University of Lleida

Master's Degree in Informatics Engineering

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SuperMUC-NG

High Performance Computing

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1 Introduction

The world of supercomputers have been increased during the last decades becoming the highest performance devices of the day that extend the limits of size, technology, power, and buyer budgets to solve technical and scientific “grand challenge” problems.

Supercomputer journey is marked by fifty-five years of amazing races from the big hardware and technological manufactures to design and build “the world’s fastest”, and usually the most costly supercomputer to solve complex calculations from various areas in less time.

The exascale competition rises as the new space race focused on scientific research like recreating the Big Bang, understanding earthquakes, protein folding, modelling of new disease, finding the God particle, among others. But, most of all, this is a story about nations. Competition still reigns - over resources, over science, over the future. And to build that future, superpowers need supercomputers.

This document aims to expand knowledge about supercomputers in today’s world in addition to conducting a comprehensive study of the *SuperMUC-NG*, based on a detailed analysis of specifications and performance compared to other computing giants.

2 Motivation

The possibility arose to carry out such a research task on a precisely interesting field, and it was then when came up the planning to deepen its knowledge. In this way, it is definitely a good starting point getting focused on areas to increase knowledge acquiring a better complete vision over the possibilities in the supercomputers world.

Moreover, would be enlightening to get focused on analyzing in detail and deepen into knowing more of one remarkable supercomputer belonging to the top 500, even doing comparisons of its performance with other supercomputers.

3 Executive summary

Supercomputers, the beasts of the computing world, occupy enormous rooms and perform trillions of calculations per second. In general, a supercomputer can be defined as a machine with high computing performance that has extremely fast processing speeds which are employed for specialized applications requiring immense amounts of mathematical calculation and logical analysis.

Besides, the purpose of this document, whether a researcher or not, is to provide a starting point as a comprehensive guide concerning the wide range of fields in the super-computing cosmos, and a reference on how detail accurately a supercomputer chosen in a comparison analysis resulting in a grasp breakdown.

Accordingly, the *SuperMUC-NG* is one of the top500 supercomputers included in the last november 2020 list giving support for innovative research in a variety of complex scientific disciplines such as astrophysics, fluid dynamics or life sciences, and, further on, is highlighted a report analysis from a critical point of view.

4 Document structure

This section looks forward to narrating what is in each section of the document to help understand and facilitate the approach to the contents.

- **Supercomputers:** Debut on the supercomputers world, defining and detailing what a supercomputer is and its purpose deepening in research interests, just as nations sympathy.
- **Why SuperMUC-NG:** Justification on the chosen selection to focus on a complete supercomputer analysis.
- **SuperMUC-NG specifications:** Describing and enumerating all the technical specifications.
- **Analysis:** Exhaustive performance analysis of the *SuperMUC-NG* supercomputer laying the groundwork for the subsequent comparison.
- **Comparison:** Discussion and comparison with other supercomputers.
- **Conclusions:** Complete end of the line resulting from the study and over the realization of this document as well as from the *SuperMUC-NG* and some contributions regarding personal opinion.

5 Supercomputers

The supercomputer, any of a class of extremely powerful computers. The term is commonly applied to the fastest high-performance systems available at any given historic time. Such computers have been used primarily for scientific and engineering work requiring exceedingly high-speed computations.

Common applications for supercomputers include testing mathematical models for complex physical phenomena or designs, such as climate and weather, the evolution of the cosmos, nuclear weapons and reactors, new chemical compounds (especially for pharmaceutical purposes), and cryptoanalysis. In this way, the supercomputer plays an important role in the field of science. As the cost of super-computing declined in the 1990s, more businesses began to use supercomputers for business research and other business-related models.

Supercomputers have specific distinguishing features. Unlike conventional computers, they usually have more than one CPU (Central Processing Unit), which contains circuits for interpreting program instructions and executing arithmetic and logic operations in sequence.

The use of several CPUs to achieve high computational rates is necessitated by the physical limits of circuit technology. Electronic signals cannot travel faster than the speed of light, which thus establishes a fundamental speed limit for signal transmission and circuit switching.

This limit has almost been reached, owing to miniaturization of circuit components, dramatic reduction in the length of wires connecting circuit boards, the transistors race over the years, and innovation in cooling techniques (e.g., in various supercomputer systems, processor and memory circuits are immersed in a cryogenic fluid to achieve the low temperatures at which they operate fastest).

