

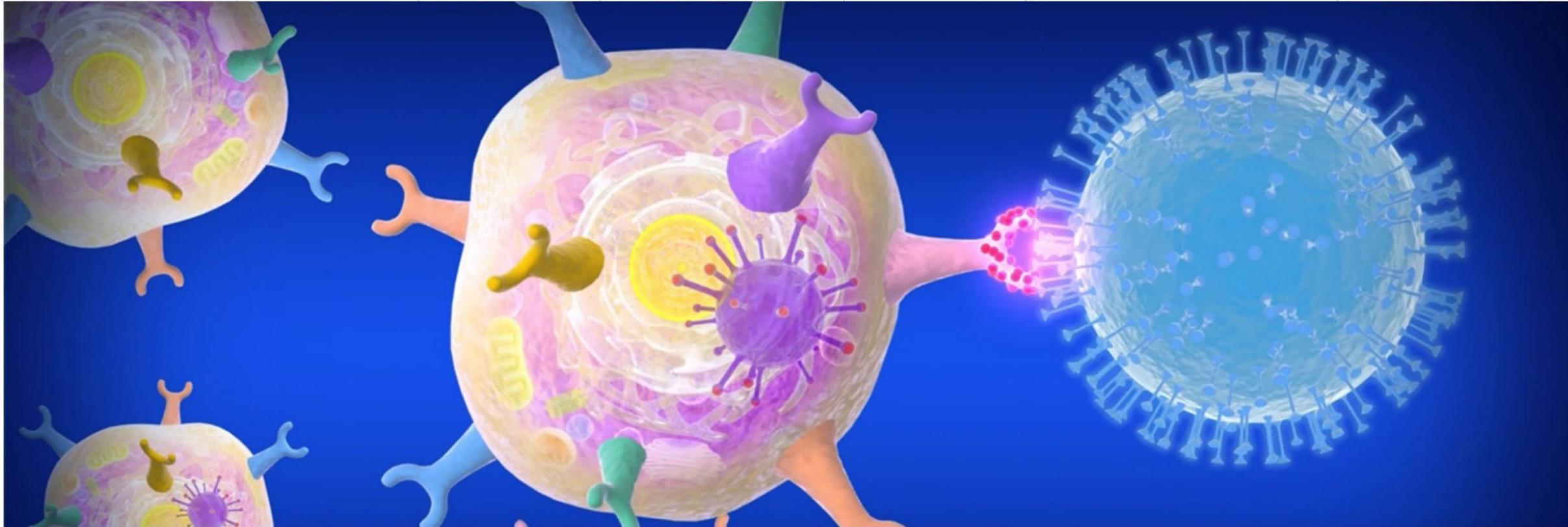


RIKEN
Center for
Computational
Science

Toshiyuki Imamura

20 June 2022, IHPCSS2022 @ Athens





> **Immune response to seasonal coronaviruses may offer protection against COVID-19**



[Research related to COVID-19 \(Updated on April 1, 2022\)](#)

