Exploring the Universe by the Next-Generation Simulations

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N. Tominaga, M. Machida, T. Moriya, and
CfCA Members

2024.12.6

Outline

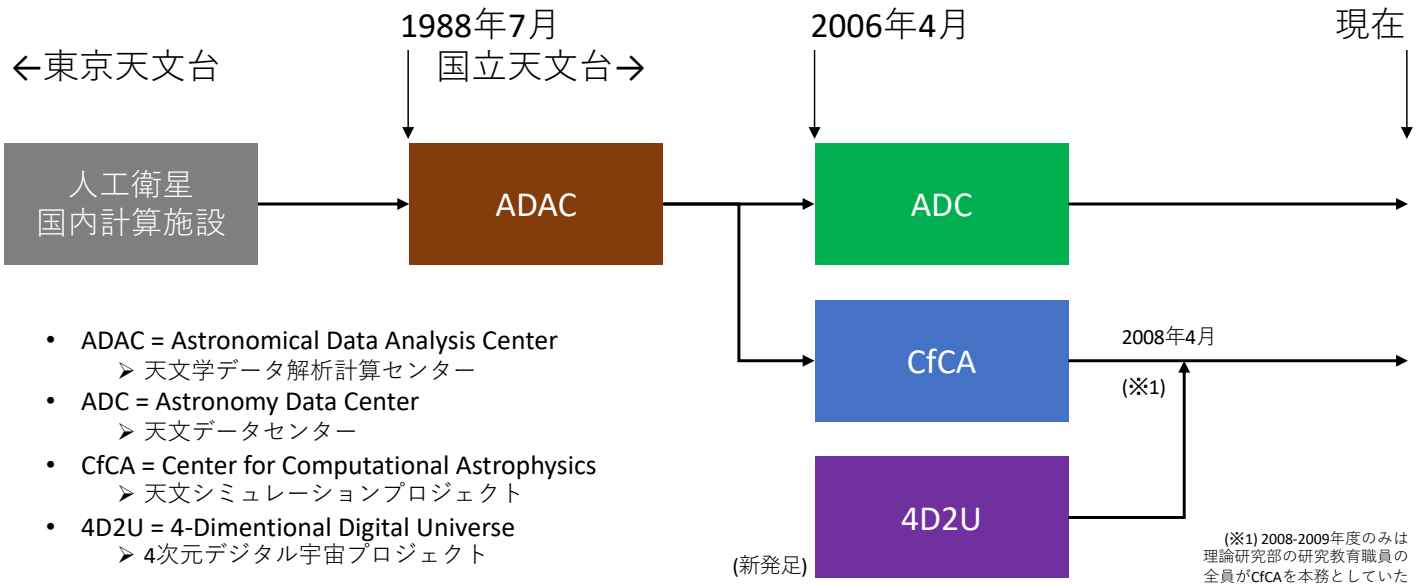
Center for Computational Astrophyics

- Scientific goals and missions
- Current status

Exploring the Universe by the Next-Generation (TNG) Simulations

- Proposal overview

Brief History



Center for Computational Astrophysics (CfCA)

- Established in 2006 as a C-type project when ADAC was split off into ADC and CfCA
- Used to be a ”center” (ADAC) until 2006
- Propsed names
  - English: Center for Computational Astrophysics
  - Japanese: **計算科学センター**

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.

NS-06 ATERUI III (HPE Cray XD2000)

Supercomputer Dedicated to Astronomy

Present Open-Use Computer Facilities

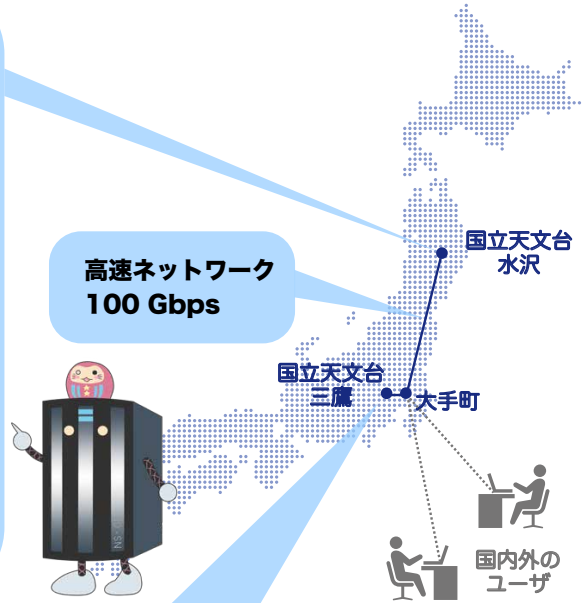
スーパーコンピュータ「アテルイIII」
(HPE Cray XD2000)

