Outline

• Discrete Convolutions
  – Cyclic vs. Linear
  – Standard vs. Centered
  – Complex vs. Hermitian

• Dealiasing
  – Zero Padding
  – Phase-shift dealiasing

• Implicit Padding in 1D, 2D, and 3D:
  – Standard Complex
  – Centered Hermitian
  – Biconvolution

• Conclusions
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 \( N \)th 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
\[
f_j = \sum_{k=0}^{N-1} \zeta_N^{jk} F_k \quad j = 0, \ldots, N - 1,
\]

- The corresponding forward transform is

\[
F_k = \frac{1}{N} \sum_{j=0}^{N-1} \zeta_N^{-kj} f_j \quad j = 0, \ldots, N - 1.
\]

- The orthogonality of this transform pair follows from

\[
\sum_{j=0}^{N-1} \zeta_N^{\ell j} = \begin{cases} 
N & \text{if } \ell = sN \text{ for } s \in \mathbb{Z}, \\
\frac{1 - \zeta_N^{\ell N}}{1 - \zeta_N^\ell} = 0 & \text{otherwise}.
\end{cases}
\]
Discrete Linear Convolution

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

- The convolution theorem states:

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

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

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

- 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 $N = 0 \mod N$.

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

- Although explicit padding seems like an obvious waste of memory and computation, the conventional wisdom on avoiding this waste is well summed up by Steven G. Johnson, coauthor of the FFTW ("Fastest Fourier Transform in the West") library [Frigo & Johnson]:

  The most common case where people seem to want a pruned FFT is for zero-padded convolutions, where roughly 50% of your inputs are zero (to get a linear convolution from an FFT-based cyclic convolution). Here, a pruned FFT is hardly worth thinking about, at least in one dimension. In higher dimensions, matters change (e.g. for a 3d zero-padded array about 1/8 of your inputs are non-zero, and one can fairly easily save a factor of two or so simply by skipping 1d sub-transforms that are zero).
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

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

- 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:

\[ N F_k = \sum_{j=0}^{N-1} \zeta_N^{-kj} f_j = \sum_{\ell=0}^{m-1} \zeta_N^{-k2\ell} f_{2\ell} + \sum_{\ell=0}^{m-1} \zeta_N^{-k(2\ell+1)} f_{2\ell+1} \]

\[ = \sum_{\ell=0}^{m-1} \zeta_m^{-k\ell} f_{2\ell} + \zeta_N^{-k} \sum_{\ell=0}^{m-1} \zeta_m^{-k\ell} f_{2\ell+1} \quad k = 0, \ldots, \frac{N}{2} - 1. \]

No bit reversal is required at the highest level.

An implicitly padded convolution is implemented as in our FFTW++ library (version 1.05) as \texttt{cconv(f,g,u,v)} computes an in-place implicitly dealiased convolution of two complex vectors \( \mathbf{f} \) and \( \mathbf{g} \) using two temporary vectors \( \mathbf{u} \) and \( \mathbf{v} \), 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 \( f \)

\[
\begin{align*}
    u &\leftarrow \text{fft}^{-1}(f); \\
v &\leftarrow \text{fft}^{-1}(g); \\
u &\leftarrow u \ast v; \\
\text{for } k = 0 \text{ to } m - 1 \text{ do} \\
    f[k] &\leftarrow \zeta_{2m}^k f[k]; \\
g[k] &\leftarrow \zeta_{2m}^k g[k]; \\
\text{end} \\
v &\leftarrow \text{fft}^{-1}(f); \\
f &\leftarrow \text{fft}^{-1}(g); \\
v &\leftarrow v \ast f; \\
f &\leftarrow \text{fft}(u); \\
u &\leftarrow \text{fft}(v); \\
\text{for } k = 0 \text{ to } m - 1 \text{ do} \\
f[k] &\leftarrow f[k] + \zeta_{2m}^{-k} u[k]; \\
\text{end} \\
\text{return } f/(2m);
\end{align*}
\]
Implicit Padding in 1D

\[ \begin{align*}
10^{-5} & \quad 10^{-4} \\
10^{-3} & \quad 10^{-2} \\
10^{-1} & \quad 10^{-0} \\
10^{0} & \quad 10^{1} \\
10^{2} & \quad 10^{3} \\
10^{4} & \quad 10^{5} \\
10^{6} & \quad 10^{7}
\end{align*} \]

\[ m \]

- explicit
- implicit
Implicit Padding in 2D

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The graph shows the relationship between the time (sec) and the parameter $m$ on a log-log scale. The graph compares three different methods:

- **explicit**
- **$y$-pruned**
- **implicit**

The x-axis represents $m$, while the y-axis represents time in seconds (sec). The data points for each method are clearly visible, with the implicit method showing the least time compared to the explicit and $y$-pruned methods.
Implicit Padding in 3D

The graph shows the time (in seconds) as a function of a parameter $m$ (from $10^{-1}$ to $10^2$) for different methods:

- **explicit**
- **xz-pruned**
- **implicit**

The x-axis represents the parameter $m$, and the y-axis represents the time in seconds, plotted on a logarithmic scale.
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 is at wavenumber zero:

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

- 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

![Graph showing time (sec) vs. m with explicit and implicit data points]

- **time (sec)**
  - $10^{-1}$
  - $10^{-2}$
  - $10^{-3}$
  - $10^{-4}$
  - $10^{-5}$
  - $10^{-6}$

- **m**
  - $10^2$
  - $10^3$
  - $10^4$
  - $10^5$
  - $10^6$

- **explicit**
- **implicit**
Implicit Hermitician Centered Padding in 2D

![Graph showing time (sec) vs. m with different lines representing explicit, y-pruned, and implicit methods.](image-url)
Biconvolutions

- The biconvolution 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 $Z_4 = N^3 \sum_j \omega^4(x_j)$ requires computing the Fourier transform of the cubic quantity $\omega^3$.

- This requires a centered Hermitian biconvolution:

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

- 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 biconvolution, implicit padding is twice as fast and uses half of the memory required by conventional explicit padding.
Implicit Biconvolution in 1D

![Graph showing comparison between explicit and implicit methods over time (sec) vs. m (for m = 10^2 to 10^6), with exponential scale on both axes. The graph demonstrates linear growth with increasing m for both methods.]
Implicit Biconvolution in 2D

![Graph showing time (sec) vs. m with explicit, y-pruned, and implicit methods.](image_url)
Conclusions

- Memory savings: in $d$ dimensions implicit padding asymptotically uses $1/2^{d-1}$ of the memory required 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

(freely available under the Lesser GNU Public License)
Asymptote Lifts \TeX{} to 3D

\[ \int_{-\infty}^{+\infty} e^{-ax^2} \, dx = \sqrt{\frac{\pi}{a}} \]

http://asymptote.sf.net

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References

