Strategic Theme 1

SCD will build and strengthen our existing capability of providing enabling computational expertise and e-infrastructure to support STFC in fulfilling its strategic goals: "world class research, world class innovation, and world class skills."

DL_POLY/DL_FIELD/DL_ANALYSER – An Integrated Software Engine for Molecular Simulations

Computational scientists at the Daresbury Laboratory have developed and integrated a series of software packages to investigate the behaviour of materials at the atomic scale. Some materials used in food packaging, for example, are composed of miniscule particles, some as small as 1000th the width of a human hair, which may be adsorbed into food and cause major concerns for human health. Other materials, such as those used in spacecraft design, can be badly damaged by tiny meteorites and debris crashing into them as they hurtle through space. Our scientists are using molecular simulations to explore the physical and chemical behaviour of these and other materials. Their work will aid the design of new materials and provide a cost-effective method of testing before materials are widely produced.

Three separately developed software packages at Daresbury Laboratory have been integrated to form an efficient computational infrastructure to investigate a variety of phenomena at atomic scales. This is achieved by inventing a new universal notation called the DL_F Notation to describe the chemical behaviour of atoms that are essential to assign the correct values for computation and enable scientists to carry out analysis that can directly relate to the behaviour of these atoms.

Two test cases have illustrated how the software can be used to answer some important science questions. In test case 1, the effects of extremely tiny particles (with sizes down to a thousandth of the width of a human hair) on human health is a major concern, in particular, how they can stick and adsorb into biological cells. In most cases, foreign particles generally bounced off because of a protective layer of water round the cell membrane. The example illustrates how a tiny polythene particle can glide and slide, making attempts to bypass these protective layers that eventually draws it into the cell layer. In test case 2, the calculations involved smashing a stone on an aluminium surface, mimicking the damage that may be caused to a spacecraft's hull as a result of a tiny meteorite impact in space. The diagrams illustrate bits of aluminium that are ejected violently into space, creating a crater on the hull. They also illustrate such a violent event can occur without making any actual damage to the valuable spacecraft itself.

Introduction

Molecular simulations are essential computational techniques to provide information on the physical and chemical behaviour of the compound materials at atomistic details that are not readily assessable by experimental means. From such, a wealth of valuable information can be extracted to provide the predictive chemical and structural behaviour of a system model. This article will briefly describe how such integration enable users to efficiently produce quality scientific output: from model setup, to simulations and finally the results analysis by using the software packages DL_FIELD, DL_POLY and DL_ANALYSER, respectively. These packages formed part of the DL_Software [1], a collective term for the scientific software packages that are developed at Daresbury Laboratory.

DL_POLY [2] is a versatile and powerful molecular dynamics (MD) program suite that can run efficiently on a variety of computer platforms, from a single-processor PC to massively parallel supercomputers. DL_FIELD [3] is a support application tool for DL_POLY, especially in setting up complex force field models. DL_ANALYSER [4] is a robust tool to carry out post analysis work on the simulation outputs produced by DL_POLY.

DL_POLY is developed to be highly agnostic in nature, whereby it can handle molecular models of varying size and complexities: from inorganic materials such as minerals, zeolites, to complex topological structure models such as graphenes, organic cages, biomolecules and even mixed component systems such as the bio-inorganic models. In case of DL_FIELD, the philosophy behind the software development is to minimise the requirement for users to understand detail knowledge and inner workings of complicated force field descriptions and preparation procedures. It is intended to serve as a user-friendly tool that automatically processes the molecular information with minimum user intervention. On the other hand, DL_ANALYSER contains a collection of unified analysis tools that can produce results in a single read through of a collection of DL_POLY's trajectory files.

Software Integration

To ensure smooth software integration and data transitions between different packages, the standard DL_F Notation [3] is implemented within DL_FIELD. This is a universal notation scheme that standardises the expression of atom types in a molecular system, of which the atom typing procedures are essential to ensure correct setup of simulation models. The DL_F notation is to provide a common solution that harmonises the atom typing which varies wildly from one force field scheme to the other. Quite often, the conversion of one force field scheme to the other is not a trivial task. The notation removes layers of complexities involving data structure conversions and ensures smooth data transition among various force field schemes.

