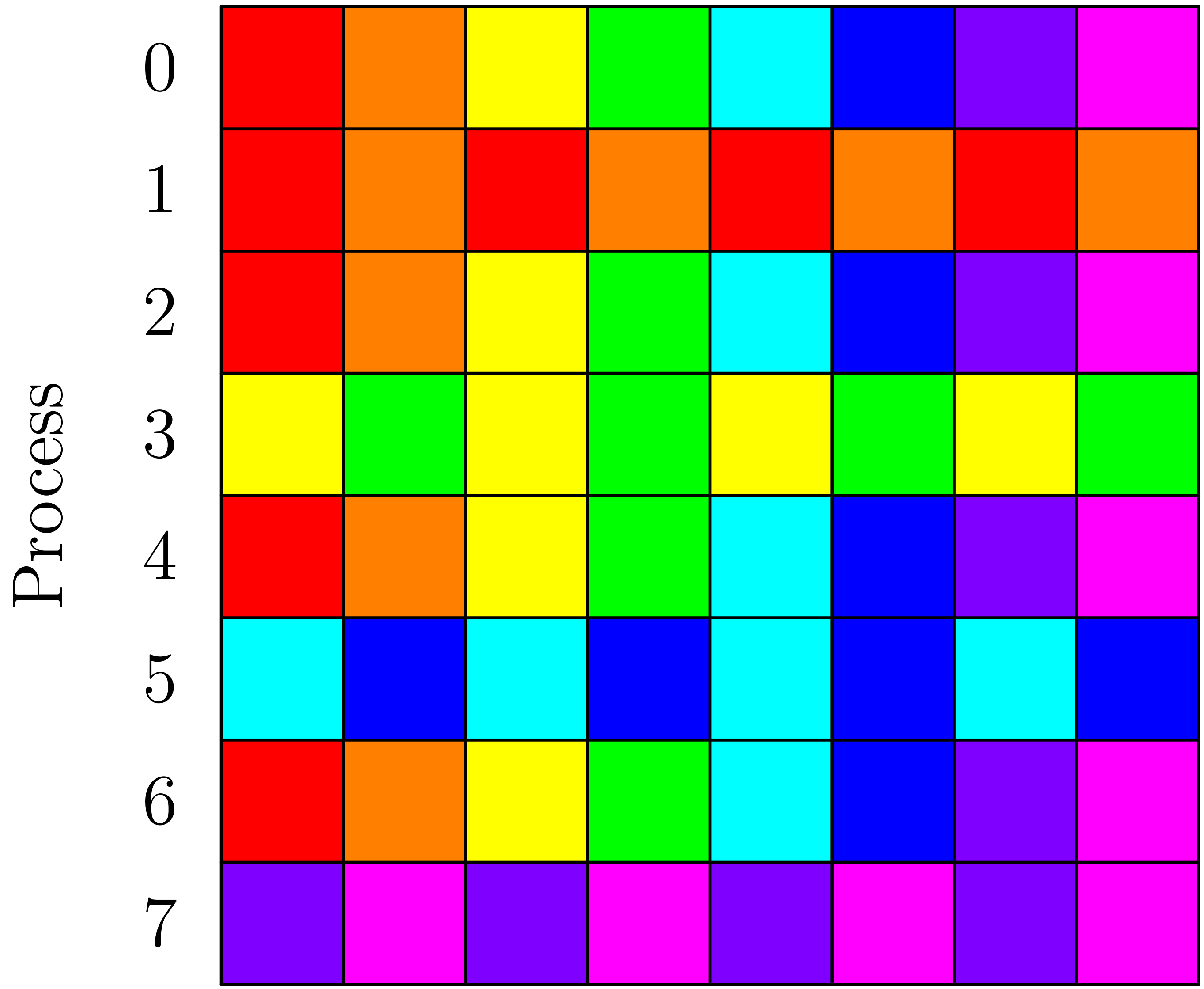

