

An Introduction to Classical Molecular Dynamics Simulation for Experimental Scattering Users

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Classical molecular dynamics simulations are a common component of multi-modal analyses from scattering measurements, such as small-angle scattering and diffraction. Users of these techniques often have no formal training in the theory and practice of molecular dynamics simulation, leading to the possibility of these being treated as a “black box” analysis technique. This work discusses an open educational resource designed to introduce classical molecular dynamics to users of scattering methods. [SAY SOMETHING ABOUT WHAT THIS RESOURCE IS / HOW “STUDENTS” USE IT?] We present a general introduction to topics including TODO. We then discuss typical sources of error in classical molecular dynamics simulations, before considering some of the approaches to using simulations in the analysis of scattering data.

I. INTRODUCTION

The use of molecular dynamics simulations to help analyse experimental data, particularly from small-angle scattering and diffraction, has grown significantly over the past ten years [1–8]. Figure I shows the percentage of small-angle scattering publications that mention molecular dynamics in recent years, reaching more than 20 % of small-angle scattering articles published in 2018.

Users of scattering and diffraction techniques often have backgrounds in experimental science, with little or no formal training in the theory or practice of computational modelling. This can lead to molecular dynamics simulations being used as a “black box”, with little understanding of the underlying methodologies, or consideration of possible sources of erroneous results. The use of molecular simulations without at least some understanding of the techniques can lead to the unintended inclusion of severe, systematic errors. The challenge of enabling researchers to use molecular dynamics simulation in their analysis of scattering data, while reducing this risk of modelling errors, has led to the development of software tools, such as WAXSiS and SASSIE,[9–11], that present easy-to-use interfaces [INTERFACES FOR WHAT?].

A complementary strategy to help avoid researchers inadvertently using erroneous simulation results is targeted educational resources and activities, such as lectures or workshops that introduce molecular simulation to audiences of scattering and diffraction users. One example is the annual ISIS Neutron Training Course, which includes a module entitled “An Introduction to Molecu-

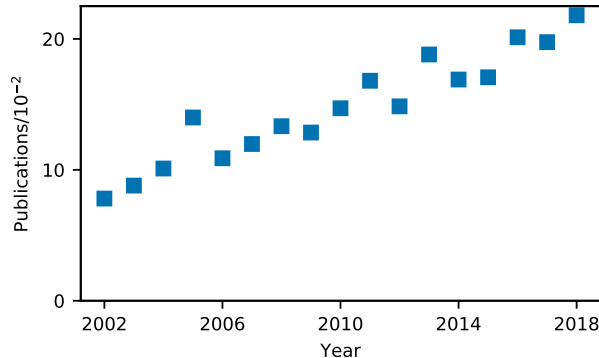


FIG. 1. The annual percentage of publications that mention “small angle scattering” that also mention “molecular dynamics”, determined from the numbers of matching Google Scholar results. [Personal quibbles: the colour is unnecessary here / Squares are uglier than filled circles]

lar Dynamics for Neutron Scattering”. [CITATION?] This covers the fundamentals of classical molecular dynamics simulation, before presenting applications of these methods in neutron science, and allowing students to gain practical experience with the SASSIE software package [11]. Lectures and workshops are certainly an important training approach, but often can be inconvenient or impractical for all interested students to attend, limiting their accessibility.

There has been a recent movement within the scientific and engineering communities towards technology-enhanced open educational resources (OERs). These are courses, lectures, or learning resources that are made freely available online for use by anyone. This allows the permission for others to engage in the “5R activities”: Retain, Reuse, Revise, Remix, and Redistribute [12].

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The act of publishing an OER increases the reach of a particular resource as it allows others to pick it up, modify it, and use the modified version in their own teaching. The availability of the Jupyter Notebook framework [13] has facilitated the availability of OERs by improving the ability for students to interact directly with the resource often, but not always, using the Python programming language [14].

Herein, we present an online, open-source, interactive learning resource aimed to introduce members of the scattering and diffraction community to molecular dynamics simulations. This open educational resource comprises of six lessons, covering classical methods, introducing molecular dynamics, and showing how this method may interact with scattering in a multi-modal fashion. We leverage the open-source Python library pylj [15] to give a visual and programmatic representation of the interactions between these two techniques. In this paper we will discuss the implementation of the resource and detail how the student may get the most from the resource (in this work *the student* refers to anyone working through the OER, regardless of career position).

