Microdroplets of suspensions are ubiquitous – recently, it has become generally obvious in a particularly unpleasant way since many of them carry biologically active material, like viruses. Efficient, quick and possibly non-contact methods of microdroplets characterisation/recognition are eagerly sought after. It is widely accepted that methods using coherent light scattering on microdroplets can provide a versatile tool. Scattering images from microdroplets of suspension consist of so-called speckles. Spatial speckles distribution is characteristic of the microdroplet properties (size, shape, refractive index) and internal structure. Unfortunately, using a scattering method usually requires solving a so-called inverse scattering problem, which is mathematically difficult. In the case of complex evaporating/condensing microdroplets, real-time solving of the inverse problem becomes an exceedingly serious issue. An alternative approach seems, however, possible. The scattering images could be in real-time directly classified with machine learning – artificial neural networks. Such an approach circumvents the issue of real-time solving of the inverse problem, by shifting it to off-line training of the classifying machine – artificial intelligence algorithm. Obviously, the internal droplet structure dynamics must be a priori understood and unambiguously linked to the scattering phenomena.

The ultimate goal of this project is to build an optical-numerical system, using machine learning, for the fast recognising of suspensions in the form of microdroplets, which in future might enable detecting the aerosol microdroplets carrying specific pathogens. The intermediate goal is to identify, with non-contact and contact methods, the possible scenarios of evolution of the suspended nanoparticles (NPs) distribution in a microdroplet and associate them with the scattering images observed in experiments.

The applicability of machine learning for optical recognition of aerosol microparticles has already been studied, as mentioned above, but the number of recognised microparticle classes was limited to just several, which must be considered insufficient for the planned application. In our experiments on NPs suspensions in a thin cuvette, we showed that even more than 100 suspension types can be quickly identified by classifying the scattering images with a so-called convolution neural network. It seems very promising in the prospect of the target tool, and the development of the neural network suitable for the project will capitalise on this experience. However, it must be kept in mind that the distribution of NPs in microdroplets is usually inhomogeneous. Microdroplets observed in a real environment usually evolve – evaporate or condense, which leads to an evolution of NPs distribution, which in turn can result in a non-trivial internal (nano)structure. Furthermore, a microdroplet constitutes an optical microresonator – resonance cavity, which very significantly modifies the distribution of light scattered by suspension in comparison to the sample in bulk (cuvette). Finally, it is known that the development of deep neural networks is in itself an experimental work – trial and error to much extent. Thus, three main issues must be addressed in the course of this project: (i) establishing possible distributions of the NPs in the microdroplet, (ii) associating them unambiguously with the classes of scattering images, (iii) constructing and training the dedicated neural network.

Remote optical characterisation of a complex particle is a difficult task. In the case of (sub)millimetre objects, especially where ray optics or physical optics can prompt something, there are established techniques, like (digital) in-line holography or rainbow refractometry that can provide fairly accurate information. Rainbow refractometry is claimed to be able – under certain assumptions – to yield the average radial distribution of the refractive index of a microdroplet. The components distribution can be inferred then.

Groups from the Institute of Physics of the Polish Academy of Sciences and Cardinal Stefan Wyszyński University in Warsaw have joined the scientific effort in the field of remote optical particle characterisation. We have developed several methods of assessing the surface and partially the internal structure of a microdroplet of suspension. Our methods are mostly based on Mie scattering imaging – analysis of the spatial distribution (evolution) of the interference pattern of light scattered by a (homogeneous) sphere. By analysing the evaporation rate evolution (also in the language of surface thermodynamics) and morphological resonances (of an optical microresonator) in detail, in many cases, we could infer how the transient composition/structure of the droplet surface evolves. In electrodynamic traps – also known as electrodynamic balances or levitators – we investigated droplets containing silica nanospheres, surfactants and fullerenes – mimicking atmospheric aerosols containing desert dust, soot and detergents. We also gained several valuable insights by performing numerical simulations of NPs aggregation in the evaporating droplet and by scanning electron microscopy of final products of microdroplet evolution – dry nanostructured microparticles.

However, it must be admitted that the methods developed so far are mostly at a loss when the distribution of the NPs below the microdroplet surface (in the microdroplet volume) is concerned. To mend that, we've started experimenting with luminescent nanoprobes and dynamic light scattering (DLS) in microdroplets and obtained promising results. Luminescent nanoprobes seem particularly predestined for this task since they can provide illumination from the inside of the microdroplet, while the light coupled to the microdroplet from outside stays mostly just below its surface. In the course of the project, we plan to develop a microdroplet characterisation method using luminescent nanoprobes, possibly in conjunction with DLS. If the method is successful, the number of identified suspended phase distributions could be significantly broadened and so the number of available scattering images classes for neural network training.