Louisiana EPSCoR
EXPERIMENTAL PROGRAM TO STIMULATE COMPETITIVE RESEARCH VOL.10 NO.2

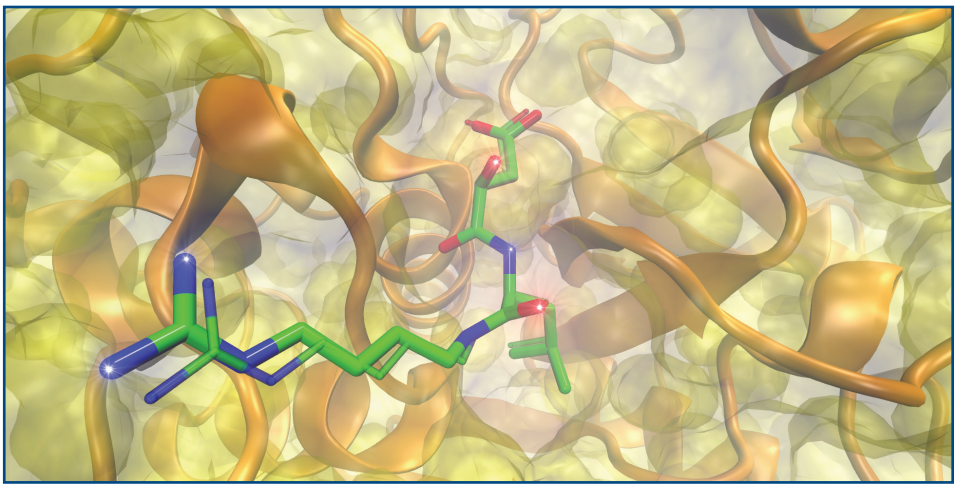
Shared Monte Carlo Computer Codes Shorten Discovery Time

Imagine a beautiful evening gambling in a casino in the French Riviera. How do you know whether to bet aggressively or play it safe? Mathematically speaking, to determine the probability of winning (or losing), you would repeatedly play the game over an extended period of time and record the results for analysis. This technique inspired the naming of a class of computational algorithms that rely on repeated random sampling to obtain numerical results, called "Monte Carlo" methods.

Monte Carlo algorithms are used in mathematics and physics computer experiments to run simulations repeatedly in order to obtain the distribution of an unknown probabilistic entity. This method is particularly effective for simulations of systems that have varying degrees of freedom or disorder, like weather, fluids, cellular structures, and strongly correlated materials. For example, in the field of astrophysics, Monte Carlo methods are used to model the evolution of galaxies. In particle physics, polymers are modeled at the molecular level to develop new methods of delivering medicines to targeted organs.

Researchers from the Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA) consortium, funded by the National Science Foundation, utilize Monte Carlo experiments to study materials science, condensed matter physics, and computational biology.

The team has successfully developed four computer programming codes to facilitate Monte Carlo experiments and have released them to the public domain at http://www.institute.loni.org/lasigma.



GeauxDock: Illustration of a "match" between a computer-generated prediction of the orientation of a drug molecule bound to a protein (thick green), and an overlay of the same structure solved by X-ray crystallography (thin green). Image by Michal Brylinski.

The codes can be utilized on desktop computers with Nvidia graphic cards and supercomputing clusters.

The four Monte Carlo codes available on the LA-SiGMA website are as follows:

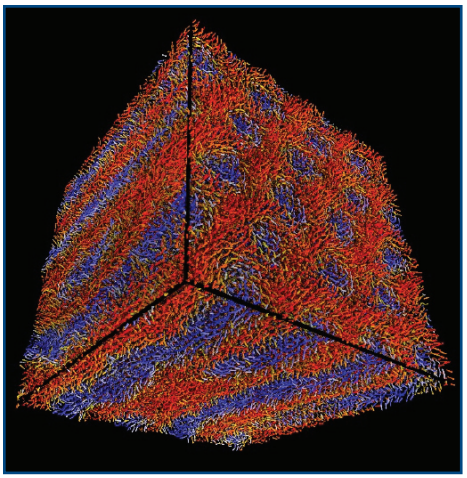
Parallel Tempering Monte Carlo

The parallel tempering Monte Carlo simulation is used for random frustrated systems. Geometrical frustration occurs when a system of interacting particles is unable to find its lowest energy state because of how the particles are arranged. "A lot of interesting problems in condensed matter physics with disorder are not well understood," said Dr. Ka-Ming Tam, Postdoctoral Researcher at Louisiana State University's Department of Physics & Astronomy. "Random frustrated systems are notoriously difficult to simulate because of the rough energy landscape. The simulation demands small memory but huge computations, averaging millions of disorder realizations. The randomness and frustration in the model lead to a very long equilibration time," added Dr. Tam.

To solve these computation bottlenecks, LA-SiGMA researchers employed various optimization algorithms and techniques to the program and have achieved world leading performance. This is the fastest code for the simulation of Edwards-Anderson model for systems with extreme sluggish dynamics, even for relatively small system sizes.

A paper on this code has been published in *Computer Physics Communications* in 2014, and another paper focusing on the Edwards-Anderson model is currently being reviewed.

continued on page 2



Parallel Tempering Monte Carlo: Electron spin configuration of a skyrmion lattice phase in manganese silicide. This material has potential applications in spintronics. Image by Jonas Wilhelm.

Variational Monte Carlo

The Variational Monte Carlo code is designed for the study of strongly correlated materials. These solid materials exhibit unusual electronic and magnetic behaviors that cannot be described by one-electron theories. High temperature superconductors are one example of a strongly correlated material.

The simulation of systems with multiple electrons suffer from the so-called "minus sign problem," which causes a bottleneck when calculating the integral over different configurations of the electrons. Unlike other Monte Carlo methods, the Variational Monte Carlo performs sampling according to the amplitude of the wave function, and therefore it is always positive. This method is widely used for the study of spin liquid, pseudogap, and superconductivity.

Hirsch-Fye Monte Carlo

The Hirsch-Fye Monte Carlo algorithm is a core tool used in computational quantum mechanical modeling, in particular, to add missing interactions to Density Functional Theory (DFT).

DFT is used to determine the electronic structure and predict complex system behavior of many-body systems like atoms and molecules. When these materials have strong electron-electron correlation, the approximation of independent electrons breaks down.

The Hirsch-Fye Monte Carlo code is a proven method to repair the DFT solutions. The team has accelerated the simulation for scenarios with multiple impurities that cause the minus sign problem and long simulation times.

GeauxDock

LA-SiGMA researchers have also created a Monte Carlo code for applications in biology and medicine, called GeauxDock. The code employs a novel hybrid force field and Monte Carlo protocol for the efficient sampling of conformational space.

This tool virtually screens for a match of which small molecules, called ligands, bind to the macromolecular receptor target of interest. This greatly speeds up the automated docking predictions that are used to develop new medicines.

In addition to developing new medicines to treat disease, researchers use the code to study how drug molecules interact with multiple targets. This field, called polypharmacology, helps researchers design more effective, but less toxic medicines.

Another research area where this code is utilized is finding new applications for existing medicines, called "drug repositioning." For example, Ropinirole was originally developed for the treatment of Parkinson's disease, and through additional studies, it was discovered that it is also an effective treatment for Restless Leg Syndrome. This provides significant cost and time savings toward research and development since the drug has already passed a significant number of toxicity and other tests.

Louisiana EPSCoR
P.O. Box 3677
Baton Rouge, LA 70821-3677
#4475