Multi-Phase Locking Value: A Generalized Method for Determining Instantaneous Multi-frequency Phase Coupling

Yuan Yang,1,2 Bhavya Vasudeva,3 Hazem H. Refai,4 and Fei He5

1Stephenson School of Biomedical Engineering, The University of Oklahoma, Tulsa, Oklahoma-74135, USA
2Department of Physical Therapy and Human Movement Sciences, Feinberg School of Medicine, Northwestern University, Chicago, Illinois-60611, USA
3Indian Statistical Institute, Kolkata, West Bengal 700108, India
4Department of Electrical and Computer Engineering, The University of Oklahoma, Tulsa, Oklahoma-74135, USA
5Centre for Data Science, Coventry University, Coventry CV1 2JH, UK

Many physical, biological and neural systems behave as coupled oscillators, with characteristic phase coupling across different frequencies. Methods such as $n : m$ phase locking value and bi-phase locking value have previously been proposed to quantify phase coupling between two resonant frequencies (e.g. $f$, $2f/3$) and across three frequencies (e.g. $f_1$, $f_2$, $f_1 + f_2$), respectively. However, the existing phase coupling metrics have their limitations and limited applications. They cannot be used to detect or quantify phase coupling across multiple frequencies (e.g. $f_1$, $f_2$, $f_3$, $f_4$, $f_1 + f_2 + f_3 - f_4$), or coupling that involves non-integer multiples of the frequencies (e.g. $f_1$, $f_2$, $2f_1/3 + f_2/3$). To address the gap, this paper proposes a generalized approach, named multi-phase locking value (M-PLV), for the quantification of various types of instantaneous multi-frequency phase coupling. Different from most instantaneous phase coupling metrics that measure the simultaneous phase coupling, the proposed M-PLV method also allows the detection of delayed phase coupling and the associated time lag between coupled oscillators. The M-PLV has been tested on cases where synthetic coupled signals are generated using white Gaussian signals, and a system comprised of multiple coupled Rössler oscillators. Results indicate that the M-PLV can provide a reliable estimation of the time window and frequency combination where the phase coupling is significant, as well as a precise determination of time lag in the case of delayed coupling. This method has the potential to become a powerful new tool for exploring phase coupling in complex nonlinear dynamic systems.

I. INTRODUCTION

Complex systems such as the human brain behave as a series of oscillators with their instantaneous phases dynamically coupled over multiple frequency bands [1-5]. Methods such as $n : m$ phase locking value (PLV) [6], bi-phase locking value (bPLV) [7] and their variants [8-10] have previously been proposed to detect and quantify different types of phase coupling. The $n : m$ PLV measures phase coupling between two resonant frequencies when $n$ cycles of one oscillatory signal are phase locked to $m$ cycles of another oscillatory signal, i.e. $m \phi(f_n, t) - n \phi(f_m, t) \leq \text{const}$ [0, 11]. The bPLV quantifies quadratic phase coupling among three frequencies, where a pair of frequencies, $f_1$ and $f_2$ are coupled to a third frequency $f_3 = f_1 + f_2$ or $f_1 - f_2$, i.e. $\phi(f_1, t) \pm \phi(f_2, t) - \phi(f_3, t) \leq \text{const}$ [7].

However, phase coupling could be shown in more complicated patterns involving more than three frequencies (e.g. $f_1$, $f_2$, $f_3$, $f_4$, $f_1 + f_2 + f_3 - f_4$) as well as their non-integer multiples (e.g. $f_1$, $f_2$, $2f_1/3 + f_2/3$), which cannot be detected or quantified by using those conventional phase coupling metrics. A novel measure called multispectral phase coherence (MSPC) has been recently developed by Yang and colleagues to provide a generalized approach for quantifying integer multi-frequency phase coupling [12]. This method has been applied to the human nervous system to advance our understanding of nonlinear neuronal processes and their functions in movement control [13, 14] and sensory perception [15]. The MSPC is a straightforward extension of bPLV based on high-order spectra [16]; however, it does not cover either the non-integer multi-frequency phase coupling (e.g. $f_1$, $f_2$, $2f_1/3 + f_2/3$) or non-integer resonant coupling (e.g. $2f_1$ coupling [17] revealed by $n : m$ PLV) problems.

