TSUBAME Grand Challenge Program
SuperCon Programming Contest

TSUBAME Grand Chalenge

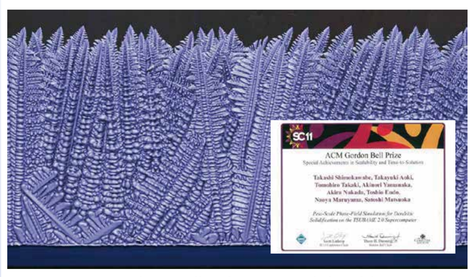
The TSUBAME Grand Challenge solicits proposals for grand challenge problems that can utilize all nodes of TSUBAME3.0 and has two categories.

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

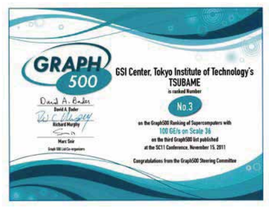
	2021		2020		2019		2018		2017		2016		2015		2014		2013		2012		2011		Total
	F	S	F	S	F	S	F	S	F	S	F	S	F	S	F	S	F	S	F	S	F	S	
Category A	0	0	0	0	0	0	0	1	2	0	1	1	1	2	1	2	0	1	2	2	3	4	23
Category B	0	2	0	1	1	2	0	2	0	1	0	1	1	3	2	2	1	1	0	0	2	0	22
Total	0	2	0	1	1	2	0	3	2	1	1	2	2	5	3	4	1	2	2	2	5	4	45

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 45 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 Solidifcation 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, 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 network analysis problem for epidemics on the Fugaku supercomputer.
The following teams won the competition:
1st place: team Citrus (Nada High School)
2nd place: team NPC (N High School)
3rd place: team Novice (Nada High School)
Below are photos from previous years when it was in person.

Teams at Tokyo Tech.

Teams at Osaka U.

Grand Challenge Project 1:
Analysis of membrane permeation process of a cyclic peptide (Cyclosporin A) by large-scale simulation based on two-dimensional replica-exchange method

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

Motivation

In order to improve the success rate of "cyclic peptide drug discovery" attracting attention from pharmaceutical companies around the world, it is an emergent task to elucidate the cell membrane permeation mechanism of large cyclic peptides with more than eight residues and to develop a method for improving membrane permeability based on the mechanism.

Method

In this study, a membrane permeation simulation for a lipid bilayer was performed for cyclosporin A (CSA), which is a large cyclic peptide with 11 residues. We performed molecular dynamics (MD) simulations for CSA membrane permeation, under nine different calculation conditions.

Results of Grand Challenge

It was clarified that the behavior of membrane permeation changes significantly when the cholesterol concentration exceeds 40%.
It was also found that the difference in force field parameters causes a difference of 10 kcal/mol or more in the estimation of the main barrier of membrane permeation.
In conclusion, we have discovered several clues for optimal calculation conditions for predicting the membrane permeability of large cyclic peptides.

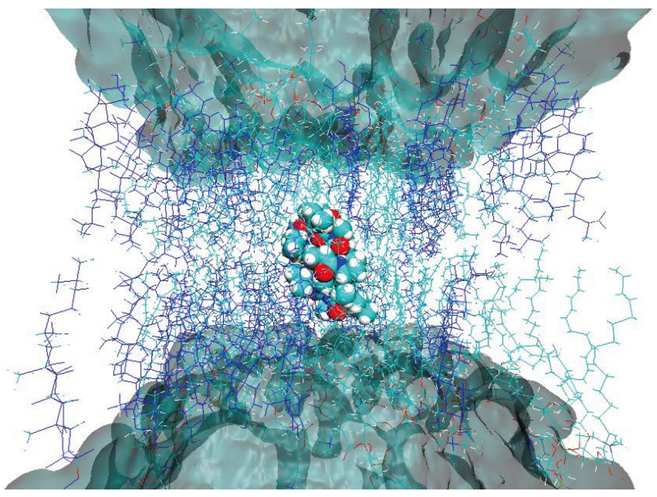


Figure: 3D structure of cyclosporin A crossing the model membrane

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

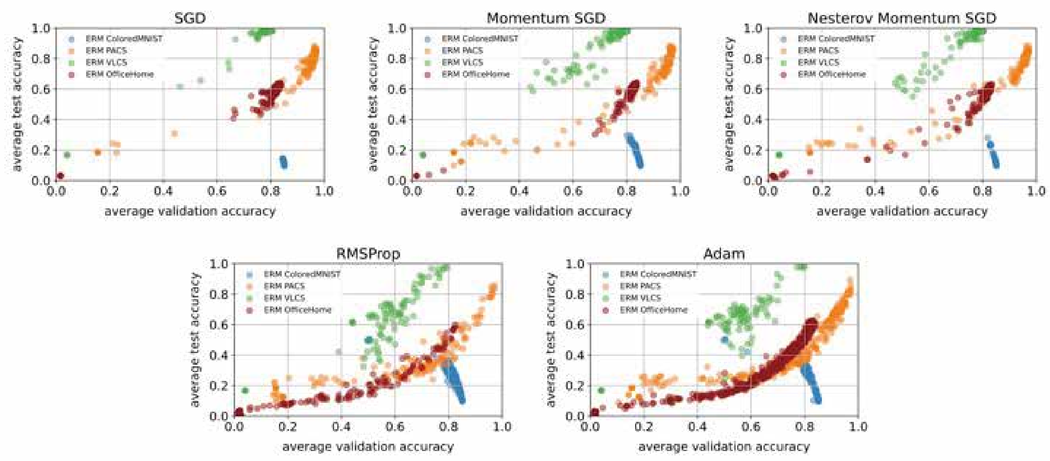
The machine learning community has studied how optimizer selection influences in-distribution generalization. However, the out-of-distribution generalization capability of the various optimization methods, which is of great importance in practical applications, is still unexplored.

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.



https://www.gsic.titech.ac.jp/sc21