Exploring the Universe by the Next-Generation Simulations

E. Kokubo, T. Ito, T. Takiwaki, K. Iwasaki,
N. Tominaga, M. Machida, T. Moriya, and
CfCA Members

2023.11.8

Center for Computational Astrophysics

Outline

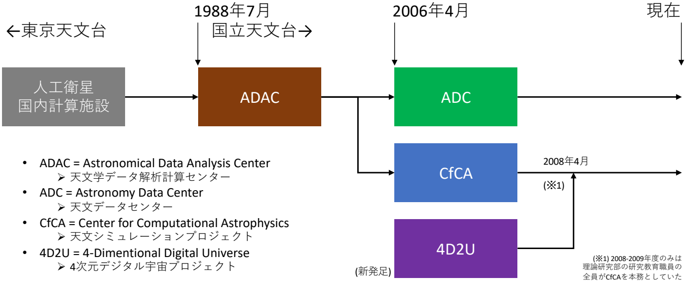
Center for Computational Astrophyics

- Scientific goals and missions
- Current status

Exploring the Universe by the Next-Generation Simulations

- Proposal overview

Brief History



Center for Computational Astrophysics (CfCA)

- Established in 2006 as a C-type project when Astronomical Data Analysis Center was split off

Scientific Goals and Missions (1)

Purpose

- The Center for Computational Astrophysics (CfCA) promotes computational astrophysics to explore the Universe as a Center of Excellence (COE) of this research area in Japan.

Missions

The missions of this project are:

1. to operate diverse computing resources, provide them to the Japanese astronomy community on an open-use basis, and support the progress of research activity in astronomy and astrophysics;
2. to produce first-rate research achievements in the area of computational astrophysics; and
3. to develop cutting-edge contents with astronomical data, and publicize the latest achievements in astronomy.

Scientific Goals and Missions (2)

Primary Scientific Goals

The primary scientific goals of this project are:

1. maintain stable operation of the open-use computing facilities, and serve as a COE for this research field in Japan;
2. carry out research and development of the hardware/software dedicated to computational astrophysics, and obtain a substantial amount of first-rate academic achievements in astrophysics; and
3. develop cutting-edge contents for the advanced 4-Dimensional Digital Universe (4D2U) program for visualization of astronomical data.

Present Open-Use Computer Systems

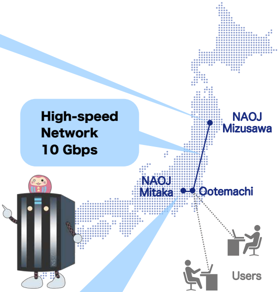
Supercomputer “ATERUI II” (Cray XC50)

Theoretical Peak Performance: 3.087 Pflops
Main Memory: 385.9 TB
Nodes: 1,005

CPU: Intel Xeon Skylake 6148
2.4 GHz, 40 cores
Total Core Number: 40,200

File server (DDN EXA Scaler)

Disk Capacity: 6.5 PB

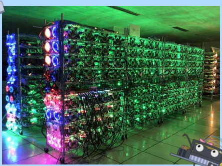


GPU server

Nodes: 6
Total GPU Number: 32
(NVIDIA A100)

Small Parallel Computers

Nodes: 10
(AMD EPYC 7402 : 6
AMD EPYC 74F3 : 4)
Total Core Number: 480



PC cluster

Nodes: 106
Total Core Number: 2,176
CPU: AMD Ryzen7
and 9 types of CPU

File server

Disk Capacity: ～ 8 PB

Analysis server

Nodes: 6
Core Number: 36（※）
Main Memory: 1 TB（※）

※ per 1 node

(2022.12)

Not only supercomputer but also simulation infrastructure!

