Implicitly Padded Convolutions on Hybrid Parallel Architectures

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June 8, 2015

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Acknowledgements: Malcolm Roberts (Université de Strasbourg)

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, 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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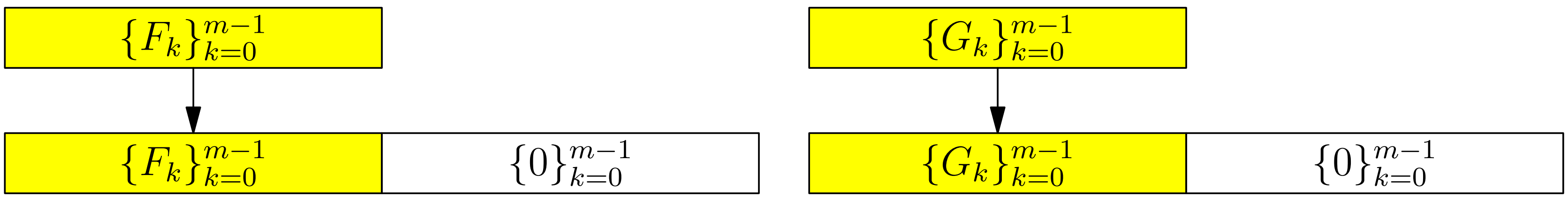

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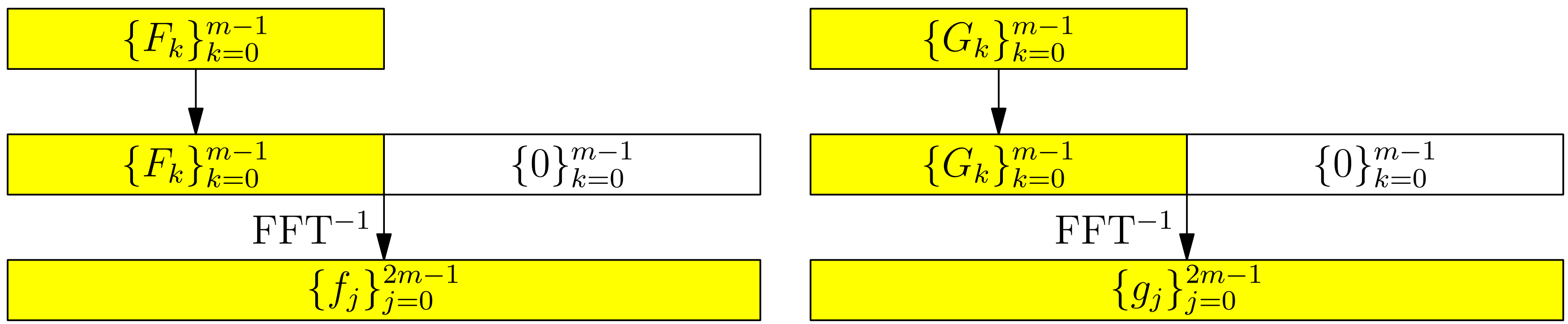

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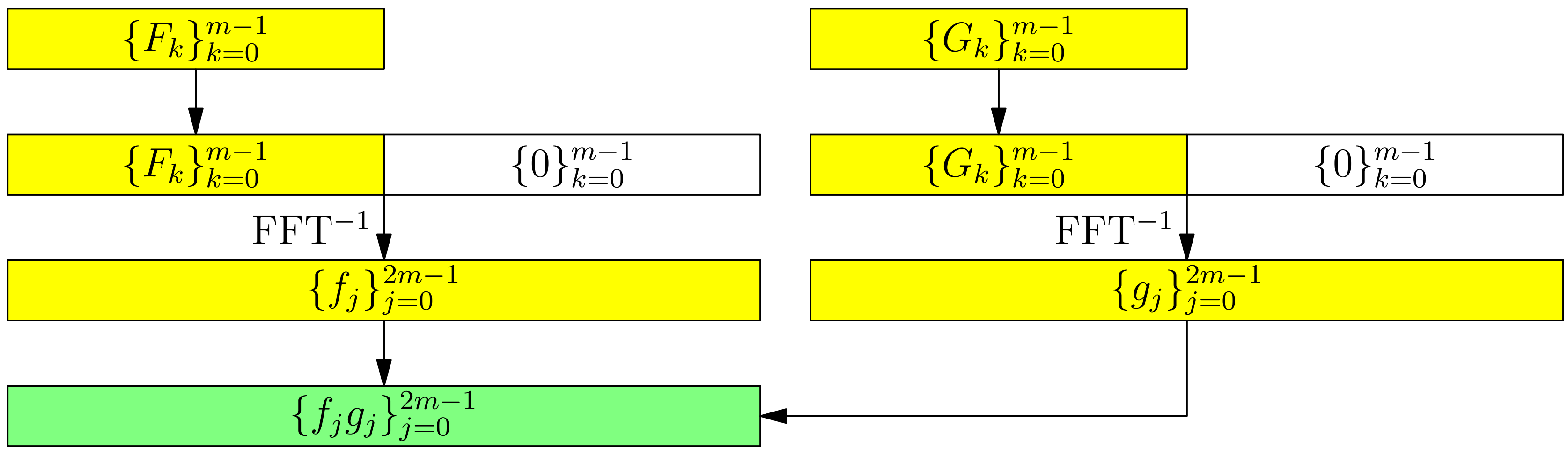

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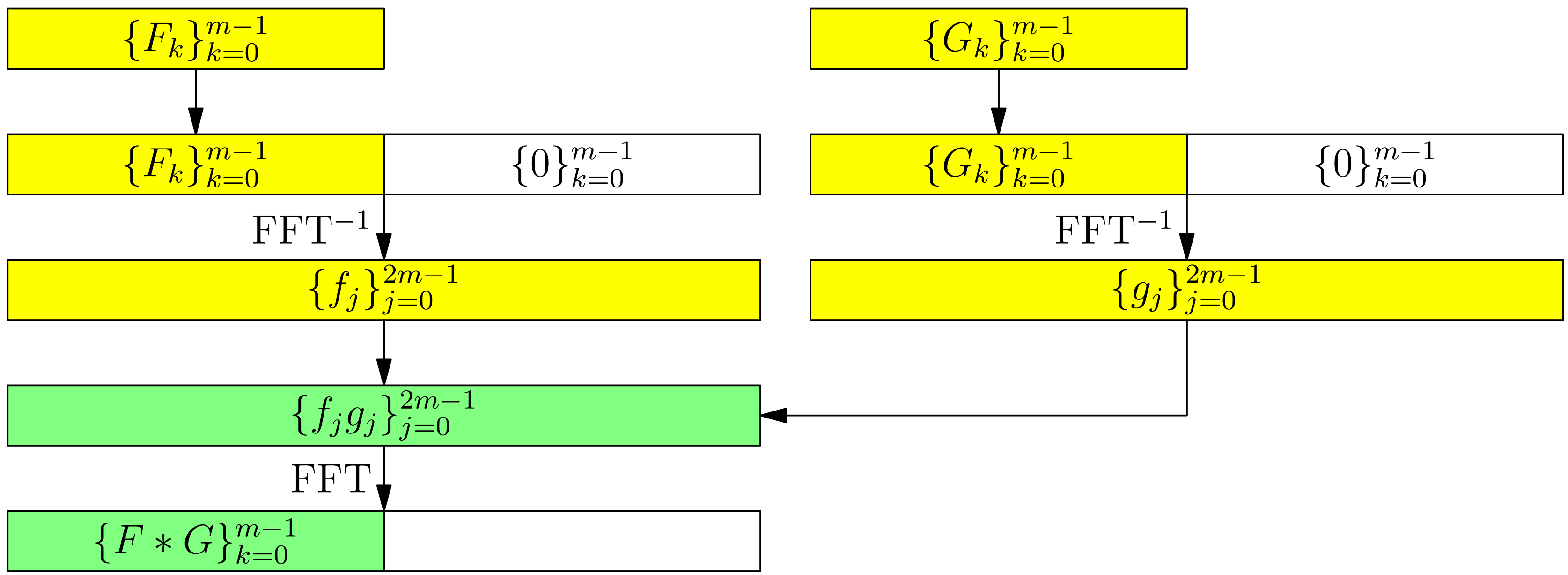

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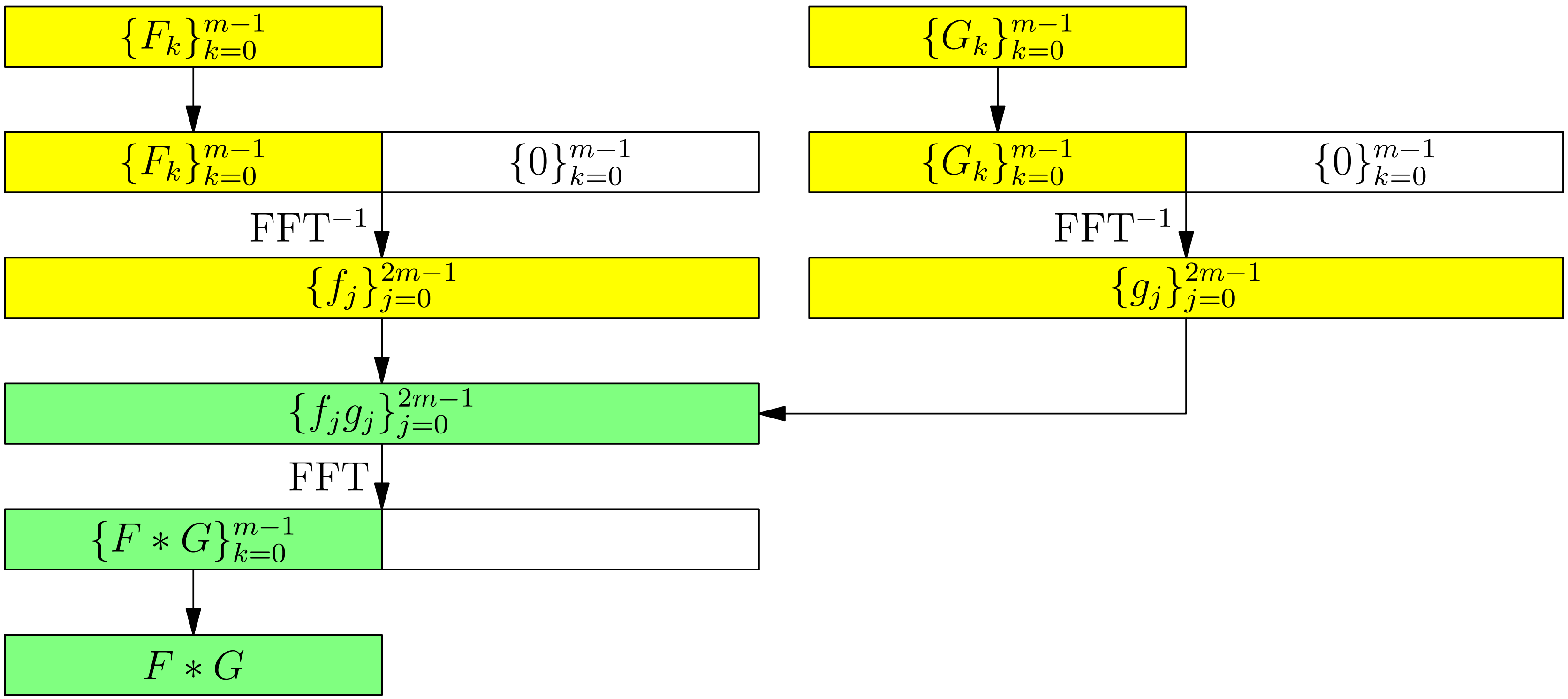

Implicit Padding

- 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:

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

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

- 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.

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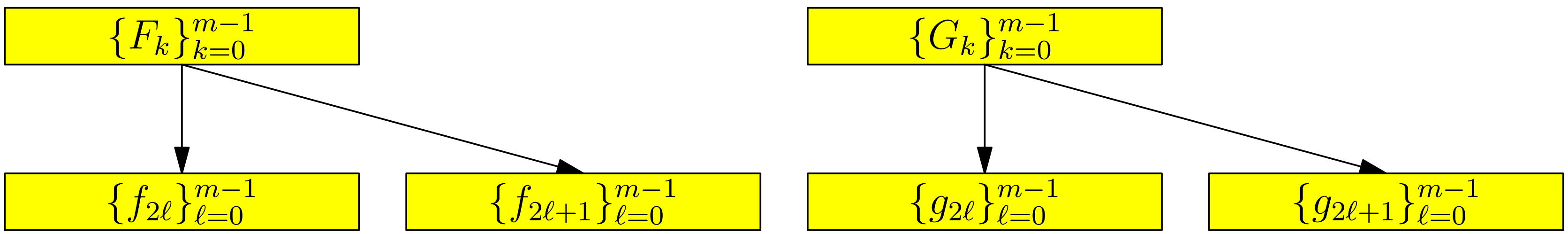