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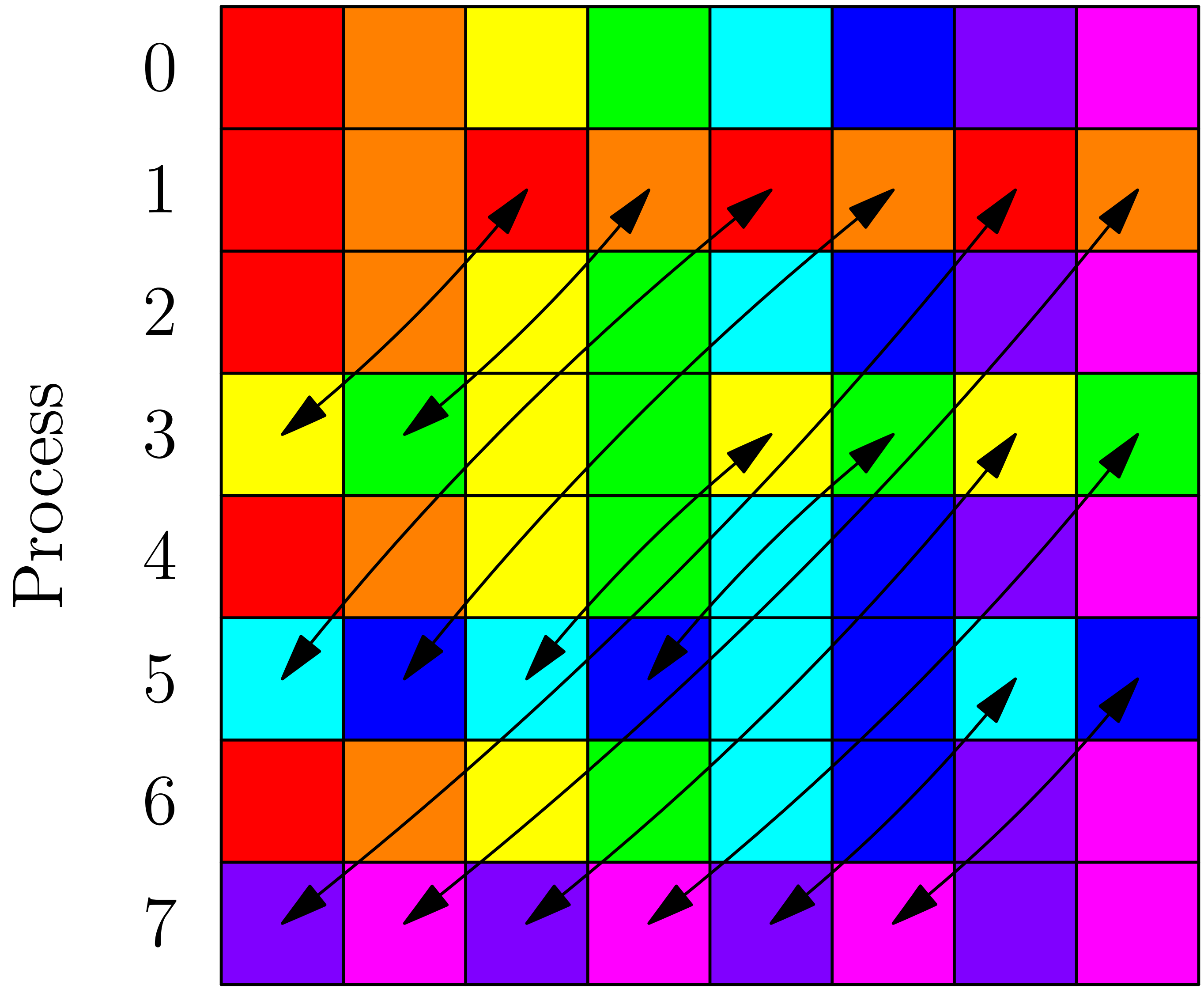