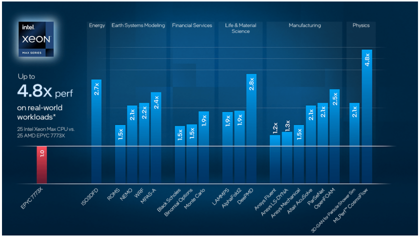
Supercomputer Replacement 2024

Schedule

- 2023.09: public announcement of bids
- 2023.11: technical review
- 2023.12: bid opening
- 2024.11: acceptance inspection
- 2024.12: operation start ($\rightarrow$ 2031.3)

New Supercomputer (ATERUI III)

- CPU: Intel Xeon Max (high-bandwidth memory)
- Budget: 350M yen/year (including electricity)



(Intel)

Background

CfCA's Missions

- Operation of open-use computer systems
- Research in computational astrophysics
- Visualization of astronomical data

Rironkon's Statement

- "The general consensus of the Theoretical Society is to support the stable operation of the supercomputer of the National Astronomical Observatory of Japan's Simulation Project (CfCA)."

Periods and Supercomputers

- ATERUI III (2024.12-2031.3)
- ATERUI TNG (2031.4?-)

TNG Supercomputer

- General-purpose computer
- Huge uncertainty in computer technology

Science Goals and Scientific Objectives

Science Goals

- Explore the formation and evolution of the universe through astrophysical simulations with the next-generation supercomputers

Scientific Objectives

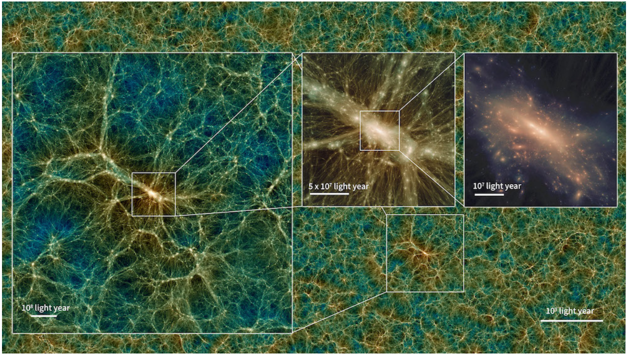
- Elucidate the formation and evolution of the large-scale structure, the milky-way galaxy, stars, and the solar system, and the mechanisms of supernova and accretion disks through large-scale simulations with realistic physics

Science Investigations (1)

（「天文学・宇宙物理学の長期計画 -2030-2040 年代のビジョン-」）

Large-Scale Structure

- Cosmological *N*-body simulations of structure formation using dark matter particles on the scale of 10-100 trillion bodies to investigate the structure formation of groups and clusters of galaxies while resolving the galaxy scale.



(Ishiyama et al. 2021)

Science Investigations (2)

Galaxies and Stellar Systems

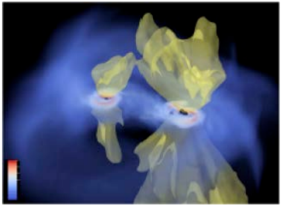
- Large-scale fluid-*N*-body simulations using more realistic gas-star system models that take into account star formation, stellar evolution, binary star evolution, chemical evolution, etc., to elucidate the formation and evolution of galaxies and star clusters.

(T. Saito)

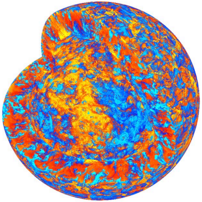
Science Investigations (3)

Star Formation and Evolution

- Sophisticated simulations of star and disk formation, taking into account not only magnetic fields and self-gravity but also realistic processes such as radiation transfer, chemical evolution, and dust evolution in order to connect star formation and planet formation.
- High-resolution simulations consistently covering a wide spatial range from the solar surface to the deep interior in order to reveal the origin of 11-year periodic variations of the solar magnetic field.



