Parallel Molecular Dynamics Simulation of Commercial Surfactants

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Extended Abstract

The Parallel Applications Centre has been working in collaboration with Unilever Research in Port Sunlight and the University of Southampton Department of Chemistry to develop a set of tools which will enable a chemist to investigate the properties of surfactant layers using the molecular dynamics simulation technique. Surfactant layers are commonly encountered in consumer chemical products such as fabric softeners, detergents, etc., in which Unilever has a strong commercial interest. At present, active ingredients for such products are developed by synthesizing and testing molecules from a very large class of candidates whose properties are only broadly understood. Success as a fabric softener (say) is difficult to quantify, so the test procedures often involve collecting subjective opinions directly from consumers, an expensive and time consuming process.

The immediate objective of the project is to support research into the detailed properties of surfactant molecules, refining the requirements for candidate molecules. A longer term objective is to use molecular dynamics simulation to screen molecules prior to synthesis, reducing the amount of consumer testing required in product development.

The systems of interest are not simple. Typical products consist of mixtures of surfactants, electrolytes, other active ingredients and water. They often act at poorly characterised interfaces such as fabrics and cell membranes. Modelling such systems requires the handling of charged particles and flexible long chain molecules. The properties and simulation conditions of interest require new algorithm development and combinations of techniques never applied before. Finally, extraction of bulk properties requires the simulation of relatively long intervals of around 1 nanosecond. Since each simulation time-step represents a few femtoseconds, it is necessary to run the simulation for least 105 to 106 steps, making this an industrial ‘Grand Challenge’ problem. Only parallel computing can provide the performance required to solve these problems in sufficient detail within reasonable timescales.

As an initial task the collaboration is directed towards the simulation of a cationic surfactant. The approach taken is to develop a code which will simulate the target molecule and a range of related molecules. The target molecule is
dimethyl-distearyl ammonium chloride. The molecule consists of a nitrogen atom bonded to two methyl and two 18 unit hydrocarbon chains. The nitrogen is positively charged and consequently requires a counter ion which in the case of this simulation is a chloride ion. In order to perform molecular dynamics a potential model must be formulated which models the atomic interactions within and between the molecules. The potential model used allows for bending of bond angles and rotation of groups about bonds, for repulsion-dispersion between unconnected atoms, and for electrostatic interactions between charged atoms.

As a starting configuration the molecules are ordered in a monolayer or bilayer in the xy plane with periodic boundary conditions applied in the x and y coordinate directions. The z-direction is bounded by the cotton surface, which is represented using a surface potential. Each unit cell contains typically 64 to 256 molecules. At present, all runs (including test runs) are allowed to proceed for 100,000 equilibration steps (in which the temperature is held constant), and then for 100,000 'production' steps at constant energy. Trajectory files are created during this latter stage which form the basis for subsequent analysis of bulk properties. The configuration set up and subsequent analysis operations use codes which have been integrated into the Biosym package, with which the users of the code are already familiar.

All the simulation code is original to the collaboration. A major objective is portability between as wide a range of machines and architectures as possible. To enable this a modular approach has been taken, in which dependencies on particular machines are restricted to a small number of routines. By combining this approach with adherence to the FORTRAN 77 standard (plus limited use of common extensions), a highly portable code has been produced. The code can be ported between different parallel systems by modifying the architecture-dependent routines only. This has allowed the code to be run successfully on the Intel iPSC/860 machine (under the NX/2 parallel operating system), an IBM SP1 machine, on workstation clusters under PVM, and on serial machines. The core computational routines have been designed for efficient execution on vector machines, so the code should perform well on traditional vector supercomputers, although this has not yet been necessary.

While deciding on the parallel implementation most appropriate for our purposes, an important consideration was that connectivity information is required during the calculation of the potentials. We believed that this was significant enough to dictate that any parallel decomposition of the data structure should not break up individual molecules. The system sizes that can reasonably be simulated with currently available computing power are small enough for an individual molecule to extend over a significant proportion of the simulation domain. The standard geometric decomposition approach would therefore have split individual molecules between processors. This fact, along with the problem of handing the long range electrostatic interactions, led us to seek an alternative parallel approach.

A more straightforward 'brute-force' parallelisation of the code was eventu-