

Quantum Chemistry on GPUs

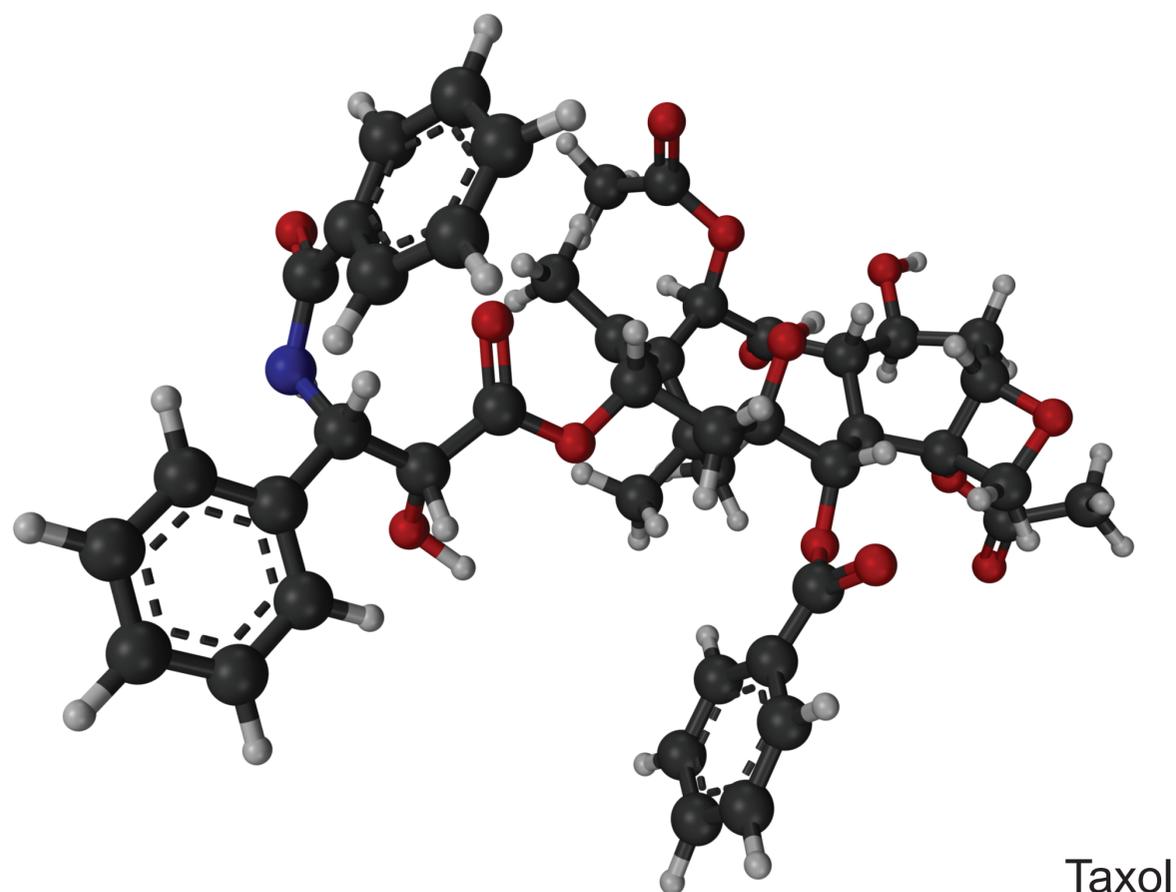
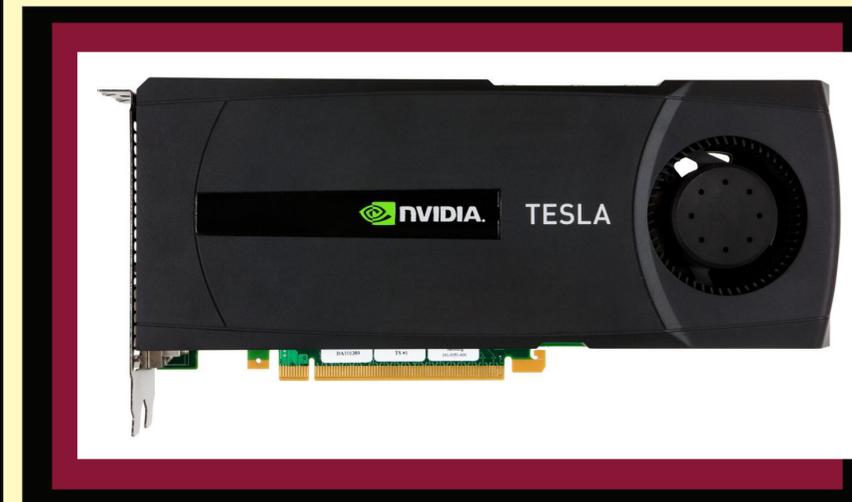
C++ Implementation

Rys quadrature two-electron integrals were implemented using C++ and automatically generated code to take advantage of modern CPU features such as SIMD. Hartree-Fock and MP2 energies were implemented to take advantage of multi-threading and to reduce memory consumption.

The GPU implementation was derived from CPU implementation reusing CPU code as much as possible.

GPU specific code amounts to approximately 1000 lines.

The amount of code is kept small by using C++ template meta-programming and BOOST libraries.



Taxol

GPU code status

Any integral with total quartet angular momentum of less than 10 can be computed.

Therefore majority of integrals, for example $\langle \text{spsp} | \text{spsp} \rangle$ or $\langle \text{dd} | \text{spf} \rangle$ can be computed.

Fock matrix is constructed directly on GPU avoiding memory transfer overhead.

Integrals which can not be computed on GPU, e.g. $\langle \text{ff} | \text{ff} \rangle$, are handled by CPU backlog queue.

Any number of CPU and GPU threads can run a single host. Hartree-Fock across multiple nodes is also possible piggy-backing on top of GAMESS.

Performance

Computations are done using double precision basically matching those of CPU code.

The Hartree-Fock energy single-iteration on Taxol using 6-311G(2df,2p) basis set takes around 10 minutes to run using 7 - 2.0 GHz cores and Fermi board.

By comparison, original GAMESS takes around 45 minutes using 8-cores.

You would need around 4 nodes running GAMESS to achieve timings of a single node with a Fermi board.

Future Work

Codes using for index transformation: CCSD(T)
Density Functional Theory implementation
Gradient implementation.