

## Press Release



April 7, 2021

The Representative for HPCI operation  
Research Organization for Information Science and Technology (RIST)

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### HPCI Urgent Call for Fighting against Infectious Diseases including COVID-19

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**Continuing from FY 2020, the call for proposals for the use of HPCI computational resources <sup>(\*)</sup> to fight against COVID-19 was issued on April 7. In FY 2021, the target research areas are expanded from COVID-19 to infectious diseases in general. HPCI supports researches on countermeasures using supercomputers against infectious diseases.**

In corporation with associating institutions, Research Organization for Information Science and Technology (RIST, President: Dr. Yasuhide Tajima), as the Representative for HPCI operation, opened the call for proposals for using HPCI resources other than Fugaku to fight against infectious diseases including COVID-19. The call is open throughout the year from April 7.

For Fugaku projects, the priority area "Research and development of infectious disease control" is set in the General Access projects in Period-B of FY 2021.

There is an urgent need for a wide range of research areas, such as bioinformatics, drug discovery and epidemiology, to fight against COVID-19. Contribution of supercomputers with ultrafast computing capability and massive amount of computational capacity are expected.

HPCI has opened the call for projects fighting against COVID-19 since 2020, targeting the use both from academia and industry. In FY 2020, 16 proposals were submitted, and 14 projects shown in the Attachment 1 was awarded. Achievements have already been reported in research areas with great urgency. Receiving continuing cooperation from associating institutions, it has been decided to open the call to provide computational resources with variety for free of charge.

The overview and the schedule are as shown below. For details, please visit the HPCI portal site:  
[https://www.hpci-office.jp/pages/e\\_hpci\\_infect](https://www.hpci-office.jp/pages/e_hpci_infect)

#### <Summary of call for proposals>

- Name of the Call : HPCI Urgent Call for Fighting against Infectious Diseases including COVID-19 for Applications
- Project Theme : Projects requiring computational resources that contribute to research on infectious disease control including COVID-19
- Resources : As shown in the table below
- Call opens : April 7, 2021
- Submission : Open throughout the year from April 14, 2021
- Project period : Up to one year until the end of March 2022
- Usage charge : Free

- User report : Submission of user report. The submitted report will be published on the HPCI portal site.
- Publication of research achievement : It is not mandatory to make reviewed publication. However, considering the intention of this call, it is expected to publicize the research achievements quickly by means of refereed papers, press release, or equivalent.

<Available HPCI supercomputers>

	Organizations engaging in the HPCI system operation	Supercomputer
1	Information Initiative Center, Hokkaido University	Grand Chariot, Polaire
2	Cyberscience Center, Tohoku University	AOBA-A (SX-Aurora TSUBASA) AOBA-B (LX406Rz-2)
3	Center for Computation Sciences, University of Tsukuba	Cygnus
4	Joint Center for Advanced High Performance Computing (JCAHPC)	Oakforest-PACS
5	Information Technology Center, The University of Tokyo	Oakbridge-CX, Wisteria-O (Odyssey)
6	Global Scientific Information and Computing Center, Tokyo Institute of Technology	TSUBAME3.0
7	Information Technology Center, Nagoya University	Type I Subsystem (FX1000), Flow Type II Subsystem (CX2570)
8	Academic Center for Computing and Media Studies (ACCMS), Kyoto University	Supercomputer Cray XC40 (SystemA)
9	Cybermedia Center, Osaka University	SQUID, OCTOPUS
10	Research Institute for Information Technology, Kyushu University	Supercomputer system ITO
11	Japan Agency for Marine-Earth Science and Technology	Earth Simulator (ES4)
12	National Institute of Advanced Industrial Science and Technology	AI Bridging Cloud Infrastructure (ABCI)
13	The University of Tokyo (Eastern Hub) / RIKEN (R-CCS) (Western Hub)	HPCI Shared Storage

(\*) HPCI (The innovative High-Performance Computing Infrastructure)

HPCI is a research platform that connects supercomputers installed at national universities and research institutions, including the supercomputer Fugaku from RIKEN R-CCS, with a high-speed network (SINET5\*) to realize an innovative shared computational environment that accommodates diversified needs of the users. For details, please see the HPCI portal site (<https://www.hpci-office.jp/folders/english>).

Note that the target of this call is for projects using HPCI computational resources other than Fugaku.