Thus, this paper aims to introduce a more generalized approach, namely multi-phase locking value (M-PLV), that integrates the concepts of MSPC and $n : m$ PLV to allow the detection and quantification of various types of phase coupling, including integer and non-integer, multi-frequency and resonant phase coupling. The proposed M-PLV provides us with a tool to explore the unreported non-integer multi-frequency phase coupling that has never been captured by existing phase coupling methods. Furthermore, different from commonly used instantaneous phase coupling metrics, the proposed method also allows the detection of delayed phase coupling and the associated time lag between coupled oscillators. We tested M-PLV on two scenarios where synthetic coupled signals are generated using white Gaussian signals, and a system comprised of multiple coupled Rössler oscillators.

The rest of this paper is organized as follows: Section II describes M-PLV, Section III summarizes the experiments used to validate the method, Section IV presents...
the results and discussion, and Section V concludes the paper.

II. MULTI-PHASE LOCKING VALUE (M-PLV): THEORY AND CALCULATION

The proposed M-PLV is a generalized approach that integrates the concept of MPLC \[12\] and \( n : m \) PLV \[6\]. It not only provides us with a formulated mathematical description for the phase coupling problems separately described by MSPC and \( n : m \) PLV, but also permits the detection and quantification of non-integer multi-frequency phase coupling that cannot be assessed by using existing phase coupling methods.

A. M-PLV

The MSPC considers the case where multiple input frequencies \( f_1, f_2, ..., f_L \) are coupled to an output frequency \( f_\Sigma \) based on an integer combination, such that \( f_\Sigma = \sum_{l=1}^{L} m_l f_l, m_l \in \mathbb{N} \):

\[
\left( \sum_{l=1}^{L} m_l \phi(f_l, t) \right) - \phi(f_\Sigma, t) \leq \text{const} \tag{1}
\]

The MSPC does not cover the case where non-integer multiples of input frequencies are coupled to the output frequency. To address this gap, the proposed M-PLV generalizes the relation between frequencies as \( n f_\Sigma = \sum_{l=1}^{L} m_l f_l \) or \( f_\Sigma = \sum_{l=1}^{L} \frac{m_l}{n} f_l \). It can be seen that although \( m_l, n \) are integers, their ratio can give real numbers. This idea is in line with the concept of \( n : m \) PLV \[6\], but allows assessment of phase coupling between multiple input frequencies and one targeted output frequency.

Moreover, there may exist a delay \( \tau \) in the system between the input and the output, such that the coupling can be detected only after this delay has been compensated by aligning the indices of all the instantaneous phases. Incorporating these factors, the proposed M-PLV aims to detect and quantify a more generalized phase coupling phenomenon that can be described as:

\[
\left( \sum_{l=1}^{L} m_l \phi(f_l, t - \tau) \right) - n \phi(f_\Sigma, t) \leq \text{const} \tag{2}
\]

Based on this theoretical definition, the formula of M-PLV (\( \Psi \)) is given as follows for the calculation:

\[
\Psi(f_1, f_2, ..., f_L; m_1, m_2, ..., m_L, n; t, \tau) = \left| \frac{1}{K} \sum_{k=1}^{K} \exp \left( j \left( \sum_{l=1}^{L} m_l \phi_k(f_l, t - \tau) - n \phi_k(f_\Sigma, t) \right) \right) \right| \tag{3}
\]

where \( K \) is the number of observations, \( \phi_k(f_l, t) \) is an instantaneous input phase at the \( k^{th} \) observation, which can be obtained from the Hilbert transform of narrow-band filtered time series with the spectrum centered at frequency \( f_l \) \[15\].

