M2 internship offer

Can Machine Learning make gas hydrate research more efficient and eco-friendly?

Supervision

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Description

Under specific conditions of pressure and temperature, the mixing of water and gas molecules can lead to the formation of nanoporous crystalline solids called clathrate hydrates. These compounds are made by a tetrahedral network of water molecules (“host”) forming cages inside of which gas molecules (“guest”) are encapsulated. Naturally abundant on Earth, gas hydrates can be observed on permafrost regions (Alaska, Siberia), on ocean floors and are generally expected to exist on icy celestial bodies (comets and planets of the solar system).

Gas hydrates, by their nature and their application fields, present at the same time promising properties regarding their abilities to store and sort gases (e.g. N2 clathrates seem to be favoured for CO2 encapsulation), and a threat concerning their stability (CH4 hydrates may represent 500 − 2500Gt on earth).

Multiple modelling approaches exist in order to unveil their properties. Among them, Density Functional Theory (DFT) has become a method of choice. However, due to its computational cost, it is impossible to access large-scale systems or long time-scale phenomena, which are crucial for accurately capturing the structural, thermodynamic, and dynamic behaviour of gas hydrates. There has been an attempt to overcome this issue by coupling such calculations with coarse-grained simulations, namely Kinetic Monte Carlo (KMC), but as it relies on DFT calculations, the issue stays the same for more complex composition. A promising state-of-the-art approach is the use of Machine Learned interatomic Potentials (MLiPs). Indeed, by taking profit of modern machine learning methods, we can now simulate systems at weaker costs while conserving a DFT like accuracy. In this project, after bibliographic research on gas hydrates field, especially on mixed gas hydrates, and on machine learning techniques in VASP software, the student will develop a methodology allowing to generate Ab-Initio quality MLiPs by coupling DFT/ML simulations. The resulting MLiP will be tested in order to recover known thermodynamic properties, and the student will establish performance metrics to assess in what extent his force-field is reliable and compare the computational gain to traditional DFT approaches.

In addition, the student will examine, quantify and compare the energetic costs (and corresponding greenhouse gas emissions) of the calculations made by traditional techniques (KMC with DFT) and by machine learning (DFT/ML). We expect this part of the study to unveil whether improving the computational efficiency also improves the climate impact of this research activity or comes with an increased climate cost.

Expected candidate profile

The candidate should pursue a master’s program in physics or in a related field, and have a taste for numerical simulations. An interest in sustainability is a plus.

Practical conditions

The student will be integrated in the UTINAM institute (https://www.utinam.cnrs.fr/), which is hosted at the Besançon observatory. This institute depends on the Université Marie et Louis Pasteur and the Centre National de la Recherche Scientifique (CNRS).

The duration of the intership is from 4 to 6 months. It can start immediately.

This master’s internship includes a monthly allowance of 625€/month.

Contact

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