

Supercomputers and Applications: ITC/JCAHPC The University of Tokyo



SC20

Atlanta, GA | more
than hpc.



東京大学
THE UNIVERSITY OF TOKYO

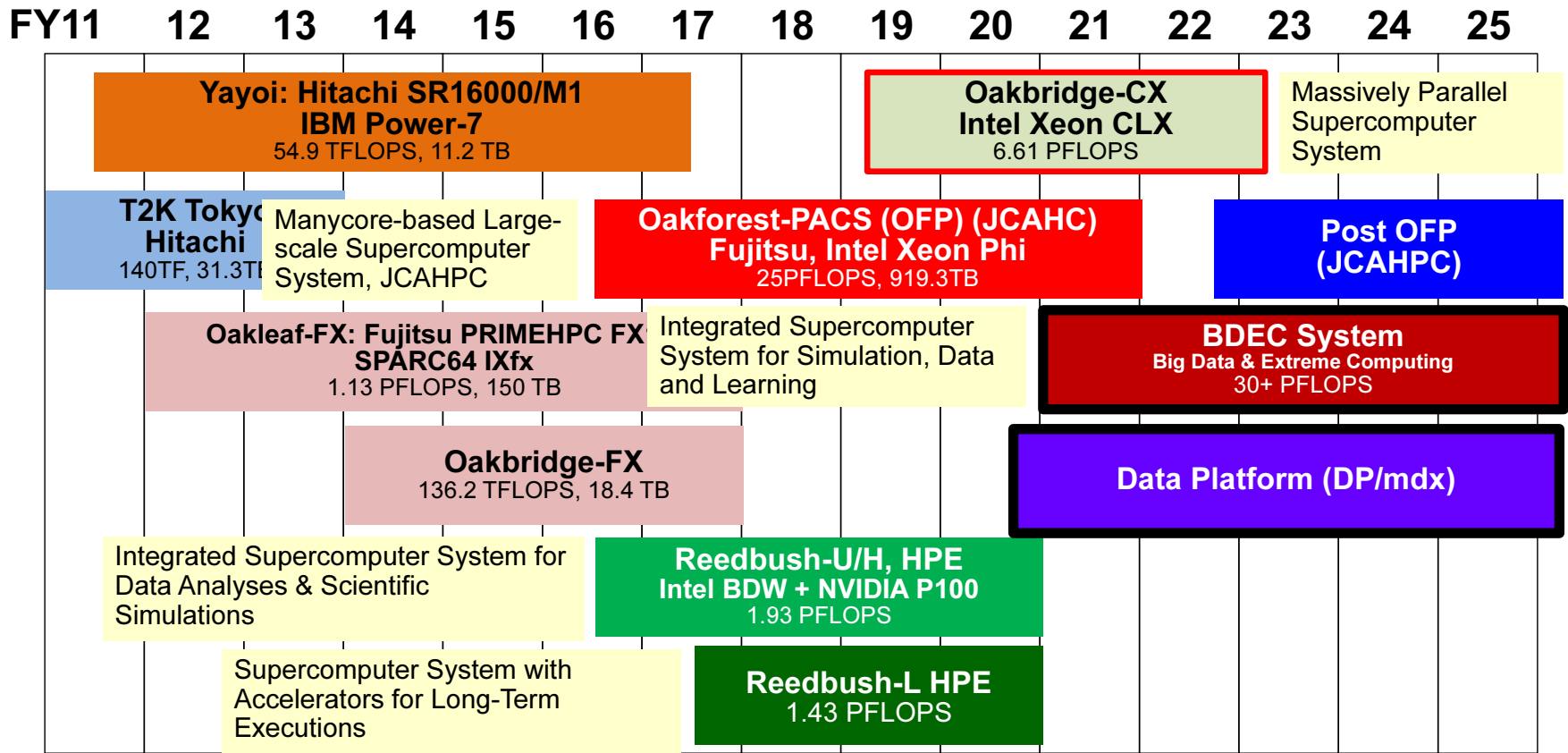


東京大学情報基盤センター
INFORMATION TECHNOLOGY CENTER, THE UNIVERSITY OF TOKYO

Supercomputing Research Division
Information Technology Center
The University of Tokyo

Supercomputers in ITC/U.Tokyo

Information Technology Center, The University of Tokyo



Now operating 3 Systems

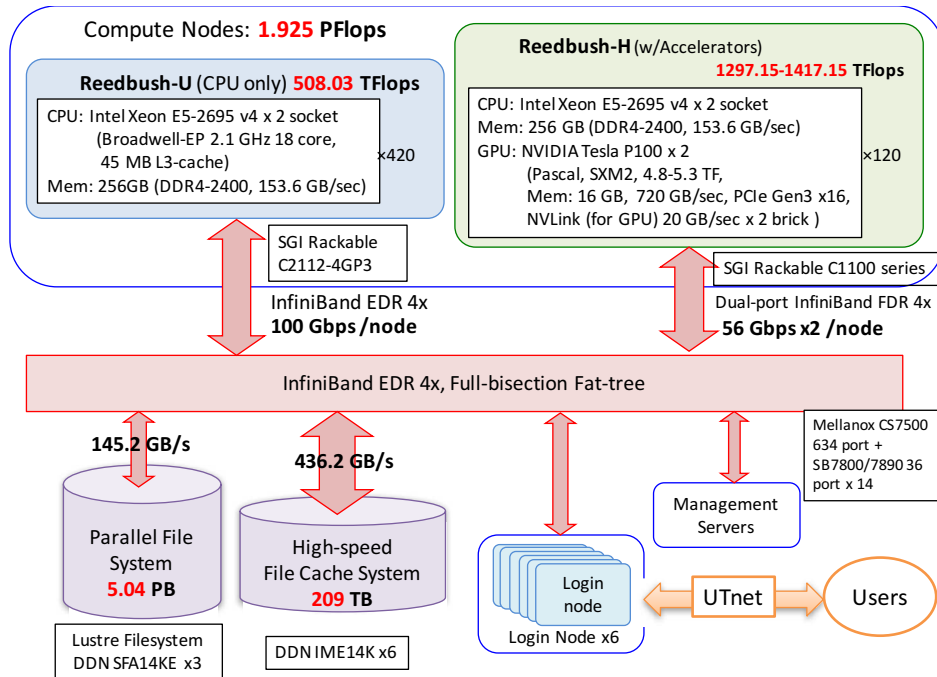
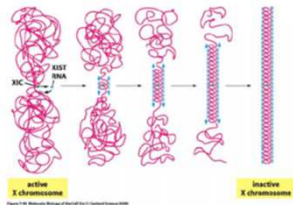
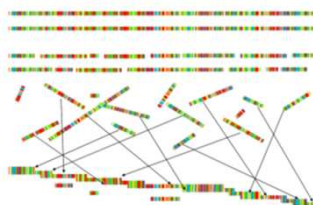
2,600+ users (55+% from outside of U.Tokyo)