(K. Sugimura)



(Hotta et al. 2021)

Science Investigations (4)

Planetary Systems

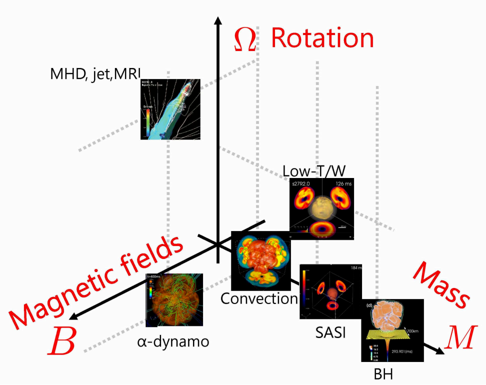
- Wide-area N-body simulations of planet accretion on tens of au scales using 10-100 million planetesimals in evolving gas disks, including planetary migration, to reveal the origin of the diversity of planetary systems.

High-Energy Astrophysics

- High-resolution simulations on supernova, kilonova, accretion disks, and jets to elucidate the detailed properties of neutron stars and black holes and their surroundings.
- A sophisticated numerical method to treat gravity, nuclear force, weak interaction, and magnetic fields is investigated and the predictions of gravitational waves, neutrinos, and electromagnetic waves are obtained for multi-messenger astronomy.

One Hundred 3D Core-Collapse Simulations

Toward Complete Understanding of Stellar Explosions

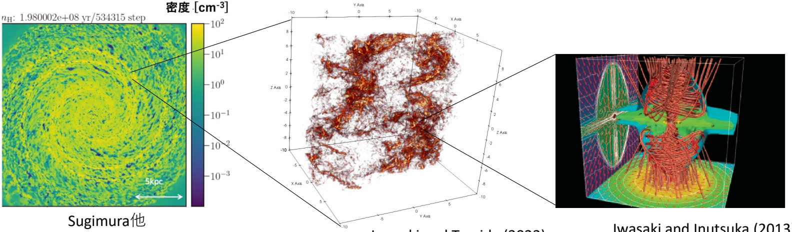


(T. Takiwaki)

- 5 × 5 × 4 models for rotation, magnetic fields, and mass
- Code: GRMHD simulations with neutrino radiation
- The mechanisms of supernovae, gamma-ray-bursts, and black-hole formation, etc. are systematically clarified.

Comprehensive Simulations Incorporating Molecular Cloud Formation

to Circum-stellar Disk Formation



Sugimura他

Iwasaki and Tomida (2022)

Iwasaki and Inutsuka (2013)

- Investigate the evolution of the interstellar medium from the atomic gas to molecular clouds and to star formation to reveal the universality and diversity of star formation processes.
  - To bridge the scale gap, use the AMR and zoom-in techniques.
- Code development: star particles, radiative transfer, establishment of Zoom-in technique on star formation simulations.

Exploring Planetary Rings with TNG Simulations

TNG Simulations

- Global
- Real-size ($\sim$ 1 m) particles
- $N \sim 10^9$-10^{10}

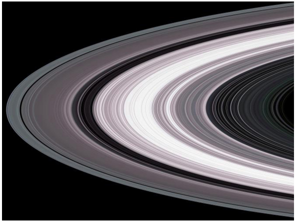
Code

- New collisional *N*-body code (Michikoshi & EK in prep.)

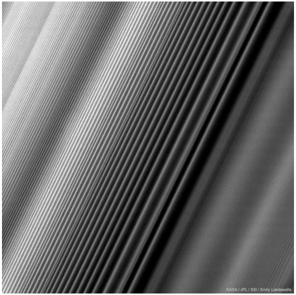
Goals

- Satellite-ring interaction
  - division/gap formation
  - density wave

Pan in the Encke gap



Mimas 2:1 Cassini division



Janus 2:1 spiral density wave (Cassini/NASA)

Instruments and Data to be Returned

Instruments

- 2018.6-2024.8: ATERUI II (3 Pflops)
- 2024.12-2031.3: ATERUI III ($\lesssim$ 3 Pflops, HBM)
- 2031.4?-: ATERUI-TNG (30 Pflops)
  - 10 times larger computational resources are required for new scientific innovations.
  - We select a suitable CPU or GPU. Following the choice of CPU or GPU, we need to develop simulation codes.

