

Supercomputing Division, Information Technology Center, The University of Tokyo



Welcome

SCD/ITC, The University of Tokyo, Japan

The Supercomputing Division, Information Technology Center, The University of Tokyo (http://www.cc.u-tokyo.ac.jp/) was originally established as the Supercomputing Center of the University of Tokyo in 1965, making it the oldest academic supercomputer center in Japan. The Information Technology Center (ITC) was organized in 1999, and the Supercomputing Center became the Supercomputing Division (SCD) of the ITC. ITC is also a core organization of the "Joint Usage/Research Center for Interdisciplinary Large-Scale Information Infrastructures (JHPCN)", and a part of HPCI (the High-Performance Computing Infrastructure) operated by the Japanese Government. The three main missions of SCD/ITC are (i) Operations of Supercomputers & Services, (ii) Research & Development, and (iii) Education & Training. Currently, SCD/ITC consists of more than 10 faculty members. SCD/ITC is now operating four supercomputer systems, "Integrated Supercomputer System for Data Analyses & Scientific Simulations (Reedbush-H/L)" by HPE with 2.85 PFLOPS, "Manycore-based Large-scale Supercomputer System (Oakforest-PACS)" by Fujitsu with 25 PFLOPS as JCAHPC, "Massively Parallel Supercomputer System (Oakbridge-CX)" by Fujitsu with 6.61 PFLOPS, and "Integrated Supercomputer System for Simulation, Data and Learning (Wisteria/BDEC-01)" by Fujitsu with 33.1 PFLOPS. The four supercomputer systems operated by SCD/ITC contain 2,600+ users; 55+% of these users are from outside the university. Their average utilization ratio is ~90%. Hands-on tutorials for parallel programming (on-line) are held 20+ times per year. Up to 10% of the total computational resources of each system are open to users from the industry.

Computational Science Alliance, the University of Tokyo

At the University of Tokyo, we established the Computational Science Alliance (*http://www.compsci-alliance.jp/*) in 2015 by collaborating with 14 departments, including ITC. The primary purpose of this alliance is to provide an interdisciplinary education program for High-Performance Computing (HPC). The alliance has started lectures since April 2017.

JHPCN: Joint Usage/Research Center for Interdisciplinary Large-scale Information Infrastructures



"JHPCN (https://jhpcn-kyoten.itc.u-tokyo.ac.jp/en/)" comprises academic supercomputer centers in Japan associated with eight national universities (Hokkaido, Tohoku, Tokyo, Tokyo Tech, Nagoya, Kyoto, Osaka, and Kyushu). This began in April 2010. The total performance of the supercomputer

systems involved is 170+ PFLOPS (May 2021). JHPCN promotes collaborative research projects using the facilities and human resources of these eight centers, including the supercomputers, storage systems, and networks; interdisciplinary projects using multiple facilities are particularly encouraged. 40 or more projects have been accepted each year. New frameworks for international and industry collaborations have been initiated since 2017.

JCAHPC: Joint Center for Advanced High Performance Computing

JCAHPC In 2013, Center for Computational Sciences, University of Tsukuba (CCS) and ITC agreed to establish the Joint Center for Advanced High-Performance Computing (JCAHPC). JCAHPC consists of more than 20 faculty and staff members of CCS and ITC. Primary mission of JCAHPC is designing, installing and operating the Oakforest-PACS system (OFP). In addition, CCS and ITC will develop system software, numerical libraries, and large-scale applications to for OFP in collaboration made possible by the establishment of JCAHPC. JCAHPC is a new model for collaboration for research and development between supercomputer centers. JCAHPC plans to introduce OFP-II with 100+ PFLOPS, the successor of OFP, which starts operation in April 2024.

