



Date of publication of the job offer – July 20th 2018

Job Title: PhD in Machine learning the drug discovery process

Job Description

This project aims to develop artificial neural networks applied to structural biology, drug discovery and computational chemistry. The aim is to go substantially beyond the state-of-the-art in the use of machine learning and GPU computing, exploring supervised, unsupervised and reinforcement learning approaches.

We expect the candidate to participate in the development of new learning approaches derived from deep learning, other brain-inspired learning algorithms, GPU and distributed computing. By working in this project, the researcher will have access to state of the art computational project like GPUGRID.net and large amount of simulation data, which will be crucial for the development and validation of novel computational protocols. This project is expected to lead to discoveries that will be publishable in the highest impact scientific journals.

Project and Institution that finance the contract

BIO2017-82628-P Ministerio de Economía, Industria y Competitividad – Agencia Estatal de Investigación, co-funded by FEDER

Official number reference BIO2017-82628-P

Skills and Experience

The candidate will preferably have a profile in physics, computer science, mathematics, chemistry and engineering, but other fields are also considered. We seek exceptional candidates with a passion for programming and computing, the capability to think out of the box, the ambition to work in very innovative projects and very good communication skills in English. Prior knowledge in neural information processing, deep learning frameworks (pyTorch, Tensorflow) is desirable, as well previous experience with CUDA programming, C/C++ and Python. This is a strongly computational position, so we encourage application of people that love algorithms, computing, programming and likes to apply it.

The candidate will be able to use <http://www.gpugrid.net>, one of the largest volunteer computing project worldwide with thousands of GPUs. The laboratory is very well equipped with access to a local GPU and CPU cluster, hundreds of TB of storage and experimental facilities.



Benefits of the opening:

The successful candidate will be offered an initial part-time contract, with salary commensurable with experience, with the possibility for an extension.

Information on the application process:

Send CV and letter of interest, to carina.oliver@upf.edu (REF: PN_GdF)

Deadline to submit applications – Sept 30th 2018

Contact: Carina Oliver (GRIB) – carina.oliver@upf.edu