OCTA (Open Computational Tool for Advanced Material Technology)

Masao Doi
Department of Computational Science and Engineering
Nagoya University, Nagoya, Japan

Summary: OCTA (Open Computational Tool for Advanced material technology) is an integrated simulation system for polymeric materials developed by a joint project of industry and academia supported by Japanese government. It aims at exploring the utility of mesoscale modelings developed in polymer science. OCTA consists of four simulation engines (molecular dynamics engine, rheology engine, interface engine, multi-phase engine) and a simulation platform. The system is designed to be open and extendable: all programs and source codes can be downloaded at http://octa.jp.

Keywords: modeling; rheology

1. Introduction

Understanding how material properties of polymers are related to its micro structures has been a central problem in polymer science. It is also a crucial question in the research and development in industries.

As computer is becoming a useful tool in the design of architectural, mechanical and electrical engineering, it is natural to expect a similar simulation tool for material engineering. To explore the possibility, we have conducted a joint project of academia and industries supported by the Japanese government. The objective of this project is to construct a simulation system which bridges the micro-structural (or molecular) characteristics of materials with the macroscopic characteristics of the materials. This objective is quite challenging.

The properties of polymers are not determined by the constituting monomers only: they depend on many other material characteristics, such as molecular weight, molecular weight distribution, branching structure, degree of chain orientation, degree of crystallization, and the states of the crystal-amorphous interfaces. The situation becomes even more complex in the case of polymer blends or composites where the dispersion state, and the interfaces

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between the component phases change the material property drastically. It is clear that no single simulator can handle such complex problem. The problem involves many length scales and many physics. Such problem is generally called multi-scale, multi physics problem, and is one of the major challenge in the current computational science and engineering.

Though difficult, the multi-scale modeling is a strategy we have to take in the modeling of polymeric materials. Polymeric materials involve many meso-scale structures, and theories have been developed in polymer science to deal with the dynamics of such structures. Therefore it would be useful to transform such theories in the form of computational codes, and make them available for researchers in the world. With such general aim, we have developed four simulation programs, i.e. (1) coarse-grained molecular dynamics, (2) reptation dynamics, (3) interfacial dynamics, (4) multiphase dynamics, and a simulation platform on which these engines run. We call this integrated system OCTA[1,2]. In this talk, I will describe the function of these program and some of its applications.

2. Simulation Engines

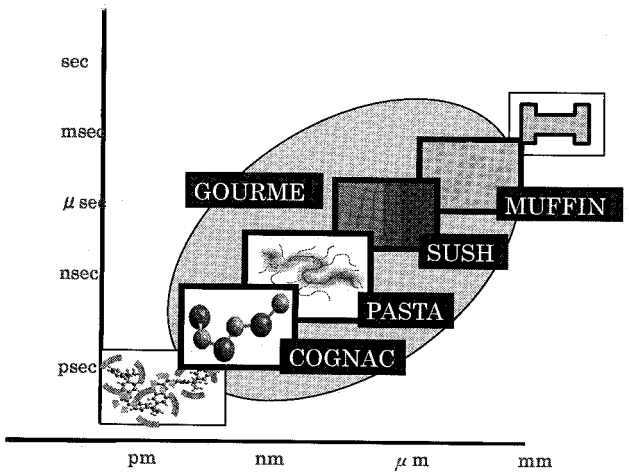
2.1 Coarse-Grained Molecular Dynamics Simulator COGNAC[3]

COGNAC is a general molecular dynamics simulation program which covers a large class of molecular models, ranging from full atomistic models to bead-spring models. Many potential functions used in coarse-grained models such as Lennard-Jones, Gay-Berne and Coulombic potentials are

available, and new potential functions can be implemented easily. COGNAC can deal with various conditions such as under constant temperature, under deformation (elongation and shear), and under external fields. COGNAC has a special function, called zooming, which is to generate the equilibrium molecular configuration for given density profile of atoms.

Examples of application

* Chain conformation of phase-separated block copolymers



* Interfacial properties of polymer blends
* Properties of semi-crystalline lamellae
* Elastic properties of network polymers
* Clay-Polymer nanocomposites
* Dynamics of confined polymer melts
* Phase transition of liquid crystals
* Ion diffusion in polyelectrolytes

2.2 Rheology Simulator PASTA[4]

PASTA is a stochastic simulation program which calculates the rheological properties of polymeric liquids of polydisperse linear and star polymers. For given molecular weight distribution, the program calculates the stress response for any history of deformation (shear and elongation). The program is based on the slip-link model, in which polymer molecules interact only through the creation and release of binary entanglements. The three important relaxation mechanisms, i.e., reptation, contour-length fluctuation and constraint

release, are taken into account.