In addition, the notation completely describes the actual chemical identity of an atom within a molecule that can be easily interpreted by both the computational modellers as well as experimentalists. This allows correlation of both cognitive and computational assessment of the simulation results and directly relates the analysis to the actual chemistry of the test structures over a range of different force field schemes. In addition, the ease of interpreting the DL_F Notation means the DL_POLY's trajectory files can be archived for analysis using DL_ANALYSER and to be assessed by other future researchers with only a minimum training requirement.

Figure 1 illustrates the integrated workflow environment of the molecular simulation software engine. In most cases, no further programming or scripting is necessary for the data transfer between packages. For instance, the input files generated by DL_FIELD via a single-step process can be used for simulation runs in DL_POLY without further modification. The dash arrow also indicates future plans to integrate other DL_Software packages by making available to other packages the wide variety of force field schemes generated by DL_FIELD.

Below illustrates two test cases that make use of the molecular simulation software engine.

Test case 1 - study of interactions between polymer nanoparticles and cell membranes.

Nanoparticles are now widely used in areas such as food sciences, materials sciences and common household applications. An understanding of the structure of nanoparticles and the interactions with biological cell membranes is important for understanding nanotoxicological effects on human and animal health and the environment. For instance, it is known that nanoparticles can easily be ingested and adsorbed into living organisms and yet studies regarding their biocompatibility and cytotoxicity effects are still quite limited.

This test case demonstrates the use of the molecular dynamics as a complementary tool to investigate the adsorption behaviour of polymer nanoparticles on cell membranes [4]. Molecular simulation can isolate and investigate systematically specific factors that contribute to the behaviour of particle interactions with the cell membranes, and the underlying atomistic mechanisms.

The simulations were carried out using DL_POLY_4 software package. The DL_FIELD software was used to set up the molecular system, with the all-atom CHARMM36 as the force field model to describe the molecular system. All results analysis was carried out using DL_ANALYSER. The visualisation and graphical outputs were generated using VMD [5].

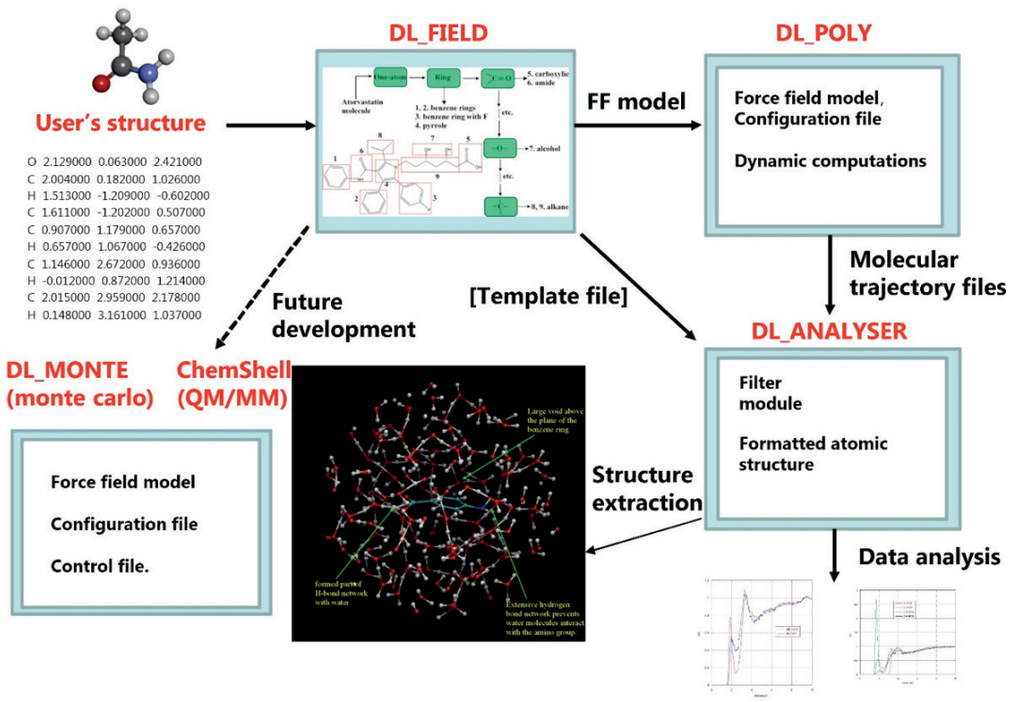

Figure 1. Diagrammatic flow chart of the integrated molecular simulation software engine. The arrows indicate the directions of the data flows.

