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Advances in Computational High-Resolution Mechanical Spectroscopy HRMS. Part II - Resonant Frequency – Young's Modulus

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Abstract. In this paper, we compare the values of the resonant frequency f_0 of free decaying oscillations computed according to the parametric OMI method (*Optimization in Multiple Intervals*) and nonparametric DFT-based (discrete Fourier transform) methods as a function of the sampling frequency. The analysis is carried out for free decaying signals embedded in an experimental noise recorded for metallic samples in a low-frequency resonant mechanical spectrometer. The Yoshida method (Y), the Agrež method (A), and new interpolated discrete Fourier transform (IpDFT) methods, that is, the Yoshida-Magalas (YM) and (YM_C) methods developed by the authors are carefully compared for the resonant frequency $f_0 = 1.12345$ Hz and the logarithmic decrement, $\delta = 0.0005$. Precise estimation of the resonant frequency (Youngs' modulus ~ f_0^2) for real experimental conditions, i.e., for exponentially damped harmonic signals embedded in an experimental noise, is a complex task. In this work, various computing methods are analyzed as a function of the sampling frequency used to digitize free decaying oscillations. The importance of computing techniques to obtain reliable and precise values of the resonant frequency (i.e. Young's modulus) in materials science is emphasized.

1. Introduction

High-resolution mechanical spectroscopy HRMS [1, 2, 12] provides excellent estimation of Young's modulus E, which is proportional to the square of the resonant frequency of harmonically oscillating sample, $E \sim f_0^2$ [3-6]. This paper focuses on the performance and the accuracy of discrete Fourier transform-based (DFT-based) methods [19-22] to obtain the resonant frequency f_0 from exponentially damped harmonic oscillations (i.e., free decaying oscillations) recorded in a low-frequency mechanical spectrometer [7]. The parametric OMI method (*Optimization in Multiple Intervals*) [8-12] and interpolated discrete Fourier transform (IpDFT) techniques [1, 2, 12-16] are used to analyze exponentially damped harmonic oscillations characterized by the following parameters: the length of the free decaying signal L, the sampling frequency f_s , the signal-to-noise ratio S/N, phase, the resonant frequency f_0 , and the damping level (i.e. the logarithmic decrement, δ). The discrete Hilbert transform-based methods are not discussed in this work [6, 17, 19].

The OMI method [8] and IpDFT methods [12-15] compute jointly the logarithmic decrement and the resonant frequency. Therefore the problem of the computations of the δ and the f_0 cannot be

discussed separately. That is why, the results concerning the δ and the f_0 are reported in this volume in two Parts.

The effect of the Zero-Point Drift (ZPD) [11, 12, 17, 18] on computations of the resonant frequency is not discussed in this work. The OMI method and the IpDFT methods are not affected by the presence of constant offsets, unlike the classical algorithms reported in the literature [3, 4, 8]. A new road to high-resolution mechanical spectroscopy takes into consideration the presence of the ZPD for all damping levels and different lengths of the signal [7, 12, 18]; these results will be reported elsewhere.

2. Resonant Frequency

The exponentially damped time-invariant harmonic oscillations embedded in an experimental noise $\mathcal{E}_w(t)$ can be described using the digitized data $A_i(t)$ and t_i from free decaying signal A(t) [1, 2]:

$$A(t) = A_0 e^{-\delta f_0 t} \cos(2\pi f_0 t + \varphi) + \mathcal{E}_w(t) + dc , \qquad (1)$$

where A_0 is the maximal strain amplitude of a sample mounted in a mechanical spectrometer, t is a continuous time in seconds, $-\pi < \varphi \le \pi$ is the phase of the signal A(t) in radians, f_0 is the resonant frequency, and dc is an offset. The noise $\mathcal{E}_w(t)$ corresponds here to the signal-to-noise ratio S/N= 32 dB [1, 2, 8, 10, 12].

It can be shown that the resonant frequency f_0 can be directly computed from the DFT spectra:

$$f_0 = \frac{Re\left(s_1 - \frac{3}{R-1}\right)}{L}.$$
(2)

The *R* parameter is defined by Yoshida [13]:

$$R = \frac{F(s_1) - 2F(s_2) + F(s_3)}{F(s_2) - 2F(s_3) + F(s_4)},$$
(3)

where $F(s_1), F(s_2), F(s_3), F(s_4)$ state for the magnitude of DFT bins [1, 2, 12, 13, 15].