理論演算性能：1.99 Pflops
ノード数：288
総コア数：32,256

CPU：Intel Xeon CPU Max 9480
（システム M，208 ノード）
Intel Xeon Platinum 8480+
（システム P， 80 ノード）

ファイルサーバ
(DDN EXA Scaler)

総容量：15.00 PB



GPU クラスタ

ノード数：7
（NVIDIA A100）

中規模サーバ

ノード数：11
総コア数：524

計算サーバ

ノード数：100
総コア数：1,064
CPU：AMD Ryzen7
および 9 の各種 CPU

ファイルサーバ

総容量：約 10.2 PB

解析サーバ

ノード数：6
コア数：36（※）
主記憶容量：1 TB（※）

※1 ノードあたり

(2024.12)

Not only supercomputer but also simulation infrastructure!

Recent Activities

FY2019-2023

FY	# of users	# of publications	XC-A adoption rate	XC50 operating ratio
2019	273	137	12/60	94%
2020	298	179	13/63	93%
2021	288	168	16/52	96%
2022	310	165	15/51	95%
2023	305	171	15/38	97%

- 10 Nature/Science papers
- Average citation count: 37.7 (Web of Science 2024.11.21)

FY2023

FY2023	total	XC50	GPU	PC cluster
users	305(34%)	243	29	67
papers	171	146	11	30

(): % of students

- 4 press releases
- 34 PhD and master theses

Internal Collaborations

- ADC (Subaru HSC), TMT, ...

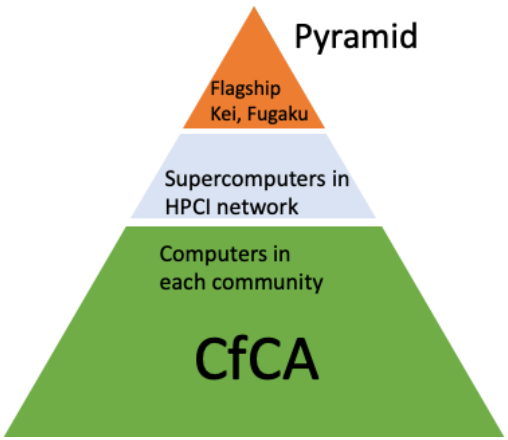
Roles of CfCA Supercomputer

MEXT HPCI Program

- 1st tier: flagship (e.g., Fugaku)
  - cutting-edge simulations
- 2nd tier: university supercomputers
- 3rd tier: supercomputers in each field (e.g., ATERUI)
  - middle-scale simulations
  - code development
  - education

Theoretical "Telescope" or "Laboratory"

- high-resolution simulations with realistic physics
  - to predict what we observe
  - to interpret what we observe



Background

CfCA's Missions

- Operation of open-use computer systems
- Research in computational astrophysics ($\rightarrow$ external fund)
- Visualization of astronomical data ($\rightarrow$ external fund)

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) (2021)."
- Yajima-san's message
  1. Keep updating the supercomputer every $\sim$5-6 years
  2. Keep CfCA & theoretical groups in NAOJ

Science Goals and Scientific Objectives

Science Goals

- Explore the formation and evolution of the universe through astrophysical simulations with the next-generation (TNG) 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

