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The Impact of Supercomputer Frontier for Scientific Research

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Abstract

This research paper will examine the powerful machine created by the Oak Ridge National Laboratory (ORNL), the Frontier supercomputer, also known as the world's first exascale supercomputer. Frontier is a key tool for studying climate change in the US, as it's the first supercomputer capable of performing over a quintillion calculations per second. This breakthrough enables more detailed and accurate study and prediction of climate patterns, helping scientists develop detailed models of weather patterns and climate systems. These models show how climate change is affecting the country, including stronger storms, rising sea levels, and other extreme weather events. Through its powerful computing capabilities, the Frontier supercomputer enables advanced climate modelling. It supports the SCREAM programme, which aims to improve the accuracy of climate predictions by simulating global weather patterns at unprecedented scales. This

paper will explore how Frontier works, what makes it so powerful, and how it helps the United States better understand and fight climate change. It will also discuss the advanced technology behind Frontier and how it solves problems that were once too complex to handle.
Keywords: *Supercomputer, SCREAM, Frontier works, modeling.*

Abstrak

Makalah penelitian ini akan membahas mesin komputasi canggih yang dikembangkan oleh *Oak Ridge National Laboratory* (ORNL), yaitu superkomputer Frontier, yang juga dikenal sebagai superkomputer eksaskala pertama di dunia. Frontier merupakan alat penting dalam mempelajari perubahan iklim di Amerika Serikat karena menjadi superkomputer pertama yang mampu melakukan lebih dari satu kuintiliun perhitungan setiap detiknya. Terobosan ini memungkinkan para ilmuwan untuk mempelajari dan memprediksi pola iklim dengan tingkat detail dan akurasi yang jauh lebih tinggi, sehingga membantu dalam membuat model terperinci mengenai pola cuaca dan sistem iklim. Model-model tersebut menunjukkan bagaimana perubahan iklim berdampak pada negara tersebut, termasuk meningkatnya intensitas badai, kenaikan permukaan laut, serta berbagai kejadian cuaca ekstrem lainnya. Melalui kemampuan komputasi yang sangat kuat, superkomputer Frontier memungkinkan pengembangan pemodelan iklim tingkat lanjut. Frontier mendukung program SCREAM, yang bertujuan untuk meningkatkan akurasi prediksi iklim dengan melakukan simulasi pola cuaca global dalam skala yang belum pernah dicapai sebelumnya. Makalah ini akan membahas bagaimana Frontier bekerja, faktor-faktor yang membuatnya memiliki kemampuan komputasi yang sangat besar, serta bagaimana teknologi ini membantu Amerika Serikat dalam memahami dan menghadapi perubahan iklim. Selain itu, makalah ini juga akan membahas teknologi canggih yang mendukung Frontier serta bagaimana

superkomputer ini mampu menyelesaikan permasalahan yang sebelumnya terlalu kompleks untuk ditangani.

Kata kunci : Superkomputer, SCREAM, cara kerja Frontier, pemodelan.

INTRODUCTION

The evolution of these powerful machines has transformed the landscape of scientific research, enabling unprecedented simulations and analyses that were once deemed impossible. Among the most notable advancements in this field is the development of the Frontier supercomputer, which has redefined the capabilities of high-performance computing. Frontier are developed by Oak Ridge National Laboratory (ORNL), is recognized as the world's first exascale supercomputer Operating under the auspices of the Energy Exascale Earth System Model E3SM collaboration, the group developed a cloud-resolving atmosphere model: Simple Cloud Resolving E3SM Atmosphere Model SCREAM [3][15]. Resolving clouds is a famously challenging task for climate models, which typically operate at resolutions too coarse to represent clouds, capable of performing over one quintillion calculations per second. This remarkable speed allows researchers to solve complex issues such as climate modeling and climate change with unparalleled accuracy and efficiency [7]. The supercomputer's architecture, which incorporates advanced graphics processing units (GPUs), has facilitated significant advancements in modeling atmospheric phenomena, including cloud formations. These capabilities have opened new avenues for understanding long-term climate patterns and predicting extreme weather events [5].

Understanding climate change requires analyzing massive datasets and running highly detailed simulations. Traditional computing methods struggle with the scale and complexity of climate models, which must factor in atmospheric dynamics, ocean currents, and long-term environmental changes. Frontier's unprecedented

computational capabilities enable researchers to enhance climate predictions, refine weather forecasting, and develop strategies for mitigating global warming. As climate change continues to pose a critical threat to global ecosystems and human societies, the role of supercomputers like Frontier becomes increasingly vital [1]. Researchers can generate insights that inform policy decisions and adaptation strategies by enabling high-resolution simulations that accurately represent cloud dynamics and precipitation patterns. The collaborative efforts behind Frontier demonstrate a commitment to leveraging cutting-edge technology for the greater good, showcasing how supercomputing can be harnessed to solve some of humanity's most daunting challenges.

