A Random Walk through the Web

Like to take random walks with molecules? The "Molecular Monte Carlo Home Page", sponsored by the Cooper Union Department of Chemistry, is meant to serve as an international information resource for those who use (or would like to use) stochastic methods based on random numbers and probability statistics to investigate molecular systems. Generally speaking, the use of Monte Carlo (MC) methods allows examination of complex chemical and physical problems that would otherwise only be soluble by approximations or might be quite intractable. MC calculations can provide essentially exact solutions to problems such as thermally averaged structural properties of atomic and molecular liquids, free energies, phase transition temperatures, reaction rate constants, charge distributions—just about anything of interest in the context of molecular computations. MC methods are actually used in a diverse number of ways. Apart from the "classical" MC method, where samples are drawn from a probability distribution to obtain thermodynamic properties, the home page mentions four other types of MC techniques, which are most commonly encountered in the context of molecular computations, such as path-integral MC to calculate finite-temperature properties of quantum systems. A rough description of these methods and introductory articles about random walks, Markov chains, simulated annealing, and random number generators to name just a few, can be found in the "MC tutorials", one of the link collections accessible from the main page. Furthermore, there is a link to MC-related conferences, reference databases (such as the Los Alamos e-print archive), and journal home pages, including the *Journal of Chemical Physics* where the Metropolis algorithm was first published. While the direct access to journals is convenient, the selection of listed conferences seems to me to be rather arbitrary and, with currently only three entries, very limited. Given the variety of problems to which MC methods are applied, I would suggest to extend the list by more general conferences on theoretical chemistry (biology) and statistical physics. The home page also contains links to online papers and books. However, as in the case of conferences, there are only few articles listed. Moreover, most of the topics are too specific to be of general interest, and altogether this link collection does not seem to be particularly useful.


Welcome to the Molecular Monte Carlo Home Page!

Last Update: **March 6, 2001.**

Electronic Computational Chemistry Conference

7

April 2-30, 2001

ECCC7's participants are...
the Molecular Monte Carlo Havens of the Months of March/April 2001!

This page, sponsored by the Cooper Union Department of Chemistry, is meant to serve as an international information resource for those who use "random walks" (stochastic methods) to simulate and analyze molecular systems. You will find links to hypertext tutorials on Monte Carlo methods here as well as software repositories and other information.

Molecular Monte Carlo: What Is It?

Although Monte Carlo methods are used in a daringly diverse number of ways, in the context of molecular computations there are five types most commonly encountered:

"classical" Monte Carlo, or CMC (samples are drawn from a probability distribution, often the classical Boltzmann distribution, to obtain thermodynamic properties, minimum-energy structures and/or rate coefficients, or perhaps just to sample conformers as part of a global conformer search algorithm);
"quantum" Monte Carlo, or QMC (random walks are used to compute quantum-mechanical energies and wavefunctions, often to solve electronic structure problems, using Schroedinger's equation as a formal starting point);
"path-integral" quantum Monte Carlo, or PIMC (quantum statistical mechanical integrals are computed to obtain thermodynamic properties, or even rate coefficients, using Feynman's path integral as a formal starting point);
"volumetric" Monte Carlo, or VMC (random and quasirandom number generators are used to generate molecular volumes and sample molecular phase-space surfaces);
"simulation" Monte Carlo, or SMC (stochastic algorithms are used to generate initial conditions for quasiclassical trajectory simulations, or to actually simulate processes using scaling arguments to establish time scales or by introducing stochastic effects into

In my opinion, the strong point of the home page is the collection of software and numerical tools as the CCP5 (Computer Simulation of Condensed Phases) library on MC and Molecular Dynamics methods. A detailed description of the code is not included, but the links provide, for example, direct access to all the source codes of Allen and Tildesley's book on "Computer Simulation of Liquids". Also, the arrangement and layout of the page are clear enough to find specific information easily.

Taken altogether, the Molecular Monte Carlo Home page appears to be a helpful source, particularly for MC novices looking for introductory articles and some practical help.

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For further information visit:
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