In recent years, there has been a rapid development of new methods of teaching deep neural networks, thanks to which they have found application in many fields of science and technology. Neural networks are now very widely used also in physics. In this project, we plan to focus on a particular application of neural networks that has been proposed in recent years: approximation of the probability distributions of states.

In order to calculate physical quantities in a statistical system, it is necessary to know the probability distribution of physical states. In the vast majority of cases considered in physics, the number of states of a system is too large to be efficiently computed numerically (often infinite). Therefore, more sophisticated numerical methods are used, e.g. Markov Chain Monte Carlo (MCMC). In MCMC, a new state of the physical system is generated by a small, random change to the previously generated configuration. Each new state can be accepted or rejected with a certain probability, which guarantees that for very long chains the states have the required probability distribution. Essentially, there are two main problems with the MCMC approach. Firstly, it is impossible to calculate some state functions, e.g. free energy and entropy, due to the fact that the method is not sensitive to the normalization of the probability distribution. Secondly, there is autocorrelation – configurations that are very close to each other in the chain are not statistically independent of each other. Autocorrelation increases the simulation error, sometimes significantly. Both of these problems can be substantially reduced by the use of neural network methods.

There are several methods of training neural networks to reproduce a given probability distribution of the states. In this project, we will focus on two that we believe are the most promising: i) Variational Autoregressive Networks (VAN), which are used in systems with discrete degrees of freedom; ii) Normalizing Flow (NF) applicable to the systems with continuous degrees of freedom. Both of these approaches have a common feature - the network simultaneously learns the probability distribution and generates the states of the system. Therefore, one does not need a set of data on which the network is trained, but only a non-normalized form of the target probability distribution is required. The learning method is based on minimizing the variational free energy, which allows estimating the state functions with very high accuracy. Moreover, a trained neural network can be used for the generation of MCMC (so-called Neural MCMC - NMCMC), where each successive state is independent of the previous one, and the only correlations may appear due to the imperfect reconstruction of the target distribution.

The main goals of this project are to develop the VAN and NF algorithms by improving their performance and applying them to various physical systems. There are models for which one of these two algorithms can be used in almost every area of physics, these are for example: physical fields of the Standard Model (e.g. quantum chromodynamics), dynamical triangulation approach to the quantum theory of gravity, spin glasses, time crystals, topological materials. The proposed project includes elements of many areas of physics and we hope to expand the knowledge in each of them.