- **Reedbush (HPE, Intel BDW + NVIDIA P100 (Pascal))**
 - Integrated Supercomputer Sys. for Data Analyses & Scientific Simulations
 - Jul.2016-Mar.2021
 - Our first GPU System, DDN IME (Burst Buffer)
 - Reedbush-U: CPU only, 420 nodes, 508 TF (Jul.2016, retired on June 30)
 - Reedbush-H: 120 nodes, 2 GPUs/node: 1.42 PF (Mar.2017)
 - Reedbush-L: 64 nodes, 4 GPUs/node: 1.43 PF (Oct.2017)
- **Oakforest-PACS (OFP) (Fujitsu, Intel Xeon Phi (KNL))**
 - JCAHPC (U.Tsukuba & U.Tokyo)
 - 25 PF, #18 in 55th TOP 500 (June 2020) (#3 in Japan)
 - Omni-Path Architecture, DDN IME (Burst Buffer)
- **Oakbridge-CX (OBCX) (Fujitsu, Intel Xeon Platinum 8280, CLX)**
 - Massively Parallel Supercomputer System
 - 6.61 PF, #60 in 55th TOP 500, July 2019-June 2023
 - SSD's are installed to 128 nodes (out of 1,368)



Reedbush: Our First System with GPU's

- Improvement of OpenACC
 - Similar Interface as OpenMP
 - Research Collaboration with NVIDIA Engineers
- Data Science, Deep Learning
 - New types of users other than traditional CSE (Computational Science & Engineering) are needed



Oakforest-PACS (OFP): KNL & OPA



- 8,208 Intel Xeon/Phi (KNL), 25 PF Peak Performance
 - Fujitsu, Full operation started in December 2016
- **TOP 500 #18 (#3 in Japan), HPCG #11 (#3) (June 2020)**
- **JCAHPC: Joint Center for Advanced High Performance**

Computing

- University of Tsukuba
- University of Tokyo
- <http://jcahpc.jp>



筑波大学
University of Tsukuba



東京大学
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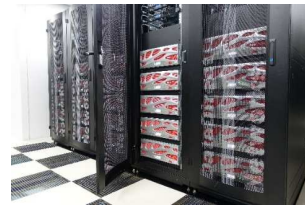
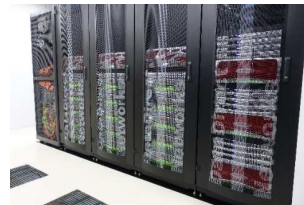


JCAHPC

- **In spite of KNL & OPA, still an excellent system for R&D on SW/Algorithms for large-scale computing**

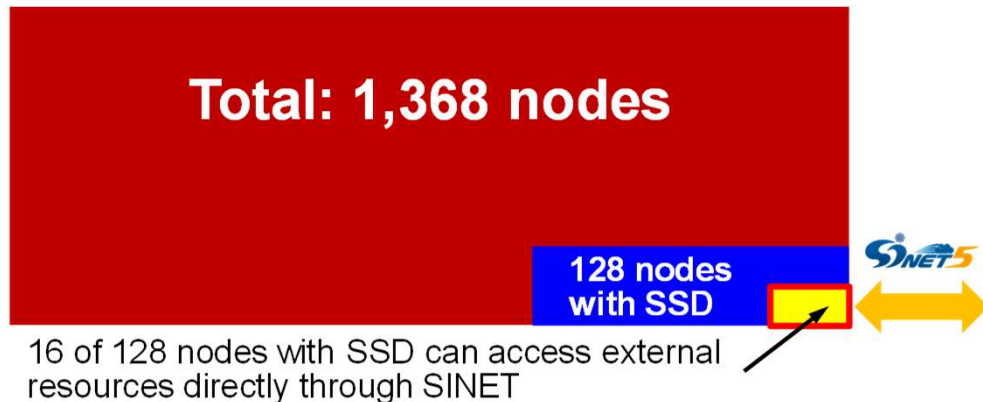
• File I/O

- Shared File System: Lustre, 26PB
- File Cache System : (DDN IME, Burst Buffer):
1+TB/sec Performance for IOR Benchmarks

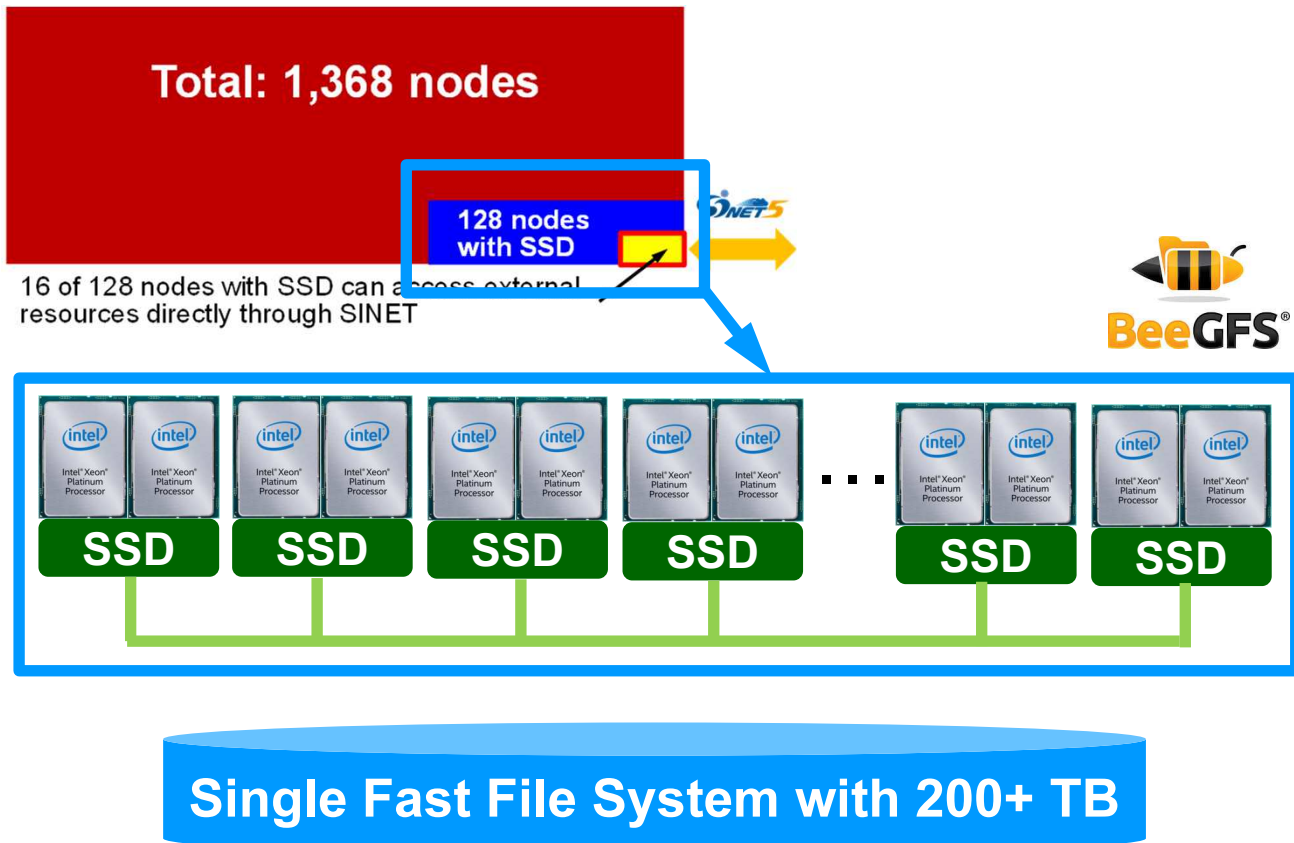


Oakbridge-CX (OBCX)

