Dealiased Convolutions without the Padding

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Outline

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Discrete Convolutions

- Discrete linear convolution sums based on the fast Fourier transform (FFT) algorithm [Gauss 1866], [Cooley & Tukey 1965] have become important tools for:
  - image filtering;
  - digital signal processing;
  - correlation analysis;
  - pseudospectral simulations.

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 $\zeta_N^N = 1$.

- 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

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

Discrete Linear Convolution

- The pseudospectral method requires a *linear convolution* since wavenumber space is not periodic.

- The convolution theorem states:

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

$$= \sum_{p=0}^{N-1} \sum_{q=0}^{N-1} F_p G_q \sum_{j=0}^{N-1} \zeta_N^{(-k+p+q)j}$$

$$= N \sum_{s} \sum_{p=0}^{N-1} F_p G_{k-p+sN}.$$

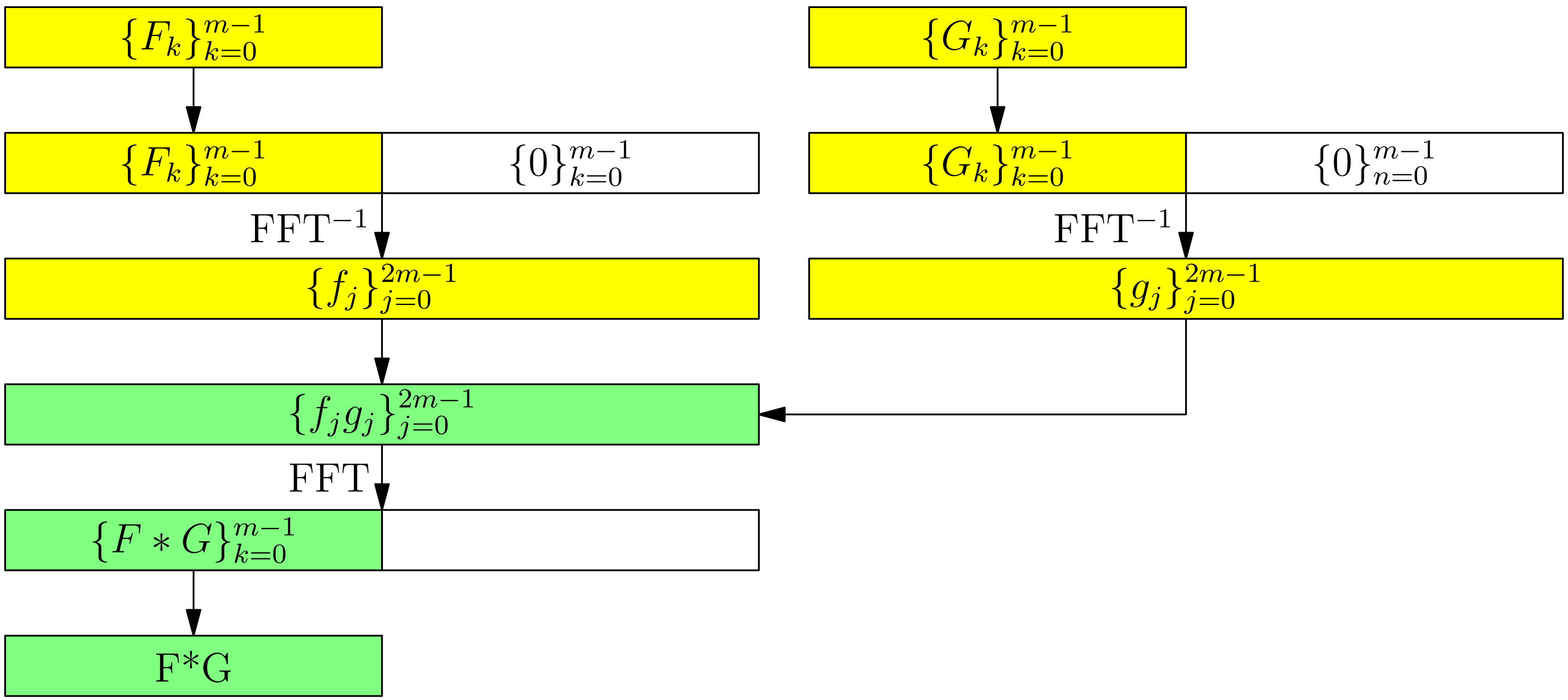
- The terms indexed by $s \neq 0$ are called *aliases*.