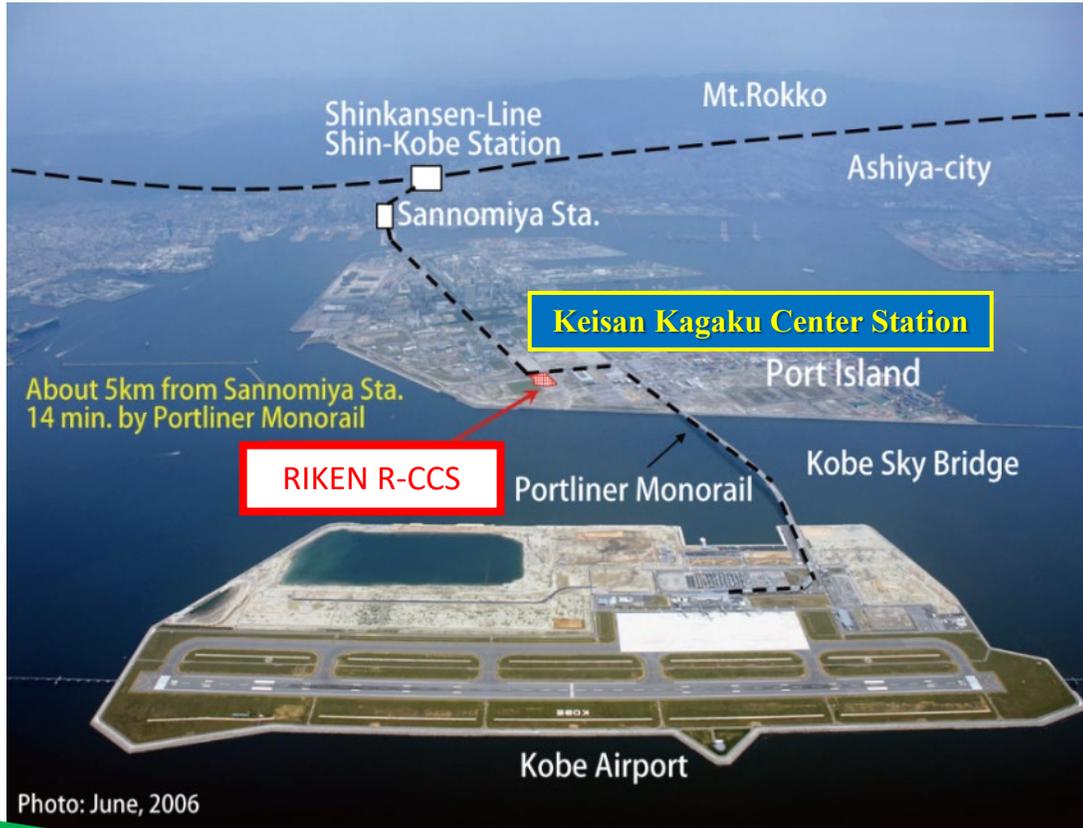
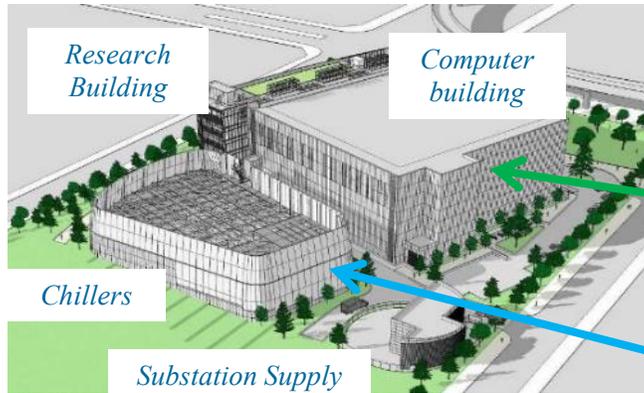
[COVID-19 Measures at RIKEN \(Updated on June 13, 2022\)](#)