Rapid retrieval of stored data and instructions is required to support the extremely high computational speed of CPUs. Therefore, most supercomputers have a very large storage capacity, as well as a very fast input/output capability which regurarly results in a bottleneck.

So, **What makes a computer turn into a SuperComputer?**

There some features introduced before, just like a vast number of processing units which empowers the computational capacity. Today's supercomputers feature several hundreds of thousands, some up to millions of processing units, CPUs, or GPUs[1] depending on the architecture, working in unison using massively parallel processing. But to measure the ratio over a normal supercomputer with just one or a few processing units is used the Floating Point Operations Per Second (FLOPS) standing as truly multiplications and divisions since they require significantly more power than additions and substractions.

Then, obviously, they will get an immense collection of RAM-type memory units. The RAM modules, although they are usually distributed across many nodes, can be treated as a single pool with multiple access, all thanks to the software middlewares applied to avoid race conditions.

[1]GPU: Graphic Processing Unit

Moreover, a high-speed interconnect between nodes. The idea is to establish a high-speed switches net, as there are a large number of nodes, and thus, make possible the communication between them. There lots of topologies when talking about nets, but they are usually connected in a non-blocking, fat-tree topology delivering not only up to 200Gb/s bandwidth between them but also in-network computing frameworks such as MPI (Message Passing Interface).

Further, this high-speed achieved is also complemented by equally powerful data writing and reading capability by using parallel file systems or via software solutions. Just because, most of them use specific software to ensure the best computing performance and high production levels from these complex systems.

Finally, this kind of supermachines must use innovative ways of cooling the processing units. Hence, thermal management of supercomputers involves intricate and efficient liquid cooling systems, hot water cooling, and immersion cooling. Keeping the processors below their throttle temperatures ensuring all nodes are available at full capacity with no performance downgrades.

On the other side, and regarding the history, these supermachines started around the 1950s, when early supercomputers were built by various companies, one individual, *Seymour R. Cray*, really defined the product almost from the start creating *the CDC 1604*, one of the first generation of commercially successful transistorized computers, and the fastest computer in the world. He was an electronic engineer and was deeply involved in every aspect of creating the computers that his companies built, but the brilliant stage rises in the 1970s.

Specifically, Cray's pioneering achievement was *the Cray-1*, introduced in 1976, which is the first successful implementation of vector processing (meaning it could operate on pairs of lists of numbers rather than on mere pairs of numbers). But, later, was released *the Cray-2* based on 4 processor liquid cooled totally immersed in a tank of *fluorine.*

Cray establishes the basis during these years, therefore, in the 90s appeared the first computers with thousands of processors which really achieve a great margin of computation power to the ones released until then. That is when massive processing rises.

Ergo, in the 90s, there were a lot of experiments and innovations and started to appear the first software to communicate via nodes and to aggregate highly parallel computing proceedings. In this manner, now, in the 21st century, we can talk about petascale computing.

But that's not all, all this work was on one hand related always to companies, such as IBM, but, the nations were aware of these amazing achievements giving contract support to those companies who investigate the world of those giants. Basically, there was for years, a hidden race since the aim was to employ, also, the capabilities that these supercomputers possess in various weapon programs, simulations of weapon systems, and in designing and modeling of high-end technologies for defense research, as using them the research is less time consuming and more efficient.

6 Why SuperMUC-NG?

It is a German Supercomputer located in Leibniz, in the state of Bavaria belonging to the Leibniz Supercomputing Centre (LRZ) of the Bavarian Academy of Sciences. It was the fastest supercomputer in Europe when it started its operation in 2012, and it has been figuring among the Top 10 of the 500 most powerful supercomputers in the world since November of 2018.

First, *SuperMUC-NG* is based on *Lenovo* and we think that the quality of the product manufactured in Germany is the best in the world. However, we interested in the *SuperMUC-NG* because it has a great optimization related to energy efficiency and it uses singular refrigeration; it uses a new form of cooling that IBM developed, called *Aquasar*, that uses hot water to cool the nodes.

In addition, it uses a *XEON Platinum* processor-based architecture which is only the one based on it. And as we know these processors are historical just because they are built over the years by Intel and they are the origins of the new one's today. Moreover, applies *the Intel Omni-Path* designed to achieve a low latency of communication, a low energy consumption, and a high ratio of performance which Intel developed this architecture specifically to great scale computing.

