HANDBOOK
OF
MOLECULAR DYNAMICS POTENTIAL FUNCTIONS

JOHN R. LLOYD
TENGFEI LUO

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HANDBOOK OF MOLECULAR DYNAMICS POTENTIAL FUNCTIONS
BY JOHN R. LLOYD AND TENGFEI LUO

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PREFACE

The process of researching and writing this handbook was undertaken because of our start-up experience when we began our molecular dynamics studies of phonon–electron interface energy transport. It was very difficult to locate proper potential functions for the particular materials we wanted to work with. The Lennard-Jones (LJ) potential function had served as the standard potential function for many materials, since it was easy to understand, easy to apply, and very well known. Every undergraduate engineering, chemistry, and physics student has seen it in their courses, and of course it has the correct general physics in it. For higher-level research though, the question soon became whether or not the LJ potential function was the best for the molecule system of interest. Thus an extensive literature search was undertaken to identify potential functions and all their empirical constants for the specific systems that were of interest to our study.

To begin our research, we dedicated time to search for and record all potential functions in all the literature we identified where MD simulations were instituted. We soon had a significant collection of potential functions, and we started to work with them in our research with confidence that previous researchers had helped establish an acceptable level of accuracy for a particular potential function for a particular system.

This handbook is a result of our research in identifying potential functions for use in MD simulation. We have listed potential functions by name and cross-listed them by the molecular systems that they have been used to simulate. We hope that this handbook will prove useful to others involved in performing MD simulations. We are continuously looking for more potential functions and information about the systems that they can describe.

This preface would not be complete without recognizing Mr. Tom Pabst, an undergraduate Mechanical Engineering student from Michigan State University, who worked a summer to initiate this collection of potential functions. His contributions to this compilation were invaluable.

Professor John Lloyd would also like to thank his wife, Mary Jane Lloyd, for her willingness to put up with his crazy hours and work schedule throughout his career. It would have been impossible for him to accomplish all that he has without her patience, support, and love.

Dr. Tengfei Luo wants to thank Professor Lloyd for bringing him to the field of molecular simulation. He also would like to thank his wife, Yuanyuan Zhu, for her continuous support in his study career.

Professor John Lloyd would like to thank Professor Arun Majumdar, who sponsored him during a sabbatical leave at UC Berkeley in 2004, where Professor Lloyd's formal research program in nanotechnology was initiated. Professors Lloyd and Majumdar obtained a grant from the National Science Foundation that supported our study at UC Berkeley and at Michigan State University.

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1. INTRODUCTION

Molecular dynamics (MD) simulation is a computational method that calculates the time-dependent behavior of atomic systems. MD simulations can provide detailed information on the fluctuation or evolution of a system given a set of initial conditions plus forces of interaction. MD simulations have long been used to investigate structure, dynamics, and thermodynamics of atomic systems such as molecules, molecular complexes, polymers, liquids and crystals. They can sometimes work as bridges between microscopic time and length scales and the macroscopic counterparts because they are capable of predicting bulk properties by simulating a small number of atoms. Because of the emerging field of nano science, technology has reached the size of a nanometer. This makes MD simulations even more valuable since they can directly simulate the behavior of nano systems.

1.1 *Ab-initio* Method

Since accurate interatomic forces are crucial for MD simulations, calculating the forces from *ab-initio* is a good way to ensure their precision.

As we know, any materials can be modeled as simply nuclei and electrons. Because electrons travel thousands of times faster than nuclei, electrons can follow any nuclear motions with almost infinitesimal time elapse. As a result, the electronic and nuclear motions can be decoupled since the electrons can respond instantaneously to any changes in nuclear coordinates. In such a condition, the electronic wavefunction only depends on the instantaneous nuclear configurations, and not on time. As a result, its behavior can be described with the time-independent Schrödinger equation. On the other hand, the nuclei are massive enough to be treated as classical particles, responding to the electronic forces according to Newton’s second law. By calculating the electronic structures "on-the-fly" at every MD step, the forces on the nuclei are obtained by taking the gradient of the total energy of the electron system.

