**Date of publication of the job offer – October 31st, 2018**

**Job Offer** :
PhD Position at the Computational Science Laboratory, University Pompeu Fabra, Barcelona. (Development of the code in particular on GPUs and distributed computing.)

**Job Description:**
This project aims to develop a code based on artificial neural networks and first principles physics applied to structural biology, drug discovery and computational chemistry. We expect the candidate to participate in the development of the code in particular on GPUs and distributed computing. By working in this project, the researcher will have access to state of the art computational project like GPUGRID.net. This project is expected to lead next generation codes that are transformative in the field and publishable in the highest impact scientific journals. There will be ample opportunities to present his/her work at international meetings and conferences and to collaborate with other research groups in USA and Europe.

**Project and Institution that finance the contract:**
The work is supported by grant: AEI-BIO2017-82628-P (FEDER/UE) FABRITIIS from the Spanish Ministry of Economy (MINECO), FEDER and Agencia Estatal de Investigación sources.

**Official number reference:**
AEI-BIO2017-82628-P (Aplicación de métodos de aprendizaje automático y de aumento de datos en el estudio de la conformación proteica y el reconocimiento molecular para el desarrollo de fármacos)

**Skills and Experience:**
The candidate will preferably have a profile in physics, computer science, mathematics, chemistry and engineering. 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 experience in deep learning frameworks (pyTorch), Python, CUDA programming, C++ is highly desirable. This is a strongly computational position, so we encourage application of people that love algorithms, computing and programming.

**Other relevant information:**
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. The molecular modelling will be using state of the art software environments in molecular modelling and simulations (http://www.playmolecule.org) developed by the research group in collaboration with the spin-off company Acellera.

**Benefits of the opening:**
The successful candidate will be offered an initial part-time contract, with an annual gross salary  around 19.000 EUR, commensurable with experience, with the possibility for an extension.

**Application process:** Fill the Google Form
**Deadline to submit applications –** Not defined
**Contact:** Gianni de Fabritiis, Head of Computational Science Lab, Universitat Pompeu Fabra.