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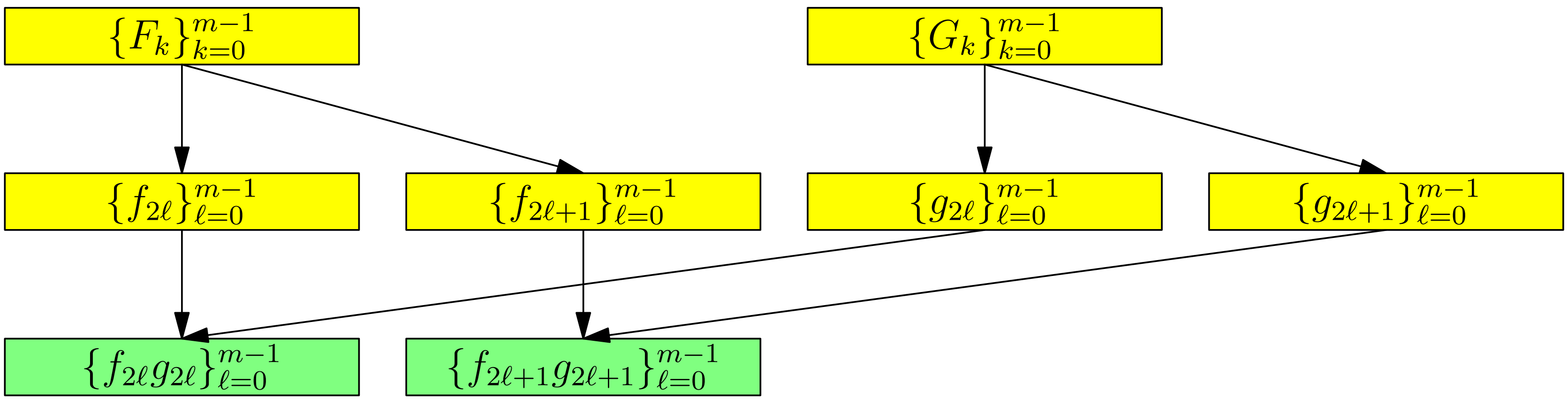

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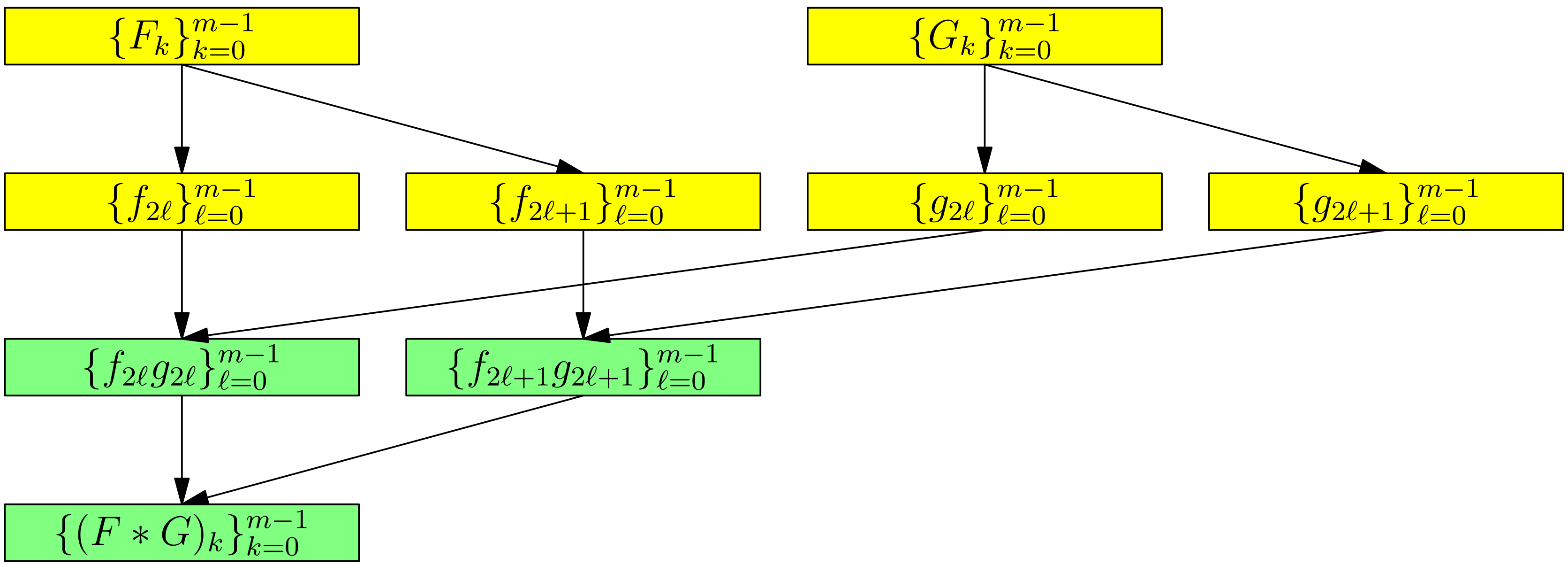

Input: vector f, vector g

Output: vector f

$\mathsf{u} \leftarrow \mathtt{fft}^{-1}(\mathsf{f})$;

$\mathsf{v} \leftarrow \mathtt{fft}^{-1}(\mathsf{g})$;

$\mathsf{u} \leftarrow \mathsf{u} * \mathsf{v}$;

for $k = 0$ **to** $m - 1$ **do**

  $\mathsf{f}[k] \leftarrow \zeta_{2m}^{k}\mathsf{f}[k]$;

  $\mathsf{g}[k] \leftarrow \zeta_{2m}^{k}\mathsf{g}[k]$;

end

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$\mathsf{v} \leftarrow \mathsf{v} * \mathsf{f}$;

$\mathsf{f} \leftarrow \mathtt{fft}(\mathsf{u})$;

$\mathsf{u} \leftarrow \mathtt{fft}(\mathsf{v})$;

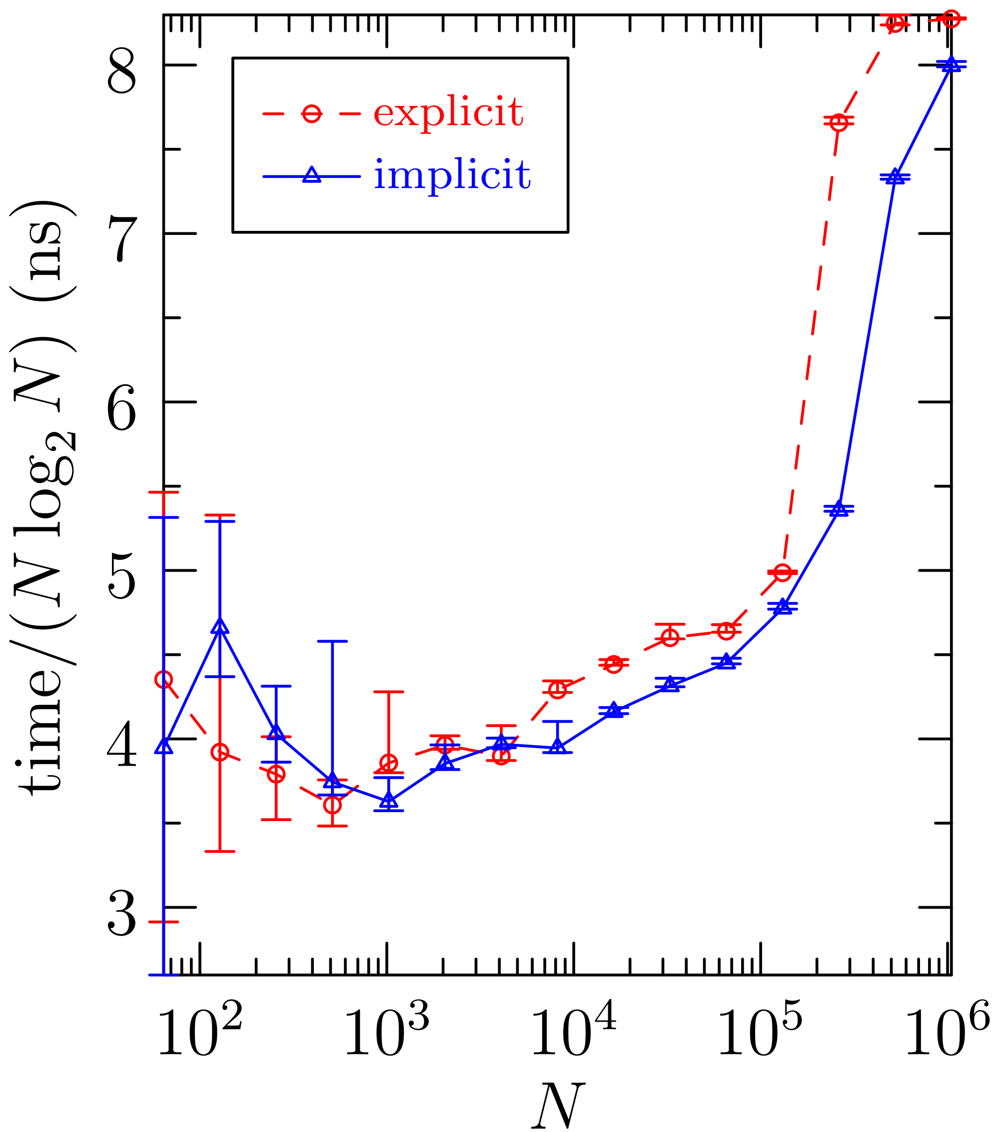
for $k = 0$ **to** $m - 1$ **do**

  $\mathsf{f}[k] \leftarrow \mathsf{f}[k] + \zeta_{2m}^{-k}\mathsf{u}[k]$;

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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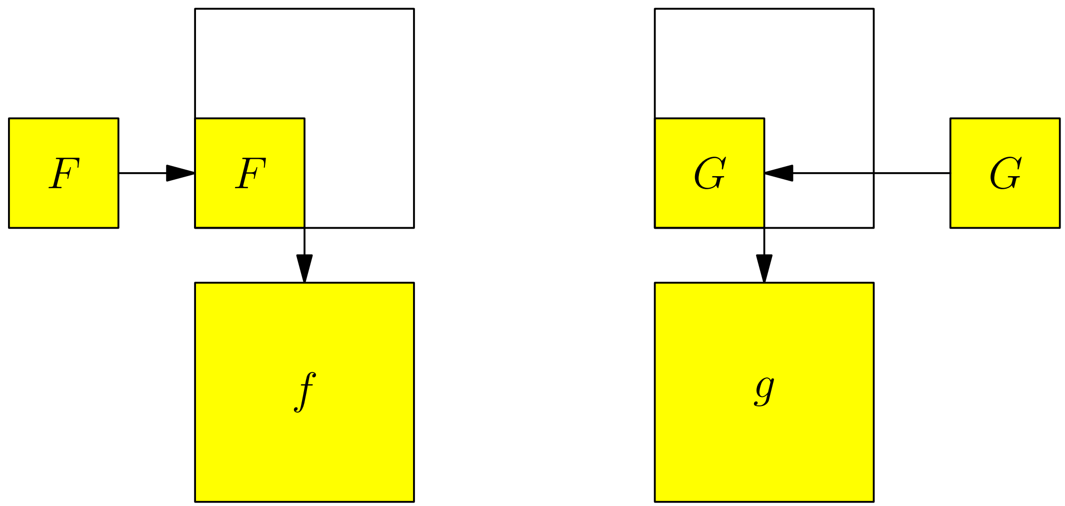

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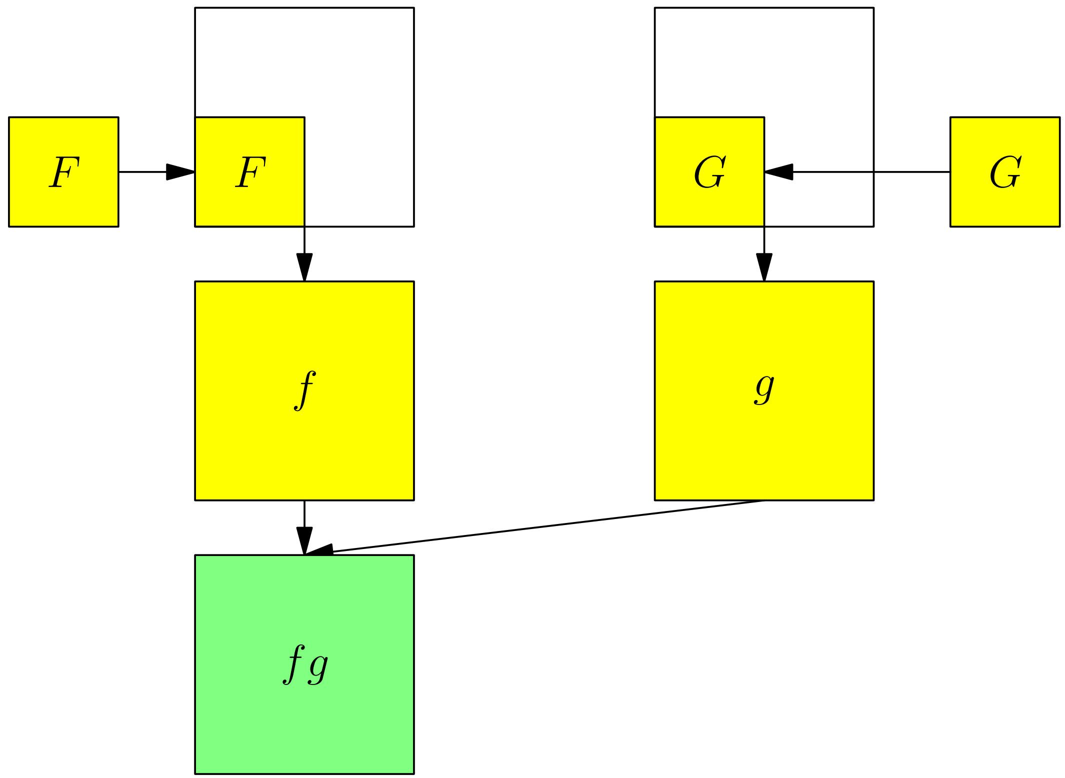

