Shining light on particle dynamics with machine learning

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Dynamics simulations can provide insight into the mechanisms responsible for observed experimental phenomenon which cannot be easily predicted from the optical force fields. For example, dynamics simulations can be used to calculate particle escape or transition rates between multiple potential wells as a function of temperature. While optical forces on particles can be calculated relatively easily and accurately using a variety of existing tools, accurate methods are not always fast enough for simulating dynamics. Simulating dynamics requires repeated calculation of the optical forces which can easily take days, months or even years of computational time [1]. The simulation time required for a particle to explore all possible configurations increases exponentially with the number of degrees of freedom. As a result, simulations of particles with many degrees of freedom, such as particles which change shape or optical properties, are almost impossible without simplifying assumptions or approximations.

One approximation method that is used for large simulations is interpolation. Interpolation involves calculating the forces at positions where the particle is most likely to be and interpolating the forces to near-by locations. For more than three degrees of freedom, the amount of memory required by this method quickly becomes excessive. In this talk, we will present an alternative method which scales well up to many degrees of freedom. The method involves training a neural network to calculate the forces on the particle. This technique is similar to a technique used in studies of biodiversity and metrology and can accurately estimates the forces with significantly less memory [2,3].

In this talk we will demonstrate how we have been using machine learning to better understand particle dynamics in optical tweezers, allowing us to study out-of-equilibrium dynamics and optical trapping of particles whose size and refractive index varies as a function of time. We will also briefly describe training of our neural network and how this technique can be easily applied to other fields and the simulation of particle dynamics.

References

[1] Bui, A. A. M., *et al.*, 2017: Theory and practice of simulation of optical tweezers. *J. Quant. Spectrosc. Radiat. Transfer* **195**, 66–75.

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