

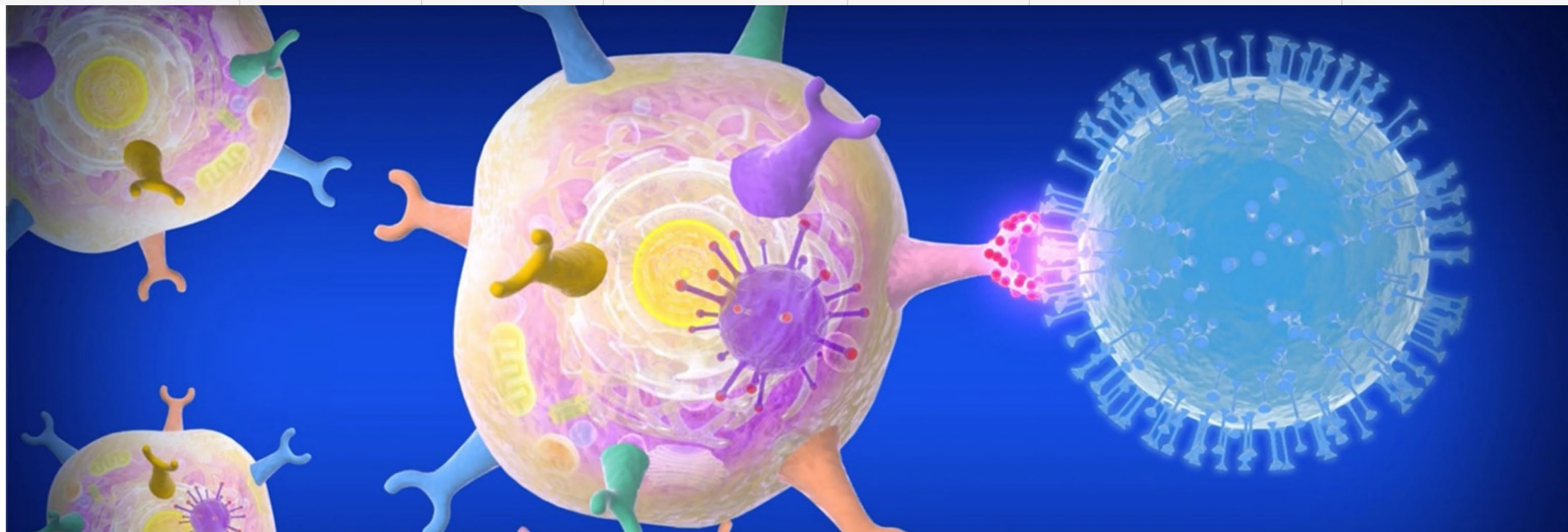
RIKEN  
Center for  
Computational  
Science

