GhostiPy: an efficient signal processing and spectral analysis toolbox for large data

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Abstract

Recent technological advances have enabled neural recordings consisting of hundreds to thousands of channels. As the pace of these developments continues to grow rapidly, it is imperative to have fast, flexible tools supporting the analysis of neural data gathered by such large scale modalities. Here we introduce **ghostipy** (general **hub of s**pectral **t**echniques **in Py**thon), a Python open source software toolbox implementing various signal processing and spectral analyses including optimal digital filters and time-frequency transforms. **ghostipy** prioritizes performance and efficiency by using parallelized, blocked algorithms. As a result, it is able to outperform commercial software in both time and space complexity for high channel count data and can handle out-of-core computation in a user-friendly manner. Overall, our software suite reduces frequently encountered bottlenecks in the experimental pipeline, and we believe this toolset will enhance both the portability and scalability of neural data analysis.

Introduction

Advancements in neural recording technologies have enabled the collection of large data in both space (high density/channel count) and time (continuous recordings). During subsequent analysis, the scale of the data induces certain challenges which may manifest

as the following scenarios: (1) analysis code takes a long time to complete (high time complexity), (2) code is unable to complete due to insufficient memory on the hardware (high spatial complexity). Moreover the scientist may have difficulty finding existing tools that address both (1) and (2) and that implement the desired analyses.

Although a potential remedy is to simply upgrade the hardware, it is not an acceptable solution for scientists desiring portability of analyses. In those situations hardware resources may be limited (e.g. using a laptop at the airport). We thus took an 11 alternate approach by efficiently implementing analyses that would trivially scale for 12 different hardware configurations. Our solution is ghostipy (general hub of spectral 13 techniques in Python), a free and open source Python toolbox that attempts to 14 optimize both time and space complexity in the context of spectral analyses. Methods 15 include linear filtering, signal envelope extraction, and spectrogram estimation, 16 according to best practices. ghostipy is designed for general purpose usage; while well 17 suited for high density continuous neural data, it works with any arbitrary array-like 18 data object.

In this paper we first describe ghostipy's software design principles to increase 20 efficiency. We then elaborate on featured methods along with code samples illustrating 21 user friendliness of the software. Finally we benchmark our software against a 22 comparable implementation, and we discuss strategies for working under an out-of-core 23 (when data cannot fit into system memory) processing context. 24

Materials and methods

An overview of implemented methods can be found in Table 1. Excluding out-of-core support, it is possible to use multiple different packages to achieve the same functionality. However the mix-and-match approach can reduce user friendliness since application programming interfaces (APIs) differ across packages and dependency management is more difficult. We believe our unified package provides an attractive solution to this challenge.

Software Design Considerations

As previously noted, successful completion of analyses may be hampered by long 33 computation times or lack of system memory. Specifically, algorithmic time and space complexity are major determinants for the efficiency and performance of a software method. In general it is difficult to optimize both simultaneously. For example, time complexity may be reduced by increasing hardware parallelization, at the expense of 37 higher space complexity (memory requirements). While we sought to lower both kinds of complexity compared to existing solutions, we gave space complexity a higher priority. Stated concretely, slow computation time is primarily a nuisance, but failure to complete an analysis due to insufficient memory is catastrophic. 41

Our design decision to prioritize space complexity was particularly critical because it directly influenced which backend library we chose for the Fast Fourier Transform (FFT), an operation used in the majority of ghostipy's methods. While investigating the different options, we saw that numpy currently uses the pocketfft backend [26, 20]. When accelerated with Intel's MKL library, it can be slightly faster than FFTW [6]. However, we have found FFTW [9, 10] superior for memory management and better suited for arbitrary length FFTs, including prime and odd numbers. An additional benefit of FFTW was its multithreaded capabilities. We therefore selected FFTW as our FFT backend.

