Date of publication of the job offer: June 7th 2022

Job Offer: Position on deep learning biomolecular simulations at the Research Programme on Biomedical Informatics (GRIB)

Job Description:

The successful candidate will work on next generation molecular simulations and neural network potentials with the goal of substantially impacting physics-based simulations and molecular dynamics. These positions involve having a key role in the development of OpenMM (http://openmm.org) of which we are co-coordinators. The candidate will contribute together with other PhDs fellows and international collaborators from academia and industry to the research lines of the Computational Science Laboratory (https://www.compscience.org/).

Depending on your skillset, you are expected to contribute to the machine learning of neural network representations for molecular potentials, improve speed in collaboration with OpenMM and Nvidia, enhance capabilities in terms of representing longer range physical terms, charges, etc.

Relevant publications: TorchMD: A deep learning framework for molecular simulations, S Doerr, M Majewski, A Pérez, A Krämer, C Clementi, F Noe, T Giorgino, … Journal of chemical theory and computation 17 (4), 2355-2363 (https://github.com/torchmd)

Project and Institution that finance the contract.

The work is supported by grant (Official number reference):
PREUR00419 - EC-H2020-CompBioMed2-Gianni de Fabritiis

Desired skills and expertise:

The candidate will have a BSc in Chemistry and a MSc in Computational Physics. We seek exceptional candidates with a passion for computing. Good knowledge of Quantum Dynamics and strong programming skills. Good communication skills in English.

Benefits of the opening:

Contract as PSR according to regulations in force.

Estimated annual gross salary: 21.700€

Timetable: part time, 22,5 hrs/week

Place of work: PRBB, Research Programme on Biomedical Informatics (GRIB)

Computational Science Group

Prof. Gianni De Fabritiis, ICREA research professor

Department of Medicine and Life Sciences (MELIS),

Universitat Pompeu Fabra

Barcelona Biomedical Research Park (PRBB)

c/ Dr. Aiguader, 88, 08003 Barcelona.

Estimate start date: 1/07/2022

Information on the application process:

To apply: please send your CV and letter of presentation to chus.donlo@upf.edu

Deadline to submit applications 22/06/22