Dynamics of Bose-Einstein Condensates in Different Random Potentials

Khang Pham, Samuel Kellar, Ka Ming Tam, Juana Moreno
Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803

LA-SiGMA
Louisiana Alliance for Simulation-Guided Materials Applications

Introduction

In classical mechanics, one can illustrate the movement of one or more particles by using their position and velocity as functions of time and from there determine the location at any time. In quantum mechanics the wave function gives a probability of the particles' location in any given region in space at any given time. Currently, my wave function is derived from a Schrodinger equation with a simple harmonic potential. Since the equation is time-dependent and nonlinear, it is a nontrivial partial differential equation. Because the equation is nontrivial, it requires the use of numerical methods which need to be programmed.

Furthermore, HPX, a run time system for C++, is used to run the program more efficiently. HPX reduces the effects of SLOW (starvation, latencies, overheads, waiting) which are four main factors that slow down the systems while performing the parallel computation. Moreover, the code will be modified to simulate a Bose Einstein Condensate (BEC), which is describe by a Schrodinger equation that relates the time derivative of the wave function with the Hamiltonian operator, as well.

Background

Bosons are particles that do not obey the Pauli Exclusion Principle. Instead Bosons follow rules which assert that two indistinguishable Boson particles can occupy the same energy level. Einstein predicted that cooling a Bosonic system to a very low temperature would cause a large fraction of the particles in the system to converge (condense) into the ground state (lowest energy level). This phenomenon is now known as the Bose-Einstein condensation (BEC). At this state, all particles share the same phase and behave coherently.

On June 5, 1995, the first ever BEC was achieved by Eric Cornell and Carl Wieman at the JILA lab. Later, Wolfgang Ketterle, a researcher at MIT, studied and demonstrated the important properties of BEC. The work earned them the 2001 Nobel Prize in Physics. The graph below illustrates the BEC.

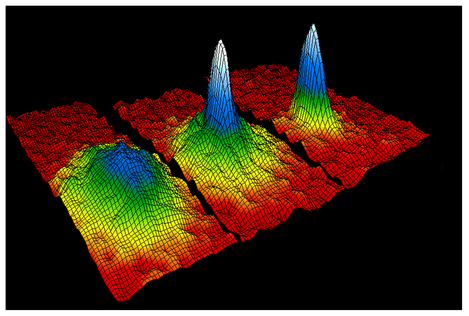


Image Credit: Quantum Physics; Bose Einstein condensate, National Institute of Standards and Technology, 95PHY001, 1995

- Velocity-distribution graph of rubidium gas with different temperatures in each frame
- The colors indicate the number of atoms at different velocities with red being the smallest and light blue being the largest.
- The velocity is lowest at the center of each frame.

High Performance ParalleX (HPX)

HPX is a runtime system implementation of the ParalleX execution model. This runtime system allows programmers to counter problems they face that slow down their parallel implementations. Four fundamental factors of those problems are SLOW: Starvation, Latencies, Overhead, and Waiting for Contention resolution. Starvation occurs when there is not enough computation for the program to maintain high performance and utilize all resources. Latencies cause stoppage in the code due to the waiting for information to be received. Overhead is the work required to manage parallel actions. Waiting for Contention resolution is the time delays for different parts of the program to get an overshared information. HPX mitigates SLOW by using tools such as future, dataflow, action. A future is a facility that carries the result of a computation. It acts as a representative for the result that is yet to be computed and suspends any threads that request the result until it becomes available. Dataflow is a local control object that is triggered when the values it depends on become available. One way to use dataflow is to use a future as its argument so that when the future's result becomes available, dataflow is triggered. An action is a function wrapper which will then allow HPX to send this packet to any node.

Method

The probability of finding a particle at any given point in time is given by the wave function, Ψ(x,t), whose result is found by solving the Schrodinger equation:

$$i\frac{\partial\Psi(x,t)}{\partial t} = -\frac{1}{2}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t)$$

V is the potential energy, which in this case is :

$$V(x)=1/2\ kx\uparrow 2$$

In order to solve this equation, I use the Crank-Nicolson numerical method since it is fairly stable and accurate.

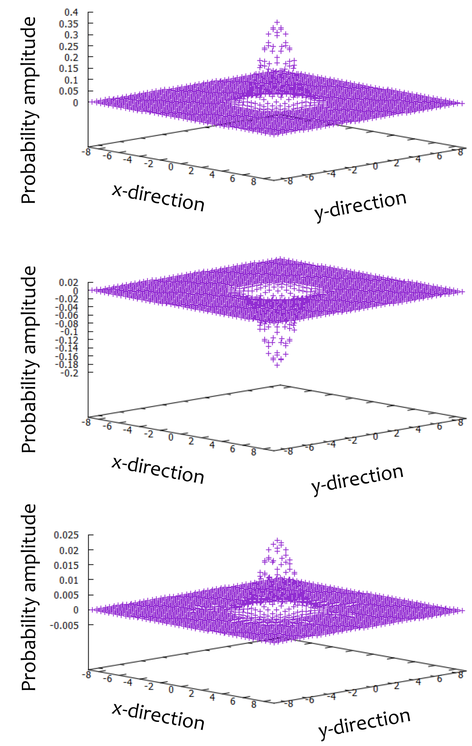
$$2\Psi\downarrow j\uparrow n+1 + iH\Delta t\Psi\downarrow j\uparrow n+1 = 2\Psi\downarrow j\uparrow n - iH\Delta t\Psi\downarrow j\uparrow n$$

This method is simply the average of the explicit and implicit Euler methods with n being the time coordinate, j being the spatial coordinate, and *H* being the Hamiltonian operator:

$$H=-1/2\ \partial\uparrow 2\ /\partial x\uparrow 2 + V(x)$$

This reduces to with a set of m equations with m unknowns.

Results



Above are the graphs at three different times with the uppermost being the earliest time and the bottom being the latest time. The graphs are showing data from the real part of the calculated wave function.

Conclusions

Through the data, we have shown that the code is fully functional and capable of simulating a system of particles within a harmonic potential. This is a step toward the goal of simulating BEC with different disorder random potentials. For future work, we are going to extend the code by adding in different random potentials.

LSU Center for Computation & Technology
Interdisciplinary | Innovative | Inventive

References and acknowledgements

Phys. Rev. Lett. 98, 210401 – Published 23 May 2007; Erratum Phys. Rev. Lett. 106, 149901 (2011)
This material is based upon work supported by the National Science Foundation under the NSF EPSCoR Cooperative Agreement No. EPS-1003897 with additional support from the Louisiana Board of Regents.