Supercomputer Systems at SCD/ITC

JCAHPC's Oakforest-PACS (OFP) by Fujitsu started its full operation in December 2016. OFP comprises compute nodes with Intel Xeon Phi processors, and has contributed to dramatic developments in new frontiers of various fields of research works in Computational Science & Engineering (CSE), especially after shutdown of K in August 2019. The Reedbush-H and Reedbush-L are by HPE with Intel Broadwell-EP (BDW) and NVIDIA Tesla P100 (Pascal). Reedbush-H (since March 2017) is our first GPU cluster, and each node includes two NVIDIA Pascal GPUs. Each node of Reedbush-L (since October 2017) has four GPUs. Oakbridge-CX (OBCX) by Fujitsu started its operation in July 2019, and it consists of compute nodes of Intel Xeon Platinum 8280 (Cascade Lake, CLX). 128 of 1,368 nodes of OBCX have fast SSDs, and are utilized for data intensive applications. In May 2021, we introduced the new system, Wisteria/BDEC-01. It is a heterogeneous system for integration of (Simulation+Data+Learning), which consists of Simulation Nodes (Odyssey) with Fujitsu A64FX, and Data/Learning Nodes (Aquarius) with Intel Xeon Platinum 8360Y (Ice Lake, ICX) and NVIDIA A100 Tensor Core GPUs. Each node of Aquarius is



re GPUS. Each node of Aquanus is equipped with eight A100 GPUs. Furthermore, we introduce series of "Large-scale Common Storage Systems (Ipomoea-X)", which can be accessed from current and future supercomputers at SCD/ITC. The first system (Ipomoea-01) with 25+PB will start its operation in January 2022. "mdx (Data Platform)" with Intel Xeon Platinum 8368 (ICX) and NVIDIA A100 was installed in March 2021.

Scientific Computing & Numerical Algorithms

Toward Establishing Compatibility Between Large-scale and Long-time Phenomena in Molecular Simulations

Molecular dynamics (MD) simulations are applied for a wide range of scientific problems, from physics and chemistry of materials & molecular biology to astrophysics. Thanks to the present status of the art where basic simulation methodology for parallel MD simulations is approaching its maturity, many open source packages are commonly available for usage on supercomputers. The problem nowadays is that MD simulations cannot be carried out for time that is long enough for describing physical processes in billion-atom-scale systems, as the increase in the clock cycles in the processors are about to peak out, and then it is now not easy to increase the number of total time steps.

We are now developing a molecular simulator that can allow computations on both large-scale and long-time. The key to realizing this is the efficient usage of machine learning for "perceiving" collective variables that appropriately describe the free-energy landscape of the system and enable unbiased long-time sampling, together with applying tree-based method for large-scale parallelism. Using the proper combinations of these methodologies, fundamental studies are ongoing regarding dynamical properties of liquid matter, including electrolytes, glasses, and other soft materials.



Left: Appropriate collective variables (q^*) that characterize the free energy landscape are necessary for realizing unbiased sampling of long-time trajectories.

Right: Tree methods are employed for effective computation of long-ranged electrostatics.

Performance Optimization of Gravitational Octree Code and Application to Galactic Archaeology

Collisionless N-body simulations are frequently employed to explore the formation and evolution of galaxies. We have developed a gravitational *N*-body code optimized for GPU: GOTHIC (Gravitational Oct-Tree code accelerated by Hlerarchical time step Controlling). GOTHIC includes both the tree method and the hierarchical time step. The code



runs entirely on GPU and is optimized for from the Fermi to the NVIDIA Ampere GPU architectures. A100, the current flagship GPU by NVIDIA, achieves a 1.3-fold acceleration compared to V100, the flagship GPU in the previous generation. The observed speed-up of 1.3 is greater than 1.2, which is the ratio of the theoretical peak performance of the two GPUs.

Stellar halos of galaxies provide fossil records of the formation and evolution of galaxies through galactic mergers. The Andromeda galaxy (M31) is an attractive laboratory for galactic archaeology due to its proximity and external perspective. *N*-body simulations using GOTHIC have reproduced stellar structures observed in the M31's halo. Stellar



streams are promising probes to detect interactions between the streams and invisible dark matter (DM) sub-halos. The further synergy of *N*-body simulations on Wisteria/BDEC-01 and dedicated observations using the Subaru telescope will unveil the nature and assembly history of the DM halo.