Although *ab-initio* MD gives high levels of accuracy, it is so computationally expensive that only a very limited number of atoms can be simulated. This method is normally applicable to chemistry and biochemistry problems where only limited numbers of atoms are necessary to study a certain phenomenon. In many current *ab-initio* codes, plane waves are used as the basis sets in order to represent the periodic part of the electron orbitals. In order to minimize the size of the plane wave basis necessary for the calculation, core electrons are replaced by pseudopotentials, which are constructed to correctly represent the long-range interactions of the core and to produce pseudo-wavefunction solutions that approach the full wavefunction outside a core radius. Inside this radius the pseudopotential and the wavefunction should be as smooth as possible, in order to allow for a small plane wave cutoff. In addition, it is desirable that a pseudopotential is transferable, which means that the same pseudopotential can be used in calculations for different systems under different conditions with comparable accuracy. Readers are referred to [1] for a more detailed discussion on *ab-initio* calculations.

Although *ab-initio* MD simulations are accurate because of the "on-the-fly" feature of force calculation, and the computation time requirement has been greatly reduced by using plane waves with appropriate cutoffs and pseudopotentials, they are still not capable of simulating large systems and large timescales. This makes the classical MD attractive in many fields where large systems and long physical times need to be simulated.

1.2 Classical Molecular Dynamics

Classical molecular dynamics simulations are different from *ab-initio* methods. *Ab-initio* methods calculate atomic forces by calculating electronic structures. Classical MD simulations employ predefined empirical potential functions to obtain the forces [see eq. (1.1)]

$$-\nabla\phi = \vec{F} = m\frac{d^2\vec{r}}{dt^2}, \tag{1}$$

where ϕ is the potential energy, $\vec{F}$ is the force, m is the atomic mass, $\vec{r}$ is the position vector, and t is the time. In principle, MD simulations can be applied to any arbitrary atomic system. However, the applicability of this method is limited by the availability of accurate empirical potential functions.

1.3 Empirical Potential

Depending on the nature of electronic structures or simply bonding characteristics, the suitable choice of potential functions is extremely important for realistic simulations. The accuracy of the potential function limits the accuracy of the simulations and thus the accuracy of any information to be extracted from the simulations. These "predefined" potentials are either based on experimental data or on independent *ab-initio* calculations and are the solution to the question of how to describe, or in practice how to approximate, the interatomic interactions which is the core problem of any MD simulation. Fortunately well-tested empirical potentials are available for many materials. Typically, the interactions are broken up into two-body, three-body, and many-body contributions, long-range and short-range terms, which have to be represented in suitable functional forms.

However, the need to devise a "predefined" potential implies serious drawbacks. First, the "predefined" potentials usually suffer from transferability problems. One potential cannot be used to simulate everything in all the different conditions. The validity of a potential should always be checked when they are used in different conditions or different systems. Second, when the electronic structures and thus the bonding patterns change qualitatively in the course of simulations, "predefined" models will not be able to represent the interactions all the time while the simulations proceed. These disadvantages limit the applicability of classical MD simulations in systems involving special processes, such as chemical reactions and phase transitions.

As a result, before any meaningful simulation being carried out, correct selection of potential functions is essential.

1.3.1 *Choosing the Right Potential Model*

The definition of "right" and "wrong" of a potential function is only valid when it is applied to a certain simulation system. Choosing the correct potential function is nontrivial, and it requires a lot of experience to choose the correct one. For example, it is appropriate for one to use the simple pariwise Lennard-Jones (LJ) potential [2] to simulate monatomic argon systems. However, LJ will fail if it is used to simulate crystalline Si due to lack of angle terms which stabilize the crystal. The Stillinger–Weber (SW) potential [3] is designed to simulate bulk crystalline semiconductors, but it cannot reproduce the surface reconfiguration of GaAs surfaces as the Tersoff potential [4] does which considers the bonding environment. Although water molecules look simple, they can be simulated using the simple LJ potential or the very sophisticated TIP6P model [5], all depending on the nature of the simulation system. In many cases, if one is unlucky, there can be no established potential functions that can model the system of interest, and construction of brand new potential functions might be necessary, which usually takes a long time.

Although there are no rules of thumb on selecting potential functions, some limited guidance can be given for beginners. For example, the LJ potential can usually be used for simple liquids. SW and Tersoff potentials are often enough for semiconductors. Embedded atom models (EAM) [6-10] are appropriate for metals, and integrated force fields like Amber [11], GROMACS [12], CHARMM [13] are optimized for molecular, protein and polymer simulations. Another criterion of choosing an appropriate potential functional is that such a potential should be adequate for the system being studied. For example, if we are to simulate a lattice at very low temperatures when atoms will only move very close to their equilibrium positions, a harmonic potential will be good enough to simulate such movements. However, if the temperature is increased, harmonic potentials will not be adequate to capture the anharmonic behavior when the atoms move further away from equilibrium, and one will then need to use anharmonic potentials, such as the Morse potentials, to describe such anharmonicity (see Fig. 1).