- We need to remove the aliases by ensuring that $G_{k-p+sN} = 0$ whenever $s \neq 0$.

- If F_p and G_{k-p+sN} are nonzero only for $0 \leq p \leq m-1$ and $0 \leq k-p+sN \leq m-1$, then we want $k+sN \leq 2m-2$ to have no solutions for positive s.

- This can be achieved by choosing $N \geq 2m-1$.

- That is, one must *zero pad* input data vectors of length m to length $N \geq 2m-1$:



- Physically, *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 $N = 2m$.

Implicit Padding

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

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

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

- 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:

$$2mF_k = \sum_{j=0}^{2m-1} \zeta_{2m}^{-kj} f_j = \sum_{\ell=0}^{m-1} \zeta_{2m}^{-k2\ell} f_{2\ell} + \sum_{\ell=0}^{m-1} \zeta_{2m}^{-k(2\ell+1)} f_{2\ell+1}$$

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

- No bit reversal is required at the highest level.

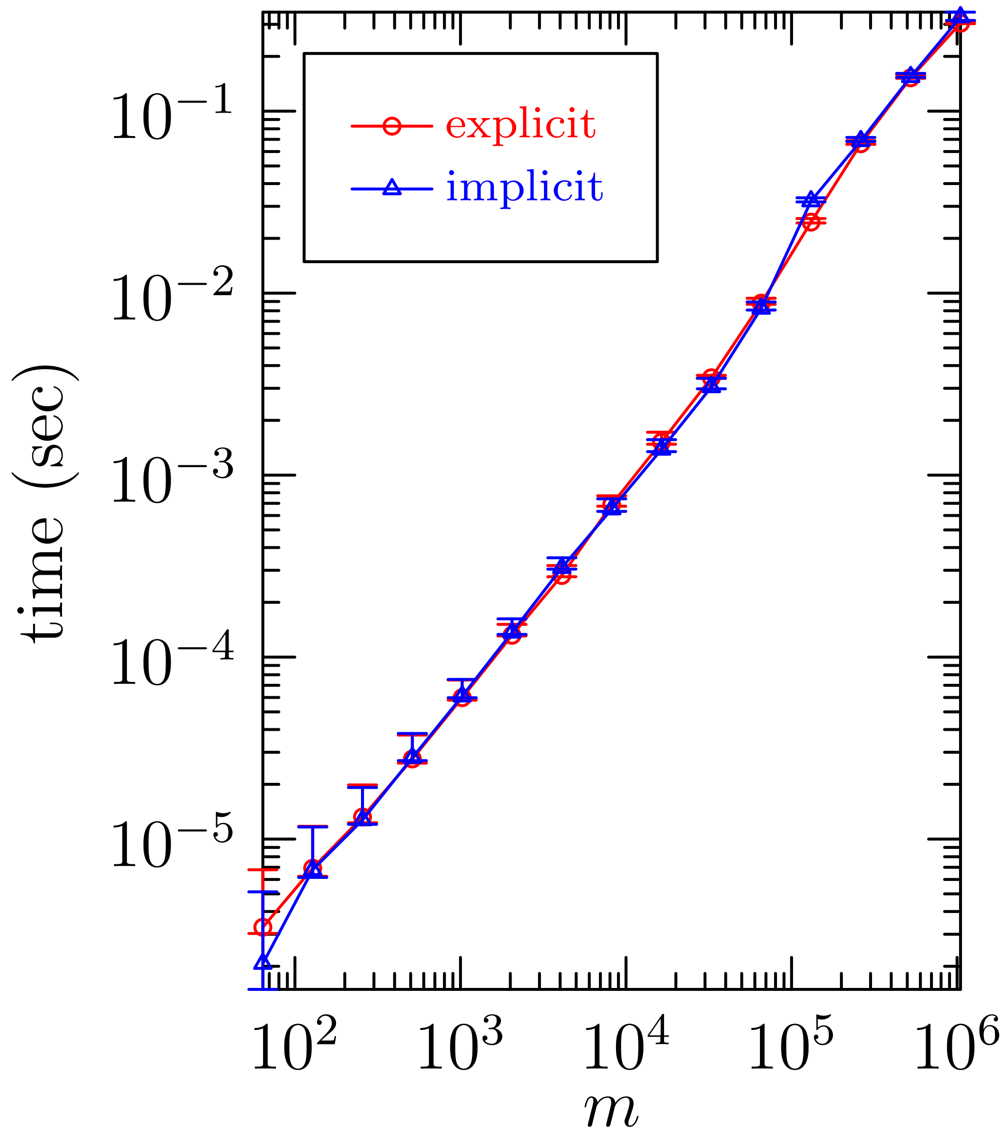
- An implicitly padded convolution is implemented as in our `FFTW++` library (version 1.07) as `cconv(f,g,u,v)` computes an in-place implicitly dealiased convolution of two complex vectors `f` and `g` using two temporary vectors `u` and `v`, each of length m.