To lower space complexity we used blocked algorithms, including overlap save convolution, which is not offered in any of the standard Python numerical computing libraries such as numpy or scipy [26, 27]. This approach enabled us to process very large data that could not fit in memory (also known as out-of-core processing). Throughout our code, we also employed other strategies such as in-place operations.

To lower the time complexity, we used efficient lengths of FFTs wherever possible, and we leveraged modern computing hardware by parallelizing our algorithms. For 57 example a wavelet transform can be trivially parallelized since the transform for each scale is not dependent on other scales.

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	Python	Overlap save convolu- tion	Multi- taper method	Hilbert Trans- form	Morse CWT	Synchro- squeezed trans- form	Out-of- core
Ghostipy	+	+	+	+	+	+	+
SciPy	+	+	-	+	-	-	-
Chronux	-	-	+	-	-	-	-
Elephant	+	+	-	+	-	-	-
Brain- storm	+	+	+	+	-	-	-
PyWt	+	-	-	-	-	+	-
Field Trip	-	+	+	+	-	-	-
MNE	+	+	+	+	-	-	-
MATLAB	-	+	+	+	+	+	-

Table 1. Features implemented by ghostipy compared to existing software [27, 1, 28, 22, 13, 18, 12]

Multitaper Method

Users often wish to perform a spectral decomposition on a signal of interest. This can be accomplished by using the multitaper method [25, 19]. The technique is well-suited to reduce the variance of a spectrum estimate, which is particularly useful when working with noisy neural data. The spectrum estimate is obtained as an average of multiple statistically independent spectrum estimators for a discrete signal x[n] with sampling frequency f_s :

$$\hat{S}_{W}^{mt}(k) = \frac{1}{L} \sum_{l=1}^{L} \hat{S}_{l,W}^{mt}(k)$$
(1)

$$\hat{S}_{l,W}^{mt}(k) = \frac{1}{f_s} \sum_{n=0}^{N-1} v_{l,W}[n] x[n] e^{-2\pi j k n/N}$$
(2)

Given the length of data N and a smoothing half-bandwidth W, the tapers $v_{l,W}[n]$ are computed by solving for vectors that satisfy the energy and orthogonality properties 668

$$\sum_{n=0}^{N-1} v_{l,W}[n] \ v_{l,W}[n] = 1$$
(3)

$$\sum_{n=0}^{N-1} v_{l,W}[n] \ v_{m,W}[n] = 0, \ l \neq m$$
(4)

An example using ghostipy is shown in Figure 1.

Continuous Wavelet Transform

Neuroscientists often use a continuous wavelet transform (CWT) to study transient 71 oscillatory activity. The CWT itself is defined in the time domain by 72

$$W(a,b) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{a}} \psi^{\star} \left(\frac{t-b}{a}\right) x(t) dt$$
(5)

where $\psi(...)$ is the mother wavelet function. The transform represents a two-dimensional decomposition in the scale (a) and time (b) planes. In the frequency domain, the CWT 74

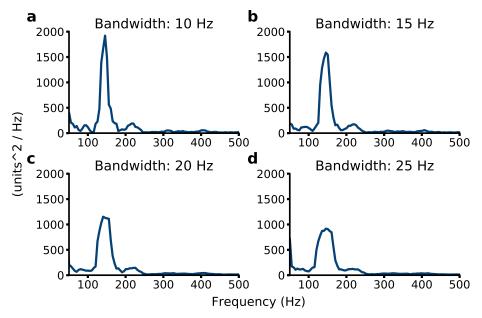


Fig 1. Mutitaper spectrum estimates can be readily generated. The example uses a sharp wave ripple event, where energy occurs mainly between 100 and 250 Hz.