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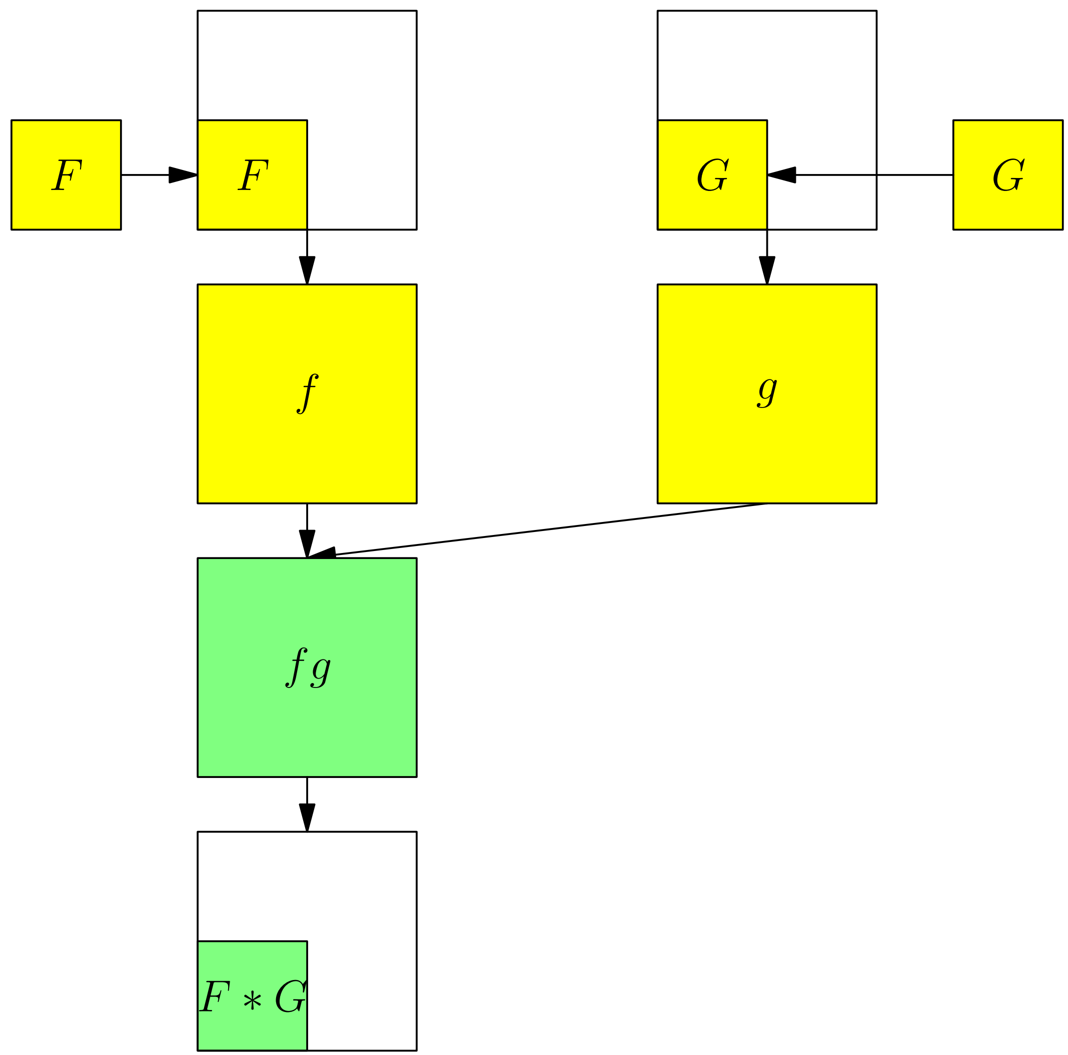

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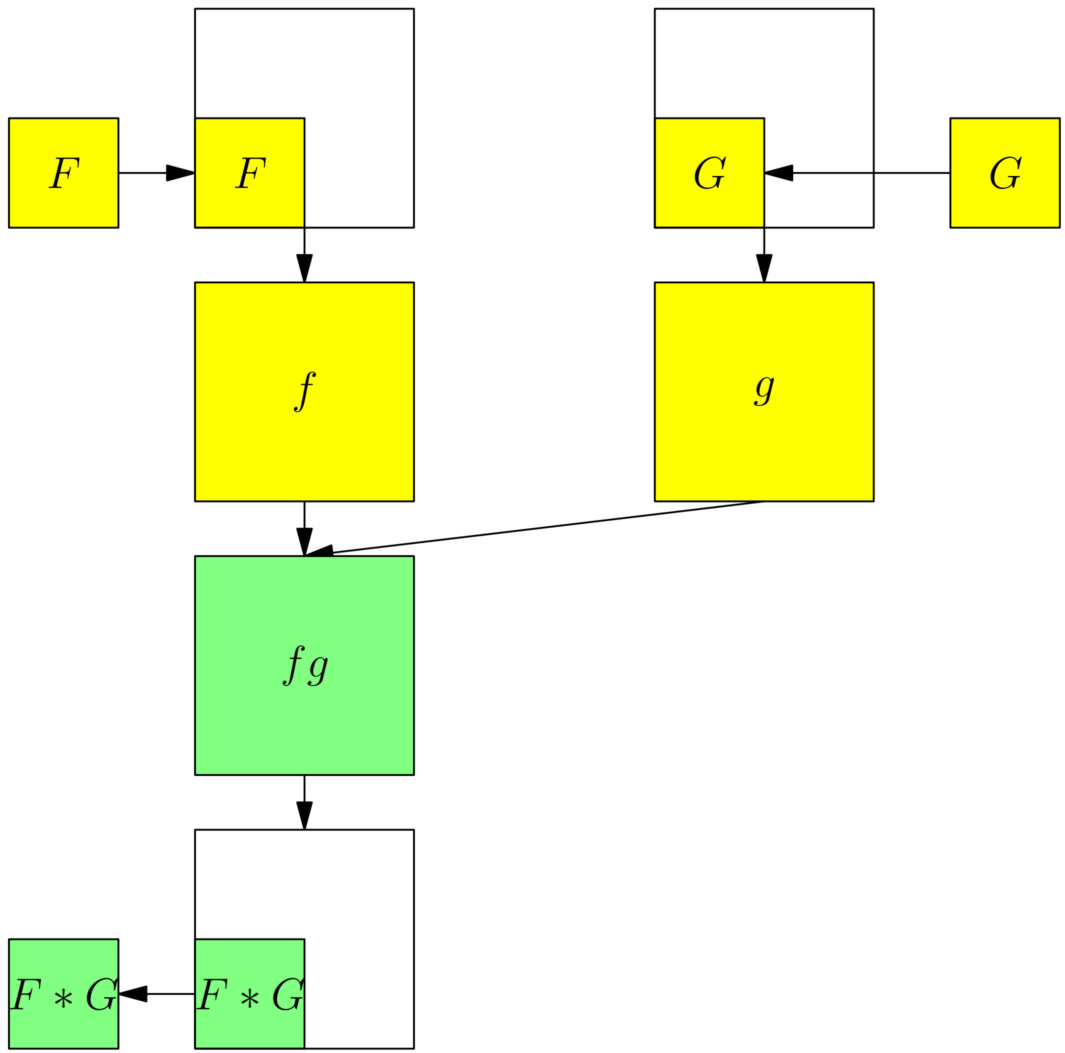


Recursive Convolution

- Naive way to compute a multiple-dimensional convolution:

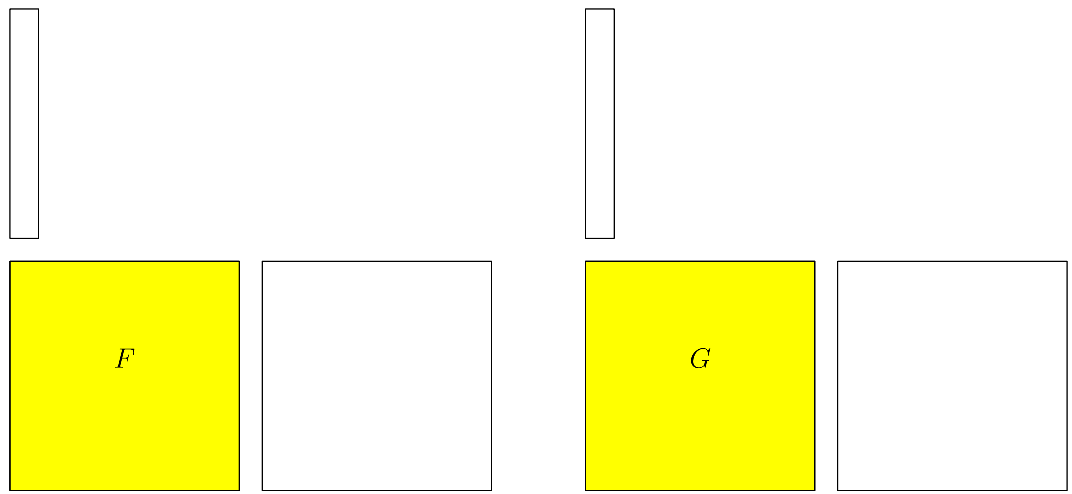
$$\boxed{\mathcal{F}_{N_1,\ldots,N_d}} \longrightarrow \boxed{\text{multiply}} \longrightarrow \boxed{\mathcal{F}^{-1}_{N_1,\ldots,N_d}}$$

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

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

Implicit Padding in 2D

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



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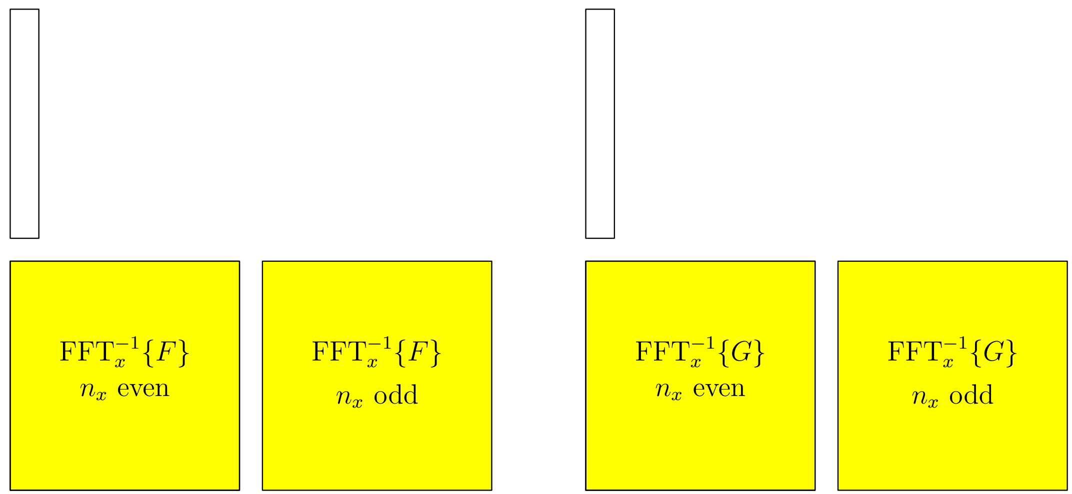

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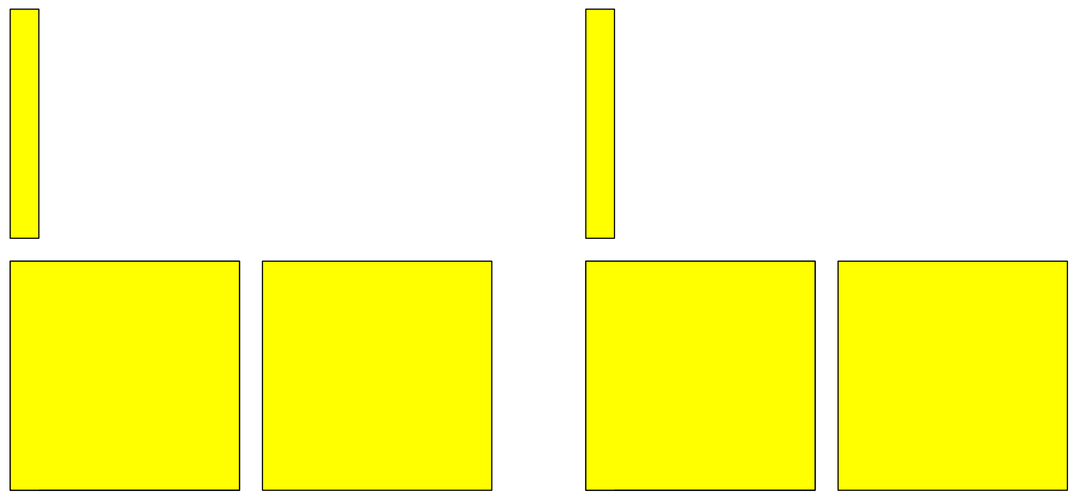

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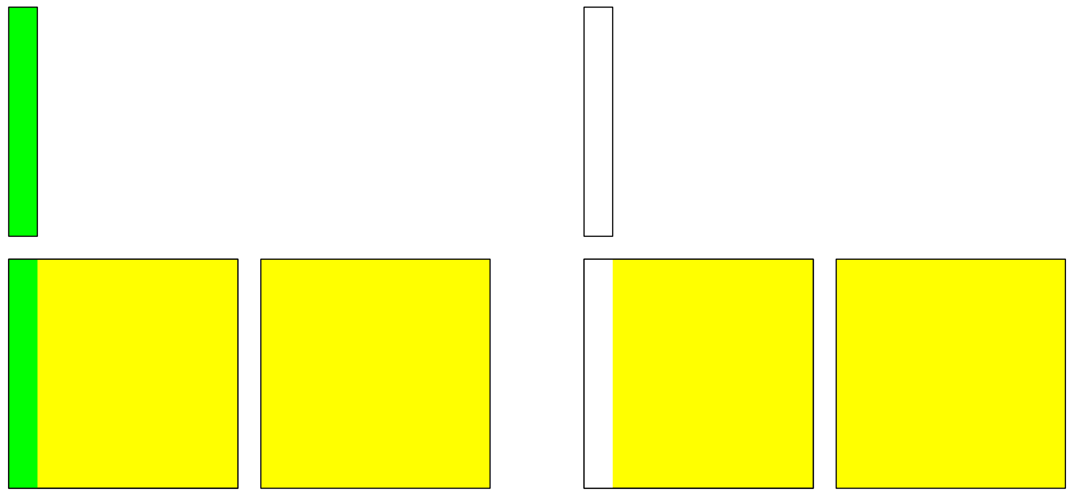

