GPU Technology Conference 2010 Sessions on Quantum Chemistry (subject to change)

IMPORTANT: Visit www.nvidia.com/gtc for the most up-to-date schedule and to enroll into sessions to ensure your spot in the most popular courses.

2128 - Hybrid Quantum Mechanics/Electrodynamics (QM/ED) Modeling of Solar Cells on a CUDA Cluster

One of the greatest challenges of the twenty-first century is the utilization of renewable energy. In providing a theoretical explanation and guidelines for computer-aided design of dye-sensitized solar cell (DSSC), we recently developed a hybrid multi-scale quantum mechanics/classical electrodynamics (QM/ED) methodology.

Our numerical simulations were tested on a CUDA enabled Linux cluster using CP2K. We extended its CUDA implementation to MPI parallel environment. Our preliminary results demonstrated a superior performance advantage of hybrid MPI/GPGPU programming that could potentially shorten the total simulation wall time by an order of magnitude.

Speaker: Hanning Chen, Northwestern University

Topics: Quantum Chemistry, Energy Exploration, Molecular Dynamics, Physics Simulation

Time: Wednesday, September, 22nd, 17:00 - 17:50