II. ASSUMED PRIOR KNOWLEDGE

The OER, entitled “*The interaction between simulation and scattering*” makes use of the Python programming language, this allows for interactive examples of the mathematical and algorithm content to be included. A result of this is that to be able to fully utilise the resource some knowledge of, or willingness to learn, Python is required. However, we have attempted to develop the resource in such a fashion that an in depth knowledge of Python is not required. It is anticipated that the users of this resource would have some familiarity with undergraduate level chemistry or physics, alongside a commensurate understanding of mathematics. This is particularly important when considering the nature, and chemical rationale, of classical interaction potentials.

III. RESOURCE CONSTRUCTION

The resource is currently available online, at http://pythoninchemistry.org/sim_and_scatt. These web-pages were written as a series of Jupyter Notebooks and Markdown files, which were then compiled using the `jupyter-book` tool [16]. This system allows Python code blocks to be included alongside the textual content, providing algorithmic details whilst also facilitating interactivity, though both Thebelab and BinderHub integrations [17–19]. Interacting with the resource in this fashion will allow the student to either run the Python code directly in the resource interface (Thebelab), or easily launch a MyBinder window to more intensive visualisations (such as pylj). [I feel at some point this could mention “literate programming” as a concept [20]]

The resource is provided under a CC-BY-SA-4.0 license [21], and builds on the growing library of open educational resources. The open-source nature of this license means that anyone may use the material to enhance their own educational platform and experts in the field may contribute to improve the resource. The source code for the resource is available at https://github.com/pythoninchemistry/sim_and_scatt.

IV. RESOURCE OUTLINE

The resource follows a simple outline to introduce important aspects of molecular dynamics simulations. Code blocks are used to gradually build up the student’s understanding of the various concepts.

A. Home

The welcome page, introduces the resource and gives the student information about how the resource may be used, including details of Thebelab and BinderHub integration. Furthermore, this page gives information about the use and sharing of the content of the resource including details of the license. This page also includes an authors and contributors list.

B. Classical methods

Following the introduction, concepts relating broadly to classical simulation methods are introduced. This includes the functional nature of potential modelling and gives some examples, such as the Lennard-Jones and Buckingham potential models [22, 23]. Potential model parameterisation is briefly covered including the use of higher accuracy quantum mechanical calculations to do so. The presence of off-the-shelf, general potential models are discussed; with particular attention paid to the caveat that they may still require system specific optimisations. Finally, we mention mixing, or combination, rules; again discussing the possible problems that a user may encounter related to system specificity.

C. Molecular dynamics

Building on the classical potential model methods the student is then presented with molecular dynamics. This is shown by using different aspects for the method to gradually build up a one-dimensional molecular dynamics simulation using NVE (Number, Volume and Energy) ensembles, the Velocity-Verlet algorithm and the Lennard-Jones potential model [22, 24]. This is introduced in terms of Newton’s laws of motion and the generalised equations of motion, which should be familiar to most students. Finally, different importance considerations for

molecular dynamics simulations are described including ensembles, the potential cut-off, and periodic boundary conditions.

D. pylj and the interaction with scattering

The final aspect of the resource is to utilise a molecular dynamics simulation to understand some scattering profiles. This is achieved using the open-source pylj package [15], which allows for a two-dimensional simulation or argon particles, interacting through a Lennard-Jones potential, to be performed. The student is firstly shown a working pylj simulation and invited to interact with the simulation and the custom plotting functionality of pylj. In the final lessons, a formulation of the Debye equation [25] is given and the student is invited to observe the effect of simulation temperature on the resulting scattering profile. There is mention of other, faster, algorithms for the determination of scattering profiles, such as the Fibonacci sequence or Golden Vectors methods [26, 27].

V. FUTURE OUTLOOK

In future, we hope that the nature of the material, as an OER, will promote interest from other parties towards reuse, and remixing the material. Furthermore, we hope to implement this material within training at the ISIS Neutron and Muon Source as well as Diamond Light Source. Finally, it is hoped, *via* student and community feedback, that the improvement of implementation, materials, and general pedagogy of the resource can be achieved, driving up the quality and depth of molecular dynamics analyses performed on results obtained from scattering and diffraction measurements.

VI. AUTHOR CONTRIBUTIONS

The open education resource was developed, and the manuscript written, by A. R. M. with input from all authors.

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