

pyFFS: A Python Library for Fast Fourier Series Computation and Interpolation with GPU Acceleration

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Summary

Fourier transforms are an often necessary component in many computational tasks, and can be approximated efficiently through the Fast Fourier Transform (FFT) algorithm (Cooley & Tukey, 1965). However, many applications involve an underlying continuous signal, and a more natural choice would be to work with e.g. the Fourier series (FS) coefficients in order to avoid the additional overhead of translating between the analog and discrete domains. Unfortunately, there exists very little literature and tools for the manipulation of FS coefficients from discrete samples in practice. This paper introduces a Python 3 library called pyFFS for efficient FS coefficient computation, convolution, and interpolation for N-D signals. While the libraries SciPy (Virtanen & others, 2020) and NumPy (Harris & others, 2020) provide efficient routines for discrete Fourier transform (DFT) coefficients via the FFT algorithm, pyFFS addresses the computation of FS coefficients through what we call the Fast Fourier Series (FFS). Moreover, pyFFS includes an FS interpolation method based on the chirp Z-transform (CZT) (Rabiner et al., 1969) that can make it more than an order of magnitude faster than the SciPy equivalent when one wishes to perform distortionless bandlimited interpolation. GPU support through the CuPy library (Okuta et al., 2017) is readily available, and allows for further acceleration: an order of magnitude faster for computing the 2-D FS coefficients of 1000×1000 samples and nearly two orders of magnitude faster for 2-D interpolation.

Statement of need

While deceptively simple, the FFS algorithm presented in this paper is surprisingly neither described in signal processing textbooks nor implemented in numerical computing libraries. For example, NumPy and SciPy in the Python ecosystem focus mainly on the DFT and related operations. We aim to change this by providing an efficient and easy-to-use interface to the FFS algorithm via our Python package pyFFS. The main motivation for working with pyFFS rather than the FFT routines from NumPy/SciPy is convenience when working with continuous-domain compactly-supported signals. The philosophy of pyFFS is to retain the continuous-domain perspective, often neglected when using numerical libraries such as NumPy and SciPy, which allows for much clearer code (as will be shown in a Fourier optics example). This can also prevent common pitfalls due to an invalid conversion between discrete and continuous domains (e.g. spectral leakage, aliasing, periodisation artefacts, etc). Beyond conveniency, pyFFS is also extremely efficient. We benchmark pyFFS with equivalent functions in SciPy, observing scenarios in which the proposed library is more than an order of magnitude faster, i.e. for 2-D convolution and for interpolation. Moreover, GPU support has been seamlessly incorporated for an even faster implementation. Just as the FFT implementation via NumPy and SciPy can be readily used for an efficient $\mathcal{O}(N\log N)$ analysis and synthesis of discrete sequences, pyFFS offers the same ease-of-use and performance capabilities for discrete representations of continuous-domain signals, along with faster interpolation

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techniques.

pyFFS has been used in (Fageot & Simeoni, 2020), where the authors make use of the FFS algorithm to efficiently compute multidimensional periodic splines. It is currently being investigated in radio-astronomy and optics projects, in which physical processes have been modeled as bandlimited. In general, pyFFS is useful for interpolating multidimensional functions efficiently. Such functions are commonplace in numerous applications, e.g. radio-astronomy, medical imaging, holography, etc. Finally, Fourier Series are an important component of the Non Uniform Fast Fourier Transform (NUFFT), extensively used in MRI imaging and other computational imaging modalities (Barnett et al., 2019).

Algorithms

In this section, we provide for reference the main definitions and results leveraged in pyFFS. For simplicity, the results are provided in the context of 1-D sequence, but pyFFS also offers N-D versions of the various algorithms/transforms below. As the purpose of this paper is to present the library, how to use it, and some benchmarking results, we refer to (Bezzam et al., 2021) for mathematical presentations and proofs of the FFS algorithm and the CZT-based interpolation.

