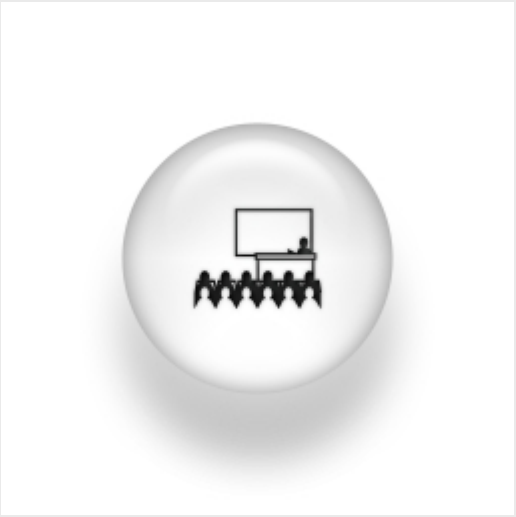
Molecular simulations in the Era of GPUs

Friday, 31 October 2008, 12:00-13.00



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The recent introduction of cost-effective accelerator processors (APs), such as the IBM Cell processor and Nvidia's graphics processing units (GPUs) represents an important technological innovation for computational science. Present accelerator processors can deliver over an order of magnitude more floating-point operations per second (flops) than standard processors, broadly equivalent to a decade of Moore's law growth. In conjunction with distributed and grid computing solutions these devices can be deployed to become a new form of supercomputing as in PS3GRID.net and GPUGRID.net, where accelerated molecular simulations are used to simulate hundreds of protein-ligand complexes with full molecular specificity, a crucial requirement of in silico drug discovery workflows.