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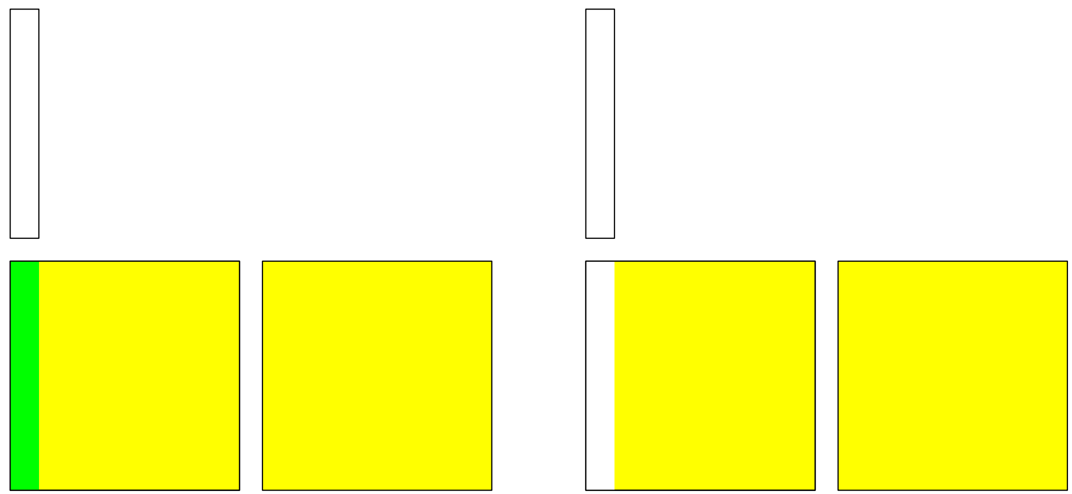

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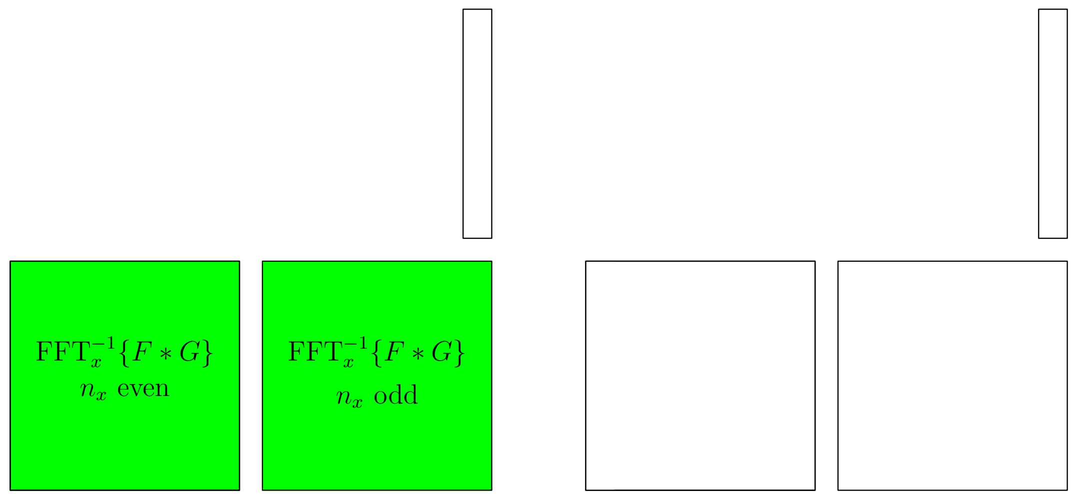

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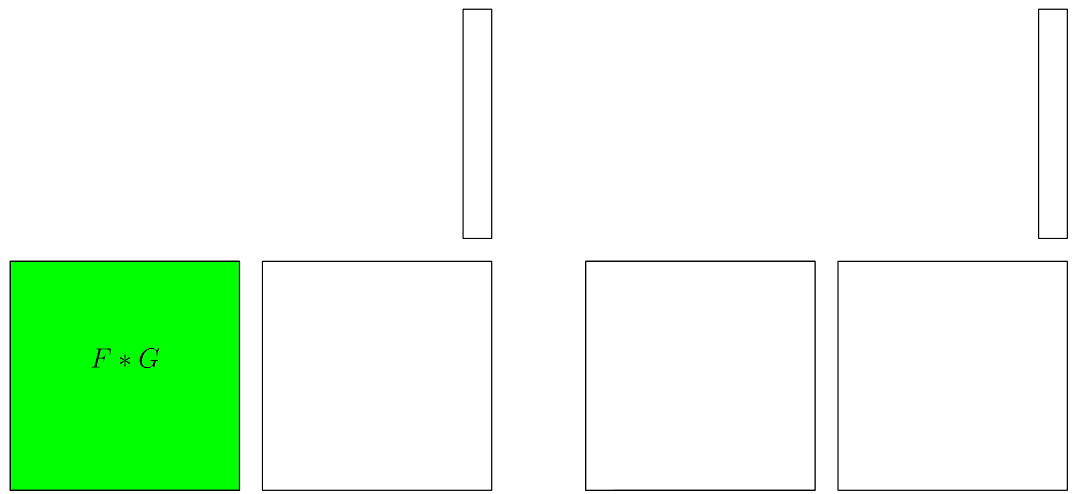

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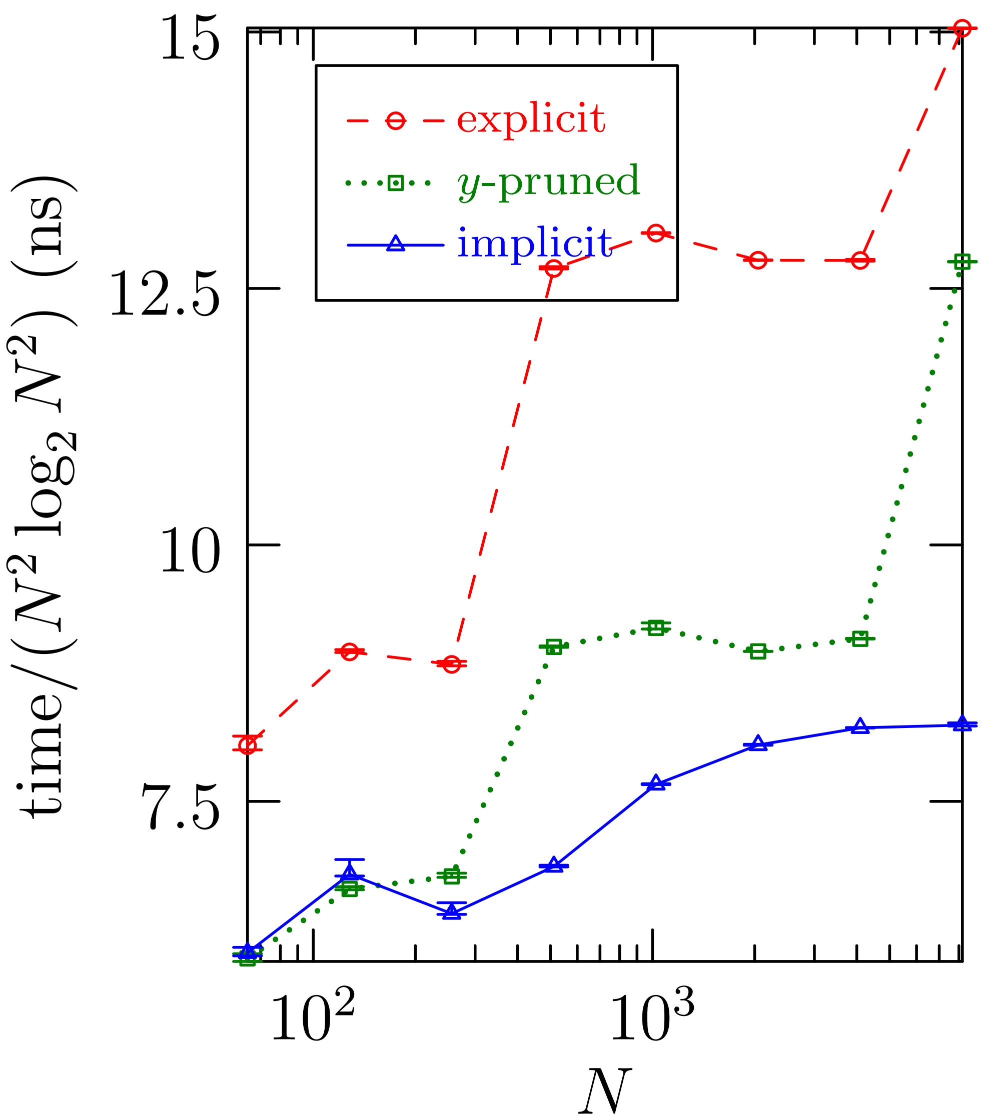
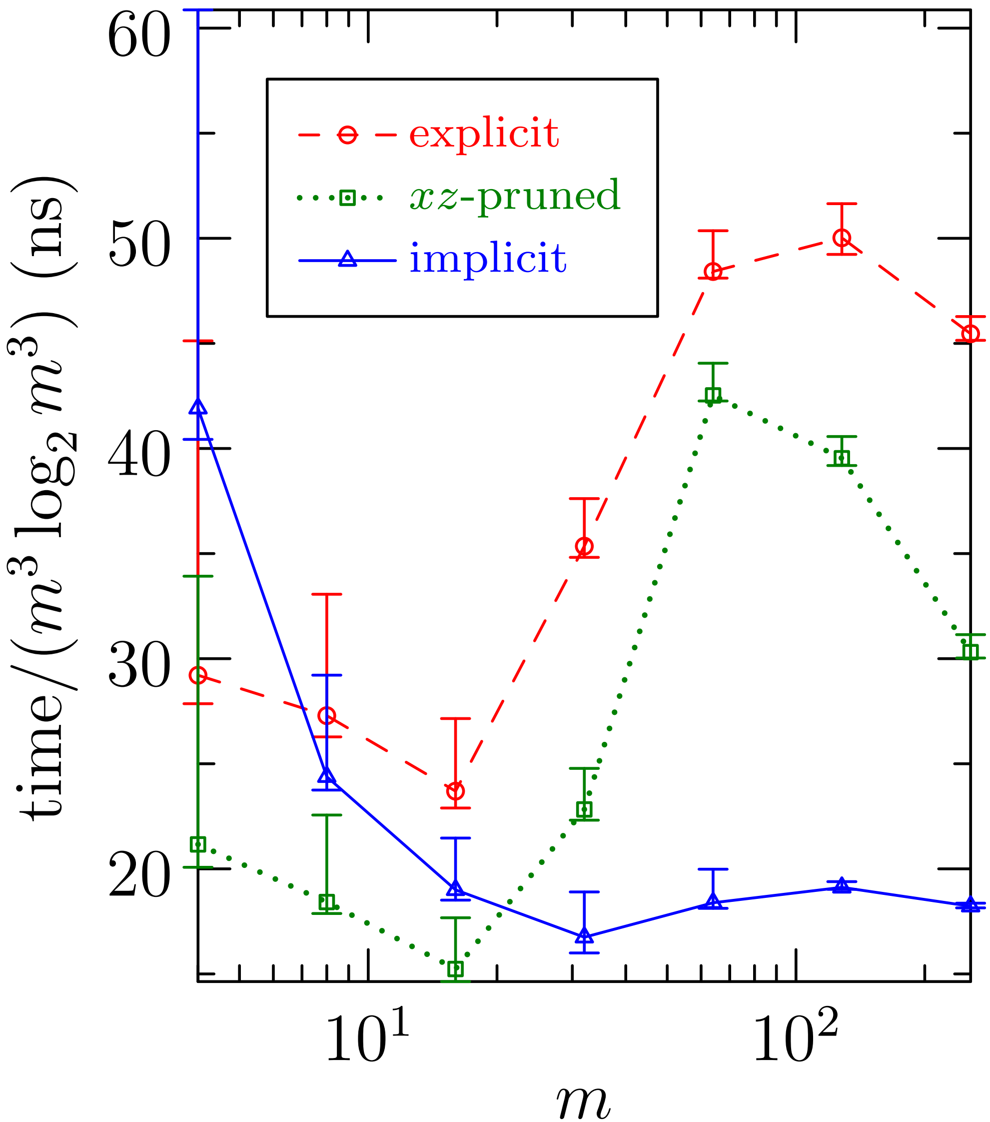


Implicit Padding in 3D



Hermitian Convolutions

- *Hermitian convolutions* arise when the input vectors are Fourier transforms of real data:

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

Centered 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 prevent mode $m-1$ from beating with itself to contaminate the most negative (first) mode, at wavenumber $-m+1$.