The Yoshida-Magalas methods (YM) and (YM_C) [1, 2, 12] and the original Yoshida method (Y) [13] use four DFT bins ($F(s_1), F(s_2), F(s_3), F(s_4)$) and a rectangular window [19, 22]. The YM method uses four optimal values of the DFT bins whereas the YM_C differs from the YM method by using a complete number of oscillations. The Yoshida method is described in [13]. The Agrež method (A) uses three DFT bins [14] and the Hann window [20, 22]. The wavelet transform gives too poor frequency resolution [16, 23-26], and is not discussed in this work.

3. Results and Discussion

The results of computing the resonant frequency f_0 according to Eqs. (2, 3) by the YM, the YM_C [1, 2, 12], and the Y methods [13] are carefully compared here with the results obtained according to the A method [14] and the parametric OMI method [8-12]. The results shown in Figs. 1 - 4 confirm that the OMI method can be considered as the 'gold standard' [1, 2, 7-12, 15].

Figure 1 shows dispersion of computed f_0 values obtained for 100 free decaying oscillations embedded in an experimental noise as a function of the length of signals, L, (in seconds and/or as a function of the number of oscillations L_{osc}) [1, 2, 10-12] for the sampling frequency $f_s = 1$ kHz. The dispersion of computed f_0 values obtained for the sampling frequency $f_s = 6$ kHz is illustrated in Fig. 3. The results obtained for 100 different free decaying oscillations ($\delta = 5 \times 10^{-4}$, $f_0 = 1.12345$ Hz, S/N = 32 dB) computed according to the following methods: OMI, YM, YM_c, A, and Y are vertically plotted in Figs. 1, 2 and Figs. 3, 4 for $f_s = 1$ kHz and $f_s = 6$ kHz, respectively.

The OMI unequivocally outperforms IpDFT methods for all lengths of free decaying signals. The Yoshida method [13] usually generates the highest dispersion in f_0 points (see Figs. 1-4.) It is noteworthy that the dispersion in f_0 values increases with decrease in the length of free decaying signals. This observation is valid for all IpDFT methods and all damping levels. The Yoshida-Magalas YM method returns the smallest dispersion in experimental points among all tested IpDFT methods. The point we should like to emphasize is that computed f_0 values are biased for signals that are too short (Figs. 1(a), 2(c), 3(a), 4(a), 4(c).)

Figures 2 and 4 show variation of the minimal $\gamma_{f_o \min}$ and the maximal $\gamma_{f_o \max}$ relative errors of the resonant frequency f_0 for two sampling frequencies: $f_s = 1$ kHz and $f_s = 6$ kHz, respectively. The computed values of the f_0 are confined within two lines: $\gamma_{f_o \min}$ and $\gamma_{f_o \max}$ corresponding to the specific method. The method which returns the best f_0 values returns simultaneously the best results for the logarithmic decrement (see Part I in this volume.)

An increase in the sampling frequency f_s from 1 kHz to 4 kHz reduces relative errors by 5-15 %. Further increase in the sampling frequency returns slightly better results only.

It is concluded that the performance of tested methods is as follows: (1) OMI – it is worthwhile to reiterate the fact that the OMI is considered as the 'gold standard', (2) the Yoshida-Magalas YM, (3) the Yoshida-Magalas YM_C, (4) the Agrež A, and (5) the Yoshida Y. The results shown in Figs. 1-4 suggest that for short and very short signals only the OMI and the YM_C can be recommended. The Agrež method, A, provides good estimation of the resonant frequency for low damping level only. For medium and higher damping levels it returns low quality unacceptable results. That is why the A method can only be used in the computations of the f_0 for relatively narrow span of low damping level. It is important to emphasize that in all investigated cases the Yoshida-Magalas YM method is slightly better as compared to the Agrež method. The potential use of the Agrež method [14] in mechanical spectroscopy and other spectroscopic techniques will be limited since it yields wrong results for the logarithmic decrement, δ .