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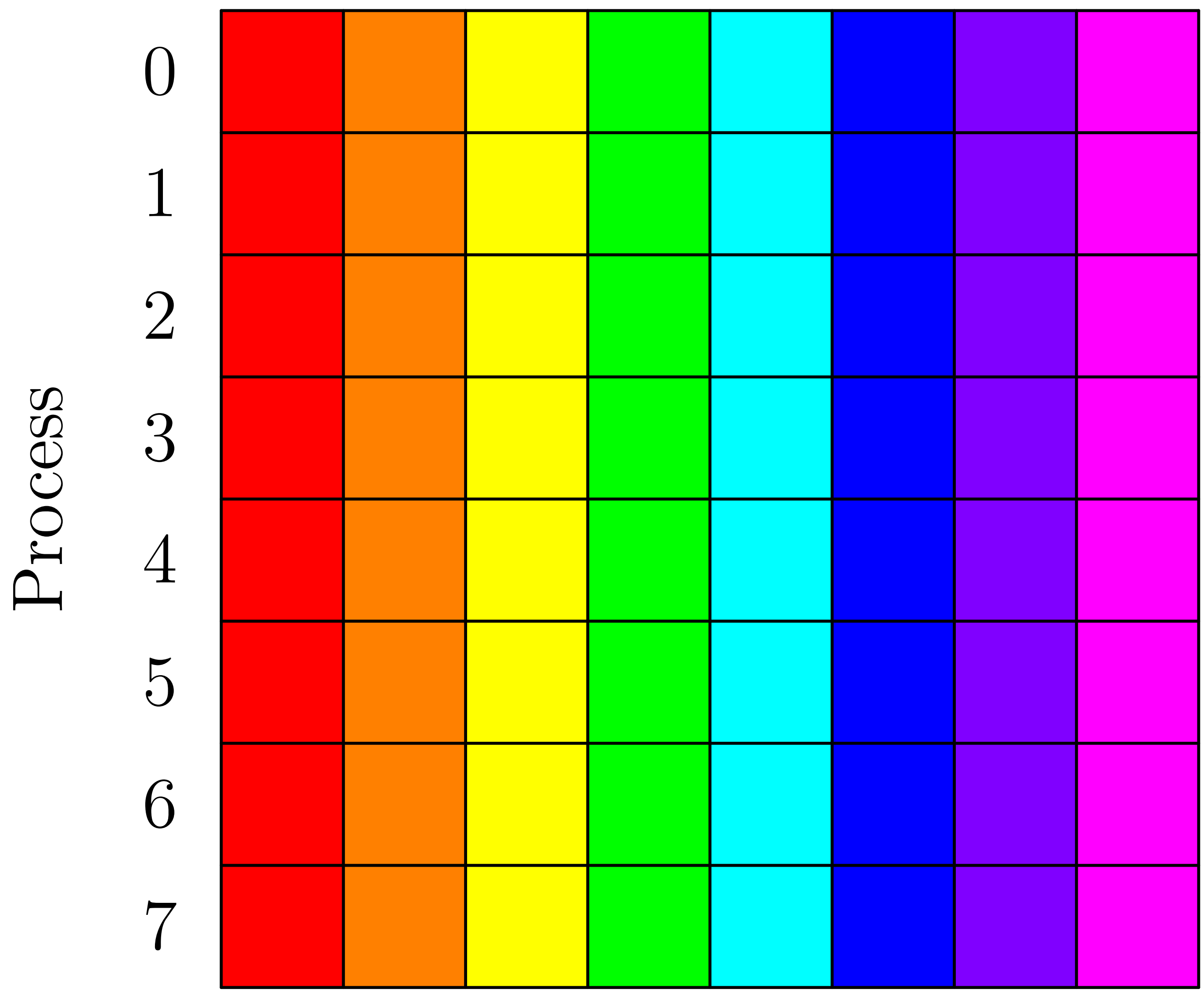

Advantages of Hybrid MPI/OpenMP

- Use hybrid OpenMPI/MPI with the optimal number of threads:

  – yields larger communication block size;