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

- The Hermiticity condition then appears as

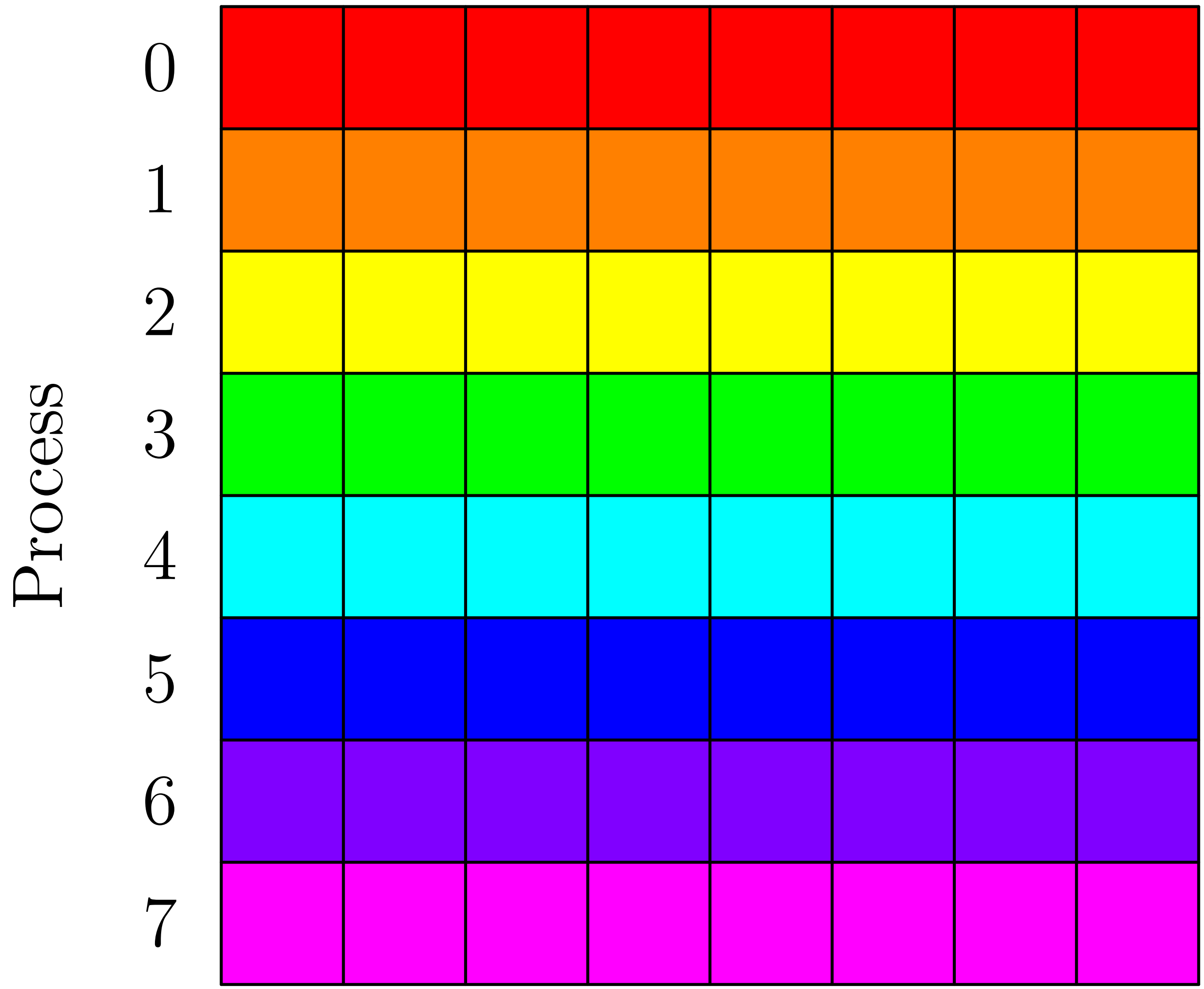
$$f_{-k} = \overline{f_k}.$$

Parallelization

- Our implicit and explicit convolution routines have been multithreaded for shared-memory architectures.
- Parallel generalized slab/pencil model implementations have recently been developed for distributed-memory architectures (available in svn repository and upcoming 1.14 release).
- The key bottleneck is the distributed matrix transpose.
- We have compared several distributed matrix transpose algorithms, both blocking and nonblocking, under both pure MPI and hybrid MPI/OpenMP architectures.
- Local transposition is not required within a single MPI node.
- Hybrid MPI/OpenMP offers a larger communication block size than pure MPI for matrix transposition.

- Hybrid MPI/OpenMP is sometimes more efficient (by a factor of 2) than pure MPI for computing distributed matrix transposes [Bowman & Roberts 2013].
- We have developed an adaptive algorithm, dynamically tuned to choose the optimal block size and number of threads.

8×8 Block Transpose over 8 processors



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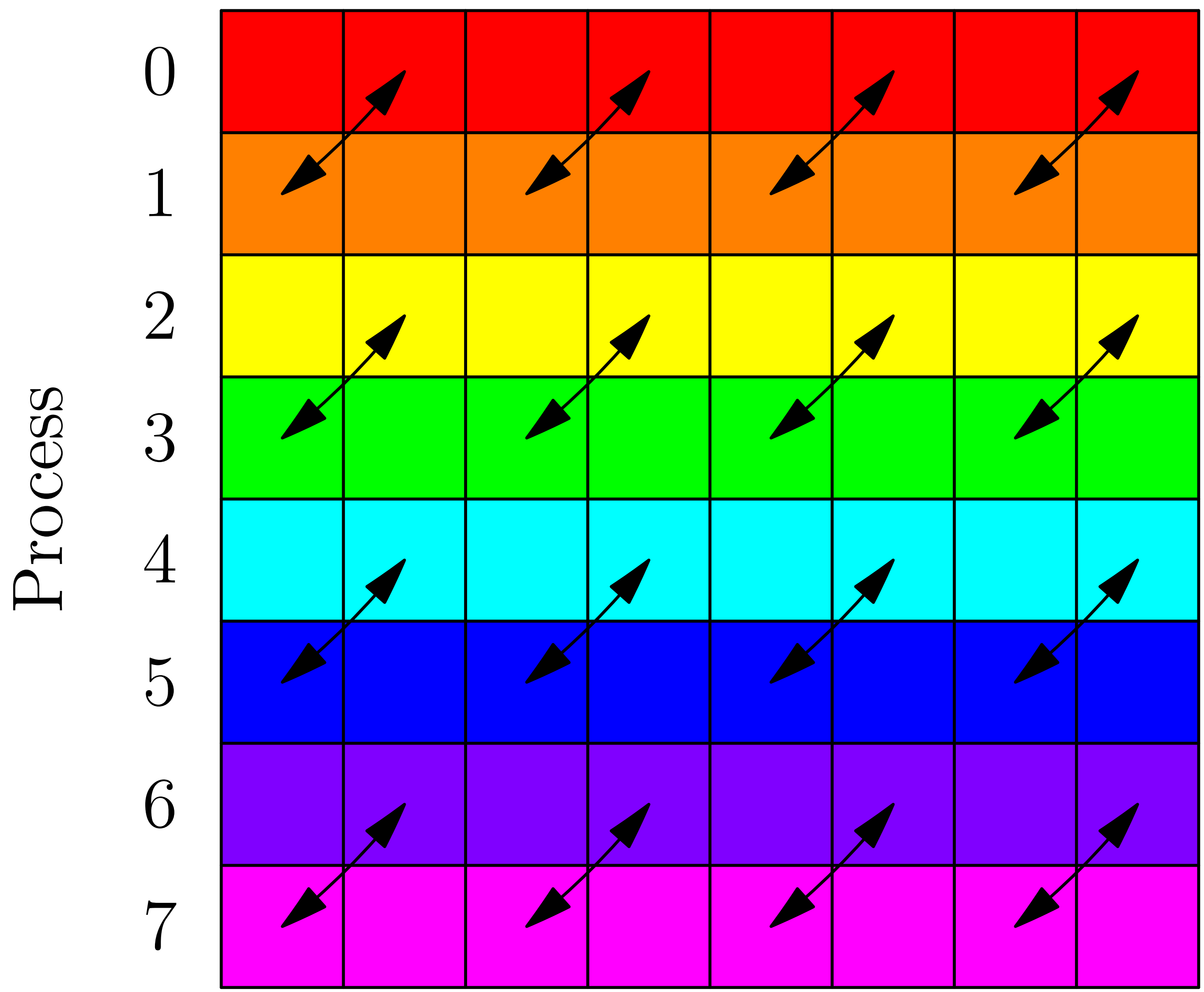

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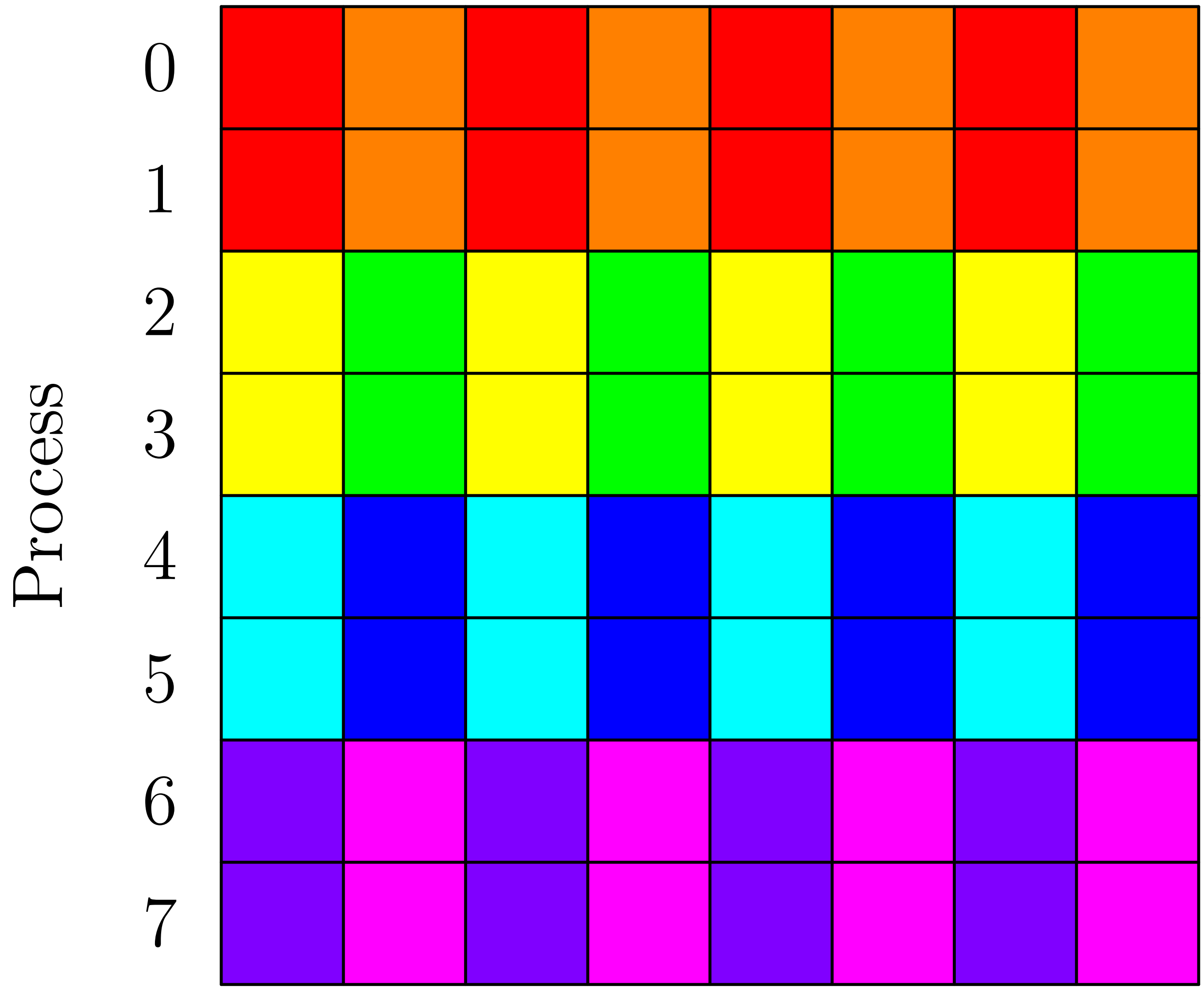
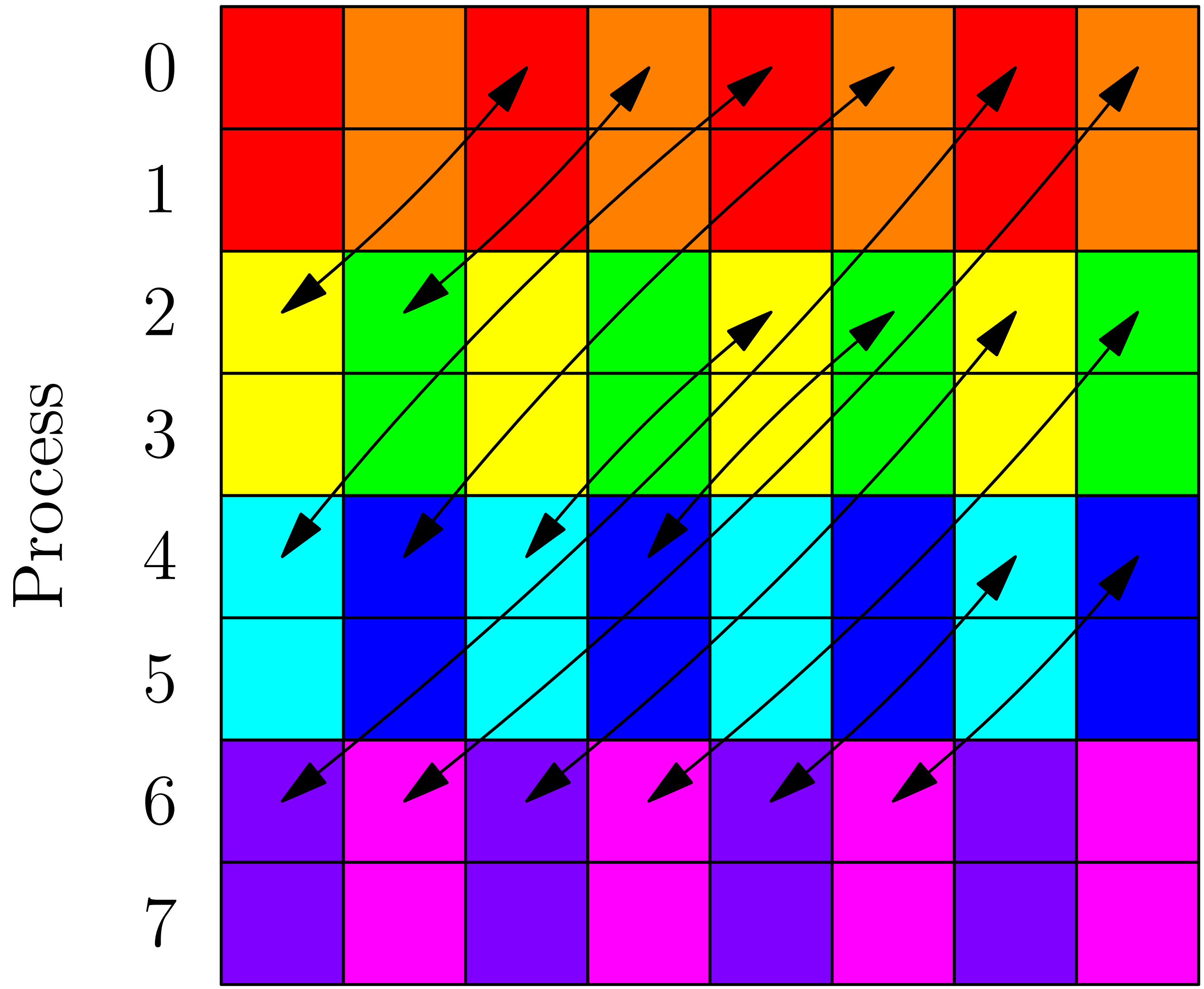