Data to be Returned

- Higher-resolution simulation data of physical quantities

Operation

Open-Use Operation Policy

- Peer review is adopted for the selection of users on all the computing facilities.
- No fee is charged.

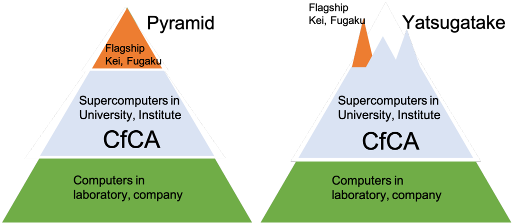
Operation of the Open-Use Facilities

- ATERUI-TNG is expected to be in operation from FY2031 to FY2036 (or FY2027) in Mizusawa(?).
- All other computing facilities other than ATERUI-TNG are installed and operated in Mitaka.
- The CfCA staff members carry out the operation of the facilities located at Mitaka.

Rationale and Trade-Off Studies

Relationship to the HPCI Program

- The HPCI has a hierarchical structure.
- CfCA's facilities are positioned in the second tier and are used for middle-scale applications or preparation for the run on flagship machine.
- Flagship machine does not always exist. The second-tier facilities play major roles in this era.
- A possible future direction: consolidating the budget for the open-use of computing facilities within NINS and introducing larger equipment.



HPCI: High-Performance Computing Infrastructure

Threshold Science

Simulation Results

- Positive correlation with available computing resources

Computing Resources

- No threshold that would make it meaningless to implement

Key Technologies

GPU

- GPU has a high performance per unit electrical power.
- In the future, many types of GPU will appear, and the role and handling of GPU could be different from the current one. For example, high bandwidth connection between GPU and CPU. GPU and CPU work in one chip.
- Programming using GPU is sometimes complicated. Can we GPU-enable our existing simulation code?

Bandwidth

- Computational speed depends on the bottleneck (slowest part) of the system. The bandwidth among arithmetic logic unit and L1–L3 caches, main memory, and other nodes is important.

AI

- With good training data, AI can be used to reduce the necessary computational resources.

Technical Risk Identification

Slowing Down of Moore's Law

- The performance of the semiconductor used to grow following an exponential curve. However, recently, that pace has slowed down. We may not obtain sufficient performance in 2031.

High Energy Consumption

- A huge amount of data is used in the computation, and that requires high electricity consumption. Electricity costs are getting higher. CO_2 emissions should be reduced. The technique to reduce the electricity consumption is important.

Separated Memory

- Current GPU has a different main memory from CPU. It is hard to efficiently co-operate both CPU and GPU. That prevents us from developing and debugging our code easily.

Risk Mitigation

Choice of Best CPU or GPU

- We select a suitable CPU or GPU from a variety of machines. We can find a better machine for astrophysical applications even if the growth of the performance of the semiconductor slows down.

GPU

- GPU is a power-efficient solution. If we can use it, we can avoid high electricity consumption.

Shared Memory

- The separated memories of GPU and CPU can be unified in the future. This technique can help our code development.

Technical Heritages, Technology Development Status and Plan

Code Development

- In this project, we primarily develop software, simulation code and do not develop hardware, CPU or GPU.
- Methods for N-body, magnetohydrodynamic, radiative transport, and special and general relativistic calculations are being developed in public and as group codes.
- GPU-enabled software is also being developed.

Acquisition Surveillance: Make or Buy

Supercomputer

- Lease

Other Facilities

- Purchase and/or build our own

Software

- New development and/or public codes

Cost Assessments, Budget Line and Status

Budget, Expenses, and Their Uncertainties

- The open-use operation does not have a fixed term. So, the budget for the facility operation should come from the regular annual budget (“hard money”), not from the external funding (“soft money”).
- The larger the scale of the computing facilities, the more users there will be, and the more research outcomes will be achieved.
- The NAOJ Executive Board decided to provide 350M yen/year until FY2031. This budget is mainly for the operation of the supercomputer including electricity fees.
- In addition, we also need budgets for updating the non-leased equipment installed at Mitaka. This is at least 20M yen/year, and hopefully more.