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Attachment 1: HPCI Covid-19 Research Access Projects Awarded for Using HPCI System in FY 2020

Project ID	Project Name	Project Representative	Affiliation (Organization / Department)	Country Name	Provider Name / Resource Name		Awarded Resources (Node Hours)
hp200142	Molecular dynamics simulation of COVID-19 virus RNA polymerase and its inhibitor candidates	Hisashi Okumura	National Institutes of Natural Sciences, Institute for Molecular Science	Japan	Global Scientific Information and Computing Center, Tokyo Institute of Technology	Cloudy, Big-Data and Green Supercomputer "TSUBAME3.0"	18,000
hp200145	Detail analysis of RNA modification from COVID19 nanopore sequence data	Hiroki Ueda	The University of Tokyo	Japan	National Institute of Advanced Industrial Science and Technology (AIST)	ABCI (AI Bridging Cloud Infrastructure)	14,000
hp200146	Fragment molecular orbital calculations on the main protease of COVID-19	Yuji Mochizuki	Rikkyo University	Japan	Joint Center for Advanced High Performance Computing (JCAHPC)	Oakforest-PACS	100,000
hp200147	Fragment molecular orbital calculations on the spike protein of COVID-19	Yuji Mochizuki	Rikkyo University	Japan	Research Institute for Information Technology, Kyushu University	ITO Subsystem A <Fixed-node>	75,000
hp200148	Computer-assisted search for inhibitory agents for SARS-CoV-2	Tyuji Hoshino	Chiba University	Japan	Information Technology Center, The University of Tokyo	Oakbridge-CX	34,560
hp200149	Study on the evaluation of arrhythmogenic risk of COVID-19 candidate drugs: chloroquine, hydroxychloroquine	Toshiaki Hisada	UT-Heart Inc.	Japan	Joint Center for Advanced High Performance Computing (JCAHPC)	Oakforest-PACS	336,000

Project ID	Project Name	Project Representative	Affiliation (Organization / Department)	Country Name	Provider Name / Resource Name		Awarded Resources (Node Hours)
	and azithromycin and its reduction measures						
hp200151	Structure modeling of SARS-CoV-2 related proteins	Takashi Ishida	Tokyo Institute of Technology	Japan	Global Scientific Information and Computing Center, Tokyo Institute of Technology	Cloudy, Big-Data and Green Supercomputer "TSUBAME3.0"	3,000
hp200152	Developing Inhibitors for COVID-19 Endoribonuclease Oligomerization	Akio Kitao	Tokyo Institute of Technology	Japan	Global Scientific Information and Computing Center, Tokyo Institute of Technology	Cloudy, Big-Data and Green Supercomputer "TSUBAME3.0"	18,000
hp200153	Prediction of dynamical structure of Spike protein of SARS-COVID19	Yuji Sugita	RIKEN	Japan	Joint Center for Advanced High Performance Computing (JCAHPC)	Oakforest-PACS	350,000
hp200154	Prediction and Countermeasure for virus droplet Infection under Indoor Environment: Case studies for massively-parallel simulation on Fugaku	Makoto Tsubokura	Kobe University	Japan	Information Technology Center, The University of Tokyo	Oakbridge-CX	172,800
hp200155	MD-based screening of drugs with novel action mechanism against COVID-19	Yasushi Okuno	Koto University	Japan	Center for Computational Sciences, University of Tsukuba	Cygnus	47,000

Project ID	Project Name	Project Representative	Affiliation (Organization / Department)	Country Name	Provider Name / Resource Name		Awarded Resources (Node Hours)
hp200156	Integrated in silico repositioning for anti-viral Covid-19 related proteins.	Yasuteru Shigeta	University of Tsukuba	Japan	Center for Computational Sciences, University of Tsukuba	Cygnus	16,000
hp200157	Spreading of polydisperse droplets in a turbulent puff of saturated exhaled air	Marco Edoardo Rosti	Okinawa Institute of Science and Technology Graduate University	Japan	Information Technology Center, The University of Tokyo	Oakbridge-CX	110,400
hp200158	Comprehensive analysis of infection rate reduction and movement restriction effect on virus transmission using multi agent simulation	Masaki Onishi	National Institute of Advanced Industrial Science and Technology (AIST)	Japan	National Institute of Advanced Industrial Science and Technology (AIST)	ABCI (AI Bridging Cloud Infrastructure)	30,000