

The Role of Fugaku Supercomputer in Advancing High-Performance Computing for COVID-19 Scientific Research

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Abstrak

Pandemi COVID-19 menuntut pendekatan komputasi berskala besar untuk mempercepat penelitian, analisis, dan pengambilan keputusan berbasis data. Fugaku, salah satu superkomputer berperforma tertinggi di dunia, memainkan peran penting dalam mendukung riset terkait COVID-19 melalui kemampuan komputasi berkecepatan tinggi. Penelitian ini bertujuan untuk mengkaji peran Fugaku dalam pemodelan komputasional COVID-19, khususnya pada simulasi transmisi aerosol dan penemuan kandidat obat. Metode penelitian yang digunakan adalah studi kualitatif melalui tinjauan sistematis terhadap literatur ilmiah, laporan teknis, dan publikasi resmi terkait pemanfaatan Fugaku dalam konteks pandemi. Hasil kajian menunjukkan bahwa Fugaku mampu mempercepat simulasi dinamika aerosol menggunakan Computational Fluid Dynamics (CFD) serta analisis interaksi protein-obat melalui simulasi molekuler, sehingga memberikan pemahaman yang lebih akurat mengenai pola penyebaran virus dan potensi terapi. Temuan ini menegaskan bahwa superkomputer Fugaku berperan signifikan dalam menjembatani high-performance computing dengan aplikasi kesehatan nyata, serta menjadi model penting bagi pengembangan riset komputasi di masa depan.

Kata kunci— Fugaku, High-Performance Computing, COVID-19, simulasi komputasional, Computational Fluid Dynamics

Abstract

The COVID-19 pandemic has demanded large-scale computational approaches to accelerate research, analysis, and data-driven decision-making. Fugaku, one of the world's highest-performance supercomputers, has played a critical role in supporting COVID-19 research through its advanced computing capabilities. This study aims to examine the role of the Fugaku supercomputer in computational modeling of COVID-19, particularly in aerosol transmission simulation and drug discovery processes. The research adopts a qualitative approach through a systematic review of peer-reviewed literature, technical reports, and official publications related to Fugaku's applications during the pandemic. The findings indicate that Fugaku significantly accelerated aerosol dynamics simulations using Computational Fluid Dynamics (CFD) and enabled large-scale molecular simulations for protein–drug interaction analysis, leading to more accurate insights into virus transmission patterns and potential therapeutic candidates. These results demonstrate that Fugaku serves as a crucial bridge between high-performance computing and real-world healthcare applications, while also highlighting its importance as a benchmark for future computational research and exascale systems.

Keywords— Fugaku, High-Performance Computing, COVID-19, computational simulation, Computational Fluid Dynamics

1. INTRODUCTION

The COVID-19 pandemic has exposed significant limitations in conventional research approaches when confronted with large-scale, rapidly evolving global crises. The urgent need to understand virus transmission mechanisms, evaluate mitigation strategies, and accelerate drug discovery processes has required computational capabilities far beyond those offered by traditional computing infrastructures. Experimental and clinical studies, while essential, are often time-consuming, costly, and constrained by physical and ethical limitations. Consequently, high-performance computing (HPC) has become an indispensable component in modern scientific research, enabling large-scale simulations, massive data analysis, and real-time scenario evaluation to support evidence-based decision making [1], [2].

In recent years, the role of HPC has expanded beyond classical numerical computation to include data-intensive workloads, artificial intelligence, and mixed-precision computing. These advances have positioned

supercomputers as critical tools for addressing complex, multi-scale problems in fields such as climate modeling, materials science, epidemiology, and biomedical engineering [3], [4]. During the COVID-19 pandemic, HPC systems played a pivotal role in accelerating computational modeling of virus transmission, molecular interactions, and population-level dynamics, demonstrating the strategic importance of supercomputing in public health emergencies [1], [5].