- Intel Xeon Platinum 8280 (Cascade Lake, CLX), Fujitsu
 - 1,368 nodes, 6.61 PF peak, 385.1 TB/sec, 4.2+ PF for HPL
 - #60 in 55th Top500 (June 2020)**
 - **Fast Cache: SSD's for 128 nodes: Intel SSD, BeeGFS: 200+TB Fast FS**
 - 1.6 TB/node, 3.20/1.32 GB/s/node for R/W
 - Staging, Check-Pointing, Data Intensive Application
 - **16 of these nodes can directly access external resources (server, storage, sensor network etc.) through SINET**
 - Network: Intel Omni-Path, 100 Gbps, Full Bi-Section
 - Storage: DDN EXAScaler (Lustre) 12.4 PB, 193.9 GB/sec
 - Power Consumption: 950.5 kVA
- **Operation Start: July 1st, 2019**



128xSSD's: Single Fast File System



55th TOP500 List (June, 2020)

<http://www.top500.org/>

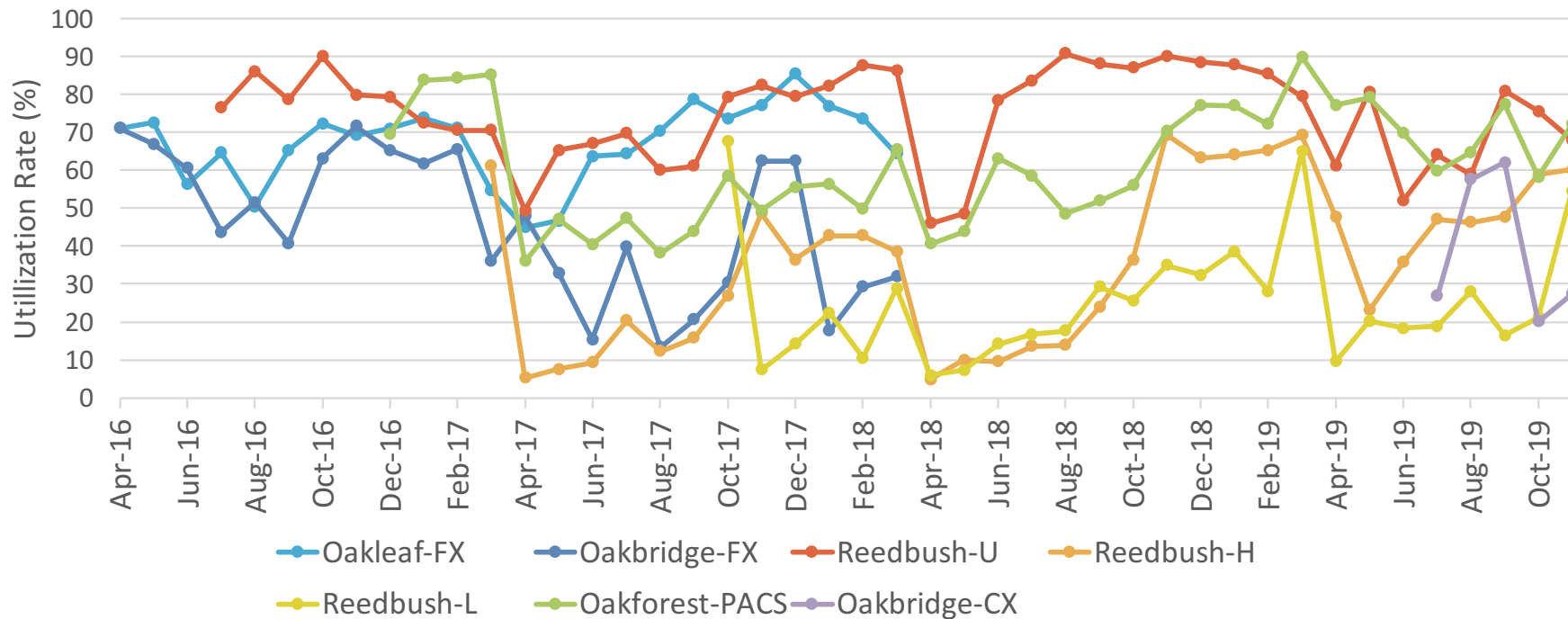
	Site	Computer/Year Vendor	Cores	R _{max} (TFLOPS)	R _{peak} (TFLOPS)	Power (kW)
1	<u>Supercomputer Fugaku, 2020, Japan</u> RIKEN Center for Computational Science (R-CCS)	Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu	7,299,072	415,530 (= 415.53 PF)	513,854.7	28,335
2	<u>Summit, 2018, USA</u> DOE/SC/Oak Ridge National Laboratory	IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband	2,414,592	148,600	200,795	10,096
3	<u>Sieera, 2018, USA</u> DOE/NNSA/LLNL	IBM Power System S922LC, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband	1,572,480	94,640	125,712	7,438
4	<u>Sunway TaihuLight, 2016, China</u> National Supercomputing Center in Wuxi	Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway	10,649,600	93,015	125,436	15,371
5	<u>Tianhe-2A, 2018, China</u> National Super Computer Center in Guangzhou	TH-IVB-FEP Cluster, Intel Xeon E5-2692v2 12C 2.2GHz, TH Express-2, Matrix-2000	4,981,760	61,445	100,679	18,482
6	<u>HPC5, 2020, Italy</u> Eni S.p.A (Ente Nazionale Idrocarburi)	PowerEdge C4140, Xeon Gold 6252 24C 2.1GHz, NVIDIA Tesla V100, Mellanox HDR Infiniband, Dell EMC	669,760	35,450	51,720.8	2,252
7	<u>Selene, 2020, USA</u> NVIDIA Corporation	DGX A100 SuperPOD, AMD EPYC 7742 64C 2.25GHz, NVIDIA A100, Mellanox HDR Infiniband	277,760	27,580	34,568.6	1,344
8	<u>Frontera, 2019, USA</u> Texas Advanced Computing Center	Dell C6420, Xeon Platinum 8280 28c 2.7GHz, Mellanox Infiniband HDR	448,448	23,516	38,746	
9	<u>Marconi-100, 2020, Italy</u> CINECA	IBM Power System AC922, IBM POWER9 16C 3GHz, Nvidia Volta V100, Dual-rail Mellanox EDR Infiniband	347,776	21,640	29,354	1,476
10	<u>Piz Daint, 2017, Switzerland</u> Swiss National Supercomputing Centre (CSCS)	Cray XC50, Xeon E5-2690v3 12C 2.6GHz, Aries interconnect , NVIDIA Tesla P100	387,872	21,230	27,154	2,384
18	<u>Oakforest-PACS, 2016, Japan</u> Joint Center for Advanced High Performance Computing	PRIMERGY CX1640 M1, Intel Xeon Phi 7250 68C 1.4GHz, Intel Omni-Path	556,104	13,556	24,913	2,719