The Discrete Fourier Transform

Let $\mathbf{x} \in \mathbb{C}^N$. The length-N Discrete Fourier Transform $\mathsf{DFT}_N\{\mathbf{x}\} \in \mathbb{C}^N$ is defined as (Vetterli et al., 2014):

$$\mathsf{DFT}_N\{\mathbf{x}\}[k] = \sum_{n=0}^{N-1} \mathbf{x}[n] W_N^{nk}, \qquad k \in \{0, \dots, N-1\},$$

with $W_N = \exp\left(-j\frac{2\pi}{N}\right)$.

The length-N inverse Discrete Fourier Transform $iDFT_N\{x\} \in \mathbb{C}^N$ is defined as:

$$\mathsf{iDFT}_N\{\mathbf{x}\}[n] = \frac{1}{N} \sum_{k=0}^{N-1} \mathbf{x}[k] W_N^{-nk}, \qquad n \in \{0,\dots,N-1\}.$$

Moreover, (i)DFT $_N$ is reversible:

$$(\mathsf{iDFT}_N \circ \mathsf{DFT}_N)\{\mathbf{x}\} = (\mathsf{DFT}_N \circ \mathsf{iDFT}_N)\{\mathbf{x}\} = \mathbf{x}.$$

The FFT (Cooley & Tukey, 1965) is a particularly efficient $\mathcal{O}(N\log N)$ algorithm to compute (i)DFT $_N$, especially if N is highly composite.

The Chirp Z-Transform

Let $\mathbf{x} \in \mathbb{C}^N$. The length-M Chirp Z-Transform $\operatorname{CZT}_N^M\{\mathbf{x}\} \in \mathbb{C}^M$ of parameters $A, W \in \mathbb{C}^*$ is defined as:

$$\mathsf{CZT}_N^M\{\mathbf{x}\}[k] = \sum_{n=0}^{N-1} \mathbf{x}[n] A^{-n} W^{nk}, \qquad k \in \{0,\dots,M-1\}.$$

The CZT is a generalization of the DFT which samples the Z plane at uniformly-spaced points along the unit circle. It can be efficiently computed using can be efficiently computed using



the DFT and iDFT in $\mathcal{O}(L\log L)$ operations, where $L \geq N+M-1$. This is done via Bluestein's algorithm (**Bluestein1970?**). A similar formulation of the CZT and its efficient computation is known as the fast fractional FT algorithm (Bailey & Swarztrauber, 1991).

Fast Fourier Series

Let $x:\mathbb{R}\to\mathbb{C}$ be a T-periodic function of bandwidth $N_{FS}=2N+1$. Then x is fully characterized by its N_{FS} Fourier Series coefficients $\{X_k^{FS}, k=-N,\dots,N\}$ (Vetterli et al., 2014)

$$x(t) = \sum_{k=-N}^{N} X_k^{FS} \exp\left(j\frac{2\pi}{T}kt\right),\,$$

where the FS coefficients $\{X_k^{FS}, k=-N,\dots,N\}$ are defined as

$$X_k^{FS} = \frac{1}{T} \int_{T_c - \frac{T}{2}}^{T_c + \frac{T}{2}} x(t) \exp\left(-j\frac{2\pi}{T}kt\right) dt, \tag{1}$$

with T_c being one of x's period mid-points.

Computing the X_k^{FS} with (1) can be prohibitive when closed-form solutions are unavailable. However, it is possible to calculate the FS coefficients exactly from $N_s=N_{FS}+Q$ judiciously-placed samples of x, where $Q\in 2\mathbb{N}$ is some arbitrary zero-padding. Then,

$$\mathbf{x} = N_s \; \mathrm{iDFT}_{N_s} \left\{ \mathbf{X}^{FS} \odot \exp \left(j \frac{2\pi}{T} T_c \right)^{\mathbf{E}_1} \right\} \odot \exp \left(-j \frac{2\pi}{N_s} \right)^{N\mathbf{E}_2},$$

