reaction "rates," and the various species concentrations are represented by continuous, single-valued functions of time. Although this deterministic formulation is adequate in most cases, there are important situations, such as a nonlinear system in the neighborhood of a chemical instability, for which its underlying physical assumptions are unrealistic and its consequent predictions are unreliable.

An approach to the chemical kinetics of spatially homogeneous systems which is somewhat more broadly applicable than the deterministic formulation is the *stochastic formulation.* Here the reaction constants are viewed not as reaction "rates" but as reaction "probabilities per unit time," and the temporal behavior of a chemically reacting system takes the form of a Markovian random walk in the N-dimensional space of the molecular populations of the N species. In the stochastic formulation of chemical kinetics the time evolution is analytically described, not by a set of N coupled differential equations for the species concentrations, but rather by a single differential-difference equation for a grand probability function in which time and the N species populations all appear as independent variables. This differential-difference equation is customarily called the master equation, and the function which satisfies that equation measures the *probability* of finding various molecular populations at each instant of time.

From a *physical* point of view, the stochastic formulation of chemical kinetics is superior to the deterministic formulation: the stochastic approach is always valid whenever the deterministic approach is valid, and is sometimes valid when the deterministic approach is not. (Some may disagree with this assertion; we shall present arguments supporting it in Section 2). From a strictly *mathematical* point of view, though, the set of deterministic reaction rate equations for a given chemical system is invariably much easier to solve than the stochastic master equation for the same system. However, if the system involves more than a few molecular species and chemical reactions, it usually turns out that *neither* formulation of chemical kinetics is tractable by purely *analytical* methods, and one is forced to consider computer-oriented *numerical* methods. Considerable success in this vein has been realized within the deterministic formulation by applying finite-time-step techniques to the coupled differential reaction rate equations. Within the framework of the stochastic formulation, though, prospects for performing numerical calculations have until now been regarded as generally unpromising.

In this paper we present what appears to be an eminently feasible method for numerically calculating the stochastic time evolution of virtually any spatially homogeneous chemical system. This computational method does *not* try to numerically solve the master equation for a given system; instead, it is a systematic, computer-oriented procedure in which rigorously derived Monte Carlo techniques are employed to *numerically simulate* the very Markov process that the master equation describes analytically. The simulation algorithm is fully equivalent to