In this research paper, we will explore the historical trajectory of supercomputers, focusing on their evolution from early machines to today's exascale systems. The development of Frontier supercomputers, their significance in the evolution of high-performance computing, and how this is changing climate research. By examining their architecture, capabilities, and contributions to climate science, we will examine how these technological advances have empowered scientists to develop sophisticated climate models that improve our understanding of climate change and its potential impacts on our world.

Background and History

Frontier is the world's first exascale supercomputer that breaks the boundaries of traditional computing by achieving exascale performance of more than 1 exaflops, or 1.1 exaflops in the High-performance Linpack benchmark [7]. One of the largest challenges during development was power consumption. Existing information pointed to hundreds of thousands of GPUs being necessary to achieve 1 exaFLOP, with a total power consumption of 150-500 MW. For the location Oak Ridge Leadership Computing Facility

and The operators from Oak Ridge National Laboratory and the U.S Department of Energy [11].

METHODOLOGY

The methodology used in this research paper focuses on how learning about the Frontier supercomputer may help mitigate climate change. In order to do this, we started by collecting data from a number of reliable sources, such as Frontier-related technical papers and reports [7]. These resources gave valuable details on its computational power, energy consumption, and climate modelling applications. Learning about Frontier's practical uses was very important for this study like how we looked at its function in the SCREAM program which generates highly accurate weather and climate predictions [3]. We also investigated how scientists can explore the impacts of climate change, including rising sea levels and extreme weather events, and simulate global weather patterns thanks to the supercomputer's massive processing power [15]. We also looked at Frontier's waste heat output and energy usage. Frontier is one of the most energy-intensive data centers which generates a significant amount of waste heat that might be used to heat campus facilities [9]. We looked at innovative solutions to the problems caused by low-grade heat, like heat pump technology, which effectively transfers and uses this waste heat to support sustainable operations [1]. We also looked at modern technologies like carbon capture and renewable energy sources that can help reduce the effects of climate change [2]. We evaluated how Frontier supports these attempts by supporting modern research and performing complex simulations [12]. By looking at all

of these aspects, we were able to get a full understanding of Frontier's energy efficiency design and contributions to minimizing the effects of climate change.

Architecture & Design

The Frontier supercomputer and related systems employ several sophisticated architectures to achieve their high performance and efficient operation. These architectures span from the overall system design down to the individual components.

System-Level Architecture

At the highest level, Frontier utilizes the HPE Cray EX supercomputer architecture. This is characterized by its dense, liquid-cooled compute cabinets, designed for maximum computational density and efficient thermal management. Frontier comprises 74 cabinets housing 9408 compute nodes, along with standard racks for support and management functions. The system is powered by AMD 64core OPtimized 3rd Gen EPYC CPUs and AMD MI250X Instinct GPUs, connected by GPE Slingshot interconnects with 200Gbe interfaces.

Cabinet and Blade Architecture

HPE Cray EX4000 Cabinet is a key component of the system. Each cabinet can hold up to 64 compute blades within 8 compute chassis and employs direct liquid cooling using a shared coolant distribution unit (CDU) to efficiently remove heat The cabinet also includes 4 power shelves, each with a maximum of 8 rectifiers.



Figure 1: HPE Cray EX4000 Cabinet Architecture

Within the cabinet, The HPE Cray EX235A blade architecture is used systems like Frontier and LUMI



Figure 2: HPE Cray EX235A Blade

From figure 2 Each blade contains two compute nodes, each equipped with one CPU and four MI250X accelerators. These blades are direct liquid cooled for all components to support high-power processors exceeding 500W.