$$\mathbf{X}^{FS} = \frac{1}{N_s} \mathsf{DFT}_{N_s} \left\{ \mathbf{x} \odot \exp \left(-j \frac{2\pi}{N_s} \right)^{-N\mathbf{E}_2} \right\} \odot \exp \left(j \frac{2\pi}{T} T_c \right)^{-\mathbf{E}_1},$$

where

$$\mathbf{x} = [x(t_0), \dots, x(t_M), x(t_{-M}), \dots, x(t_{-1})] \in \mathbb{C}^{N_s},$$

$$\mathbf{X}^{FS} = \left[X_{-N}^{FS}, \dots, X_{N}^{FS}, \mathbf{0}_{Q}\right] \in \mathbb{C}^{N_{s}}, \qquad t_{n} = T_{c} + \frac{T}{N_{s}}n, \quad n \in \mathbb{N},$$

$$\mathbf{E}_1 = [-N, \dots, N, \mathbf{0}_Q] \in \mathbb{Z}^{N_s}, \qquad \mathbf{E}_2 = [0, \dots, (N_s - 1)/2, -(N_s - 1)/2, \dots, -1] \in \mathbb{Z}^{N_s}.$$

A proof of this result as well as the case $Q \in 2\mathbb{N} + 1$ is available in (Bezzam et al., 2021).

Fast Interpolation of FS Coefficients

Let $0 \le a < b \le T \in \mathbb{R}$ be the end-points of an interval on which we want to evaluate M equi-spaced samples of x. Then

$$\mathbf{x} = A^N \mathsf{CZT}^M_{N_{FS}}(\mathbf{X}^{FS}) \odot W^{-N\mathbf{E}},$$

where

$$\mathbf{x} = [x(t_0), \dots, x(t_{M-1})] \in \mathbb{C}^M$$



$$\begin{split} \mathbf{X}^{FS} &= \frac{1}{N_s} \mathsf{DFT}_{N_s} \left\{ \mathbf{x} \odot \exp \left(-j \frac{2\pi}{N_s} \right)^{-N\mathbf{E}_2} \right\} \odot \exp \left(j \frac{2\pi}{T} T_c \right)^{-\mathbf{E}_1}, \\ t_n &= a + \frac{b-a}{M-1} n, \quad n \in \{0, \dots, M-1\}, \\ A &= \exp \left(-j \frac{2\pi}{T} a \right), \qquad W = \exp \left(j \frac{2\pi}{T} \frac{b-a}{M-1} \right), \qquad \mathbf{E} = [0, \dots, M-1] \in \mathbb{N}^M, \end{split}$$

and where the CZT has parameters A,W. With this result, one can interpolate sub-sections of a period efficiently. More-over, it is possible to perform DFTs of a smaller length than what would be normally required with a more standard iDFT interpolation approach, namely zero-padding the DFT coefficients and taking a longer iDFT for an increase in temporal resolution across the entire period. Again, the proof of this result is available in (Bezzam et al., 2021).

pyFFS Overview and Usage

pyFFS is a Python library for performing efficient and distortionless FS coefficient computation, convolution, and interpolation for periodic/compactly-supported, bandlimited signals. The goal is to provide an intuitive tool to numerically work with such signals of any dimension \$ D \$. Just as the FFT functions from NumPy and SciPy can be used without too much thought about the internal details, we have created a a user interface for FS computations that can also be used out-of-the-box for the appropriate scenario.

