danceroom Spectroscopy: Interactive quantum molecular dynamics accelerated on GPU architectures using OpenCL

David R. Glowacki,[1,2]* Philip Tew,[2] Thomas Mitchell,[3] James Price,[4] and Simon McIntosh-Smith[4]

[1]School of Chemistry, University of Bristol, Bristol, BS2 9LG, UK; [2]Pervasive Media Studio, Watershed, 1 Canons Rd, Bristol BS1 5TX, UK; [3]Computer Science and Creative Technologies, University of the West of England, Bristol BS16 1QY, [4]Department of Computer Science, University of Bristol, BS2 9LG, UK

*drglowacki@gmail.com

danceroom Spectroscopy (dS) is an interactive audiovisual installation and performance tool built from algorithms commonly used to simulate and analyze quantum molecular dynamics. Using an array of up to seven simultaneous depth sensors, dS literally interprets and renders humans as "energy landscapes". The result is an interactive system where movement is interpreted as perturbations in a virtual energy field. This interpretative leap (i.e., imagining humans as "energy fields") allows users to perceive the emergent physics arising from their movement within a real-time simulation of an atomic ensemble. Graphically, users perceive this interaction via projections of their energy field embedded in a simulation of thousands of interactive particles that fluidly react to the real-time motion of their fields. In addition, we have developed a flexible suite of algorithms for analyzing the particle dynamics to detect transient structures amidst the chaos. The data are packaged into appropriate structures, and sent to an electronica musician for sonification, allowing users to hear the sonic effect of their field perturbations within the atomic nano-physics.

dS has appeared at the London 2012 Cultural Olympiad and London's Barbican Arts Centre. The interactivity that we have so far achieved with dS relies on a high-performance custom-built workstation. Our code utilizes OpenCL C# wrappers run on a heterogeneous platform that includes an Intel i7 hexacore hyper-threaded CPU and two NVIDIA GTX 590 GPUs. One of the GPUs is reserved exclusively for DirectX 11 graphics, and the other for real-time physics computations and mathematical analysis. Using profiling tools, we ported a number of our most intense computations to the physics GPU, including calculation of the external and internal forces acting on the atoms, propagation of atomic positions and velocities, collision detection, and construction/updating of an ensemble-averaged velocity autocorrelation function. We left on the CPU less computationally intensive tasks that benefitted from fast access to global atomic ensemble data (e.g., several of the sonification algorithms). Our GPU accelerated code allowed us to substantially increase the performance of the system and reliably simulate up to 10,000 interactive quantum particles, compared to fewer than 300 with CPU-only physics computations. In this presentation, we will demonstrate the dS system, and discuss the parallel design driving those portions of the code that led to maximum performance enhancements when porting to the GPUs.