Will Your Next Shampoo Be Developed on GPUs?

Temple University Researchers Help Procter & Gamble Design Better Models for Cleaning Products; Two NVIDIA Tesla GPUs Beat 1024 CPU BlueGene/L Cluster

SANTA CLARA, CA -- Improving the cleaning power of shampoos and liquid detergents and making them more environmentally friendly is as much a computer problem as it is a balance of chemicals. By harnessing the parallel processing power of NVIDIA(R) Tesla(TM) GPUs, researchers at Temple University are developing a computer simulation model which provides companies like Procter and Gamble with a fast, cost effective and accurate tool for research and development of surfactant molecules.

Surfactants have many uses; for example they provide the cleaning capacity and texture of shampoos, laundry detergents, and many other cleaning products. Their job is to attach themselves to dirt and make it mix with water, and their effectiveness in this process determines their ability to clean. The process of finding new, better surfactants and testing their effectiveness in laboratories is time consuming and costly.

"The computer models needed to accurately simulate surfactant properties are extremely demanding in terms of computational power," said Axel Kohlmeyer of the Institute for Computational Molecular Science at Temple University. "We discovered that by adding just two NVIDIA Tesla C1060 GPUs, each node in our newest cluster can do 16 times more work, and thus multiplies our local compute capacity far beyond what we could previously get through the national supercomputing centers."

"To put this into context, we can run a single GPU-optimized molecular dynamics simulation on two Tesla GPUs as fast as we can on 128 CPU cores of a Cray XT3 supercomputer or on 1024 CPUs of an IBM BlueGene/L machine with conventional software," continues Dr. Kohlmeyer. "With the NVIDIA Tesla GPU-based solution, we now have a more powerful, cost-effective solution that will enable us to advance critical research at a much faster pace. We're moving rapidly ahead to deploy a larger Tesla GPU cluster at Temple, which will give another huge boost to our work."

The Temple researchers are using GPU-accelerated HOOMD (Highly Optimized Object Oriented Molecular Dynamics) simulation software, written by researchers at the Department of Energy's Ames Laboratory to leverage the NVIDIA GPUs.

In addition to deploying a small local GPU cluster, the university team will also look to scale its work using the NCSA Lincoln cluster, where the computational output has been boosted to 47 TeraFLOPS through the addition of Tesla S1070 1U GPU systems.

For more information:

Video of the Temple University team discussing their work in surfactant research Molecular dynamics using GPUs Institute for Computational Molecular Science at Temple University The HOOMD application from Ames Lab

NCSA Supercomputer

About NVIDIA

NVIDIA (NASDAQ: NVDA) awakened the world to the power of computer graphics when it invented the graphics processing unit (GPU) in 1999. Since then, it has consistently set new standards in visual computing with breathtaking, interactive graphics. Expertise in programmable GPUs has led to breakthroughs in parallel processing which make supercomputing inexpensive and widely accessible. Fortune magazine has ranked NVIDIA #1 in innovation in the semiconductor industry for two years in a row. For more information, see www.nvidia.com

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About NVIDIA

Since 1993, NVIDIA (NASDAQ : NVDA) has pioneered the art and science of visual computing. The company's technologies are transforming a world of displays into a world of interactive discovery — for everyone from gamers to scientists, and consumers to enterprise customers. More information

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