FFTW++: A Hybrid OpenMP/MPI Implementation of FFTs and Implicitly Dealiased Convolutions

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Discrete Cyclic Convolution

- The FFT provides an efficient tool for computing the *discrete cyclic convolution*

  $$\sum_{p=0}^{N-1} F_p G_{k-p},$$

  where the vectors F and G have period N.

- Define the *Nth primitive root of unity:*

  $$\zeta_N = \exp\left(\frac{2\pi i}{N}\right).$$

- 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

$$f_j \doteq \sum_{k=0}^{N-1} \zeta_N^{jk} F_k \qquad j = 0, \ldots, N-1.$$

- The corresponding *forward transform is*

$$F_k \doteq \frac{1}{N} \sum_{j=0}^{N-1} \zeta_N^{-kj} f_j \qquad k = 0, \ldots, N-1.$$

- 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

$$\begin{aligned}
\sum_{j=0}^{N-1} f_j g_j \zeta_N^{-jk} &= \sum_{j=0}^{N-1} \zeta_N^{-jk} \left(\sum_{p=0}^{N-1} \zeta_N^{jp} F_p \right) \left(\sum_{q=0}^{N-1} \zeta_N^{jq} G_q \right) \\
&= \sum_{p=0}^{N-1} \sum_{q=0}^{N-1} F_p G_q \sum_{j=0}^{N-1} \zeta_N^{(-k+p+q)j} \\
&= N \sum_s \sum_{p=0}^{N-1} F_p G_{k-p+sN}.
\end{aligned}$$

- The terms indexed by $s \neq 0$ are *aliases;* we need to remove them!

- If only the first m entries of the input vectors are nonzero, aliases can be avoided by *zero padding* input data vectors of length m to length $N \geq 2m-1$.

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

● Since FFT sizes with small prime factors in practice yield the most efficient implementations, the padding is normally extended to $N = 2m$:

$\{F_k\}_{k=0}^{m-1}$

$\{G_k\}_{k=0}^{m-1}$

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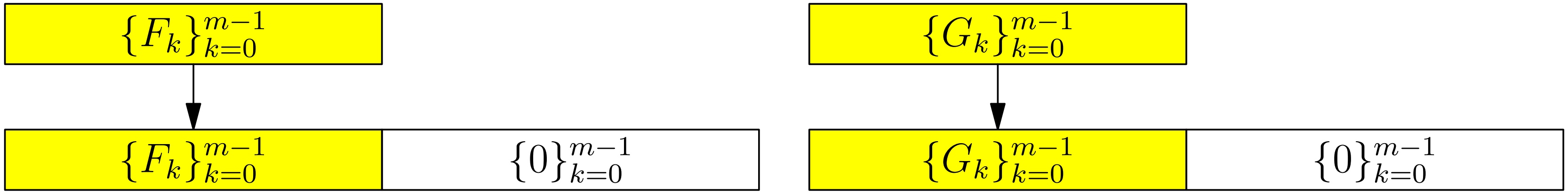

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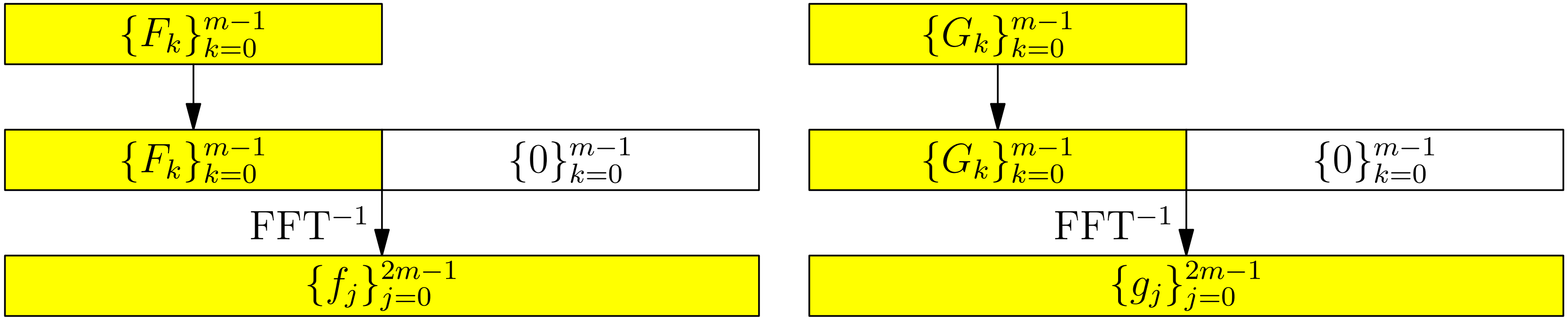

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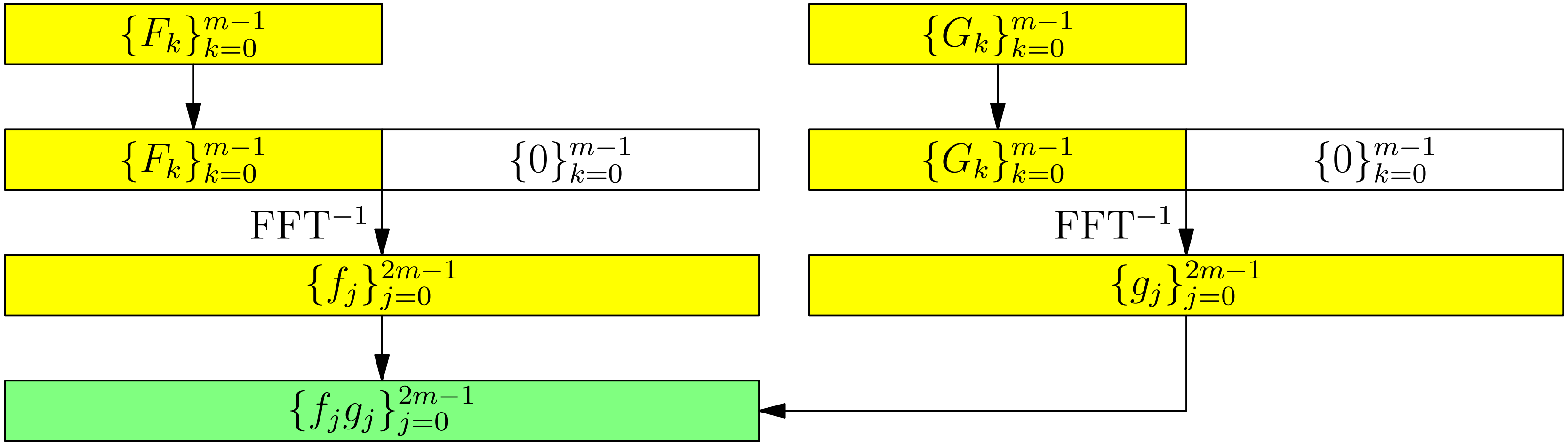

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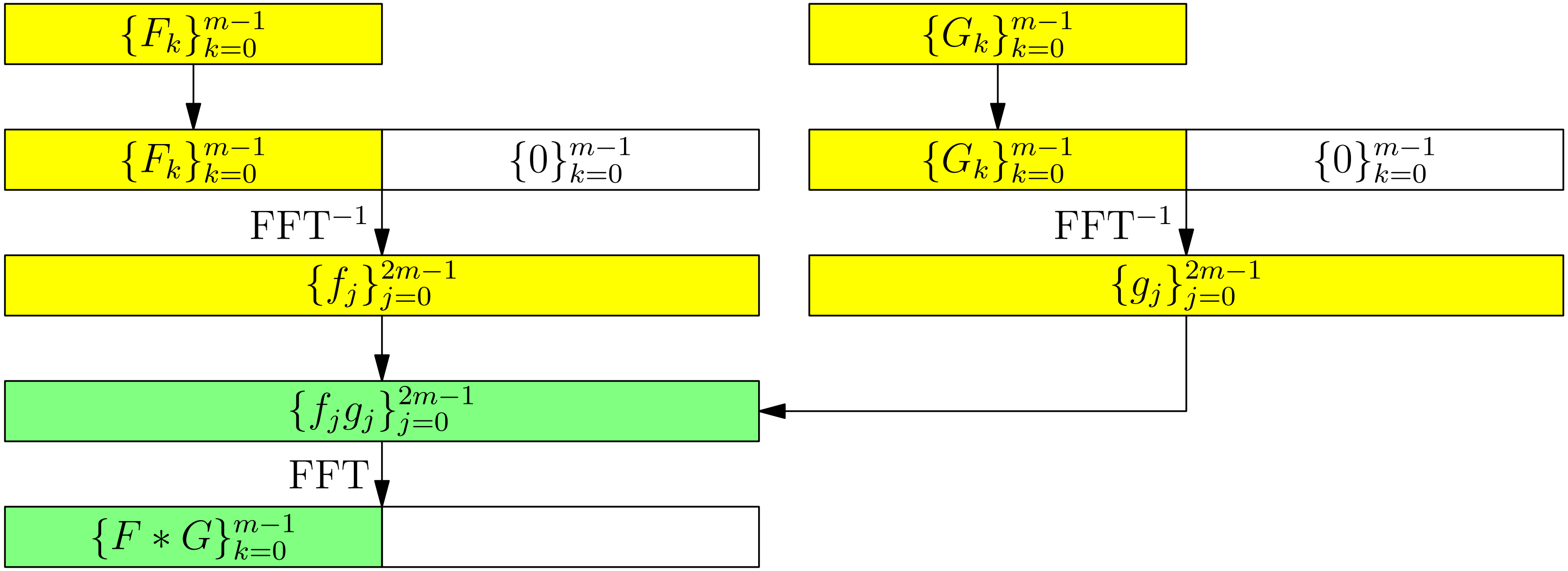

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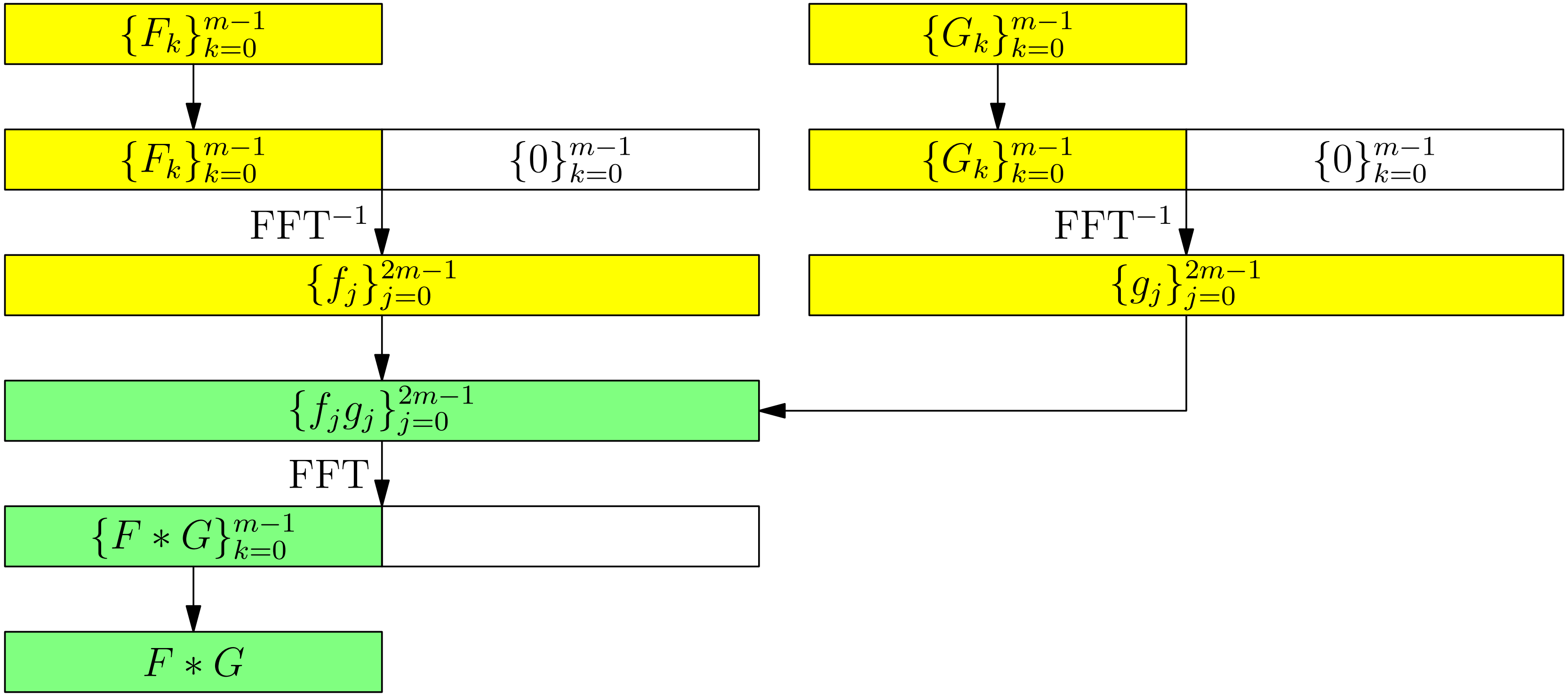

$\{F_k\}_{k=0}^{m-1}$

$\{G_k\}_{k=0}^{m-1}$

$\{F_k\}_{k=0}^{m-1}$ $\{0\}_{k=0}^{m-1}$

$\{G_k\}_{k=0}^{m-1}$ $\{0\}_{k=0}^{m-1}$

FFT^{-1}

FFT^{-1}

$\{f_j\}_{j=0}^{2m-1}$

$\{g_j\}_{j=0}^{2m-1}$

$\{f_j g_j\}_{j=0}^{2m-1}$

FFT

$\{F * G\}_{k=0}^{m-1}$

$F * G$

Implicit Padding

- Let $N = 2m$. For $j = 0, \ldots, 2m-1$ we want to compute

$$f_j = \sum_{k=0}^{2m-1} \zeta_{2m}^{jk} F_k.$$

- If $F_k = 0$ for $k \geq m$, one can easily avoid looping over the unwanted zero Fourier modes by decimating in wavenumber:

$$f_{2\ell} = \sum_{k=0}^{m-1} \zeta_{2m}^{2\ell k} F_k = \sum_{k=0}^{m-1} \zeta_m^{\ell k} F_k, \quad \ell = 0, 1, \ldots m-1.$$

$$f_{2\ell+1} = \sum_{k=0}^{m-1} \zeta_{2m}^{(2\ell+1)k} F_k = \sum_{k=0}^{m-1} \zeta_m^{\ell k} \zeta_{2m}^{k} F_k,$$

- 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:

$$\begin{aligned}
2mF_k &= \sum_{j=0}^{2m-1} \zeta_{2m}^{-kj} f_j \\
&= \sum_{\ell=0}^{m-1} \zeta_{2m}^{-k2\ell} f_{2\ell} + \sum_{\ell=0}^{m-1} \zeta_{2m}^{-k(2\ell+1)} f_{2\ell+1} \\
&= \sum_{\ell=0}^{m-1} \zeta_{m}^{-k\ell} f_{2\ell} + \zeta_{2m}^{-k} \sum_{\ell=0}^{m-1} \zeta_{m}^{-k\ell} f_{2\ell+1} \qquad k = 0, \ldots, m-1.
\end{aligned}$$

- 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.