Imprints of past DM sub-halo collision to stellar stream.

 $\frac{-40-20}{x(\text{pc})} \frac{20}{20} \frac{40}{40} - \frac{-40-20}{x(\text{pc})} \frac{20}{20} \frac{40}{40} - \frac{-40-20}{x(\text{pc})} \frac{20}{20} \frac{40}{40} - \frac{-40-20}{x(\text{pc})} \frac{20}{20} \frac{40}{x(\text{pc})}$ Time evolution of torus-shaped gas surrounding the massive black hole during a head-on

galaxy collision. (from Miki et al. 2021 https://doi.org/10.1038/s41550-020-01286-9)

Development of Methods to Predict Fluid Simulation Results by Deep Learning

Computational fluid dynamics (CFD) is widely used in science and engineering. However, since CFD simulations require a large number of grid points and particles for these calculations, these kinds of simulations demand a large amount of computational resources such as supercomputers.

Recently, deep learning has attracted attention as a surrogate method for obtaining calculation results by CFD simulation approximately at high speed. We are working on a project to develop a parallelization method to make it possible to apply the surrogate method based on the deep learning to large scale geometry. Unlike the model parallel computing, the method we are currently developing predicts large-scale steady flow simulation results by dividing the input geometry into multiple parts and applying a single small neural network to each part in parallel. This method is developed based on considering the characteristics of CFD simulation and the consistency of the boundary condition of each divided subdomain. By using the physical values on the adjacent subdomains as boundary conditions, applying deep learning to each subdomain can predict simulation results consistently in the entire computational domain. It is possible to predict the simulation results in about 36.9 seconds by the developed method, compared to about 286.4 seconds by the conventional numerical method. In addition to this, we are also attempting to develop a method for fast prediction of time evolution calculations using deep learning.



Comparison of the flow velocity results obtained by the conventional simulation (upper figure) and the prediction of these results by deep learning (lower figure).

System, Tools & Hardware

Studying Usability of Arbitrary Precisions

In recent years, the usefulness of low-precision floating-point representation has been studied in various fields such as machine learning. Low accuracy can be expected to have effects such as shortening calculation time and reducing power consumption. For example, in an application with a memory bandwidth bottleneck, the effect of reducing the calculation time by reducing the amount of memory transfer is significant. However, in fields such as iterative methods, it is common to use FP64 because the calculation accuracy strongly affects the convergence, and there are few application examples of low-precision arithmetic. This study investigates the applicability of low-precision representation to the Krylov subspace and stationary iterative methods. In this research, we focus on the FP32, FP16, and FP42, FP21, which are not standardized by IEEE754.

$\mathcal H$ -matrices Library for Many-core Processors

Hierarchical matrices (\mathcal{H} -matrices) are an approximation technique for dense matrices, such as the coefficient matrix of the boundary element method (BEM). An \mathcal{H} -matrix is expressed by a set of low-rank approximated and small dense sub-matrices, each of which has various ranks. The use of \mathcal{H} -matrices reduces the required memory footprint of dense matrices from O(N2) to O(NlogN) and is suitable for manycore processors that have relatively small memory capacities compared to traditional CPUs.

However, existing parallel adaptive cross approximation (ACA) algorithms, which are low-rank approximation algorithms used to construct \mathcal{H} -matrices, are not designed to exploit many-core processors in terms of load balancing.

In existing parallel algorithms, the ACA process is independently applied to each sub-matrix. The computational load of the ACA process for each



Low-rank sub-matrix



sub-matrix depends on the sub-matrix's rank; however, the rank is defined after the ACA process is applied. This makes it difficult to balance the load.

We propose load-balancing-aware parallel ACA algorithms for \mathcal{H} -matrices that focus on many-core processors. We implemented the proposed algorithms into \mathcal{H} ACApK, which is an open-source \mathcal{H} -matrix library originally developed for CPU-based clusters.