- This in-place convolution requires six out-of-place transforms, thereby avoiding bit reversal at all levels.

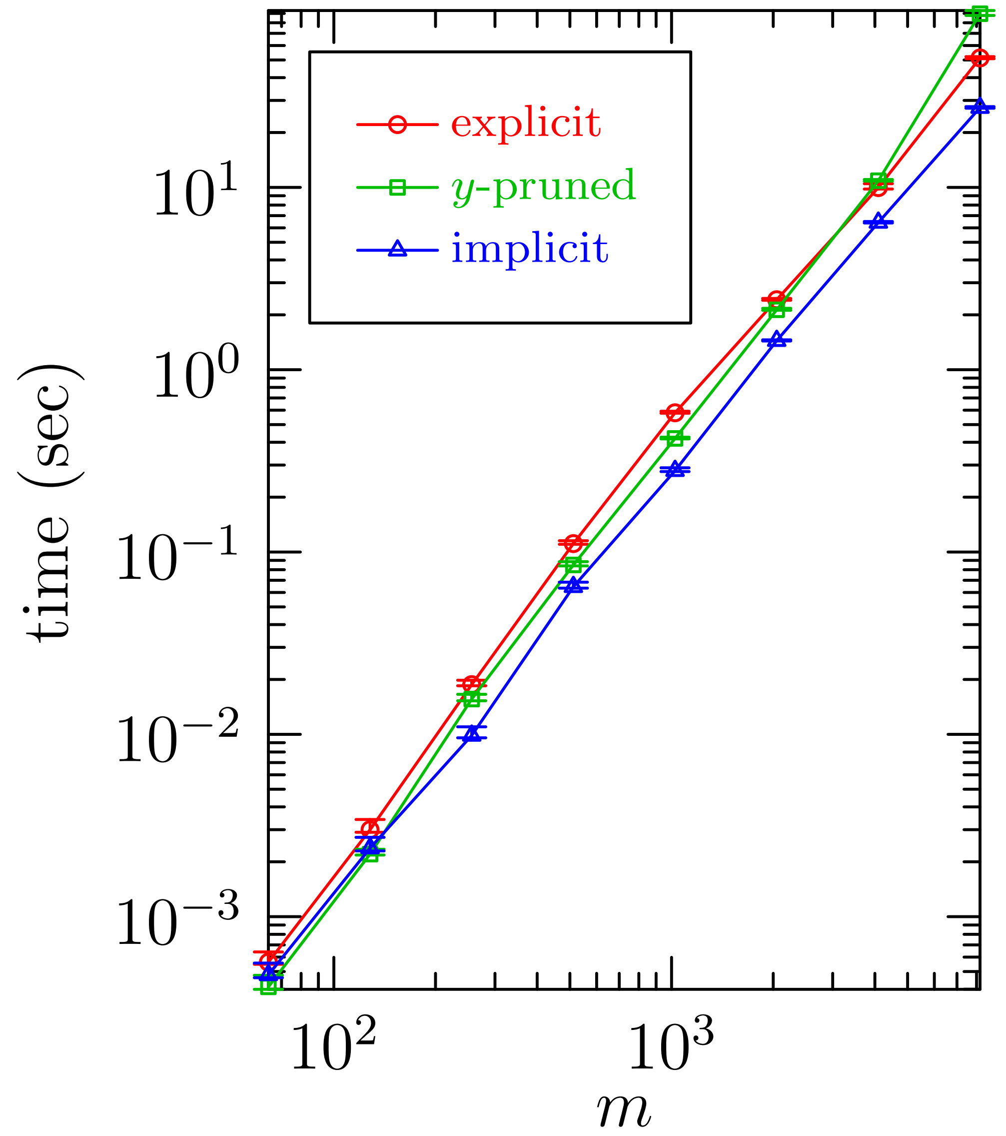
Input: vector f, vector g
Output: vector f

