Chemical Computation on Future Computers

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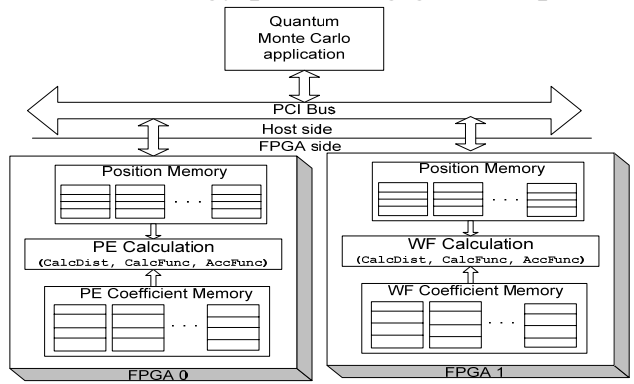
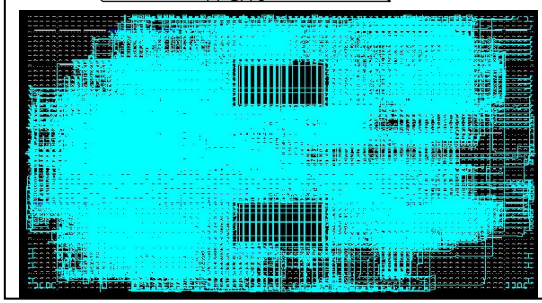
Computer technology is a major enabling factor in scientific simulation, and the beginning of the 21st century marked the end of sequential computing. No longer will ever faster processors accelerate our simulations. In the future, most performance improvement will come from increased parallelism and use of specialized accelerators that promise huge speedups over commodity processors. Our multi-university collaboration of chemists, computer scientists, and electrical engineers aims to resolve the theoretical, algorithmic and technical problems resulting from these new technologies.

A suite kernels from chemistry algorithms, including quantum Monte Carlo, Gaussian and plane-wave density functional theory, and two-electron integral evaluation, are being used to evaluate general purpose graphical processing units (GPGPU), field programmable gate arrays (FPGA) and multi-core chips. Ultimately, new algorithms will be deployed in widely used chemistry codes and the design of future systems made more relevant to chemistry.

UT and UIUC/NCSA are exploring the use of FPGAs in chemical computation. Combining some advantages of special purpose silicon and programmable processors FPGAs have accelerated some quantum Monte Carlo and other kernels by 2x to 30x with new technology promising greater speeds.





Left is the routing of the QMC kernel on a Xilinx FPGA. The two large ares in the center are PowerPC cores. The green lines are the circuit.

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