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is given by the inverse Fourier transform of

$$W(a) = X(\omega)\Psi^{\star}(a\omega) \tag{6}$$

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for a given scale (a), where X and Ψ are the Fourier transforms of x and ψ , respectively. 76

Many mother wavelet functions have been investigated in the literature, but we have focused on the analytic wavelets, as they are found to be superior, particularly for estimating phase [17, 14, 16, 15]. We have implemented the analytic Morse, Morlet, and Bump wavelets, whose respective frequency domain definitions are

$$\Psi(a\omega) = 2 \ e^{-(a\omega - \omega_0)^2/2} \ H(\omega), \tag{7}$$

$$\Psi(a\omega) = 2 \left(\frac{e\gamma}{\beta}\right)^{\frac{\beta}{\gamma}} (a\omega)^{\beta} e^{-(a\omega)^{\gamma}} H(\omega)$$
(8)

$$\Psi(a\omega) = 2 \ e^{1 - \left(1 - \left(\frac{\mu - \sigma}{a}\right)^2\right)^{-1}} \ \mathbb{1}_{(\mu - \sigma)/a, (\mu + \sigma)/a} \tag{9}$$

where $\mathbb{1}_{(\mu-\sigma)/a,(\mu+\sigma)/a}$ is the indicator function for the interval $(\mu-\sigma)/a \leq \omega \leq (\mu+\sigma)/a$ and $H(\omega)$ is the Heaviside step function. In our implementation, we use Equation 6 to compute the CWT.

Note that in practice the timeseries x(t) is sampled, and the CWT is likewise sampled. Then equation 6 becomes a pointwise complex multiplication of discrete Fourier transforms, where the discretized angular frequencies ω_k are determined by

$$\omega_k = \frac{2\pi k}{N\Delta t} \tag{10}$$

where N is the number of data samples and Δt is the sampling interval.

For electrophysiological data, a typical wavelet analysis will require computing Equation 6 for 50-500 scales. This is an obvious candidate for parallelization since the wavelet transform for each scale can be computed independently of the others. We use a backend powered by **dask** to carry out the parallelization [21]. Users can set the number of parallel computations to execute and thereby leverage the multicore capabilities offered by modern computing hardware.

Synchrosqueezing Transform

One disadvantage of the wavelet transform is that its frequency resolution decreases as the temporal resolution increases. Strictly speaking the CWT results in information contained in the (time, scale) plane, but a single frequency is typically assigned to each scale. Regardless, spectral smearing can be observed for at higher frequencies/lower scales. However, [4, 24] showed the synchrosqueezing transform (SST) could mitigate this issue by transferring a CWT's (time, scale) plane information to the (time, frequency) plane.

The synchrosqueezing transform proceeds as the following. For every scale a:

- 1. Compute the CWT W(a) using equation 6 103
- 2. Compute the partial derivative

$$\partial_b W(a) = j\omega X(\omega) \Psi(a\omega) \tag{11}$$

3. Compute the phase transform

$$\omega_f(a) = \frac{1}{2\pi} \Im\left(\frac{\partial_b W(a)}{W(a)}\right) \tag{12}$$

The phase transform contains the real frequencies each point in the CWT matrix should be assigned to. In practice the real frequency space is discretized, so the CWT points are assigned to frequency bins. Note that multiple CWT points at a given time coordinate *b* may map to the same frequency bin. In this situation, a given frequency bin is a simple additive accumulation of CWT points.

Note the similarity of the SST to the spectral reassignment algorithms in [11, 8]. However an important distinction is that the SST only operates along the scale dimension. In addition to preserving the temporal resolution of the CWT, this makes SST data easy to work with since uniform sampling can be maintained.

Overall, the spectrogram methods implemented by ghostipy give an experimenter a more complete picture of the time-varying spectral content of neural data. Figure 2 116 illustrates using the scipy standard spectrogram method along with ghostipy's 117 methods.