- The computational complexity is $6Km\log_2 m$.
- The numerical error is similar to explicit padding and the memory usage is identical.

$\{F_k\}_{k=0}^{m-1}$

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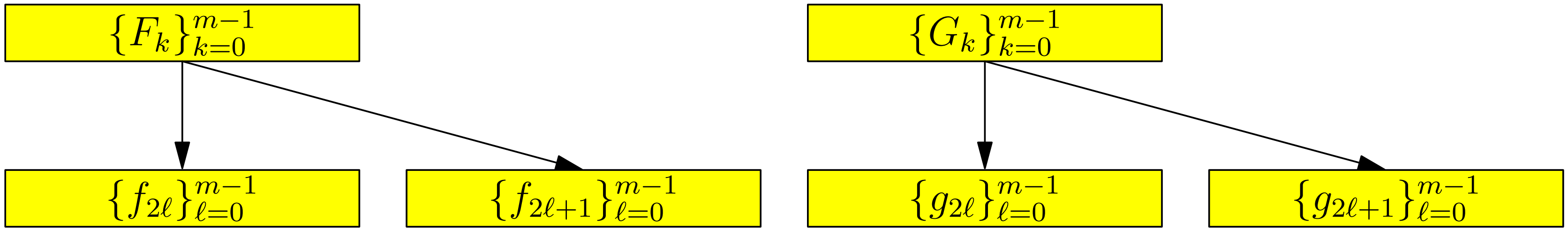

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$\{f_{2\ell+1}\}_{\ell=0}^{m-1}$

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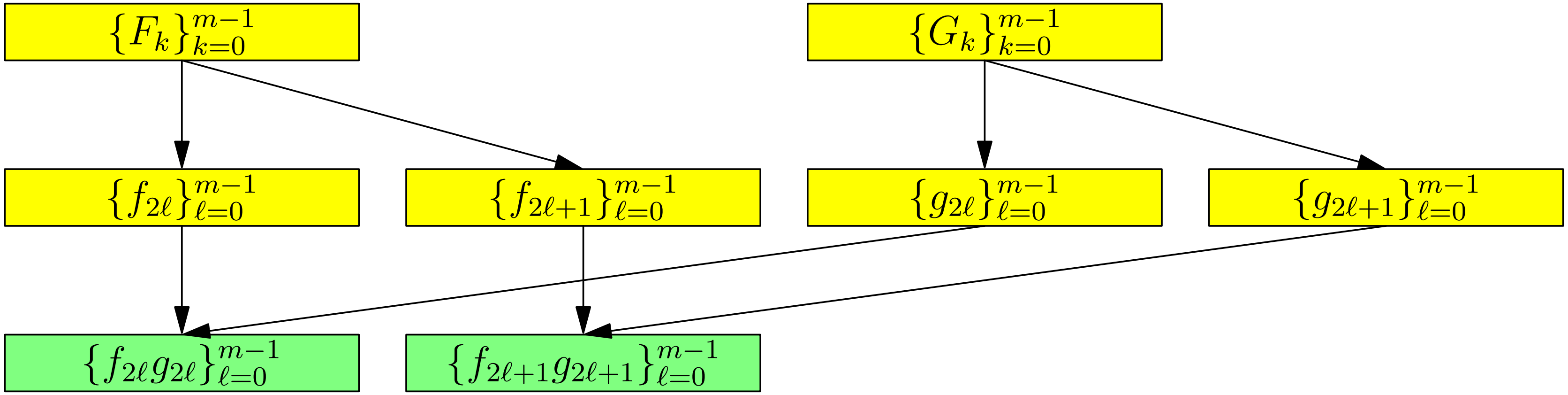
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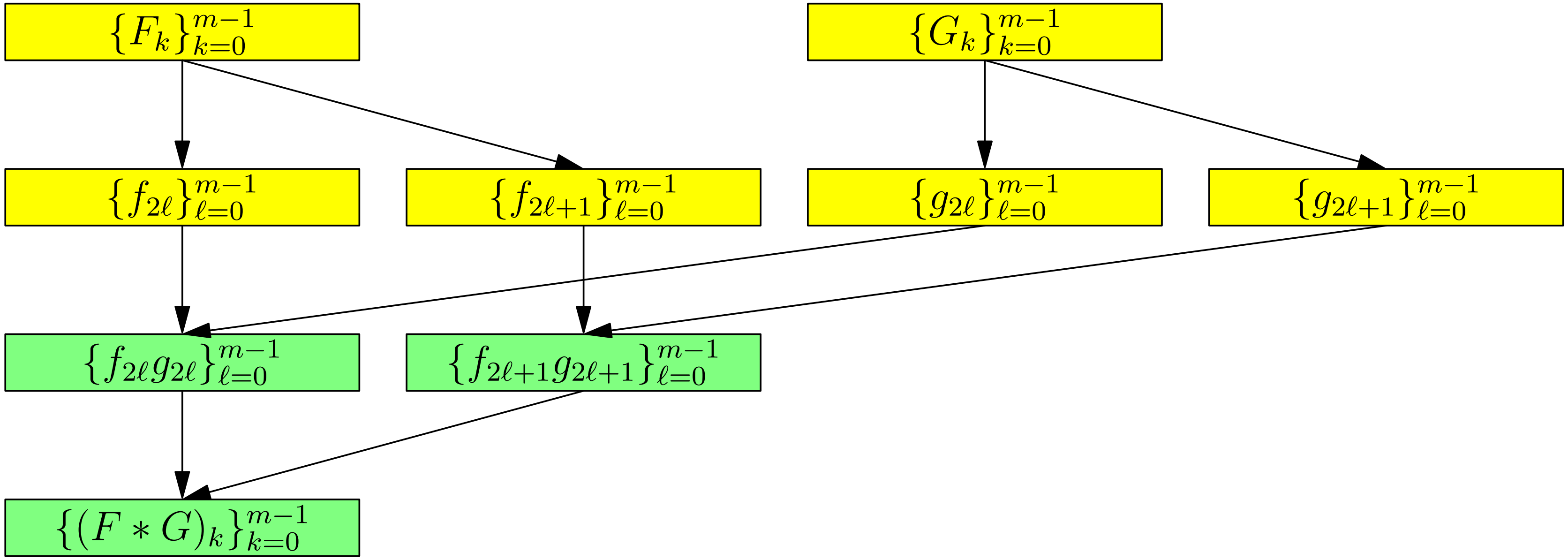

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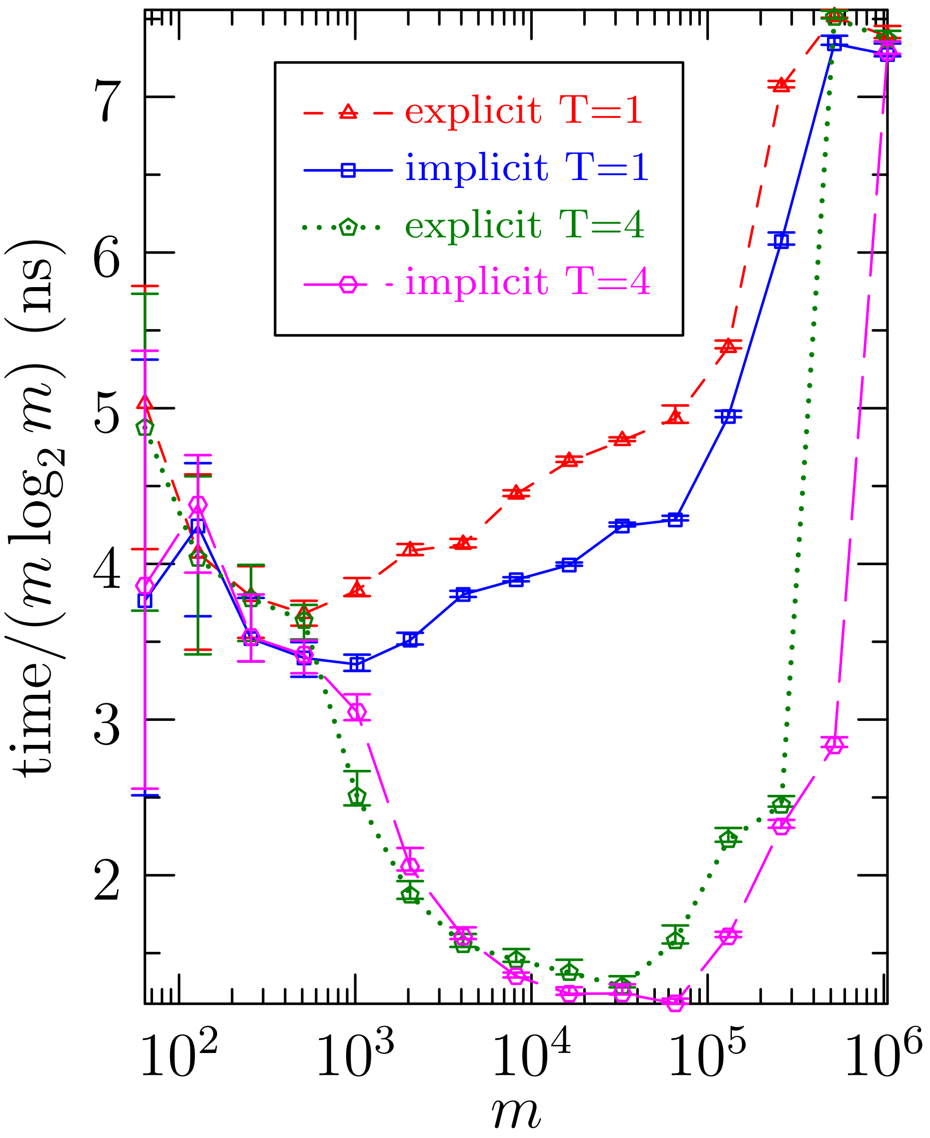
$\{(F*G)_k\}_{k=0}^{m-1}$

```
**Input**: vector f, vector g
**Output**: vector f
$u \leftarrow \texttt{fft}^{-1}(f)$;
$v \leftarrow \texttt{fft}^{-1}(g)$;
$u \leftarrow u * v$;
for $k = 0$ to $m - 1$ do
    $f[k] \leftarrow \zeta_{2m}^{k} f[k]$;
    $g[k] \leftarrow \zeta_{2m}^{k} g[k]$;
end
$v \leftarrow \texttt{fft}^{-1}(f)$;
$f \leftarrow \texttt{fft}^{-1}(g)$;
$v \leftarrow v * f$;
$f \leftarrow \texttt{fft}(u)$;
$u \leftarrow \texttt{fft}(v)$;
for $k = 0$ to $m - 1$ do
    $f[k] \leftarrow f[k] + \zeta_{2m}^{-k} u[k]$;
end
return f/(2m);
```

Implicit Padding in 1D



Convolutions in Higher Dimensions

- An explicitly padded convolution in 2 dimensions requires 12 padded FFTs, and 4 times the memory of a cyclic convolution.

