Modeling a Boltzmann Distribution: Simbo (Simulated Boltzmann)

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Modeling a Boltzmann Distribution: Simbo (Simulated Boltzmann), a Computer Laboratory Exercise

A Software Program Included in Advanced Chemistry Collection, 3rd Edition, Special Issue 28, a CD-ROM for Students

Modeling a Boltzmann Distribution: Simbo (Simulated Boltzmann), a Computer Laboratory Exercise

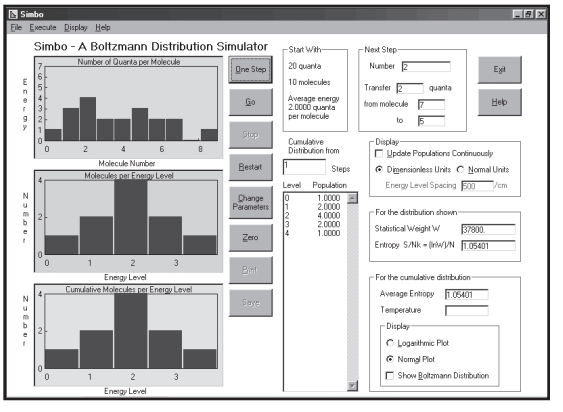
Alexander P. Lyubartsev, Division of Physical Chemistry, Arrhenius Lab., Stockholm University, 106 91 Stockholm, Sweden; Emerson F. Heald, Department of Chemistry, Thiel College, Greenville, PA 16125-2181; Richard W. York, Department of Chemistry, Wittenberg University, Springfield, OH 45501

Derivation of the probability distribution in the canonical ensemble (Boltzmann distribution) is one of the more difficult topics in statistical mechanics or statistical thermodynamics courses. The approach taken in most textbooks consists of calculating the most probable distribution over energy levels with given constraints. This derivation uses some mathematical techniques that many chemistry students find difficult. On the other hand, the concept of canonical distribution is the basis of statistical thermodynamics, and its understanding is important for all chemistry students, not only for those specializing in theoretical chemistry.

The Windows-compatible simulation program, Simbo, uses a simple model to illustrate the appearance of the exponential Boltzmann distribution of energy levels, and gives some insight into the fundamentals of statistical thermodynamics. We consider a model of N harmonic oscillators, which may represent vibrational energy levels in a system of weakly interacting diatomic molecules (ideal diatomic gas), or vibrational excitations in the Einstein model of crystals. The whole system is isolated—that is, the total energy is kept constant, but energies of individual molecules can change randomly. One can see that, at sufficiently large number of molecules and after proper equilibration, the distribution over energy levels for individual molecules becomes exponential. The program provides the possibility of exploring in detail the appearance of the statistical laws and of checking some statements that students usually have to take on faith when the theory is explained in the conventional way. Temperature, entropy, and other thermodynamic quantities may be determined from this distribution. Moreover, the second law of thermodynamics (the increasing of entropy with time) can be illustrated.

Simbo has been used as a computer laboratory exercise within the statistical thermodynamics portion of the advanced course Quantum Chemistry and Spectroscopy at the department of Physical Chemistry, Stockholm University. It may also be used as an illustrative tool during lectures or exercises on the theory of statistical ensembles.

Two versions of Simbo are included in the Advanced Chemistry Collection. The version that uses Visual Basic is recommended for most users. The other version performs the same simulation but is written in Tcl script language and uses a graphical library (BLT), currently available for Windows, Unix, and Linux platforms. *JCE Software* cannot support Simbo on the Unix and Linux platforms.



A screen from Simbo for Windows.