R-CCS with Supercomputer Fugaku



423 km (263 miles)
west of Tokyo



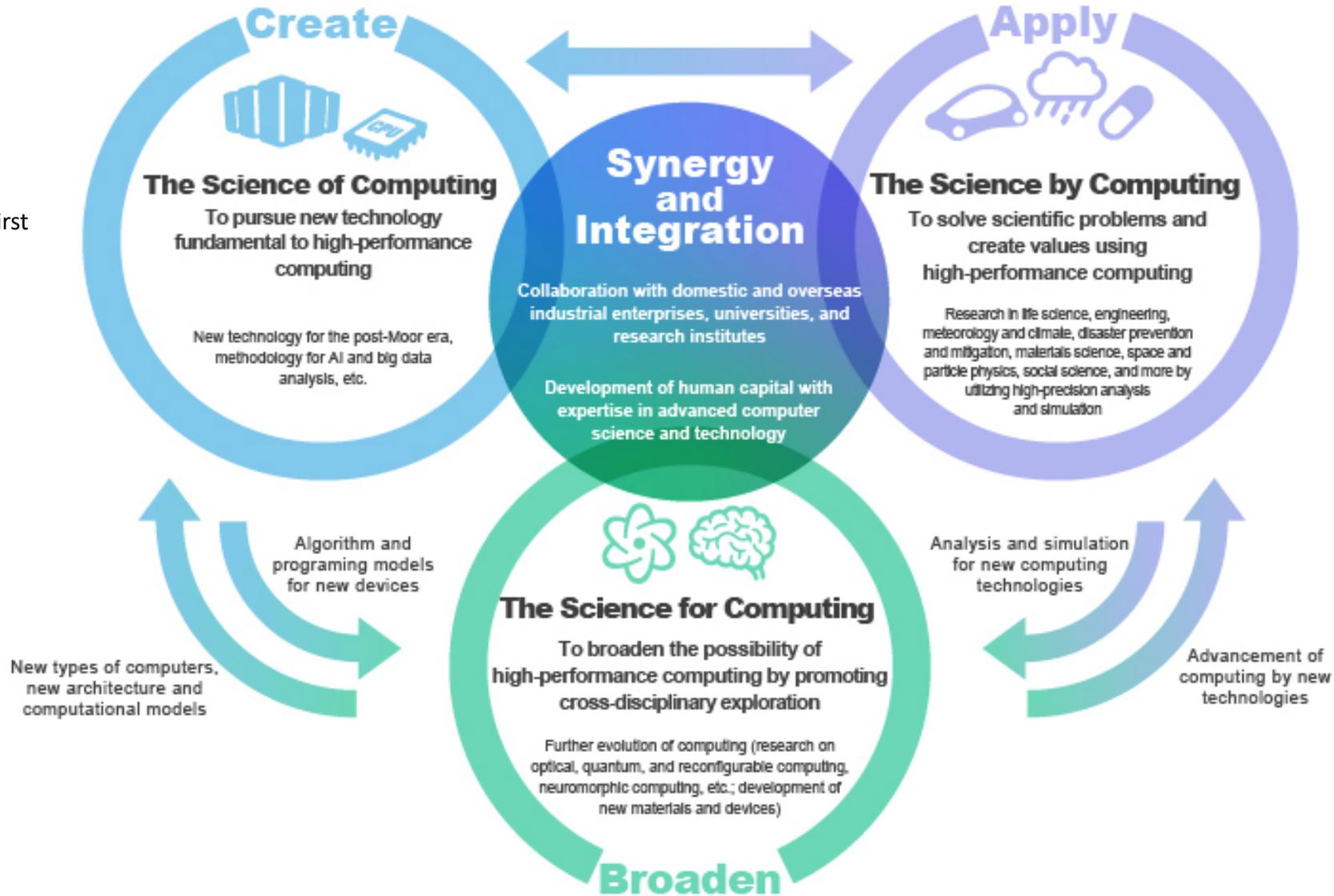
Computer room 50 m x 60 m = 3,000 m²
Electric power up to 37 MW
Water cooling system

Gas-turbine co-generation 5 MW x 2

Striving for excellence in science and becoming the cornerstone of Society 5.0



A research center out of 13 centers in RIKEN. The tier first national HPC center.





Deputy Director
M. Sato

Computer Science



Programming Environment
M. Sato



Next Gen High Performance Architecture
M. Kondo



Advanced Processor Architectures
K. Sano



High Performance Big Data Systems
K. Sato



Parallel Numerical Technology
T. Imamura

From April 2022

High Performance AI Systems
Mohamed WAHIB

New Teams JFY2022 (plan)

**(New Team)
Supercomputing Performance Research**

**(New Team)
S5-Digital twin**



Director
S. Matsuoka

Computational Science



Field Theory
Y. Aoki



Biophysics
Y. Sugita



Data Assimilation
T. Miyoshi



Discrete Event Simulation
N. Ito



Climate Science
H. Tomita



Structural Biology
F. Tama



Molecular Science
T. Nakajima



HPC Engineering Applications
M. Tsubokura



Disaster Mitigation & Reduction
S. Oishi



Quantum Physics
S. Yunoki



Deputy Director
K. Nakajima

HPC-and AI-driven Drug Development Platform Division



Biomedical Computational Intelligence Unit
Yasushi Okuno



Medicinal Chemistry Applied AI Unit
Teruki Honma



Molecular Design Computational Intelligence Unit
Mitsunori Ikeguchi



AI-driven Drug Discovery Collaborative Unit
Yasushi Okuno

Office of the Fugaku Society 5.0 initiative



Director
S. Matsuoka



Deputy Director
M. Shinano

Operations and Computer Technologies



Facility Operations & Development
T. Tsukamoto



System Operations & Development
A. Uno



Software Development Technology Unit
H. Murai



HPC Usability Development
F. Shoji



Advanced Operation Technologies
K. Yamamoto

The "Fugaku" 富岳 "Exascale" "Applications First" Supercomputer for Society 5.0

*Mt. Fuji representing
the ideal of supercomputing*

High-Peak --- Acceleration of
Large Scale Application
(Capability)