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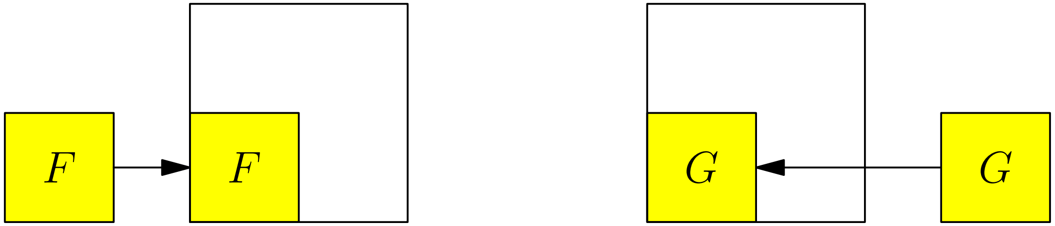

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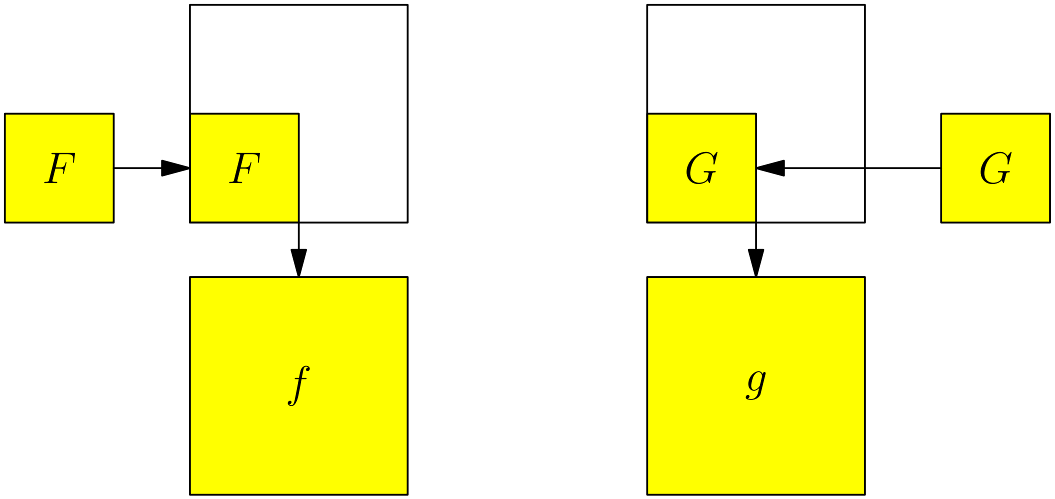

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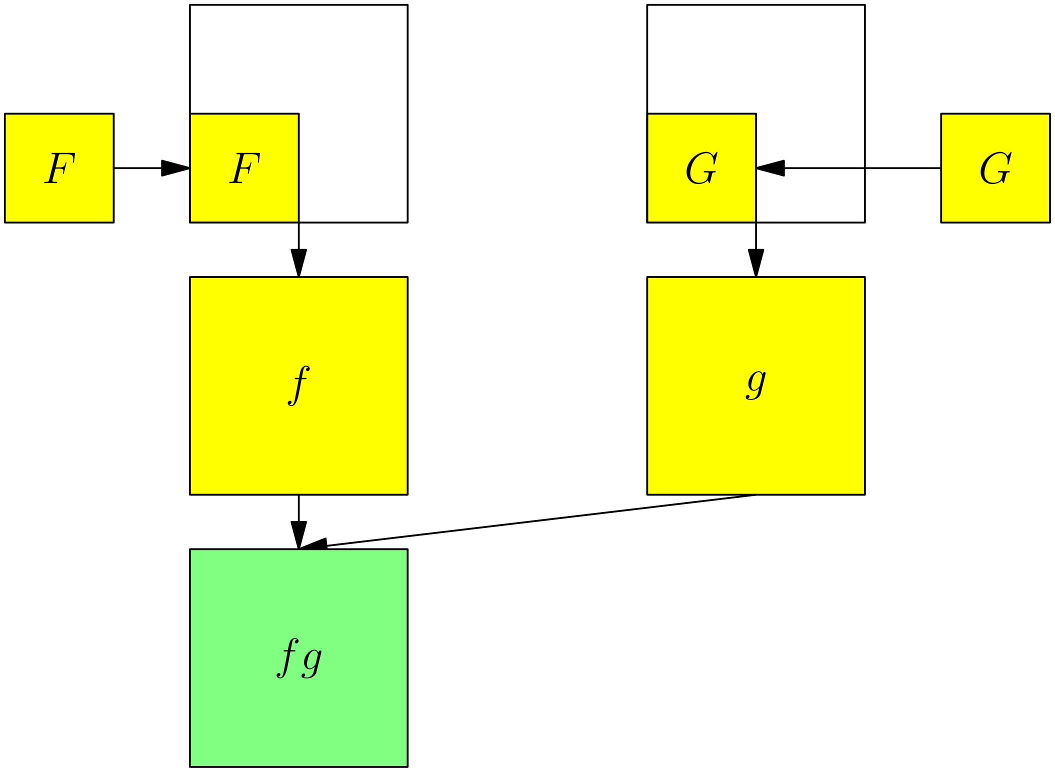

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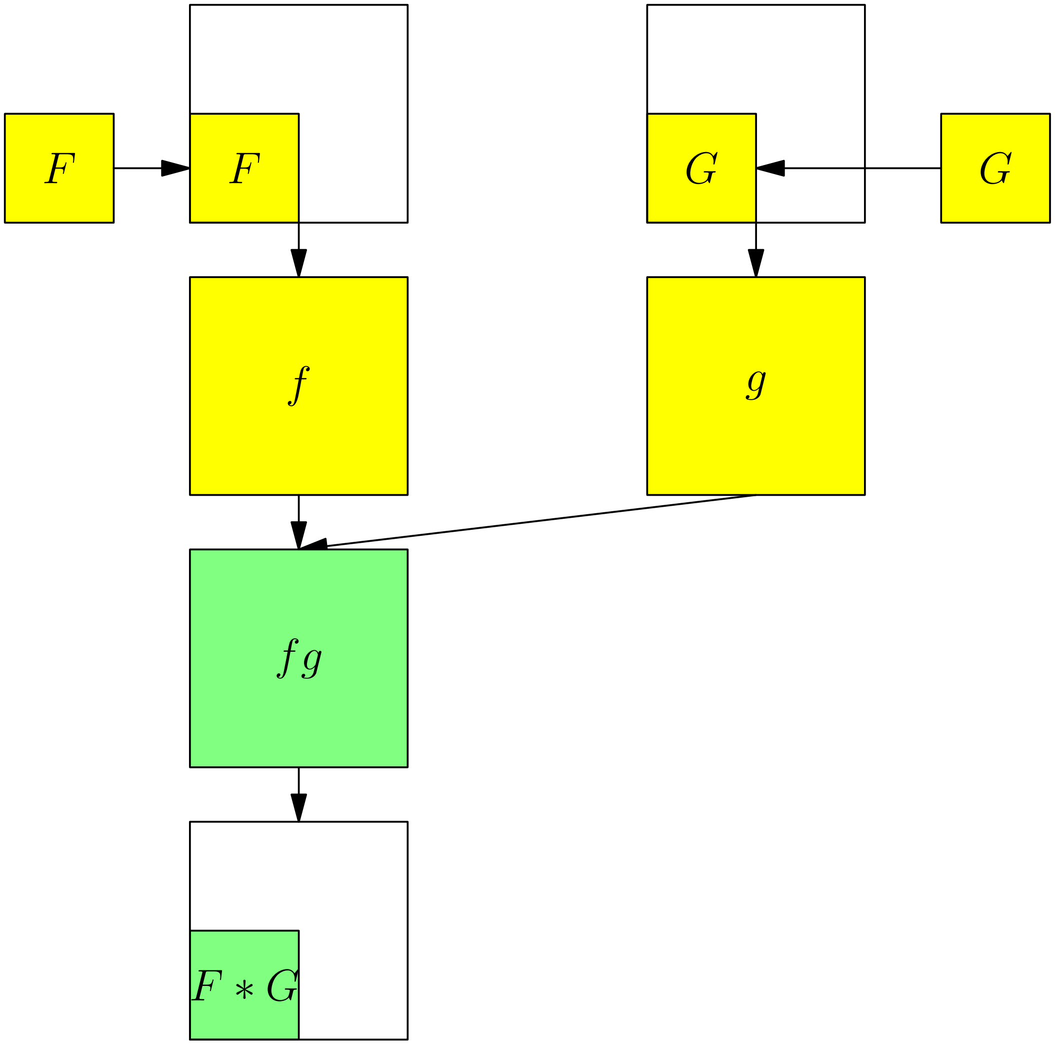

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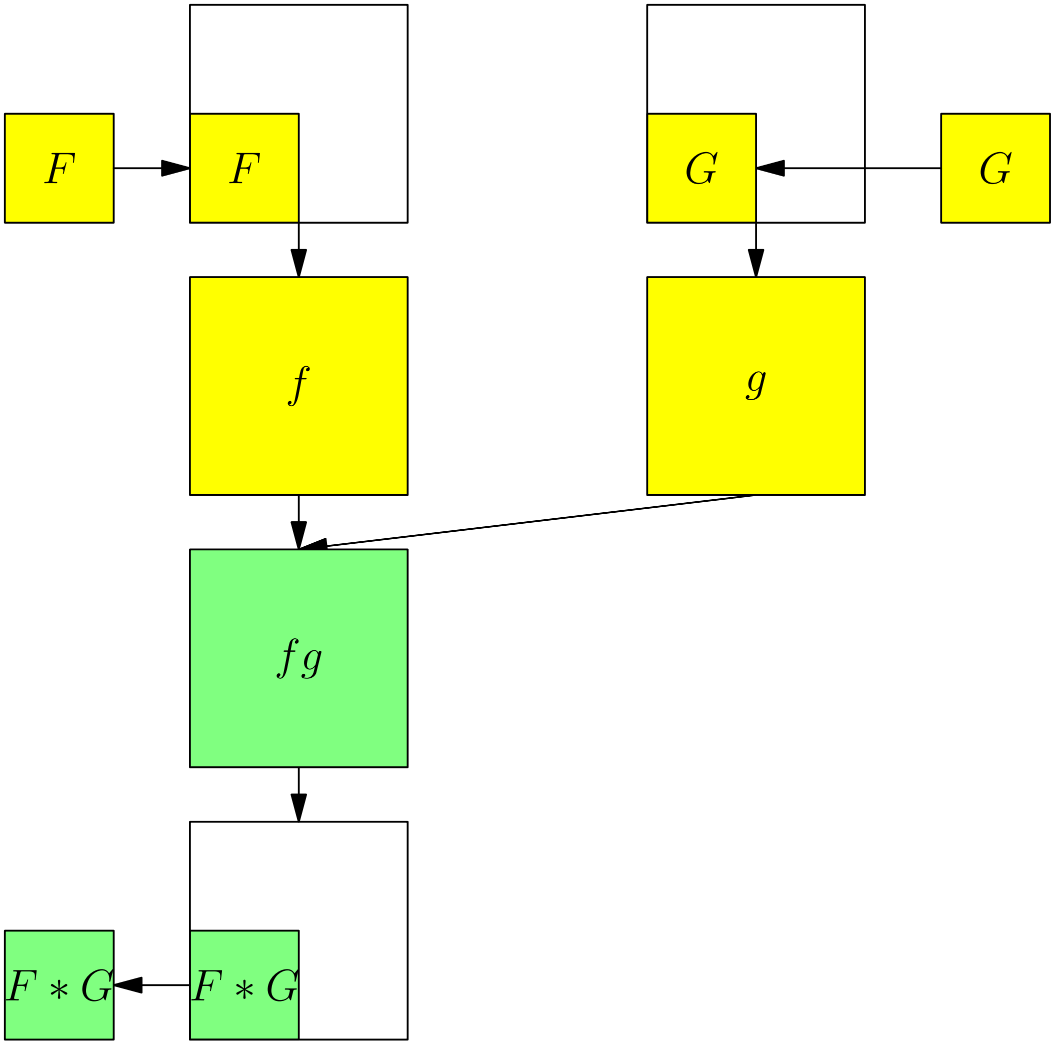
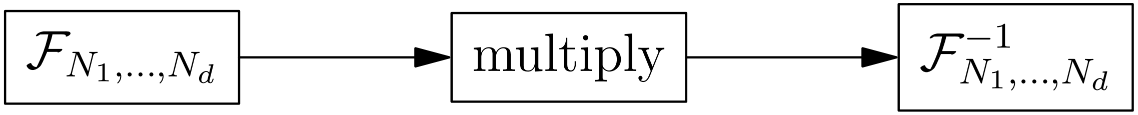


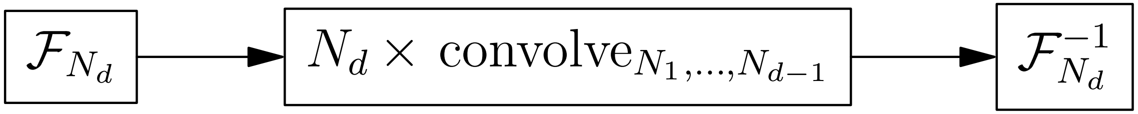
Recursive Convolution

- Naive way to compute a multiple-dimensional convolution:



$\mathcal{F}_{N_1,\ldots,N_d}$ → multiply → $\mathcal{F}^{-1}_{N_1,\ldots,N_d}$

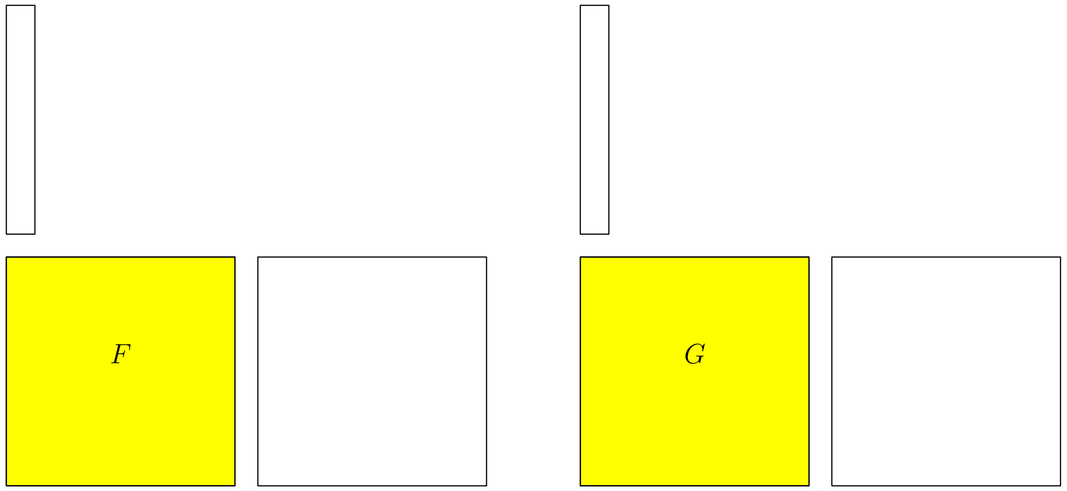
- The technique of *recursive convolution* allows one to avoid computing and storing the entire Fourier image of the data:



$\mathcal{F}_{N_d}$ → $N_d \times$ convolve$_{N_1,\ldots,N_{d-1}}$ → $\mathcal{F}^{-1}_{N_d}$

Implicit Padding in 2D

- Extra work memory need not be contiguous with the data.



