# FORMA: Force Reconstruction via Maximum-likelihood-estimator Analysis

**Laura Pérez García[1,2], Jaime Donlucas Pérez[1], Giorgio Volpe[3], Alejandro V. Arzola[1], and Giovanni Volpe[2]**

*[1]Instituto de Física, Universidad Nacional Autónoma de México Apdo. Postal 20-364. Cd. México, México.*
*[2] Department of Physics, University of Gothenburg, 41296 Gothenburg, Sweeden.*
*[3]Department of Chemistry, University College London, 20 Gordon Street, London WC1H OAJ, United Kingdom.*

*Author e-mail address: laup@ciencias.unam.mx*

**Abstract:** We propose an algorithm to retrieve the conservative and non-conservative components of a force field acting on a Brownian particle from the analysis of its displacements with important advantages over established techniques.

## 1. The Challenges of Microscopic Force Characterization

Microscopic force characterization is often done by using a microscopic colloidal particle which probes local forces. These particles are often held by a harmonic trapping potential with stiffness $k$ so that a homogeneous force acting on the particle results in a displacement $\Delta x$ from the equilibrium position and the force can, therefore, be measured as $k\Delta x$. To perform such measurement, it is necessary to determine the value of $k$, which is often done by measuring the Brownian fluctuations of the particle around its stable equilibrium position. This is achieved by measuring the particle position as a function of time, $x(t)$, and then using some calibrations algorithms; the most commonly employed techniques are the potential analysis that relies on the fact that the force is derived from a potential; and the power spectral density (PSD) and the auto-correlation function (ACF) methods that require a regular sampling in time. Besides the previous requirements, all methods depend on the choice of some analysis parameters [1]. This has inhibited the applicability of force measurement methods to characterize force fields with non-conservative components or where the particle freely explores an extended potential landscape.

We propose a method for Force Reconstruction via Maximum-likelihood-estimator Analysis (FORMA) that exploits the fact that in the proximity of an equilibrium position the force field can be approximated by a linear form and, therefore, optimally estimated using a linear Maximum-likelihood-estimator (MLE).

## 2. Exploiting Linearity

Using the overdamped Langevin equation and the Taylor series expansion around 0 of the force field, we can obtain the average viscous friction in the $n$-th interval around an equilibrium point:

$$\boldsymbol{f}_n = \gamma \frac{\Delta \boldsymbol{r}_n}{\Delta t_n} = \boldsymbol{J}_0 \boldsymbol{r}_n + \sqrt{\frac{2D\gamma^2}{\Delta t_n}}\,\omega_n. \qquad (1)$$

where $\mathbf{J_0}=\mathbf{J}(\mathbf{0})$ is the Jacobian at $\mathbf{0}$, $\boldsymbol{\omega}_n$ is an array of independent random numbers with zero mean and variance $\Delta t_{-1}$ . Equation (1) is a linear regression model, and can be solved for $\mathbf{J_0}$ using a linear Maximum-likelihood-estimator (MLE):

$$\boldsymbol{J}_0^* = [\boldsymbol{r}^T \boldsymbol{r}]^{-1} \boldsymbol{r}^T \boldsymbol{f}\,, \qquad (2)$$

where $\boldsymbol{r} = (\boldsymbol{r}_n)$ and $\boldsymbol{f} = (\boldsymbol{f}_n)$ are matrices with $N\times2$ elements. Extracting the conservative and non-conservative components from the Jacobian $\boldsymbol{J}_0$, we can obtain the angle of the principal axes $\theta$; the stiffness of the force field along the principal axes $k_1$ and $k_2$ ; and the angular velocity due to the angular momentum of the trap $\Omega$ . It is important to notice that FORMA is parameter-free, does not impose a conservative nature to the force field and the particle position sampling does not require to be regular in time. FORMA's performance was compared with the other methods available, calibrating a single beam optical tweezer. FORMA showed to produce less error, compute in less time and converge with fewer data to the expected values.

## 3. Characterization of Generic Force Fields in 2D

We have used FORMA to characterize the force fields of focused Laguerre Gaussian beams with different polarization states. We obtained equations that suggest that the orbital angular momentum and spin angular momentum contribute equally to the rotation of the particle [2].

Also, we tested FORMA with more complex force fields, the first example is a double well potential generated with a spatial light modulator which separates the beam into two components. It is interesting to observe that with FORMA we obtain 5 equilibrium points rather than the three that are expected, this has been previously reported in the literature [3]. Also, we managed to characterize the non-stable equilibrium points, which is not possible with PSF and ACF.