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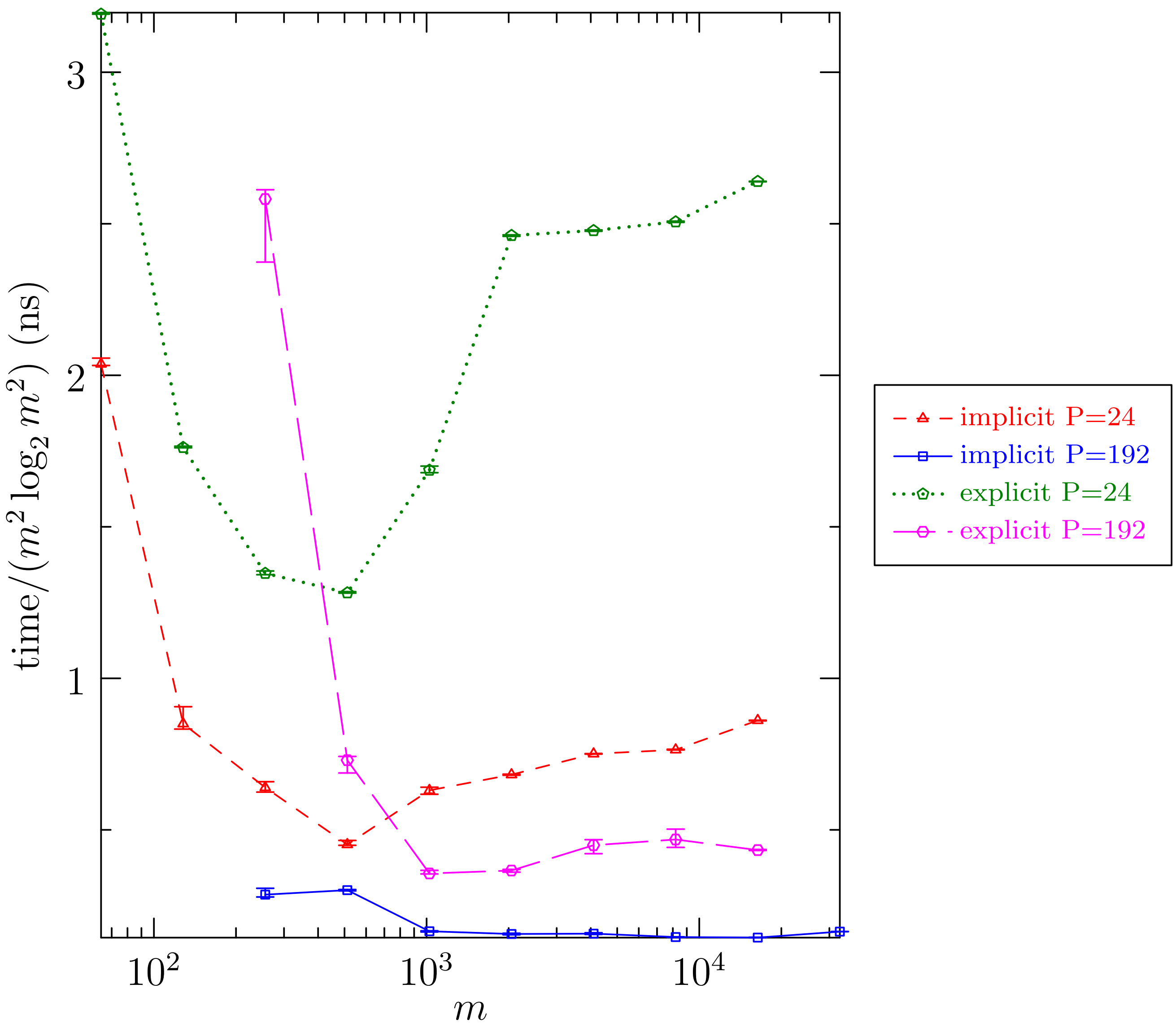
- The use of nonblocking MPI communications allows us to overlap computation with communication: this can yield up to an additional 32% performance gain for implicitly dealiased convolutions, for which a natural parallelism exists between communication and computation.