HPCG Ranking (June, 2020)

<http://www.top500.org/>

	Computer	Cores	HPL Rmax (Pflop/s)	TOP500 Rank	HPCG (Pflop/s)
1	Fugaku	7,299,072	415.530	1	13.400
2	Summit	2,414,592	148.600	2	2.926
3	Sierra	1,572,480	94.640	3	1.796
4	HPC5	669,760	35.450	6	0.860
5	Trinity	979,072	20.159	11	0.546
6	Selene	277,760	27.580	7	0.509
7	ABCI	391,680	19.880	12	0.509
8	Piz Daint	387,872	21.230	10	0.497
9	Sunway TaihuLight	10,649,600	93.015	4	0.481
10	Nurion (KISTI, Korea)	570,020	13.929	17	0.391
11	Oakforest-PACS	556,104	13.555	18	0.385

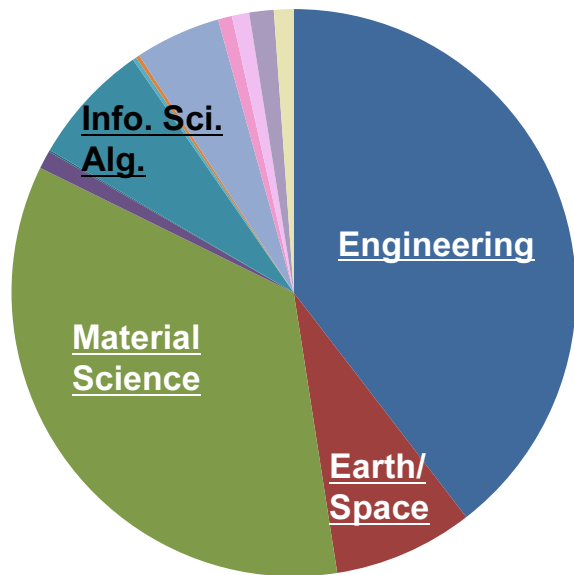
Utilization Rate (Apr. 2016 - Nov. 2019)



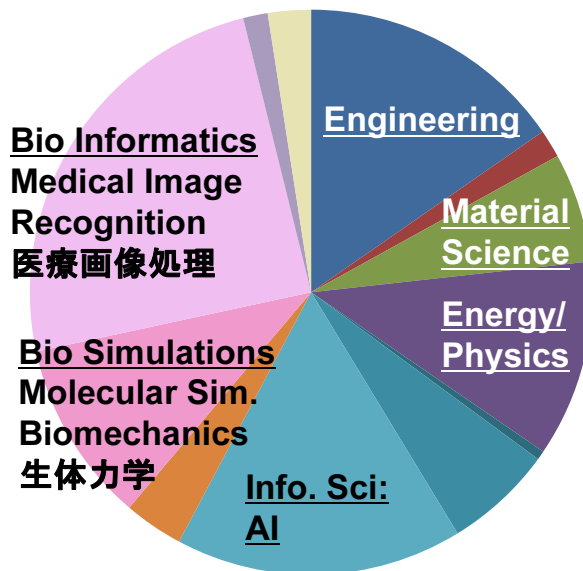
JPY (=Watt)/GFLOPS, GFLOPS/W (Green 500)

System	JPY/GFLOPS Small is Good	GFLOPS/W Large is Good
Oakleaf-FX/Oakbridge-FX (Fujitsu) (Fujitsu SPARC64 IXfx)	125	0.8663
Reedbush-U (HPE) (Intel BDW)	61.9	2.310
Reedbush-H (HPE) (Intel BDW+NVIDIA P100x2/node)	15.9	8.575
Reedbush-L (HPE) (Intel BDW+NVIDIA P100x4/node)	13.4	10.167
Oakforest-PACS (Fujitsu) (Intel Xeon Phi/Knights Landing)	16.5	4.986
Oakbridge-CX (Fujitsu) (Intel Cascade Lake (CLX))	20.7	5.076

Research Area based on CPU Hours (FY.2019)



Multicore Cluster
Intel BDW Only
(Reedbush-U)

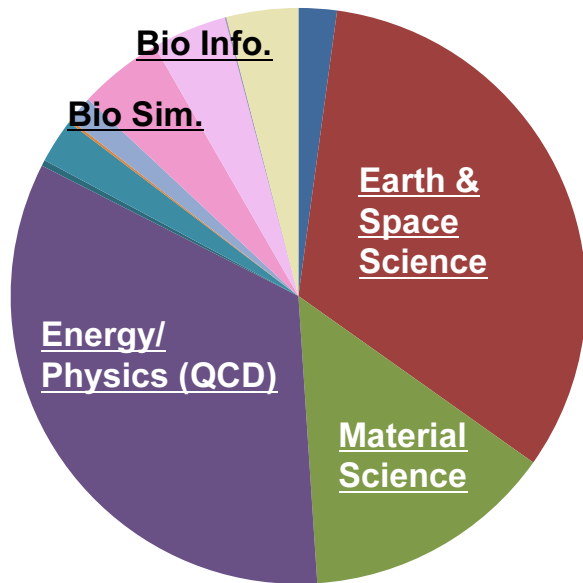


GPU Cluster
Intel BDW + NVIDIA P100
(Reedbush-H)

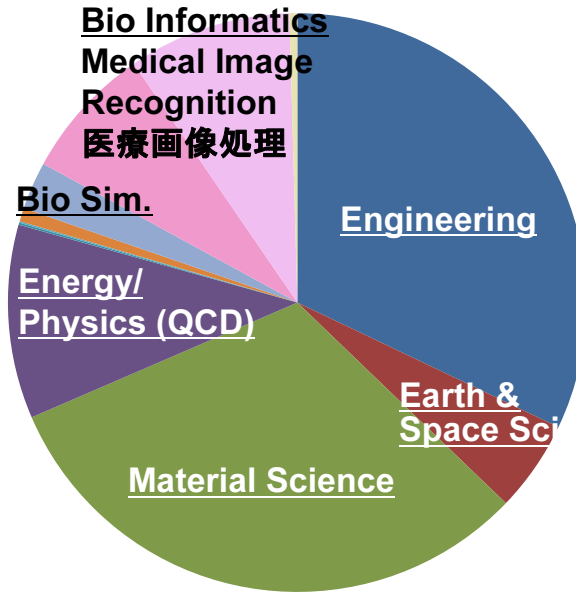
- Engineering
- Earth/Space
- Material
- Energy/Physics
- Info. Sci. : System
- Info. Sci. : Algorithms
- Info. Sci. : AI
- Education
- Industry
- Bio
- Bioinformatics
- Social Sci. & Economics
- Data