Figure 2 illustrates the adsorption process of a polyethylene nanoparticle into the POPC biological membrane. It was found that the whole nanoparticle reoriented in such a way that the folded polymer main backbone chain aligned approximately to those of hydrocarbon chains in the membrane, while at the same time the nanoparticle chain slides and glides against each other as the particle is immersed into the membrane. Perhaps such knowledge would be crucial in nanoparticles manufacturing and fabrication by altering the chemical structure in order to prevent these interactions from occurring.

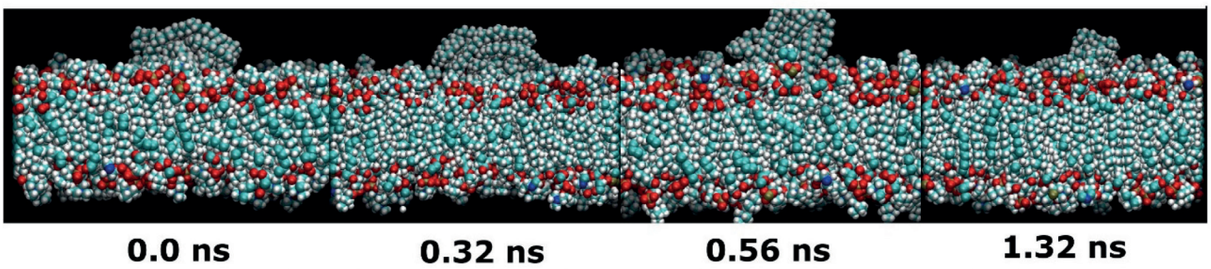

Figure 2. Four movie snapshots of the molecular configurations of polyethylene nanoparticle adsorption on the POPC membrane surface that illustrates the process of particle insertion into the membrane.

Test case 2 – Energetic nanocluster impact on metal surfaces.

We are interested in the damage and corrosion mechanism of surface materials due to orbital debris and micro-meteoritic bombardment in space. The extreme environment of interplanetary space provides an ultimate testing ground to the performance and endurance of materials that are used to construct satellites and space crafts. The particle debris can achieve an impact velocity in the order of 10 km/s. Such collision can cause permanent damage and degrade the material performances in terms of structure and chemical and mechanical behaviour. Testing materials on Earth present a challenge in recreating the appropriate conditions of outer space, as it is very difficult for experiments to capture the dynamics of these highly transient events at atomic scales.

In this test case, an aluminium (Al) surface was bombarded by a magnesium oxide (MgO) nanoparticle with an impact velocity corresponds to 1 keV. Aluminium is the most common construction material in the space industry. MgO represents a typical 'stony' meteorite material that is largely consisted of some mineral oxides and silicates.

The model consists of an Al surface that was large enough to contain the energetic event (in the order of several 105 atoms). A custom-made force field was constructed (Morse splined with Moliere potentials) for the interactions between the metal surface and the meteorite and tabulated in DL_POLY. The large-size trajectory files that subsequently produced were analysed using DL_ANALYSER.

Figure 3 illustrates the sequence of the transient impact process, which occurred in the sub-picosecond time frame. The time = 0.0 ps marked the beginning of the impacting process. During the process at time = 0.23 ps to 2.58 ps after impact, a large amount of energy was imparted into a small area of the surface, which subsequently caused the impact area to implode, while those atoms near to the surface were ejected violently into space as sputtered species. At the final time = 32.0 ps after impact, the surface was eventually cooled as the energy was dissipated to the bulk. Partial healing to the Al surface was also evident with some of the Al atoms re-deposited and solidified as adatoms on the surface. The projectile was also fragmented and embedded near to the impact crater.