Supercomputers

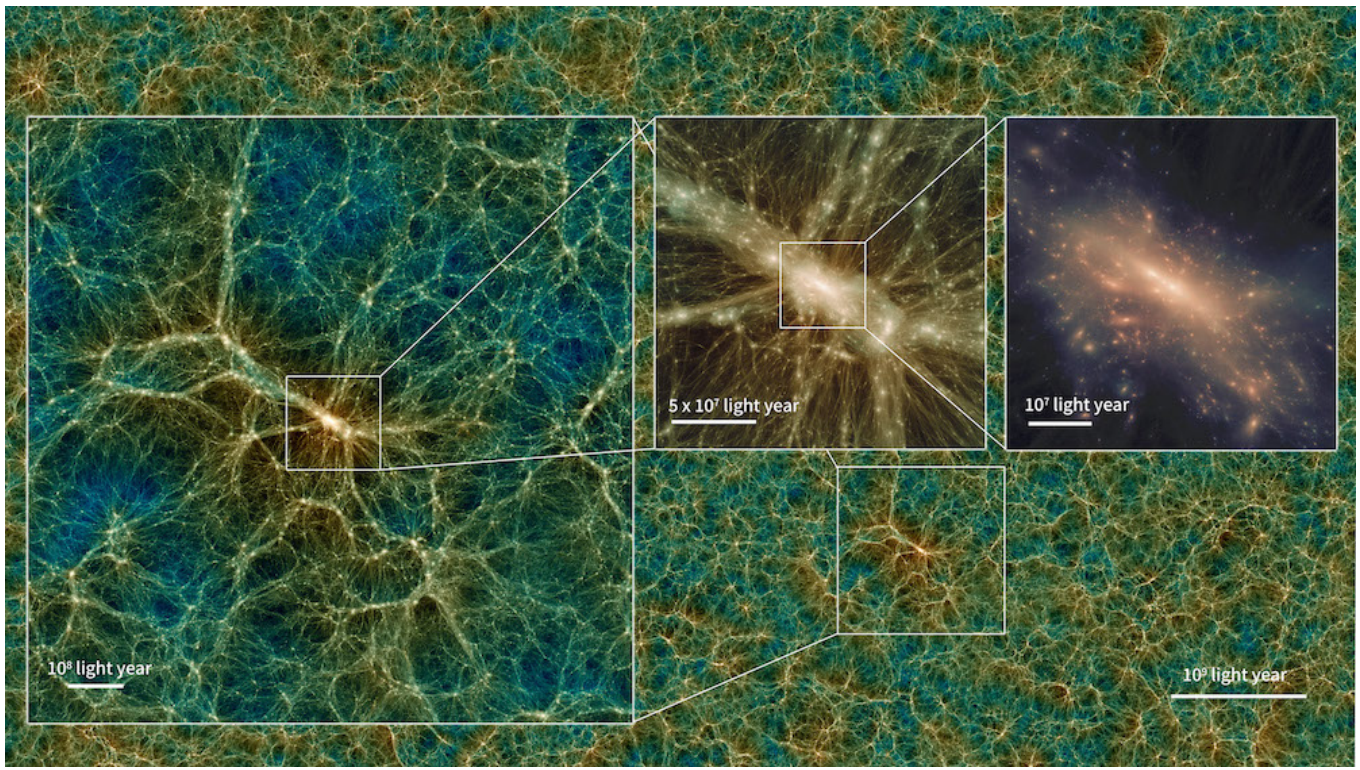
- ATERUI III (2024.12-2031.3)
- ATERUI TNG (2031.4?-?)

Science Investigations (1)

(Long-Term Plan for Astronomy and Astrophysics – Vision for the 2030s and 2040s)

Large-Scale Structure

- Cosmological *N*-body simulations of structure formation using dark matter particles on the scale of 10^{13}-10^{14} 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

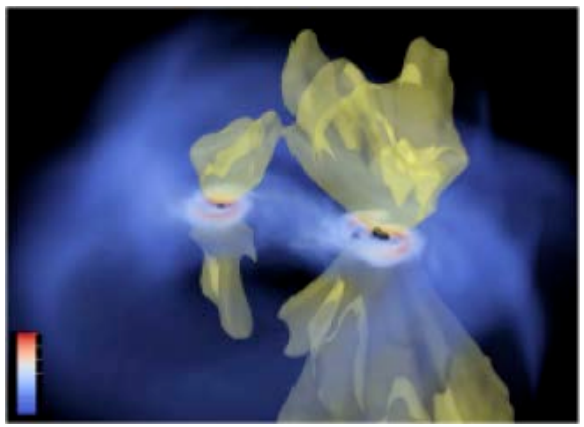
- Large-scale fluid-*N*-body simulations using more realistic gas-star system models that take into account star formation, stellar evolution, binary star evolution, chemical evolution, etc., to elucidate the formation and evolution of galaxies and star clusters.

(T. Saito)

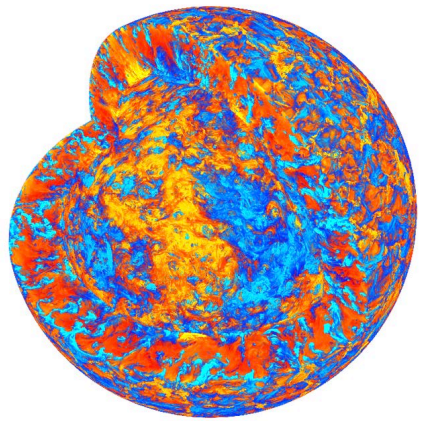
Science Investigations (3)