Research Area based on CPU Hours (FY.2019)

OBCX: 9 months (October 2019~September 2020)



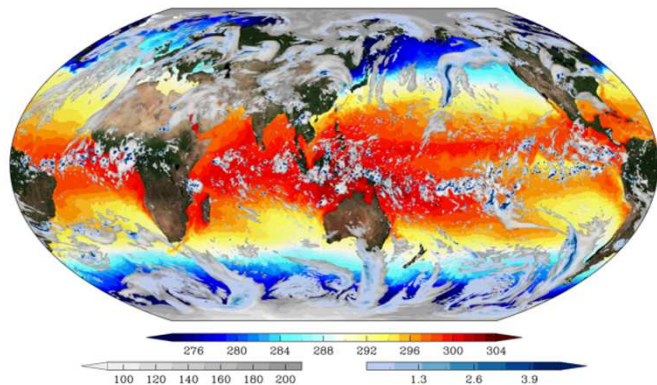
Manycore Cluster
Intel Xeon Phi
(Oakforest-PACS) (OFP)



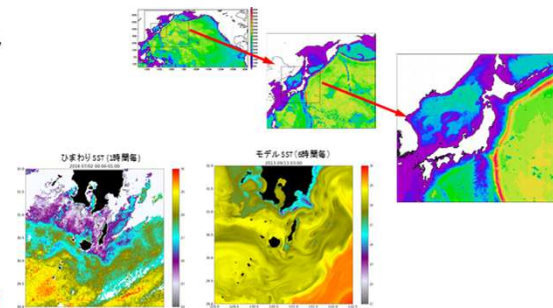
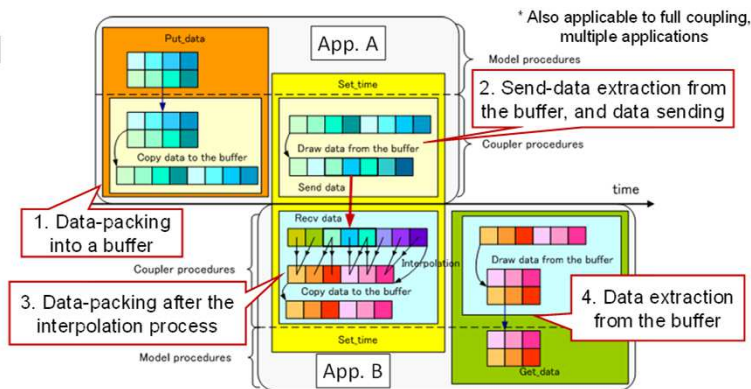
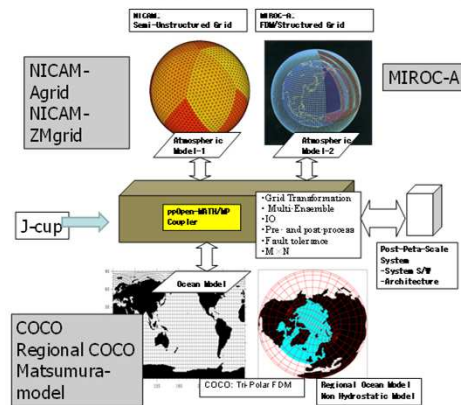
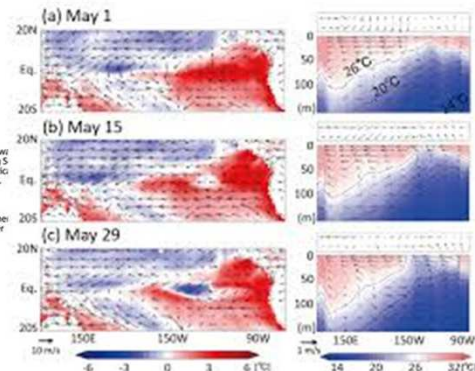
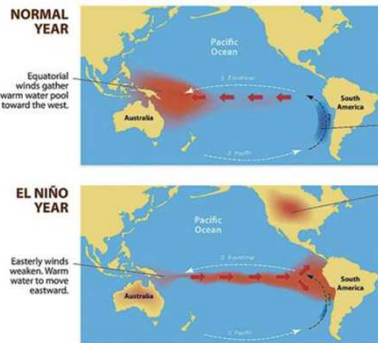
Multicore Cluster
Intel Xeon CLX
(Oakbridge-CX) (OBCX)

- Engineering
- Earth/Space
- Material
- Energy/Physics
- Info. Sci. : System
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- Social Sci. & Economics
- Data

Global Atmosphere-Ocean Coupled Simulations



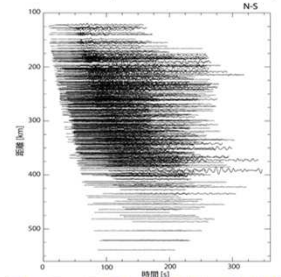
THE EL NIÑO PHENOMENON



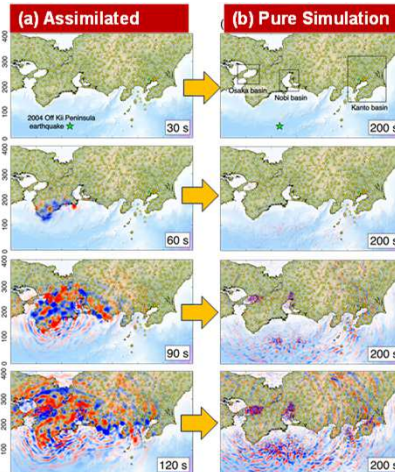
[c/o Prof. M. Sato, Prof. H. Hasumi (AORI/U.Tokyo)]

Solid Earth & Earthquake Simulations

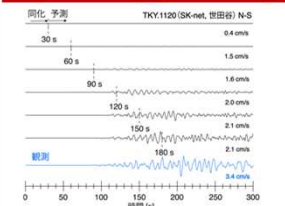
○ Observation (K-NET, KIK-net 446 pts)



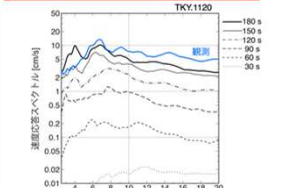
Assimilation at 90 sec. → Pure Simulation



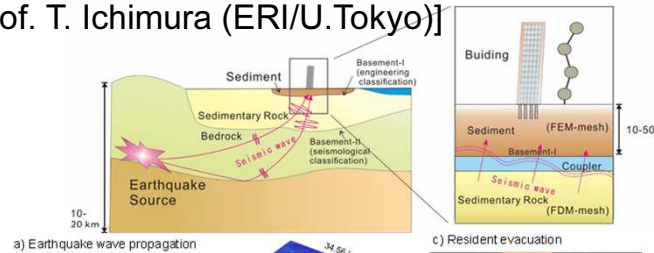
Long Wave Propagation in Tokyo



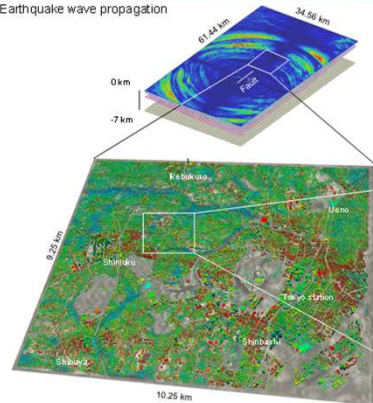
Response Spectrum



[c/o Prof. T. Furumura,
Prof. T. Ichimura (ERI/U.Tokyo)]



