How did the world's most powerful supercomputer help science fight the Covid-19 epidemic?

Thanks to breakthroughs in computer technology in recent years, it is easy for us to breathe a little during the Covid-19 pandemic.

Even in the first months of 2020, scientists faced a rare challenge: to speed up the study of SARS-CoV-2 virus to keep pace with its spread. Fortunately, supporting scientists is supercomputer technology has achieved many remarkable milestones in recent years.

Summit, the world's most powerful supercomputer, can perform 200 million billion, or 200,000,000,000,000,000 calculations / second. With a brain that can think like lightning, Summit runs thousands of simulations at once to analyze the effective anti-Covid-19 drug.

By the time this article was published, Summit had identified 77 such drugs out of a total of 8,000 types of drugs being reviewed. This is a big step in the race to find a vaccine for Covid-19.

Researchers at Oak Ridge National Laboratory published what Summit found in the chemistry journal ChemRxiv.

This is the original purpose when people created Summit, is to solve the problems that the community encounters. In the past, Summit has helped us identify the cell structure that appeared before Alzheimer's disease was formed, analyzed the genes causing opioid analgesics, and predicted extreme weather events based on available information. have about climate.

This is how Summit fights SARS-CoV-2 virus

Viruses cause disease in cells through spikes containing genetic material. Summit's job is to find a combination of drugs that can attach to those spikes, preventing the virus from spreading. Researcher Micholas Smith created a model of corona virus spines, based on how atoms and particles in the viral protein interact with drug combinations.

The supercomputer runs an emulation program of 8,000 drugs that can attach to protein spikes. And after hours of analysis, Summit discovered 77 drugs that have the potential to contain the Covid-19 pandemic.

After getting the results, the team will run the Summit supercomputer again, with more accurate protein spikes. They also published their findings in Science.

But the strength of the Summit is limited, and research is currently limited. However, it still provides a stepping stone for further analysis, finding effective doses. Further studies are needed to confirm the ability of 77 drugs to prevent SARS-CoV-2 virus.

' *This does not mean we have found a cure* ,' says Jeremy Smith, director of the Molecular Physiology division at Oak Ridge National Laboratory. But this will be the basis for creating the most effective vaccine against Covid-19.