Press Release

Keio University NIT, Sendai College

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Keio University
National Institute of Technology, Sendai College

Computational Method for Evaluating the Frictional Properties of Various Lubricants: Scientists now able to estimate frictional properties from molecular movements by combining molecular dynamics with machine learning

In a recent study, a team of researchers successfully evaluated the frictional properties of multiple types of lubricants by using their new proposed method of combining machine learning and molecular dynamics. The research team included first-year doctoral student Ikki Yasuda and second-year doctoral student (at the time of this study) Katsuhiro Endo from the Keio University Graduate School of Science and Technology, as well as Assistant Professor (at the time of this study) Yusei Kobayashi, Associate Professor Noriyoshi Arai, and Professor Kenji Yasuoka from the same university. The remaining members of the research group, Associate Professor Kazuhiko Fujiwara, Professor Kuniaki Yajima, and the late Professor Yoshihiro Hayakawa were from the National Institute of Technology, Sendai College.

Lubricants are used in mechanical interfaces to reduce any friction that may occur. It is a well-known fact that the speed of mechanical processes has an impact on lubricants' frictional properties. However, it has been difficult for scientists to use molecular dynamics to perform exhaustive analyses on these frictional properties for lubricants with diverse molecular structures. In this study, the team of researchers was able to decipher the molecular movements associated with common frictional properties in various molecules by using a method that employs machine learning to analyze the molecular dynamics of the molecules in lubricants. The research method proposed in this study provides a new way of performing a simplified and comprehensive analysis of various lubricants' characteristics. It is expected to make considerable contributions to a wide range of industries that rely on lubricants.

The outcomes of this study were published in the international academic journal, *ACS Applied Materials & Interfaces,* on January 30, 2023.

1. Main Points of Research

- Proposed a method to analyze data about molecular movements in a variety of confined lubricants (Note 1) through automated machine learning. Using this method, the researchers were able to identify factors related to the lubricants' frictional properties from their molecular movements.
- Results demonstrated that it is possible to efficiently predict frictional properties in a short period of time through calculations based on molecular dynamics.

2. Background of Research

In recent years, environmental awareness has led to a call for energy conservation. It is estimated that approximately 20% of the world's energy consumption is caused by friction which occurs between machine parts, making improvements to lubricant technology and refinements to frictional properties essential issues. However, frictional properties can be influenced by a great number of factors including the molecular composition of lubricants, the speed at which machines operate, and interactions between lubricants and machine surfaces. This makes it difficult to identify the role molecular movements play in influencing differences in frictional properties.

3. Research Design and Findings

This research used molecular simulations to recreated the conditions that are present at the interfaces between mechanical parts. The molecular movement obtained from the simulation data were then

analyzed by an unsupervised machine learning model (Note 2) in which the given data was not marked with correct answers (refer to figure 1. (a) and (b)). Through this method, unsupervised machine learning classified differences in the motion of representative points for diverse forms of molecules at varying shear velocities. The results demonstrated that it is possible to draw distinctions between movement factors that were related to the frictional properties of the lubricants as compared to the movement factors that were related to the molecule type. Furthermore, the research team was able to show that it is possible to predict the frictional properties from molecular movements even when the molecular structures significantly differ.

4. Future Developments

Because the research method proposed in this study provides a new way of performing simplified and comprehensive analyses of various lubricants' characteristics, it is expected to make considerable contributions to a wide range of industries that rely on lubricants. In particular, the researchers plan to further explore practical applications for their findings, including how additives might change the frictional properties of materials.

Details of Journal Article

Article Title: Combining Molecular Dynamics and Machine Learning to Analyze Shear Thinning for Alkane and Globular Lubricants in the Low Shear Regime
Authors: Ikki Yasuda, Yusei Kobayashi, Katsuhiro Endo, Yoshihiro Hayakawa, Kazuhiko Fujiwara, Kuniaki Yajima, Noriyoshi Arai, and Kenji Yasuoka
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Glossary

(Note 1) The state at which lubricant exists in an extremely narrow space only as wide as a single molecule (a thickness of mere tens of nanometers). The experiments conducted for this study simulated the behavior of lubricant when confined by walls of mica.

(Note 2) In most cases, supervised machine learning is used to predict new input values after learning the corresponding relationships between input values and correct output data. In contrast, unsupervised machine learning tries to perform desired tasks using only input values. An example would be feature extraction, a process that simplifies complex data. For this study, the researchers extracted simplified features from the complex movement data associated with the lubricants.

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