Institution: Nicolaus Copernicus University; Faculty of Physics, Astronomy and Informatics

City: Toruń, Poland

Position: PhD student

Research field: Physics

Posted: 18 Jul 2022

Expires: 10 Sep 2022, 23:59 - Europe/Brussels

Envisaged job starting date: 1 Oct 2022

Number of offers: 1

Type of contract: Temporary

Job status: Full-time

Hours per week: 40

Offer description:

This PhD student position will be an appointment for the project entitled *Statistical Learning of Slow Collective Variables from Atomistic Simulations* lead by Dr. Jakub Rydzewski at the Institute of Physics, Nicolaus Copernicus University in Toruń, Poland. The project is financed by National Science Center (NCN Sonata).

Modeling the long-timescale dynamics of complex systems is a fundamental task in the physical sciences. Molecular dynamics (MD) simulations allow to probe the spatiotemporal details of molecular processes, but the so-called sampling problem severely limits their usefulness in practice. The sampling problem comes from the fact that a typical energy landscape consists of many metastable states separated by barriers much higher than thermal energy. As such, on the timescale one can simulate, barrier crossings are rare events, and the system remains kinetically trapped in a metastable state.

One way to alleviate the sampling problem is to employ enhanced sampling simulations in which fluctuations of few degrees of freedom, called collective variables (CVs), are boosted. Typically, CVs are selected using intuition. However, it may not be trivial to find CVs that quantify the essential characteristics of a rare event. In this project, we consider crucial problems related to the methodology of estimating CVs for complex physical systems: How to construct the CVs without resorting to system-specific expert knowledge? Is it possible to construct the slow CVs directly from enhanced sampling simulations?

By improving our recent method, multiscale reweighted stochastic embedding (MRSE) [J. Phys. Chem. A, 2021, 125], we will devise a tool that will be able to learn slow CVs in a near-blind manner, making it accessible to many users without detailed knowledge about enhanced sampling theory. We expect the method will have a large impact on the current state of the MD community and be applicable to long-timescale processes in chemistry, physics, and biology.

Should you have any questions, you can contact Dr. Jakub Rydzewski (jr@umk.pl).

Selection process:

Applications received before September 10th, 2022 will be given full consideration, but will continue to be accepted until the position is filled. Selected applicants will be asked to participate in interviews held in the NCU or via teleconference call.

Required documents:

• Curriculum vitae

- Scan of the master's degree diploma

- Cover letter

- Contact details of people who can provide references

Skills/Qualifications:

- Basic knowledge about molecular dynamics simulations

- Programming (e.g., C++, Python), Linux operating systems, and data analysis will be an advantage.

Benefits:

- The Ph.D. stipend in the project is 5000 PLN (~1040 euro)/month (much higher than standard stipend for PhD students in Poland) for 36 months. It is required that the student has successfully obtained the status of a PhD student at the Nicolaus Copernicus University till 1st October 2022.

- Opportunity to train and develop in a rapidly developing research area

- Access to vast computing infrastructure, new notebook

- Participation in scientific or skills courses, conferences, and R&D trainings.

Offer requirements:

- Required education level: Master's degree (or equivalent) in physics, mathematics, computer science, or similar

- Required languages: English

Specific Requirements:

- Have the qualification for being enrolled to the Doctoral School called Academia Scientiarum Thoruniensis (AST) at Nicolaus Copernicus University (https://www.phd.umk.pl/ast/).

Additional information: Documents should be submitted to Dr. Jakub Rydzewski at: jr@umk.pl before 1 Sep 2022. The applicants will be contacted for interview to schedule time.

Please include the following statement in your application:

"I hereby give consent for my personal data included in my application to be processed for the purposes of the recruitment process under the Personal Data Protection Act as of 10 May 2018 (consolidated text: Journal of Laws 2019, item 1781) and pursuant to art. 6 § 1a GDPR (General Data Protection Regulation - EU 2016/279)."