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```
import scipy.signal as sig
fs = asa.fs
nperseg = 64
noverlap = 16
w = 25
f_spect, t_spect, psd_spect
                                 = sig.spectrogram(data, fs=fs,
                                                    nperseg=nperseg,
                                                    noverlap=noverlap)
psd_mtm, f_mtm, t_mtm
                                   gsp.mtm_spectrogram(data, w, fs=fs,
                                 =
                                                        nperseg=nperseg,
                                                        noverlap=noverlap)
                                 = gsp.cwt(data, fs=fs, freq_limits=[1, 500])
coefs_cwt, _, f_cwt, t_cwt, _
coefs_wsst, _, f_wsst, t_wsst, _ =
                                   gsp.wsst(data, fs=fs, freq_limits=[1, 500],
                                           voices_per_octave=32)
```

psd_cwt = np.abs(coefs_cwt)**2 / fs
psd_wsst = np.abs(coefs_wsst)**2 / fs

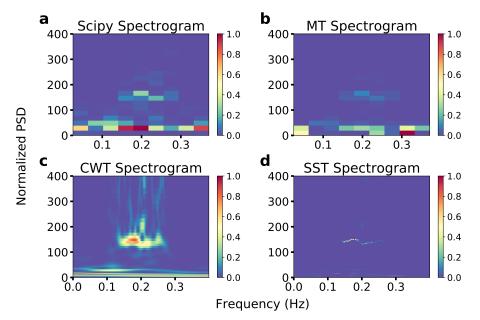


Fig 2. Users can leverage scipy's spectrogram along with ghostipy's methods to determine different time-frequency representations. The synchrosqueezed transform in (d) gives the overall sharpest time and frequency resolution.

FIR Filter Design

In addition to the time-frequency transforms described above, ghostipy provides 120 classical signal processing capabilities such as filtering data, using the efficient overlap 121 save convolution. Filtering data is an ubiquitous operation, but before this stage, the 122 filter must itself be designed. While this step may appear somewhat trivial, it can make 123 a significant difference. Consider theta-gamma phase amplitude coupling (PAC), a 124 phenomenon in which the amplitude of the gamma band (approximately 30-120 Hz) 125 oscillation is modulated by the phase of the theta band (approximately 6-10 Hz) 126 oscillation. [7] states that "It is not possible to measure significant amounts of PAC 127 with amplitudes filtered with narrower bandwidths than the frequency of the 128 modulatory rhythm", but one of the early studies documenting theta-gamma coupling 129 used 4 Hz bandwidth filters [3]. How could theta-gamma PAC have been discovered if 130 the filters were nominally 4 Hz in bandwidth? The answer was that the software library 131 used by the seminal paper scaled the transition bandwidth according to the passband 132 center frequency, so the effective bandwidth was larger than the initially requested 4 Hz 133 [7]. Theta-gamma coupling was thus a serendipitous discovery. Clearly it is important 134 to control the transition bands of the filter, not just the passband. Existing packages 135 such as scipy and MNE offer a variety of FIR filter design methods [27, 12]. However 136 they suffer from certain issues, as documented below: 137

- Least squares method: A solution may result in a filter with magnitude response
 effectively zero throughout. This situation is more common when designing filters
 with passband relatively low compared to the sampling rate.
- 2. Remez exchange method: The algorithm may simply fail to converge.
- Window method: The transition bands cannot be controlled exactly, and
 optimality can not be defined, as is the case for the least squares (L2 optimal) and
 Remez exchange (L1 optimal)

Therefore ghostipy's filter design uses the method defined in [2] for the following reasons:

1. It is simple to design. The computational complexity is similar to that of a ¹⁴⁷ window method and can be implemented on embedded hardware if desired. ¹⁴⁸

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- 2. Optimality can be defined, as it is optimal in the L2 sense.