8 × 8 Block Transpose over 8 processors



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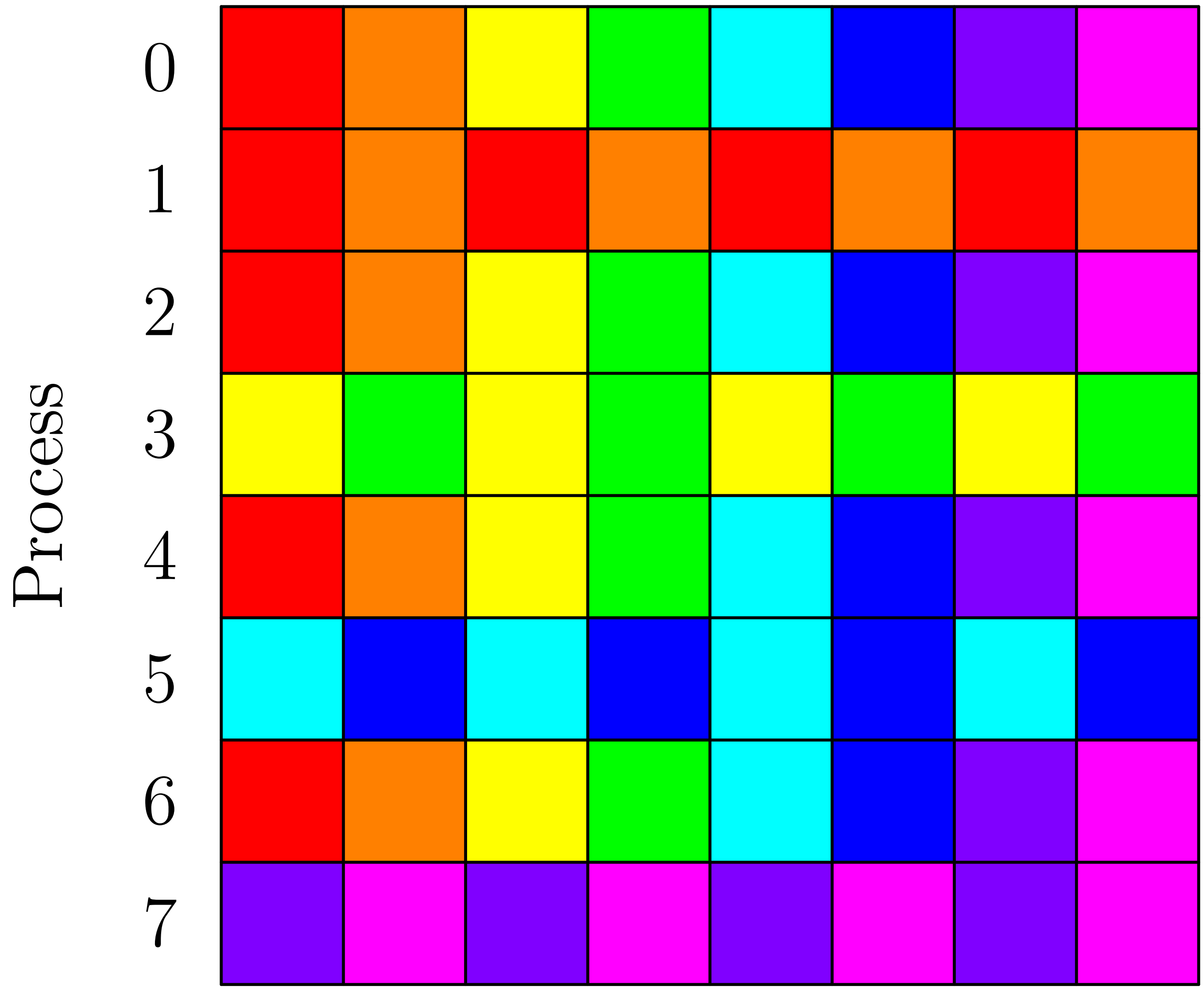

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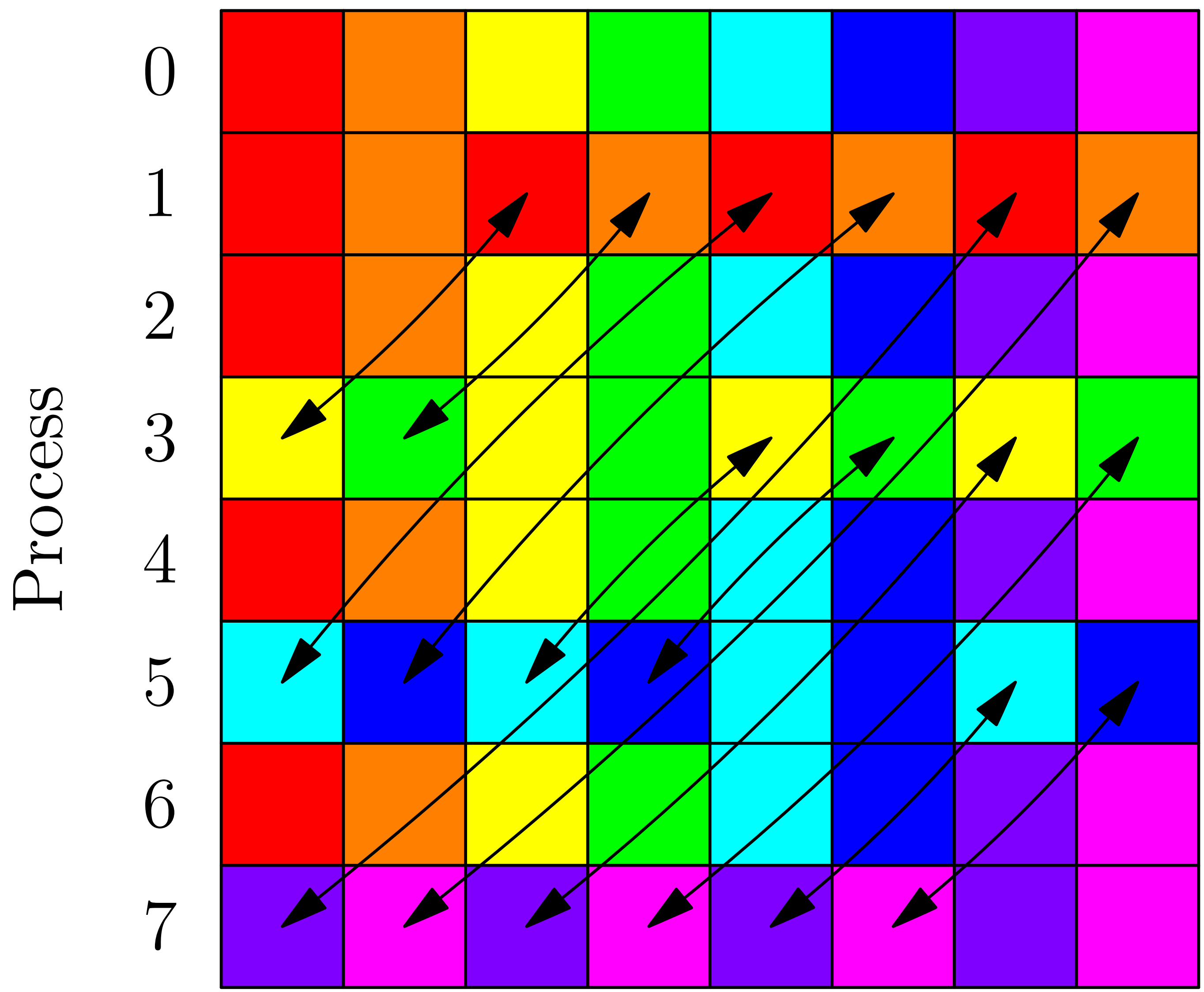

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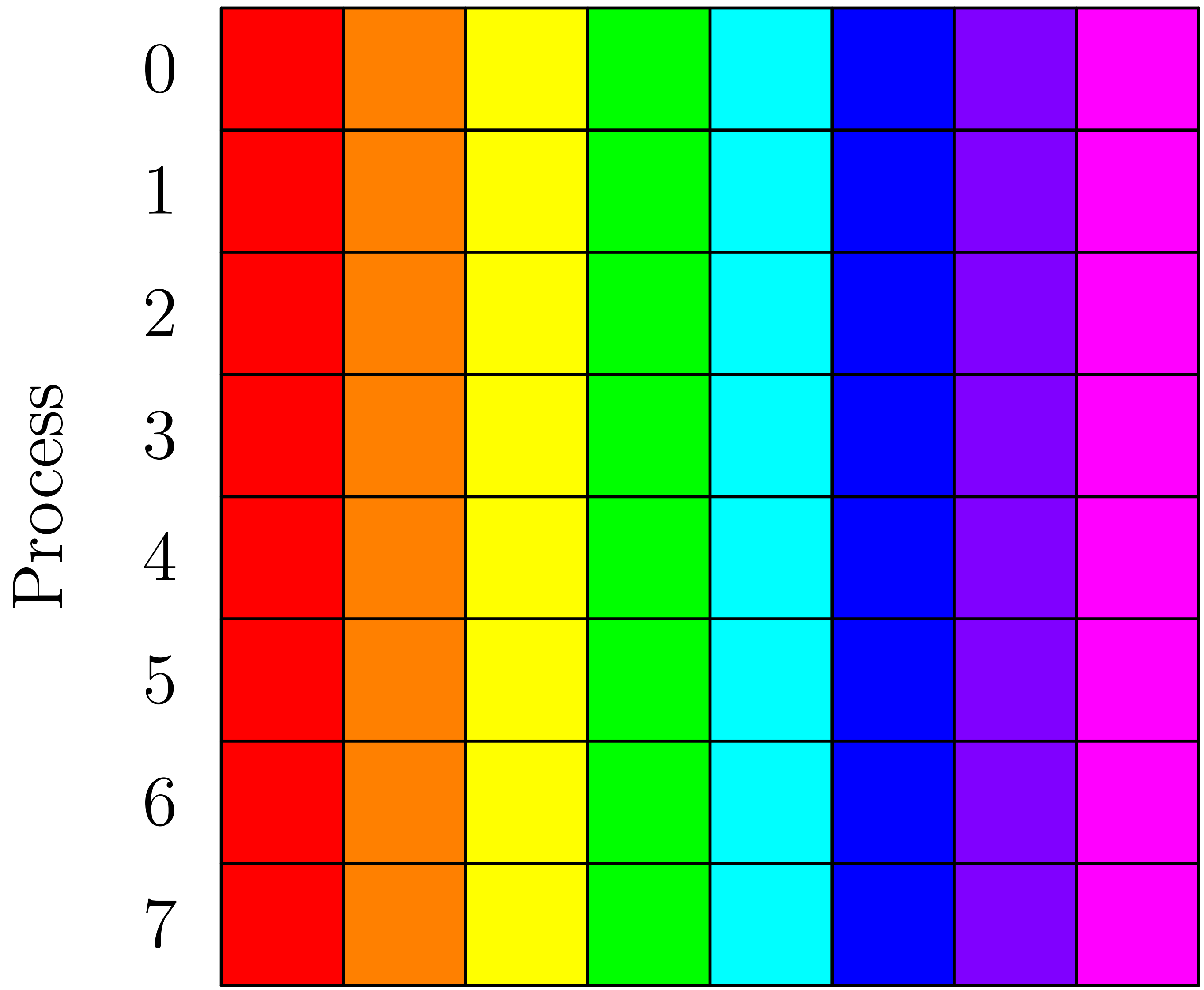
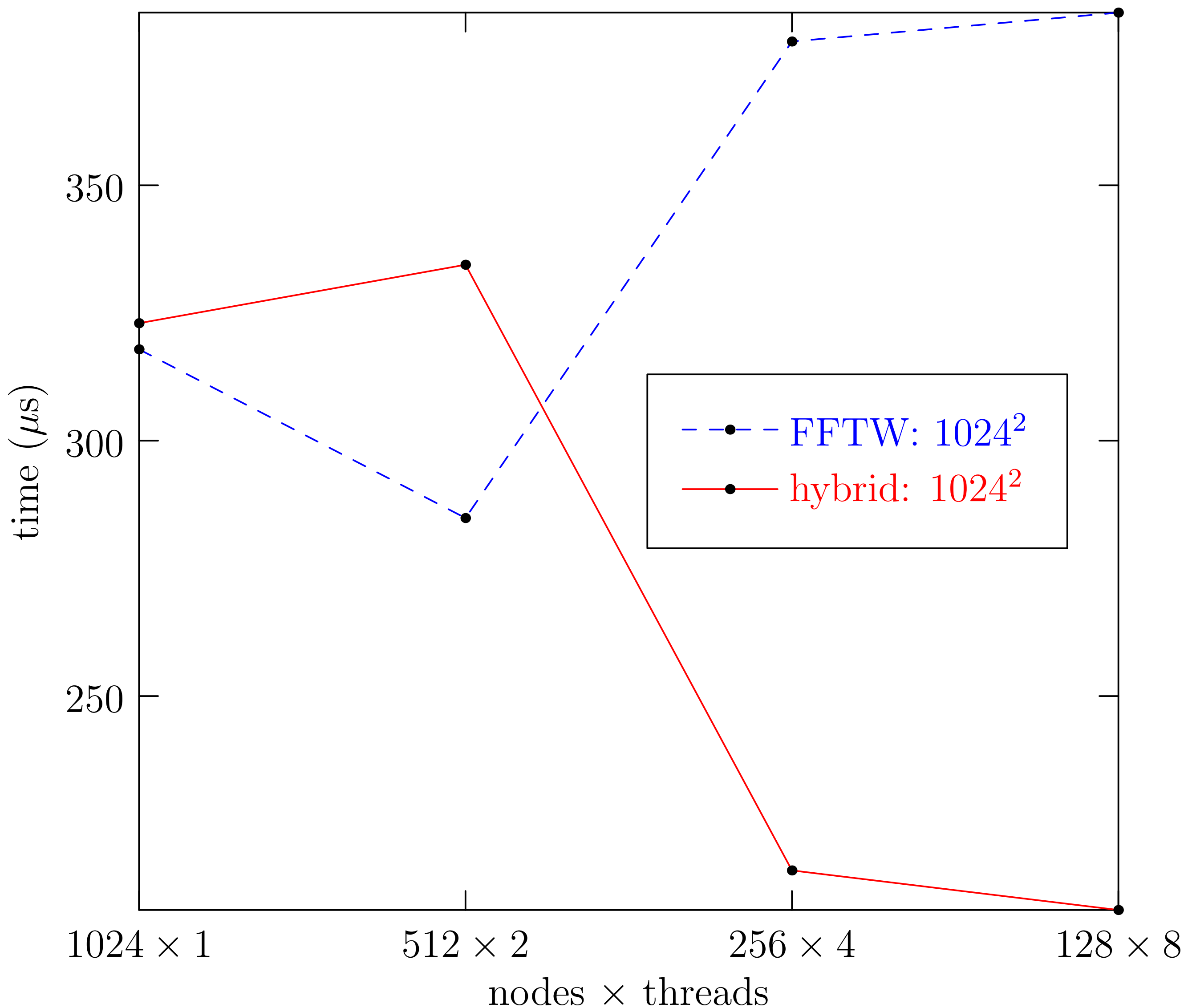