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

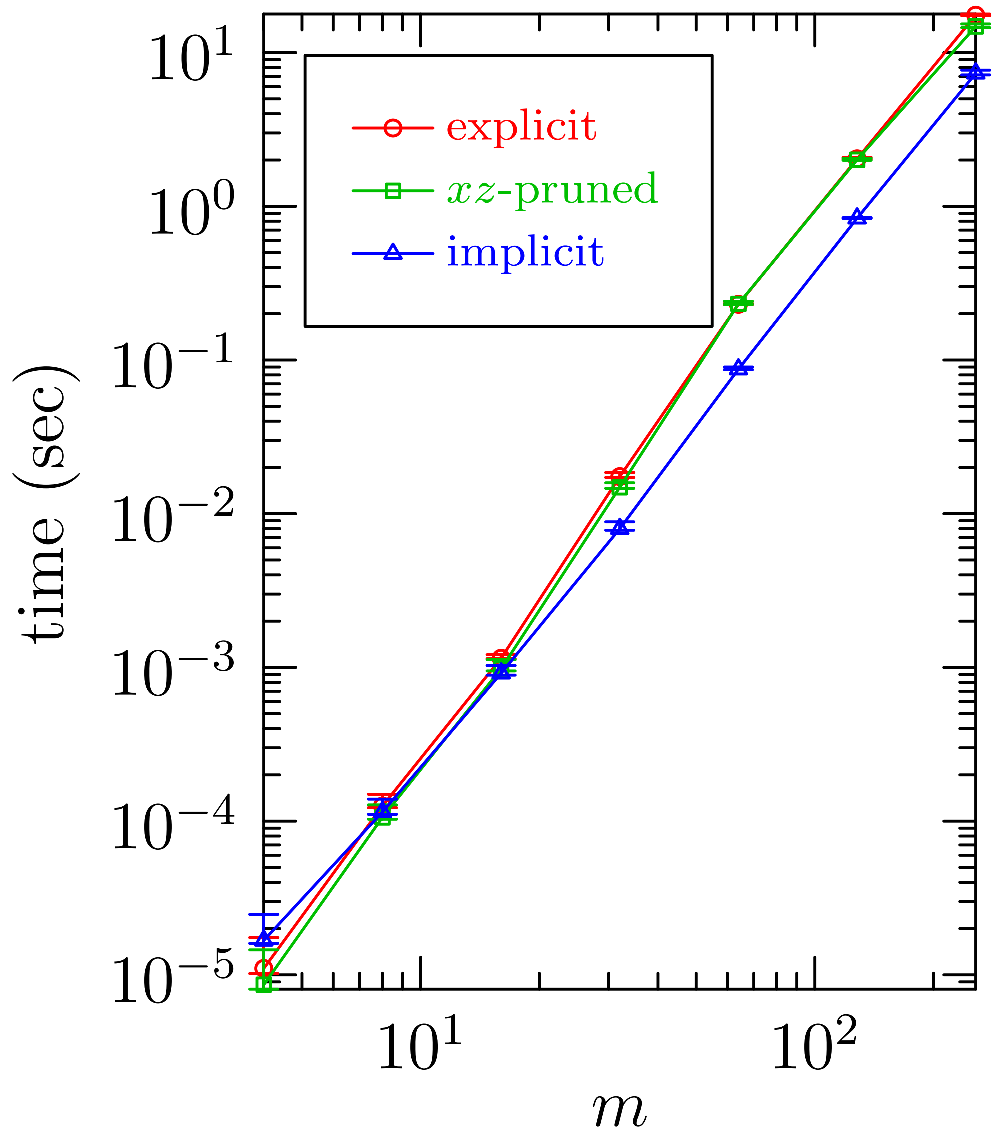
Implicit Padding in 1D



Implicit Padding in 2D



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:

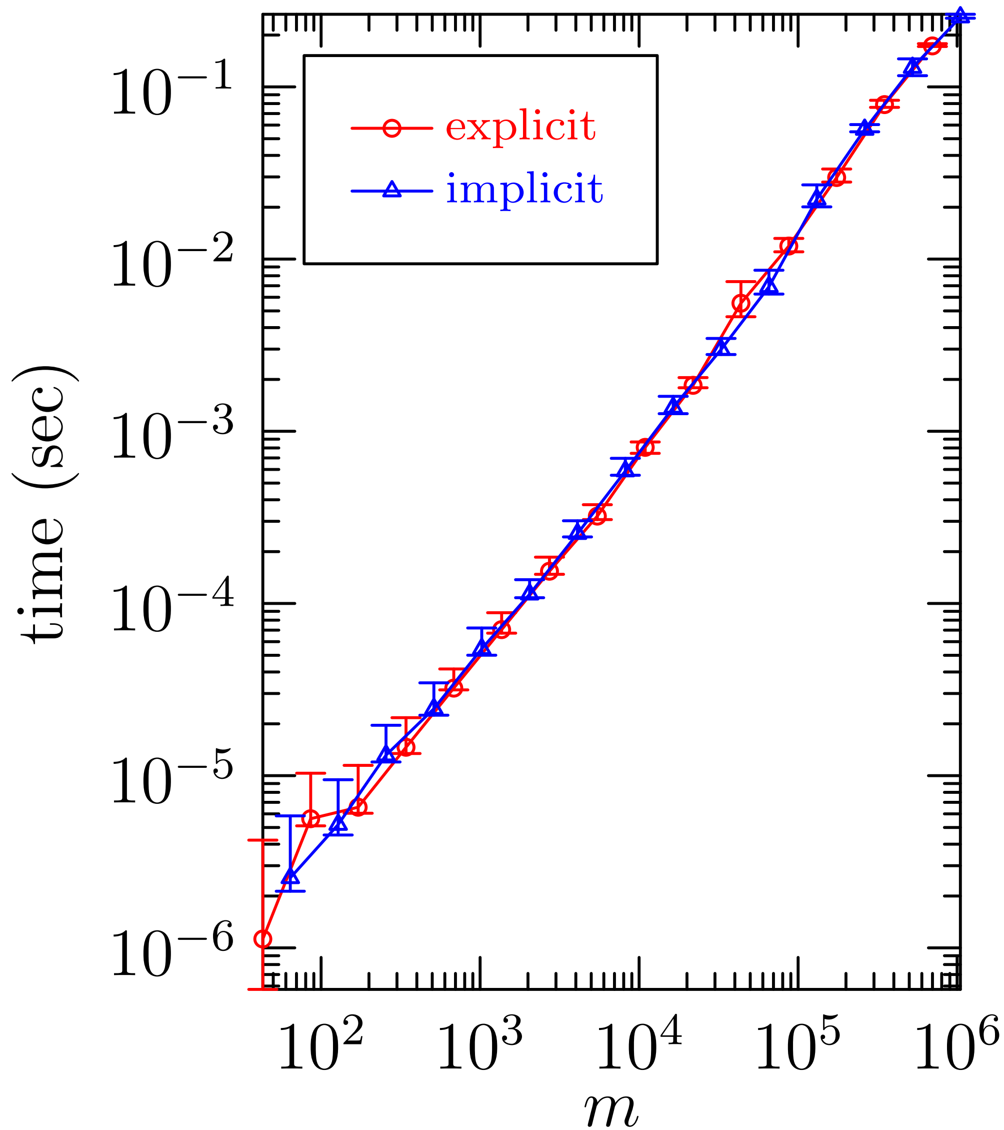
$$\sum_{p=k-m+1}^{m-1} f_p g_{k-p}$$

- Here, one needs to pad to $N \geq 3m - 2$ to prevent mode $m - 1$ from beating with itself to contaminate the most negative (first) mode, corresponding to wavenumber $-m + 1$. Since the ratio of the number of physical to total modes, $(2m - 1)/(3m - 2)$ is asymptotic to 2/3 for large m, this padding scheme is often referred to as the *2/3 padding rule.*

