`PFMCal`: Photonic force microscopy calibration extended for its application in high-frequency micro-rheology

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Abstract

The present document is an update of the previously published MatLab code for the calibration of optical tweezers in the high-resolution detection of the Brownian motion of non-spherical probes [1]. In this instance, an alternative version of the original code, based on the same physical theory [2], is outlined, but this is focused on the automation of the calibration of measurements using spherical probes. The new added code is quite useful for high-frequency micro-rheology studies, where the probe radius is known but the viscosity of the surrounding fluid maybe not. This extended calibration methodology is almost automatic, without the need of a user's interface. A code for calibration by means of thermal noise analysis [3] is also included; this is a method that can be applied when using viscoelastic fluids if the spring constant of the trap is previously estimated [4]. The new code can be executed in MatLab and using GNU Octave.

Keywords: Calibration of optical tweezers, Brownian motion, Power spectral density (PSD), Mean square displacement (MSD), Velocity autocorrelation function (VAF)

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NEW VERSION PROGRAM SUMMARY

Program Title: PFMCal

Licensing provisions: GPLv3

Programming language: MatLab 2016a (MathWorks Inc.) and GNU Octave 4.0

Operating system: Linux and Windows.

Supplementary material: A new document `README.pdf` *includes basic running instructions for the new code.*

Journal reference of previous version: Computer Physics Communications, 196 (2015) 599

Does the new version supersede the previous version?: No. It adds alternative but compatible code while providing similar calibration factors.

Nature of problem (approx. 50-250 words): The original code uses a MatLab-provided user's interface, which is not available in GNU Octave, and cannot be used outside of a proprietary software as MatLab. Besides, the process of calibration when using spherical probes needs of an automatic method when calibrating long amounts of different data focused to micro-rheology.

Solution method (approx. 50-250 words): The new code can be executed in the latest version of MatLab and using GNU Octave, a free and open-source alternative to MatLab. This code generates an almost automatic calibration process with small interaction of the user. Additionally, we include a calibration method based on thermal noise statistics, which can be used with viscoelastic fluids if the trap stiffness is previously estimated.

Reasons for the new version: This version extends the functionality of `PFMCal` *for the particular case of spherical probes and unknown fluid viscosities.*

Summary of revisions: The original MatLab program in the previous version, which is executed by `PFMCal.m`*, is not changed. Here, we have added two additional main archives named* `PFMCal_auto.m` *and* `PFMCal_histo.m`*, which implement automatic calculations of the calibration process and calibration through*

Fluid	η	k	β_{MSD}	β_{VAF}	β_{PSD}	β_{σ^2}	β_E
Water	0.94	6.3	12.3	11.3	13.1	11.8 ± 0.2	12.1 ± 0.2
`PFMCal`	[0.99]	[illegible].5	$\beta = 11.8$				
Acetone	0.33	6.1	10.0	9.8	9.7	9.06 ± 0.12	9.24 ± 0.11
`PFMCal`	[0.32]	5.9	$\beta = 9.9$				

Table 1: Comparison between calibration factors and trap stiffnesses, β (μm/V) and k (μN/m), for interferometry-based optical tweezers, calculated for spherical probes with radius $a = 0.94$ μm in water or acetone at 21°C by using the automatic methods here exposed and by means of the GUI-based original code `PFMCal`. Values between square brackets are fixed inputs. The extended calibration methodology provides the expected zero-shear viscosities η (mPa.s) values. Obtained values for β and k using all methods available are compatible between them.

Boltzmann statistics, respectively. The process of calibration using this code for spherical beads is described in the ***README.pdf*** *file provided in the new code submission. Here, we obtain different calibration factors, β (given in μm/V), according to [2], related to two statistical quantities: the mean-squared displacement (MSD), β_{MSD}, and the velocity autocorrelation function (VAF), β_{VAF}. Using that methodology, the trap stiffness, k, and the zero-shear viscosity of the fluid, η, can be calculated if the value of the particle's radius, a, is previously known. For comparison, we include here also the ~~classic~~ method of calibration using the corner frequency of the power-spectral density (PSD) [5], providing a calibration factor β_{PSD}.*

Besides, ~~if we are able to obtain an estimation of k,~~ along with the known value of the particle's radius, we can use thermal noise statistics to obtain calibration factors according to the quadratic form of the optical potential. We define two β factors, one ~~related to the quadratic form of the~~ potential, β_E, whereas the other is ~~related to~~ the Gaussian distribution of the bead's position~~s~~, β_{σ^2}. This method has been ~~observed~~ to be applicable to the calibration of optical tweezers when using non-Newtonian viscoelastic polymeric liquids [4].

An example of the results using this calibration process is summarized in Table 1. Using the data provided in the new code submission, for water and acetone fluids, we calculate all the calibration factors by using the original ***PFMCal.m*** *and by the new non-GUI code* ***PFMCal_auto.m*** *and* ***PFMCal_histo.m****. Regarding the new code,* ***PFMCal_auto.m*** *returns η, k, β_{MSD}, β_{VAF} and β_{PSD}, while* ***PFMCal_histo.m*** *provides β_{σ^2} and β_E. Table 1 shows how we obtain the expected viscosity of the two fluids at this temperature and how the different methods provide good agreement between trap stiffnesses and calibration factors.*

Additional comments including Restrictions and Unusual features (approx. 50-250 words): The original code, `PFMCal.m`*, runs under MatLab using the Statistics Toolbox. The extended code,* `PFMCal_auto.m` *and* `PFMCal_histo.m`*, can be executed without modification using MatLab or GNU Octave. The code has been tested in Linux and Windows operating systems.*

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