Ioannis Ypsilantis

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CS677

Project Proposal

Problem Description

For this project I want to simulate atoms by modelling both electrons and protons as elementary particles. A neutron is formed by the direct contact between an electron and a proton. By Grand unified theory, there are three forces that explain the motion of these particles: strong forces, weak forces, and electromagnetic forces. For the purposes of this project, I intend to model strong forces and electromagnetic forces. Weak forces are best explained using quarks and other sub particles, a level of precision outside of the scope presented. To have better control over the environment I wish to model both external gravity and electromagnetic waves.

Quantitatively, strong forces only exist within a very small distance (roughly 1-3 femtometers, 10^{-15} meters). At this range strong forces are roughly 100 times stronger than electromagnetic forces.

The electromagnetic forces between atoms can be solved using Coulomb's law:

$$|F| = k_e \frac{|q_1||q_2|}{r^2}$$

Where k_e is a constant, q_1 and q_2 are the charges of the particles and r is the distance between the particles. The Force of a particle within a magnetic field can be calculated using Lorentz force equation:

$$F = q(E + v \; x \; B)$$

Where q is the charge, E is the direction of the electric field, v is the velocity of the particle, and B is the Magnetic field. Gravitation force exists simply as a force in the desired direction. The force on any single particle is calculated by summing all forces because of all other particles and external forces in the system.

Suitability for GPU acceleration

This computation is inherently suitable for GPU acceleration. Each particle within the simulation can be solved in parallel. The only serial code in this application is the code spent sending information to/from the host. All particle calculations can be done in parallel.

The main data overhead for this project is sending the particle data to host for visualization. Initially, the host must send over the initial state data for all particle, this includes it location in 3D space, instantaneous velocity, intrinsics, etc. At every timestep in the simulation the host will need to receive only the location in 3D space of each particle to be sent for visualization.

Evaluation

This project deals with trying to simulate everyday atomic processes in the computer environment. Evaluation for success is dependent on successfully modelling reality. A few tests of interest:

- Form nuclei and have electrons “orbit” nuclei.
- Form molecules, i.e. two hydrogen atoms form a bond to create stable molecule.
- View the system in different phases of matter. I.e. water moves from solid to liquid to gas.
- Fission/Fusion. Create an extreme environment that allows for fission/fusion to occur. In the case of fusion this involves getting the materials into a plasma state.

Intellectual Challenges

This problem is interesting because it requires both understanding quantum mechanics as well as simulation coding. There are various complex interactions that occur in parallel. Optimizing the particle-to-particle interactions is the main area for speedup. Testing and experimentation are required to try different strategies such as the Barnes-Hut algorithm for simulation to find an option that works and provides the best speedup. A brute force strategy is guaranteed to work; however, optimizations may not succeed when compared with more conventional simulators. Ensuring that the optimizations are applicable is an important aspect of this project. Another consideration is the necessary precision for this simulation, what precision is suitable and how accurate functions must be when solving.