A Case Study of the Application of COTS Components in a Molecular Dynamics Software

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Abstract—Commercial Off-The-Shelf (COTS) components are widely used in many software industries and also in scientific computing. This paper first considers the definition of the term COTS and then tries to explore how it typically manifests itself in a software used for Molecular dynamical calculations. Some details regarding a popular software used for such calculations, viz., GROMACS are furnished. Since this is a freely downloadable program and a non-commercial one, it is better to consider this as an example of Scientific Off –The-Shelf (SOTS) components, a newly coined acronym.

Index Terms—COTS, GROMACS software, molecular dynamics, SOTS.

I. INTRODUCTION

COTS components are defined as “*components which are bought from third party vendors and integrated into the system*”. However, a more detailed and expanded view of COTS components should be taken. A COTS component could be as small as a routine that computes the square root of a number or as large as a credit card validation software. The important thing is that a COTS component already exists and was created by people outside the software development organization that will actually use it.

A commercial off-the-shelf component can therefore be defined as, “any software component that already exists, that was created by people outside the organization that will be using it, and that was purchased from a third party vendor” [1].

The above definition leads to the following conclusions [1]:

- 1) The source code can never be made available to the component user, unlike an in-house component. A COTS component is like a black box. The user can view the component only through its interfaces and outputs.
- 2) There are possibilities that a complete description of the component’s behavior may not be given by the vendor to the user. This may result in problems during component integration.
- 3) Maintenance can become an issue because the vendor

may not correct defects or add enhancements according to the component’s specification.

- 4) Sometimes the vendors can provide updated components that do not integrate with the earlier version of the application.

Component-based development offers several focus of reuse. Some common sources from where one can acquire components are:

- 1) External component libraries
- 2) Commercial off-the-shelf (COTS) components
- 3) Open source software (OSS) components
- 4) In-house component infrastructure
- 5) Mining components from legacy systems

Almost without exception, every software-related endeavour will utilize a significant percentage of COTS software components. The application of COTS components in crystallographic softwares was evaluated by us earlier [2], [3]. In another contribution, the case of the mathematical software viz., SCILAB was taken up as a case study [4]. In this paper, the case of a molecular dynamics software is taken up for detailed study. Since the program package to be discussed in the following sections is freely downloadable from websites and a non-commercial one, it is better to consider this as an example of **Scientific Off-The-Shelf (SOTS)** components, a newly coined acronym.

II. ENERGY MINIMIZATION

In computational chemistry or physics, energy minimization (also called energy optimization or geometry optimization) methods are used to compute the equilibrium configuration of molecules and solids. Starting from a non-equilibrium molecular geometry, energy minimization employs the mathematical procedure of optimization to move atoms so as to reduce the net forces on the atoms until they become negligible. A well established algorithm of energy minimization can be an efficient tool for molecular structure optimization.

The algorithms of gradient are the most popular methods for energy minimization. The basic idea of gradient methods is to move atoms by the total net forces acting on them. The force on atoms is calculated as the negative gradient of total potential energy of the system. An analytical formula of the gradient potential energy is preferentially required by the gradient methods. If not, one needs to calculate numerically the derivatives of the energy function from the potential. Fig. 1 shows the schematics of the algorithm used [5].

Molecular modeling methods are now routinely used to investigate the structure, dynamics, surface properties and thermodynamics of inorganic, biological and polymeric

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systems. The types of biological activities that have been investigated using molecular modeling include protein folding, enzyme catalysis, protein stability, conformational changes associated with bio-molecular function and molecular recognition of proteins, DNA and membrane complexes.

Fig. 1. Schematics of a computational self consistent energy minimization procedure.

III. SOFTWARES FOR MOLECULAR MODELING

There are numerous software packages for the above calculations in molecular dynamics. Some of the popular packages are AMBER, Auto Dock, CHARMM, VASP, GAUSSIAN, GROMACS, Materials Studio, Sirius, etc. In the following sections, some of the features of the software: GROMACS [5] are discussed.

A. The GROMACS Software

GROMACS (Groningen Machine for Chemical Simulations) is a molecular dynamics simulation package originally developed in the University of Groningen. It is written in C, C++ and Assembly languages and may be used in Solaris, Linux, MacOS X, Windows and Unix operating systems.

- 1) GROMACS is an engine to perform molecular dynamics simulations and energy minimization.
- 2) A high performance Molecular Dynamics Program.
- 3) It is reasonably well optimized for low memory usage.
- 4) The highly optimized code makes GROMACS the fastest program for molecular simulations.
- 5) The support of different force fields and the open source (GPL) character make GROMACS very flexible.
- 6) It is a high performance research tool which can be run on almost every platform.
- 7) This program is a free software; it can be redistributed.

IV. COMPUTATIONS INVOLVED

Several steps of energy minimization may be necessary, which consist of the following cycles of computations.

Generating topologies and coordinates, running a simulation, converting pdb files to topology and coordinate files, generating a primitive topology from coordinates, editing the box and writing subgroups, solvating a system, generating mono atomic ions on energetically favorable positions, multiplying a conformation in 'random' orientations, generating position restraints or distance restraints for index groups, protonating structures, making a run input file, making a run input file for restarting a crashed run and performing a simulation.

From the details given in the above paragraph, it is easy to understand that one has to go through several computations, step by step to arrive at the minimum energy structure of the molecule, using the data available. Suitable computer programs have been written and are available for the different steps of the calculations, stated above. The modern software package such as GROMACS incorporates all the above programs in a unique way and helps the scientists in arriving at the minimum energy configuration of the molecules. No one knows the details of the programs used in the above packages and they remain black boxes, but help the scientists!

V. CONCLUSIONS

One could easily visualize the usage of (Non) Commercial Off-The-Shelf (COTS) technology in the above example. The modern packages are very versatile in their functioning and the quality is not compromised in utilizing the above software package. Hence, the above example could be considered as a positive usage of COTS components, in designing a software package for the usage of a group of scientists. Since the program package discussed above is freely downloadable from websites and a non-commercial one, it will be more appropriate to consider this as an example of **Scientific Off-The-Shelf (SOTS)** components, an acronym coined by us.

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