MOLECULAR SIMULATIONS

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Contents

Summary

Providing the link to microscopic processes taking place at the atomic level, molecular simulation methods have developed to an indispensable tool for elucidating structure-property-processing relationships in all fields of materials science and engineering. Although continuum models of materials and of their macroscopic behavior continue to be important in chemical, pharmaceutical and biotechnology industries, life sciences are becoming clearly linked today to concepts referring to molecular phenomena. The two main thrusts are *molecular simulations* and *computational quantum chemistry*, coupled with modeling and interpretation of the results (*informatics*). Molecular simulation is based on classical Newtonian physics, modeling interactions within or between

molecules using interaction forces (force fields). Systems are modeled either deterministically (molecular dynamics, which integrates classical equations of motion) or stochastically (Monte Carlo methods). In contrast, computational quantum chemistry is based on quantum physics, primarily applied to the electronic structure of atoms or molecules. The immediate results are wavefunctions or probability density functionals describing electron states. This chapter reviews the two classical molecular simulations methods (molecular dynamics and Monte Carlo) capable of probing structure and dynamics at the atomistic level. A review of the dissipative particle dynamics (DPD) method, which is suitable for the mesoscale modeling of material domains (it finds extensive applications in the study of biological membranes), is also included.

1. Introduction

In recent years chemical engineers have become increasingly involved in the design and synthesis of new materials and products based on complex molecules as well as in the development of biological processes and biomaterials. Most of these applications often demand that one understands the molecular mechanisms shaping the physicochemical properties of these systems so that the product properties are controlled with precision. Molecular modeling, simulating chemical and molecular structures or processes by computer, significantly aids scientists in this endeavor. Typical applications of theoretical and computational methods to specific chemical engineering technologies today include: (1) the bottom-up and top-down design of self-organizing materials (by understanding e.g. the mechanisms and principles of peptide self-assembly into α-sheet tapes) and of bio-inspired materials for multifunctional biomedical applications, (2) manipulating structure and properties in high-performance, nanostructured materials for the design of systems for a variety of chemical, physical, and biological technologies, (3) understanding and modeling the kinetics of chemical reactions which is crucial to any research and development effort aimed at process optimization and innovation (e.g., the quantum modeling of elementary-reaction kinetics in flames, PECVD plasmas, polymer decomposition, and homogeneous catalysis; the first-principles simulation of heterogeneous catalysis using density functional theory; computational chemistry approaches to industrial chlorination and automotive lubricant additives; hybrid quantum chemistry/molecular mechanics approaches to solvated homogeneous catalysts; and computational spectroscopy methods for quantitative thermochemistry), (4) predicting the mechanical behavior of glassy materials and of ceramic and nanophase composites and understanding the microscopic electronic processes controlling the properties of ferroelectric and photonic materials and semiconductors, (5) simulating pattern formation in systems undergoing phase transitions, and (6) understanding the molecular origin of polymer viscoelasticity which governs the rheological properties of complex, chain-like molecules. Being broadly applicable because "everything" is made of atoms and molecules, in all these fields, molecular modeling is the limit of the reductionist approach to chemical engineering. And its power is growing rapidly with the continuing development of computer power, new algorithms, and the availability of software. Today, molecular modeling: (a) can provide useful estimates of the properties and behavior of materials even before they have been synthesized, (b) can provide useful estimates of the parameters and behavior needed to do traditional chemical engineering process development and design, and (c) is often the most efficient way to obtain these estimates. It is thus considered the best partner of experiments and of the traditional estimation and design approaches, something that all chemical engineers should be aware of. But we ought to state that even in molecular modeling certain approximations are usually employed, whose validity varies with the method and with the system considered. Some approximations are quite valid for some systems and one can expect useful results when a suitable method is used to predict some subset of properties for those systems. We should not blindly apply a given method to all systems and rationally expect useful answers. A given method will typically supply only some of the properties and information needed to solve a given problem. Thus, although molecular modeling can and does replace some unnecessary experimentation (often leading to insights which initiate new experiments), molecular modeling techniques are most useful when used in combination with each other and with experiment.

