Simulating the Atomic World

by Madhurrya Talukdar - Tuesday, January 12, 2016

http://gonitsora.com/simulating-atomic-world/

Computer simulation, in the present day scientific scenario, has become one of the primary tools in both basic and applied sciences. With the escalating advancement of science in the last few decades experiments have become more complex with the use of sophisticated scientific instruments. And understanding such complex scientific phenomena in a realistic and lucid manner needs more than just pen and paper. Moreover co-relation of experiment with its proposed theory is another bigger task. And this is where simulation comes into existence. It acts as a bridge between mathematical theories and practical experiments. The world of scientific simulation is far too immense to sum up in an article. However a humble attempt has been made to give a glimpse of its usefulness in the physical science.

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Science in general and physics in particular has been trying to study the heart of matter, our magnificent universe, the complex interactions between atoms and sub atomic particles, how various physical systems behave etc. from centuries now. The great minds like Galileo and Newton, using only pure intuition and available math then, tried to explain our physical surroundings in the most justifiable manner. Then with the development of new and innovative mathematics, theories became more precise with approximations giving to nearly accurate results with experiments. It was with the advent of Quantum Mechanics in early 20^{th} century that physics became more intricate with complex mathematics explaining the different phenomena occurring in the sub atomic regime. But experimenting with such minute systems was rather impossible at that time. Nevertheless, this did not restrain the theorists from exploiting deeper into nature's delicate arrangement with mathematical elegance. The air was heated up with new theories explaining newer phenomena in all branches of physics. Some of these predictions are still being tested today for better accuracy with experiments.

Experiments can never lie, it shows results of whatever one wants to uncover provided the right instrumental approach has been applied. But the underlying mechanism about how the results have been achieved through various atomic and sub atomic interactions in the system with time cannot be shown by experiments, urging the need of simulation for a complete understanding.

Simulation involves construction of detailed algorithms in compliance with proposed mathematical theories. The algorithms are made as such so to have minimum error factor for better accuracy. These algorithms are then introduced into powerful supercomputers and calculations are allowed to run. Depending on the algorithm and its complexity in calculation the amount of run time varies. In simulating an experiment the system is introduced virtually into the computer and different boundary conditions are given as input for the system to follow accordingly. There are mainly two broad classes of simulation for the atomic world i.e. Classical which includes Molecular Dynamics simulation, Monte Carlo etc., and Quantum simulations using Density Functional calculations. Through these simulations one can study the behaviour of different thermodynamic systems, their varied interactions at every step, stable atomic configurations and predicting the results accordingly.

Classical atomic physics simulations mainly deal with the interaction potentials, kinetic energy and potential energy of atoms by creating a system virtually and observing the interplay of these potentials within the atoms virtually which converges to some end results which are more or less crude. It can be used to study simple systems two body or three body problems, statistical mechanics problems involving probability as in case of atomic systems taking the smallest indivisible entity to be the atom . On the other hand the more recently developed Quantum Simulations is more complex involving a range of different potentials (known as functionals) to the minutest details involving perturbations to the level of different atomic orbitals of a single atom. Calculations involving two interacting atoms with so many electrons with each one having different atomic orbitals so huge in itself that one can hardly complete it manually in a lifetime!!. Then think of calculating real systems with billions of atoms! These complex calculations require massive computation impossible in our simple personal computers. This is where supercomputers get to work. With very high processing speed these computers can work 24x7 and give us the results making an impossible feat possible.

Today a good quality and complete research finding must be accompanied by theory, experiment and simulation as well. It is a growing and completely different branch of scientific study in all the sciences. One of the most important facets of simulation is to develop our research methodology in the future to a level so as to divest ourselves of the trial and error of performing different experiments and their associated costs by finding the perfect set up for experiment computationally which would give sure shot results. The future of computational physics is very extensive and developments are going on in this direction with much more needed to be done.