Pure MPI 2D Convolutions



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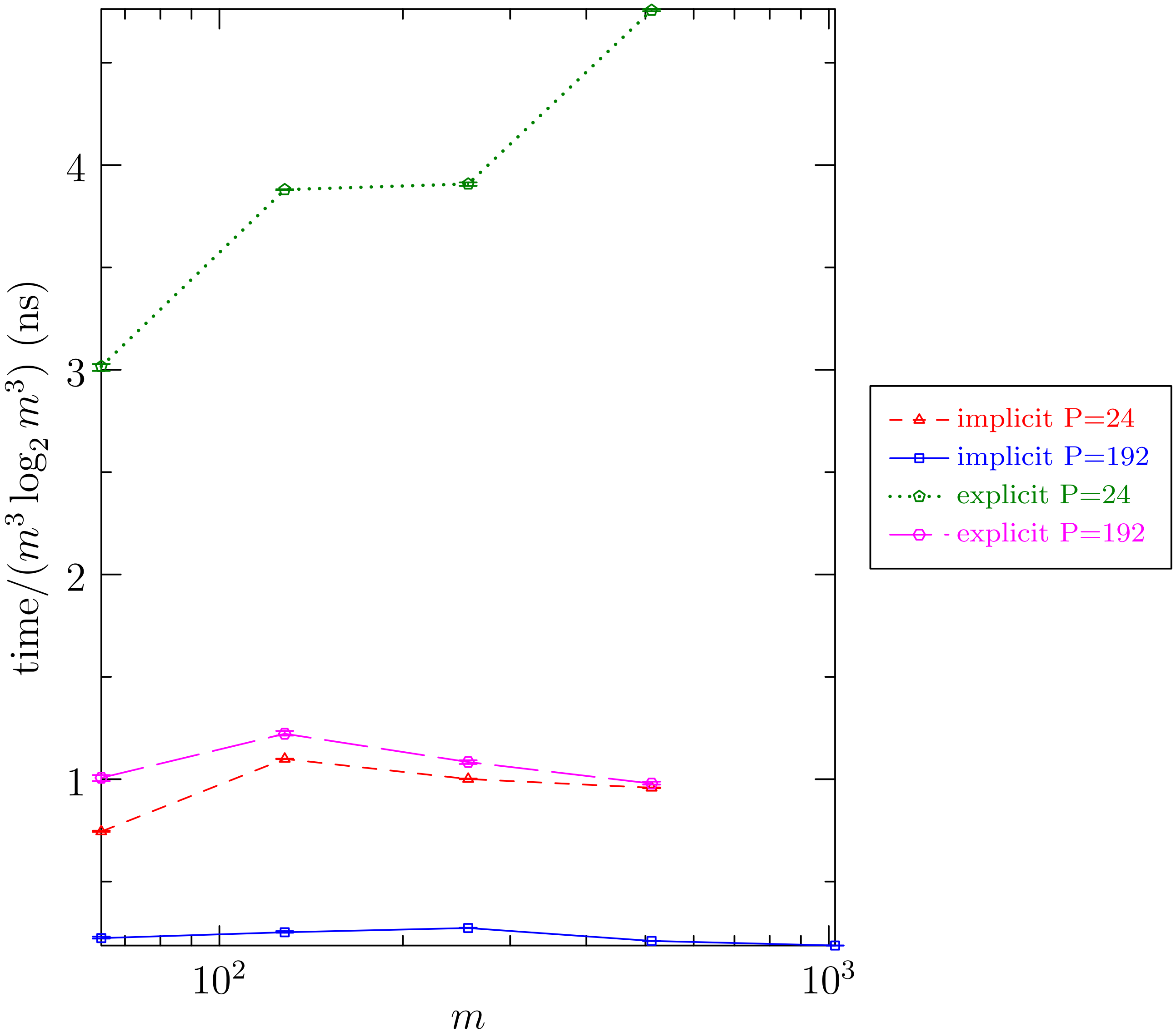
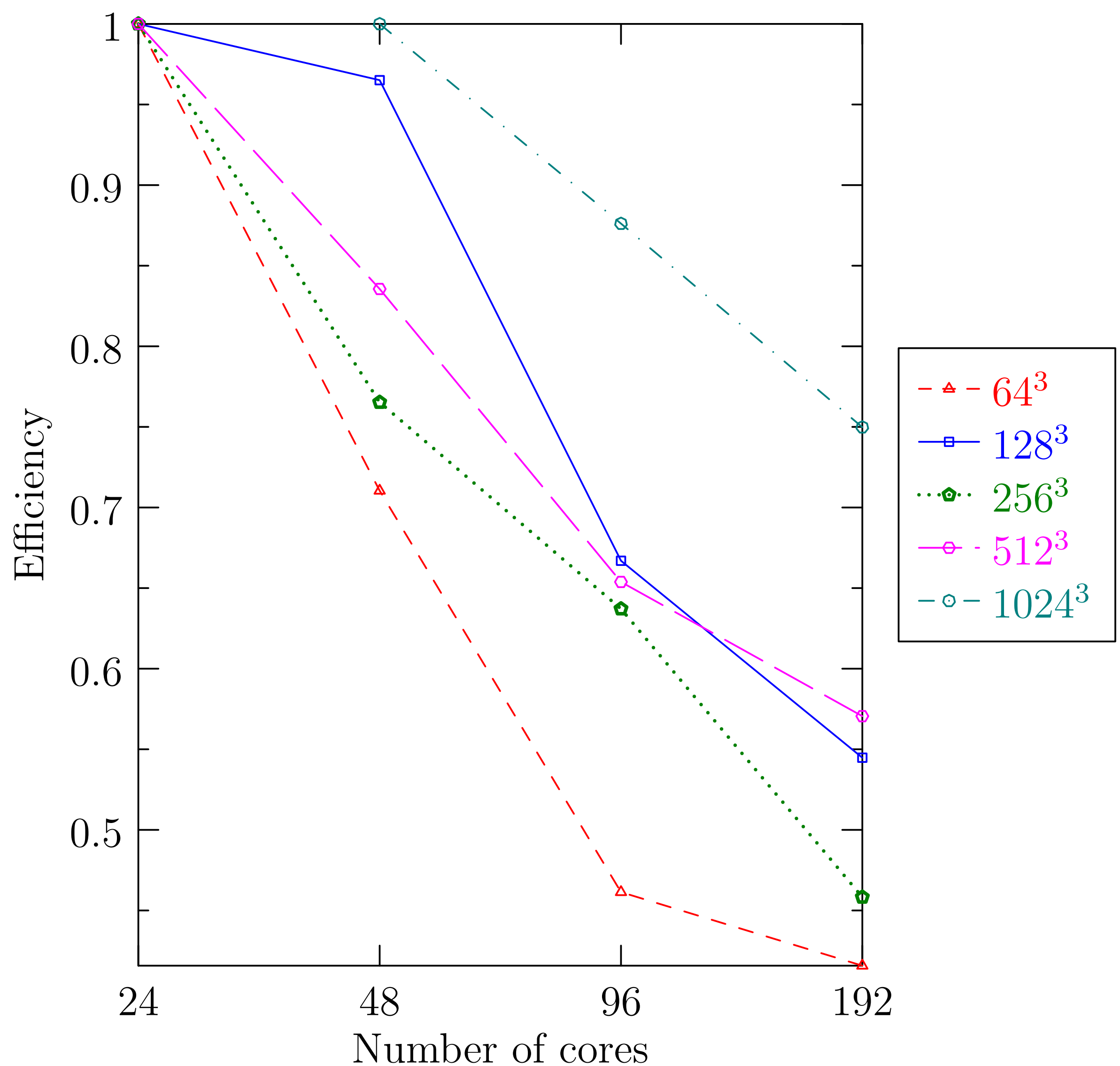


