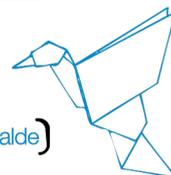


Postdoctoral Fellowship in ML-driven Atomistic Simulations for Energy & Health

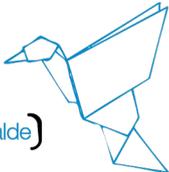
Job Offer	
Topics:	<p>In the framework of the BCAM “<i>Maths & Artificial Intelligence</i>” strategy, a series of projects in this field is launched in different areas of Applied Mathematics.</p> <p>The project “Machine-Learning-Driven Atomistic Simulations for Energy and Biomedical Applications” will be led by the group of Modelling & Simulation in Life & Materials Sciences at BCAM, Basque Country and the MS2Discovery Interdisciplinary Research Institute at Wilfrid Laurier University in Waterloo, Canada. Both groups are involved in the International Consortium on Multiscale Modelling of Advanced Energy Materials and collaborate extensively with physicists, mathematicians, theoretical/experimental chemists and engineers from a number of institutions around the world.</p> <p>The objective of the aforementioned project is to enable efficient and tractable simulations of several important classes of complex atomistic systems through the use of novel Machine Learning (ML) techniques, paying particular attention to those cases where state of the art Molecular Dynamics (MD) algorithms are lagging behind the current needs of challenging applications in energy and health. Many such applications require the modelling based on local atomic interactions for better understanding properties of the underlying structures and systems. Such interactions, often derived from quantum mechanical representations, are prohibitively expensive to simulate. ML algorithms provide a natural tool to address this challenge, and thus one of the underlying ideas of the project is to train neural networks efficiently or to use other ML tools in order to reproduce results of density functional theory calculations at a much lower cost.</p>
PI in charge:	Elena Akhmatkaya (BCAM) & Roderick Melnik (Wilfrid Laurier University)
Salary and conditions:	<p>The gross annual salary of the Fellowship will be 28.000 - 32.000€.</p> <p>It will then be on your own responsibility to make your yearly income declaration at the Bizkaia Treasury</p>



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	<p>Agency.</p> <p>There is a moving allowance for those researchers that come from a research institution outside the Basque Country from EUR 1.000 to EUR 2.000 gross.</p> <p><i>Free access to the Public Health System in Spain is provided to all employees.</i></p>
No Positions offered:	#1
Contract and offer:	1 year at BCAM, extensible 1 year more at Wilfrid Laurier University, contingent upon the availability of funds and candidate's credentials.
Deadline:	September 13th 2019, 14:00 CET (UTC+1)
How to apply:	Applications must be submitted on-line at: http://www.bcamath.org/en/research/job

Scientific Profile Requested	
Requirements:	<ul style="list-style-type: none"> • Promising young researchers. • Applicants must have their PhD preferable in Applied Mathematics, Computational Statistics, Computer Science, Physics, Electrical Engineering or related fields.
Skills and track-record:	<ul style="list-style-type: none"> • Good interpersonal skills. • A proven track record in quality research, as evidenced by research publications in top scientific journals and conferences. • Demonstrated ability to work independently and as part of a collaborative research team. • Ability to present and publish research outcomes in spoken (talks) and written (papers) form. • Ability to effectively communicate and present research ideas to researchers and stakeholders with different backgrounds. • Fluency in spoken and written English.
Scientific Profile:	<p>The preferred candidate will have:</p> <ul style="list-style-type: none"> • Strong background in computational statistics, applied mathematics and statistical mechanics. • Demonstrated knowledge in ML techniques, Monte Carlo methods, Molecular Dynamics, DFT. • Good programming skills in C/C++, Python as well as good software development practices (e.g. version control software usage and embedded tests). • Experience in high performance computing. • Research experience in Applied Statistics in



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	interdisciplinary applications (e.g.: Health, Energy).
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Application and Selection Process

Formal Requirements:	<p>The selected candidate must have applied before the application deadline online at the webpage http://www.bcamath.org/en/research/job</p> <p>The candidates that do not fulfil the mandatory requirements will not be evaluated with respect to their scientific profile.</p>
Application:	<p>Required documents:</p> <ul style="list-style-type: none"> ▪ CV ▪ Letter of interest ▪ 2 recommendation letters ▪ Statement of past and proposed future research (2-3 pages)
Evaluation:	<p>Based on the provided application documents of each candidate, the evaluation committee will evaluate qualitatively: the adaption of the previous training and career to the profile offered, the recommendation letters, the main results achieved (papers, proceedings, etc.), the statement of past and proposed future research and other merits; taking in account the alignment of these items to the topic offered.</p>

Incorporation:	<p>November 2019 or as soon as possible thereafter</p> <p><i>The BCAM postdoctoral contract will start when the selected candidate has finished the PhD, i.e. after dissertation defence.</i></p>
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