Among existing HPC systems, the Fugaku supercomputer, jointly developed by RIKEN and Fujitsu, represents a significant milestone in the evolution of modern supercomputing. Since its full-scale operation began in 2021, Fugaku has consistently maintained leading positions in global performance benchmarks, including HPCG and Graph500, highlighting its superior capability in handling both compute-intensive and data-centric workloads [6]–[9]. Built on the A64FX processor architecture, Fugaku integrates massive parallelism with high memory bandwidth and exceptional energy efficiency, addressing one of the most critical challenges in contemporary HPC development—achieving high performance while minimizing power consumption [10], [11].

Fugaku’s flexible and scalable architecture enables efficient execution of diverse computational workloads, ranging from computational fluid dynamics (CFD) and molecular dynamics simulations to artificial intelligence and deep learning applications. Its support for mixed-precision computation allows researchers to balance numerical accuracy and computational speed, making Fugaku particularly suitable for large-scale scientific simulations that require both precision and performance [12], [13]. These architectural features have positioned Fugaku as a benchmark platform for next-generation exascale and post-exascale computing systems [14].



Figure 1. Japan's Fugaku keeps position as world's fastest supercomputer

One of Fugaku’s most impactful applications has been its contribution to research supporting the global response to the COVID-19 pandemic. Through large-scale CFD simulations, Fugaku enabled detailed analysis of aerosol and droplet transmission in various real-world environments, including offices, public transportation, healthcare facilities, and educational spaces. These simulations provided quantitative insights into airflow patterns, ventilation effectiveness, mask efficiency, and physical distancing measures, directly informing public health guidelines and risk mitigation strategies [1], [2], [15]. Unlike simplified analytical models, the high spatial and temporal resolution achieved through Fugaku-based simulations allowed for more accurate representation of complex environmental conditions and human behavior [16].

In parallel, Fugaku has been extensively utilized for large-scale molecular simulations aimed at accelerating drug discovery and therapeutic development. By simulating protein–drug interactions at unprecedented scale and speed, Fugaku significantly reduced the time required to identify potential antiviral compounds targeting SARS-CoV-2. This computational approach complemented laboratory experiments by narrowing down candidate molecules, thereby optimizing resource allocation and accelerating subsequent experimental validation [17], [18]. Such integration of HPC-driven molecular modeling into biomedical research highlights the transformative role of supercomputing in modern drug discovery pipelines [19].

Beyond its immediate impact on COVID-19 research, Fugaku’s success illustrates the broader potential of HPC systems to bridge the gap between computational science and real-world applications. The ability to rapidly process massive datasets, perform high-fidelity simulations, and support interdisciplinary collaboration underscores the strategic importance of supercomputing infrastructures in addressing global challenges. Therefore, this study focuses on analyzing the role of the Fugaku supercomputer in computational modeling of COVID-19, with particular emphasis on its architectural characteristics, performance capabilities, and

applications in aerosol transmission analysis and molecular simulation. By synthesizing recent literature and technical reports, this research aims to demonstrate how HPC platforms such as Fugaku can serve as foundational tools for future scientific innovation and large-scale problem solving [14], [20].

2. RESEARCH METHODS

2.1. Research Design

This study employs a qualitative research design with a systematic computational review approach to analyze the role of the Fugaku supercomputer in supporting COVID-19 research. This design is appropriate for synthesizing existing computational and technical evidence without conducting new experimental or clinical trials, following established qualitative research and systematic review guidelines in computer science and engineering research [21], [22]. The study focuses on examining Fugaku's computational architecture, performance characteristics, and its applications in large-scale simulations related to aerosol transmission and drug discovery.

2.2. Data Sources and Literature Selection

Data were collected from peer-reviewed journals, international conference proceedings, technical reports, and official documentation published between 2022 and 2026 to ensure the relevance and currency of the analysis. Major digital libraries and repositories used in this study include IEEE Xplore, ACM Digital Library, ScienceDirect, SpringerLink, Wiley Online Library, and official publications from RIKEN and Fujitsu [23], [24].

The literature selection process followed predefined inclusion criteria [22], [25]:

1. Publications that explicitly discuss Fugaku supercomputer architecture or performance.
2. Studies utilizing high-performance computing (HPC) for COVID-19-related simulations, including aerosol transmission modeling and molecular simulations.
3. Articles published in reputable journals or conferences indexed in Scopus, Web of Science, or IEEE Xplore.
4. Publications written in English and released within the specified time range.

