Use of Graphics Cards (GPU) to Simulate Atoms, Molecules and Nucleus.

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Monte Carlo Techniques

Quantum Monte Carlo (QMC) methods solve the Schrödinger Equation by casting it as an integral and evaluating it through stocastic sampling.

$$\hat{H}\psi = E\psi$$

Application of QMC

Description of the physical properties of the microscopic systems with a finite number of particles: nuclei, atoms and molecules, isolated or confined inside of molecular complexes.

Paralellism

Quantum Monte Carlo:

- Computationally expensive
- Well suited to paralellization (Higher sampling implies higher statistic)

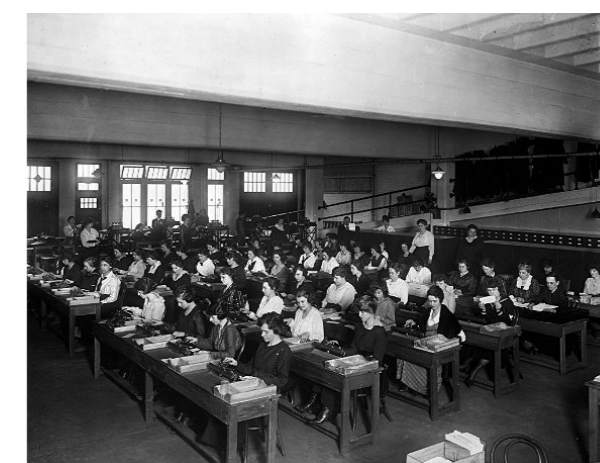Paralellization in CPU or in GPU ?

GPU vs CPU

·CPU:
- Up to 8 processors
- Optimized for sequential serial processing

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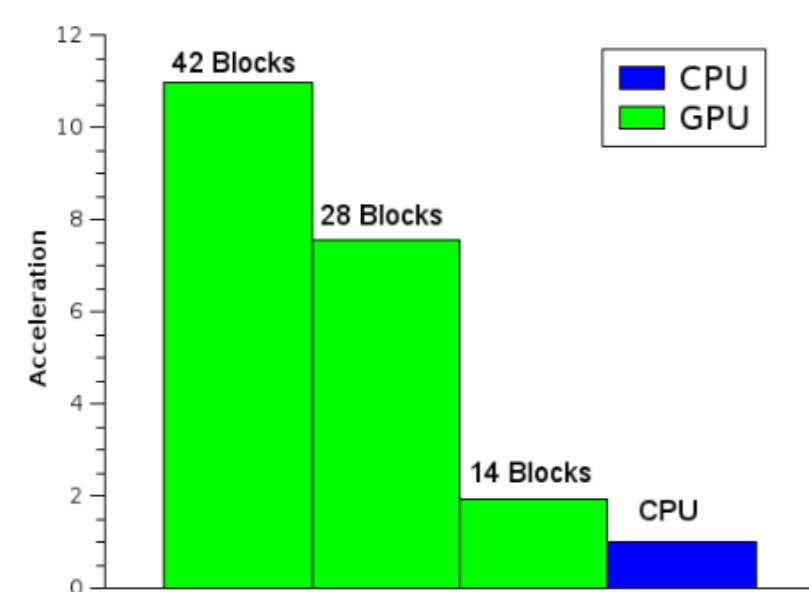
·GPU:
- Up to hundreds of light processors
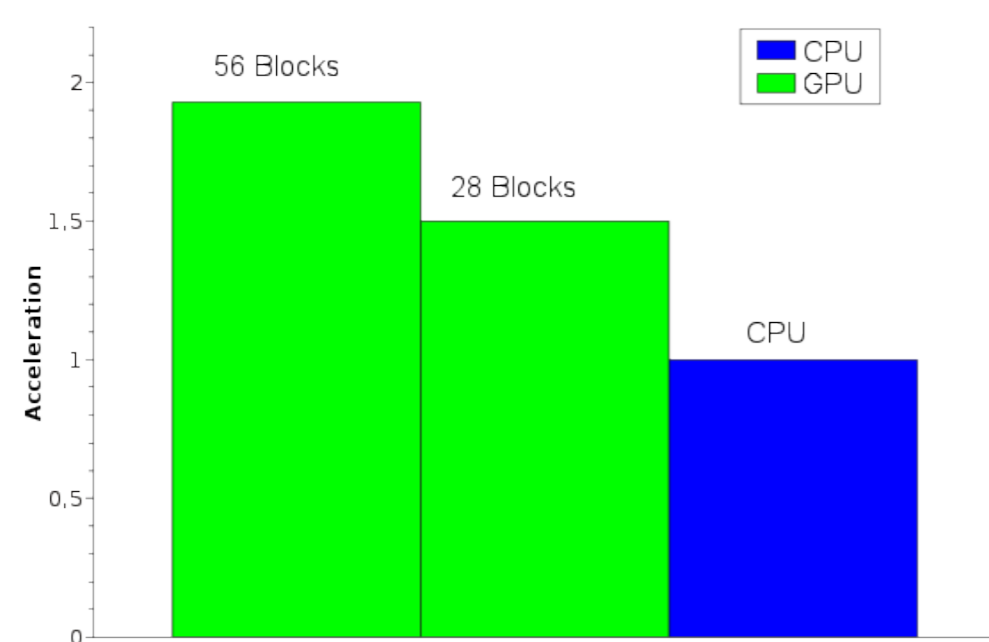- Specialized for highly parallel computation

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Some Examples

H atom Ground State Calculation with QMC Variational

Morse Potential Calculation with QMC Path Integral

GPU= Nvidia® GeForce GTX 470
CPU= Intel® Core™ i3-530

$$Acceleration = \frac{Exec.\,Time}{Exec.\,Time\,CPU}$$

Future Work:

- QMC Variational for Many electrons atoms
- Diffusion Monte Carlo (DMC) for fermionic systems

References
Quantum Confinement of the Covalent Bond beyond the Born−Oppenheimer Approximation.(2013) A. Sarsa. J. M. Alcaraz-Pelegrina, C. Le Sech,and S. A. Cruz.J. Phys. Chem. B, 117, 7270−7276
Fast quantum Monte Carlo on a GPU.(2015).Y. Lutsyshyn. Computer Physics Communications 187, 162−174