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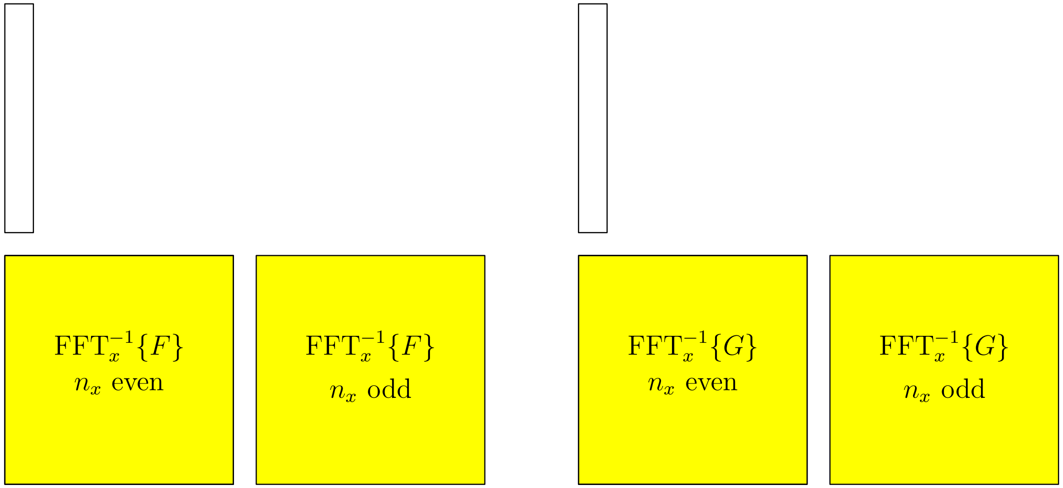
$\mathrm{FFT}_x^{-1}\{F\}$
n_x even
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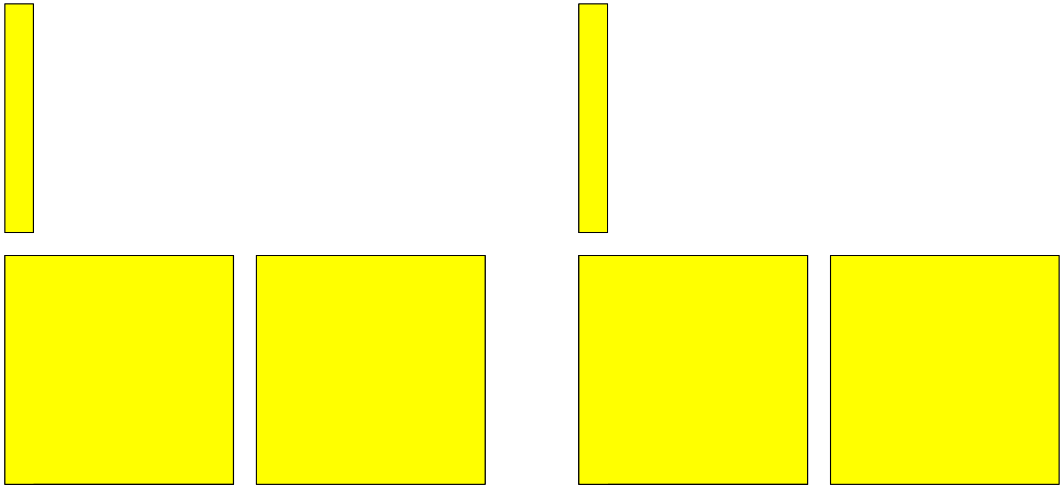

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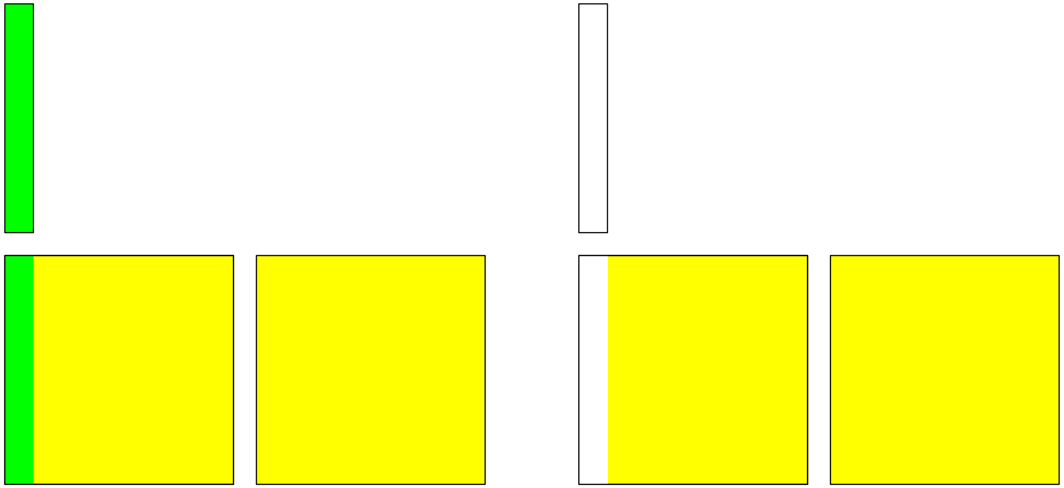

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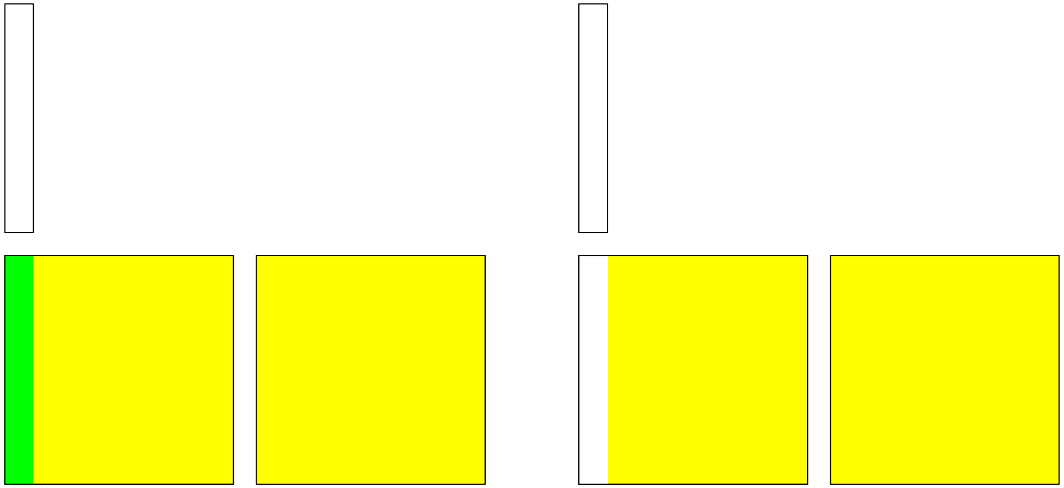

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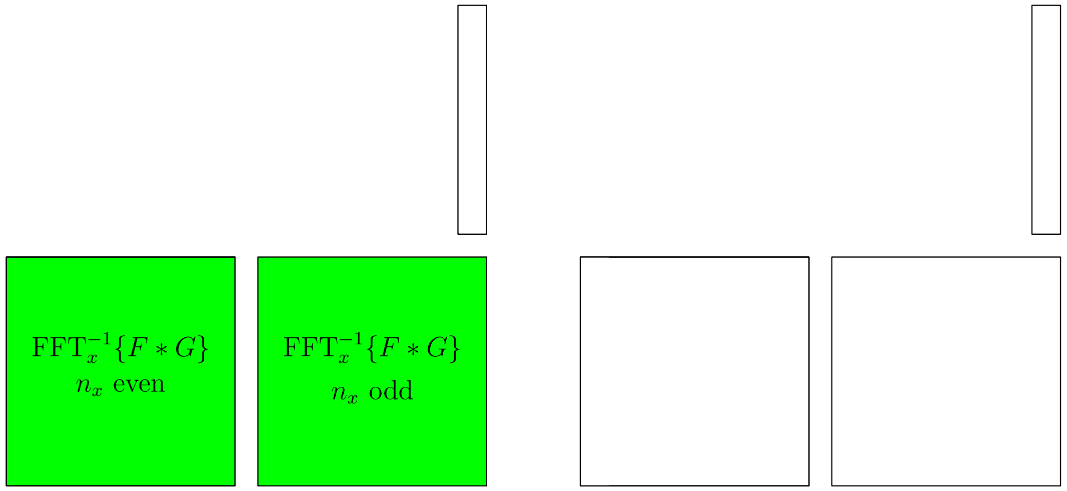
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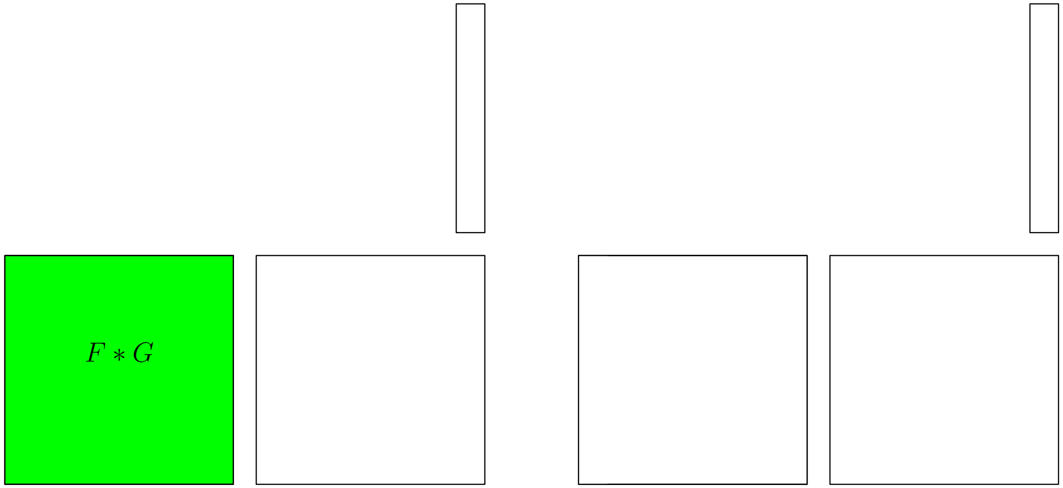

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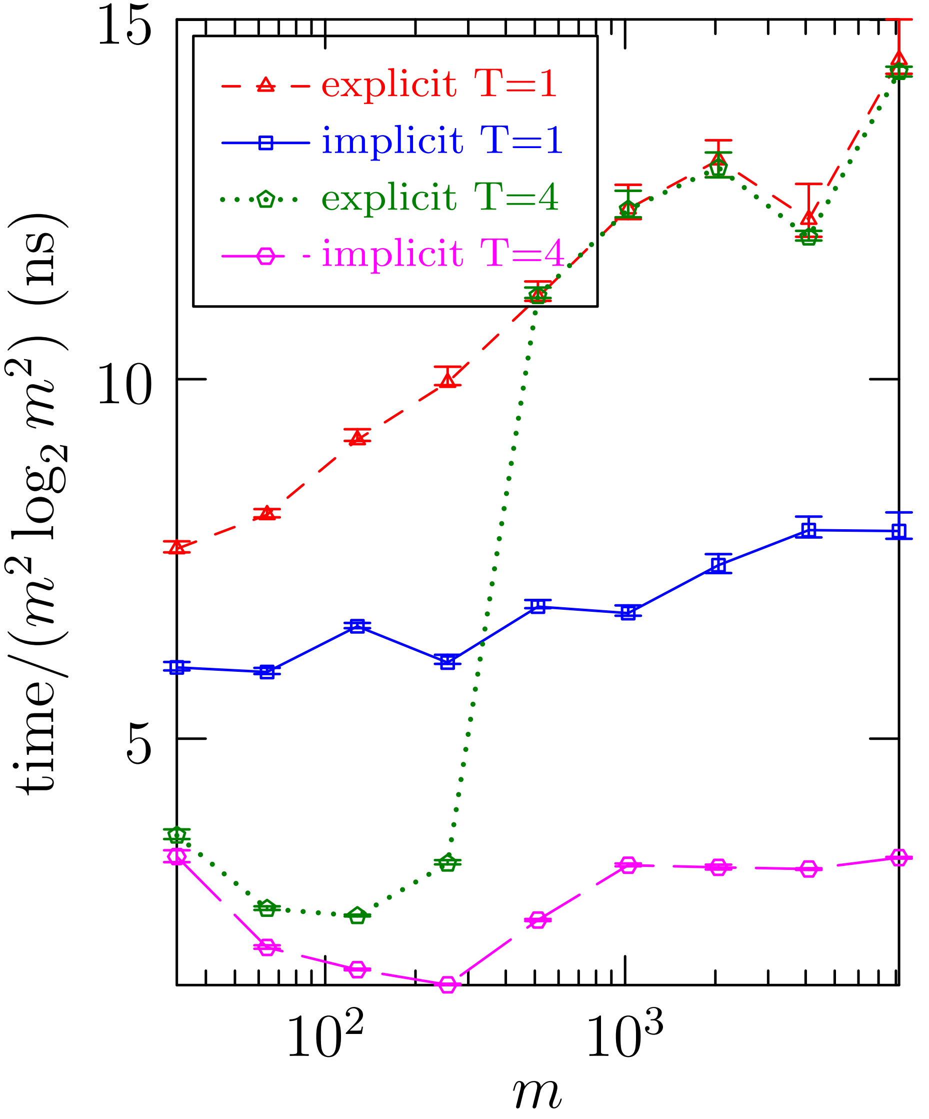
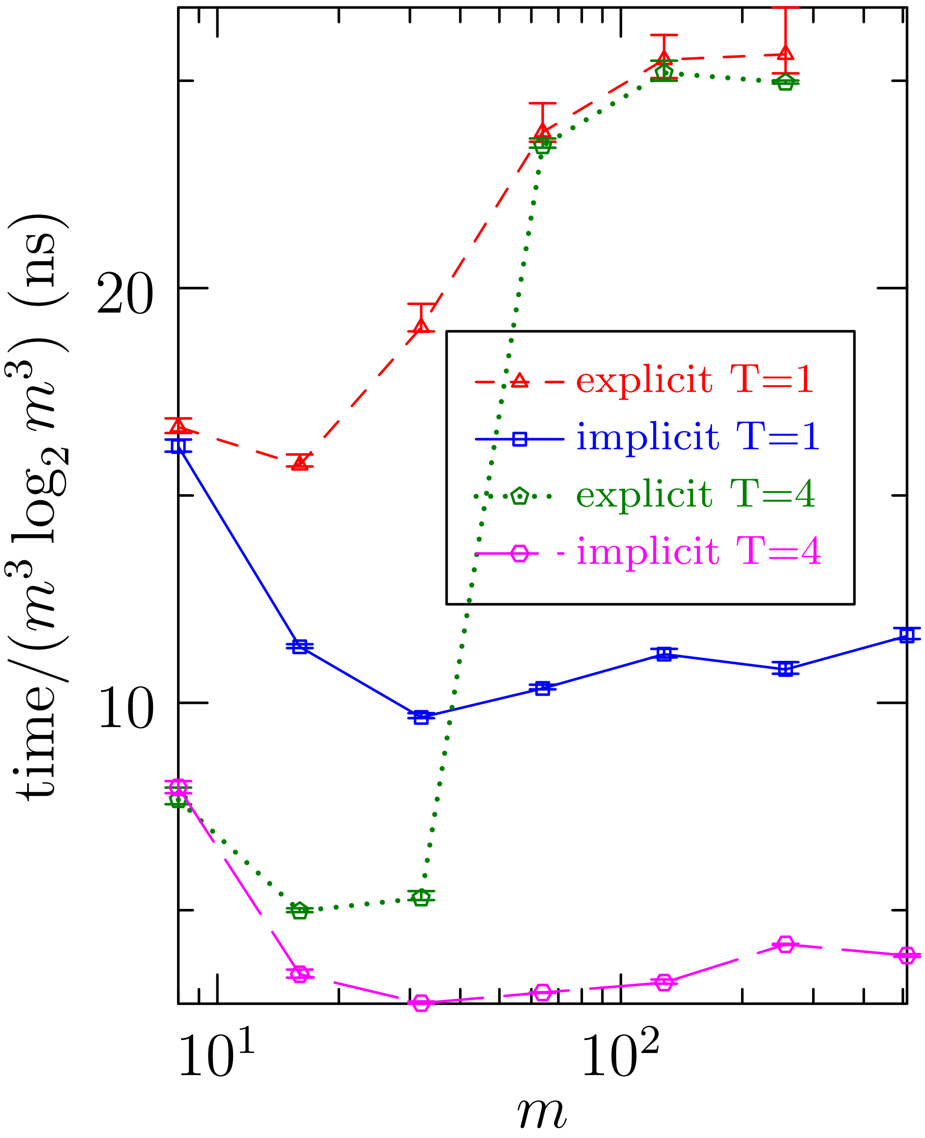