Studies that lacked technical relevance, did not involve HPC-based analysis, or focused solely on clinical outcomes without computational modeling were excluded.

2.3. Data Analysis Method

The selected literature was analyzed using thematic analysis, a well-established qualitative method for identifying recurring patterns and technical themes across complex datasets [26]. The analysis was structured into three dimensions commonly used in high-performance computing (HPC) system studies [27], [28]. The analysis focused on three primary dimensions:

1. Computational Architecture Analysis

This dimension examines Fugaku's system architecture, including processor design (A64FX), interconnect topology, memory hierarchy, and energy efficiency. Performance metrics such as HPL, HPCG, and Graph500 benchmarks were reviewed to assess Fugaku's computational capabilities relative to other HPC systems [29], [30].

2. Simulation and Modeling Analysis

This analysis evaluates the use of Fugaku in large-scale computational fluid dynamics (CFD) simulations for aerosol transmission studies and molecular dynamics simulations for protein-drug interaction analysis. Parameters such as simulation scale, resolution, computational precision, and execution efficiency were examined to assess Fugaku's suitability for COVID-19-related modeling [31], [32].

3. Application Impact Analysis

This dimension analyzes how Fugaku-based simulations contributed to practical outcomes, including public health risk assessment, ventilation optimization, and acceleration of drug discovery workflows. The analysis emphasizes the role of HPC-driven insights in supporting data-driven decision making [33], [34].

2.4. Validation and Reliability

To enhance the reliability of the findings, cross-source validation was performed by comparing results across multiple independent studies and technical reports. Consistency of findings related to Fugaku's performance and application outcomes was used as an indicator of reliability [21], [26]. Additionally, benchmark results reported in different sources were cross-checked to minimize bias and ensure

methodological robustness.

2.5. Research Workflow

The research workflow follows a structured review process adapted from systematic review and mapping study methodologies in software and systems engineering [22], [25], consisting of scope definition, literature collection, classification, thematic analysis, and synthesis. The overall research workflow consists of the following steps:

1. Identification of research scope and computational focus.
2. Systematic collection of relevant literature and technical documentation.
3. Classification of studies based on computational methods and application domains.
4. Thematic analysis of architectural features, simulation methodologies, and application outcomes.
5. Synthesis of findings to evaluate Fugaku’s role in COVID-19 computational research.

2.6. Research Limitations

This study relies on secondary data and previously published research and does not involve direct execution of simulations on the Fugaku system. Such limitations are inherent in systematic review-based research; however, the use of validated benchmark data and peer-reviewed sources ensures analytical reliability and scientific rigor [22], [27].

3. RESULTS AND DISCUSSION

This section presents and discusses the key findings of the study regarding the role of the Fugaku supercomputer in supporting COVID-19–related research and technological development. The results are derived from a systematic analysis of selected studies and technical reports focusing on Fugaku’s computational architecture, large-scale simulation capabilities, and real-world applications. Rather than merely reporting numerical outcomes, this section integrates the findings with interpretative discussion to highlight their broader scientific and practical implications.

The discussion emphasizes how Fugaku’s high-performance computing capabilities enable advanced simulations that are not feasible on conventional systems. Particular attention is given to its applications in aerosol transmission modeling, molecular simulations for drug discovery, and data-driven decision support. By comparing computational approaches and observed outcomes across multiple studies, this section illustrates how Fugaku contributes to accelerating research workflows, improving analytical accuracy, and supporting evidence-based strategies in public health and scientific innovation.

1. Specification

The specifications of Fugaku will be listed in this the table below:

Table 1. Specification Fugaku Supercomputer Basic

Performance Modes	Normal Mode: <i>Double Precision (64 bit) 488 Petaflops</i> <i>Single Precision (32 bit) 977 Petaflops</i> <i>Half Precision (16 bit) 1.95 Exaflops</i> <i>Integer (8 bit) 3.90 Exa Exaops</i>
	Boost Mode: <i>Double Precision (64 bit) 537 Petaflops</i> <i>Single Precision (32 bit) 1.07 Exaflops</i> <i>Half Precision (16 bit) 2.15 Exaflops</i> <i>Integer (8 bit) 4.30 Exaops</i>
Total Memory	4,85 PiB(pebibyte) or 1,126 Terabyte
Total Memory Bandwidth	163 PB/s approximate 166.912 TB/s
Cores	48 Cores
Memory	HBM2 32 GiB, 1024 GB/s