Examples of application

* Prediction of the rheological properties
- Relaxation moduli
- Shear viscosities
- Uniaxial, biaxial and planar elongational viscosities
* Dielectric relaxation of linear type-A chain (e.g. PI)
* Self diffusion constants
* Double step shear deformations

2.3 Interface Simulator SUSHI[5]

SUSHI calculates the equilibrium and non-equilibrium structures in polymer blends and block copolymers by solving the self-consistent Edwards equation. SUSHI can deal with a variety of polymers, linear polymer, branched polymers with any topology, copolymers with any monomer sequence (block, random, tapered random) and the polymers grafted on solid surfaces. SUSHI can be used to study the surface modification caused by polymer grafting or polymer adsorption, and the self-assembly of block polymers (micellar formation).

Examples of applications

* Micro phase separation of polymer blends
* Interfacial tension of polymer blends
* Micelle and critical micelle concentration
* Polymer brush on a solid surface
* Polymer adsorption to a solid surface
* Polymer thin film on a solid surface
* Reaction-induced phase separation

2.4 Multiphase Simulator MUFFIN[6]

MUFFIN is a general solver for the continuum models for the dynamics of soft materials

based on finite difference method (FDM) or finite element method (FEM). MUFFIN includes six packages, Elastica, ElaDyna and GelDyna, Electrolyte, MEMFluid and PhaseSeparation, and can deal with various problems in soft materials, such as the elasticity of multi-phase materials, swelling and deswelling of gels, ion transport in charged colloids, reaction and diffusion in narrow channels, phase separation and droplets deformation in shear and electric field. MUFFIN can take the multi-phase structure obtained by SUSHI and can calculate various properties such as the effective elastic modulus of the system.

Examples of applications

* Phase separation of polymeric fluids under shear flow
* Spin Coating
* Electro-rheological fluid
* Electrophoresis and Electroosmosis
* Micro-reactors and micro-fluid chips
* Soft-actuators using electrolyte gels and DDS using pH-sensitive gels

3. Simulation Platform GOURMET[2]

To integrate such simulation engines each based on different physical model and requiring different input files, we have developed a simulation platform GOURMET. GOURMET provides a common graphic user interface for all engines: it is an editor of the input data, a viewer of the output data, a tool

to make graphs and animations, and most importantly a place for various engines to meet and exchange the information they have. These services are provided if the engines use a certain flexible text format (called UDF; User Definable Format).

UDF is a text file format consisting of two parts, the definition of the data structure, and the data itself. The data definition part states the name, type and unit of the data plus some additional information for the users. The UDF file can be regarded as a file in data base. All data in the UDF file are named, and can be accessed by their names. User can thus take an arbitrary part in the data file, process the information (averaging, doing fourier transform etc), and output the result into the other UDF file for the use of the other engines. The data

manipulation can be programmed by the script language Python.

GOURMET also controls running simulation programs: monitoring the output of the programs, one can stop, change parameters and restart again. Using GOURMET one can run various simulation programs with the same interface. Any simulation programs can be incorporated in the system, if it uses the input and output files written in UDF.

4. Collaborative Operation of Engines

The platform can be used as a base of operating various engines collaboratively. Such activity may be regarded as a prototype of zooming, namely going from one level of description to the other. In our project, we made several prototypes of zooming. Here I describe just an example, which is to predict the mechanical properties of block polymers. Other applications can be seen in the home page of OCTA.

Block polymers form various micro domain structures of lamellar, cylindrical, spherical and bicontinuous forms. These structures depend on many parameters such as the monomeric characteristics (the so called chi parameter, bond length, specific volume etc), the connectivity of the blocks, and the mixing ratio etc. Predicting the equilibrium structure by molecular dynamics alone is practically impossible since the ordering takes place in a extremely large time scale (ca 10^3s) compared with the characteristic time scale of molecular dynamics (ca 10^{-12}s). To overcome the difficulty, we first used the interfacial engines (SUSHI) to calculate the spatial distribution of monomer density at equilibrium. We then passed this information to COGNAC, and generated the equilibrium configuration of polymer chains. We then calculated the stress-strain curve of the block-copolymers by the molecular dynamics. We can also study the permeability of gas molecules through such structures using the function of MUFFIN.

So far, such collaborative operation has been done manually. The work may become easier with GOURMET, but one has to write certain programs (by python or C++). In future, the operations may be automated, but , at this stage we left the task to users. We did this deliberately as we believe that the "zooming" is an operation which needs deep understanding of the problem, and that much validation work needs to be done before the

operation is automated.

5. Conclusion

In the OCTA system, we purposely tried to remove any mechanism which forces engine programmers to participate in zooming. The activity of zooming is basically left to the user who uses OCTA for a particular system. The platform only provides an environment which facilitates engine programmers to make his program understandable for others, and for them to use the programs made by others. This is because we thought that the what is currently needed for our multi-scale modeling is actually a mechanism which facilitates the collaboration of many simulation programs, which essentially means the collaboration of people. We hope that OCTA will become a base for such collaboration.

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