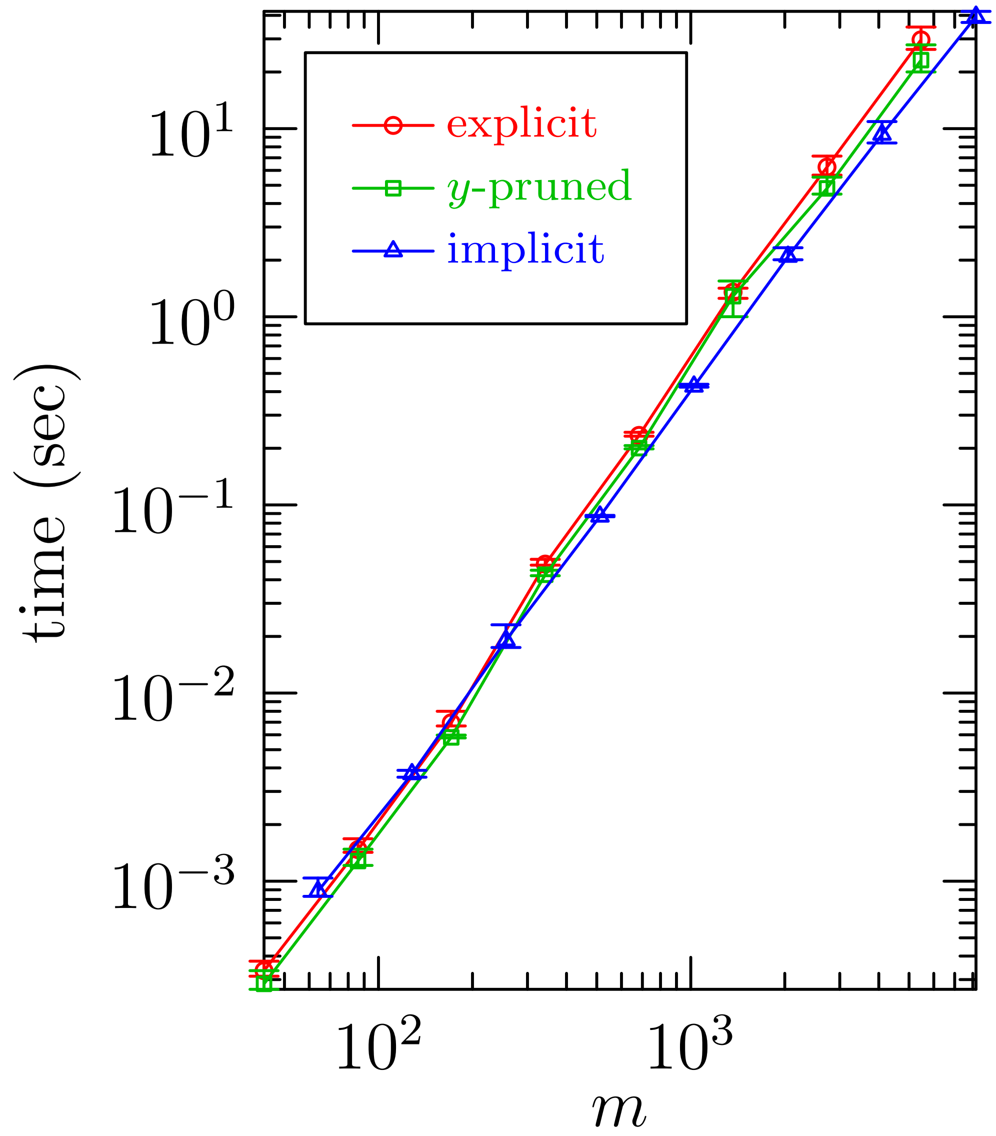
- The Hermiticity condition then appears as

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

Implicit Hermitician Centered Padding in 1D



Implicit Hermitician Centered Padding in 2D



Ternary convolution

- The *ternary convolution* of three vectors F, G, and H is

$$\sum_{p=0}^{N-1}\sum_{q=0}^{N-1} F_p G_q H_{k-p-q}.$$

- Computing the transfer function for $Z_4 = N^3\sum_{\boldsymbol{j}}\omega^4(x_{\boldsymbol{j}})$ requires computing the Fourier transform of the cubic quantity ω^3.

- This requires a centered Hermitian ternary convolution:

$$\sum_{p=-m+1}^{m-1}\sum_{q=-m+1}^{m-1}\sum_{r=-m+1}^{m-1} F_p G_q H_r \delta_{p+q+r,k}.$$