Technology	7nm FinFET
Compiler	Fortran2008 & Fortran2018 subset
	C11 & GNU and Clang extensions
	C++14 & C++17 subset
	OpenMP 4.5 & OpenMP 5.0 subset
	Python + Numpy + Scipy, Ruby
Operating System	Red Hat Enterprise Linux 8
	McKernel
MPI	Fujitsu MPI (Based on OpenMPI), RIKEN-MPICH (Based on MPICH)

2. Fugaku's Architecture

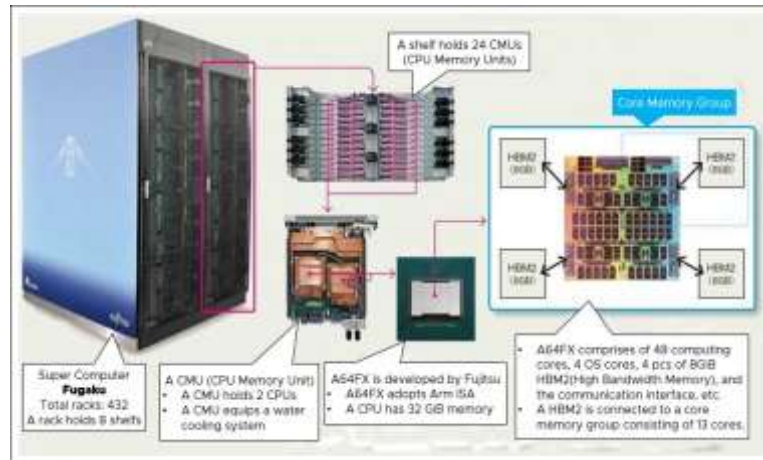


Figure 2. Fugaku's Architecture taken from hacarus.com

This image shows the detailed architecture of the Fugaku supercomputer, where each rack is composed of multiple shelves that hold CPU Memory Units (CMUs). Each CMU integrates a Fujitsu A64FX processor, high-bandwidth HBM2 memory directly connected to the CPU, and a water-cooling system to maintain efficiency at scale. The A64FX processor is based on the ARM instruction set architecture and contains multiple computing cores, operating system cores, and memory and communication cores, all organized into core memory groups. By tightly coupling computation, memory, and cooling within a highly modular rack design, Fugaku achieves extremely high performance, low latency, and excellent scalability for advanced simulations, artificial intelligence, and data-intensive scientific research.

3. Documentation

To use the Supercomputer Fugaku, you need to use the Fugaku website and login node. Here describes the installation procedure of client certificate which is required for using the Fugaku website, and the creation and registration procedure of SSH public key which is required to connect the login node. The flow of setting is as follows:

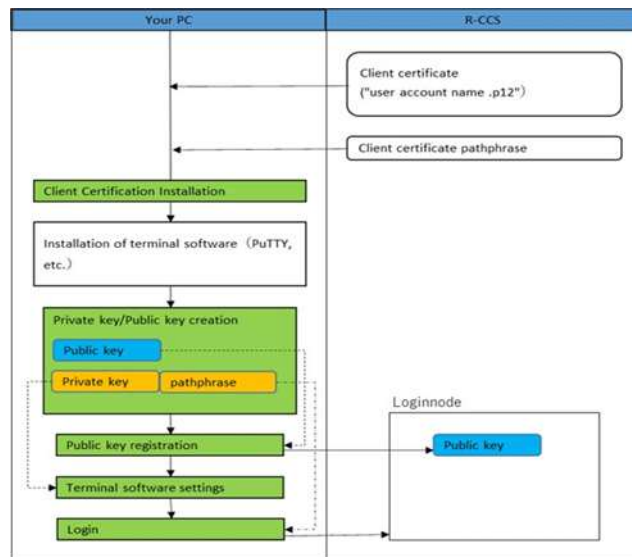


Figure 3. Workflow diagram of the authentication login process to the R-CCS system