Fourier series analysis and synthesis

The user interface for 1-D functions is shown below. Note that the samples provided to ffs are not in chronological order (see previous section). The method ffs_sample returns the timestamps and indices necessary for ensuring the samples provided to ffs are in the expected order.

```
# determine appropriate timestamps and indices for rearranging input
sample_points, idx = pyffs.ffs_sample(
          # function period
          # function bandwidth, i.e. number of FS coefficients (odd)
  N FS,
  Тc,
          # function center
          # number of samples
  N_s
# sample a known function at the correctly ordered timestamps
x = pyffs.func.dirichlet(sample_points, T, T_c, N_FS)
# OR rearrange ordered samples using `idx
\# x = x_{orig}[idx]
# compute FS coefficients
x_FS = pyffs.ffs(x, T, T_c, N_FS)
# back to samples with inverse transform
x_r = pyffs.iffs(x_FS, T, T_c, N_FS)
                                       # equivalent to x
```

The user interface for the general N-D case is shown below, with the specific example of 2-D. As in the 1-D case, samples provided to ffsn are not in increasing order of the input variables. The method ffsn_sample returns the locations and indices necessary for making sure the samples provided to ffsn are in the expected order. Alternatively, the method ffs_shift can be used to reorder the samples.



```
T = [T_x, T_y]
                      # list of periods for each dimension
                      # list of function centers for each dimension
T_c = [T_cx, T_cy]
N_FS = [N_FSx, N_FSy] # list of function bandwidths for each dimension
N_s = [N_sx, N_sy]
                     # number of samples per dimension
# determine appropriate timestamps and indices for rearranging input
sample_points, idx = pyffs.ffsn_sample(T=T, N_FS=N_FS, T_c=T_c, N_s=N_s)
# sample a known function at the correctly ordered timestamps
x = pyffs.func.dirichlet_2D(sample_points, T, T_c, N_FS)
# OR rearrange ordered samples
\# x = pyffs.ffs\_shift(x\_orig)
# compute FS coefficients
x_FS = pyffs.ffsn(x, T=T, T_c=T_c, N_FS=N_FS)
# go back to samples
x_r = pyffs.iffsn(x_FS, T=T, T_c=T_c, N_FS=N_FS)
                                                  # equivalent to x
```

Circular convolution

The user interface for N-D circular convolutions is shown below.

```
out = pyffs.convolve(
   f=f, # samples of one function in the convolution
   h=h, # samples of the other function in the convolution
   T=T, # period(s) of both functions along all dimensions
   T_c=T_c, # period center(s) of both functions along all dimensions
   N_FS=N_FS, # number of FS coefficients for both functions
        # along all dimensions
   reorder=True # whether input samples should be reordered into
        # expected order for ffsn
)
```

Samples can be provided in their natural order or in the order expected by ffsn. By default, the argument reorder is set to True, such that samples are expected in their natural order and are reordered internally. The output samples are returned in the same order as the inputs.

Bandlimited interpoloation

The user interface for 1-D badnlimited interpolation is shown below.

```
x_interp = pyffs.fs_interp(
  x_FS,  # FS coefficients in increasing order of index
  T,  # period
  a,  # start time
  b,  # stop stop
  M  # number of points
)
```

The user interface for the general N-D bandlimited interpolation is shown below, with the specific example of 2-D.



```
M=[M_x, M_y] # number of samples per dimension
```

In both cases, the provided FS coefficients must be ordered such that the indices are in increasing order, as returned by ffs and ffsn.

GPU usage

GPU support is available through the CuPy library (Okuta et al., 2017). This library supports many of NumPy and SciPy's functionality in order to perform equivalent operations on CUDA. If the appropriate version of CuPy is installed, nearly all array operations will take place on the GPU if the provided input is a CuPy array, as shown below. In general, pyFFS' functions can be used for both CPU and CUDA by simply passing NumPy or CuPy arrays (respectively) as inputs to the corresponding pyFFS functions.

```
import cupy as cp

x_cp = cp.array(x)  # convert existing `numpy` array to `cupy` array

# apply functions like before, array operations take place on GPU

x_FS = pyffs.ffs(x_cp, T, T_c, N_FS)  # compute FS coefficients

x_r = pyffs.iffs(x_FS, T, T_c, N_FS)  # back to samples

y = pyffs.convolve(x_cp, x_cp, T, T_c, N_FS)  # convolve

x_interp = pyffs.fs_interp(x_FS, T, a, b, M)  # interpolate
```

Note that converting between CuPy and NumPy requires data transfer between the CPU and GPU, which could be costly for large arrays. Therefore, if passing CuPy arrays to pyFFS, it is recommended to perform as much pre-processing and post-processing as possible on the GPU in order to limit such data transfer.