Implicit Padding in 3D



Centered (Pseudospectral) Convolutions

- For a *centered convolution,* the Fourier origin ($k = 0$) is centered in the domain:

$$\sum_{p=k-m+1}^{m-1} f_p g_{k-p}$$

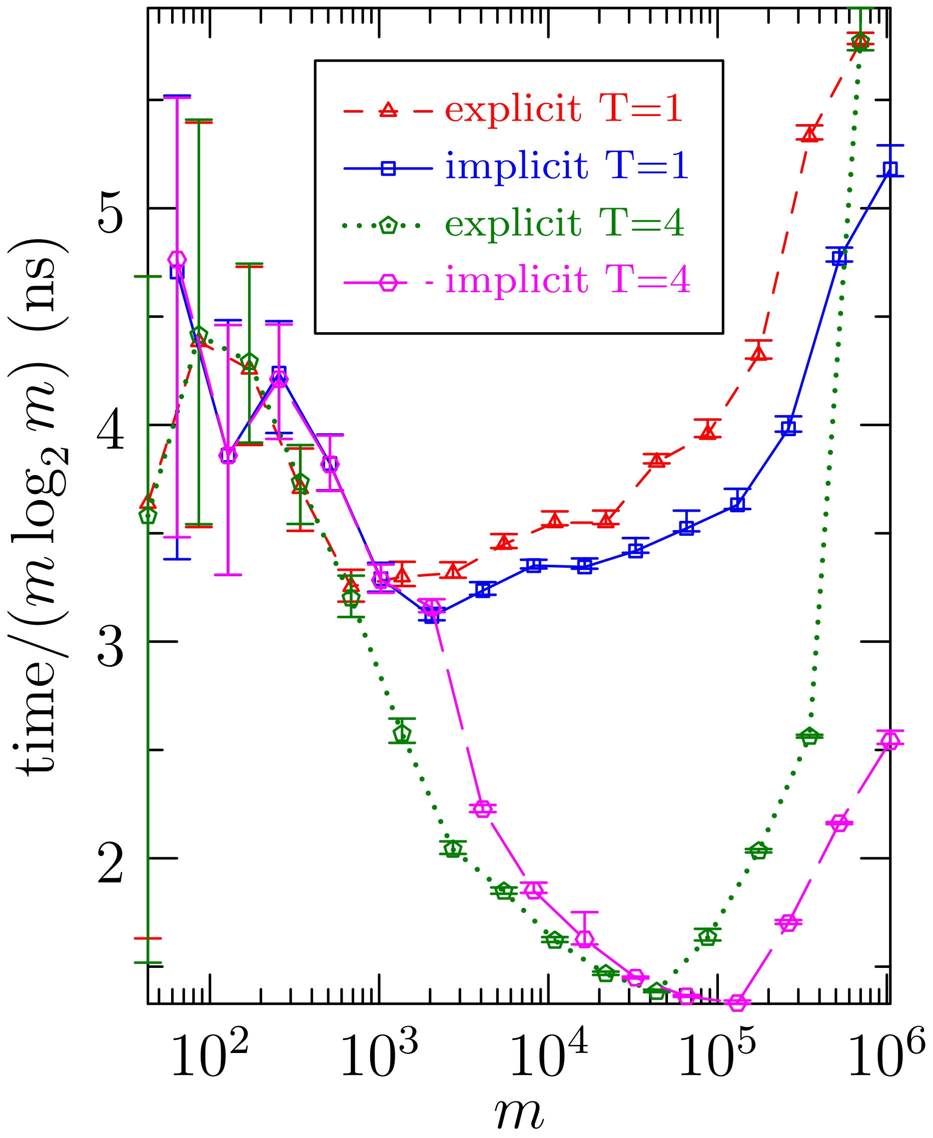
- Need to pad to $N \geq 3m - 2$ to remove aliases.

- The ratio $(2m-1)/(3m-2)$ of the number of physical to total modes is asymptotic to $2/3$ for large m .

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

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

1D Implicit Hermitian Convolution



Distributed-Memory Parallelization

- The pseudospectral method uses a matrix transpose to localize the computation of the multi-dimensional FFTs onto individual processors.

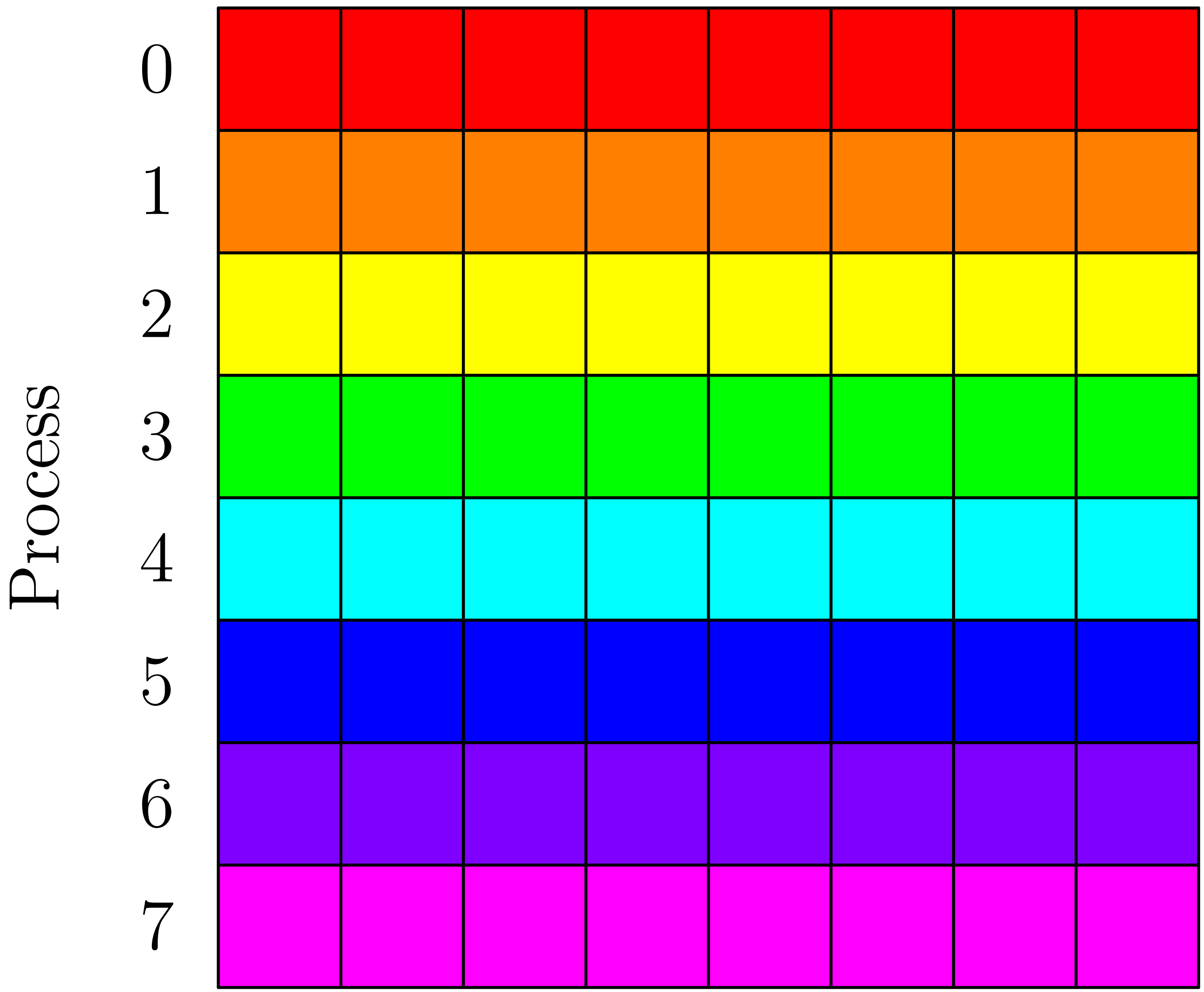
- Parallel generalized slab/pencil decompositions have recently been developed for distributed-memory architectures.

- We have compared several distributed matrix transpose algorithms, both blocking and nonblocking, under pure MPI and hybrid MPI/OpenMP architectures.

- 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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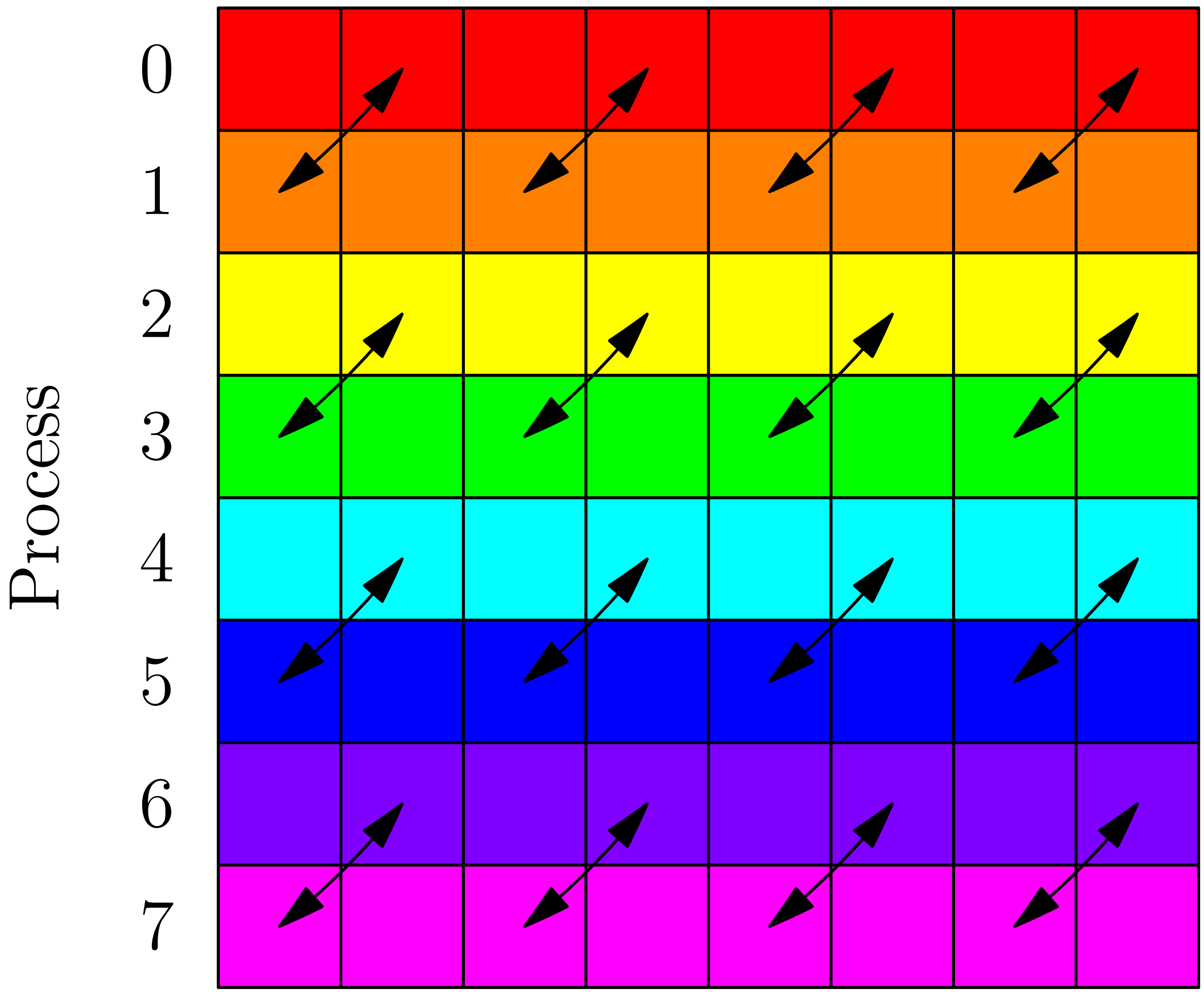