Toshiyuki Imamura

20 June 2022, IHPCSS2022 @ Athens







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



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

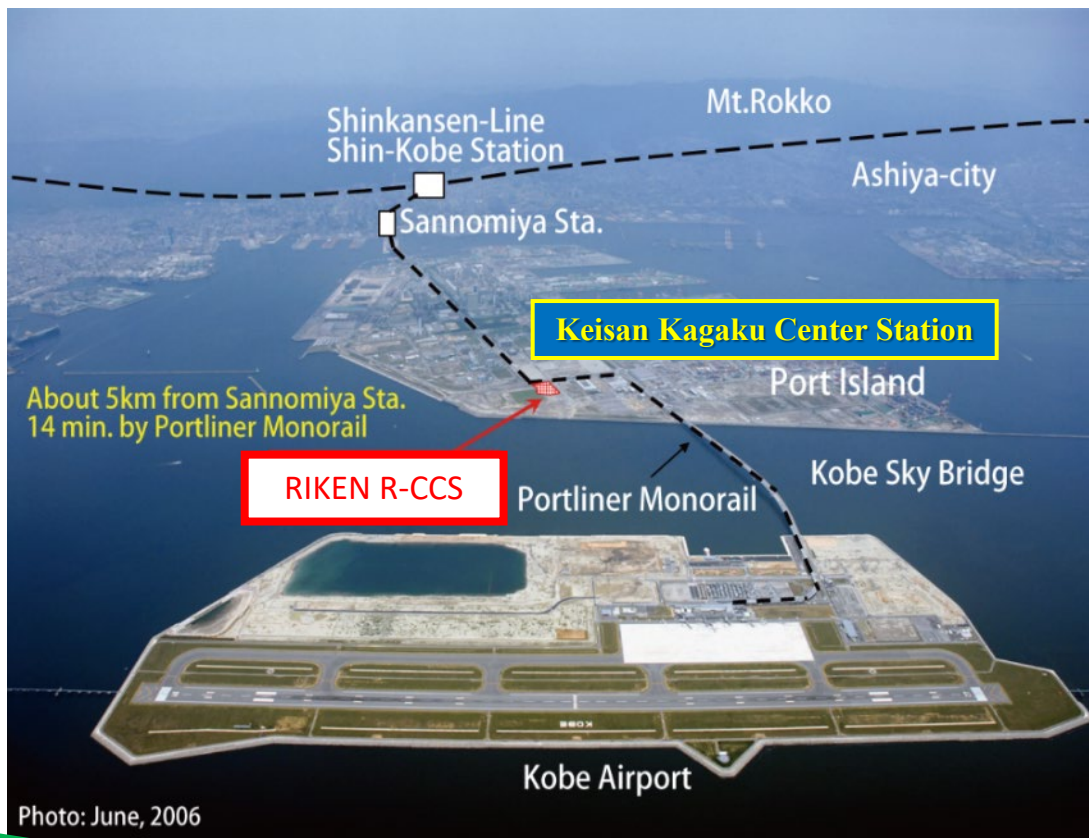
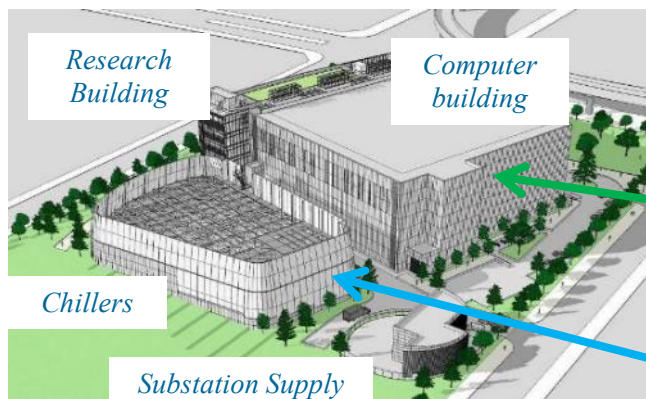
[COVID-19 Measures at RIKEN \(Updated on June 13, 2022\)](#)