2. Molecular Simulations

Molecular simulations differ from other forms of numerical computation in that the computer with which the calculations are carried out is not merely a machine but the virtual laboratory in which the system is studied. In such a “laboratory”, understanding is achieved by constructing first a theoretical model of molecular behavior able to reproduce and predict experimental observations and then solving it using a suitable algorithm or a computer program. Molecular dynamics (MD) and Monte Carlo (MC) are two such methods capable of providing accurate predictions of the thermodynamic, mechanical, permeability, electrical, optical and other properties of materials. For systems coarse-grained to the level of soft particles, an appropriate method to use is dissipative particle dynamics (DPD).

MD is a deterministic method at the heart of which is the solution of Newton’s classical equations of motion; these are integrated numerically to give information for the positions and velocities of atoms in the system. Let us consider a system consisting of N interacting atoms or atomistic units described by a potential energy function U, which depends in general on the position vectors $\mathbf{r}_i$ of all atoms present in the system:

$$U = U(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) \qquad (1)$$

Then, Newton’s equations of motion read:

$$m_i \ddot{\mathbf{r}}_i = \mathbf{F}_i, \quad i = 1, 2, ..., N \qquad (2)$$

i.e.,

$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = -\frac{\partial U(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N)}{\partial \mathbf{r}_i}, \quad i = 1, 2, ..., N \qquad (3)$$

where m_i is the mass of atom i, $\mathbf{r}_i$ its position vector, $\mathbf{F}_i$ the force acting on it and t the time. Solving the equations of motion then involves the integration of the $3N$ second-order differential equations (Newton's equations).

The classical equations of motion possess some interesting properties, the most important one being the conservation law. If the kinetic energy K and the potential energy V of the system do not depend explicitly on time, then it is straightforward to verify that $\dot{H}\left(=\frac{dH}{dt}\right)$ is zero [1], where H is the Hamiltonian of the system, i.e., the sum of K and U, $H = K + U$; consequently, H is a constant of the motion. In actual calculations, this conservation law is satisfied if there exist no forces acting on the system that depend explicitly on time or velocities. A second important property is that the corresponding equations of motion for the generalized coordinates (Hamilton's equations) are reversible in time. This means that changing the signs of all velocities will cause the atoms to retrace their trajectories backwards. The computer-generated trajectories should also possess this property.

MC, on the other hand, is a computing method for simulating the properties of matter that relies on probabilities. In contrast to MD, however, where the atoms are moved according to the inter- and intra-molecular forces derived from the potential function U by solving Newton's equations of motion, MC is a stochastic method based on transition probabilities between different states of the simulated system [2,3]. These transitions are traced through a scheme that involves three (3) main steps: (a) generation of an initial configuration, (b) trial of a randomly generated system configuration, and (c) evaluation of an "acceptance criterion" for the trial configuration and comparison to a random number to decide whether the trial configuration will be accepted or not. The acceptance criterion is usually formulated in terms of the potential energy change between trial (new) and existing (old) states and some other properties of the new and old configurations, depending on how the trial transition is implemented.

Being a stochastic method, MC cannot of course provide any information about the true dynamics of the system. Despite this, however, it has developed in the last years to a powerful tool for simulating the properties of matter, because of the unique capability it offers to accelerate system equilibration through the implementation of moves that have nothing to do with the natural trajectory followed by the system. In fact, one can devise totally unphysical ways for moving atoms that substantially depart the system from its natural trajectory. By cutting through energy barriers obstructing structural rearrangements, such cleverly-designed, unphysical moves can accelerate (by many orders of magnitude, in some cases) thermal equilibration at the conditions of the computational experiment, rendering MC a more efficient method for simulating the system than MD. For systems of chain molecules (e.g., synthetic polymers, branched macromolecules, and biopolymers), whose equilibration is hindered by the problem of long relaxation times, namely the fast increase in the longest relaxation time with chain length, this is of paramount importance.

For systems represented as a set of point particles whose distribution and density is determined by a set of prescribed forces, a mesoscale method that can be used to study their properties is dissipative particle dynamics (DPD). The method shares features of both molecular dynamics and lattice gas automata and closely resembles the structure of Brownian dynamics, assuming stochastic, dissipative, and conservative forces. The action of conservative forces is to distribute the beads in space as evenly as possible in order to minimize the free energy of the system. The dissipative forces represent friction and their action is to reduce velocity differences between the beads. The stochastic forces account for the degrees of freedom that were eliminated in the coarse-grained model. The magnitude of the stochastic and dissipative forces is coupled by the fluctuation-dissipation theorem and this serves as a thermostat for the system. The method is ideal for simulating among others the self-assembly behavior of amphiphilic micelles and bilayers, structure and morphology in systems containing microphase separating diblock copolymers and nanoparticles, and the interfacial properties of immiscible polymer blends.