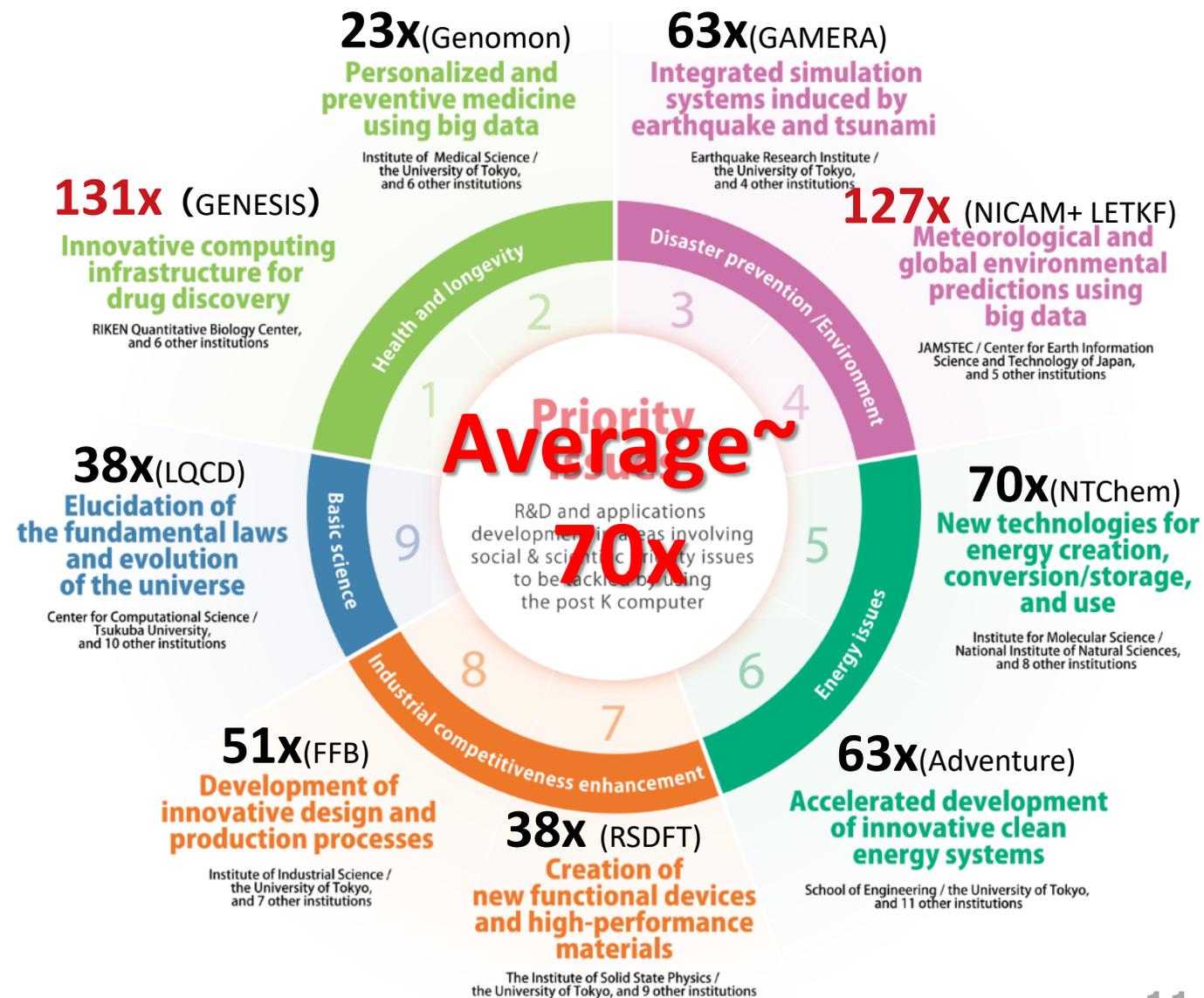


Broad Base --- Applicability & Capacity
Broad Applications: Simulation, Data Science, AI, ...
Broad User Base: Academia, Industry, Cloud Startups, ...
For Society 5.0

“Applications First” Exascale R&D

Fugaku Target Applications – Priority Research Areas

- **Advanced Applications Co-Design Program to Parallel Fugaku R&D**
- **Select one representative app from 9 priority areas**
 - Health & Medicine
 - Environment & Disaster
 - Energy
 - Materials & Manufacturing
 - Basic Sciences
- **Up to 100x speedup c.f. K-Computer => achieved!**