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Node and Processor

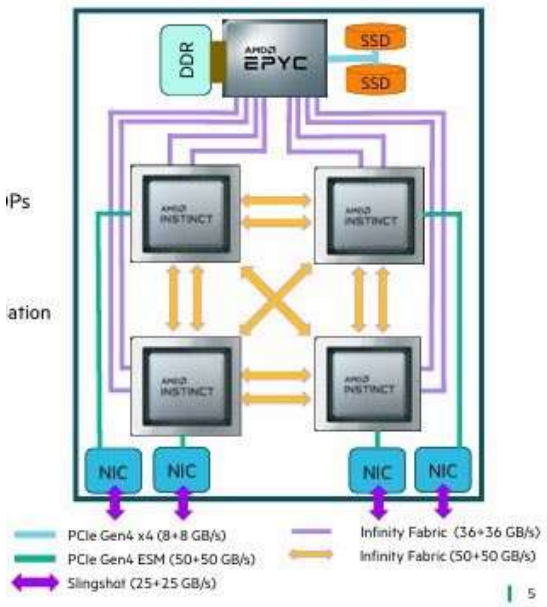


Figure 3: Frontier Compute Node Design

The Frontier compute node architecture is where the core processing occurs. Each node features 1 AMD Optimized 3rd Gen EPYC 64core processor with 2 hardware threads per core, a 2,0GHz base clock, and a 3.7GHz boost clock. It also includes 512 GB of DDR4 memory with 205 GB/s peak bandwidth, 2 NVMe 2 TB SSDs, and 4 AMD MI250X Instict GPUs. The AMD MI250X Instinct GPUs have 128 GB of high bandwidth memory (HBM2E) and 3.2 TB/s peak bandwidth. The GPU delivers 53 TFLOPS double-precision peaks for modeling and simulation. AMD Infinity Fabric is used for high-speed connections between the CPU and GPUs and between the MI250X Gpus. The CPU and all GPUs have coherent memory. Each node has 4 HPE Slingshot Interconnect 200 Gbe NICs

for internode communication. Each MI250Z has two Graphic Compute Dies (GCDs) per module, resulting in 8 GCDs per node. Each GPU has 64 GB of HBM and 1.6 TB/s of HBM peak bandwidth containing 110 compute units and delivering 26.5 TFLOPS double-precision peak. The GPUs are connected to each other and the CPU via AMD Infinity Fabric links.

The Frontier Compute Node

The Frontier supercomputer's exceptional performance is underpinned by the design of its compute nodes, the fundamental building blocks of the system. These nodes are complex and powerful units, featuring a heterogeneous architecture optimized for high-performance computing.

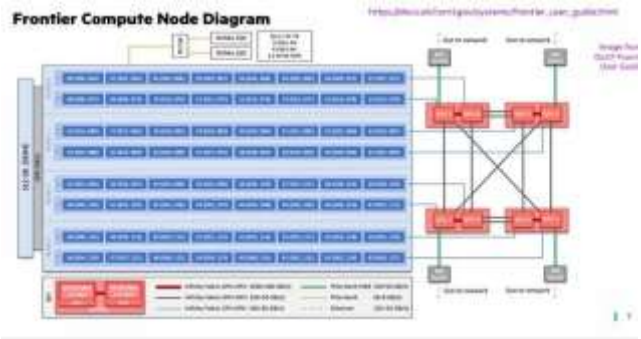


Figure 4: Frontier Compute Node Diagram

The Frontier Compute Node's Diagram has many things design principles. Heterogeneous Computing. By combining CPUs and GPUs, the node leverages the strengths of both types of processors. CPUs excel at general-purpose tasks, while GPUs are highly efficient at parallel computations, enabling the node to handle a wide range

of workloads effectively Emphasis on Interconnects. The high-speed interconnect, particularly use of AMD Infinity Fabric and PCIe Gen4, are critical for the node's performance memory Capacity and Bandwidth. The node's large memory capacity and high memory bandwidth are essential for handling the massive datasets and complex computations involved in exascale computing. At the heart of each Frontier compute node lies a heterogeneous architecture, combining different types of processing units to handle a wide range of computational tasks efficiently. The primary components include: AMD EPYS 7755HX CPU, 512 GB DDR4 Memory, NVme SSDs, And AMD MI250X Instict GPUs. Interconnect has different speeds and storage, efficiency and performance of the compute node heavily rely on the high-speed interconnections between its various components. Frontier employs several advanced interconnect technologies. Infinity Fabric GPU-GPU (200+200 GB/s). The diagram highlights the very high-speed connections between the two GPUs located within the same MI250X module and this Infinity provides 200 GB/s bandwidth in each direction, enabling bidirectional bandwidth. This enables the dual-die accelerator to act as a unified, high-performance computing node, facilitating seamless peer-to-peer communication and large-scale parallel workload execution.