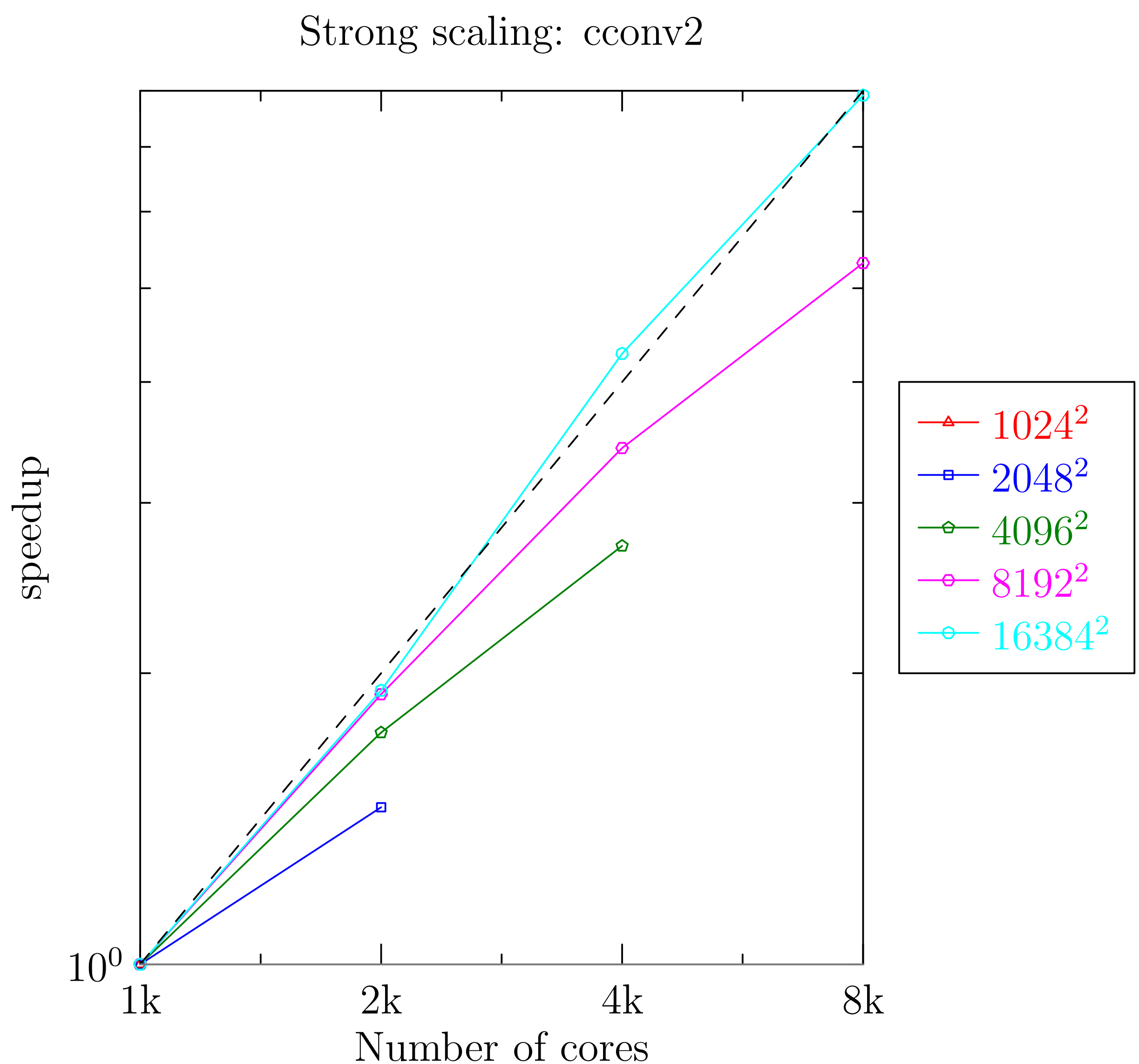
Matrix Transpose: Optimal Number of Threads



Advantages of Hybrid MPI/OpenMP

- Smaller problems sizes to be distributed over a large number of processors;
- More slab-like than pencil-like model; this reduces the size of or even eliminates the need for the second transpose.
- Overlapping computation with communication can yield a 10% speedup for 3D implicitly dealiased convolutions, where a natural parallelism exists between communication and computation.

Pure MPI Scaling of 2D Implicit Convolutions



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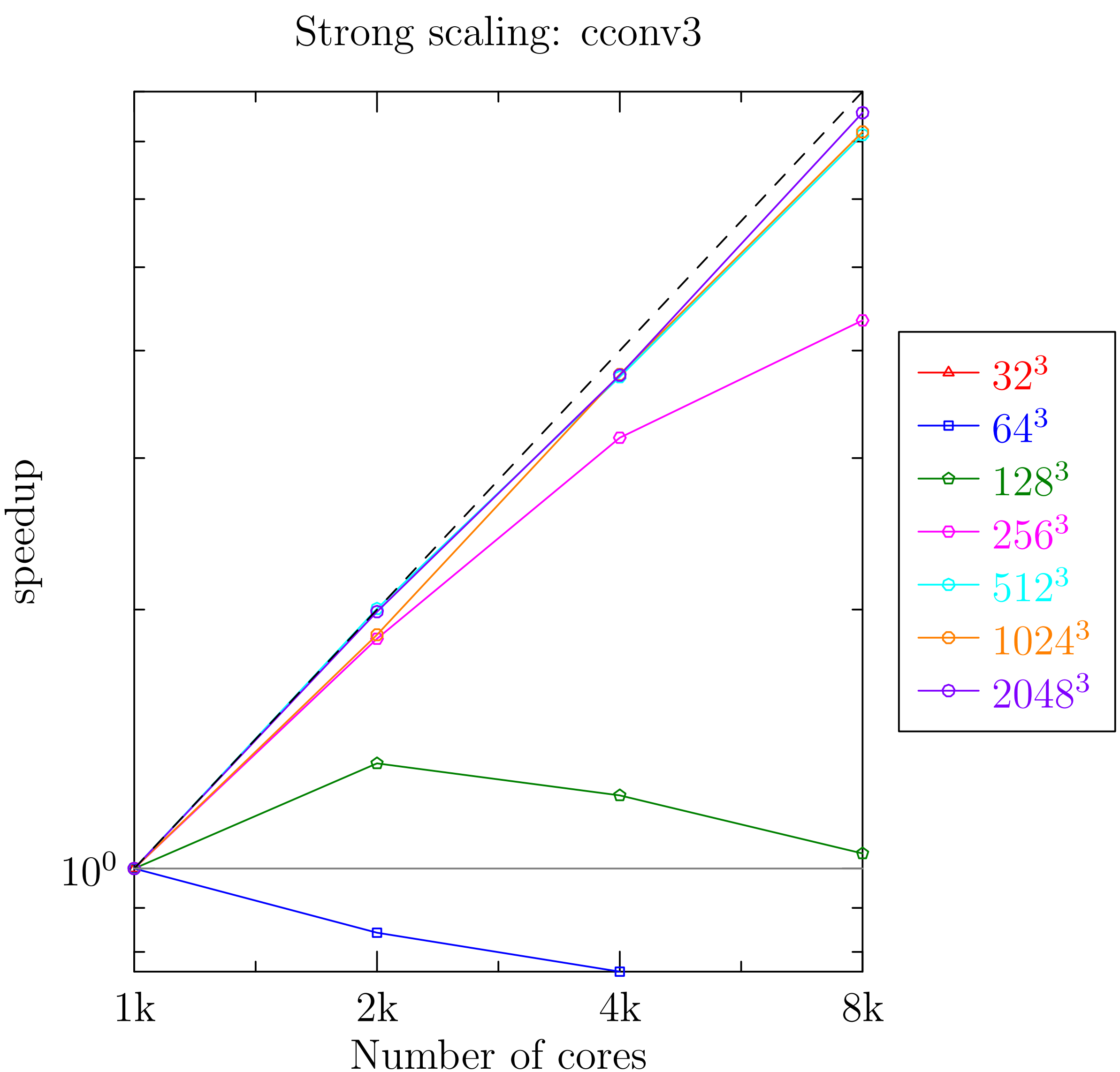


Multithreaded Hermitian Convolution

- 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

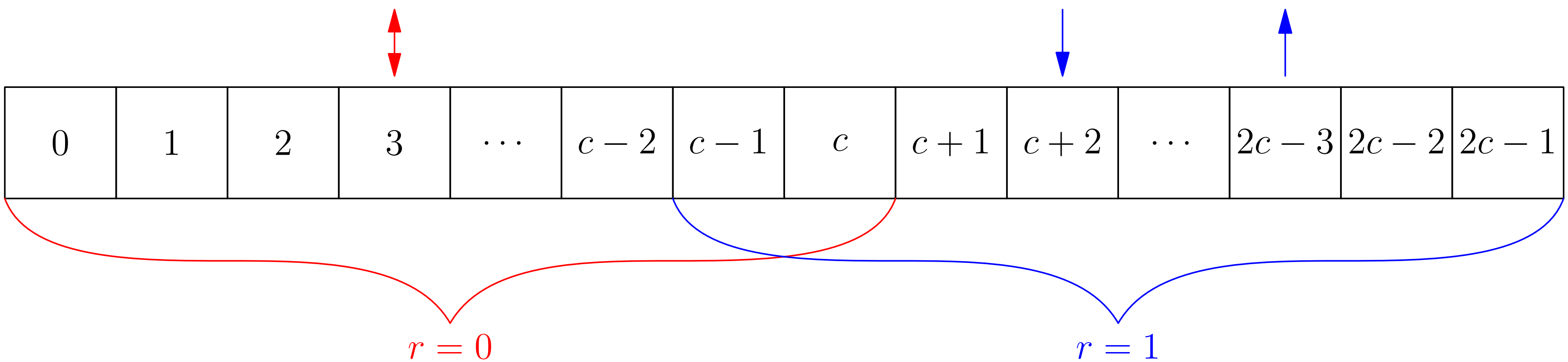
$$w_{k,r} \doteq \begin{cases} U_0 & \text{if } k = 0, \\ \zeta_{3m}^{rk}\left(U_k + \zeta_3^{-r}\overline{U_{m-k}}\right) & \text{if } 1 \le k \le m-1. \end{cases}$$

- 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.

- To facilitate an in-place implementation, in our original paper (SIAM, 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.

Multithreaded Hermitian Convolution

- 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.



