Master 2: ***International Centre for Fundamental Physics***

INTERNSHIP PROPOSAL

(One page maximum)

Laboratory name: LRI (to become LISN)
CNRS identification code: UMR CNRS 8623
Internship director'surname: François Landes
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Web page: http://lptms.u-psud.fr/francois-landes/internships-phd/
Internship location: Paris-Saclay, LRI

Thesis possibility after internship: **YES**/NO
Funding: YES/**NO** If YES, which type of funding:

(Deep) Graph Neural Networks for Fundamental Physics:
the case of Glassy liquids

The idea of using Machine Learning to attack the problem of Structural Glasses is rather recent, the first works dating from 2015 [*Attractive versus truncated repulsive supercooled liquids: The dynamics is encoded in the pair correlation function, Physical Review E, 2020*]
However most of these works rely on simple, yet robust ML technology: concretely, binary classification using SVMs (shallow learning). In a previous (short) internship, it has been shown that a regression approach performed equally well as the corresponding binary classification approach. This opens the way to methodological changes in the approach.
Independently and very recently, GNNs have been demonstrated to perform better than previous models to predict the local state (liquid/solid) in supercooled liquids [*Unveiling the predictive power of static structure in glassy systems,* Nature Physics, April 2020].
The internship's goal is to understand and critically assess the performance of past GNNs, and ultimately design new ones, taking into account the specificities of the problem at hand. Depending on the interests and abilities of the trainee, this task may be attacked more or less directly.
At first, the trainee will be expected to get acquainted with the physics literature on glassy dynamics (for this, the previous internship report may help, along with more thorough reviews). To get a grasp of the concrete problem, one may then use the available software and data (from our team) of Molecular Dynamics simulations, which may also help in strengthening the knowledge of fundamentals of ML.
Then, before designing novel GNNs architectures, one may use the available code from literature [cited above, Nature Physics, April 2020] to get acquainted with GNNs (and DNNs in general) and reproduce past experiments. Using this vanilla GNN as a base, the trainee will be able to propose more advanced or entirely novel architectures to better tackle the problem. This goal is ambitious, and if it is reached it may of course lead to a publication.
The trainee is expected to be proficient in python, and/or C++ (an imperative language). A good knowledge of Machine Learning, and a strong interest in it, is needed. The ideal candidate will have some prior knowledge of Deep Learning, and of a standard library (TensorFlow or PyTorch). Of course a Physics background implies advanced understanding of Statistical Physics.
More details on the offer on my website.

Please, indicate which speciality(ies) seem(s) to be more adapted to the subject:

Condensed Matter Physics: **YES** Soft Matter and Biological Physics: **YES**
Quantum Physics: YES Theoretical Physics: **YES**