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

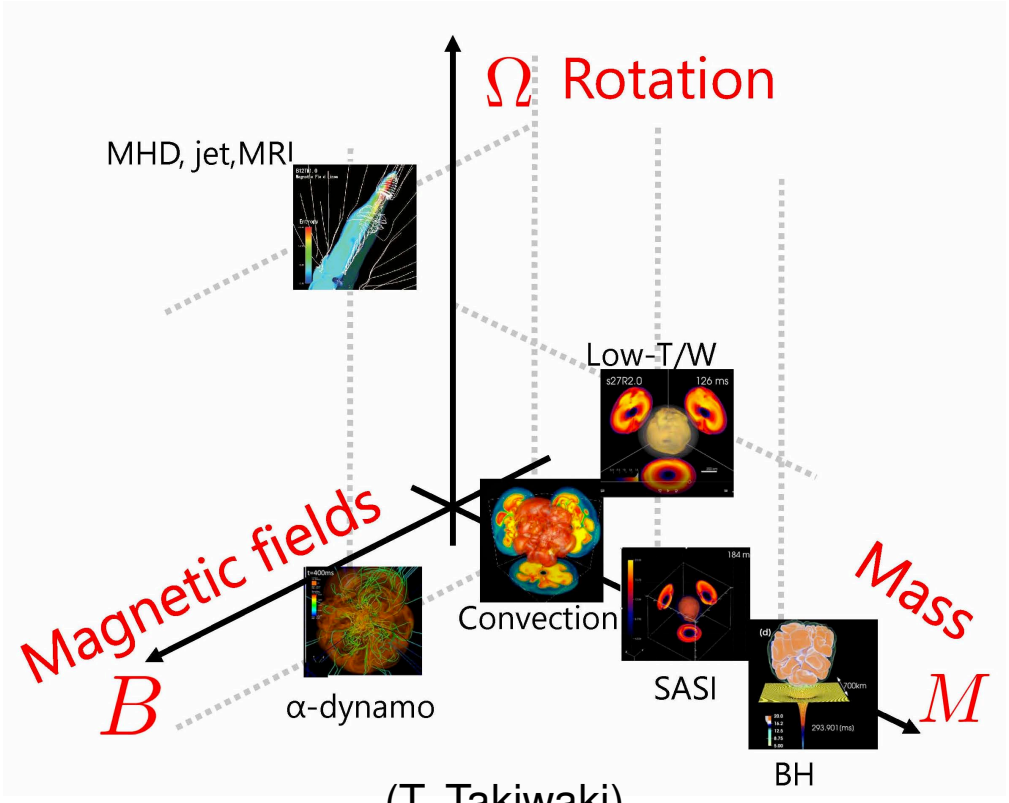
- Wide-area *N*-body simulations of planet accretion on tens of au scales using 10^7-10^8 planetesimals in evolving gas disks, including planetary migration, to reveal the origin of the diversity of planetary systems.

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.

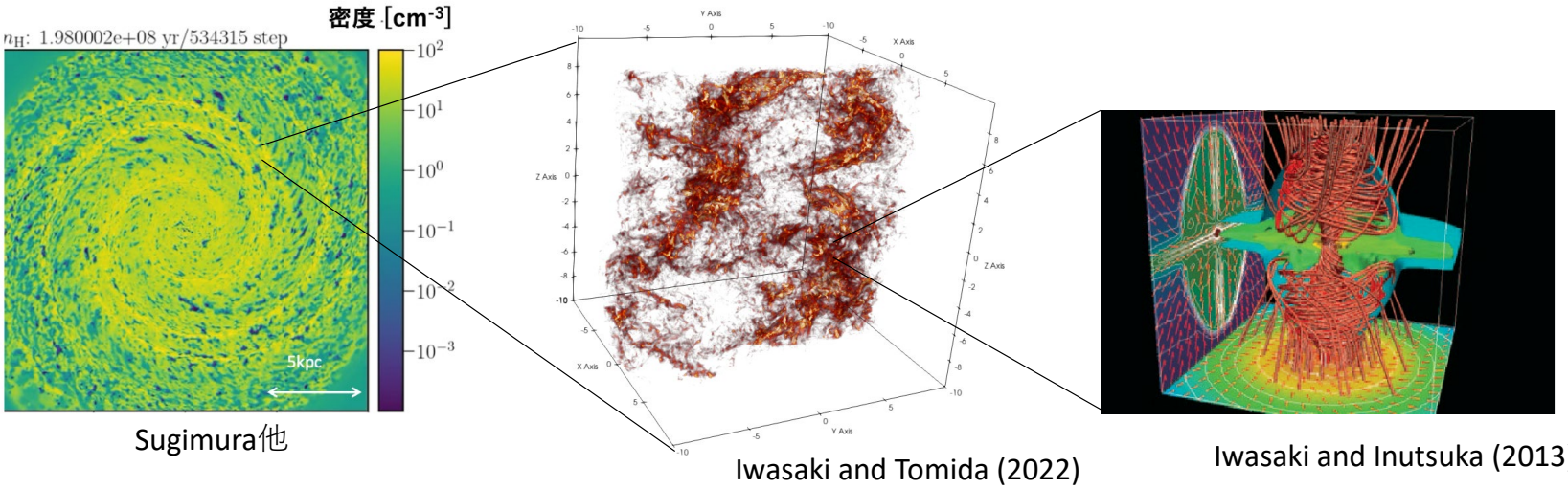
One Hundred 3D Core-Collapse Simulations