In the next Sections of this Chapter, we discuss in detail how the three methods are employed in simulations of soft matter physics systems with an emphasis on their applications, i.e., on the properties that can be computed with them. Before this, however, we will present some important issues related with the way a molecular simulation is carried out in a simulation box.

3. The Concept of the Amorphous Cell and of the Molecular Model

Atomistic simulations are executed by using either a detailed molecular model in which all atoms are represented explicitly or a less detailed one in which entire groups of atoms are lumped into single quasiatomic entities. For polyethylene, for example, the former (explicit-atom, EA) description requires treating hydrogen (H) and carbon (C) atoms separately as individual sites while the latter (united-atom, UA) allows considering each CH_3, CH_2 and CH unit as a single, united pseudoatom [4]. In simulations with a united-atom model, the total number of interacting sites present in the system is drastically reduced; however, the results that are obtained are less accurate than those with an explicit-atom model. To improve the accuracy of a UA representation, anisotropic united-atom (AUA) models are sometimes introduced, in which the centers of the non-bonded interactions are moved slightly away from the carbon centers of the united pseudoatoms.

As far as the potential energy function U is concerned, this in general involves a large number of terms accounting for the bonded (bond-stretching, bond angle bending, and dihedral angles) and non-bonded (intra- and intermolecular) interactions, and their couplings. A typical form is as follows [5]:

$$
\begin{aligned}
U = {} & \sum_{l} k_{l,2}\left(l-l_0\right)^2 + k_{l,3}\left(l-l_0\right)^3 + k_{l,4}\left(l-l_0\right)^4 + \\
& \sum_{\theta} k_{\theta,2}\left(\theta-\theta_0\right)^2 + k_{\theta,3}\left(\theta-\theta_0\right)^3 + k_{\theta,4}\left(\theta-\theta_0\right)^4 + \\
& \sum_{\phi} k_{\phi,1}\left[1-\cos\left(\phi-\phi_1^0\right)\phi\right] + k_{\phi,2}\left[1-\cos\left(2\phi-\phi_2^0\right)\right] + k_{\phi,3}\left[1-\cos\left(3\phi-\phi_3^0\right)\right] + \\
& \sum_{\chi} k_{\chi}\chi^2 + \\
& \sum_{l}\sum_{l'} k_{ll'}\left(l-l_0\right)\left(l'-l'_0\right) + \sum_{\theta}\sum_{\theta'} k_{\theta\theta'}\left(\theta-\theta_0\right)\left(\theta'-\theta'_0\right) + \\
& \sum_{l}\sum_{\theta} k_{l\theta}\left(l-l_0\right)\left(\theta-\theta_0\right) + \sum_{l}\sum_{\phi}\left(l-l_0\right)\left[V_1\cos\phi + V_2\cos 2\phi + V_3\cos 3\phi\right] + \\
& \sum_{\theta}\sum_{\phi}\left(\theta-\theta_0\right)\left[V_1\cos\phi + V_2\cos 2\phi + V_3\cos 3\phi\right] + \\
& \sum_{i}\sum_{j>i}\frac{q_i q_j}{\varepsilon r_{ij}} + \\
& \sum_{i}\sum_{j>i}\left(\frac{a_{ij}}{r_{ij}^9} - \frac{b_{ij}}{r_{ij}^{12}}\right)
\end{aligned}
\qquad (4)
$$

where l and l' denote bond lengths, θ and θ' bond angles, ϕ dihedral angles, and r_{ij} interatomic distances. Also,

$k_{l,2}, k_{l,3}, k_{l,4}, l_0, k_{\theta,2}, k_{\theta,3}, k_{\theta,4}, \theta_0, k_{\phi,1}, k_{\phi,2}, k_{\phi,3}, \phi_1^0, {}_2^0,$

$\phi_3^0, k_{\chi}, k_{ll'}, l'_0, k_{\theta\theta'}, \theta'_0, k_{l\theta}, V_1, V_2, V_3, a_{ij}$, and b_{ij}

are numerical constants of the model, q_i denotes the electric charge on atom i, and ε the dielectric constant of the medium.