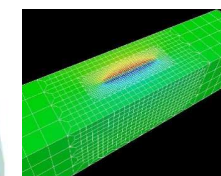
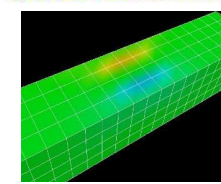
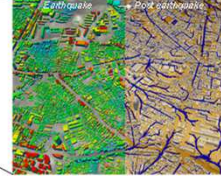
a) Earthquake wave propagation



b) City response simulation



c) Resident evacuation



[c/o Prof. R.
Ando (U.Tokyo)]

Simulation of Geologic CO₂ Storage

[c/o Dr. Hajime Yamamoto
(Taisei Corporation)]

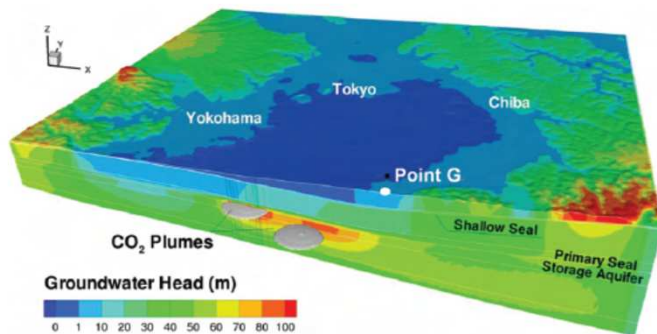
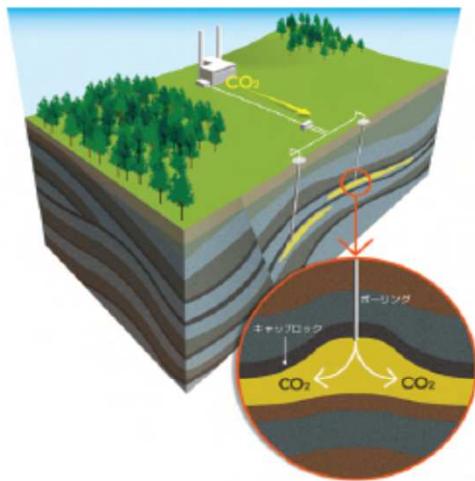
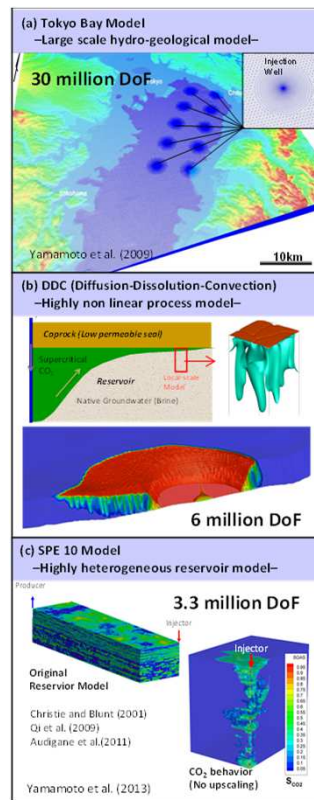
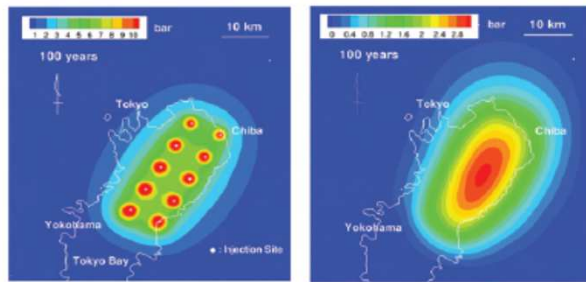


図-4 CO₂ 圧入後の地下水圧（全水頭換算）の分布（100 年後）



※DOF: degrees of freedom



(a) 深部遮蔽層下面 (b) 浅部遮蔽層下面

図-5 圧力上昇量の平面分布（初期状態からの増分、圧入開始から 100 年後）

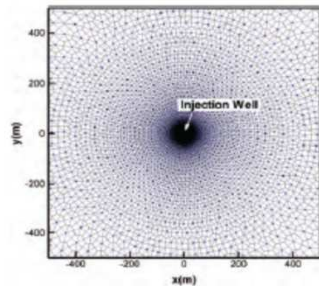
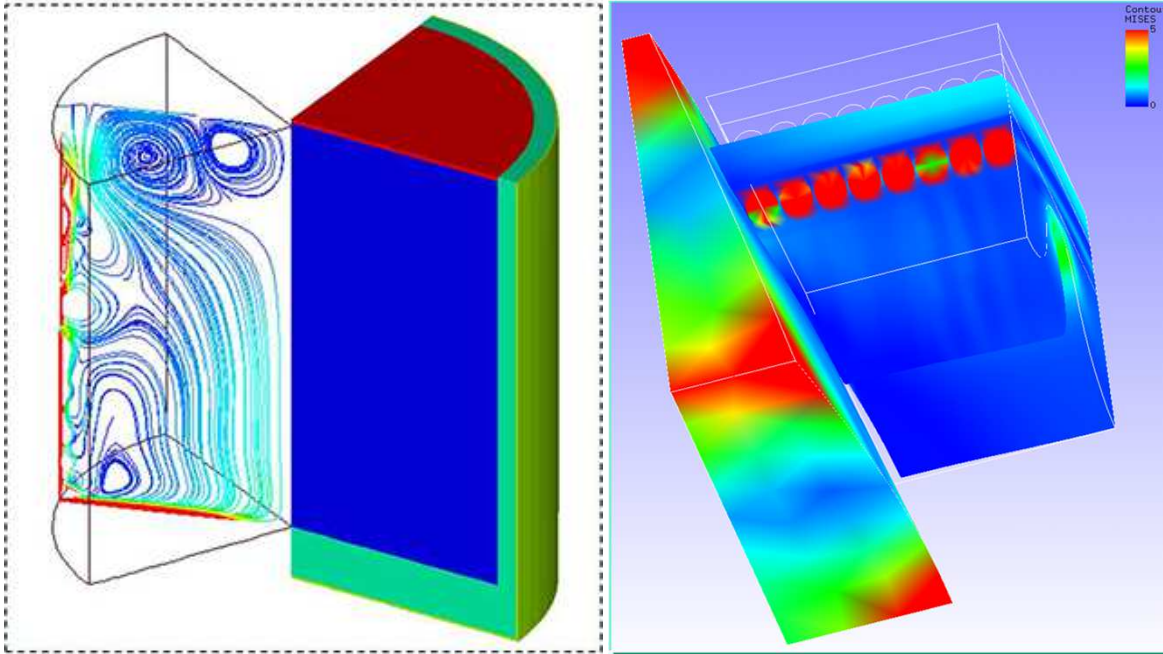
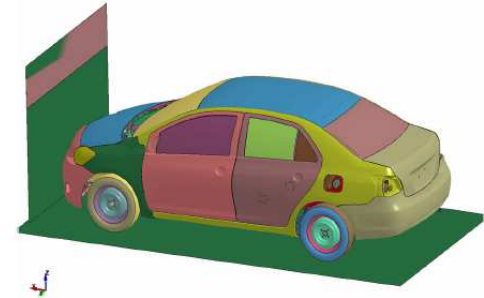