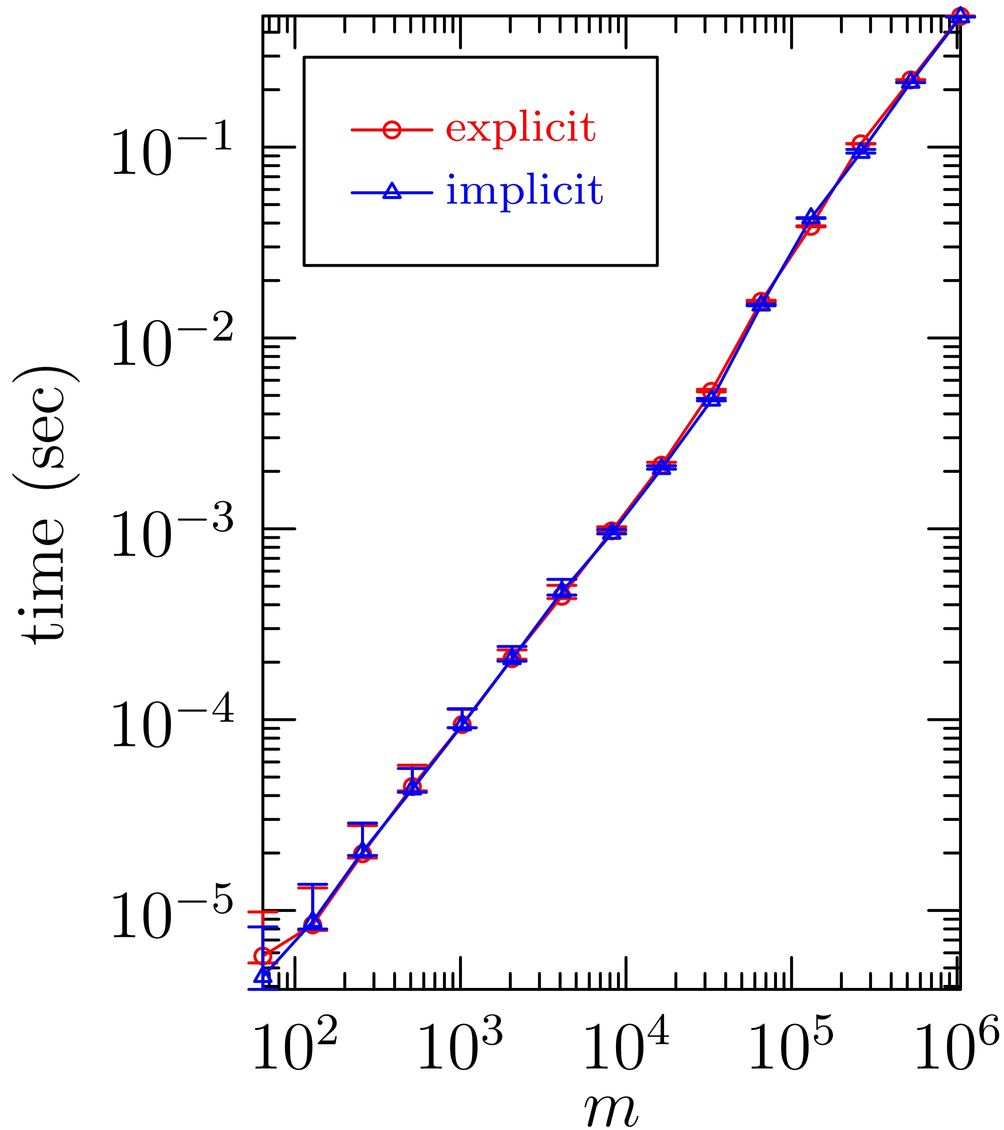
- Correctly dealiasing requires a 2/4 zero padding rule (instead of the usual 2/3 rule for a single convolution).