API Scope

The following table summarises pyFFS' API and compares it with functions from SciPy offering similar functionalities (Virtanen & others, 2020).

| pyFFS | SciPy |
|-----------------------------|--|
| pyffs.ffs | scipy.fft.fft |
| pyffs.iffs | scipy.fft.ifft |
| pyffs.ffsn | scipy.fft.fftn |
| pyffs.iffsn | scipy.fft.ifftn |
| pyffs.convolve | scipy.signal.fftconvolve |
| pyffs.fs_interp | scipy.signal.resample |
| <pre>pyffs.fs_interpn</pre> | - |
| | pyffs.ffs pyffs.iffs pyffs.ffsn pyffs.iffsn pyffs.convolve pyffs.fs_interp |

Benchmarking

Convolution

Note that SciPy's scipy.fft.fftconvolve zero-pads inputs in order to approximate a linear convolution, while pyFFS performs a circular convolution. Within SciPy, circular convolution is only supported for 2-D by calling scipy.signal.convolve2d with the parameter boun dary = wrap. This method can be considerably slower than pyFFS' pyffs.convolve for modest size inputs, as shown below. All benchmarking is performed on a Lenovo ThinkPad P15 Gen 1 laptop, with an Intel i7-10850H six-core processor.



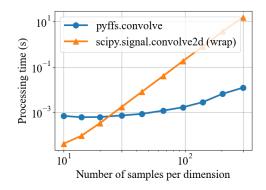


Figure 1: 2-D bandlimited circular convolution.

For N-D bandlimited interpolation with SciPy, it is possible to use scipy.signal.resample along each dimension. However, there is no one-shot function. Below we benchmark 1-D and 2-D interpolation as we vary the width of the interval over which we interpolate.

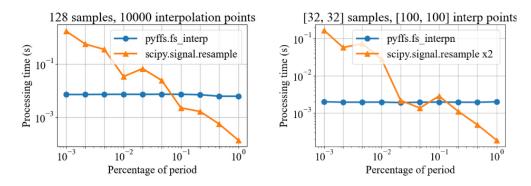


Figure 2: Bandlimited interpolation: (left) 1-D and (right) 2-D.

As can be observed above, the complexity of pyFFS's interpolation stays constant as we vary the size of the interpolation region. That is because the CZT-based approach of pyFFS performs interpolation solely in the region of interest. SciPy's interpolation, on the other hand, interpolates by zero-padding the DFT coefficients and taking an inverse DFT over the full period, requiring operations outside the region of interest. The complexity of SciPy's approach is $\mathcal{O}(N_t \log N_t)$, where $N_t = \lceil T/\Delta t \rceil$, T is the period, and Δt is the desired resolution. The complexity of the pyFFS method is defined by that of the CZT (Rabiner et al., 1969), namely $\mathcal{O}((M+N)\log(M+N))$ where M is the number of interpolation points and N is the number of FS coefficients.

In the benchmark below, we interpolate a 2% region of a 2-D function, of which we have 256×256 samples. As we vary the resolution of the interpolation, we notice that the pyFFS function is consistently more efficient.



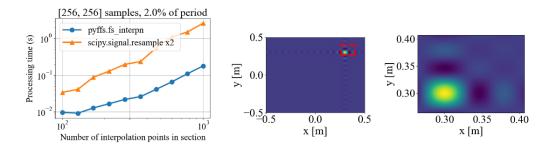


Figure 3: 2-D bandlimited interpolation: (left) profiling increasing resolution for 2% region; (middle) visualization of corresponding region; (right) 2% region of middle plot.