To increase algorithm execution, many terms in this expression are usually omitted; for example, most of the higher-order terms as well as the majority of the coupling ones are neglected (if it is judged that their effect on the property of interest of the system under study is minimal). For example, if one is interested in the PVT properties or in the long-time diffusion or in the calculation of the free volume distribution, then one can employ a simplified version of Eq. (4) of the form:

$$
\begin{aligned}
U = {} & \sum_{l} k_{l,2}\left(l-l_0\right)^2 + \sum_{\theta} k_{\theta,2}\left(\theta-\theta_0\right)^2 + \sum_{\phi} k_{\phi,1}\left[1-\cos\left(\phi-\phi_2^0\right)\phi\right] + \\
& \sum_{i}\sum_{j>i}\frac{q_i q_j}{\varepsilon r_{ij}} + \sum_{i}\sum_{j>i}\left(\frac{a_{ij}}{r_{ij}^9} - \frac{b_{ij}}{r_{ij}^{12}}\right)
\end{aligned}
\qquad (5)
$$

in which only the very basic terms are kept. On the other hand, if one wants to explore the very short-time scale dynamics of the system (local or segmental dynamics) or to elucidate fine details of the local structure or couplings which give rise to specific patterns in (e.g.) the measured IR and Raman spectra, then one should work with the most accurate expression for the potential energy available; in such a case, keeping all terms in Eq. (4) above is “a must”.

After having specified the form of the force field, one has to choose an initial configuration for the system with which the molecular simulation will be carried out. Usually the simulation is carried out in a small cell (the simulation box) filled up with a large number of molecules (of the substance to be simulated) so that its density is close to the experimentally measured one at the pressure and temperature conditions of interest. Typically, the total number of interacting sites present in the simulation box ranges from 10^3 to 2×10^4 for runs that are executed serially, with corresponding box dimensions on the order of 30 to 80Å. For parallel runs (executed on a cluster of CPUs), these numbers can be considerably different (higher) by up to two orders of magnitude in some cases. Before subjecting the initially generated configuration to MD or MC, it is imperative that the potential energy be properly minimized (in order to avoid undesirable atom overlaps and the concomitant numerical errors) by resorting, for example, to the three-stage, constant-density Molecular Mechanics (MM) technique (the amorphous cell method) of Theodorou and Suter [6], subject to a set of appropriate (periodic) boundary conditions depending on the presence or not of interfaces. To generate an initial configuration for practically any physical system and to minimize its potential energy, a number of tools are available today in the form of commercial, user-friendly software packages, such as the Materials Studio of Accelrys [5], LAMMPS, [7] GROMOS [8], AMBER [9], NAMD [10], etc.

4. The Molecular Dynamics Method

The molecular dynamics (MD) method [11] provides system trajectories in real time by solving the system of 3*N* second order differential equations, Eq. (3), usually with a finite difference method, given the initial (at time $t=0$) atomic positions and velocities. In general, one can distinguish between two families of MD algorithms for the integration of classical equations of motion: higher-order (Gear) methods and Verlet algorithms.

4.1. Higher-Order (Gear) Methods

These are predictor-corrector methods which obtain an estimate of the atomic positions and velocities at time $t+dt$ by performing a Taylor expansion around time t:

$$\mathbf{r}^{\mathrm{p}}(t+dt)=\mathbf{r}(t)+dt\mathbf{v}(t)+\frac{dt^2}{2}\ddot{\mathbf{r}}(t)+\frac{dt^3}{6}\dddot{\mathbf{r}}(t)+\frac{dt^4}{24}\ddddot{\mathbf{r}}(t)+\ldots \qquad (6a)$$

$$\mathbf{v}^{\mathrm{p}}(t+dt)=\mathbf{v}(t)+dt\ddot{\mathbf{r}}(t)+\frac{dt^2}{2}\dddot{\mathbf{r}}(t)+\frac{dt^3}{6}\ddddot{\mathbf{r}}(t)+\ldots \qquad (6b)$$

$$\ddot{\mathbf{r}}^{\mathrm{p}}(t+dt)=\ddot{\mathbf{r}}(t)+dt\dddot{\mathbf{r}}(t)+\frac{dt^2}{2}\ddddot{\mathbf{r}}(t)+\ldots \qquad (6c)$$