When \( \tau = 0 \), the proposed method can be used for detecting and quantifying the simultaneous multi-frequency phase coupling. Additionally, if \( n = 1 \), M-PLV is further reduced to MSPC, for measuring simultaneous integer multi-frequency phase coupling:

\[
\text{MSPC}(f_1, f_2, ..., f_L; m_1, m_2, ..., m_L; t) = \left| \frac{1}{K} \sum_{k=1}^{K} \exp \left( j \left( \sum_{l=1}^{L} m_l \phi_k(f_l, t) - \phi_k(f_\Sigma, t) \right) \right) \right| \tag{4}
\]

Noteworthy, bPLV \[7\] is basically a special form of MSPC or M-PLV when the interest is in determining quadratic phase coupling:

\[
\text{bPLV}(f_1, f_2; t) = \left| \frac{1}{K} \sum_{k=1}^{K} \exp \left( j \left( \phi_k(f_1, t) + \phi_k(f_2, t) - \phi_k(f_1 + f_2, t) \right) \right) \right| \tag{5}
\]

When \( L = 1 \), M-PLV can also be reduced to \( n : m \) PLV:

\[
\text{PLV}_{n:m}(f_n, f_m; m, n; t) = \left| \frac{1}{K} \sum_{k=1}^{K} \exp \left( j \left( m \phi_k(f_n, t) - n \phi_k(f_m, t) \right) \right) \right| \tag{6}
\]

As such, M-PLV not only allows the detection and quantification of non-integer multi-frequency coupling, but also provides a generic mathematical framework that can accommodate all common forms of phase coupling in the existing literature.

B. Detecting significant M-PLV

In order to detect the time window and frequency at which phase coupling is significant, a reference threshold value of M-PLV is required. For this purpose, the 95% significance threshold is obtained by a Monte Carlo simulation \[12\]. The null hypothesis is that the phase difference \( \Delta \phi(t; k) \) is completely random so that the cyclic phase difference \( \Delta \phi(t; k) = \Delta \phi(t; k) \mod 2\pi \) will be uniformly and randomly distributed in the interval \([0, 2\pi]\). The M-PLV corresponding to other frequency combinations for all instants \( t \) as well as those corresponding to the combination of interest for the instants \( t' = t - t_c \) (\( t_c \) is the estimated coupling window) are taken as surrogate data of uniformly and randomly distributed phase
values of $\Delta\phi(t;k)$. This procedure is repeated $N$ (e.g. 1000) times to obtain the statistical distribution of M-PLV values for the different number of observations, $K$, (e.g. $K = 50, 100, \ldots, 600$) and the threshold is determined as the minimum value greater than 95% of the sum of all the values in the distribution.

C. Delay Estimation

In order to estimate the delay $\tau$, the M-PLV for different values $\tau_i$ within a given range calculated. The value of $\tau_i$ corresponding to the maximum value of M-PLV is the estimated delay $\hat{\tau}$ of the system.

III. EXPERIMENTS

We tested M-PLV on two scenarios where synthetic coupled signals are generated satisfying (1) using white Gaussian signals alone, as well as (2) from a system comprised of multiple coupled Rössler oscillators. In the following simulations, the sampling frequency is 1 kHz.

A. Coupled white Gaussian signals

In this case, $x(t)$ and $y(t)$ are two independent white Gaussian signals (zero mean and unit variance). The synthetic signal, $y_c(t)$ is generated as follows:

$$y_c(t) = y(t) - y(f_\Sigma, t_c) + \frac{x[|m_1|](f_1, t_c)x[|m_2|](f_2, t_c)}{A_x[|m_1|](f_1, t_c)A_x[|m_2|](f_2, t_c)} A_y(f_\Sigma, t_c)$$

where $t$ is in the range of $[0.001, 10]$ s, $x(t_c)$ represents $x(t)$ in the phase coupling time window $t_c = [2.501, 7.5]$ s. $x(f_1, t_c)$ is a narrowband signal with the spectrum centered at frequency $f_1$, which is obtained after $x(t_c)$ is passed through a Butterworth band-pass filter centered at frequency $f_1$ (bandwidth: 2 Hz, 6th order). $A_x(f_1, t_c)$ is the envelope of the Hilbert transform of $x(f_1, t_c)$. In order to eliminate the effect of filter on the signal phase, zero-phase shift filter (Matlab function: filtfilt.m) is used in this study. The normalization of the signal $x(f_1, t_c)$ by its envelope $A_x(f_1, t_c)$ prevents abrupt changes in its amplitude.

In these designed signals, there is phase coupling between $y_c(t)$ and $x(t)$ in the time interval $t_c$, following the rule $f_\Sigma = m_1 f_1 + m_2 f_2$, serving as the ground truth in this “white” box problem for testing the M-PLV for integer ($n = 1$) multi-frequency phase coupling with zero delay ($\tau = 0$).