- 3. Transition bands can be defined exactly, and the steepness of the passband rolloff ¹⁵⁰ can be controlled by the spline power parameter. ¹⁵¹
- The filter impulse response can be defined analytically. Consequently its
 computation does not suffer from the failure modes of the least squares or Remez
 exchange methods, as those must solve systems of linear equations. In other
 words, the design process is reliable and stable.

This method designs a low pass filter according to

$$h(n) = \frac{\sin(\omega_0 n)}{\pi n} \left[\frac{\sin(\Delta n/p)}{\Delta n/p} \right]^p$$
(13)

$$\omega_0 = \frac{\omega_2 + \omega_1}{2} \tag{14}$$

$$\Delta = \omega_2 - \omega_1 \tag{15}$$

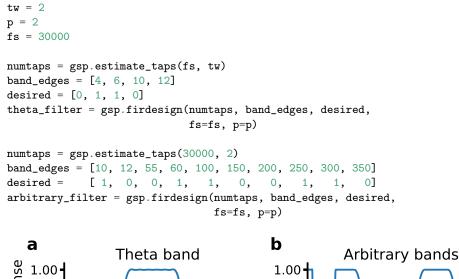
where ω_1 and ω_2 are radian frequencies defining the transition band boundaries. ¹⁵⁷

ghostipy uses the low pass filter defined in 13 as a prototype to design more158complicated filters. As a result, users can request filters with arbitrary magnitude159response. Two examples are shown in Figure 3.160

Results

Spectral analysis is ubiquitous in systems neuroscience experiments involving 162 electrophysiology. One of the primary goals of our development was to facilitate clear 163 and simple workflows with high performance. Of special note is that our tool enables 164 wavelet-based spectral analysis using the Morse wavelet [15], a feature that has 165 previously only been conveniently available in commercial tools such as Matlab. In 166 particular, the Morse wavelet is exactly analytic and nicely parameterized to tradeoff 167 frequency and temporal resolution. For very long data, most investigators will not be 168 interested in the sub-Hz frequency components, and performance can be improved by 169 restricting the frequencies/scales that are actually used for the transform. 170

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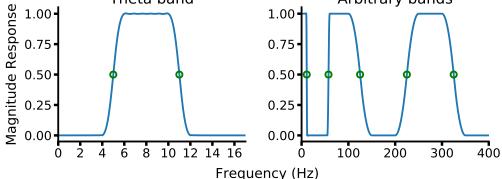


Fig 3. (a) A theta band filter designed for full bandwidth data. The specification of the transition bands allows for easy determination of critical frequencies. The -6 dB points are exactly the midpoints of the transition bands. (b) Filters with arbitrary pass and stop bands may also be designed.

A naive implementation of the Morse wavelet transform calculates untruncated 171 wavelets the same length as the input data. This is often inefficient because it is 172 equivalent to convolving the data with a time-domain wavelet mainly consisting of 173 leading and trailing zeros. In our approach we exploit the fact that wavelets are finite in 174 time and frequency, and we use an overlap-save algorithm to compute the CWT purely 175 in the frequency domain. Note that the latter point is particularly critical: Due to the 176 Gibbs phenomenon, using any time-domain representation of the wavelet may violate 177 numerical analyticity for wavelet center frequencies near the Nyquist frequency. It is 178 therefore necessary to use only the frequency domain representation of the wavelet. 179 While we offer both traditional/naive and blockwise convolution implementations, the 180 latter will give superior performance for longer-duration data. We believe that this is a 181 valuable option for researchers and that this is the first tool which uses blockwise 182

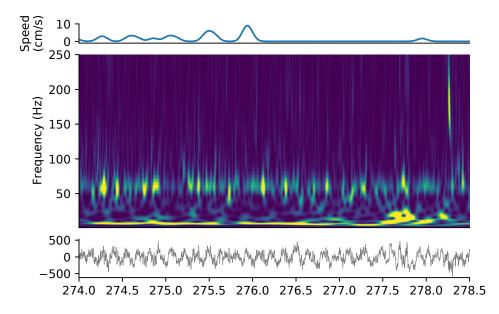


Fig 4. Spectrogram of local field potential recordings from area CA1 of the hippocampus of a rat during exploration (middle), with movement speed (top) and the raw electrophysiological signal (bottom). A number of features of the hippocampal rhythms can be noted in this example, including the pervasive theta oscillation (~ 8 Hz), theta-nested gamma oscillations (~ 60 Hz) during movement, and, towards the end, a sharp wave ripple (~ 200 Hz). An example notebook replicating this figure can be found online.