1.3.2 *Determination of Potential Parameters*

Having chosen appropriate potential functional forms, the next step is to determine a set of potential parameters, which is also a critical issue to ensure the accuracy of MD simulations.

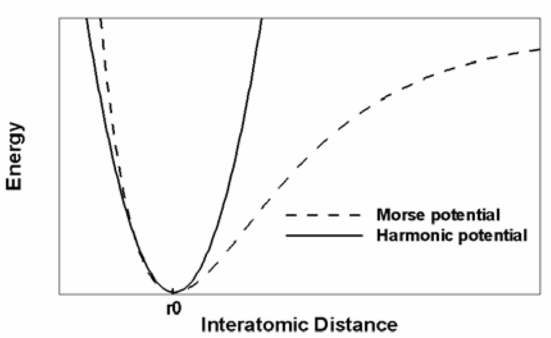

Figure 1 Morse potential and harmonic potential

These parameters are usually fitted so that the potential models can reproduce one or several properties of the system obtained either by higher order calculations such as *ab-initio* calculations or from experimental measurements. A good example would be the potential fitting for a crystalline Bi2Te3 in [14], where Morse and LJ potentials are chosen to model the bonded and van der Waals interactions, respectively. By fitting the energy hypersurface obtained from *ab-initio* calculations, the parameters of the Morse potential are determined. However, van de Waals interactions cannot be fitted to *ab-initio* calculations since they cannot correctly describe such kinds of dispersion forces. As a result, the LJ parameters are fitted to experimental elastic and structure constants. It should also be noted that the fitting is usually not a one step mission but an iterative process which involves iterative fittings to *ab-initio* and experimental data. Different from crystalline systems, the fitting of potential parameters for molecular systems are much more complicated due to different conformations of molecular systems. Interested readers are encouraged to read some references, such as the development of the COMPASS potential [15–17], to become familiar with different fitting techniques.

1.3.3 *Transferability*

As has been pointed out, most commonly potential parameters are fitted so that a potential model can reproduce certain properties under certain conditions of systems. However, the number of properties that can be fitted is always limited. If these fitted potential models are used to calculate properties other than those they are designed for, or under conditions that are different from the fitting conditions, one should always check their transferability. For example, the SW potential is usually used to predict bulk properties of crystalline Si [3, 18]. However, when studying phase transition, researchers often prefer the bond-order Tersoff potential [4, 19–21] to take into account the concept of local environment, with bond strengths depending on it. Another example is that it is widely accepted that in bio-molecular simulations, the united atom model, such as found in [22, 23], can usually give valuable information on molecular structures and conformations while saving a lot of computational time. However, when the system involves chemical reactions, more sophisticated potentials such as the Brenner potential [24, 25] or REAX potential [26, 27] are necessary to include bond breaking and forming processes.

1.4 Objective of This Book

Our objective of writing this handbook is to present molecular modeling researchers a library of potential functions and available parameters found in the literature. This handbook includes as many references as the authors are aware of. It aims at saving researcher’s time on searching the available potential models. The potential models are categorized into 2-body, 3-body, 4-body potentials and integrated force fields. The 2-body potential section includes not only general potential functionals, but also specific models for specific systems, which may involve 3- and 4-body terms. The 3- and 4-body potential sections are intended to provide general 3- and 4-body functionals. The integrated force fields section includes a number of widely used force fields that have been applied to various systems. The potential models are listed by name and are cross-listed by the system to which they are applied. The related references are listed at the end of each potential model. Due to the limitation of authors’ knowledge, it is clearly recognized by the authors that it is not possible to include all existing potentials in this handbook. We regard this book as a starting point for constructing a potential library, and it will be a continuing process to expand our database to include more and more potentials. Readers are more than welcome to contact us on anything about this book, especially missing potential models. We hope you find this handbook useful to your research.

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Part I Two-Body Potentials

4th Power Potential → General Purpose Potential → Symbols

Symbol	
E	Potential energy
r	Interatomic distance
r_0	Equilibrium interatomic distance
K	Force constants

4th Power Potential → General Purpose Potential → Function

$$E = \frac{1}{2} K_2 \left(r - r_o \right)^2 + \frac{1}{6} K_3 \left(r - r_o \right)^3 + \frac{1}{24} K_3 \left(r - r_o \right)^4$$

Comment

The 4th power potential is a variation of the harmonic potential which is often used in simulations of polymer and bio-molecular systems.