The Compiler

Frontier, the exascale supercomputer at Oak Ridge National Laboratory, provides Cray, AMD, and GCC compilers for developing and optimizing high-performance applications. Cray and AMD compilers, based on LLVM/Clang, are specifically tuned for Frontier's architecture, while GCC offers broader compatibility. Developers use compilers extremely fast communication and data transfer between these closely related GPUs

Infinity Fabric GPU-GPU (50+50 GB/s). The node also features Infinity Fabric connections between GPUs located in different MI250X modules Infinity Fabric CPU-GPU (36+36 GB/s). Efficient data transfer between the CPU and GPUs is crucial, The node uses Infinity Fabric links to connect the CPU to each of the four GPUs, providing a bandwidth of 36 GB/s in each direction PCIe Gen4 ESM (50+50 GB/s). This likely refers to PCIe Gen4 connections for Enhanced Switch Modules. PCIe Gen4 is a high-speed interface standard, and these connections likely provide pathways for the GPUs to communicate with other components within the system via the PCIe bus. PCIe Gen4 Ethernet (25+25 GB/s). High-speed network connectivity is essential for a supercomputer. The node utilizes PCIe Gen4 to connect to the e¥Ethernet network interfaces, providing 25 GB/s bandwidth in each direction. NIC (Network Interface Controller). The node is equipped with Network Interface Controllers (NICs), which are the physical interfaces that connect the node to the network wrappers like **C, C++**, and **Fortran** to streamline compilation and ensure optimal performance. These compilers support scientific applications, including climate modeling and molecular simulations, by enhancing code efficiency and scalability across thousands of nodes. Through advanced optimization features, Frontier's compilers enable researchers to maximize the system's computational power for scientific purposes.

Cooling System

The Frontier supercomputer at Oak Ridge National Laboratory employs an advanced warm-water cooling system to manage the substantial heat generated by its highperformance components. This system circulates approximately 6,000 gallons of water per minute through the supercomputer's more than 9,000 nodes, effectively dissipating heat without the need for pre-chilled water. This approach enhances energy

efficiency by eliminating the energy-intensive process of precooling the water. The cooling infrastructure includes CoolIT's Direct Liquid Cooling technology, which is integrated into the system to ensure optimal thermal management. Additionally, the system's design minimizes air-side cooling requirements, as the watercooled cabinets operate quietly without the need for internal fans. This warm-water cooling strategy not only reduces operational costs but also contributes to a quieter and more efficient data center environment, aligning with modern hardware. [9]

DISCUSSION AND RESULT

Frontier's Capabilities and Impact on Climate Modeling

Frontier's Significance stems from its extraordinary computational capabilities, which are in the realm of "Exascale computing" This means it can perform calculations at an exascale level, a quintilion calculations per second. Frontier is the Exascale Computing for Climate change Insights. It capability is directly applied to Climate science It allows for simulations and predictions of climate patterns with unprecedented details and accuracy, frontier handling, massive Climate Datasets, it will help research that involves enormous amounts of data.

Technological Advancements

Frontier's capabilities aren't just about throwing more processors at the problem, Frontier to Heterogeneous Computing for Climate Modeling that doesn't rely solely on CPUs, which are the "Brains" of most computers, It combines AMD EPCY 7713 "Trento" CPUs, which are powerful general-purpose processors, with AMD Instinct MI250X GPUs High-speed Interconnect for data Flow in a computer, the different parts need to communicate rapidly. The HPE Slingshot interconnect is the high-speed network thath enables this communication and has Advanced Cooling for performance because supercomputer generate a lot of heat. Frontier uses liquid cooling, which is much

more effective than air cooling, and this allows he components to operate at optimal temperatures, preventing them from overheating and ensuring reliable performance.

Impact on Climate Predictions and Understanding

Frontier's power and technology translate into significant advancements in climate science, and more Accurate Climate Predictions. Frontier allows scientists to create more detailed and sophisticated climate models, These models can simulate global and regional weather patterns with greater precision, This leads to more accurate predictions of future climate scenarios, such as temperature changes, rainfall patterns, sea-level rise, and extreme weather events. The insights gained from Frontier's climate modeling are essential for informing decisions about climate change mitigation and adaptation.

CONCLUSION

Exascale supercomputers like the Frontier system at Oak Ridge National Laboratory (ORNL) have revolutionized climate modeling by enabling highly detailed, cloud-resolving simulations that enhance understanding of atmospheric and oceanic processes. With the ability to process vast datasets at exceptional speeds, these systems reduce uncertainties in climate projections, improving predictive accuracy. Machine learning applications further aid in analyzing complex data, supporting informed decision-making for policymakers and scientists. Collaborative advancements in computational science have accelerated progress in this field, making exascale supercomputing a vital tool in the fight against climate change. Through more accurate simulations and predictions, these technologies contribute to global efforts to mitigate and adapt to the impacts of a changing climate.

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