$$\dddot{\mathbf{r}}^{\mathrm{p}}(t+dt)=\dddot{\mathbf{r}}(t)+dt\,\ddddot{\mathbf{r}}(t)+\ldots \tag{6d}$$

with the superscript p denoting "predicted" values. The equations of motion are introduced in the next or "corrector" step as follows: From the predicted positions, the forces are calculated at time $t+dt$ and, consequently, also the accelerations at time $t+dt$, $\ddot{\mathbf{r}}^{\mathrm{c}}(t+dt)$. The latter are used to estimate the size of the error in the "predictor" step:

$$\Delta\mathbf{x}\equiv\ddot{\mathbf{r}}^{\mathrm{c}}(t+dt)-\ddot{\mathbf{r}}^{\mathrm{p}}(t+dt)=\ddot{\mathbf{r}}(\mathbf{r}^{\mathrm{p}}(t+dt))-\ddot{\mathbf{r}}^{\mathrm{p}}(t+dt) \tag{7}$$

Then, the so called Gear coefficients $c_0,\ c_1,\ c_2,\ c_3,\ \ldots$ are used to correct positions, velocities, accelerations and higher order derivatives in the corrector step, as follows:

$$\mathbf{r}^{\mathrm{c}}(t+dt)=\mathbf{r}^{\mathrm{p}}(t+dt)+c_0\Delta\mathbf{x} \tag{8a}$$

$$\mathbf{v}^{\mathrm{c}}(t+dt)=\mathbf{v}^{\mathrm{p}}(t+dt)+c_1\Delta\mathbf{x} \tag{8b}$$

$$\ddot{\mathbf{r}}^{\mathrm{c}}(t+dt)=\ddot{\mathbf{r}}^{\mathrm{p}}(t+dt)+c_2\Delta\mathbf{x} \tag{8c}$$

$$\dddot{\mathbf{r}}^{\mathrm{c}}(t+dt)=\dddot{\mathbf{r}}^{\mathrm{p}}(t+dt)+c_3\Delta\mathbf{x} \tag{8d}$$

These are considered as a better approximation of the true variables, and the iterations are continued so as to further refine the solution, until convergence is achieved. Given that the evaluation of the forces (i.e., of the accelerations) from the atomic positions is computationally quite demanding, usually one or (at most) two corrector iterations are carried out.

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Biographical Sketch

Vlasis Mavrantzas received his Diploma in Chemical Engineering from the National Technical University of Athens, Greece, in 1988 and his Ph.D. from the University of Delaware, Department of Chemical Engineering, in 1994. In 1996 he joined the research team of Prof. Doros Theodorou in Patras as a post-doctoral fellow. In 1997 he was appointed associate researcher at the Institute of Chemical Engineering and High-Temperature Chemical Processes (FORTH-ICE/HT) where in 2001 he was promoted to associate researcher. In 2002 he was elected associate professor at the University of Patras where he has been the director of the Laboratory of Statistical Thermodynamics and Macromolecules in the Department of Chemical Engineering. He has been visiting researcher of the Dow Chemical Company in Midland, U.S.A., of the Institute for Polymers at ETH-Z, Switzerland, in the group of Prof. Hans Christian Öttinger (February 2000, February 2002, January 2008) and of the Department of Applied Physics at the University of Tokyo (June-July 2005) in the group of Prof. Masao Doi through a scholarship by the Japan Society for the Promotion of Science and Technology. Vlasis Mavrantzas is the author of about 60 scientific papers in the field of polymer modeling and simulation, of about 7 chapters in Books, of 1 book in Greek on Statistical Thermodynamics for the Hellenic Open University, and the Editor (with A.N. Beris and Th. Tzavaras) of a Special Volume in the Journal of non-Newtonian Fluid Mechanics (2008) published by Elsevier on “non-Equilibrium Thermodynamics and Complex Fluids”. He has served as President of the Hellenic Society of Rheology (2004-2006), and for the last 5 years he has been the Scientific Director of the Inter-departmental Program of graduate studies on Polymer Science and Technology at the University of Patras. Since 2005 he has been on the International Advisory Board of “Macromolecular Theory and Simulation”.