convolution to implement the CWT.

An example spectrogram of local field potentials recorded in area CA1 of the rat hippocampus is shown in figure 4. Clearly apparent are the theta oscillation, theta-nested gamma oscillations, and a sharp-wave-ripple, which occurs after the animal has stopped moving.

Performance and Complexity

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The calculation of the CWT is computationally intensive and consequently a good 189 method to benchmark performance. Of the software packages listed in Table 1, only 190 MATLAB offered an equivalent solution. It was thus chosen as the reference to compare 191 our implementation against. Figure 5 shows that our implementation results in faster 192 computation times and better memory usage. 193

It is not entirely clear what accounts for the higher jaggedness in the MATLAB curves ¹⁹⁴ from Figure 5. A possible explanation is that the FFT computation is less efficient for ¹⁹⁵

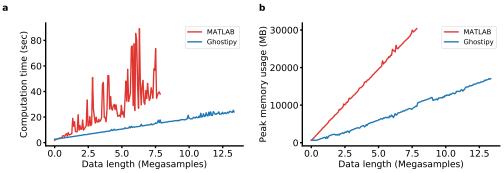


Fig 5. Our implementation of the Morse continuous wavelet transform outperforms MATLAB's in both (a) time and (b) space complexity. Note that MATLAB was unable to complete execution for the full range of the test parameter (data length) due to out-of-memory exceptions. The test machine was an Intel Core i7-4790 (8 hyperthreads) equipped with 32 GB RAM.

an odd-length transform, but the magnitude of the spikes in the curve is surprising 196 given that MATLAB's FFT backend also uses FFTW. Regardless, we have demonstrated 197 that our implementation is able to achieve lower time and space complexity. When 198 using the functionality offered by **ghostipy**, three primary scenarios arise with regards 199 to the sizes of data involved in the processing: 200

- 1. both the input and output data fit into core memory
- 2. the input fits into core memory but the output does not
- 3. neither the input nor the output fit

In all of the previous examples, we have restricted ourselves to case 1. However, with 204 the ever-increasing sizes of data, the other cases will inevitably be encountered. Case 2 205 may arise when attempting to generate spectrograms. As the input is a single channel, 206 memory constraints are rarely an issue. For example, even a 10 hr LFP recording 207 sampled at 1 kHz and saved as 64-bit floating point values will require less than 300 208 MiB of memory. However, the size of a wavelet spectrogram computed from this data 209 will be directly proportional to the number of scales/frequencies. For a typical range of 210 1 to 350 Hz at 10 voices per octave, this amount to a space requirement of 85 times that 211 of the input data. Given that this can well exceed the core memory size of a machine, 212 ghostipy's CWT routine can also accept a pre-allocated output array that is stored on 213 disk (Figure 6). 214

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Fig 6. Example code when the output array is too large for main memory. The CWT method is first executed as a dry run to compute the necessary array sizes.

Case 3 may arise when a user wishes to filter many channels of full bandwidth data. ²¹⁵ One use case is a 1 hour recording for a 256 channel probe sampled at 30 kHz and stored ²¹⁶ as a 2-byte signed integer type; already this requires 51 GiB. Our strategy is similar to ²¹⁷ case 2, where an output array is allocated and stored on disk. As for the input, it is ²¹⁸ read in chunks, and the size of these can be chosen to lower memory usage, although ²¹⁹ potentially at a cost to computation time. The code in Figure 7 illustrates an example: ²²⁰