Toward Complete Understanding of Stellar Explosions



- Code: GRMHD simulations with neutrino radiation
- Model: 100 models for rotation, magnetic fields, and mass
- Goal: Systematic understanding of the mechanisms of supernovae, gamma-ray-bursts, black-hole formation, etc

Comprehensive Simulations from Galactic Disks to Circumstellar Disks



- Code: AMR with star particles and radiative transfer, zoom-in technique on star formation
- Goal: Evolution of the interstellar medium from the atomic gas through molecular clouds to stars and circumstellar disks to reveal the universality and diversity of star formation processes

Exploring Planetary Rings with TNG Simulations

TNG Simulations

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

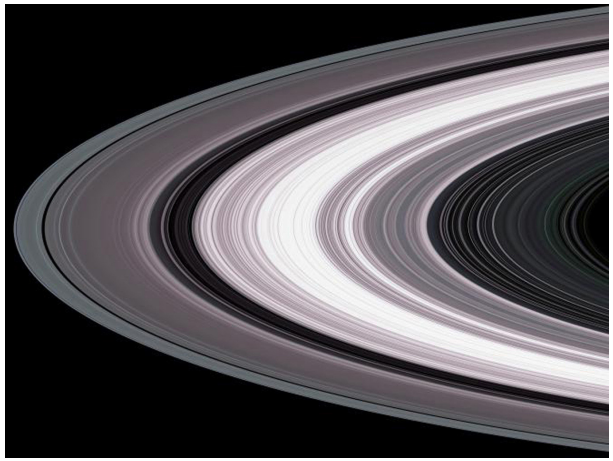
Code

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

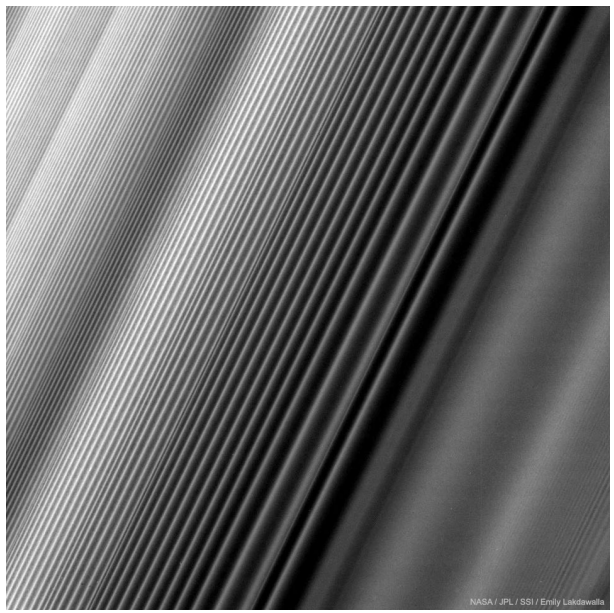
Goals

- 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)

Threshold Science

Research Outcomes

- Positive correlation with available computing resources

Computing Resources

- No threshold that would make it meaningless to implement

Threshold Science

- World's standard-level simulations
- One Hundred 3D Core-Collapse Simulations
  - 3D simulations with 100^3 resolution. M1 closure neutrino radiation with ≥ 10 energy groups. 5 models per year.
- Comprehensive Simulations from Galactic Disks to Circumstellar Disks
  - molecular cloud formation simulations with $\sim 20\ \mathrm{pc}$, the origin of stellar IMF is investigated with maximum resolution of $10\ \mathrm{au}$.
- Exploring Planetary Rings with TNG Simulations
  - elementary process of resonant satellite-ring interaction with $N = 10^9$ particles

Instruments and Data to be Returned

Instruments

- 2024.12-2031.3: ATERUI III (2 Pflops)
- 2031.4?-?: ATERUI TNG ($\gtrsim$ 30 Pflops?)
  - $\sim$10 times larger computational resources required for new scientific innovations
  - selection of a suitable CPU or GPU
  - use of AI to speed up simulations

Data to be Returned

- ”Digital Twins” of astronomical objects
  - higher-resolution physical quantities
  - multi-wavelength radiation flux
  - isotope and chemical abundance
  - dust size distribution
  - longer-term evolution
  - ...