In order to check for the phase coupling between $x(t)$ and $y_c(t)$, M-PLV is calculated based on Eq. (5), and the set of input frequencies includes $f_1$ and $f_2$.

B. Coupled Rössler oscillators

In this case, $y(t)$ is white Gaussian signal, while $x_i(t)$ are obtained from a system comprised of coupled Rössler oscillators, which consists of $N - 1$ independent oscillators coupled to the $N^{th}$ oscillator. The system is characterized by the following equations:

$$\dot{x}_i = -\left(\sum_{j=1}^{N-1} \frac{m_j \omega_j}{n}\right) x_i - z_i + \varepsilon_i \left(\sum_{j=1}^{N-1} \frac{m_j x_j}{n} - x_i\right)$$

$$\dot{z}_i = c + z_i (x_i - b)$$

$$\dot{u}_i = \omega x_i + au_i$$

where $\varepsilon_i = 0$ for $i < N$ and $\omega_j = 2\pi f_j$. These coupled oscillators are designed to mimic a multi-input-single-output (MISO) system. In this case, Eq. (7) can be generalized to include a larger number of signals coupled at different frequencies, so that $n f_\Sigma = \sum_{i=1}^{N} m_i f_i$ and the coupled signal can be obtained as follows:

$$y_c(t) = y(t) - y(n f_\Sigma, t_c) + \sum_{i=1}^{N} \frac{x[|m_i|](f_i, t_c)}{A_x[|m_i|](f_i, t_c)} A_y(f_i, t_c)$$

where $x_i(f_j, t_c)$ is obtained after $x(t_c)$ is passed through a Butterworth band-pass filter centered at frequency $f_j$ (bandwidth: 2 Hz, 6th order). In order to introduce a delay $\tau$ in the system, $t_c$ can be replaced by $t_c - \tau$ in the above equation. The coupling is evaluated between $x_N(t)$ and $y_c(t)$ by calculating the M-PLV according to Eq. (3).

The 95% significance threshold and delay $\tau$ can be estimated through the procedure described in Section II.B.

IV. RESULTS AND DISCUSSION

A. Coupled white Gaussian signals: integer ($n = 1$) multi-frequency phase coupling with zero delay ($\tau = 0$)

The results are shown for $f_1 = 29$ Hz, $f_2 = 13$ Hz, $m_1 = 2$, and $m_2 = -1$, so that $f_\Sigma = 2 \times 29 - 1 \times 13 = 45$ Hz. Fig. 4 shows M-PLV plotted as a function of time and frequency for varying numbers of epoches $K$ ($K = 500, 750, 900$). M-PLV is calculated for all possible combinations of the frequencies $f_1 = 29$ and $f_2 = 13$ Hz to examine whether the significant M-PLV is only detected on the target frequency 45 Hz rather than other frequencies. It is observed that M-PLV shows significant values for $f_\Sigma = 45\text{Hz}$ in the time window $t'_c \sim t_c = [2.501, 7.5]$, i.e., the interval $t'_c = [2.492, 7.511]$ s, [2.421, 7.461] s, and
for \( f = 500, 750, \) and \( 900, \) respectively. The error of time window estimation can be defined as the difference between \( t_c' \) and \( t_c \), and divided by the window size. The errors are below \( 5\% \) for all tested \( K \) values. To further demonstrate the performance of M-PLV, Fig. 2 shows a few of example plots of M-PLV for \( K = 600 \) for some possible combination frequencies of \( f_1 = 29 \) and \( f_2 = 13 \text{ Hz} \). Significant M-PLV is only detected at the targeted frequency \( f_2 = 45 \text{ Hz} \) within the coupled time window.

## B. Coupled Rössler oscillators: multi-frequency phase coupling with a delay

In these simulations, we set \( K = 400 \), \( N = 3 \), and the parameters of the coupled Rössler oscillators (Eq. 10) as \( a = 0.15 \), \( c = 0.2 \), \( b = 10 \), and \( \varepsilon_N = 0.1 \).

