**Name:** Aditya Pandey

**UTA ID:** 1001405034

**Course Number:** CSE 5351

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**Professor:** Ishfaq Ahmad

**Report Subject: Supercomputer- Mira, Blue Gene/Q by IBM**

**Abstract:**

Mira is an IBM Blue Gene/Q supercomputer which was developed so that it could be used at Argonne Leadership Computing Facility. After its release in 2012, Mira became one of the fastest supercomputers around that time. In June 2013, it was named as the world’s 5th fastest supercomputer as of then. On June 2017, it is still there as number 9th in the top supercomputers list. Some of its ridiculously superb specifications includes, 10-petaflops, which in fact is capable of 10 quadrillion calculations per second. With this computing power, Mira can do in one day what it would take an average personal computer 20 year to achieve. It consists of 48 racks 786,432 processors, and 768 terabytes of memory, Mira is 20 times faster than Intrepid, its IBM Blue Gene/P predecessor at the ALCF.

In addition to being one of the fastest computers in the world, Mira is also among the most energy efficient. By fitting more cores onto a single chip, Mira speeds the communication between cores and saves the energy lost when transporting data across long distances. Mira’s water-cooling system uses copper tubes to pipe cold water directly alongside the chips, saving power by eliminating an extra cooling step. Overall, the new system operates five times more efficiently than Intrepid, and roughly within the same footprint.

The Blue Gene/Q system also features a quad floating-point unit (FPU) that can be used to execute scalar floating-point instructions, four-wide SIMD instructions, or two-wide complex arithmetic SIMD instructions. This quad FPU provides higher single thread performance for some applications.

**Applications and Experimental Origins:**

**Application 1: Discovery of a new material and concept, super-lubricity (eliminating friction).**

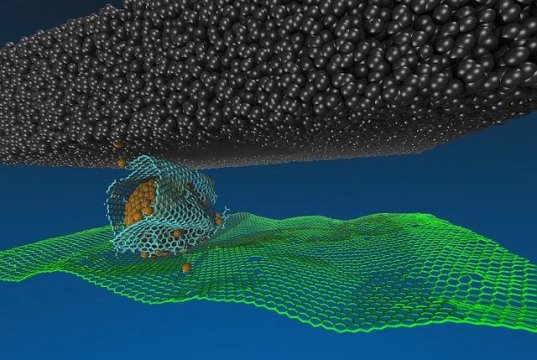
Argonne scientists used Mira to identify and improve a new mechanism for eliminating friction, which fed into the development of a hybrid material that exhibited superlubricity at the macroscale for the first time. Argonne Leadership Computing Facility (ALCF) researchers helped enable the groundbreaking simulations by overcoming a performance bottleneck that doubled the speed of the team's code.

While reviewing the simulation results of a promising new lubricant material, Argonne researcher Sanket Deshmukh stumbled upon a phenomenon that had never been observed before. Subramanian Sankaranarayanan, Argonne computational nanoscientist, who led the simulation work at the Argonne Leadership Computing Facility (ALCF), a DOE Office of Science User Facility was baffled by this new lubricant material.

What the computer simulations revealed was when the lubricant materials--graphene and diamond-like carbon (DLC)--slid against each other, the graphene began rolling up to form hollow cylindrical "scrolls" that helped to practically eliminate friction. These so-called nanoscrolls represented a completely new mechanism for superlubricity, a state in which friction essentially disappears. These nanoscrolls combat friction in very much the same way that ball bearings do by creating separation between surfaces.

Superlubricity is a highly desirable property. Considering that nearly one-third of every fuel tank is spent overcoming friction in automobiles, a material that can achieve superlubricity would greatly benefit industry and consumers alike. Such materials could also help increase the lifetime of countless mechanical components that wear down due to incessant friction.

All these was inspired form a certain serendipity, before the Mira simulations were done, , Argonne scientists were studying the hybrid material in laboratory experiments at Argonne's Tribology Laboratory and the Center for Nanoscale Materials, a DOE Office of Science User Facility. The experimental setup consisted of small patches of graphene (a two-dimensional single-sheet form of pure carbon) sliding against a DLC-coated steel ball. This combination was registering a very low friction coefficient, but the friction levels were fluctuating up and down for no apparent reason. The experimentalists were also puzzled to find that humid environments were causing the friction coefficient to shoot up to levels that were nearly 100 times greater than measured in dry environments.