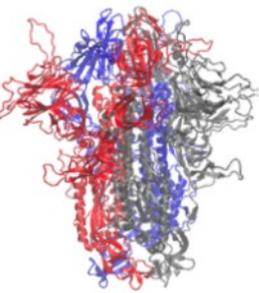
MEXT Fugaku Program: Fight Against COVID19

Fugaku resources made available a year ahead of general production
(more research topics under international solicitation,
also joined US-lead COVID-19 High Performance Computing Consortium)



Medical-Pharma

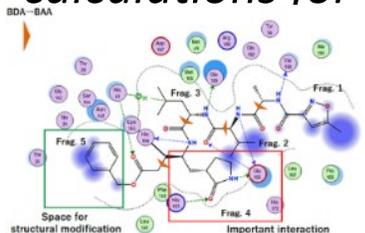
Prediction of conformational dynamics of proteins on the surface of SARS-Cov-2



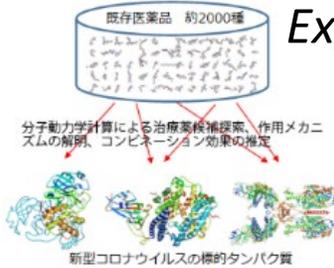
GENESIS MD to interpolate unknown experimentally undetectable dynamic behavior of spike proteins, whose static behavior has been identified via Cryo-EM

((Yuji Sugita, RIKEN))

Fragment molecular orbital calculations for COVID-19 proteins



(Yuji Mochizuki, Rikkyo University)



Exploring new drug candidates for COVID-19

Large-scale MD to search & identify therapeutic drug candidates showing high affinity for COVID-19 target proteins from 2000 existing drugs

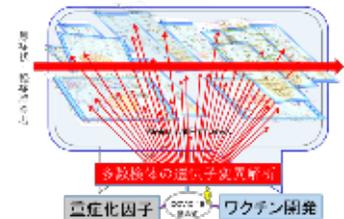
(Yasushi Okuno, RIKEN / Kyoto University)



Host genetic analysis for severe COVID-19

Whole-genome sequencing of severe cases of COVID-19 and mild or asymptomatic infections, and identify risk-associated genetic variants for severe disease

(Satoru Miyano, Tokyo Medical and Dental University)



Societal-Epidemiology

Prediction and Countermeasure for Virus Droplet Infection under the Indoor Environment



Simulation analysis of pandemic phenomena

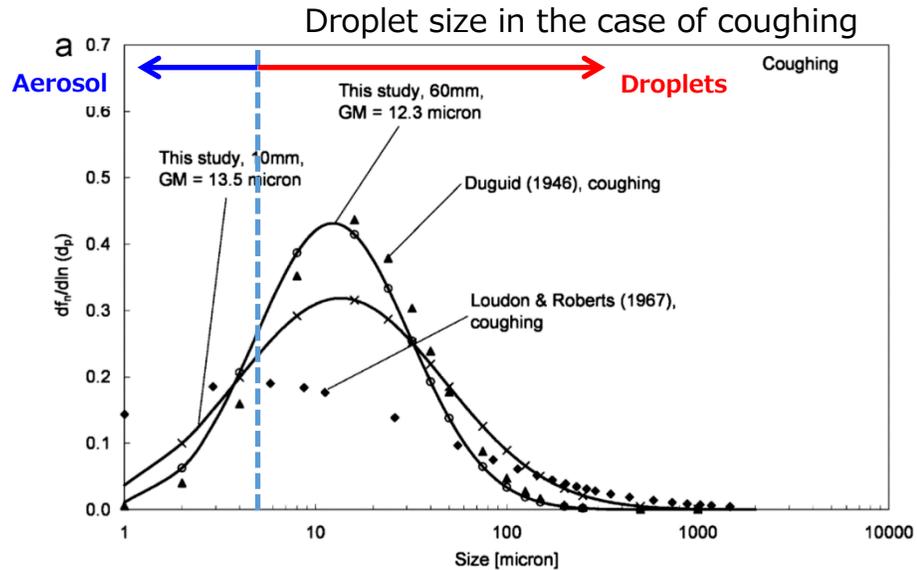
Combining simulations & analytics of disease propagation w/contact tracing apps, economic effects of lockdown, and reflections social media, for effective mitigation policies

(Nobuyasu Ito, RIKEN)



Difficulty in COVID 19 transmission

- Basically the risk of airborne transmission can be determined by four factors:
 - Behavior (breathing, speaking, singing...), Staying time, Room volume, Ventilation rate
- How droplets disperse in the air?