2/4 Padding Rule

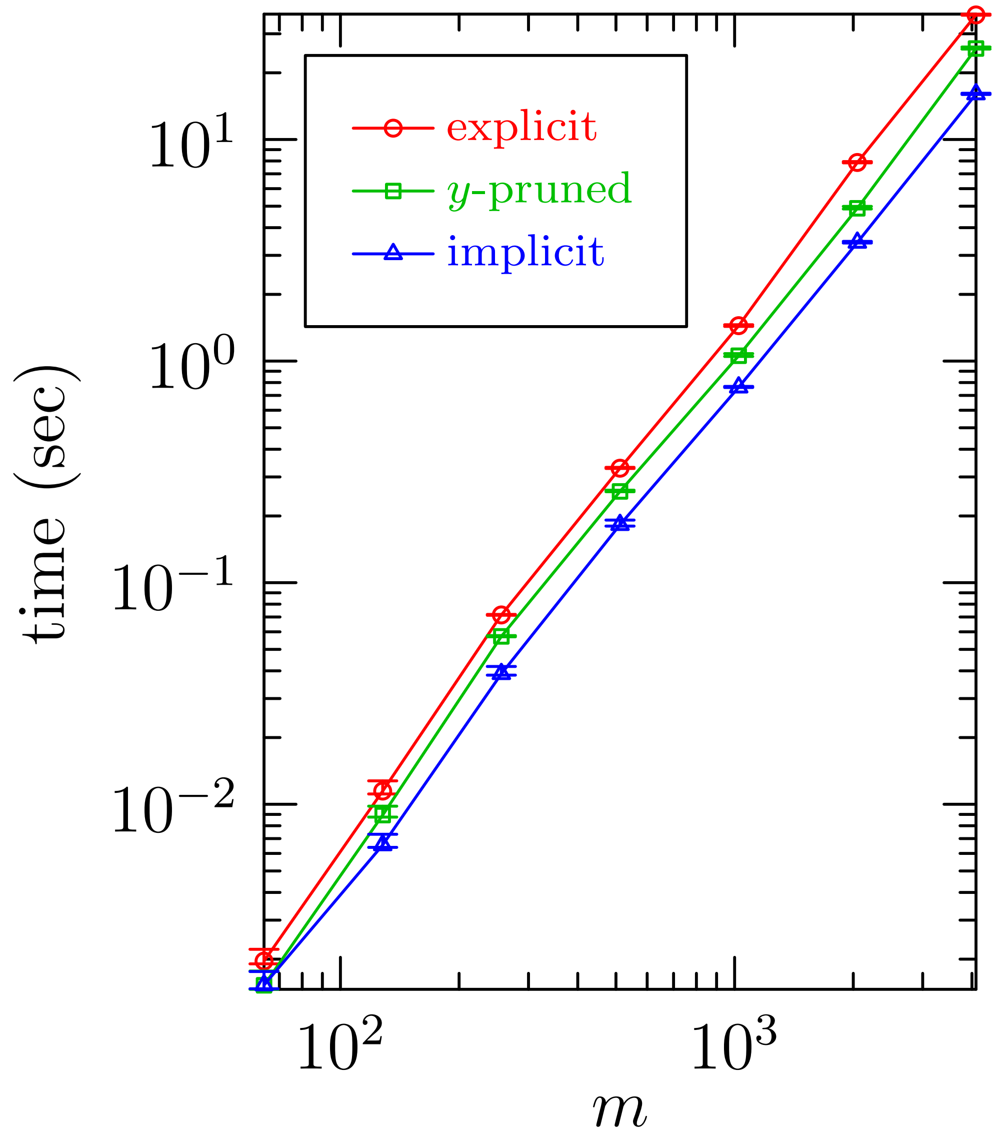
- Computing the transfer function for Z_4 with a 2/4 padding rule means that in a 2048×2048 pseudospectral simulation, the maximum physical wavenumber retained in each direction is only 512.

- For a centered Hermitian ternary convolution, implicit padding is twice as fast and uses half of the memory required by conventional explicit padding.

Implicit Ternary Convolution in 1D



Implicit Ternary Convolution in 2D



Conclusions

- Memory savings: in d dimensions implicit padding asymptotically uses $1/2^{d-1}$ of the memory require by conventional explicit padding.
- Computational savings due to increased data locality: about a factor of two.
- Highly optimized versions of these routines have been implemented as a software layer `FFTW++` on top of the `FFTW` library and released under the Lesser GNU Public License.
- With the advent of this `FFTW++` library, writing a high-performance dealiased pseudospectral code is now a relatively straightforward exercise.

Asymptote: 2D & 3D Vector Graphics Language

Andy Hammerlindl, John C. Bowman, Tom Prince

`http://asymptote.sf.net`

Asymptote Lifts TEX to 3D

$$\int_{-\infty}^{+\infty} e^{-\alpha x^2}\, dx = \sqrt{\frac{\pi}{\alpha}}$$

http://asymptote.sf.net

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References

[Cooley & Tukey 1965] J. W. Cooley & J. W. Tukey, Mathematics of Computation, **19**:297, 1965.

[Frigo & Johnson] "M. Frigo & S. G. Johnson, `http://www.fftw.org/pruned.html`.

[Gauss 1866] C. F. Gauss, "Nachlass: Theoria interpolationis methodo nova tractata," in *Carl Friedrich Gauss Werke*, volume 3, pp. 265–330, Königliche Gesellschaft der Wissenschaften, Göttingen, 1866.