GPU acceleration

There are two important considerations when using a GPU. Firstly, if the application permits, it is recommended to work with float32/complex64 arrays for less memory consumption and potentially faster computation. By default, NumPy and CuPy create float64 / comple x128 arrays, e.g. when initializing an array with np.zeros, so casting the arrays accordingly is recommended. In the benchmarking tests below, we use float32/complex64 arrays. Secondly, the benefits of using a GPU typically emerge when the processed arrays are larger than the CPU cache. So the crossover between CPU and GPU performance can be very hardware-dependent. All benchmarking below is performed on a Lenovo ThinkPad P15 Gen 1 laptop, with an Intel i7-10850H six-core processor and an NVIDIA Quadro RTX 3000 GPU.

Figure 4 compares the processing time between a CPU and a GPU for computing an increasing number of FS coefficients.

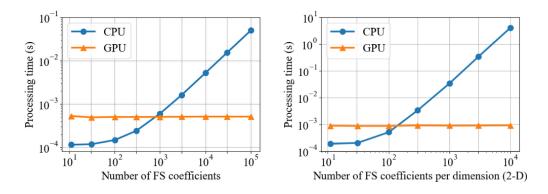


Figure 4: Profiling Fourier series computation: (left) 1-D and (right) 2-D.

In 1-D, for more than 1'000 coefficients it starts to become beneficial to use a GPU, and at around 10'000 coefficients it is an order of magnitude faster to use a GPU. In 2-D, the crossover point is at around 100 coefficients per dimension, and at around 1'000 coefficients per dimension it is more than an order of magnitude faster to use a GPU. From the 1-D and 2-D cases, it is clear that using a GPU scales well as the input increases in size. When considering a 2-D or even a 3-D object, where input sizes quickly grow, it is attractive to make use of a GPU for even modest input sizes.

Figure 5 profiles the processing time for 1-D FS interpolation. Using a GPU becomes more attractive as the number of coefficients and number of samples exceeds 300. As mentioned earlier, this is probably the point when the arrays and computation can no longer fit on the CPU cache.



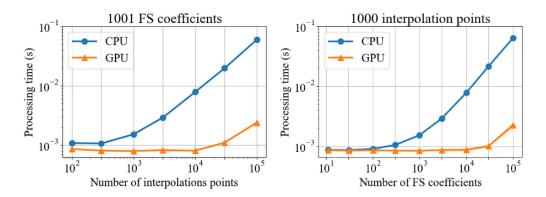


Figure 5: Profiling 1-D Fourier series interpolation.

Figure 6 profiles the processing time for 2-D FS interpolation. Using a GPU consistently provides two orders of magnitude faster computation for a varying number of FS coefficients and varying number of interpolation points per dimension. The benefits of using a GPU are even more prominent in 2-D as input sizes quickly grow when considering multidimensional scenarios.

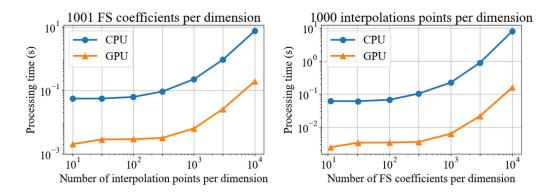


Figure 6: Profiling 2-D Fourier series interpolation.

Example application: Fourier optics

In Fourier optics, we are often interested in the propagation of light between two planes, i.e. a source plane and a target plane as shown in Figure 7(a). Given an aperture function or phase pattern at the source plane, we would like to determine the pattern at the target plane, as predicted by the Rayleigh-Sommerfeld diffraction formula. This propagation is often modeled with one of three approaches that make use of the FFT for an efficient simulation: Fraunhofer approximation, Fresnel approximation, or the angular spectrum method (Goodman, 2005). The choice between these three approaches typically depends on the requirements of the application, e.g. the distance between the two planes, the desired sampling rate at the input or output, and the size of input and output regions (Schmidt, 2010). For all approaches, we again find ourselves with a continuous-domain phenomenon that can be considered bandlimited and periodic. Bandlimited as in practice we consider finite input and output regions, lending to a restricted set of angles and therefore a bandlimited spatial frequency response between the source and target planes. This restriction of angles is shown in Figure 7(b). Even though our input may not be bandlimited, the resulting output will be bandlimited after convolution with such a response (Matsushima & Shimobaba, 2009). Finally, we can frame the optical



simulation as periodic as the input and output regions have a compact support and can thus be replicated to form periodic signals.

