PD2021MD: Postdoctoral position on deep learning applied to molecular simulations

at the Computational Science Laboratory, University Pompeu Fabra, Barcelona

Prof. Gianni De Fabritiis, ICREA research professor (https://es.linkedin.com/in/gdefabritiis), is looking to recruit a postdoctoral scientist to work **on next generation molecular simulations and neural network potentials with the goal of extending the applicability of the method to new areas and .** This involves having a key role in the development of OpenMM (http://openmm.org). 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/).

[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](#)

[Coarse graining molecular dynamics with graph neural networks BE Husic, NE Charron, D Lemm, J Wang, A Pérez, M Majewski, A Krämer, ...The Journal of Chemical Physics 153 (19), 194101](#)

[Lab's publications](#)

What you will do. 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.

What you need. The candidate will preferably have a profile in physics, computer science, mathematics or similar. However, primarily, we seek exceptional candidates with a passion for computing, the capability to think out of the box, and the ambition to work in very innovative projects more than specific profiles. Very good communication skills in English. A solid previous experience in any of the following: molecular simulations, quantum chemistry, machine learning. Python proficiency and coding skills, knowledge of Pytorch, familiarity with Linux and the ability to work with version control systems (e.g. git) are required. An excellent publication record during the PhD.

Location. The laboratory is located in the Barcelona Biomedical Research Park ([PRBB](#)) which, with a privileged location on the shoreline of the Mediterranean sea, constitutes one of the most exciting interdisciplinary research centres in Southern Europe with more than 1000 scientists in the building alone. The PRBB is more than just a research institution, it is a unique creative space that connects science and diversity. By becoming a member of its research community, the candidate will have access to conferences, networking opportunities and training events.

Facilities. Access to state of the art computational resources and large amounts of simulation data, which will be crucial for the development and validation of novel computational protocols. The lab is equipped with a cluster with state-of-the-art GPUs and has exclusive access to GPUGRID.net, a distributed computing project with 5000 GPUs.

Eligibility: Please send an email to gianni.defabritiis@upf.edu with subject "JOB PD2021DL" with a CV and a cover letter together with the names of up to three contacts for references. recommendations. We will contact you only if you are selected for a presentation.

Salary. We offer a competitive salary, depending on experience.

Duration. Initially 1-year contract with the possibility of extension to up to 3-5 years in total

Deadline: Until filled - expected starting date anytime by the end of 2021