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Review

Computer simulation techniques for food science and engineering: Simulating atomic scale and coarse-grained models

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ABSTRACT

We describe computer simulation techniques that have been, or can be, used in Food Science and Engineering. We describe models which cannot be utilized without employing computer simulation but do not explicitly address models such as self consistent field approaches or DLVO theory. We describe techniques which either continue to play fundamental roles in computer simulation of soft matter and fluids, or newer developments which have shown increased use in the last decade. Here we outline the background to statistical mechanics followed by descriptions with selected examples of Molecular Dynamics, Coarse-Grained modeling, Monte Carlo techniques, Dissipative Particle Dynamics and Lattice–Boltzmann theory.

Contents

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1. Introduction

Computer simulation of physical and chemical processes and especially engineering applications, have played leading roles in creating understanding and knowledge and in the design of fabricated structures. The use of computer simulation techniques spans all areas of physics, and many areas of chemistry and engineering. Yet there is one area in which computer simulation does not yet play a role equivalent to that played in those fields – food science. In this we do not refer to the design of factories or equipment but to the use of computer simulation in designing new or better foods. It might be argued that the science of designing food is essentially satisfied by trial-and-error: that the accumulated wisdom of at least 10^3 centuries of cooking activities will not be significantly advanced by any attempted mathematical modeling and computer simulation of, e.g., a *Schwarzwaldkirschtorte* or a *Davanagere Benne Dosa*. This comment would miss the point and the cases of (i) protein folding and (ii) edible oil structures illustrate that.

1.1. *Protein folding*

Proteins catalyze nearly all reactions in organisms, contribute to structure, and perform many other functions necessary for the existence of life. The amino acids are linked sequentially and fold into the diversity of protein structures. The problem of predicting how a 3-Dimensional (3D) protein folds from a 1-Dimensional (1D) sequence has been called the "Protein-Folding Problem" (PFP). The role of proteins in disease processes (Fabrizio and Dobson, 2006; Murakami, Nakashima, Yamashita, & Yamaguchi, 2002; Selkoe, 2001) and drug design (Noble, Endicott, & Johnson, 2004; Yuriev & Ramsland, 2013) is of immense interest. We now turn to briefly highlighting how such a fundamental problem is addressed. There has been considerable progress in the last 50 years with the elucidation of about 84,000 experimental structures found in the Protein Data Bank (PDB) (Bernstein et al., 1977) which have identified the key molecular interactions for the diversity of structures. Experimental techniques such as X-ray crystallography (Bernado et al., 2005), NMR spectroscopy (Dyson & Wright, 2005) and cryo-electron microscopy (Jimenez et al., 2002) have provided the most information into protein structure. Experimental probes into the search for mechanisms of protein-folding have spurred the development of sophisticated Temperature-Jump methods using fluorescence of specific amino acids and even single molecules have been investigated on time-scales of $>1\,\mu s$ (Callender, Dyer, Gilmanshin, & Woodruff, 1998). Today, the plethora of experimental data contained in numerous bioinformatics databases (Gromiha, 2010) enables structure prediction which is predicated on the idea that similar sequences may result in similar structures utilizing sophisticated algorithms like machine learning and neural networks (Gromiha, 2010). To gain insights into the physics of the process, a variety of physical models capturing molecular interactions (via force fields) (MacKerell, 2004) and the development of lattice-based models (Bryngelson & Wolynes, 1987) have been used on highly parallel computers among other novel computational techniques (Dill, Ozkan, Shell, & Weikl, 2008). Despite advances in experimental and computer-based techniques, however, the PFP is still largely unresolved and has been summarized by Dill and MacCallum (2012): (i) What is the folding code? How does a 1D sequence fold into a 3D structure?, (ii) What is the mechanism and kinetics of folding? and (iii) Can a computer algorithm be used to predict it? The literature on protein-folding is vast (Dill & MacCallum, 2012; Gromiha, 2010). The PFP highlights and underscores the difficulty of simulating biological molecules.