MPI 3D Implicit Parallel Efficiency



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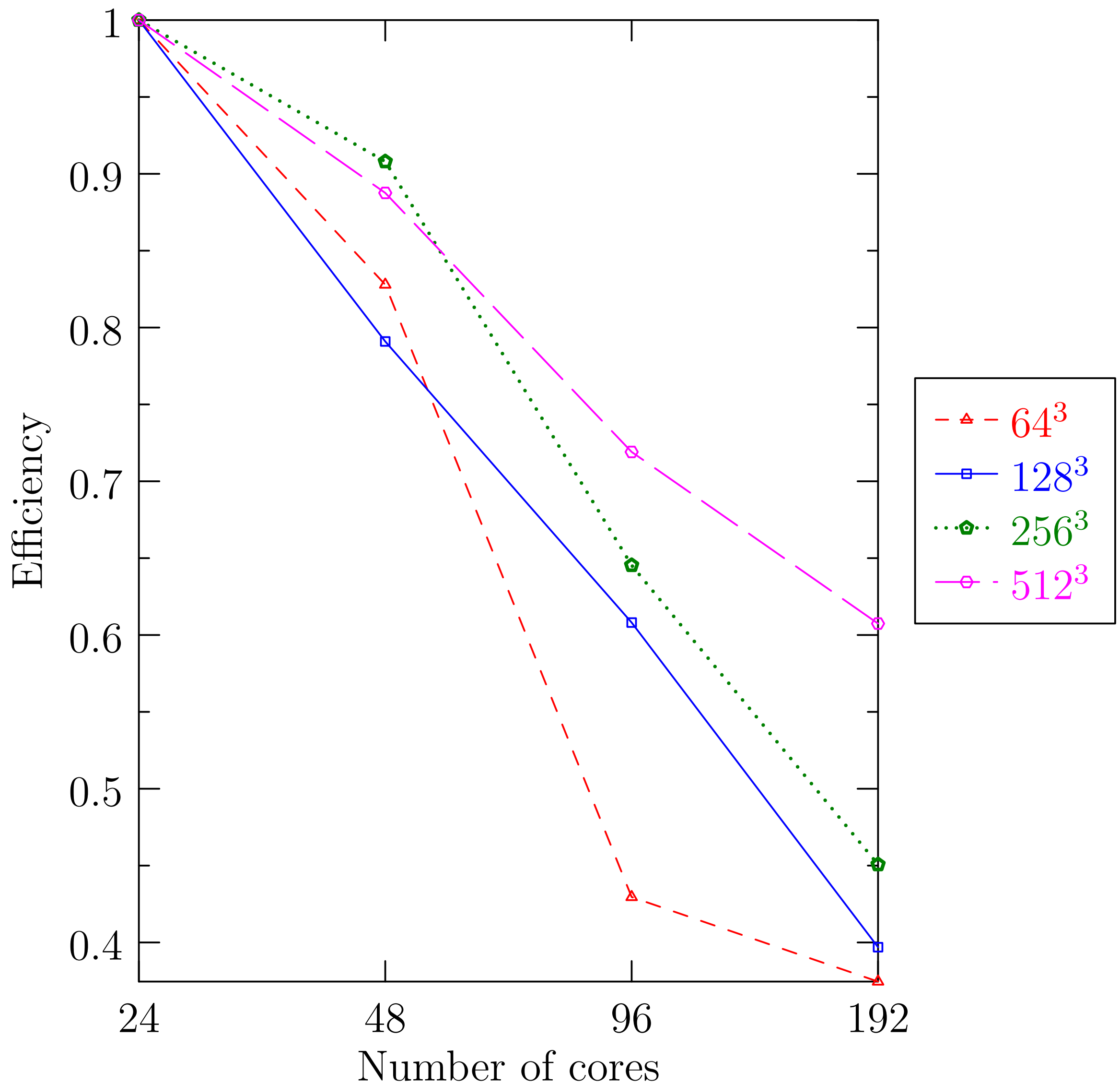

Communication Costs: Direct Transpose

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Block Transpose

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- Outer: Over each team of a processes, transpose the $a \times a$ matrix of $N/a \times M/a$ blocks.

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- Let $L = \tau_\ell/\tau_d$ be the effective communication block length.

Direct vs. Block Transposes

- Since

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- For $NM < P^2 L$, we see that T_B is convex, with a minimum at $a = \sqrt{P}$.