UT-Helper: Support for HPC and Data Analysis Utilizing Unused Cores

In recent years, CPU performance improvement is achieved by increasing the number of cores. However, using all the cores in the CPU may not be optimal to get best performance due to the restriction, such as memory bandwidth, power budget, and thermal dissipation.

To maximize the total performance, we assume the "unused cores" and let them support the main task.

In this study, we are developing the framework "UTHelper" for utilizing unused cores as the command line tools and libraries and want to realize this mechanism without special modification of the existing system.

In UT Helper, to investigate and manage optimal core assignments and appropriate numbers of parallelism, we are implementing the tool based on SystemTap that can provide the dynamic optimization for the target function without modification of the source code and recompile. In addition, the helper threads that support properly the sub functions including communication and file IO are implemented.

This work is supported by Japanese Government from FY.2020 to FY.2022 (JSPS Grant-in-Aid for Scientific Research (A), P.I.: Toshihiro Hanawa (ITC/U.Tokyo)).



Current plan

- In-situ performance profiling
- No additional codes is necessary for instruments
- Measure behavior of main calculation and observe impact of helper functions
- Auto-adjust parallelism
- Cache prefetching
- Auto-adjust power budget
- Hiding communication and file IO
 Apply to numerical library
- On-the-fly analysis during simulation and in-situ visualization
- Language extension using directive
 - · Specify prefetch data, policies, QoS



Supercomputers at SCD/ITC

HPCI: High Performance Computing Infrastructure

High performance computing infrastructure (HPCI) is an environment that enables easy usage of flagship "Fugaku" supercomputer and other computation resources (tier-2) in Japan. In addition, HPCI is expected to match a user's needs and computational resources to accelerate exploratory research, large-scale research, and industrial use of HPC. HPCI comprises 13 computational resource providers; nine are supercomputing centers at national universities, and four are governmental research institutes. These resource suppliers are connected via SINET5, which is a high-speed academic backbone network with 100 Gbps. SCD/ITC participates in this project as a hub resource provider in the Kanto region (the HPCI EAST Hub). The HPCI EAST Hub provides a 50-PB storage system integrated with the WEST Hub by Gfarm file system.



Oakforest-PACS (Fujitsu PRIMERGY)

Oakforest-PACS is the first supercomputer introduced by JCAHPC (Joint Center for Advanced HPC) which is established by SCD/ITC and Center for Computational Sciences, U. Tsukuba (CCS). The system consists of 8,208 nodes of Intel Xeon Phi (Knights Landing) as a host processor, and Omni-Path Architecture provides 100 Gbps interconnection. In addition, the system employs the parallel file system with 26 PB, and file cache system of 940 TB with BW of over 1.5 TB/sec. This system is located at Kashiwa campus and operated by Fujitsu since December 2016. Oakforest-PACS has been offering computing resource to researchers in Japan and their international collaborators through various types of programs, such as by HPCI, by MEXT's Joint Usage/Research Centers, and by each of CCS and ITC. It is expected to contribute to drastic developments of new frontiers of various field of studies, including computational science and engineering (CSE). This system is utilized for education and training of students and young researchers in both CSE and high-performance computing (HPC) as well. Both of CCS and ITC continue to make further social contributions through operations of Oakforest-PACS.

g Theoretical peak	25 PFLOPS				
Main memory	128TB (High BW)+ 770 TB (Low BW)				
Number of nodes	8,208				
Compute node	Fujitsu PRIMERGY CX600 M1 + CX1640 M1				
Processor	Intel Xeon Phi (Knights Landing) 7250				
CPU (Core)	68 core, 1.4 GHz, 2 x AVX512				
Theoretical peak	3.05 TFLOPS				
Main memory	16 GB (High BW) + 96 GB (Low BW)				
Memory bandwidth	490 GB/sec (High BW, effective) +				
	115 GB/sec (Low BW)				
Cache memory	L2: 1 MB / tile (2 cores)				
Interconnect	Intel OmniPath Architecture (100 Gbps)				
Interconnect Topology	Full-bisection BW Fat Tree				
Parallel file system	Lustre Filesystem(DDN SFA14KE x10) 26PB, 500GB/sec				
File cache system	Burst buffer(DDN IME14K x25) 940TB, 1560GB/sec				
NSXI IV					