# R-CCS with Supercomputer Fugaku



423 km (263 miles)  
west of Tokyo



**Computer room 50 m x 60 m = 3,000 m<sup>2</sup>**  
**Electric power up to 37 MW**  
**Water cooling system**

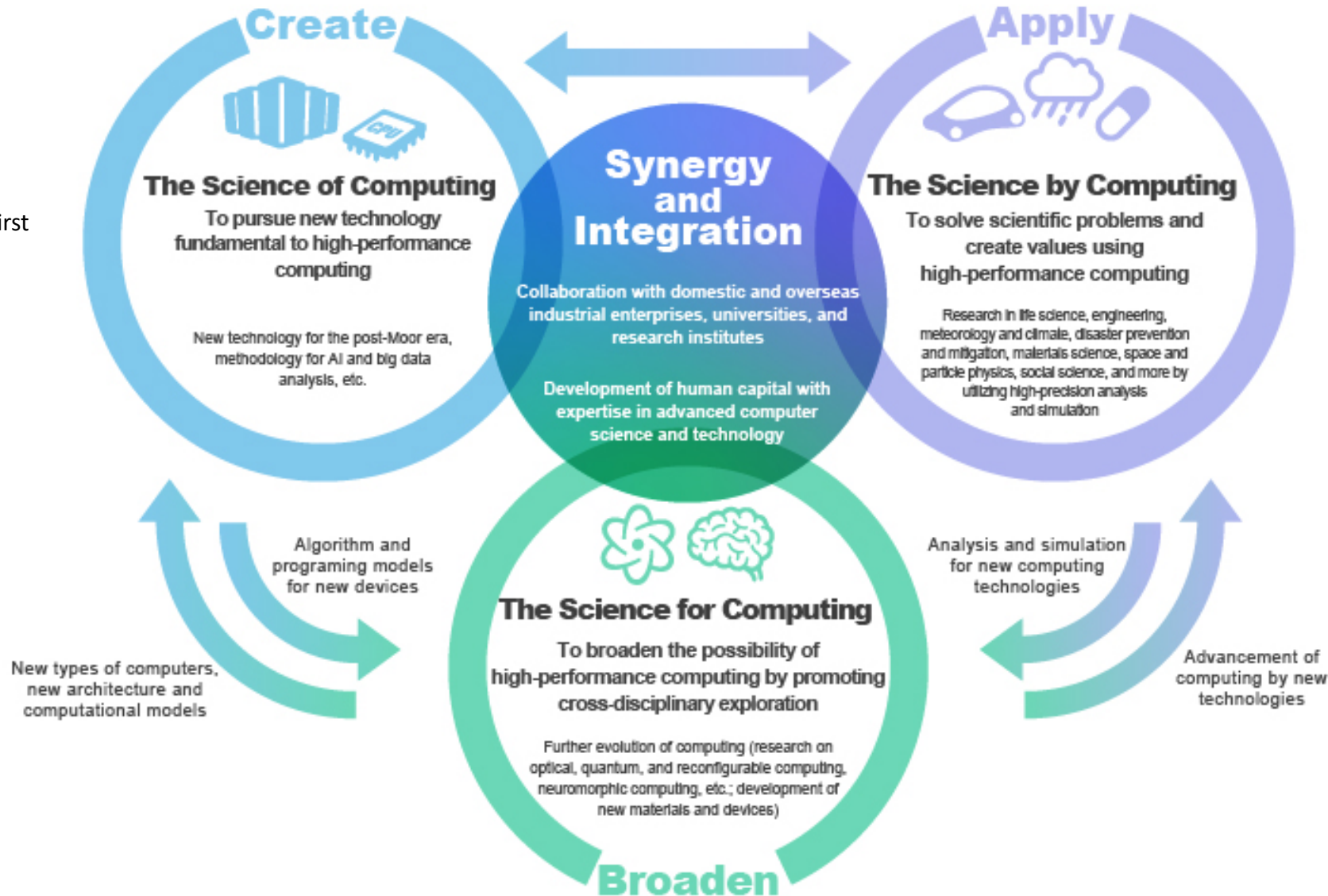
**Gas-turbine co-generation 5 MW x 2**



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



Advanced Processor  
Architectures  
K. Sano



Parallel Numerical  
Technology  
T. Imamura

New Teams JFY2022 (plan)

(New Team)  
Supercomputing  
Performance Research

(New Team)  
S5-Digital twin

From April 2022



High Performance  
AI Systems  
Mohamed WAHIB



Director  
S. Matsuoka

Computational Science



Field Theory  
Y. Aoki



Discrete Event  
Simulation  
N. Ito



Molecular  
Science  
T. Nakajima



Quantum  
Physics  
S. Yunoki



Biophysics  
Y. Sugita



Climate  
Science  
H. Tomita



HPC  
Engineering  
Applications  
M. Tsubokura



Data  
Assimilation  
T. Miyoshi



Structural  
Biology  
F. Tama



Disaster  
Mitigation &  
Reduction  
S. Oishi



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)