Originality and International Competitiveness

All-in-One System, Do-It-Yourself On-Premises Facilities

- CfCA provides analysis servers and storage, all connected through a high-bandwidth network. The system is optimized for organizing and visualizing numerical output, supporting academic publications.
- Building smaller computer systems in a DIY manner reduces costs.

Strong Community, Codes and Their Developers

- Since 1996, supported by Rironkon, NAOJ has provided supercomputers for numerical simulations. The number of users has steadily increased, now approaching 300.
- A number of codes have been developed and are actively used by the Japanese research community, such as 3DnSNe, ASURA, Athena++, CANS+, FDPS, GPLUM, GreeM, GRQKNT, NR-RMHD, R2D2, RAIKOU, RAMNES, Sfumato, VLASOV, and many more.

Current Status

ATERUI III

- Massively parallel scalar computer (HPE Cray XD2000)
- 288 nodes, 32,256 cores
  - System M (high memory bandwidth)
    208 nodes, 23,296 cores (Xeon Max)
  - System P (high memory capacity)
    80 nodes, 8,960 cores (Xeon Platinum)
- Theoretical peak performance: 2 Pflops (ref. Fugaku 488 Pflops)
- Operation period: 2024.12-2031.3
- Users: 235 (as of 2024.12.5)
  - 1/3 graduate students
  - main computer for 73% users
- Budget: 350 Myen/year

ATERUI TNG

- Project activated

Towards ATERUI TNG

ATERUI TNG

- parallel scalar computer with accelerators?

Installation Strategy

- budget: minimum 350 Myen/year
- with ”frontier” project?
- joint procurement with other institutes?
- inter-NINS supercomputer: consolidating the budget for the open-use supercomputers within NINS and introducing a larger supercomputer?
- cloud computing?
- private financing from billionaires?
- ...

Preparation for TNG

- use of accelerators (e.g., GPUs)
- application of ML, AI, Big Data, ...
- ...

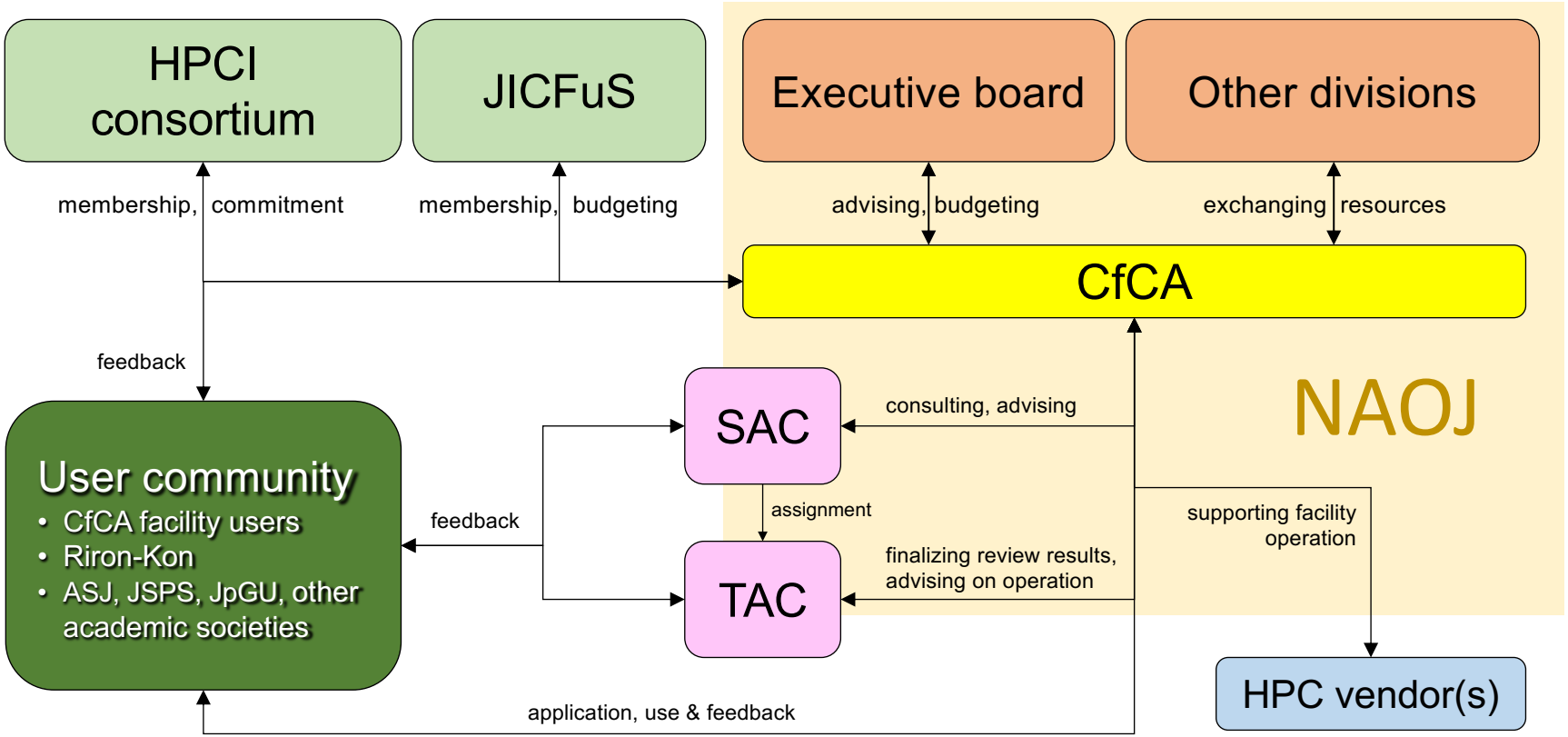
Cost Assessments, Budget Line and Status

