



Machine learning inverse problems in soft matter systems

Daniel de las Heras

Theoretical Physics II & V, Universität Bayreuth, Germany

Colloids are nano- to micron-sized particles suspended in a solvent and subject to thermal motion. A precise control over the flow and the structural properties of the colloidal particles is a requisite in applications such as cargo delivery with colloidal carriers and lab-on-a-chip processing. External fields are often used to generate structure and to sustain flows in colloidal systems. However, the response of the colloids to external perturbations is often complex due to the many-body internal interactions between the particles.

Here, we use a neural network to learn the exact functional mapping predicted in power functional theory from the density and velocity one-body profiles to the one-body internal force field. Using the network, we can reconstruct the external force field required to generate the desired dynamical evolution of a many-body system. This constitutes the solution of an inverse problem in statistical physics that can help us to improve lab-on-a-chip devices, to study memory effects, and to calculate transport coefficients and relaxation times.

Moreover, we use a local learning approach which allows us to study systems much larger than the initial ones used in the training stage, opening a route to describe macroscopic systems with microscopic resolution.