A. Preparation and Installation

- Ensure you have the client certificate file “user account name.p12
- Open the firefox browser on your computer, then click on (options) and select (privacy account and security)

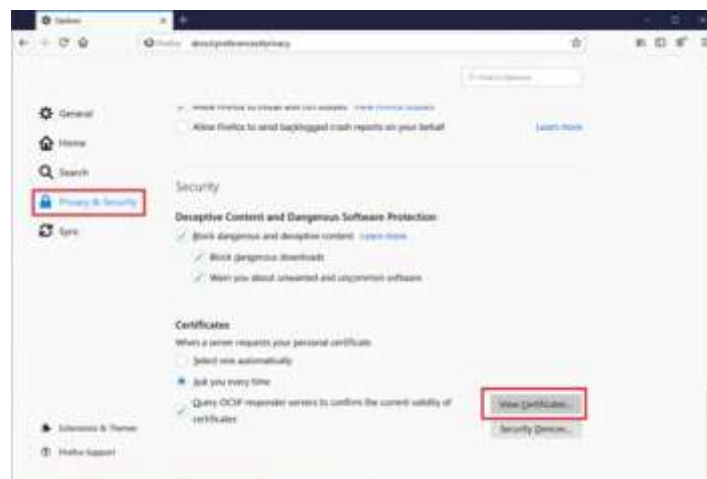


Figure 4. Preparation and Installation

- Click on (view certificates) and click (import)

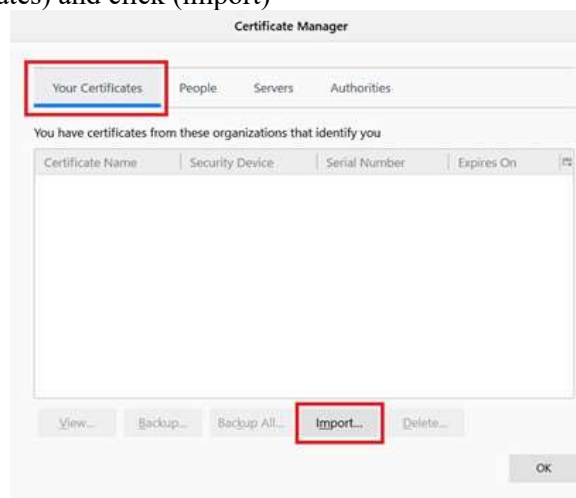


Figure 5. View certificates

- Choose the “local account name.p12 file” and click open

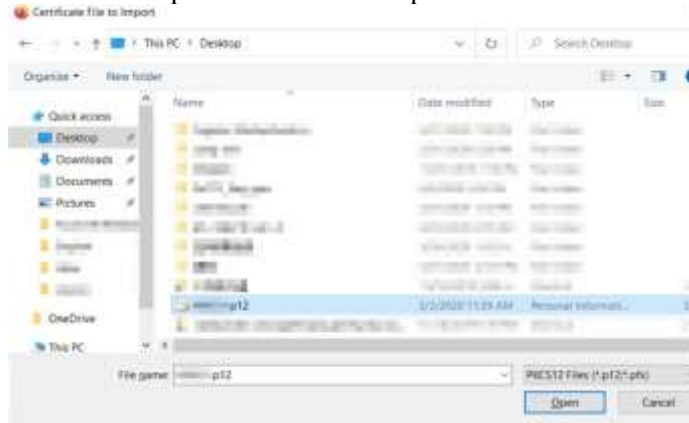


Figure 6. Local account name.p12 file

- Enter the client passphrase in the Password field and click [OK].