Work Breakdown Structure

Open-Use Computational Resources

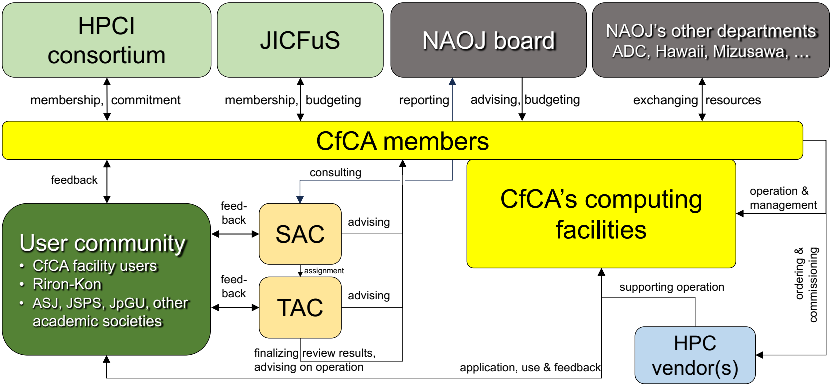
- Large-Scale Parallel Computers
  - Hardware
    - Examination of computer specifications necessary to carry out the research plan (CPU, GPU, Memory, Memory and Network bandwidths...)
    - Gathering opinions from the user community
    - Survey of the vendors' roadmap.
    - Gathering opinions from the vendors
  - Software
    - Development of modules required to carry out the research plan based on the public codes
    - Software development with a view to moving to a system that includes an accelerator.
  - Operation
- Small Parallel Computers, PC Clusters, GPU Clusters

Computational Resources for Data Analyses

- Continuous reinforcement of large-scale parallel super-computers as their performance improves

Project Organization (1)

CfCA in Relation to Other Organizations



Project Organization (2)

Personnel

- As of October 2023, CfCA is operating the computing facilities with the workforce described in p. 31.

Science Advisory Committee

- The most official channel to the user community is the CfCA Science Advisory Committee (SAC).

Time Allocation Committee

- The Time Allocation Committee (TAC) under SAC decides on the acceptance of users' applications for the supercomputer.

Users' Meeting

- At the annual CfCA Users Meeting, the activities of the SAC and TAC are shared with the participants.

Project Organization (3)

Rironkon

- CfCA keeps the cooperation with Rironkon.

Other Academic Societies

- CfCA sends out open calls for the application of computing facilities to academic societies regularly such as ASJ, JSPS, and JpGU.

HPCI Program Related Organization

- There are two channels to the community under the HPCI program:
  - Joint Institute for Computational Fundamental Science
  - The HPCI consortium.

Project Organization (4)

Human Resources beyond FY2031

- Currently, CfCA has $\sim$4 FTE of workforce for facility operation (excluding research and admin staff members such as professors or secretaries):
  - $\sim$0.5 FTE for the operation support of the supercomputer
  - $\sim$2.0 FTE for the operation of the facilities in Mitaka
  - $\sim$0.8 FTE for user registration and web management
  - $\sim$0.7 FTE for procurement of the supercomputer lease
- However, this number is not enough for long-term, stable operation, and we would need $+$1.5 FTE of workforce in the near future, even before FY2031:
  - $\sim$1.0 FTE for the operation support of supercomputer
  - $\sim$3.0 FTE for the operation of the facilities in Mitaka
  - $\sim$1.5 FTE for user registration and web management
- We have not decided as to where we will find this workforce: employing contract employees in NAOJ or relying on external workforce from outside NAOJ.