Parallel File System U. Tokyo U. Tokyo <th>Omni-Path Architecture (100 Gbps), Full-bisection BW Fat-tree 1560 GB/s DDN IME14KE x25 File Cache System 940 TB 500 GB/s Lustre File system DDN SFA14KE x10</th> <th>Compute Nodes 25 PFlops Fujitsu PRIMERGY CX-600 + CX-1640</th> <th>JCAHPC</th> <th>Oakfores</th> <th></th>	Omni-Path Architecture (100 Gbps), Full-bisection BW Fat-tree 1560 GB/s DDN IME14KE x25 File Cache System 940 TB 500 GB/s Lustre File system DDN SFA14KE x10	Compute Nodes 25 PFlops Fujitsu PRIMERGY CX-600 + CX-1640	JCAHPC	Oakfores	
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Supercomputers at SCD/ITC

Oakbridge-CX (Fujitsu PRIMERGY)

Oakbridge-CX (OBCX) is the Massively Parallel Supercomputer System using Intel Xeon Cascade Lake CPUs with the total performance of 6.61 PFLOPS. It has started operation since July 2019. The 128 nodes of compute node employ an NVMe SSD in each node for supporting staging, checkpointing, and data-intensive applications. Moreover, SSDs on designated nodes can be dynamically converged as a single shared

file system using BeeGFS on Demand (BeeOND). Moreover, 16 of these 128 nodes are directly connected to external network (SINET, Japan) and can access external resources (e.g. servers, storages, sensor networks etc.). OBCX was a prototype of Wisteria/BDEC-01, which is a platform for the integration of "Simulation+Data+Learning".



mdx: Infrastructure for Leveraging Data (Fujitsu PRIMERGY)

CPU

GPU

Memory

Storage

/irtualization

Towards Society 5.0, infrastructure for sophisticated data exchanging. sharing, and analysis is important, and HPC systems would play a significant role to offer such functions. We designed and constructed the "mdx" system as the cloud-like supercomputer towards leveraging data as the nation-wide infrastructure which realizes aggregated data collection, rapid and flexible build-up of the Proof-of-Concept (PoC) environment. The "mdx" is managed and operated by the collaboration among nine national universities and two national research institutes. The "mdx" system aims at the following features:

- 1. Provide a storage and computing infrastructure with secure, large-scale, and high-performance.
- 2. Provide flexible and secure network configuration collaborating with wide-area data acquisition networks.
- 3. Provide a platform for easy prototyping of the platform.





Society 5.0 by Wisteria/BDEC-01 and h3-Open-BDEC

What is Society 5.0 ?

https://www8.cao.go.jp/cstp/english/ society5_0/index.html

Society 5.0 was proposed in the 5th Science and Technology Basic Plan by the Cabinet Office of Japan as a future society that Japan should aspire to. It follows the hunting society (Society 1.0), agricultural society (2.0), industrial society (3.0), and information society (4.0). Society 5.0 is a human-centered society that balances economic advancement with the resolution of social problems by a system that highly integrates cyberspace and physical space, and will be achieved by Digital Innovation, such as IoT, AI, Big Data and etc.

New Directions in Supercomputing

Majority of SCD/ITC supercomputer system users belong to the fields of CSE, including engineering simulations (fluid dynamics, structural dynamics, and electromagnetics), earth sciences (atmosphere, ocean, solid earth, and earthquakes), and material sciences, as shown in the pie chart A, which shows usage rate of each research area on Reedbush-U with Intel BDW based on CPU hours in FY.2019. Recently, the number of users related to data science, machine learning, and artificial intelligence (AI) has been increasing, as shown in the pie chart B, which shows usage rate on Reedbush-H system with GPU's in FY.2019. Examples of new research topics are weather prediction by data assimilation, medical image recognition, and human genome analyses. Towards Society 5.0, a new type of method for solving scientific problems by integrations of "Simulation (S)", "Data (D)" and "Learning (L)" (S+D+L) is emerging.