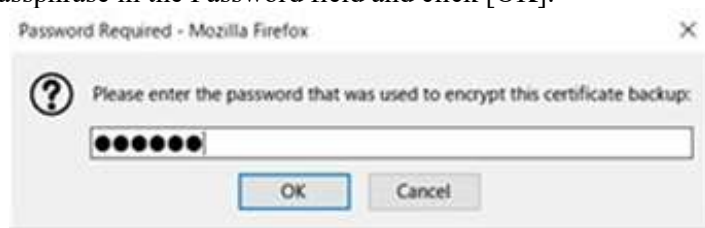


Figure 7. Password field

B. Accessing steps to the Fugaku website. This indicates how to access to the Fugaku website.

- Open the browser and access to the following:
URL. <https://www.r-ccs.riken.jp/en/fugaku/>
- Once the client certificate selection is shown, select the using local account’s client certificate.
The example of firefox

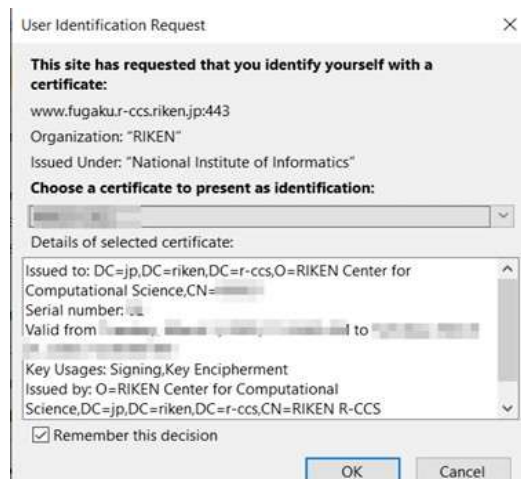


Figure 8. Client certificate

- In the password input dialog, enter the password of the private key registered when the client certificate was installed. The example of firefox

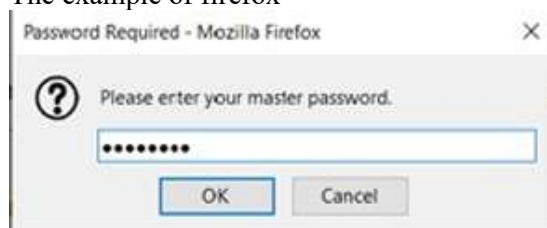


Figure 9. Password input dialog

- If the client certificate is successfully authenticated, the following screen will be displayed



Figure 10. Client certificate is successfully authenticated

- Login
Log in into Supercomputer Fugaku by using local account with using SSH (Secure Shell) Version2 (public authentication)
Create an SSH key (public key and private key) on the user terminal in advance and register the public key from the Fugaku website screen. Register only the public key. When a private key is registered, processing such as temporary suspension of login may be performed as a security measure.

4. Modules

Default supercomputer works in a shared system, which oftentimes needs a way to manage software environments more atomic and dynamically. Modules were there to instigate the process, which involved loading and unloading packages in an efficient manner. Fugaku's module supports different types of shells and script languages, including bash, ksh, zsh, sh, csh, tcsh, fish, cmd, pwsh, plus several languages such tcl, perl, python, ruby, cmake, and r. Modules used are also supported in managing different versions of these languages(Python 3.8 or Python 3.10). These are the lists of modules used during the commanding of Fugaku using bash as its language.

A. Initiating compiler environment using module

- Module load ... (any compiler name -for example gcc/12.4.0)
- Module load gcc/12.4.0 → sets up specific environment for the compiler at hand along with the specified compiler version (12.4.0)
- Module switch gcc/14 → switch version to 14.0
- Module unload gcc → to remove the current module compiler