Also, Francesc read the thesis *"Meta-Heuristics for Scheduling in Cluster Federated Environments"* by Dr. Eloi Gabaldon Ponsa, this thesis is related to the *Cluster Federated Environment* and our energy consumption and efficiency. We think that could be interesting to analyze this supercomputer because it has well energy efficiency, and the documentation is easy to find and very well texted.

Figure 1: SuperMUC-NG

7 SuperMUC-NG Specifications & Analysis

7.1 Overview

SUPERMUC-NG - THINKSYSTEM SD650, XEON PLATINUM 8174 24C 3.1GHZ, INTEL OMNI-PATH

Site:	Leibniz Rechenzentrum
System URL:	https://www.lrz.de/services/compute/supermuc/supermuc-ng/
Manufacturer:	Lenovo
Cores:	305,856
Memory:	75,840 GB
Processor:	Xeon Platinum 8174 24C 3.1GHz
Interconnect:	Intel Omni-Path
Performance	
Linpack Performance (Rmax)	19,476.6 TFlop/s
Theoretical Peak (Rpeak)	26,873.9 TFlop/s
Nmax	8,402,688
HPCG [TFlop/s]	207.844
Software	
Operating System:	SUSE Linux Enterprise Server 12 SP3

Figure 2: Overview SuperMUC-NG

As we can see in the above figure, it is an overview of *SuperMUC-NG*. This supercomputer is located in Garching, Germany (Operators: Leibniz-Rechenzentrum) and manufactured by *Lenovo*. It uses *Xeon Platinium* 8174 24C 3.1GHz as a processor and it has 305.856 cores and 75.840 GB of memory.

Related to the performance it has 19.476,6 TFlop/s of Linpack Performance (Rmax), 26.873.9 TFlop/s of Theoretical Peak (Rpeak), 8.402.688 of Nmax and 207.844 HPCG [TFlop/s]. Also, like Operating System uses SUSE Linux Enterprise Server 12 SP3 and the internal interconnect is an Omni-Path network that works with 100 Gbit/s (the connection between the islands has 1:4 of pruning factor).

7.2 Specifications

The figure below describes all the compute nodes, file systems, infrastructure, and software that *SuperMUC-NG* has.

Hardware of SuperMUC-NG

ComputeNodes	Thin Nodes	Fat Nodes	Total (Thin + Fat)
Processor	Intel Skylake Xeon Platinum 8174	Intel Skylake Xeon Platinum 8174	Intel Skylake Xeon Platinum 8174
Cores per Node	48	48	48
Memory per node (GByte)	96	768	NA
Number of Nodes	6,336	144	6,480
Number of Cores	304,128	6,912	311,040
PEAK @ nominal (PFlop/s)	26.3	0.6	26.9
Linpack (Pflop/s)	TBD	TBD	19.476
Memory (TByte)	608	111	719
Number of Islands	8	1	9
Nodes per Island	792	144	NA
Filesystems			
High Performance Parallel Filesystem	50 PB @ 500 GB/s		
Data Science Storage	20 PB @ 70 GB/s		
Home Filesystem	256 TB		
Infrastructure			
Cooling	Direct warm water cooling		
Waste Heat Reuse	Reuse for producing cold water with adsorption coolers		
Software			
Operating System	Suse Linux (SLES)		
Batch Scheduling System	SLURM		
High Performance Parallel Filesystem	IBM Spectrum Scale (GPFS)		
Programming Environment	Intel Parallel Studio XE GNU compilers		
Message Passing	Intel MPI, (OpenMPI).		

Figure 3: SuperMUC-NG Specs

SuperMUC-NG has**6.336 Thin** (8 Islands * 792 Nodes per Island) compute nodes with 48 cores and **144 Fat** (1 Island * 144 Nodes per Island) compute nodes with 48 cores. Related to the memory it has 96 GB of memory for each Thin node and 768 GB for memory for each Fat node.

It has the total of 311.040 cores distributed in 304.128 Thin cores (48 Cores per Node * 6.336 Thin Nodes) and 6.912 Fat cores (48 Cores per Node * 144 Fat Nodes). Related to the memory, it has 96GBytes for each Thin node and 768GByte for each Fat node.