図-5 圧力上昇量の平面分布（初期状態からの増分、圧入開始から 100 年後）

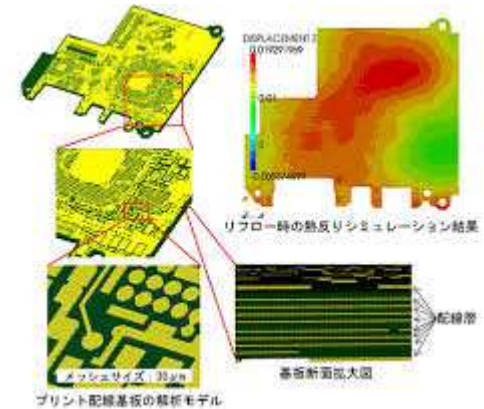
Engineering Simulations (CFD, Structural Analysis)



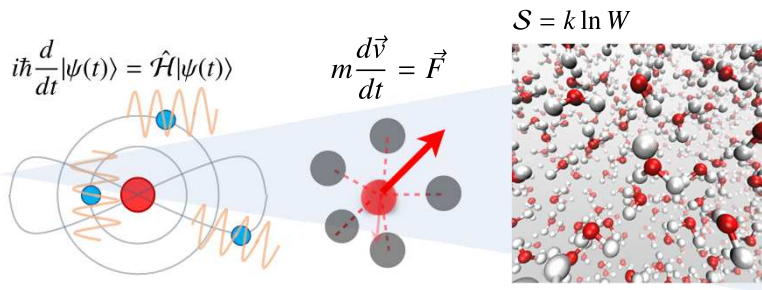
[c/o Prof. H. Okuda (U.Tokyo)]



[c/o JAMA]

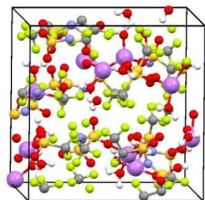


Simulations of Condensed Matter



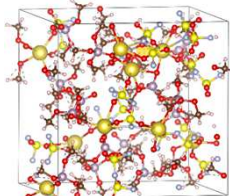
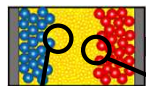
DFT-MD simulation

Novel electrolyte liquids for rechargeable batteries



Concentrated aqueous electrolytes

Nature Energy 2016

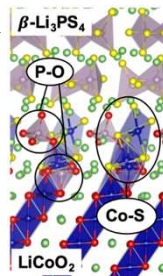


Fire-extinguishing organic electrolytes

Nature Energy 2018

DFT simulation

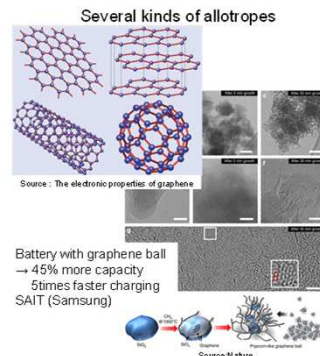
Electrode/electrolyte interface of all-solid-state batteries



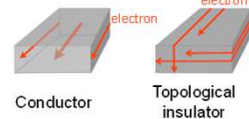
Chem. Mater. 2020

Courtesy of Prof. A. Yamada (UTokyo) & Dr. Y. Tateyama (NIMS)

Tight-binding model simulations for Dirac electrons / topological insulators



A new material which has special properties
Inside: insulation Outside: Conduction

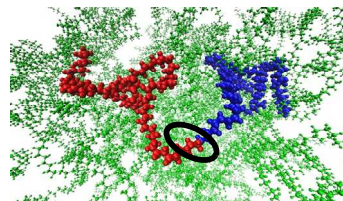


Sample of the topological insulator (SmB6)



Courtesy of Prof. Dr. Gerhard Wellein (FAU, Germany)

Free-Energy Computation of a Polymer with All-Atom MD Simulations

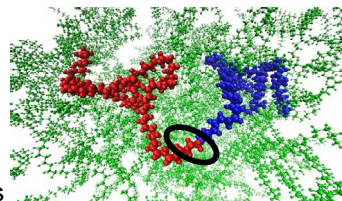


Macromolecules 2020

Chain increment

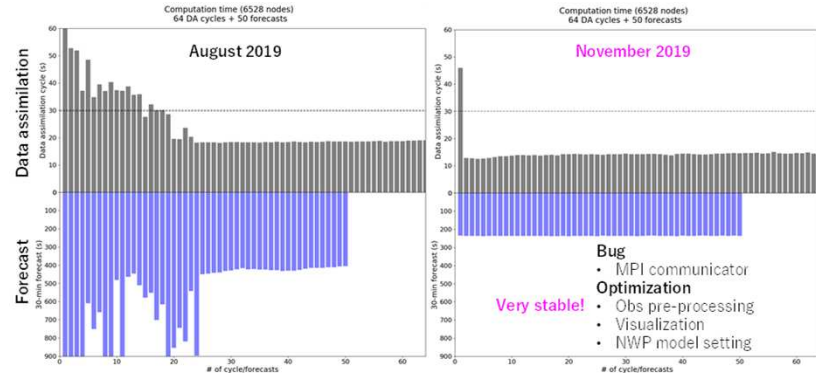
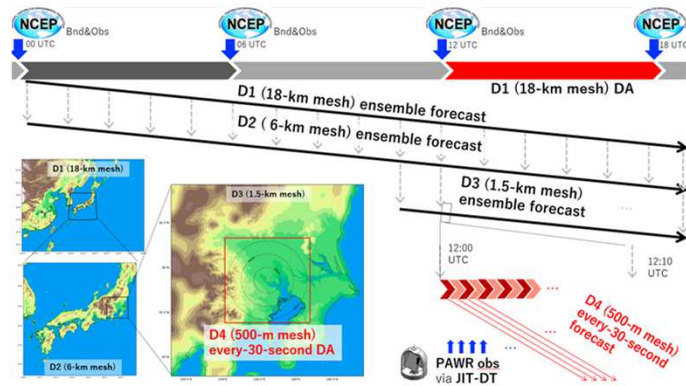
Interaction