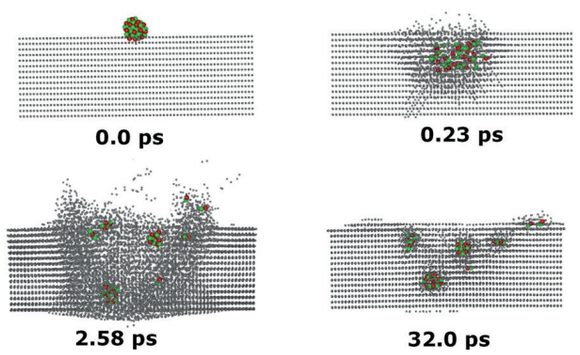

Figure 3. Four movie snapshots of the lateral views of the system configuration. The projectiles have been exaggerated as green and red spheres, representing the magnesium and oxide ions respectively. For clarity purposes, only a small section of the model is shown. The reference time = 0.0 ps indicates the moment when the particle comes into contact with the surface.

Fig. 4 shows the centre of mass velocity component along y-direction (perpendicular to the surface orientation), for the atoms located in the respective Regions as a function of time. The Regions are alphabetically labelled from A to E, as shown in Fig. 4 on the right, which are defined by a series of hemispheres each with the center O, which is the point of impact. Larger spheres are successively drawn out, each with an increase of the radius by a value Ri. Negative velocity component means the average Al atoms in a given region are moving into the surface, whereas positive velocity component means they are moving away from the surface. It can be seen that the successive peaks labelled from B to E reveal the nature of the energy deposition as the energy front travels from one Region into another. The magnitude of the peaks become smaller as the energy is deposited to a greater number of Al atoms. The initial speed of propagation was estimated to be 9000 ms_{-1} and reduced to 6500 ms_{-1} at region E. Assuming the speed of sound in Al is 6400 ms_{-1}, this means that shock waves were generated during the energy propagation.

Conclusions

This article highlights the capabilities of the molecular simulation software engine developed at Daresbury Laboratory by making references to two test cases that are very different in nature. The first test case refers to the complex biological systems specifically in the areas of nanotoxicology, while the second test case refers to the large system models that are relevant to the areas of materials science. The article also illustrates how a variety of system models can be efficiently investigated to produce scientific results in a cost effective way.

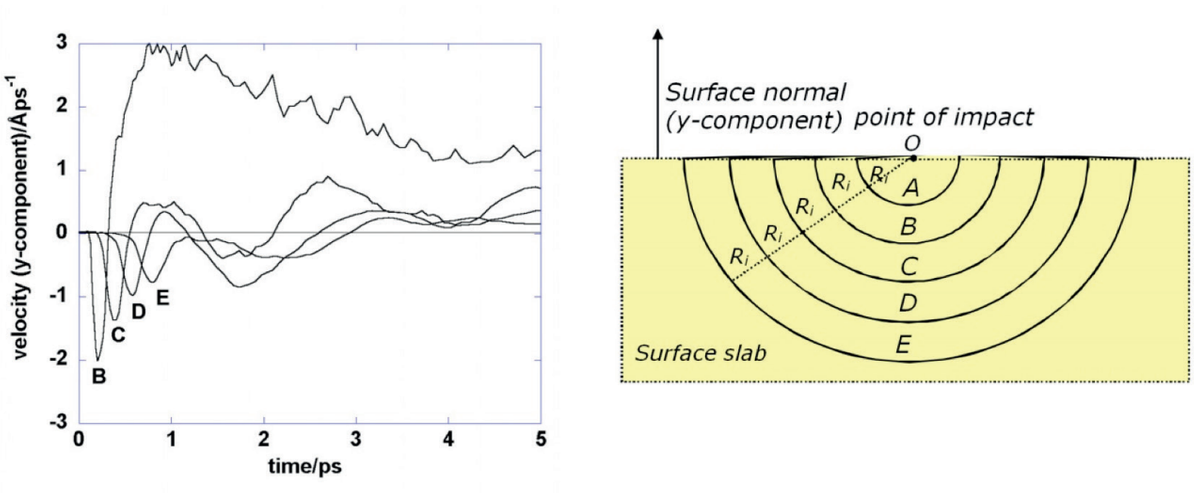

Figure 4. Centre of mass velocity along y-component as a function of time. Each profile corresponds to the velocity component in different Regions as marked by the alphabets. Profiles for Region A are omitted for clarity purposes.

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References

[1] DL_Software is the collective term for a range of scientific software suites developed at the Computational Chemistry Group at Daresbury Laboratory, spanning across multi-length and time scales, from quantum mechanics to mesoscopic scales. (http://www.ccp5.ac.uk/software).
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