Nvidia GPUs boost molecular biology research

Dr. Klaus Schulten of the University of Illinois is tapping GPU-powered computing to increase the speed and accuracy of microscopy-based simulations.

"We've benefitted a lot from GPUs. It's definitely led to several scientific discoveries and advances," Schulten said during a second day keynote speech at Nvidia's Technology Conference.

"For example, GPUs reduced the time required to compute radial distribution functions - which are measurements of atomic density - from 15 hours to 10 minutes."

Schulten also noted that his team had harnessed the power of Nvidia's GPUs to learn how viruses attach themselves to cells and respond to the effects of atomic microscopy.

In addition, GPU computing helped researchers capture high-res snapshots of ribosomes in action and the subsequent synthesis of proteins.

"Previously, we were only able to take low-resolution static images using CPU-configurations," he noted.

Finally, Schulten explained that GPUs had allowed scientists to render electron clouds in real time, thereby accelerating the computing of molecular dynamics by up to 400x.

"In comparison, CPUs require an entire working day to get a single snapshot of an electron cloud.

"[Yes], this [type of research] turns out to be heaven for GPUs. Scientists and GPUs, well, they truly go hand-in-hand."