```
with h5py.File(input_filepath, 'r') as infile:
    with h5py.File(output_filepath, 'w') as outfile:
```

```
ds = 300
K = filter_delay
N = infile['chdata'].shape[1]
shape, dtype = gsp.filter_data_fir(infile['chdata'],
                                 theta_filter,
                                 axis=1,
                                 ds=ds,
                                 output_index_bounds=[K, K+N],
                                 describe_dims=True)
outdata = outfile.create_dataset('theta_data',
                                   shape=shape,
                                   dtype=dtype)
gsp.filter_data_fir(infile['chdata'],
                    theta_filter,
                    axis=1,
                    ds=ds.
                    output_index_bounds=[K, K+N],
                    outarray=outdata)
```

Fig 7. Filtering data from a large array stored on disk and likewise storing the output on disk. Similar to the CWT out-of-core features, the method is called once as a dry run to compute array sizes, which the user can then pass in to store the result. The filtering method also allows to correct for the delay of the filter and to downsample without storing any intermediate results. Although example uses the h5py library, any object that behaves like an array can be used.

Several points can be made about the scheme in Figure 7. Our method allows for downsampling during the convolution, which can reduce the number of stages in a computational scheme. Given full bandwidth data, a traditional strategy to filter to the theta band would look like the following: 224

1.	Apply an anti-aliasing filter.	225
2.	Downsample to obtain LFP.	226
3.	Store the LFP to disk.	227
4.	Apply a theta-band filter.	228
5.	Downsample this output.	229
6.	Save the result.	230

Using ghostipy's method, it is not necessary to generate the intermediate LFP. To our knowledge, we do not know of other software that allows out-of-core filtering and downsampling in a single function call. The result is a simultaneous reduction in time and space complexity, by storing only the downsampled result and by filtering only once. Filtering to the theta band is now simplified to the following steps: 231

- 1. Apply a theta filter to the full bandwidth data. 236
- 2. Downsample the result.
- 3. Save the result to disk.

Conclusion

We have described the key features of ghostipy and given examples of its ease of use to perform computations efficiently. Users can thus conduct exploratory spectral analyses quickly across a range of parameters while reducing their concerns for running out of memory, especially since out-of-core computation is supported for many of the methods. Thus we believe ghostipy is well-suited to handle the ever-increasing size of experimental data.

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In the future we plan to improve **ghostipy** with various enhancements. For example, 246 currently the methods are designed to offer the user a lot of low level control over areas 247 such as multithreading, and to work with raw array types. However, users may desire a 248 higher-level API. For this reason we believe it would be a worthwhile endeavor to 249 incorporate our work into frameworks such as NWB [23]; this would also facilitate more 250 widespread adoption. Lastly, there are other analyses we could implement, including the 251 adaptive multitaper method [19] and other time-frequency reassignment techniques 252 similar to the synchrosqueezing transform [5]. 253

Our primary contribution is improving the ease and speed at which data analysis 254 can be conducted, by developing user-friendly software implementing efficient 255 algorithms well-suited for large data sizes. This point is specifically demonstrated by 256 our ability to outperform existing solutions in space and time complexity, and to run 257 computations even in out-of-core memory conditions, which enables machines with 1-10s 258 of GBs of memory to process data on the scale of 10-100s GBs and higher. In these 259 ways, we have increased the accessibility of neural data analysis by enabling it to be run 260 on hardware such as laptops, a scenario that often was not previously possible. 261

Lastly, the software we developed has a much larger potential impact than the scope 262 described in this paper. Although many of the examples given in this paper were 263 specific to extracellular rodent hippocampal data, the functionality we implemented is 264 intentionally generic and applicable to many fields. As an example, our code can easily 265 be adapted for use in real-time processing, whether running on embedded hardware or 266 on a laptop in a clinical EEG setting. Given the functionality already developed and the 267 full scope of our work, we are optimistic that ghostipy can help accelerate modern 268 scientific progress. 269

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