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Monte Carlo (MC), method of

In mathematics, a method originally used for calculating multiple integrals by means of a random sample. The method is used for numerical modelling of many-particle chemical systems, in particular liquids; it is based on the equilibrium statistical mechanics theory. Observables A are calculated as mean values over a great number ($\cong 10^5 - 10^6$) of instant configurations as determined by coordinates of the particles.

$$< A > = \frac{1}{N} \sum_{i=1}^{N} A\{r_i\}$$

where N is the number of configurations. At the first stage, various configurations are randomly generated and then those energetically un-realizable eliminated. An efficient search for the most probable configurations to be entered into the above expression is provided by the Metropolis algorithm based on the principle of Markov's chain theory. While being elaborated for the study of equilibrium chemical systems, MC method is also applied to studies of the dynamics of chemical reactions.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1952