Above figure: In this schematic of the superlubricity system, the gold represents nanodiamond particles; the blue is a graphene nanoscroll; green shows underlying graphene on silicon dioxide; and the black structures are the diamond-like carbon interface. *Credit: Sanket Deshmukh, Joseph Insley, and Subramanian Sankaranarayanan, Argonne National Laboratory*

To shed light on these mysterious behaviors, they turned to Sankaranarayanan and Deshmukh for computational help. Using Mira, the ALCF's 10-petaflops IBM Blue Gene/Q supercomputer, the researchers replicated the experimental conditions with large-scale molecular dynamics simulations aimed at understanding the underlying mechanisms of superlubricity at an atomistic level.

This led to their discovery of the graphene nanoscrolls, which helped to fill in the blanks. The material's fluctuating friction levels were explained by the fact that the nanoscrolls themselves were not stable. The researchers observed a repeating pattern in which the hollow nanoscrolls would form, and then cave in and collapse under the pressure of the load.

It was said that the friction was dipping to very low values now the scroll formation took place and then it would jump back up to higher values when the graphene patches were in an unscrolled state.

The computational scientists had an idea to overcome this issue. They tried incorporating nanodiamond particles into their simulations to see if the hard material could help stabilize the nanoscrolls and make them more permanent.

Sure enough, the simulations proved successful. The graphene patches spontaneously rolled around the nanodiamonds, which held the scrolls in place and resulted in sustained superlubricity. The simulation results fed into a new set of experiments with nanodiamonds that confirmed the same.

Because of this discovery is that we could see sustained superlubricity at the macroscale for the first time, proving this mechanism can be used at engineering scales for real-world applications. This collaborative effort is a perfect example of how computation can help in the design and discovery of new materials.

Drawbacks of this hybrid material: Not slippery when wet

The addition of nanodiamonds did not address the material's aversion to water. The simulations showed that water suppresses the formation of scrolls by increasing the adhesion of graphene to the surface. While this greatly limits the hybrid material's potential applications, its ability to maintain superlubricity in dry environments is a significant breakthrough in itself.

The research team is in the process of seeking a patent for the hybrid material, which could potentially be used for applications in dry environments, such as computer hard drives, wind turbine gears, and mechanical rotating seals for microelectromechanical and nanoelectromechanical systems.

Taking this disadvantage to our advantage using drop casting, which involves spraying solutions of the materials on moving mechanical parts. When the solutions evaporate, it would leave the graphene and nanodiamonds on one side of a moving part, and diamond-like carbon on the other side. If we can repel water, the graphene nanoscrolls could potentially work in humid environments as well.

The team's groundbreaking nanoscroll discovery would not have been possible without a supercomputer like Mira. Replicating the experimental setup required simulating up to 1.2 million atoms for dry environments and up to 10 million atoms for humid environments.

**Application 2: Simulating the entire Universe**

Mira used to be the third fastest computer in the world in 2012. This was the reason Mira could handle quadrillions of computations per second to accomplish some of the most difficult and complex tasks. One of the biggest problem for the physicist and cosmologist was how our universe evolved after the big bang. Hence, they took Mira to the test.

The main question was if Mira could perform such a feat and how much time it will take to perform such task, simulating our 13 billion years of universe history after the famous big bang.

Such a task would simply be impossible for conventional computers, given the sheer number of computations that are required to be done. Mira can do so only because it is juiced up with 768,000 cores which furnish 10 petaflops of processing power for this monstrous computer!

Until now, creating a simulation of a process as complex as the creation of universe itself had been impossible due to computing restraints. But with the processing power Mira commands, cosmologists are finally optimistic that such a feat can be accomplished.

Their aim is to discern the movements of trillions of particles through the universe, their collisions with each other and the consequent creation or disruption of structures. The simulation lasted for a fortnight and was studied to gauge the veracity of the prevalent theories of astrophysics.

The whole project was being hosted at Argonne National Laboratory and everything went well, the researchers were finally able to validate, or debunk, our current understanding of the universe’s development.

With the help of the code optimizations in place, they could model the phenomena in real experimental systems more accurately. The famous scientist Deshmukh said, "The simulations on Mira showed us some amazing things that could not be seen in laboratory tests."

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