In addition, the processor SKU used in *SuperMUC-NG* is a 24 core model dubbed *Intel Xeon Platinum 8174*. It supports both a 205 and 240W operational TDP mode, in regular operation however only the former is used, due to energy usage constraints.

The infrastructure to cooling the supercomputer uses direct warm water, this technology directly cools active components in the system such as processors and memory modules with coolant temperatures and it reuse for producing cold water with adsorption coolers.

Additionally to *SuperMUC-NG* itself, some cloud nodes have been purchased. The Compute Cloud currently consists of:

Cloud Node Type	Number of Nodes	CPU (Cores)	RAM (GB)	GPUs
Cloud Compute Node	82	40 (@ 2.4 GHz)	192 GB	
Cloud GPU Node	32	40 (@ 2.4 GHz)	768 GB	2x Nvidia Tesla V100 16 GB
Cloud Huge Node	1	192 (@ 2.1 GHz)	6.000 GB	

Figure 4: SuperMUC-NG Cloud Node

The compute cloud nodes are composed by 82 nodes and 192GB of RAM. According to the GPU, it has 32 GPU nodes with 2 NVidia Tesla V100 16GB and 768GB of RAM, both with 40 cores and one huge memory node with 6 TB and 192 cores.

8 Comparison

After this brief presentation about the *SuperMUC-NG* supercomputer specifications, we must be aware of his position at the top500 supercomputers list and compare it with the most powerful ones. Regarding the position, the *SuperMUC-NG* has obtained the 15th most powerful supercomputer position in the World but they used to be at position 9th in November 2019.

Then, we are doing this comparison with the first 4 current supercomputers, Fugaku, Summit, Sierra, and Sunway TaihuLight. Also, to see in perspective how in the recent years *SuperMUC-NG* got to position 15 as the technology evolves in comparison to the nowadays big giants.

First, there several parameters to compare like the number of cores when there exists a clear difference between some of them, but this doesn't mean directly that the performance is better as there are lots of factors interacting. So, the next chart shows a quick view across the number of cores for each supercomputer.

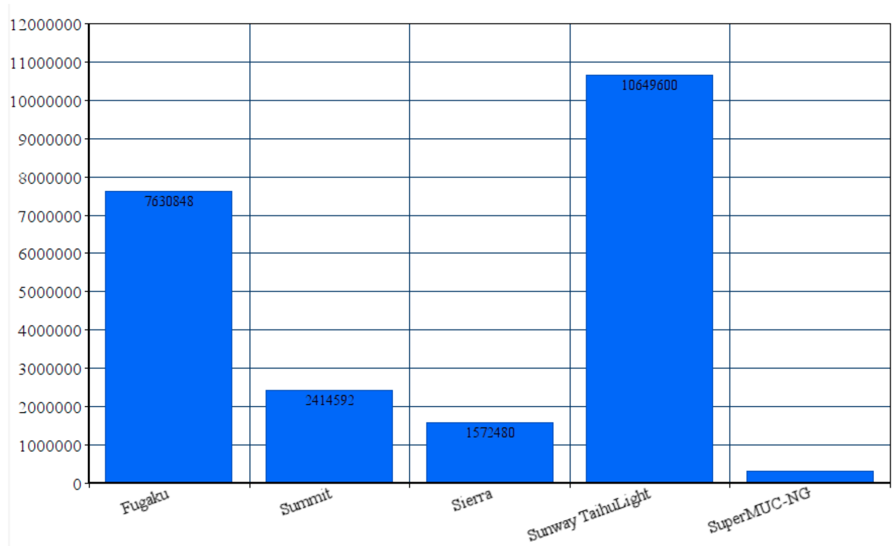

Figure 5: Cores per supercomputer

As said, there two clearly getting higher than others, and our *SuperMUC*is becoming small as years past. Even compared in November 2019, it has lower cores than others supercomputers regarding its level of power.

Later, some parameters are focused on the performance when executing the *LINPACK* benchmark. On one hand, there is the system's *Rmax* score describing its maximal achieved performance, and on the other, the *Rpeak* score which describes its theoretical peak performance. Values for both are usually presented in teraFLOPS or petaFLOPS.

Also, while it has 3.1Ghz per core, the other supercomputers doesn't exceed this by far, just like the top1 which is based on 2.2GHz per core. But obviously, the amount of them and being well parallel combined results in the major performance seen i the following charts.