Optimal Number of Threads

- The minimum value of T_B is

$$
\begin{aligned}
T_B(\sqrt{P}) \; &= \; 2\tau_d\left(\sqrt{P} - 1\right)\left(L + \frac{NM}{P^{3/2}}\right) \\
&\sim 2\,\tau_d\sqrt{P}\left(L + \frac{NM}{P^{3/2}}\right), \qquad P \gg 1.
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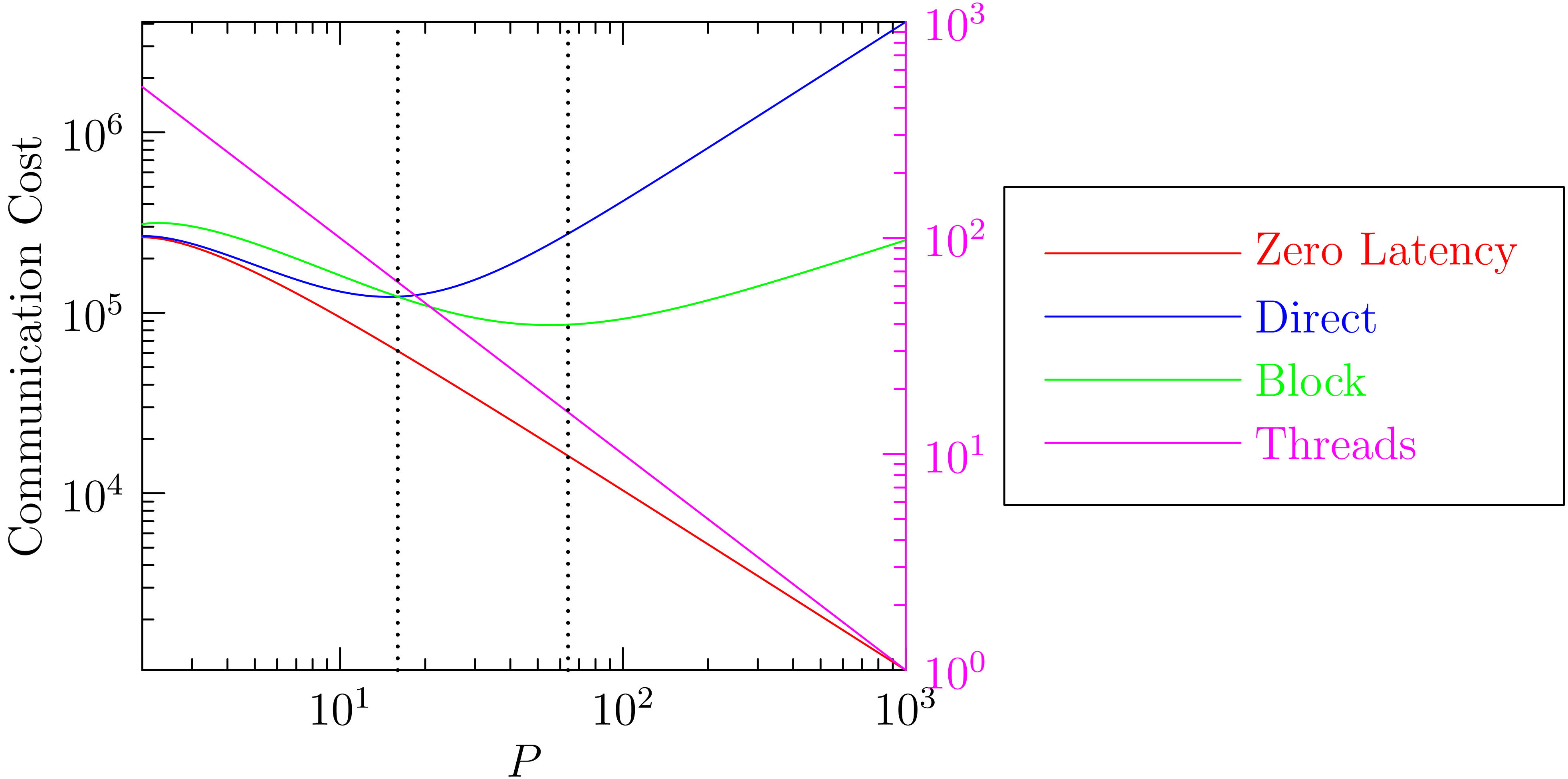
- If the matrix dimensions satisfy $NM > L$, as is typically the case, this minimum occurs above the transition value $(NM/L)^{1/2}$.

Transpose Communication Costs



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- The hybrid paradigm provides an optimal setting for nonlocal computationally intensive operations found in applications like the fast Fourier transform.
- The advent of implicit dealiasing of convolutions makes overlapping transposition with FFT computation feasible.

- Writing of a high-performance dealiased pseudospectral code is now a relatively straightforward exercise. For example, see the `protodns` project at

  `http://github.com/dealias/dns`

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