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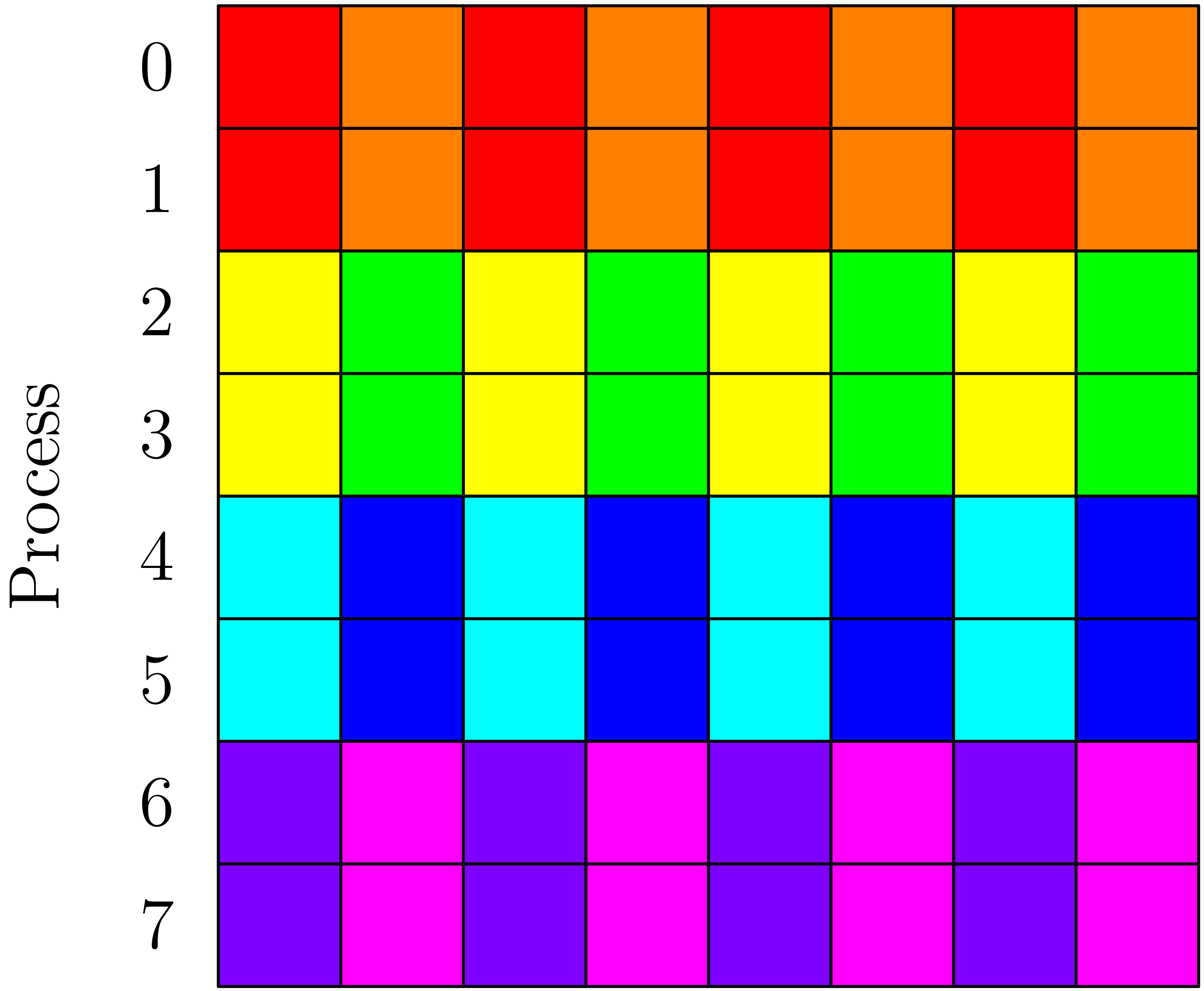

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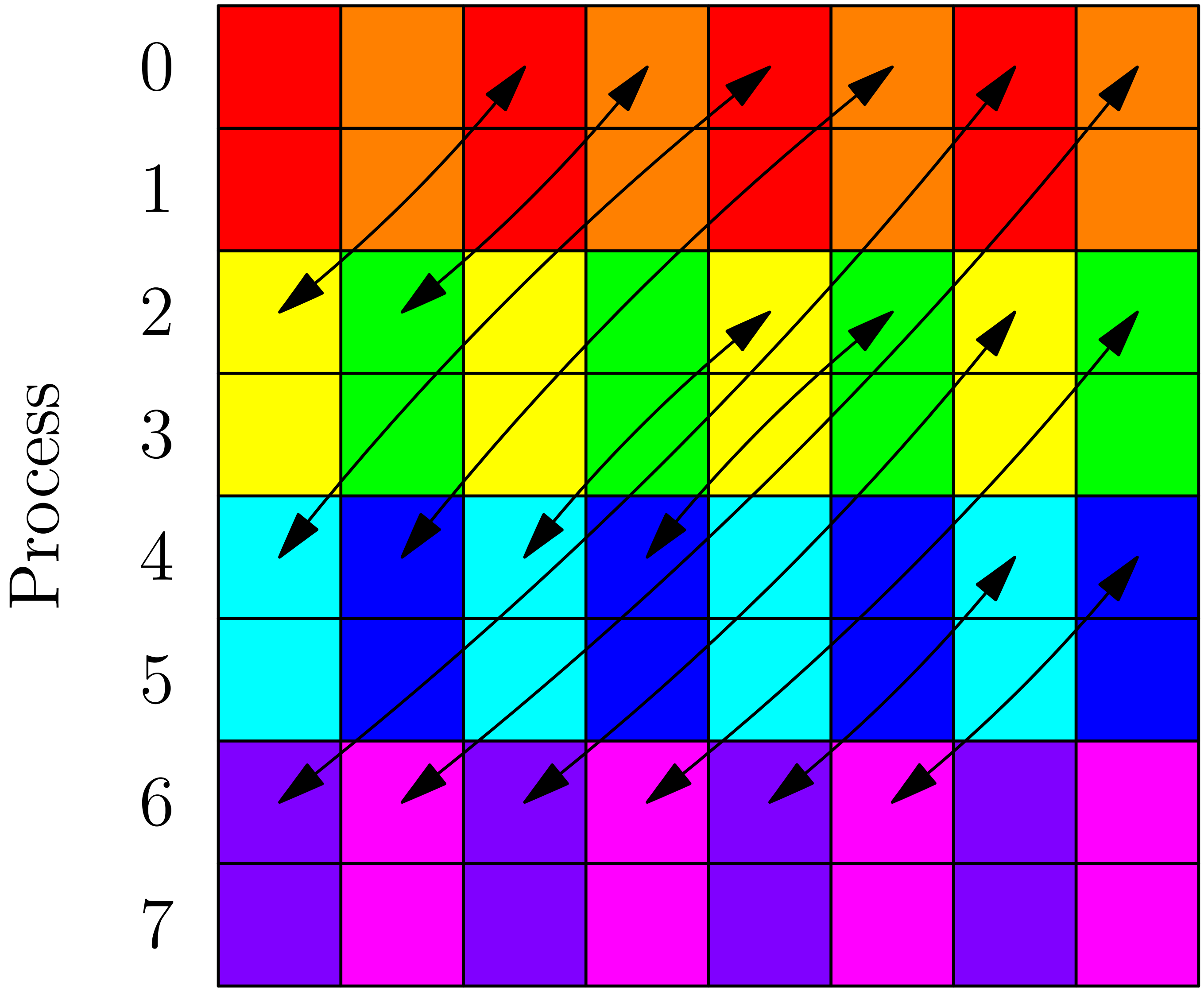

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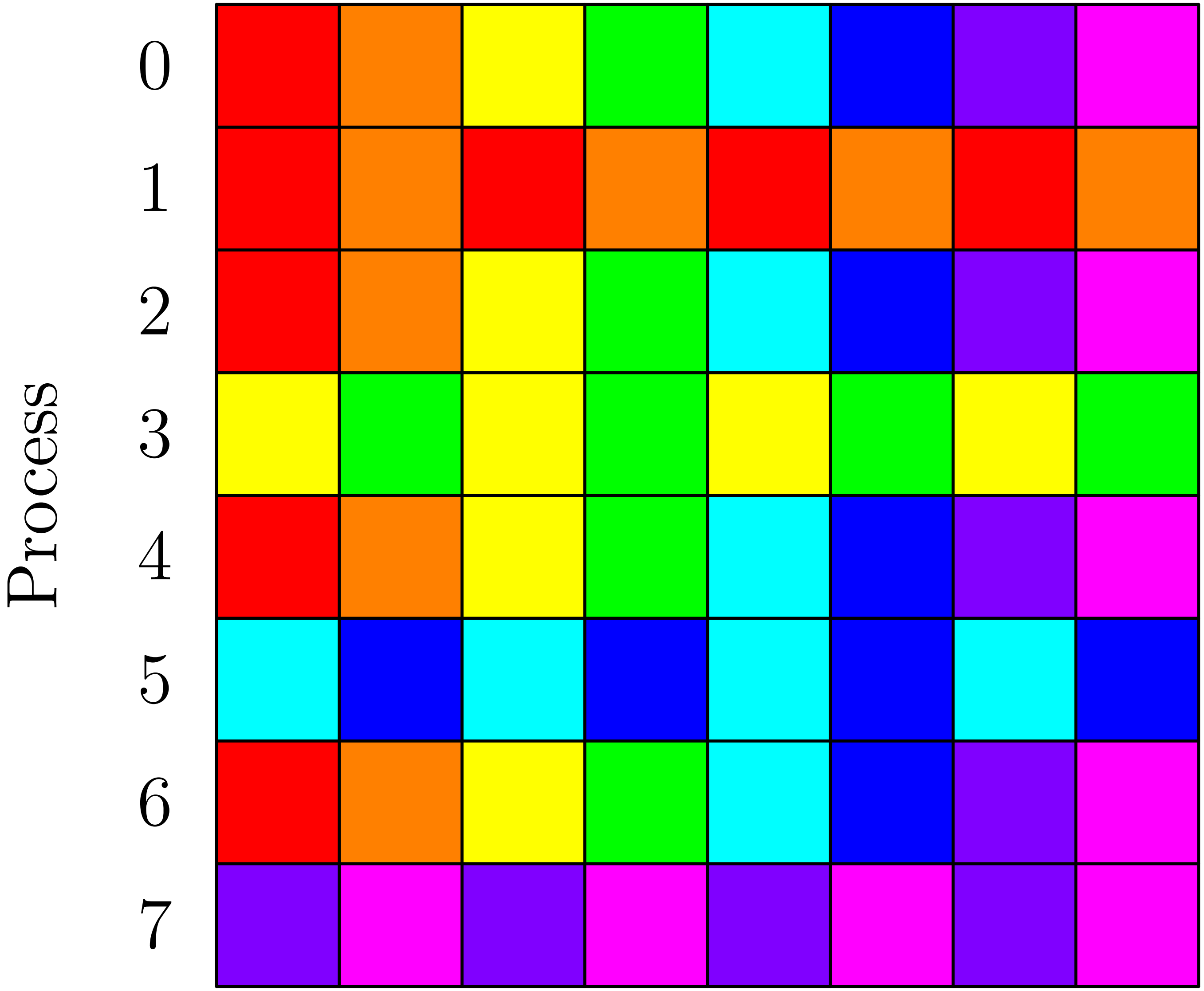

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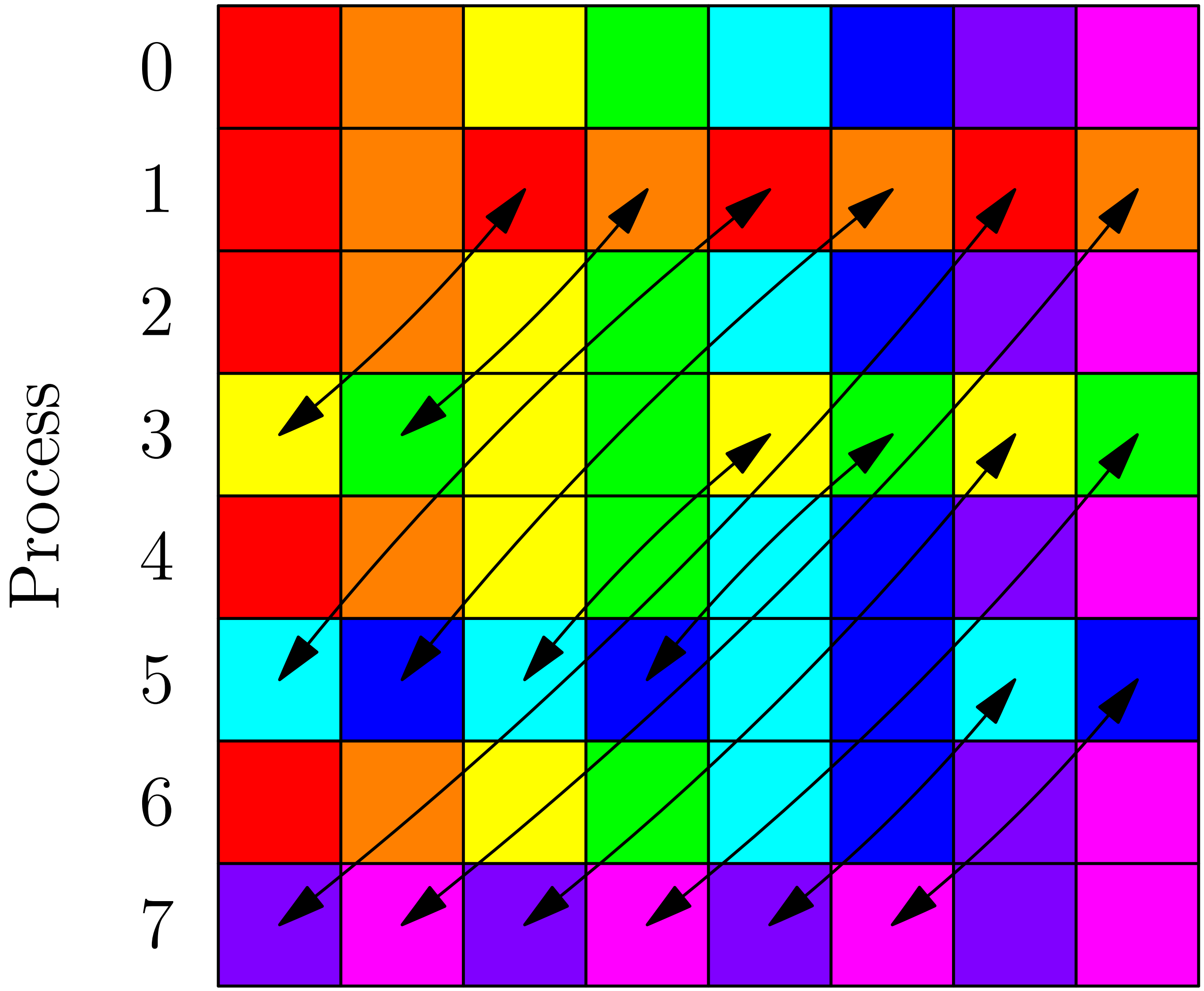