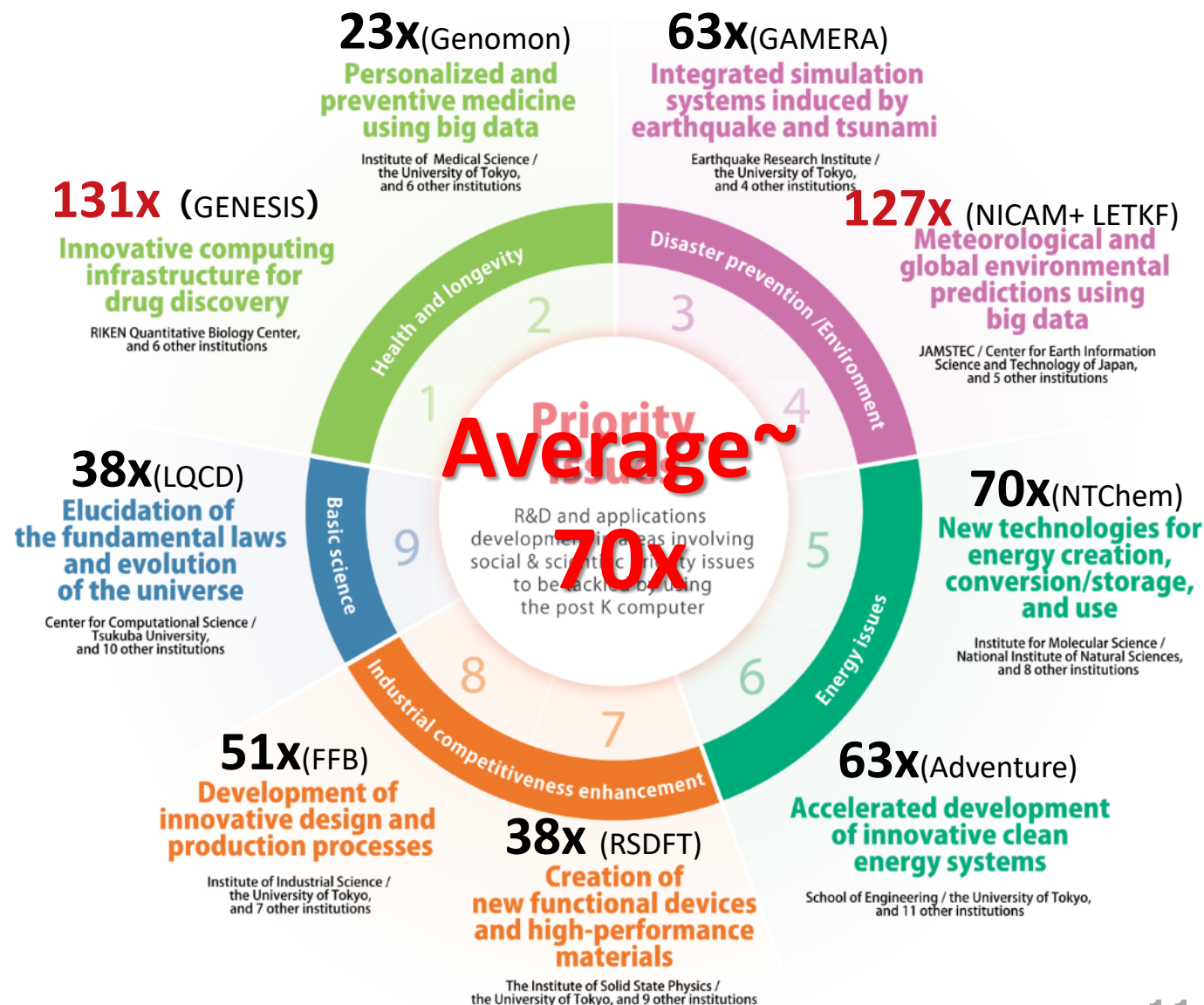
**Broad Base --- Applicability & Capacity**  
**Broad Applications: Simulation, Data Science, AI, ...**  
**Broad User Base: Academia, Industry, Cloud Startups, ...**  
**For Society 5.0**



# “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

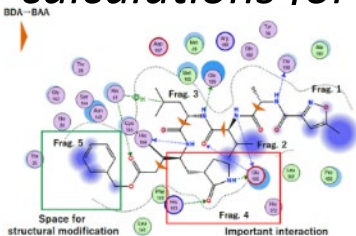
*Prediction of conformational dynamics of proteins on the surface of SARS-Cov-2*



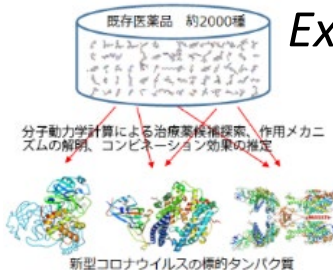
GENESIS MD to interpolate unknown experimentally undetectable dynamic behavior of spike proteins, whose static behavior has been identified via Cryo-EM

((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

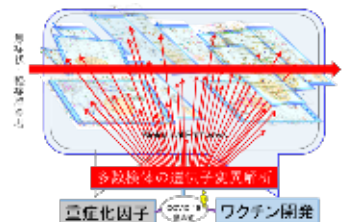
(Yasushi Okuno, RIKEN / Kyoto University)



*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*

Massive parallel simulation of virus droplet scattering and hat transmission in indoor environment, trains, office, hospital room  
(Miyazaki University)



