TSUBAME Grand Challenge Program
SuperCon Programming Contest

TSUBAME Grand Chalenge

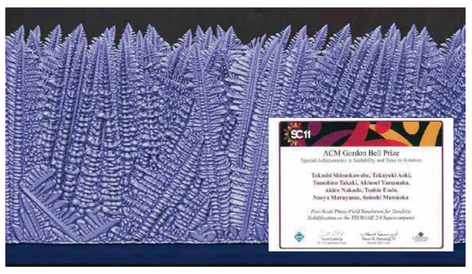
The TSUBAME Grand Challenge solicits proposals for grand challenge problems that can utilize all nodes of TSUBAME3.0 and has two categories.

Category A Exclusive use of all nodes for 24 hours
Category B Exclusive use of 1/3 of the nodes for up to 1 week

Number of Accepted Proposals

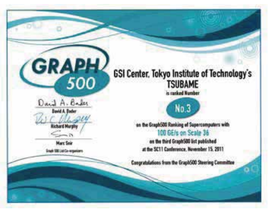
	2023		2022		2021		2020		2019		2018		2017		2016		2015		2014		2013		2012		2011		Total
	F	S	F	S	F	S	F	S	F	S	F	S	F	S	F	S	F	S	F	S	F	S	F	S	F	S	
Category A	0	0	0	0	0	0	0	0	0	0	0	1	2	0	1	1	1	2	1	2	0	1	2	2	3	4	23
Category B	0	1	0	1	0	2	0	1	1	2	0	2	0	1	0	1	1	3	2	2	1	1	0	0	2	0	24
Total	0	1	0	1	0	2	0	1	1	2	0	3	2	1	1	2	2	5	3	4	1	2	2	2	5	4	47

We started this program in 2011, and have continued to perform the Grand Challenge runs twice a year.
Under this program, we have adopted total 47 grand challenge projects some of which were awarded Gordon Bell prizes as below.



2011 ACM Gordon Bell Prize: Special Achievements in Scalability and Time-to-Solution
“Peta-scale Phase-Field Simulation for Dendritic Solidification on the TSUBAME 2.0 Supercomputer”

2011 ACM Gordon Bell Prize: Honorable Mention
Large scale biofluidics simulations on TSUBAME2



2011 Graph500 Challenge on TSUBAME 2.0

SuperCon Programming Contest

The SuperCon programming context is held every summer in cooperation with Osaka University and RIKEN, where high school students come to our campuses to compete in a programming context using our supercomputers. SuperCon started back in 1995 and has been held yearly. There is a qualifying round where students use their local environment to solve a given problem. About 10 teams consisting of 2-3 members each, will go on to the final round, which is held at Tokyo Tech, and Osaka University, for teams from the east and west side of Japan, respectively.

This year the students solved a Closest Pair of Points problem on the Fugaku supercomputer.
The following teams won the competition:
1st place: team KMB76 (Nada High School)
2nd place: team honyanya (Kaisei High School)
3rd place: team prism (High School at Komaba, University of Tsukuba)
Below are photos from previous years when it was in person.


Teams at Tokyo Tech.


Teams at Osaka U.

Grand Challenge Project 1:
Development of a method to accelerate convergence of large-scale simulations of membrane permeation processes of cyclic peptides based on a two-dimensional replica exchange method.

Yuudai Noso, Takuya Fujie, Masatake Sugita, Keisuke Yanagisawa, Masahito Ohue, Yutaka Akiyama (Tokyo Institute of Technology)

Motivation

Cyclic peptide drug discovery is of interest to pharmaceutical companies worldwide. To improve the success rate of the discovery, we are developing a molecular dynamics simulation protocol to predict membrane permeability.

Method

In this calculation, several hundred ns are dedicated to convergence of the lipid membrane structure and the interaction between the lipid membrane and the peptide, which are closely related to the convergence of the whole calculation.