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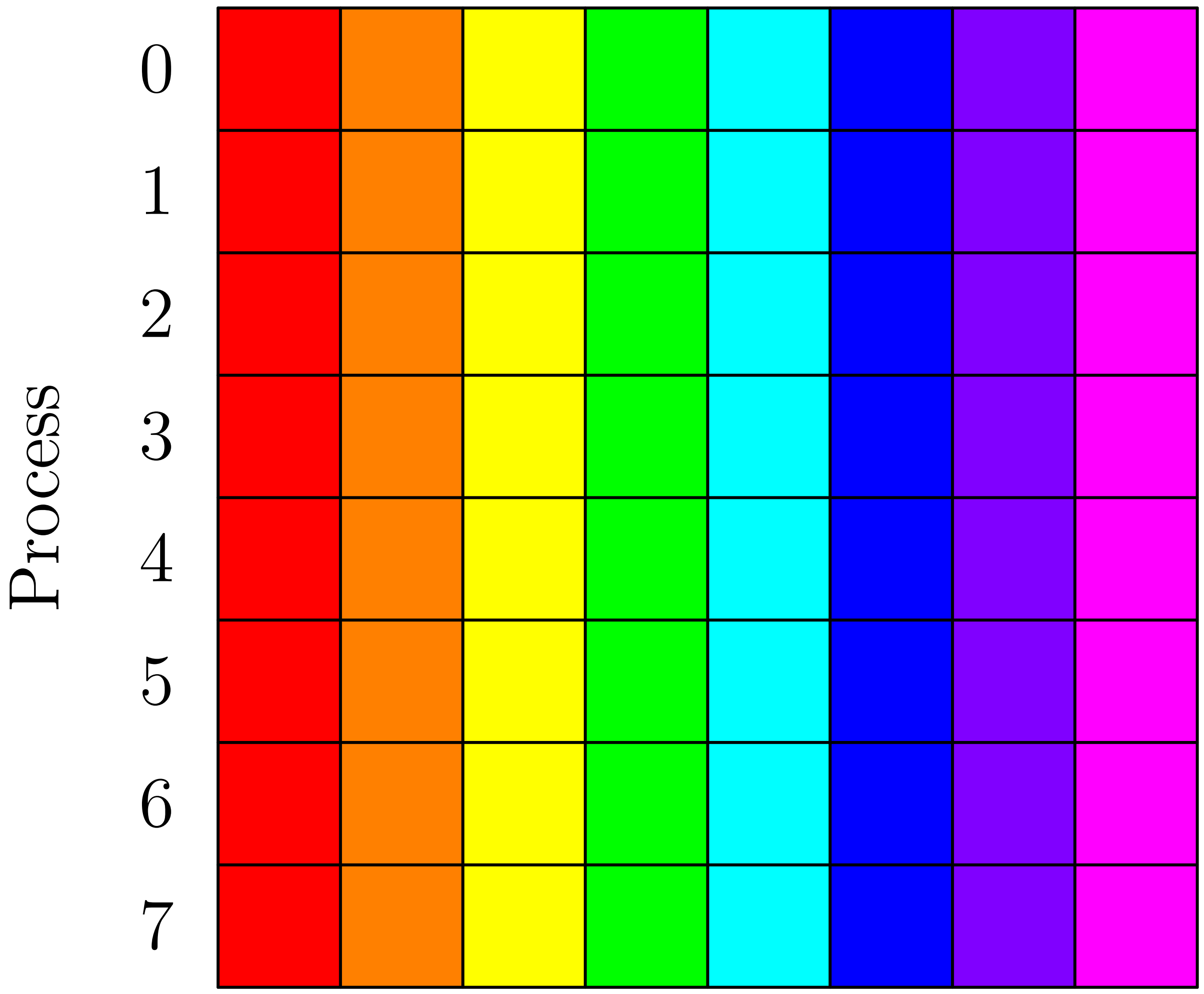


Advantages of Hybrid MPI/OpenMP

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

  – yields larger communication block size;

  – local transposition is not required within a single MPI node;

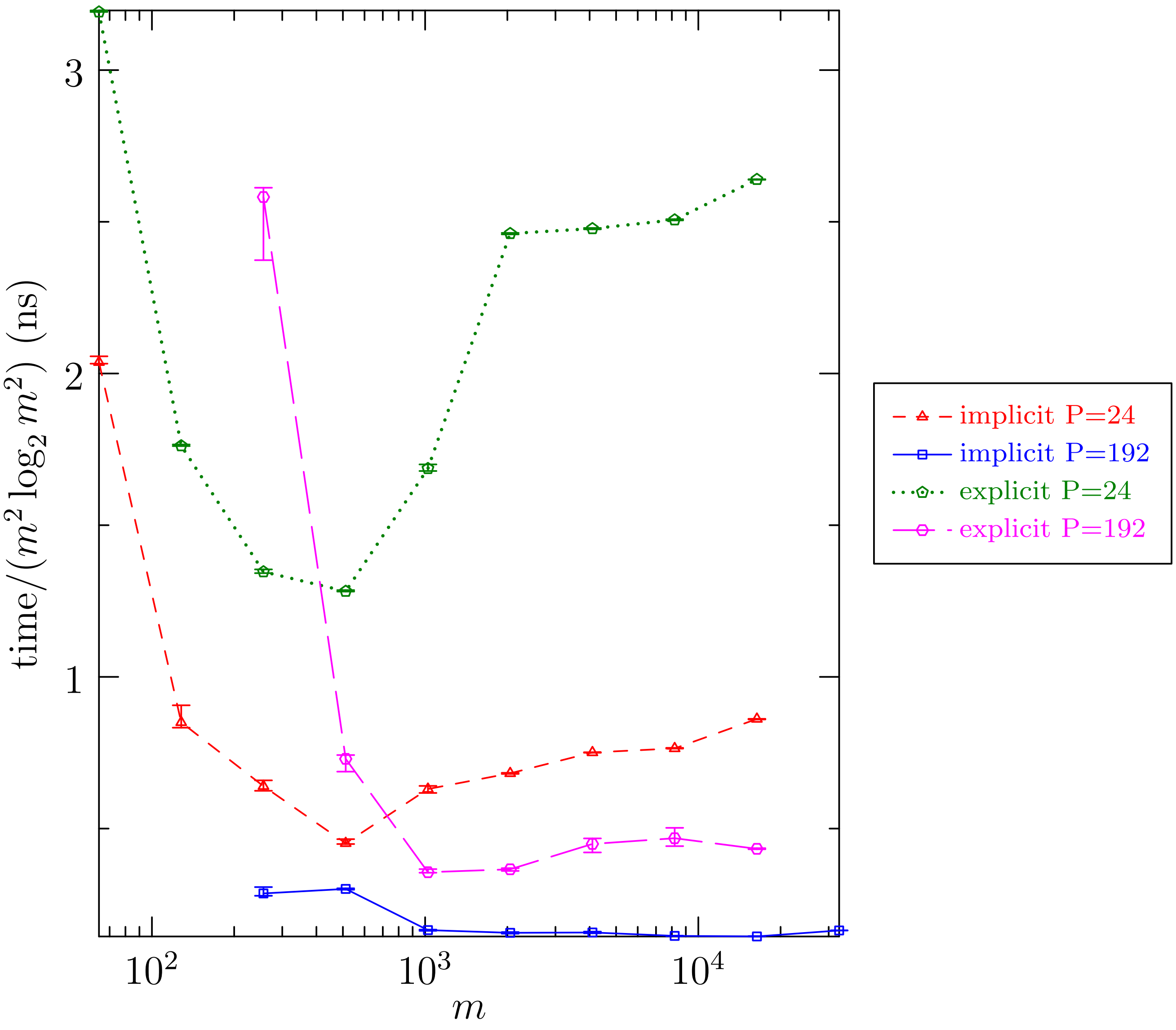
  – allows smaller problems to be distributed over a large number of processors;

  – for 3D FFTs, allows for more slab-like than pencil-like models, reducing the size of or even eliminating the need for a second transpose;

  – sometimes more efficient (by a factor of 2) than pure MPI.

