

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

City: Toruń, Poland

Position: PhD student

Research field: Physics

Posted: Extended 12 Sep 2022 (Initial date: 18 Jul 2022)

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

Envisaged job starting date: 1 Nov 2022

Number of offers: 1

Type of contract: Temporary

Job status: Full-time

Hours per week: 40

Offer description:

This Ph.D. student position will be an appointment for the project entitled "Statistical Learning of Slow Collective Variables from Atomistic Simulations," led 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.

One way to alleviate the sampling problem is to employ enhanced sampling simulations in which fluctuations of a few degrees of freedom, called collective variables (CVs), are boosted. Finding CVs that quantify the essential characteristics of a rare event may not be trivial. In this project, we consider crucial problems related to 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?

We will devise a tool that can 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 significantly impact the MD community's current state and apply to long-timescale processes in chemistry, physics, and biology.

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

Selection process:

Applications received before October 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 Nov 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 10 Oct 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)."