Results of Grand Challenge

It has been recognized that reduction of the computational time spent on this process is important for industrial applications. In this project, we tried to accelerate the convergence of the conformations of lipid molecules by raising the temperature of the entire system in the early stages of the simulation, thereby significantly reducing the time required for the convergence of the calculation. The protocol was tested by performing 500ns simulations on six peptides, utilizing 56 node taking up approximately 85 hours per peptide. As a result, it was confirmed that the error of potential mean force (PMF) was remarkably reduced for four out of six peptides. We are currently analyzing the degree of conformational convergence of peptides and membranes in detail to find a way to improve the performance of our calculations.

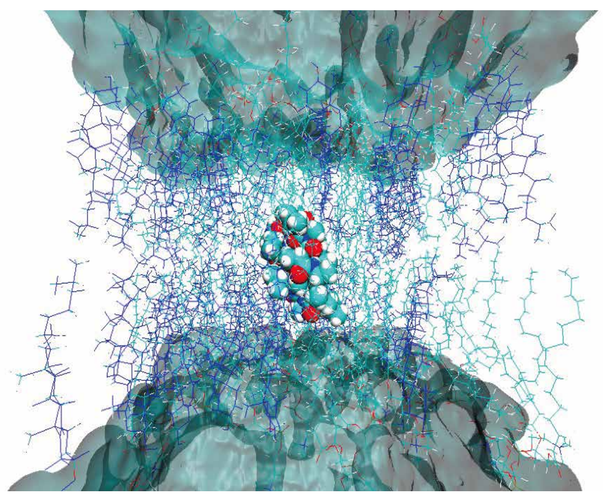


Figure: 3D structure of cyclosporin A crossing the model membrane

Grand Challenge Project 2:
An Exhaustive Study of Optimizer Characteristics for OOD Generalization on the ImageNet Scale

Hiroki Naganuma, Ioannis Mitliagkas (Université de Montréal, Mila)
Tetsuya Motokawa (Retty), Kota Ishikawa (Denso IT Laboratory)
Ikuro Sato (Tokyo Institute of Technology)

Motivation

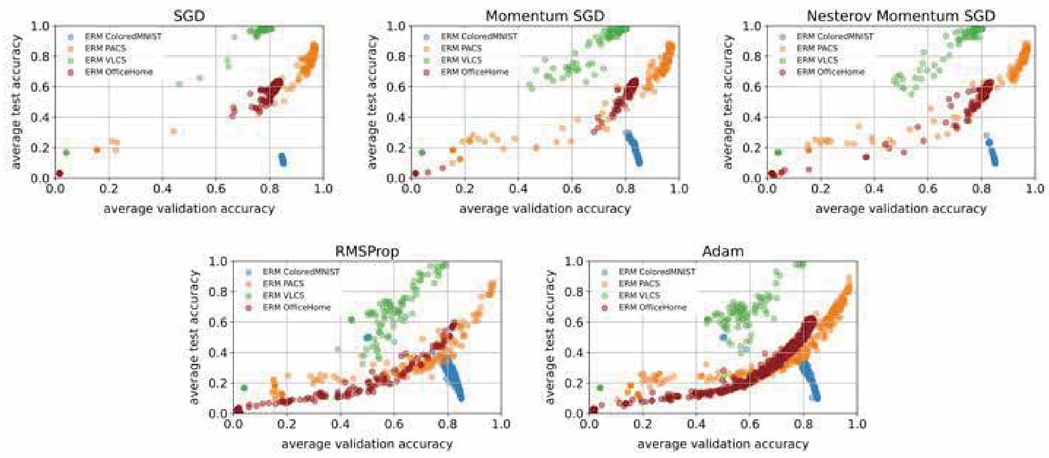
The machine learning community has studied how optimizer selection influences in-distribution generalization. However, the out-of-distribution generalization capability of the various optimization methods, which is of great importance in practical applications, is still unexplored.

Method

We investigate the relationship between in-distribution accuracy and out-of-distribution accuracy for different choices of optimizers.
We search over a wide range of hyperparameters and examine the classification accuracy (in and out-of-distribution) for over 20,000 models.

Key results

Our findings show that the out-of-distribution test accuracy of SGD is correlated with the in-distribution test accuracy, while Adam has a weaker correlation. This result implies the in-distribution test accuracy of adaptive optimizers may not always be a reliable indicator of out-of-distribution test accuracy.



http://www.gsic.titech.ac.jp/sc23