In *the TOP500 List* table, the computers are ordered first by their *Rmax* value. In the case of equal performances (Rmax value) for different computers, we have chosen to order by *Rpeak*. So, what really counts is the *Rmax* which is the real performance, and also, the *Nmax* set as the problem size for achieving the *Rmax*. In this manner, the next charts show the differences in performance for each of the supercomputers.

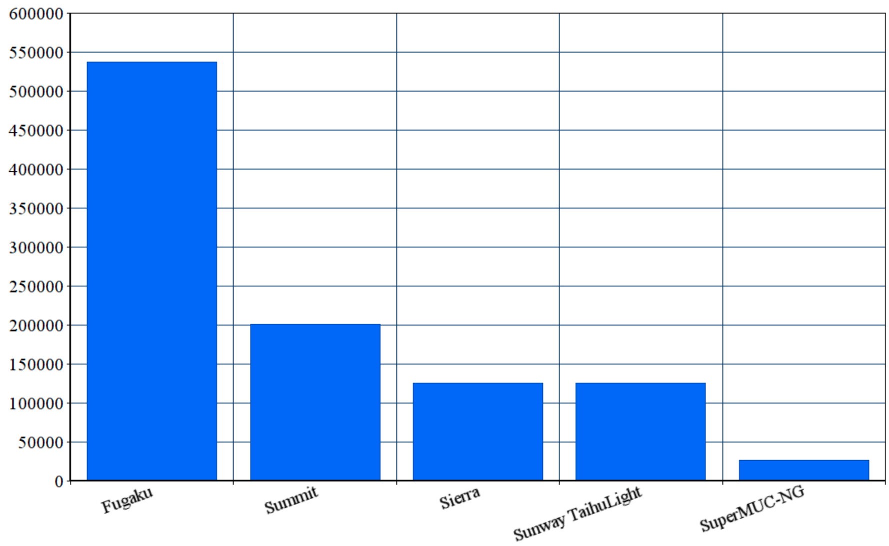

Figure 6: Rpeak (TFlop/s) performance

In this chart you may see how the theorical performance for each of the supercomputers, and there is a clear difference among them, but even our supercomputer has lower cores by far its performance is quite good compared to the others, maybe for its architecture or the highest clock speeds per core with so good efficiency.

But regarding the memory RAM this is similar and the interconnection link also with bandwidths up to 100Gbit/s in the network. Even though, other deterministic point could be the operating system or the middlewares running in each, because doesn't matter have so many cores if they are not well-optimized.

A more realistic measure, comes with the next chart which this one shows exactly the performance calculated over the *LINPACK* benchmark, seeing more or less the same results but more precisely. And in addition, we included a chart in the figure 8 showing the *Nmax* problem size for each of the supercomputers to get a better view of the complexity.

Even in this one, we can take into account the cooling systems and how well they apply into the supercomputer's architectures. The supercomputers can reach extreme speeds, but with that speeds comes extreme heat on the nodes, that is why the importance to cool down the system. Basically they can consume as much power as a small city (up to dozens of MegaWatts), which this really affects the overall performance.