- COVID 19 does not cause as strong airborne infections as tuberculosis and measles, and thought to be at high risk of inhaling droplets especially smaller than 5 microns at close range to the infected person.
- Evaluation based on “instantaneous homogeneous dispersion” does not work!

International Collaborations (1)

- **ADAC (Accelerated Data Analysis Computing Institute)**

The purpose of ADAC is to collaborate and leverage their respective investments in application software readiness in order to expand the breadth of applications capable of running on accelerated architectures.

- Partners: Oak Ridge National Laboratory (ORNL), Lawrence Livermore National Laboratory (LLNL), **ETH Zurich**, Jülich Supercomputing Centre, Tokyo Institute of Technology, The University of Tokyo, Argonne National Laboratory and RIKEN.

- Workshop:

12th ADAC Virtual Workshop, in August 2022

11th ADAC Virtual Workshop, in Jan. 2022

10th ADAC Virtual Workshop, in May 2021

9th ADAC Virtual Workshop, in September 2020

8th ADAC Workshop, Kashiwa, Japan in Oct, 2019

7th ADAC Workshop, Tennessee, USA in March 2019



International Collaborations (2)

● International HPC Summer School

The summer school familiarize the best students in computational sciences with major state-of-the-art aspects of HPC for a variety of scientific disciplines, catalyze the formation of networks, provide advanced mentoring, facilitate international exchange and open up further career options.

● Partners:



PRACE (Partnership for Advanced Computing in Europe)

XSEDE (The Extreme Science and Engineering Discovery Environment)

SciNet (University of Toronto)

RIKEN (RIKEN Center for Computational Science)

● Events (Past 5 years) :

Athens, Greece in June 2022 (upcoming)

Digital event in July 2021

Kobe, Japan in 2019

Ostrava, Czech Republic in 2018

Boulder, Colorado in 2017

Ljubljana, Slovenia in 2016

Toronto, Canada in 2015



Researcher Development 1

- **RIKEN International HPC Summer School (2018-)**
For early-career researchers in computational science
Scientists from R-CCS provide lectures in English, and the supercomputer Fugaku is used for hands-on training. Now we are opening a call for the FY2022 virtual school.

Application deadline: 5 pm, July 22, 2022(JST); see <https://www.r-ccs.riken.jp/en/outreach/schools/20220912-1/>

- **KOBE Spring (2014-) and Summer School (2011-)**
Five days at Kobe Univ., Hyogo Pref. Univ., or R-CCS to learn the basics of programming for parallel computing. For graduate students and post-docs, and technical college students in Japan
About 20-30 participants every year



- **EU-ASEAN HPC school (2021-)**

<https://www.hpcschool.net/>

Co-supported sending lectures and hands-on sessions on the Fugaku system



- **International Internship Program (2017-)**

Three months at R-CCS Research Division

Approximately five graduate students will participate.

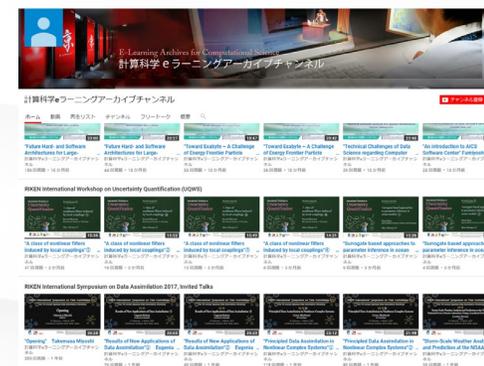
Unfortunately, the program was suspended due to the Covid19 outbreak in FY2021. We partly accept online/on-site participation in this year; please contact us.



- **E-Learning Website (2014-)**

Online, Videos of lectures, presentations, hands-on and slides on the web

The main target is graduate students





Thank you

**Further information
will be provided by consulting during this summer school and
online/virtual consulting the school afterward.**

**For example,
Fostering programs, internships, schools, and job
opportunities**