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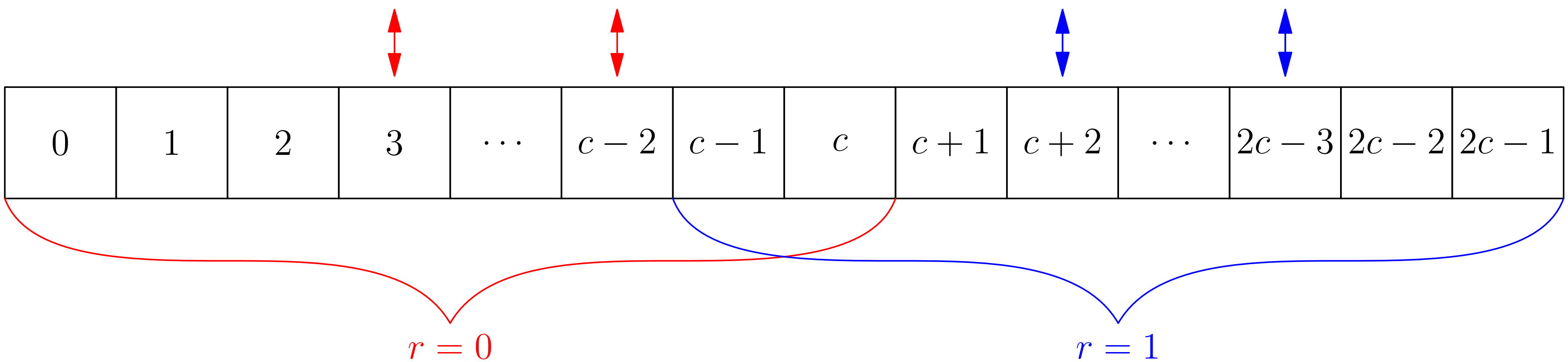
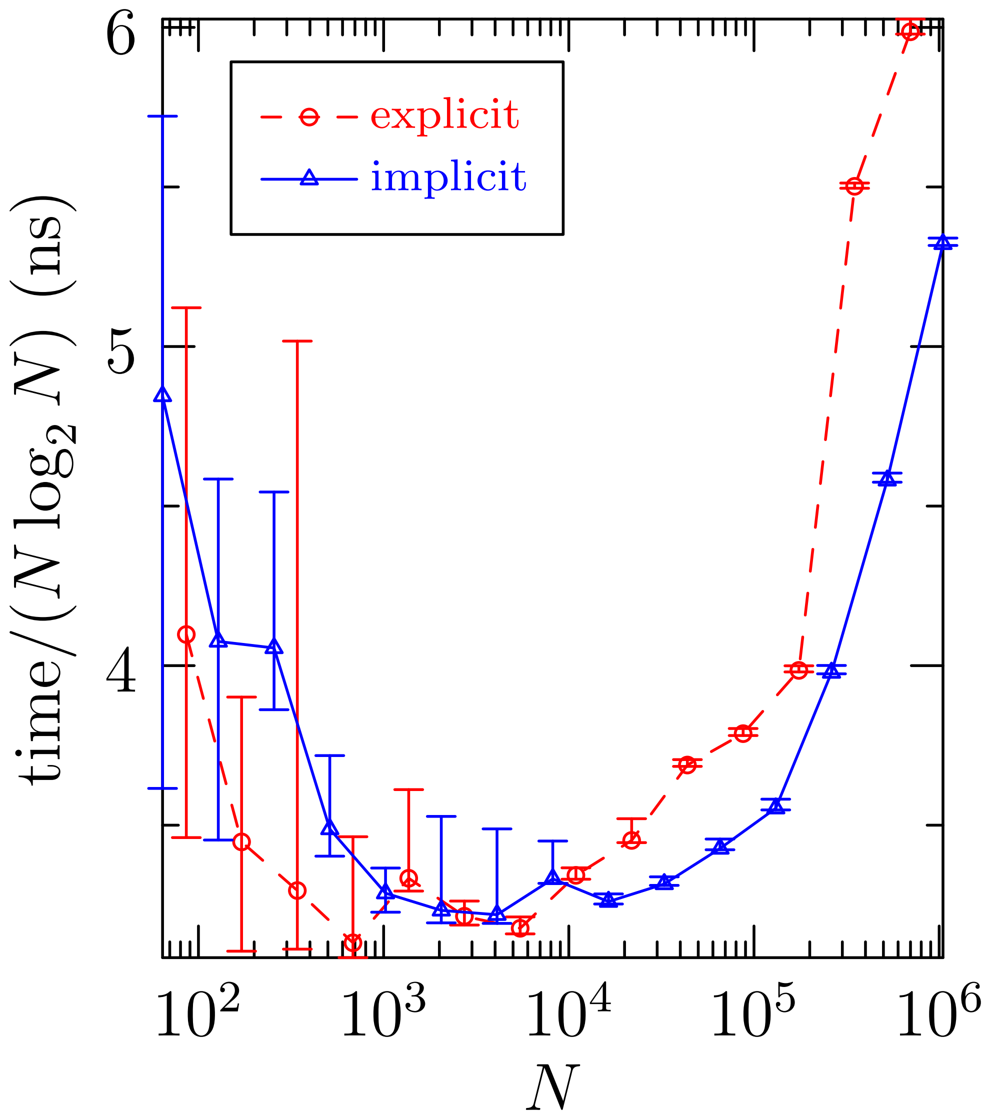
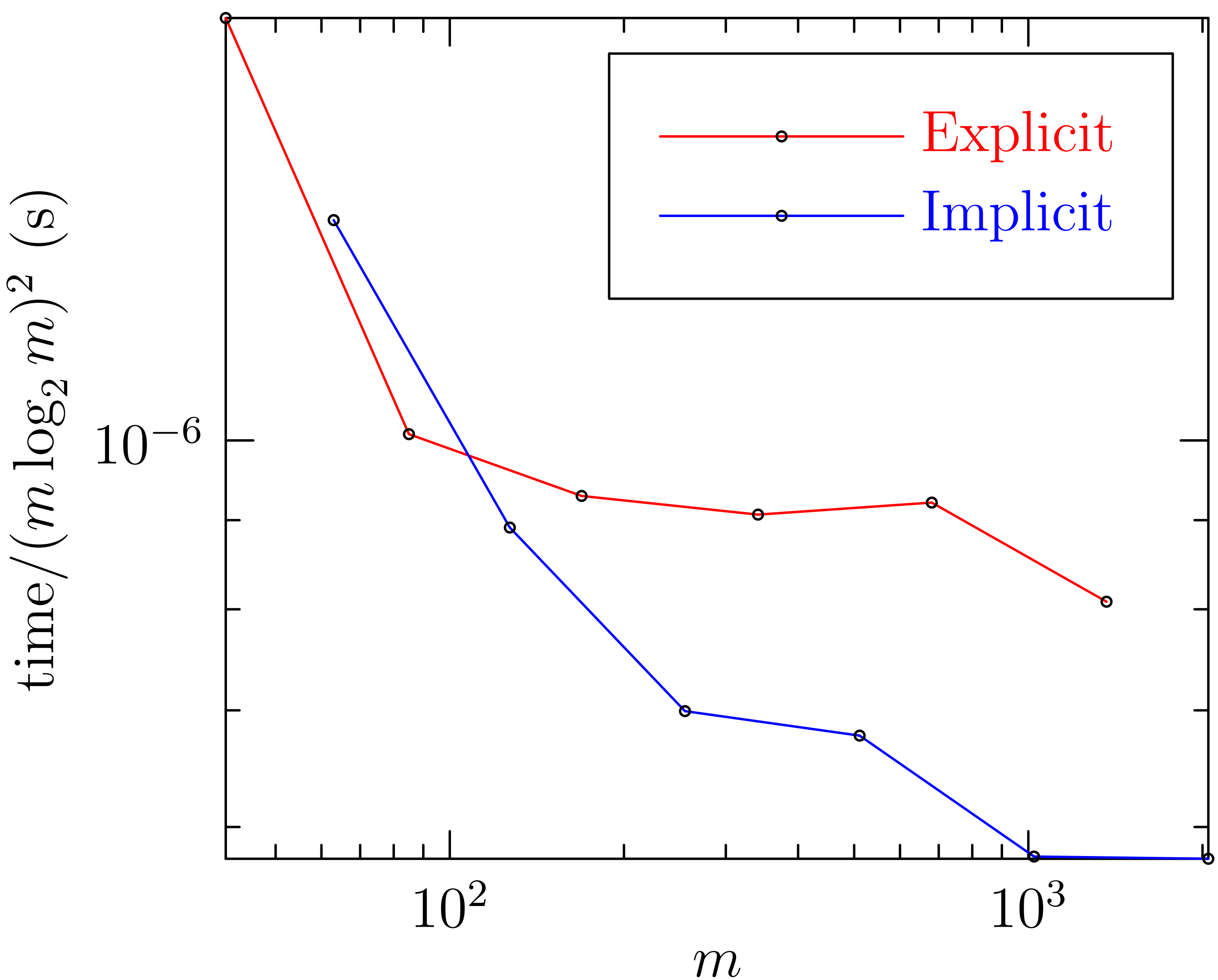


- As a result, even in 1D, implicit dealiasing of pseudospectral convolutions is now significantly faster than explicit zero padding.

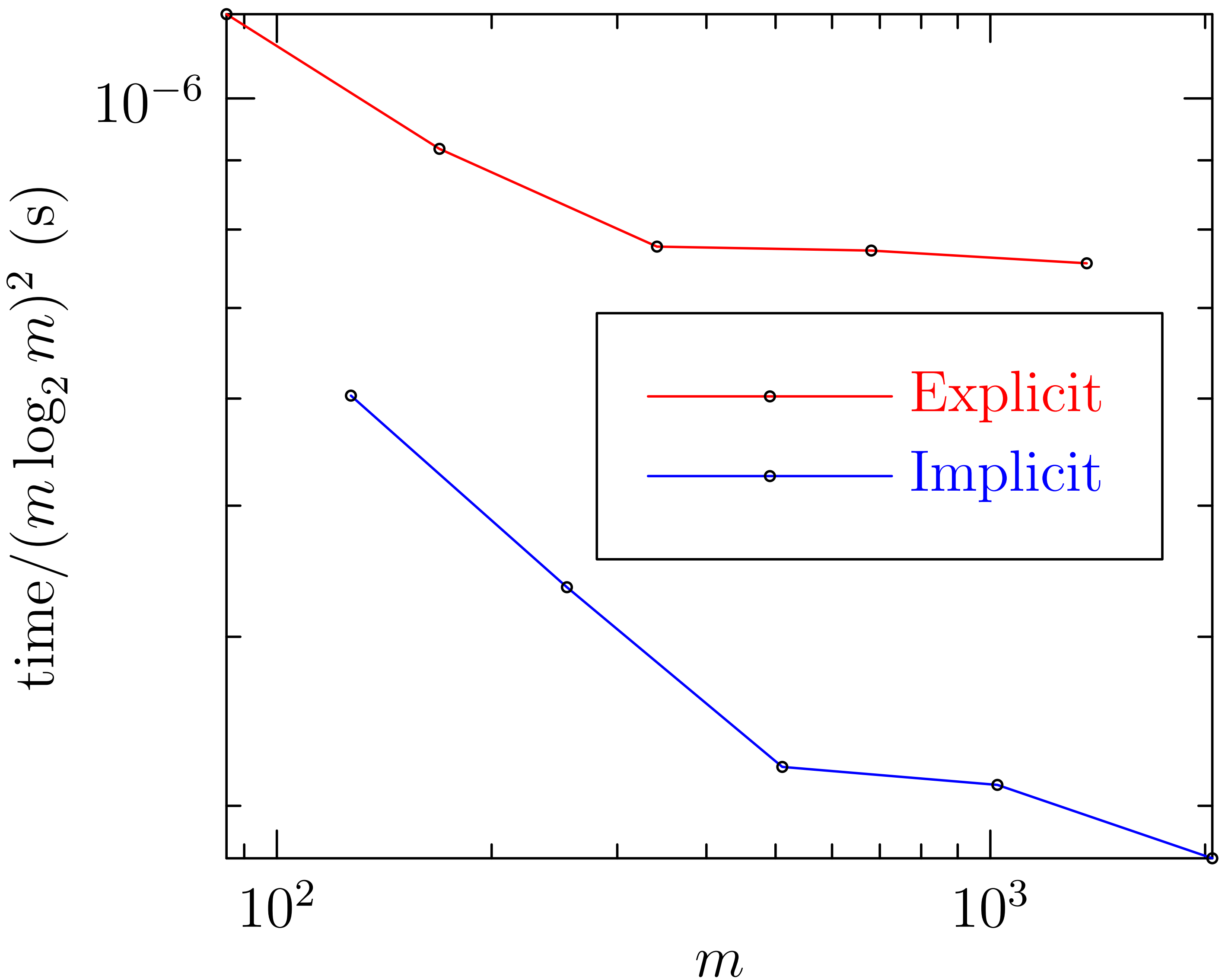
1D Implicit Hermitian Convolution



2D Pseudospectral Collocation [1 thread]



2D Pseudospectral Collocation [4 threads]



Conclusions

- Memory savings: in d dimensions implicit padding asymptotically uses $1/2^{d-1}$ [for centered convolutions $(2/3)^{d-1}$] of the memory required by conventional explicit padding.
- The factor of 2 speedup with implicit dealiasing is largely due to increased data locality.
- Highly optimized and parallelized implicit dealiasing routines have been implemented as a software layer `FFTW++` on top of the `FFTW` library and released under the Lesser GNU Public License: `http://fftwpp.sourceforge.net/`
- Writing a high-performance dealiased pseudospectral code is now a relatively straightforward exercise!
- Implicit dealiasing has been extended to handle nested convolutions and autocorrelations.
- Implicit dealiasing can also be applied to signal denoising and image filtering.

References

[Bowman & Roberts 2011] J. C. Bowman & M. Roberts, SIAM J. Sci. Comput., **33**:386, 2011.

[Bowman & Roberts 2013] J. C. Bowman & M. Roberts, "Adaptive matrix transpose algorithms for distributed multicore processors," in *Springer Proceedings of the Applied Mathematics, Modeling and Computational Science*, Springer, 2013.