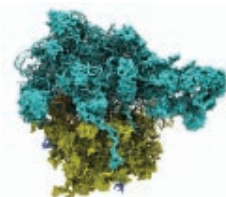# GPU Computing
UIUC | Molecular Dynamics

May 24, 2007

CHALLENGE

The University of Illinois at Urbana-Champaign's (UIUC) Nanoscale Molecular Dynamics (NAMD) and Visual Molecular Dynamics (VMD) are powerful and widely used tools for simulating and visualizing biomolecular processes. Simulating complex molecular systems is time consuming and requires large, sophisticated clusters of computers.

SOLUTION

To boost performance, the UIUC researchers ported the "cionize" ion placement tool to an NVIDIA GPU computing solution. The goal was to accelerate the computationally intensive kernels for calculating the interaction of biological molecules and ions. In doing so, UIUC researchers achieved speedups on ion simulations over 100 times that of an 18-CPU cluster (based on total CPU time vs total GPU time).

With a three-GPU workstation, a similar calculation for time-averaged electrostatics in the VMD tool reaches 705 gigaflops of realized performance. This remarkable performance allows any bioscience researcher to have the equivalent of a computing cluster on their workstation.
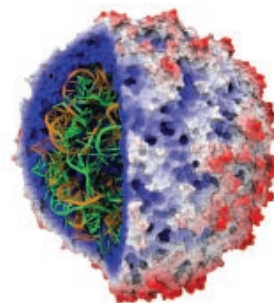
IMPACT
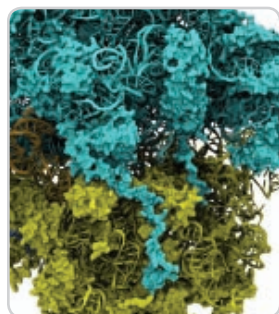
With GPU computing, these molecular simulations are no longer restricted to clusters in server rooms. By running the simulations on workstations in individual labs and desktops, projects are no longer competing with one another for scarce computing resources and the researchers are getting the results when they need them, as opposed to when they can be scheduled.

Furthermore, with GPUs in large-scale server clusters, new classes of problems can be addressed for which the necessary computing power was only a dream a year ago.

The combination of NAMD and NVIDIA computing solutions is a marriage of cutting-edge research and software development, aimed at harnessing the nation's fastest supercomputers to decipher the tiniest components of living cells. These new computing tools are quickening the pace of drug discovery and other vital research in unraveling biological processes.

For more information, visit: http://www.ks.uiuc.edu/
For more information about NVIDIA GPU computing solutions, visit www.nvidia.com/tesla