

Departament de Ciències Experimentals i de la Salut



Generalitat de Catalunya

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Job Offer:

# PD2021AI: Postdoctoral Position on Artificial Intelligence at the Computational Science Laboratory, University Pompeu Fabra, Barcelona

Job Description:

Lab website: <a href="http://www.compscience.org/">http://www.compscience.org/</a>

Relevant References: <u>https://scholar.google.es/citations?hl=en&user=-</u> \_kX4kMAAAAJ&view op=list works&sortby=pubdate

#### Research line 1: Model-based reinforcement learning

The human brain is a complex problem solver machine, but initially evolved by the strong survival pressure for navigation. Lifeforms went from the capacity to sense and react to gradients of concentrations, to developing the capacity to compute and update their orientation and position for motion planning. It is currently known that this calculation is performed by grid cells in the entorhinal cortex to represent the location of the body relative to its environment. Recent experimental evidence suggests that grid cells might also be present in the neocortex and have evolved to represent location and movements of other objects analogously, e.g. in object manipulation. We are interested in testing this hypothesis from a machine learning perspective in the context of model-based reinforcement learning and robotics to understand if this can be one of the key fingerprints of human intelligence.

#### **Research line 2: Cooperative intelligence**

Intelligence is usually associated with the human brain and the neo-cortex. Nevertheless, the brain's intelligence of a single human is limited. Something as simple as the invention of the wheel was invented only 5500 years ago. Furthermore, a single human brain is not going to be able to produce anything substantial outside of the context of human society and collaboration. Society also allows for multiplicative effects such that the type of exponential knowledge growth in knowledge can happen. While the brain is the key substrate for it, learning in the context of a population of agents is a key ingredient for the outcome of intelligent behaviour. We plan to use a large population of RL agents running on the distributed computing infrastructure GPUGRID to learn. The challenge is how to communicate basis between them in order to exchange knowledge. We plan to demonstrate our improved capabilities on challenges to easily demonstrate pioneering methods.

The computational science laboratory, led by Gianni De Fabritiis has been successfully applying deep learning approaches on fundamental problems in these areas, such as proteinligand docking, affinity prediction, protein folding and more general artificial intelligence



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problems, winning several international challenges. Currently, we are focused on developing intelligent agents that can outperform human on specific problems.

Location: The laboratory is located in the Barcelona Biomedical Research Park 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.

## Project and Institution that finance the contract:

The work is supported by grants: PO00321 - 2020 DI BIOMEDICINA (AGAUR, Generalitat de Catalunya)

Official number references: PO00321 - 2020 DI BIOMEDICINA: Gianni de Fabritiis

## Skills and Experience:

- The candidate will preferably have a profile in computer science, physics or mathematics. However, 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.
- The capability to think out of the box, the ambition to work in very innovative projects and very good communication skills in English.
- Previous experience in reinforcement learning and related fields, Python proficiency and coding skills, knowledge of Tensorflow or pytorch, familiarity with Linux and the ability to work with version control systems (e.g. git) are required.

Facilities: Access to state of the art computational resources and large amount 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.

### Benefits of the opening:

We offer a competitive salary (30k-35k EUR), depending on experience. Initially 1-year contract with the possibility of extension to 3 years in total.

### Information on the application process:

Please send an email to <u>gianni.defabritiis@upf.edu</u> with subject "**JOB PD2021AI**" with a CV and a cover letter together with the names of up to three contacts for requesting recommendations.