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 can be accommodated, and the more research outcomes will be achieved.
- The NAOJ Executive committee decided to provide 350 Myen/year until FY2031. This budget is for the operation of the supercomputer including electricity fees.

Project Organization (1)

CfCA in Relation to Other Organizations



Project Organization (2)

Personnel

- As of December 2024, CfCA is operating the computing facilities with the workforce described in p. 6–7

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

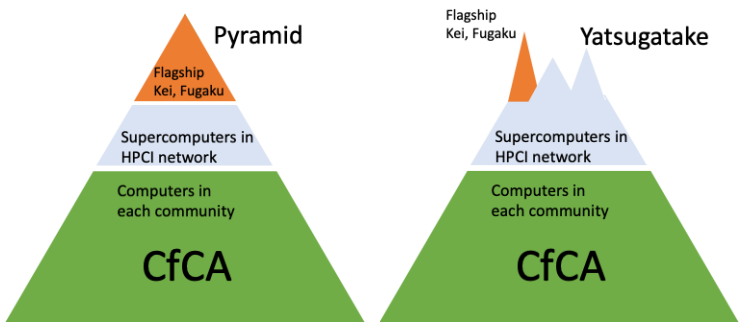
- CfCA keeps the cooperation with Rironkon.

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.

Why NAOJ?

Supercomputer in Astronomical Observatory

- synergy with telescopes
  - to predict what we observe
  - to interpret what we observe

Inter-University Research Institute Corporation

- to operate the open-use computer system as a basic HPC infrastructure of computational astrophysics

MEXT HPCI Program

- 3rd-tier supercomputer dedicated to astronomy
  (1st: flagship, 2nd: university computer centers)

Summary of the Proposal

CfCA's Most Important Mission

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

Exploring the Universe by TNG Simulations

- Period: FY2031-
- Goal: Explore the formation and evolution of the universe through astrophysical simulations with TNG supercomputers
- Examples of CfCA's focus subjects
  - supernova explosion
  - star and disk formation
  - planetary ring dynamics
  - (many others)
- Instrument: ATERUI TNG - 3rd-tier supercomputer dedicated to astronomy ($\gtrsim$ 350 Myen/year)

Appendix

Members (Tenured)

Professors (2)

- E. Kokubo (Director), N. Tominaga

Associate Professors (2)

- T. Takiwaki, M. Machida

Associate Professor (Senior Lecturer) (1)

- T. Ito (Deputy Director)

Assistant Professors (2)

- K. Iwasaki, T. Moriya

Research Engineer (1)

- M. Shizugami

Engineer (1)

- K. Takahashi

(joint appointment from DoS, Mizusawa, and ADC/ALMA)

Members (Fixed-Term/Age-Limit Retirement)

Research Expert (1)

- H. Nakayama

Senior Specialists (5)

- H. Fukushi, T. Takeda, H. Hohokabe, M. Isogai, N. Tanaka

Project Researchers (5)

- Y. Huang, S. Ideguchi, Z. Keszthelyi, Y. Matsumoto, Y. Misugi

Research Supporters (3)