Finally, we used FORMA for the characterization of the force fields generated by a speckle pattern which impinges on a colloidal particle. This is the first time that non-conservative force components due to the presence of optical vortices have been characterized in speckle fields [4].

## 4. References


[1] Jones, P. H., Maragò, O. M. & Volpe, G. Optical tweezers: Principles and applications (Cambridge University Press, Cambridge, 2015).

2] Simpson, N. B., Dholakia, K., Allen, L. & Padgett, M. J. Mechanical equivalence of spin and orbital angular momentum of light: An optical spanner. Opt. Lett. 22, 52 (1997).

[3] Stilgoe, A. B., Heckenberg, N. R., Nieminen, T. A. & Rubinsztein-Dunlop, H. Phase-transition-like properties of double-beam optical tweezers. Phys. Rev. Lett. 107, 248101 (2011).

[4] Goodman, J. W. Speckle phenomena in optics: Theory and applications (Roberts and Company Publishers, 2007).

[5] García, Laura Pérez, et al. "High-performance reconstruction of microscopic force fields from Brownian trajectories." *arXiv preprint arXiv:1808.05468.* (2018).

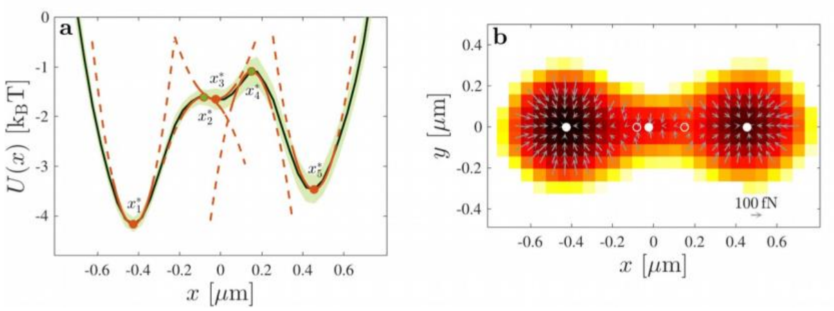


Fig 1. Reconstruction of stable and unstable equilibrium points in a multiwell optical potential. (a) Multiwell optical potential generated by two focused Gaussian beams slightly displaced along the *x*-direction. FORMA identifies three stable ($x_1$, $x_3$, $x_5$; full circles) and two unstable ($x_2$, $x_4$; empty circles) equilibrium points, and measures their stiffness (orange solid and dashed lines). The corresponding *x*-potential obtained from the potential method is shown by the green solid line (the green shaded area represents the standard deviation). (b) 2D plot of the force field measured with FORMA (arrows) and of the potential measured with the potential analysis (background color). Figure adapted from [5].

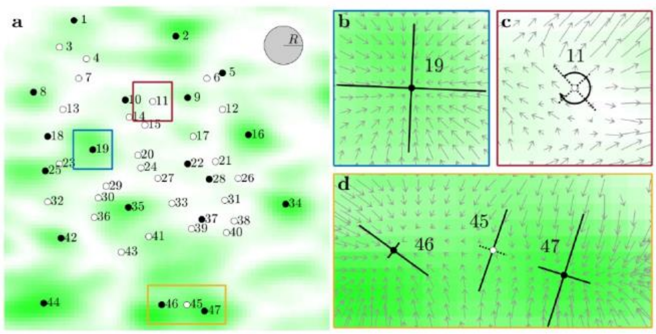


Fig 2. Reconstruction of the equilibrium points in a speckle pattern. (a) The intensity of the speckle (green background) is approximately proportional to the potential depth of the optical potential felt by a particle whose size (particle diameter 1.00 ±0.04 µm) is similar to the specklem) is similar to the speckle characteristic size (2.8 µm) is similar to the specklem). FORMA identifies several stable (full circles) and unstable (empty circles) equilibrium points and measures the orientation of the principal axes (θ), the stiffnesses along them (k), the stiffnesses along them ($k_1$ and $k_2$), and angular frequency (Ω). (b-d) Examples of reconstructed force). (b-d) Examples of reconstructed force fields around (b) a stable point, (c) an unstable point with a significant rotational component (indicated by the arrow), and (d) two stable points with a saddle in between; the grey arrows plot the 2D force field measured with FORMA and are scaled by a different factor in each plot. Figure adapted from [5].