To demonstrate the performance of the method for integer \((n = 1)\) multi-frequency phase coupling with zero delay \((\tau = 0)\) in a MISO system, the oscillators are simulated for 80 seconds and two sets of 30,000 samples are obtained from the simulated signals, with \( t = [10001, 40] \) s, \( t_c = [17501, 325] \) s for the first set and \( t = t + 40 \) s, \( t_c = t_c + 40 \) s = \([57501, 725] \) s for the second set. In this case, \( f_1 = 3 \text{ Hz} \), \( f_2 = 5 \text{ Hz} \), \( m_1 = -1 \), \( m_2 = 2 \), so that \( f_3 = -1 \times 3 + 2 \times 5 = 7 \text{ Hz} \). M-PLV is calculated for possible combinations of the frequencies \( f_1 = 3 \text{ Hz} \), \( f_2 = 5 \text{ Hz} \) to examine whether the significant M-PLV is only detected on the target frequency 7 Hz rather than others (e.g. \( 2 \times 3 - 5 = 1 \), \( 2 \times 3 + 5 = 11 \), etc.). Fig. 3 and Fig. 4 show M-PLV for the first and second time set, respectively. The coupling is detected in the time window \( t_c' = [17383, 32286] \) s (error: 2.2\%) for the first set and \( t_c' = [57484, 72279] \) s (error: 1.6\%) for the second set.

To demonstrate the performance of the method for non-integer multi-frequency phase coupling, the procedure is repeated for another case where \( f_1 = 7 \text{ Hz} \), \( f_2 = 13 \text{ Hz} \), \( m_1 = 1 \), \( m_2 = 1 \), and \( n = 5 \) so that \( f_3 = \frac{1 \times 7 + 1 \times 13}{5} = 4 \text{ Hz} \). Also, \( t = [10001, 40] \) s and \( t_c = [17501, 325] \) s. Fig. 5 shows the results obtained for \( f_2 = 4 \text{ Hz} \). Using the 95\% significance threshold, \( t_c' = [17295, 32444] \) s (error: 1.7\%).

To demonstrate the performance of the method for delay estimation, the synthetic signal is generated after \( \tau \) is set as 1 s. In this case, \( t = [10001, 40] \) s, \( t_c = [17501, 325] \) s, \( f_1 = 29 \text{ Hz} \), \( f_2 = 13 \text{ Hz} \), \( m_1 = 2 \), and \( m_2 = -1 \), so that \( f_3 = 45 \). Fig. 6 shows the average M-PLV obtained for varying \( \tau \). The estimated local maxima over 10 such simulations is \( \tau = 0.994 \pm 0.0568 \) s, with an average error less than 5\%.

## V. CONCLUSION

In this paper, a new method for quantifying multi-frequency phase coupling has been proposed. This method addresses the limitation of existing approaches that only allow the detection of coupling between two resonant frequencies (i.e. \( n : m \text{ PLV} \)) or quadratic coupling between three frequencies (i.e. \( b\text{PLV} \)). The M-PLV allows us to quantify various types of phase coupling, including both integer and non-integer phase coupling across multiple frequencies, so as to permit the exploration of more complicated, even unreported phase coupling phenomena in the real world. Simulation studies have been performed on synthetic coupled signals generated using white Gaussian signals, and a complex system comprised of multiple coupled Rössler oscillators. Our results suggest that the proposed method can achieve a reliable estimate of the frequency combination as well as the time window during which phase coupling is present. Furthermore, this method can be used for a precise estimation of the delay between the input and the output when delayed phase coupling is present between the oscillators.

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FIG. 1: M-PLV as a function of time and frequency for $K = (a) 500$, (b) 750 and (c) 900.

FIG. 2: M-PLV for $K = 600$ as a function of time (unit: ms) for the set of frequencies (a) 3, (b) 39, (c) 45, (d) 55, (e) 71, and (f) 87 Hz.

FIG. 3: M-PLV for the first set of values of the coupled Rössler oscillators, as a function of time, for the set of frequencies (a) 1, (b) 7, (c) 9, (d) 11, (e) 13, and (f) 15 Hz.


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FIG. 6: Average M-PLV as a function of delay $\tau$. The local maxima occurs at $\hat{\tau} = 1.02$ s in this case.