- 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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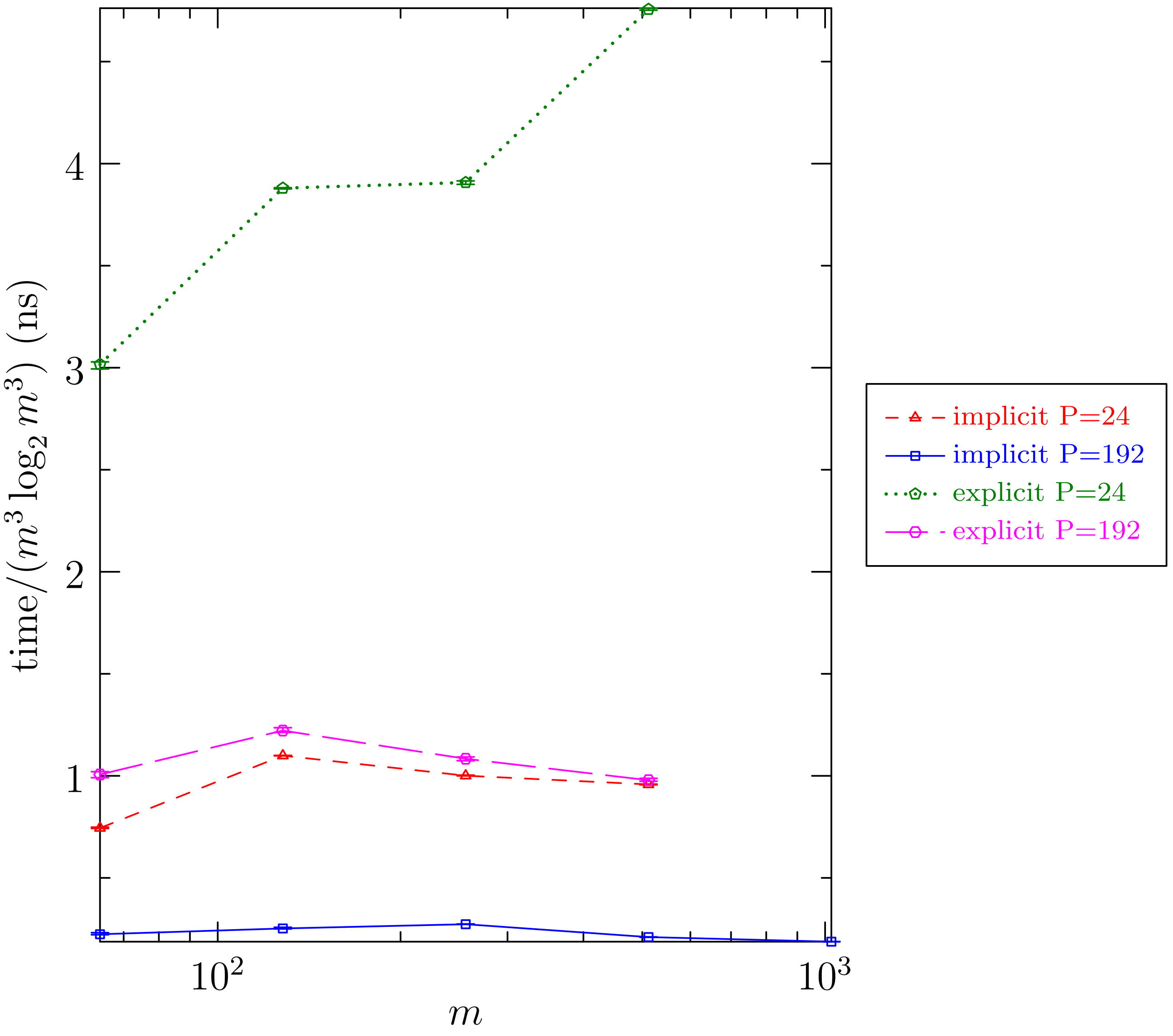
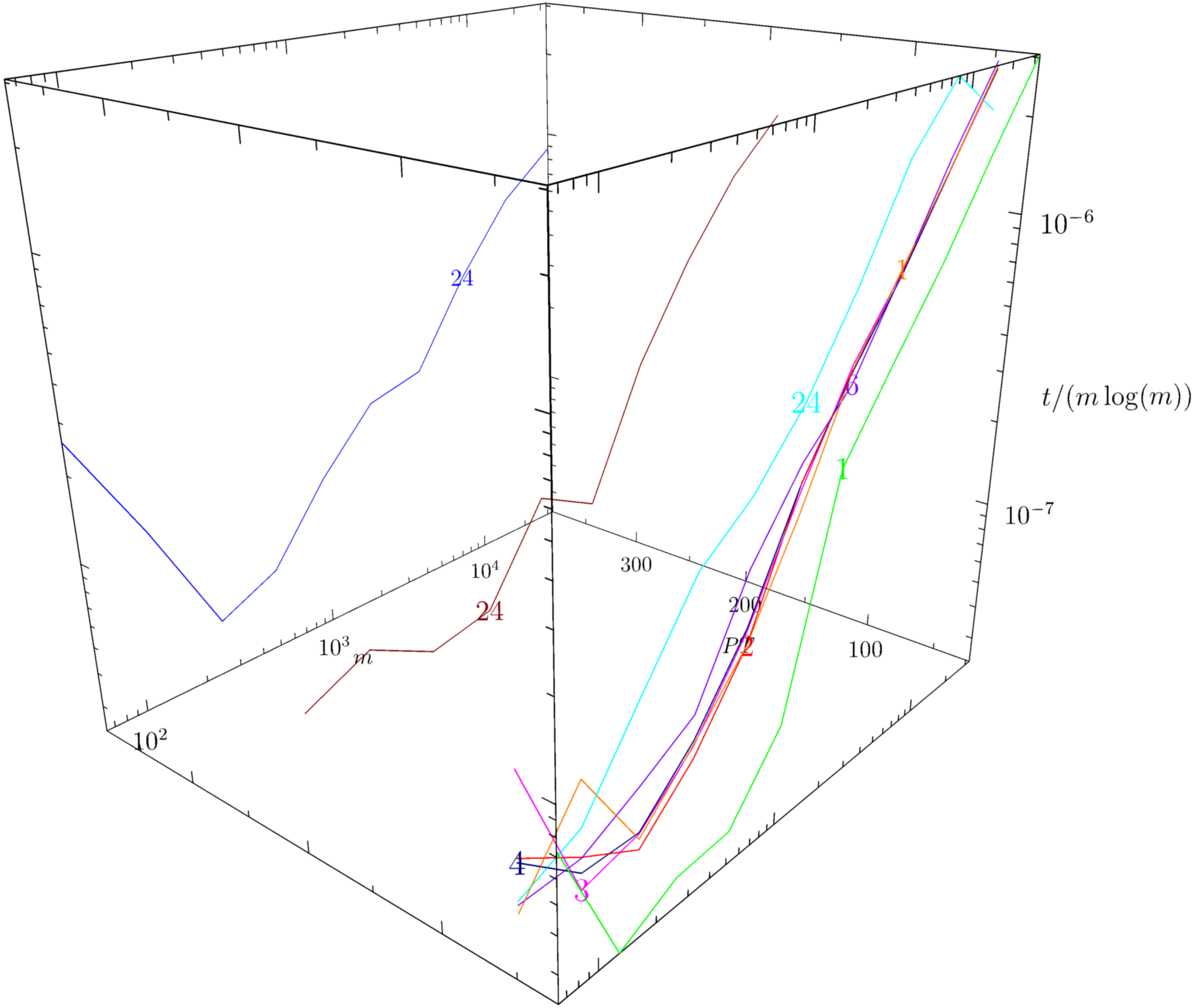
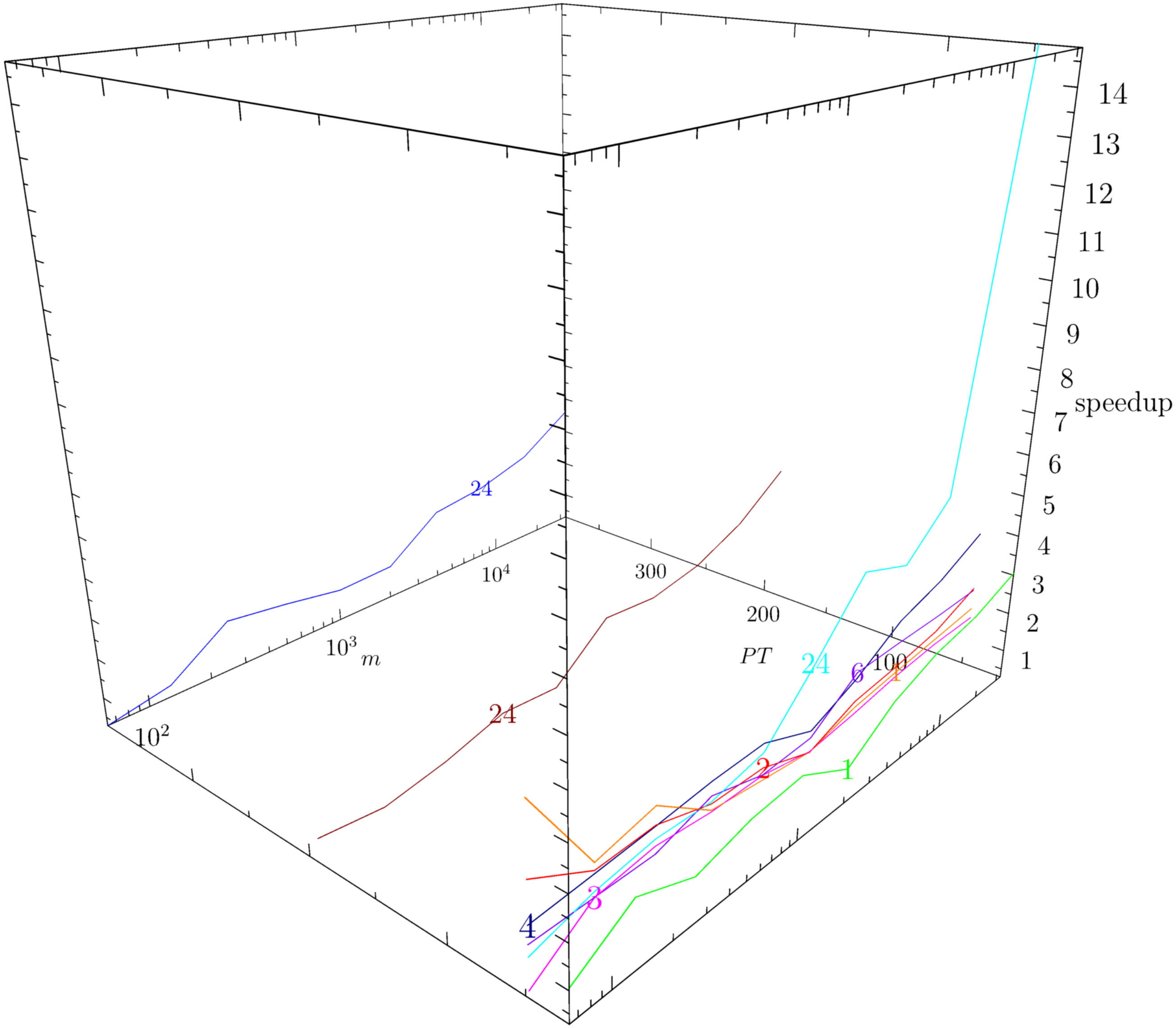


Hybrid MPI 3D Adaptive Transpose Timing



Hybrid MPI 3D Adaptive Transpose Speedup



Communication Costs: Direct Transpose

- Suppose an $N \times N$ matrix is distributed over P processes with $P \mid N$.

- Direct transposition involves $P-1$ communications per process, each of size N^2/P^2, for a total per-process data transfer of

$$\frac{P-1}{P^2}N^2.$$

Block Transpose

- Let $P = ab$. Subdivide $N \times M$ matrix into $a \times a$ blocks each of size $N/a \times M/a$.

- Inner: Over each team of b processes, transpose the a individual $N/a \times M/a$ matrices, grouping all a communications with the same source and destination together.

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

Communication Costs

- Let τ_ℓ be the typical latency of a message and τ_d be the time required to send each matrix element, so that the time to send a message consisting of n matrix elements is
$$\tau_\ell + n\tau_d$$
.

- The time required to perform a direct transpose is
$$T_D = \tau_\ell(P-1) + \tau_d \frac{P-1}{P^2} NM = (P-1)\left(\tau_\ell + \tau_d \frac{NM}{P^2}\right),$$
whereas a block transpose requires
$$T_B(a) = \tau_\ell\left(a + \frac{P}{a} - 2\right) + \tau_d\left(2P - a - \frac{P}{a}\right)\frac{NM}{P^2}.$$

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

Direct vs. Block Transposes

- Since

$$T_D - T_B = \tau_d \left(P + 1 - a - \frac{P}{a} \right) \left(L - \frac{NM}{P^2} \right),$$

  we see that a direct transpose is preferred when $NM \geq P^2 L$, whereas a block transpose should be used when $NM < P^2 L$.

- To find the optimal value of a for a block transpose consider

$$T_B'(a) = \tau_d \left(1 - \frac{P}{a^2} \right) \left(L - \frac{NM}{P^2} \right).$$

- 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

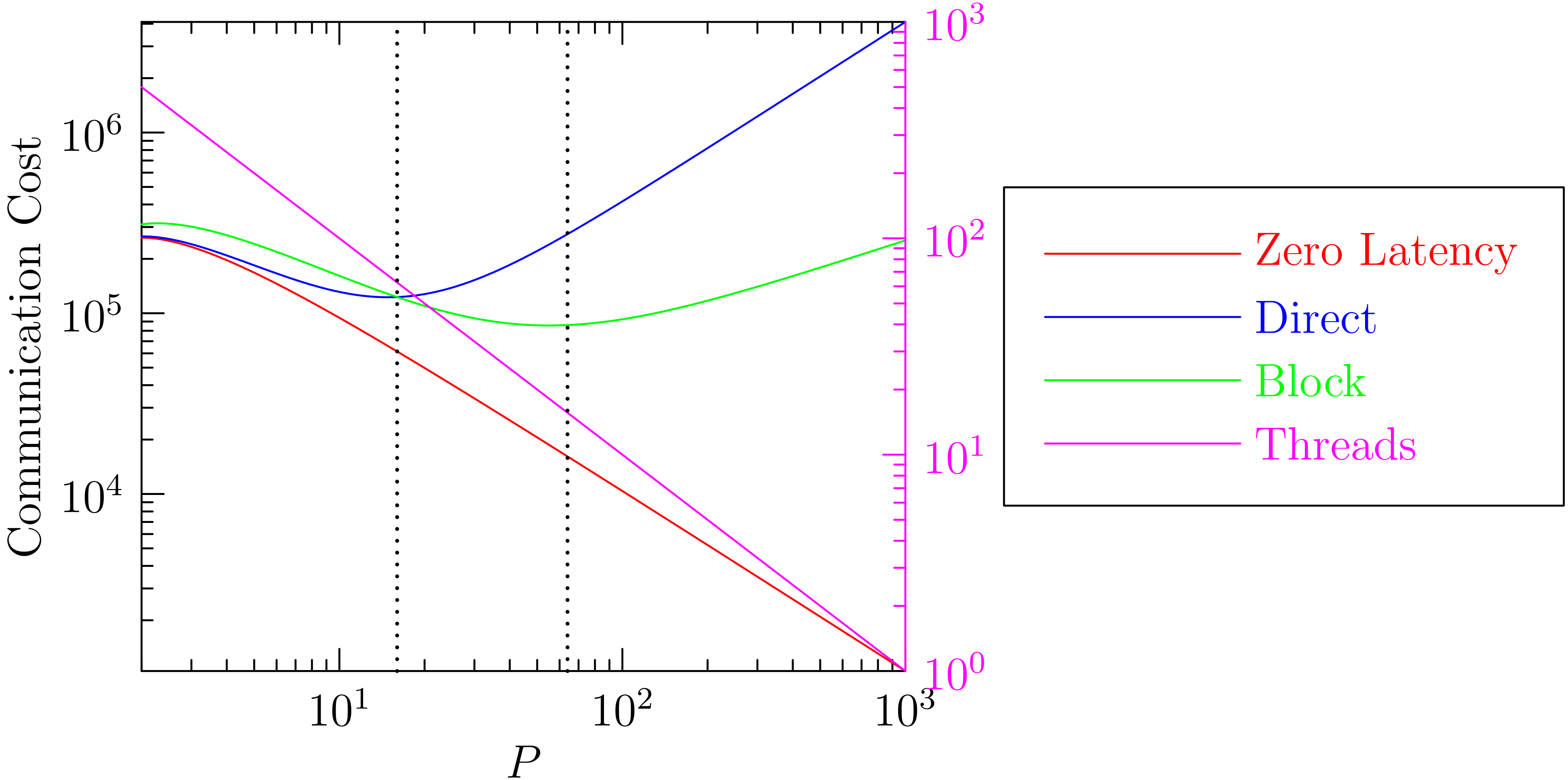
$$\begin{aligned} T_B(\sqrt{P}) &= 2\tau_d\left(\sqrt{P}-1\right)\left(L+\frac{NM}{P^{3/2}}\right) \\ &\sim 2\ \tau_d\sqrt{P}\left(L+\frac{NM}{P^{3/2}}\right), \qquad P \gg 1. \end{aligned}$$

- The global minimum of T_B over both a and P occurs at

$$P \approx (2NM/L)^{2/3}.$$

- 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



Conclusions

- For centered convolutions in d dimensions implicit padding asymptotically uses $(2/3)^{d-1}$ of the conventional storage.

- The factor of 2 speedup is largely due to increased data locality.

- Highly optimized and parallelized implicit dealiasing routines have been implemented as a software layer `FFTW++` (v 2.05) on top of the `FFTW` library and released under the Lesser GNU Public License: `http://fftwpp.sourceforge.net/`

- Hybrid MPI/OpenMP is often more efficient than pure MPI for distributed matrix transposes.

- 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`

References

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