Summary

CfCA's Most Important Mission

- Operation of open-use computers (support from Rironkon)

Exploring the Universe by the Next-Generation Simulations

- Period: FY2031-
- Goal: Explore the formation and evolution of the universe through astrophysical simulations with the next-generation supercomputers
- CfCA's focus subjects
  - supernova explosion
  - star and disk formation
  - planetary ring dynamics
- Instrument: ATERUI TNG - 2nd-tier supercomputer dedicated for astronomy

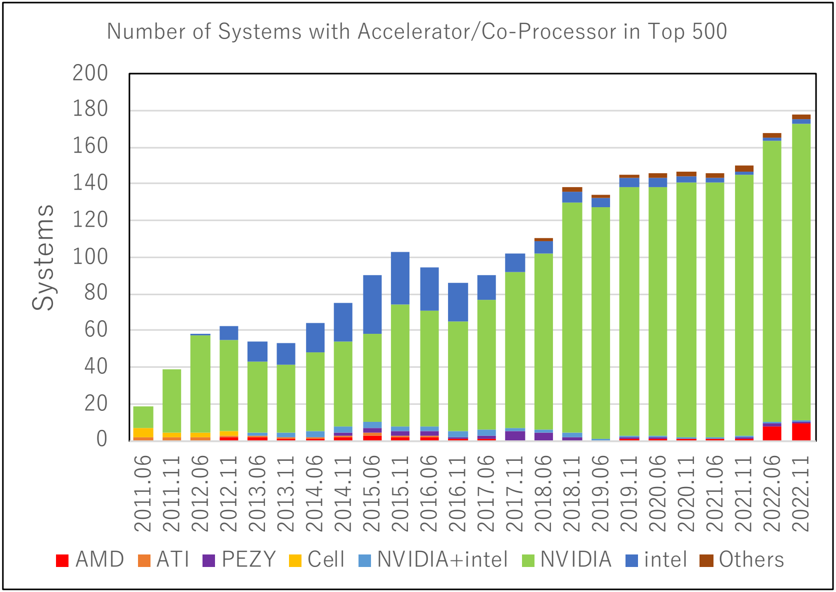
Appendix

Green500 Ranking (November 2022)

https://www.top500.org/

	TOP 500 Rank	System	Accelerator	Cores	HPL Rmax (PFlop/s)	Power (kW)	GFLOPS/ W
1	405	Henri, Flatiron Institute, USA	NVIDIA H100 PCIe	5,920	2.04	31	65.091
2	32	Frontier TDS, ORNL, USA	AMD Instinct MI250X	120,832	19.20	309	62.684
3	11	Adastra, GENCI-CINES, France	AMD Instinct MI250X	319,072	46.10	921	58.021
4	15	Setonix, Pawsey, Australia	AMD Instinct MI250X	181,248	27.16	477	56.983
5	68	Dardel GPU, KTH, Sweden	AMD Instinct MI250X	52,864	8.26	146	56.491
6	1	Frontier, ORNL, USA	AMD Instinct MI250X	8,730,112	1,102.00	21,100	52.227
7	3	LUMI, EuroHPC/CSC, Finland	AMD Instinct MI250X	2,220,288	309.10	6,016	51.382
8	159	ATOS THX.A.B, Atos, France	NVIDIA A100 SXM	25,056	3.50	86	41.411
9	359	MN-3, Preferred Networks, Japan	MN-Core	1,664	2.18	53	40.901
10	331	Champollion, HPE, France	NVIDIA A100 SXM	19,840	2.32	60	38.555
43	2	Supercomputer Fugaku, R-CCS, Japan	(CPU-only: Fujitsu A64FX)	7,630,848	442.01	29,899	15.418
70	340	MeluXina – Cluster Module, LuxProvide, Luxembourg	(x86 CPU-only: AMD EPYC 7H12)	73,344	2.29	377	6.062

- GPUs tend to have 10 times better performance per W than CPU.



- Share of GPUs is increasing and reaches 36%.