

GPU-accelerated implementation of phase-amplitude coupling

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Abstract

Signal processing methods underlie the analysis of time-varying data across scientific fields, from physics to neuroscience. Phase-amplitude coupling (PAC), which quantifies interactions between frequency components in neural oscillations, serves as a fundamental biomarker for pathological brain activity and information processing in the brain. While PAC analysis has provided crucial insights into neural computation and communication, its computational complexity has historically limited applications to large-scale datasets that are increasingly common in modern neuroscience. Here we present TorchPAC, a GPU-accelerated framework that enables rapid PAC calculation through parallel processing and optimized algorithms. Our implementation achieved a 100-fold speedup compared to conventional CPU-based methods while maintaining computational accuracy, enabling real-time PAC calculation and successfully processing terabyte-scale neural recordings from multiple brain regions. This improvement in processing speed enabled comprehensive cross-frequency coupling analyses across unprecedented scales of neural data, revealing previously undetectable patterns of brain rhythmic interactions. Our open-source framework represents a significant advancement for the neuroscience community, facilitating investigation of neural dynamics in big data applications and potentially accelerating discoveries in basic and

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30 clinical neuroscience research.

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32 ~ 1 figures, 0 tables, 176 words for abstract, and 462 words for main
33 text

34 1. Introduction

35 Introduction here

36 2. Methods

37 2.1. Synthetic Data

38 We utilized synthetic data for profiling computational speed and accuracy.

39 2.2. Physiological Data

40 Additionally, we verified our method using physiological recordings from
41 [fixme ->] XXX [<- fixme] for event-related analyses.

42 2.3. Implementation of GPU-accelerated PAC

43 To enable seamless integration with artificial intelligence (AI) training
44 frameworks, we developed a graphics processing unit (GPU)-accelerated phase-
45 amplitude coupling (PAC) implementation using PyTorch as the computa-
46 tional foundation. The implementation comprises three primary components:
47 bandpass filtering, Hilbert transformation, and mutual information index
48 calculations, which are modularly integrated into a unified PAC class and
49 function. This implementation is publicly available in the mngs package, an
50 open-source Python toolbox (<https://github.com/ywata1989/mngs/dsp>).

51 GPU-accelerated PAC calculation can be executed with three lines of
52 code:

```
53 import mngs  
54 signal, _time, fs = mngs.dsp.demo_sig()  
55 pac, freqs pha, freqs_amp = mngs.dsp.pac(signal, fs, batch_size=1, batch_size_ch=1
```

56 where **signal** represents the input time series data ($\mathbb{R}^{n_{\text{samples}} \times n_{\text{channels}} \times n_{\text{sequence}}}$),
 57 **_time** contains the corresponding time points, **fs** specifies the sampling frequency in Hz, **batch_size** defines the number of temporal segments processed simultaneously, **batch_size_ch** specifies the number of channels processed in parallel, **n_perm** indicates the number of permutations for surrogate testing, **pac** returns the calculated PAC values, and **freqs_pha** and **freqs_amp** represent the frequency bands for phase and amplitude components, respectively.

64 2.4. Machine Specification

65 All computations were performed on a workstation running Rocky Linux
 66 9.4 with an AMD Ryzen 9 7950X 16-core/32-thread CPU (maximum frequency: 5.88 GHz) and 61.7 GiB of RAM. GPU acceleration was implemented using an NVIDIA GeForce RTX 4090 with CUDA 12.6.20. Our
 68 implementation utilized PyTorch [fixme ->] version X.X.X [<- fixme] and
 69 was tested on both CPU and GPU configurations.

71 2.5. Calculation Quality

72 Mean squared error (MSE) was employed to measure calculation differences between our implementation and an existing PAC calculation package,
 73 TensorPAC.

75 2.6. Speed Comparison

76 Performance benchmarking was conducted using a baseline data chunk
 77 of dimensions $(n_{\text{samples}}, n_{\text{channels}}, n_{\text{sequence}}) = (4, 19, 2^8)$. Each condition was
 78 measured three times with the following parameters:

79 - Batch size: $2^3, 2^4, 2^5, 2^6$ - Number of channels: $2^3, 2^4, 2^5, 2^6$ - Number
 80 of segments: $2^0, 2^1, 2^2, 2^3, 2^4$ - Time duration: $2^0, 2^1, 2^2, 2^3$ seconds - Sampling rate: $2^9, 2^{10}$ Hz - Phase frequency bands: 10, 30, 50, 70, 10^2 - Amplitude frequency bands: 10, 30, 50, 70, 10^2 - Number of permutations: $2^0, 2^1, 2^2$ -
 81 Chunk size: $2^0, 2^1, 2^2, 2^3$ - FP16 precision: enabled, disabled - Gradient calculation: enabled, disabled - In-place operations: enabled, disabled - Model

85 trainability: enabled, disabled - Computing device: CPU, GPU (CUDA) -
86 Multi-threading: enabled, disabled - Number of calculations: $2^0, 2^1, 2^2, 2^3$
87 Computation times were compared between TensorPAC and our mngs
88 package implementation across all parameter combinations to assess relative
89 performance advantages.

90 2.7. Statistical Evaluation

91 Both the Brunner–Munzel test and the Kruskal–Wallis test were executed
92 using the SciPy package in Python [?]. Correlational analysis was conducted
93 by determining the rank of the observed correlation coefficient within its
94 associated set-size-shuffled surrogate using a customized Python script. The
95 bootstrap test was implemented with an in-house Python script.

96 3. Results

97 3.1. Result Headline #1

98 Result here.

99 3.2. Result Headline #2

100 Result here.

101 You might want to use *textit*, ¹, and ??.

102 4. Discussion

103 Discussion here.

104 Data Availability Statement

105 Data and code used in this study is available on <https://github.com/ywatanabe1989/torchPAC>.

¹footnote

106 **References**

107 **Ethics Declarations**

108 All study participants provided their written informed consent ...

109 **Author Contributions**

110 Y.W. and T.Y. conceptualized the study ...

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113 **Declaration of Interests**

114 The authors declare that they have no competing interests.

115 **Inclusion and Diversity Statement**

116 We support inclusive, diverse, and equitable conduct of research.

117 **Declaration of Generative AI in Scientific Writing**

118 The authors employed ChatGPT, provided by OpenAI, for enhancing the
119 manuscript's English language quality. After incorporating the suggested
120 improvements, the authors meticulously revised the content. Ultimate re-
121 sponsibility for the final content of this publication rests entirely with the
122 authors.

Figure 1 – Figure 1

A. Figure legend here.