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Figure 1. The effect of the sampling frequency $f_s = 1$ kHz on dispersion of 100 values of the resonant frequency f_0 computed according to OMI, YM, YM_c, A, and Y methods as a function of the length of free decaying signals (i.e. the number of oscillations L_{osc}.) (a) L_{osc} = 5, 10, 15, (b) L_{osc} = 20, 25, 30, (c) L_{osc} = 40, 50, 60, 70, (d) L_{osc} = 80, 90, and 100.

Computed values of the f_0 , displayed on vertical plots, correspond to a set of 100 different free decaying noisy oscillations (S/N = 32 dB) characterized by the same value of the δ = 0.0005 and the resonant frequency f_0 = 1.12345 Hz.

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Figure 2. The effect of the sampling frequency $f_s = 1$ kHz on the minimal $\gamma_{f_{0 \text{ min}}}$ and the maximal $\gamma_{f_0 \text{ max}}$ relative errors obtained for computations of the resonant frequency f_0 shown in Fig. 1. (a), (c) $L_{osc} = 5, 10, 15$; (b), (d) $L_{osc} = 20, 25, 30, 40, 50, 60, 70, 80, 90$, and 100.

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Figure 3. The effect of the sampling frequency $f_s = 6$ kHz on dispersion of 100 values of the resonant frequency f_0 computed according to OMI, YM, YM_c, A, and Y methods as a function of the length of free decaying signals (i.e. the number of oscillations L_{osc}.) (a) L_{osc} = 5, 10, 15, (b) L_{osc} = 20, 25, 30, (c) L_{osc} = 40, 50, 60, 70, (d) L_{osc} = 80, 90, and 100.

Computed values of the f_0 , displayed on vertical plots, correspond to a set of 100 different free decaying noisy oscillations (S/N = 32 dB) characterized by the same value of the δ = 0.0005 and the resonant frequency f_0 = 1.12345 Hz.

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Figure 4. The effect of the sampling frequency $f_s = 6$ kHz on the minimal $\gamma_{f_{0 \text{ min}}}$ and the maximal $\gamma_{f_0 \text{ max}}$ relative errors obtained for computations of the resonant frequency f_0 shown in Fig. 3. (a), (c) $L_{osc} = 5, 10, 15$; (b), (d) $L_{osc} = 20, 25, 30, 40, 50, 60, 70, 80, 90$, and 100.

4. Conclusions

The results are primarily reported here to highlight new methods to compute the resonant frequency, f_0 , and the logarithmic decrement, δ , in resonant high-resolution mechanical spectroscopy, HRMS.

The performance of different methods and algorithms to compute the resonant frequency for low damping level (e.g. $\delta = 5 \times 10^{-4}$) is listed in the following order: (1) the OMI, (2) the Yoshida-Magalas YM, (3) the Yoshida-Magalas YM_C, (4) the Agrež A, and finally (5) the Yoshida Y. The Yoshida-Magalas YM method [1, 2] outperforms other IpDFT methods. The YM method yields the smallest dispersion in experimental points of the resonant frequency for different lengths of free decaying oscillations and different sampling frequencies. The effect of the sampling frequency on precision in the computations of the resonant frequency and the logarithmic decrement has received scant attention to date [8] and deserves more.

The parametric OMI method is considered as the 'gold standard' in low-frequency high-resolution mechanical spectroscopy, HRMS. The point we should like to emphasize is that the sampling frequency is a key factor to reduce dispersion of experimental points computed according to the OMI and IpDFT methods. It is demonstrated that the sampling frequency $f_s = 6$ kHz readily yields better results as compared to usually used $f_s = 1$ kHz in low-frequency mechanical spectrometers operating around the resonant frequency $f_0 \approx 1$ Hz.

To conclude, the OMI method (*Optimization in Multiple Intervals*) and the Yoshida-Magalas YM method are recommended to compute the resonant frequency from the exponentially damped time-invariant harmonic oscillations embedded in an experimental noise. It is not difficult to show, by means of the experimental results reported in [1, 2] and the results described in this volume that the OMI and the YM methods pave the way toward high-resolution mechanical spectroscopy, HRMS.

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