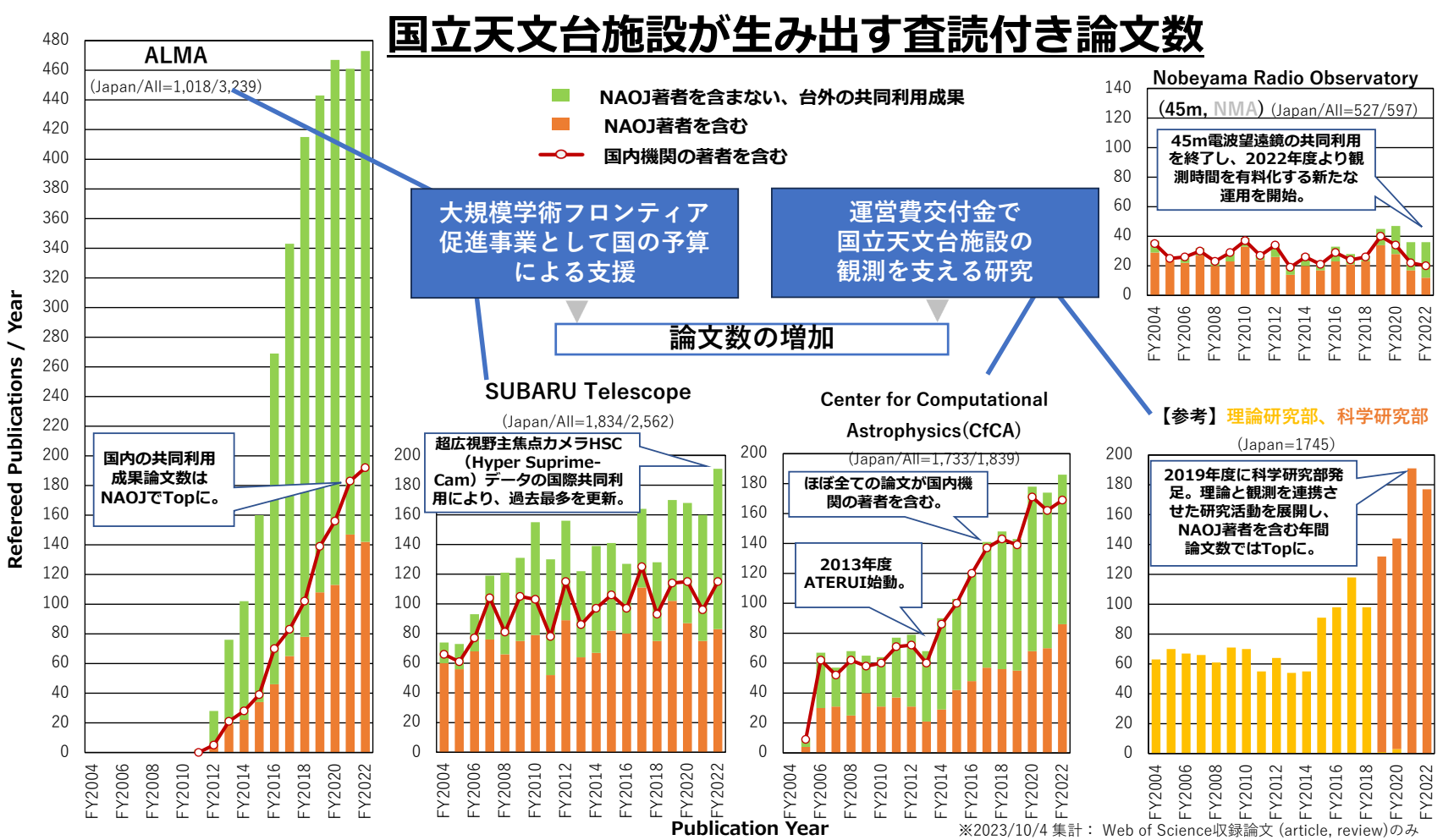
- S. Hasegawa, K. Kano, C. Kimura

Administrative Expert (1)

- M. Masuyama

(4D2U)

Papers from NAOJ



(Tsuneta 2023.12)

Renaming the Department Name in Japanese

Better Consistency between the E/J Project Names

- CfCA's is named as 天文シミュレーションプロジェクト in Japanese. Obviously, the English and Japanese names are inconsistent, and this has been the case from the beginning of the division history (2006-present).
- Along with an inquiry by the NAOJ Executive Board, we have proposed to change our Japanese name as 計算科学センター (hopefully from FY2024) while keeping the English name (CfCA) intact.
- CfCA has served as a center for numerical astrophysicists in domestic and international communities. The English name (Center for Computational Astrophysics) is completely consistent with our role.
- Japanese name should reflect this fact as well, and people will be better aware of what CfCA is for in this community.