*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

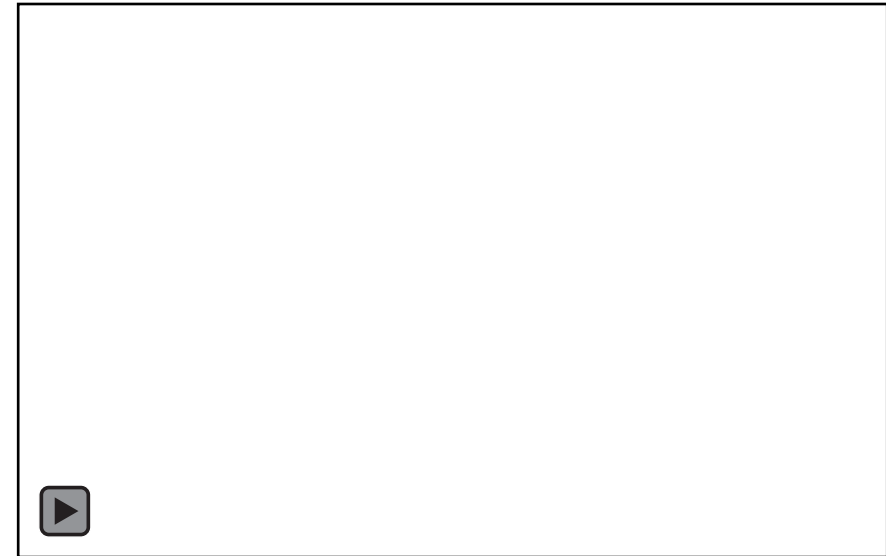
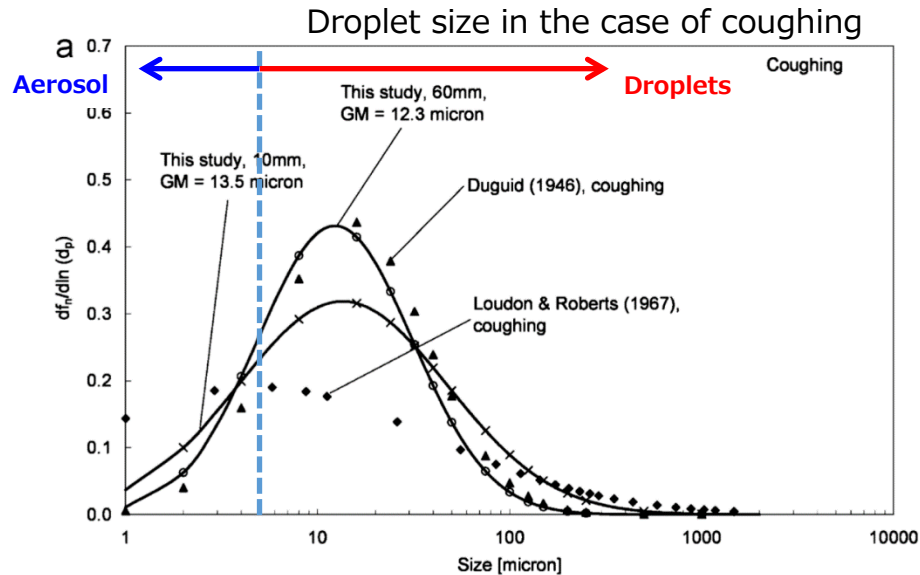
(Nobuyasu Ito, RIKEN)





# 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





# Researcher Development 2

- **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.

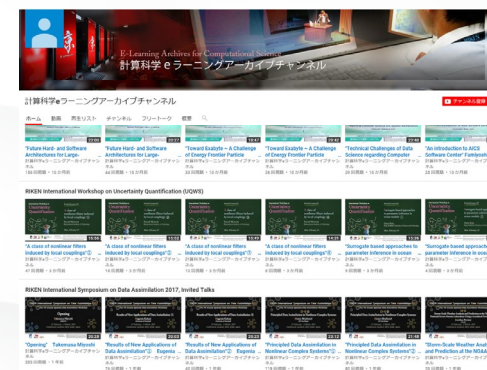
**Unfortunately, the program was suspended due to the Covid19 outbreak in FY2021. We partly accept online/on-site participation in this year; please contact us.**



- **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**