B. Several ommands list for type modulefile (Tool Command Language)

```
break → acts as stop sign
chdir directory → changes where the file system is stored
conflict → prevents incompatible compiler, or incompatible version of the
compiler to run at the sametime
continue → continues code execution unto the next line
exit → immediately terminate the commands
family → specifies the module category, thus preventing redundant module
getenv → retrieves environment variable
e.g. set mypath [getenv HOME]
    puts "Your home directory is $mypath"
getvariant → get module variant information
- e.g. set var [getvariant]
    puts "Module variant: $var"
hide-modulefile → hides module being display in module avail
- e.g. hide-modulefile mymodule
hide-version → hide the specific module version
- e.g. hide-version mymodule/1.2
is-avail → check if module version is available
- e.g. if {[is-avail gcc/12.4]} {
    puts "GCC 12.4 is available!"
}
```

```
}
is-loaded → check if module is loaded
- e.g. if {[is-loaded gcc]} {
puts "GCC is already loaded."
}
is-saved → check if module is in secure environment
- e.g. if {[is-saved mymodule]} {
puts "mymodule is in the saved list."
}
is-used → check if module is currently in used
- e.g. if {[is-used mymodule]} { puts "mymodule is in use."
}
lsb-release field - get system information details
- e.g, set os_version [lsb-release version]
puts "OS version: $os_version"
module-alias → creates alias for module name
- e.g, module-alias gfortran gcc
module-forbid → disallows loading of the specific module
- e.g. module-forbid oldmodule
prereq-all (modules...) → load all listed modules
- e.g. prereq-all gcc openmpi
prereq-any → request at least one module
- e.g. prereq-any gcc clang
pushenv → temporarily sets environment table
- e.g. pushenv PATH
/opt/mysoftware/bin
puts → prints message
- e.g. puts "Hello, user!"
remove-path → removes a specific file location
- e.g. remove-path PATH
/opt/oldsoftware/bin
reportWarning string → display warning message but allows module to load
- e.g. reportWarning "Warning: This module is deprecated."
```

5. Future Prospects

Fugaku's technology of exascale level computing must be developed, knowing possibilities of future systems that may exceed exaflop level, therefore Fugaku's future development may relate to the increase in processing power yet efficient in energy consumption and/or scalability. Based on extremetech.com, Japan -which is where Fugaku originated- is actively pursuing next level supercomputing technologies aiming to a scale beyond, called **zettascale** level by 2030 a technology exceeding 1,000 times better compared to current processing level. The Ministry of Education, Culture, Sports, Science, and Technology (MEXT), announced the new Fugaku called to be 'Fugaku Next', during this preparation the design of 2nm processor said intended for the new computer is currently in progress, with codenamed 'Monaka', were pursued to be done in the end of 2028.

4. CONCLUSION

This study provides a comprehensive analysis of the strategic role of the Fugaku supercomputer as a high-performance computing infrastructure capable of addressing the increasing complexity of modern, multidisciplinary research. Through its exceptional processing speed, energy efficiency, and scalable architecture, Fugaku has established a new benchmark in the development of exascale computing systems. The findings demonstrate that these technical advantages not only enhance computational performance but also directly improve the quality, speed, and reliability of scientific research outcomes.

From a scientific perspective, this research highlights how Fugaku enables large-scale, high-resolution simulations that were previously difficult or impractical to perform. In the context of pandemic response and environmental modeling, Fugaku has significantly contributed to advancing the understanding of complex phenomena such as aerosol transmission dynamics, molecular interactions, and nonlinear environmental systems. These capabilities strengthen computational research methodologies by complementing experimental and observational approaches with highly detailed and accurate simulations.

In terms of practical impact, the results show that Fugaku substantially accelerates research workflows,

from early-stage exploration to data-driven decision making. This acceleration leads to more efficient use of time and resources, particularly in urgent global situations such as public health crises. Moreover, the application of Fugaku in supporting policy formulation and strategic planning demonstrates that modern supercomputers have evolved beyond purely academic tools to become essential instruments for evidence-based decision support.

The study also emphasizes Fugaku's role in fostering interdisciplinary and inter-institutional collaboration. By providing a flexible and powerful computational platform accessible to diverse scientific domains, Fugaku facilitates the integration of high-performance computing, artificial intelligence, and large-scale data analytics. This convergence creates new opportunities for scientific innovation while strengthening a collaborative and sustainable research ecosystem.

From a strategic standpoint, the findings offer important insights for the design and development of future supercomputing systems. The experience of Fugaku underscores the need for next-generation HPC architectures to balance extreme computational performance with energy efficiency, sustainability, and application flexibility. Consequently, this research contributes not only to the understanding of Fugaku as a technological achievement but also to shaping future policies and infrastructure planning for high-performance computing.

Overall, this study confirms that Fugaku represents a transformative shift in the role of supercomputers in addressing global challenges. The insights gained from this research are expected to support informed decision making in HPC development and to encourage the effective utilization of supercomputing technologies in advancing scientific innovation, global resilience, and sustainable development.

DAFTAR PUSTAKA

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