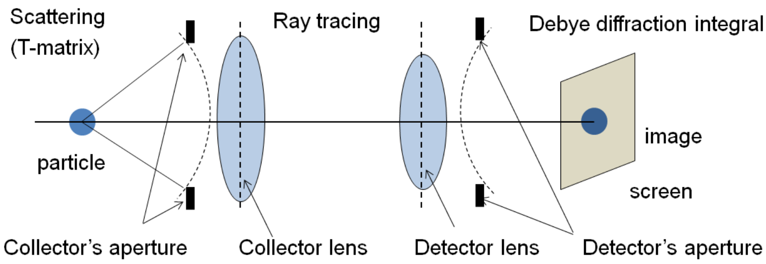

Fig. 1: Optical scheme implemented in the particle visualization module.

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Characterization of single particles from light-scattering profiles using parametric shape models

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Measurement of angle-resolved light-scattering profiles (LSPs) of single particles provides unique capabilities for detailed and accurate characterization of disperse media. A prominent example of instrument for such measurements is a scanning flow cytometer (SFC) [1]. This talk reviews our results of developing characterization methods for various kinds of particles, mostly focusing on parametric inverse light-scattering problems, i.e. when the particle model is specified up to a few free parameters. The first class of particles (homogeneous and concentric spheres) allow for fast solution of the direct problem (using the Mie theory). The characterization is then based on the direct fit (non-linear regression) using a global optimization technique, which also provides standard errors of estimated characteristics. It has been successfully applied to polystyrene beads, milk fat globules, extracellular vesicles, and lymphocytes.

Unfortunately, such approach is not practical for other particle shapes that require slower solution methods (e.g., the discrete dipole approximation). For this class of particles, we developed a method based on the nearest-neighbor interpolation using a database of simulated LSPs [2]. It also provides standard errors of characteristics and can be accelerated using hierarchical clustering of the database. This general approach has been successfully applied to blood platelets, erythrocytes, vesicles aggregates, and E. Coli bacteria. The applications of the developed methods are all based on measurements of LSPs of single particles in water using a SFC. However, the same methodology can be applied to other experimental set-ups.

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Discrete dipole approximation for electromagnetic scattering simulations

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Light scattering is widely used in remote sensing of various objects ranging from metal nano-particles and macromolecules to atmospheric aerosols and interstellar dust. Moreover, the structure of electromagnetic fields near a particle is of major importance for other phenomena, such as surface-enhanced Raman scattering (SERS) or electron energy-loss spectroscopy (EELS). All these applications require accurate simulations of interaction of electromagnetic fields with particles of arbitrary shape and internal structure. The discrete dipole approximation (DDA) is one of the general methods to handle such problems [1].

The DDA is a numerically exact method derived from the volume-integral form of frequency-domain Maxwell's equation for the electric field [2], and is a special case of method of moments. It commonly employs a regular rectangular grid of dipoles, leading to the computational complexity (and required memory) linear in number of dipoles. This allows one to solve the problems with up to 1 billion dipoles using modern supercomputers. Overall, the DDA is widely use for light-scattering and near-field simulations, thanks to the availability of robust and easy-to-used open-source codes, such as DDSCAT and ADDA.

Importantly, the DDA can be applied to a broad range of electromagnetic applications apart from the standard problem of far-field scattering by single isolated particles. This includes complicated environments (e.g., particles on substrate) and unusual incident fields (leading to SERS and EELS). The DDA can even be applied to simulate fluctuation phenomena, i.e. near-field radiative transfer and Casimir forces, which are related to the Green's tensor in the presence of a particle. The only drawback is that the latter applications require much larger computational resources.