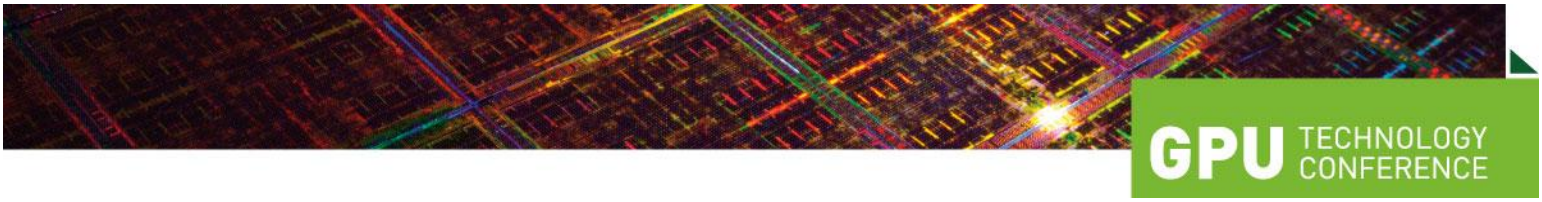

GPU Technology Conference, May 14-17, 2012
McEnery Convention Center, San Jose, California
www.gputechconf.com

Sessions on Quantum Chemistry (subject to change)

IMPORTANT: Visit http://www.gputechconf.com/page/sessions.html for the most up-to-date schedule.

S0343 - A Quantum Chemistry Domain-Specific Language for Heterogeneous Clusters
Antonino Tumeo (Pacific Northwest National Laboratory), Oreste Villa (Pacific Northwest National Laboratory)
Day: Tuesday, 05/15 | **Time:** 10:00 am - 10:25 am
Topic Areas: Quantum Chemistry; Supercomputing
Session Level: Intermediate

This talk discuss the development of a Domain-Specific Language (DSL), the tools and the related runtime for efficiently generating Tensor Contractions (generalized matrix multiplications), an important part of many quantum chemistry methods (e.g. Coupled Cluster Theory). Starting from a high level description of the computation, the tool analyses it and generates optimized C, OpenCL or CUDA implementations. The runtime, supporting a task based computation model, is then able to execute the generated code on GPU-accelerated heterogeneous large scale clusters, maximizing the utilization of the processing elements and minimizing communication costs.

S0378 - VASP Accelerated with GPUs
Maxwell Hutchinson (University of Chicago)
Day: Thursday, 05/17 | **Time:** 2:00 pm - 2:50 pm
Topic Areas: Quantum Chemistry; Application Design & Porting Techniques; Computational Physics
Session Level: Intermediate

This session will detail the performance and capabilities of GPU-accelerated VASP, explain design decisions made in porting VASP to CUDA, and present a roadmap for GPU accelerated VASP development. We've achieved performance improvements up to around 20x on systems of around 100 ions and have implemented exact-exchange. We are working on ports of more conventional functionality.

S0429 - Quantum Chemistry: Automated Code Generation and Optimization for GPU Kernels
Alexey Titov (Stanford), Ivan Ufimtsev (Stanford)
Day: Thursday, 05/17 | **Time:** 3:00 pm - 3:25 pm
Topic Areas: Quantum Chemistry
Session Level: Advanced

In this session we discuss the challenges encountered in development of quantum chemistry software for GPUs from scratch and optimization of the kernels for the best performance. We attempt to create a unified framework for automatic generation of efficient quantum chemistry codes tailored individually for various GPU (NVidia, ATI) and CPU architectures and programming (CUDA, OpenCL, C/C++) languages using a meta-programming approach based on a computer algebra system. We demonstrate its utility by generating highly optimized GPU and CPU kernels dealing with various integrals over Gaussian basis functions implemented in the TeraChem quantum chemistry package.

S0392 - Large-Scale First Principle Pseudopotential DFT Calculations on GPU Clusters
WeiLe Jia (Supercomputing Center of CNIC, Chinese Academy of Sciences), Long Wang (Supercomputing Center of CNIC, Chinese Academy of Sciences)
Day: Thursday, 05/17 | **Time:** 3:30 pm - 4:20 pm
Topic Areas: Quantum Chemistry; General Interest
Session Level: Advanced

In this session, we will present a series of work on density functional theory (DFT) plane wave pseudopotential (PWP) calculations on GPU clusters. The GPU version is developed based on a CPU DFT-PWP code: PEtot, which can calculate ~1000 atoms on thousands of processors. Our test indicates that the GPU version can have a ~20 times speedup over CPU code. A detail analysis of the speed-up and the scaling on the number of CPU/GPU (up to 256) will be presented. As far as we know, this is the first GPU DFT-PWP code scalable to large number of CPU/GPU.

S0220 - Enabling Faster Material Science Modeling Using the Accelerated Quantum ESPRESSO
Filippo Spiga (Irish Centre for High-End Computing)
Day: Thursday, 05/17 | **Time:** 4:30 pm - 5:20 pm
Topic Areas: Quantum Chemistry; Supercomputing; Application Design & Porting Techniques
Session Level: Intermediate

The goal of this session is to present the advantages of mixing CUDA libraries and CUDA kernels to deliver a robust community package for material science modeling that fully exploits multi-core systems equipped with GPUs. The Plane-Wave Self-Consistent Field (PWscf) code of the Quantum ESPRESSO suite is the focus of this work. During the session the main computation-dependent components, that also represent fundamental building blocks for many other quantum chemistry codes, will be discussed and analyzed. Subsequently an in-depth performance assessment of several realistic scientific cases will be presented, starting from single workstations to large clusters equipped with hundreds of GPUs.