Wisteria/BDEC-01

We started discussions on the BDEC system (Big Data & Extreme Computing) as a platform for integration of (S+D+L) since 2015. Wisteria/BDEC-01, which started its operation in May 2021, is the first BDEC system. Wisteria/BDEC-01 is a Hierarchical, Hybrid, Heterogeneous (h3) system, and it consists of two types of node groups for computing, Simulation Nodes (Odyssey) and Data/Learning Nodes (Aquarius), Shared File System (25.8 PB) and Fast File System (1.0 PB). Total peak performance is 33.1 PFLOPS, and aggregated memory bandwidth is 8.38 PB/sec. The system is constructed by Fujitsu. Simulation nodes for HPC (Odyssey) with more than 25 Peta FLOPS is based on Fujitsu's PRIMEHPC FX 1000 with A64FX with High Bandwidth Memory. This part has the same architecture as that of the Fugaku supercomputer. Data/Learning nodes (Aquarius) are GPU cluster consisting of Intel Xeon Ice Lake and NVIDIA A100 Tensor Core GPUs, with 7.2 Peta FLOPS for Data Analytics, AI and Machine Learning Workloads. Some of Data/Learning nodes are connected to external resources directly through SINET, Japan. Odyssey and Aquarius are connected through InfiniBand-EDR network with 2 TB/sec.



h3-Open-BDEC: Innovative Software Platform

Integration of (S+D+L) on Wisteria/BDEC-01 is done by optimization of parameters for large-scale simulations on Odyssey using data analyses, data assimilation and machine learning on Aquarius.

We develop an innovative software platform "h3-Open-BDEC" for integration of (S+D+L), and evaluate the effects of integration of (S+D+L) on Wisteria/BDEC-01. The h3-Open-BDEC is designed for extracting the maximum performance of the supercomputers with minimum energy consumption focusing on (1) innovative method for numerical analysis with high-performance/high-reliability/power-saving based on the new principle of computing by adaptive precision, accuracy verification and automatic tuning, and (2) Hierarchical Data Driven Approach (*h*DDA) based on machine learning. This work is supported by Japanese Government from FY.2019 to FY.2023 (JSPS Grant-in-Aid for Scientific Research (S), P.I.: Kengo Nakajima (ITC/U.Tokyo)).



Overview of h3-Open-BDEC

The h3-Open-BDEC is the first innovative software platform to realize integration of (S+D+L) on supercomputers in the Exascale Era, where computational scientists can achieve such integration without supports by other experts. Source codes and documents are open to public for various kinds of computational environments. This integration by h3-Open-BDEC enables significant reduction of computations and power consumptions, compared to those by conventional simulations. Possible applications using h3-Open-BDEC are combined simulations/data assimilations for climate/weather simulations and earthquake simulations, and real-time disaster simulations, such as flood, earthquake and tsunami.

Integration of 3D Earthquake Simulations with Real-Time Data Observation & Assimilation

JDXnet is the seismic observation data exchange and distribution network in Japan, and it distributes the seismic observation data of the nine national universities, JMA, NIED, JAMSTEC, AIST etc. at more than 2,000 points. We utilize the observation data obtained from JDXnet for integration of 3D earthquake simulation in strong motion and real-time data assimilation. We developed a prototype of this integrated simulations with real-time data assimilation on OBCX, and we are now porting the code on Wisteria/BDEC-01.





Numerical Weather Prediction System: SCALE-LETKF c/o T. Miyoshi & T. Honda (RIKEN R-CCS)



Visit our website for more information https://www.cc.u-tokyo.ac.jp/en/public/pamphlet.php



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SCD/ITC Supercomputing Division, Information Technology Center, The University of Tokyo