btwn. monomers



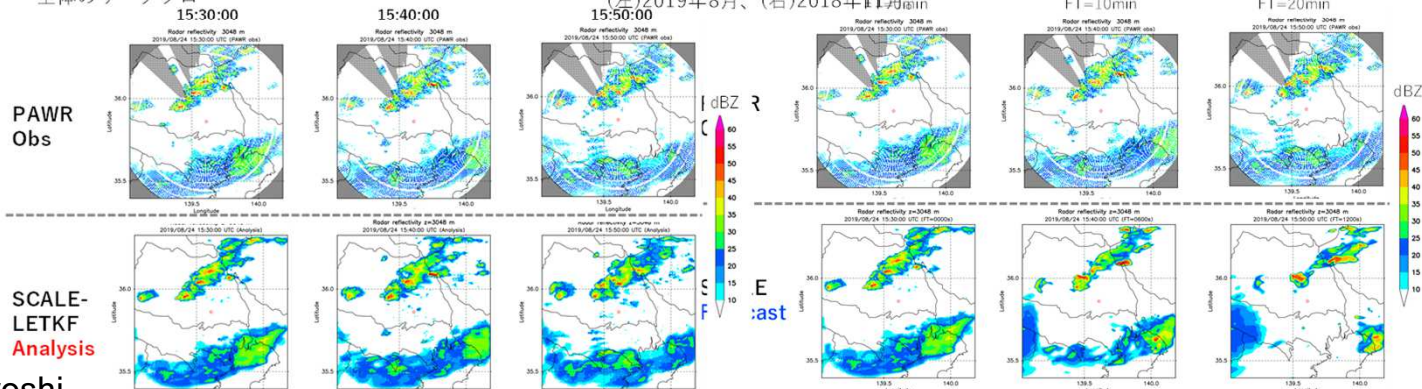
Courtesy of Prof. N. Matubayasi (Osaka)

Real-Time Prediction of Severe Rainstorm



計算性能の向上。上段はデータ同化、下段は30分予報にかかった時間(秒)。

(左)2019年8月、(右)2018年11月



[c/o Dr. Takemasa Miyoshi
(RIKEN R-CCS)]

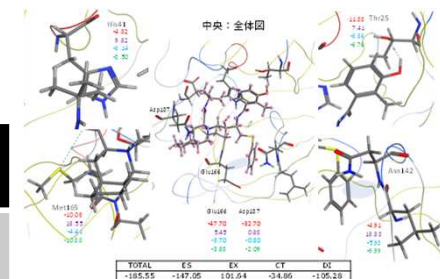
2019年8月24日の事例についてのテスト結果。(上)レーダー観測と(下)SCALE-LETKFによる解析で得られたレーダー反射強度(dBZ)を示す。

2019年8月24日の事例についてのテスト結果。(上)レーダー観測と(下)SCALE-LETKFによる予報で得られたレーダー反射強度(dBZ)を示す。

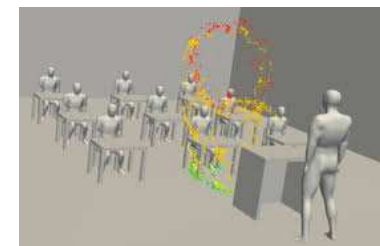
HPCI Urgent Call for Fighting against COVID-19 in Japan

by 8 SC Centers of Natl. Univ., AIST etc.

6 of 14 accepted projects use U.Tokyo's Systems



[c/o Prof. Y. Mochizuki (Rikkyo U.)]



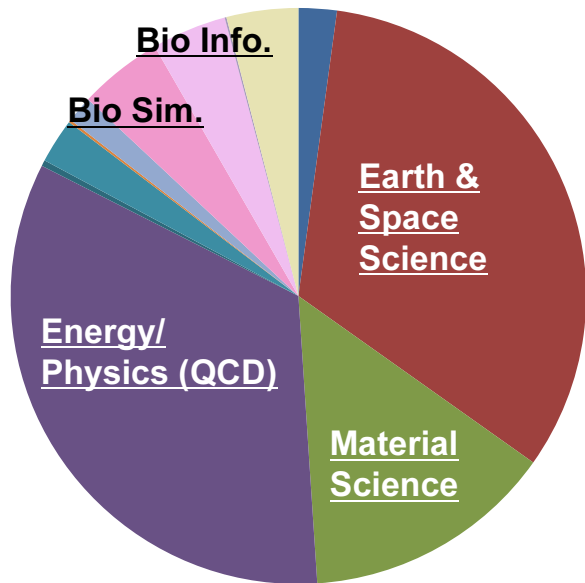
[c/o Prof. M.Tsubokura (Kobe U.)]

Project Name	PI	System
Fragment molecular orbital calculations on the main protease of COVID-19	Yuji Mochizuki (Rikkyo U.)	OFP
Study on the evaluation of arrhythmogenic risk of COVID-19 candidate drugs	Toshiaki Hisada (UT Heart)	
Prediction of dynamical structure of Spike protein of SARS-COV19	Yuji Sugita (RIKEN)	
Computer-assisted search for inhibitory agents for SARS-CoV-2	Tyuji Hoshino (Chiba U.)	OBCX
Prediction and Countermeasure for virus droplet Infection under Indoor Environment: Case studies for massively-parallel simulation on Fugaku	Makoto Tsubokura (Kobe U.)	
Spreading of polydisperse droplets in a turbulent puff of saturated exhaled air	Marco Edoardo Rosti (OIST)	

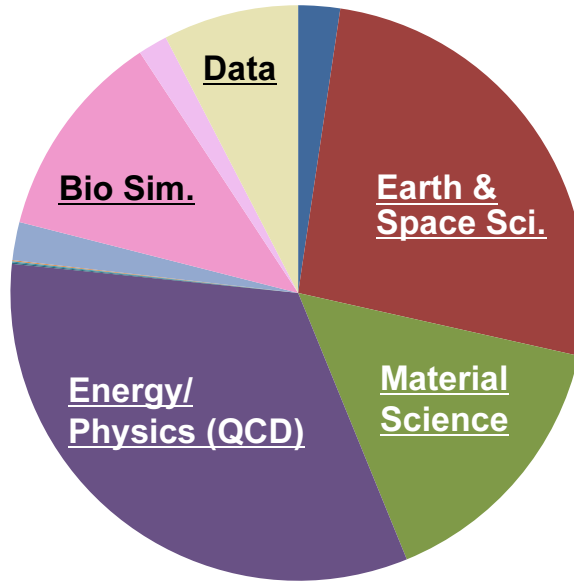
Research Area based on CPU Hours

Oakforest-PACS (Intel Xeon Phi Cluster)

FY.2019
(Apr.2019-Mar.2020)



FY.2020
(Apr.2020-Sep.2020)



- Engineering
- Earth/Space
- Material
- Energy/Physics
- Info. Sci. : System
- Info. Sci. : Algorithms
- Info. Sci. : AI
- Education
- Industry
- Bio** **COVID-19**
- Bioinformatics
- Social Sci. & Economics
- Data** **Rain Storm**