Chemical Reaction Pathway Analysis by Ising Computing

Yuta Mizuno

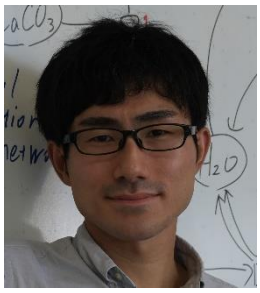
Research Institute for Electronic Science, Hokkaido University, Sapporo, Japan

Institute for Chemical Reaction Design and Discovery, Hokkaido University, Sapporo, Japan

PRESTO, Japan Science and Technology Agency, Kawaguchi, Japan

mizuno@es.hokudai.ac.jp

Chemical reaction pathway analysis on chemical reaction networks, such as organic synthetic pathway optimization and metabolic pathway analysis, involves combinatorial optimization problems that rapidly become harder to solve due to combinatorial explosion as the network size increases. In recent years, novel-type computers dedicated to solving such hard combinatorial optimization problems, called Ising computers, have been developed. Ising computers sample low energy states of Ising-type Hamiltonians by quantum or quantum-inspired processes. A lot of combinatorial optimization problems are equivalent to minimization of Ising-type Hamiltonians, thus Ising computers are expected to sample approximate solutions of combinatorial optimization problems in practical time. Toward practical applications of chemical reaction pathway analysis on large-size chemical reaction networks, we have developed a computational framework for chemical reaction pathway analysis using Ising computers and evaluated its performance. In this talk, I will present the computational framework and show the performance evaluation results.



Assistant Professor Yuta Mizuno
Research Institute for Electronic Science, Hokkaido University,
Sapporo, Japan
E-mail: mizuno@es.hokudai.ac.jp

Education/Career

2020-now	PRESTO Researcher, Japan Science and Technology Agency
2019-now	Assistant Professor (concurrent), Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University
2019-now	Assistant Professor, Research Institute for Electronic Science, Hokkaido University
2017-2019	JSPS Research Fellow, Japan Society for the Promotion of Science
2015-2018	Ph.D., Graduate School of Arts and Sciences, The University of Tokyo

Research Interest

Chemical reaction network, chemical reaction dynamics and kinetics, dynamical systems