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Theory and practice of simulation of optical tweezers

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ABSTRACT

Computational modelling has made many useful contributions to the field of optical tweezers. One aspect in which it can be applied is the simulation of the dynamics of particles in optical tweezers. This can be useful for systems with many degrees of freedom, and for the simulation of experiments. While modelling of the optical force is a prerequisite for simulation of the motion of particles in optical traps, non-optical forces must also be included; the most important are usually Brownian motion and viscous drag. We discuss some applications and examples of such simulations. We review the theory and practical principles of simulation of optical tweezers, including the choice of method of calculation of optical force, numerical solution of the equations of motion of the particle, and finish with a discussion of a range of open problems.

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1. Introduction

The optical forces in optical tweezers result from the interaction of the trapping beam with the trapped particle. Thus, the computation of optical forces and torques is a light scattering problem. While this is a challenging problem, and much work remains to be done, there has been a great deal of progress, and for many situations, it is straightforward to obtain the optical force and torque. However, if we wish to simulate the behaviour of particles within optical tweezers, the optical force is only one of the necessary ingredients. We will discuss some applications and

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examples of such simulations, and review the theory and principles of simulation of optical tweezers.

1.1. The need for simulations

Since it is usually straightforward to calculate the optical force on a trapped particle, it is possible to characterise the trap by determining the optical force as a function of particle position (and orientation if the particle is non-spherical). At first glance, this appears to provide complete information about the trap, and we might ask what need there is to perform simulations. There are two main answers to this question. First, it is not always feasible to generate such a force map of the trap. Second, while a force map of this type does contain complete information about the trap in some sense, it doesn't directly answer all questions we might have about the trap. In particular, the dynamics of a particle in the trap depend on its interaction with the surrounding environment as well as the optical force. The dominant elements of that interaction are often Brownian motion and viscous drag, but other types of interaction can also be important. Where the dynamics themselves are the object of study (e.g., escape probabilities, synchronised dynamics of trapped particles, etc.) or have a major impact on the behaviour of interest (e.g., in the simulation of measurements to test calibration procedures), it is necessary to take these non-optical forces into account.

The first of these cases results from situations with many degrees of freedom. To map the force as a function of position with useful (but not high) resolution typically requires about 30 steps along each degree of freedom (giving about 10 steps as forces change from zero to a maximum value). If it takes 1 second to calculate the optical force at a single position, this will give required computational times for different degrees of freedom (DOF) of:

- 1 DOF Example: calculating axial and/or radial force–position curves; finding equilibrium position along beam axis, and axial and radial spring constants. 30 to 60 points. Time: 0.5–1 minute.
- 2 DOF Example: mapping force for a spherical particle in a rotationally symmetric trap (e.g., circularly polarised Gaussian beam). $30^2 \approx 1000$ points. Time: ≈ 15 minutes.
- 3 DOF Example: mapping force for a spherical particle in a trap lacking rotational symmetry (e.g., linearly polarised Gaussian beam). $30^3 \approx 30,000$ points. Time: ≈ 8 hours.
- 4 DOF Example: mapping force for a rotationally symmetric non-spherical particle in a rotationally symmetric trap. $30^4 \approx 10^6$ points. Time: ≈ 10 days.
- 5 DOF Example: mapping force for a rotationally symmetric non-spherical particle in a trap lacking rotational symmetry; two spherical particles in a rotationally symmetry trap. $30^5 \approx 3 \times 10^7$ points. Time: ≈ 1 year.
- 6 DOF Example: mapping force for a non-spherical particle lacking rotational symmetry in a trap lacking rotational symmetry; two spherical particles in a trap lacking rotational symmetry. $30^6 \approx 10^9$ points. Time: ≈ 30 years.

Additional particles will add 2–3 translational degrees of freedom (depending on the symmetry of the trap) and 0, 2, or 3 rotational degrees of freedom (depending on the symmetry of the particle). If the trapping beam varies in time, this adds another degree of freedom, although if the time variation consists of switching between a small number of fixed positions, this will only multiply the number of required calculations and the computational time by a small number.

The above times do not take parallelisation of the calculations into account—this can readily bring one or two more degrees of freedom into feasibility. However, even with parallelisation, we will still rapidly run into the limits of practicality due to the exponential growth of computational time with the number of degrees of freedom. Therefore, it can be necessary to resort to simulation to obtain information we might prefer to find from a complete force map. This will typically involve non-spherical particles or multiple particles.

On the other hand, even if it is feasible to calculate a complete optical force map for the trap, we might still wish to perform simulations. In particular, a force map doesn't contain information about the dynamics of a particle in the trap. While the optical force —which the force map provides—is a key factor in the dynamics of the particle, the particle is also influenced by other forces: viscous drag, thermal forces (driving Brownian motion), and possibly interaction with other parts of the environment. If the dynamics are of interest, we can use simulation to uncover it.

To explore the dynamics of a particle in the trap, it can be possible, and advantageous, to use a pre-calculated force map. If it is feasible to calculate a complete force map with reasonable resolution, the optical force at any position can be found by interpolating between the points in the force map where the forces are known. This interpolation can be performed very quickly (the computational implementation should avoid copying the force map to perform the interpolation). The required accuracy of the interpolated force will determine the minimum resolution of the force map. This resolution of the force map, along with the required spatial extent of the simulation, determines the number of points required in the force map. If this exceed the number of time steps required in the simulation, then direct calculation will be more efficient. However, often the number of time steps will be much greater, and using a force map to find the optical force will be much more efficient. This will often be the case for optical traps with 2 or 3 degrees of freedom. An extreme case of this is where the particle remains very close to its equilibrium position, and the trap can be represented in terms of a spring constant (which will generally be a diagonal tensor, with different spring constants in different directions, or even a non-diagonal tensor).

1.2. Applications of simulations

There are many possible applications of this. Most fall into three broad categories: simulations to understand experiments that have been performed, simulations to predict the results of potential experiments, and simulations to explore optical traps and the dynamics of trapped particles in ways that are not accessible experimentally.

The first of these, simulations of experiments that have been performed, can be simply seeing if a simulated experiment matches measured results. This can be very useful if the experimental results are surprising. If agreement between simulated and measured results is obtained, the physics and models used in the simulation adequately model reality. If agreement is not obtained, then the model is either incomplete (e.g., physics not included significantly affect the measured results) or elements of the model are incorrect (invalid approximations, mathematical errors, incorrect implementation in software, numerical errors).

For example, [79] observed the appearance of a third trapping equilibrium position as two optical traps were moved close together. In this case, simulations were valuable for confirming that the third trap can be produced in this two-beam configuration, even if the two trapping beams are not mutually coherent, i.e., the third trap doesn't depend on interference between the two trapping beams.

[33] used a combination of experiment and simulation to explore the transition from overdamped motion to underdamped motion as the size of trapped particles was reduced.