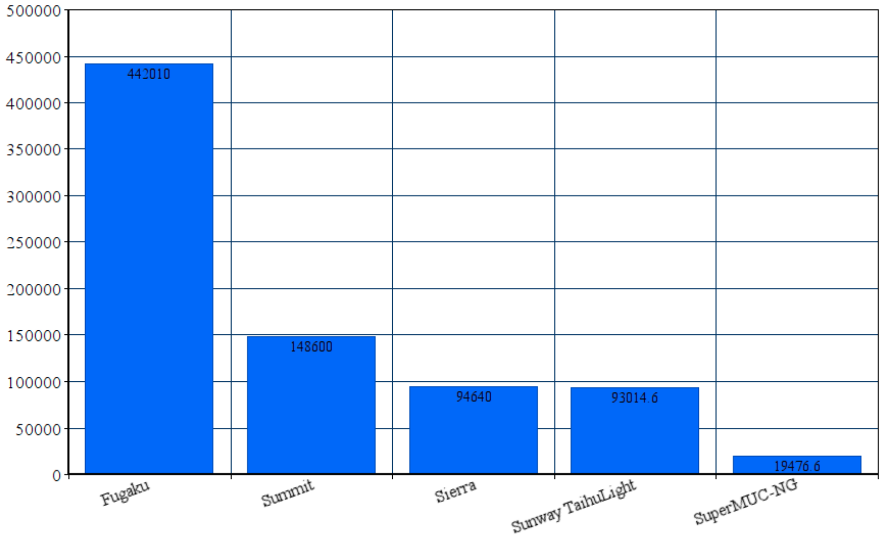

Figure 7: Rmax (TFlop/s) performance

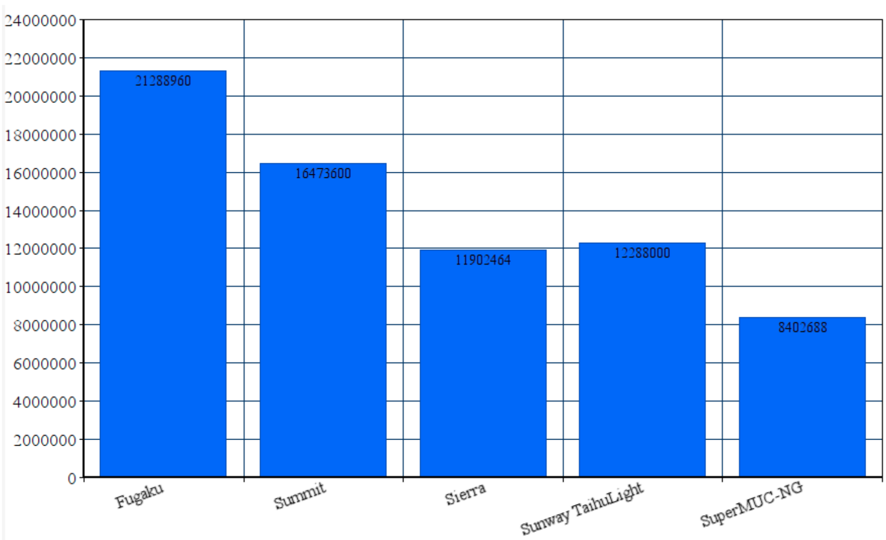

Figure 8: Nmax problem size to Rmax

With that in mind, we want to highlight that the *SuperMUC-NG*, just like most of the other Top 10 supercomputers in the world, makes use of liquid cooling to avoid the system's overheating - in this case, warm water. However unlike all of the others, the waste heat produced by the it is reused in many ways, like heating local pools and market gardens, heating asparagus crops, and driving Stirling motors and absorption chillers. And most importantly the *SuperMUC-NG* runs entirely on renewable energy sources.

9 Conclusions

The key was not to examine the *SuperMUC-NG* but to finally know how to analyze a supercomputer and also to compare it.

This work was enriching from both, we got centered not only on knowing more about the *SuperMUC-NG* but also to know better the measures used to test the performance just like the *Rmax* or *Rpeak*.

Plus, the supercomputer's history is so exciting. Now, we are accommodated to see all these kinds of machines but not only talking about supercomputers but also mobile or any kind of technology. What we are trying to state, is that sometimes is really great to know the origins and the evolution. All the steps taken for our ancestors, all the fabulous successes to finally get to where we are.

Additionally, it is surprising to see the performance compared to a home computer, and also all of the infrastructure and hardware present in this. It is also very interesting to know how much effort was put into making it energy-efficient via hardware architecture or cooling ways and that it is available to be used by researchers across Europe, making us wonder what intriguing research it might be executing right now.

To conclude, we were very pleased to be able to put in practice our knowledge acquired by doing the comparison and studying these giants, as learning more about this fascinating world of high-performance which is our near future.

References

[1] TOP 500 SuperComputers List - November 2020

[2] Meta-Heuristics for Scheduling in Cluster Federated Environmentsddd

[3] Supercomputers: The Amazing Race

[4] SUPERCOMPUTERCAPABILITIES: INTERPRETINGITS ROLE IN DEFENCE

[5] Exascale computing

[6] The 5 fastest supercomputers in the world

[7] The race to exascale: A story of superpowers and supercomputers

[8] SuperMUC-NG

[9] Supercomputer article

[10] Supercomputer article - Wikipedia

[11] Supercomputador article - Viquipèdia

[12] Features of supercomputer

[13] Top500 Description