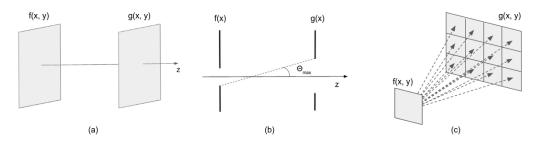


Figure 7: Visualization of optical wave propagation setup.

The application of the CZT, or equivalently the fractional FT (Bailey & Swarztrauber, 1991), for interpolation has already found its use in Fourier optics to resample the output plane outside of the grid defined by the FFT (Muffoletto et al., 2007), as demonstrated with pyFFS in Figure 2.

Below we show how the pyFFS interface can be used in optical wave propagation for efficient simulation and interpolation.

```
# pad input and reorder
f_pad = numpy.pad(f, pad_width=pad_width)
f_pad_reorder = pyffs.ffs_shift(f_pad)

# compute FS coefficients of input
F = pyffs.ffsn(f_pad_reorder, T, T_c, N_FS)

# convolution in frequency domain with free space transfer function
G = F * H

# interpolate at the desired location and resolution
# a and b specify the region while N_out specifies the resolution
g = pyffs.fs_interpn(G, T, a, b, N_out)
```

The free space propagation transfer function H in the above code listing can be obtained by evaluating the analytic expression for the Fresnel approximation or the angular spectrum method transfer functions at the appropriate frequency values (Goodman, 2005).

One may wish to simulate an output window with the same size as the input but at a finer resolution. In order to circumvent the much larger FFT that this may require, an approach known as rectangular tiling (Muffoletto et al., 2007), as shown in Figure 7(c), can be used to split up the output window into tiles. In its original proposition, the tiles are simulated sequentially, but with a GPU they could be computed in parallel for a significantly shorter simulation time: pyFFS's GPU support enables this possibility. Moreover, rectangular tiling in its original proposition requires that each tile has the same number of samples as the input window. This restriction is removed by the interpolation approach of pyFFS.

Conclusion

import pyffs

In this paper we have presented pyFFS, a Python library for efficient Fourier series (FS) coefficient computation, convolution, and interpolation. The intended use of this package is



when working with discrete samples that arise from a continuous-domain signal. When the underlying signal is periodic (or has finite support and can be periodized) and bandlimited, its FS coefficients can be computed and interpolated in a straightforward and distortionless fashion with pyFFS. If either periodicity or bandlimitedness is not met, the same workarounds as when applying the discrete Fourier transform can be used, namely windowing to taper discontinuous boundaries or bandlimiting by FS coefficient truncation.

As computation is posed in the continuous-domain, accuracy loss that may arise from switching between the discrete- and the continuous-domain can be minimized. Moreover, this package serves as a handy continuous-domain complement to the functionalities already available in SciPy, where the focus is primarily on discrete signals. We also provide functionality not available in SciPy, namely N-D circular convolution, N-D bandlimited interpolation, and a bandlimited interpolation technique based on the chirp Z-transform. As shown in our benchmarking results, the latter can be more than an order of magnitude faster when interpolating sub-regions of a 1-D or 2-D periodic function. Similar results can be expected for a general N-D function. Furthermore, GPU support has been seamlessly integrated through the CuPy package, offering more than an order of magnitude reduction when computing and interpolating a large number of FS coefficients.

In summary, pyFFS offers researchers and engineers a convenient and efficient interface for working with FS coefficients. The source code is made available on GitHub and can be easily installed for Python through PyPi.More extensive and up-to-date documentation can be found at pyffs.readthedocs.io.

Acknowledgements

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