Project Year
2014-2015

Project Title
Development of a Comprehensive Online Resource for Training in Molecular Dynamics Simulations

Project Team
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Audience
The purpose of this project is to create a comprehensive electronic resource to train both students and professional researchers in molecular dynamics simulations. The resource will be applicable to undergraduate and graduate students, experimental and medical scientists, and anyone else interested in adding molecular simulations to their portfolio of research techniques. In particular, this resource will allow students to judge if simulation techniques are suited for their future careers and to enable them to utilize simulations as part of their research projects. The resource will be piloted in the Fall *Biomaterials Laboratory* (510.430).

Pedagogical Issue
Computer simulation of biological systems is a rapidly expanding field. Due to continuing growth in computer-hardware performance and methodological developments molecular dynamics techniques have advanced greatly in the past few years and now represent a powerful tool to complement experimental approaches. While many areas of molecular biology and nanotechnology are now within the reach of this method, setting up and running molecular simulations remains an intimidating and frustrating experience, even for seasoned scientists. This is due to the inherent complexities associated with amalgamating the relevant knowledge from the wide range of different disciplines that the method entails. Furthermore, although there is growing student interest in these methods, no training material on molecular dynamics or related simulation techniques currently exists in the Johns Hopkins University curriculum.

Solution
The resource propose will consist of an easy to understand summary of the all necessary background material required to fully understand all aspects of molecular simulations, starting with basic computer knowhow, then summarizing the mathematics, physics, chemistry, and computer science that underpin the molecular simulation technique, and finishing by providing practical guidance to enable students to set up and run their own simulations. The resource will be structured as a fully online course, focusing on timed practical exercises, and supported by clear and succinct summaries of relevant background information in the form of video podcasts and downloadable PDFs.

The resource will be developed by the student over the summer and tested on the Materials Science Department's Biomaterials Lab course to obtain feedback and spot potential for improvement. After successful implementation the resource will be hosted on a web-server for public access.

Assessment Strategy

The impact of the resource will be assessed via tracking how the various components of the resource are utilized and assessing the overall understanding through in-built quizzes. These features, which are available on teaching platforms such as Blackboard, allow for continuing improvement of the course material. After initial completion of the resource it will be tested as part of the Materials Science and Engineering Biomaterials laboratory class. For this purpose we will design a particular spreadsheet with questions for students to answer. Key questions to assess are whether all background knowledge has been provided, if this information has been presented lucidly, if practical projects are timed well, and finally if the choice of sample projects is suitably interesting for students to use the tool in teaching themselves.

The wider impact on training in the field of molecular simulation is more difficult to assess. However, given the growing interested in this technique, which was the recipient of three Nobel prizes in 2013, we are confident that it will be highly useful for Johns Hopkins, especially for the Engineering and Medical Schools.

Faculty Statement

Understanding molecular simulations requires knowledge of a range of scientific fields. The aim of the resource is to provide a thorough understanding of the complex interplay between the laws of physics, their algorithmic implementation, and the chemical parameterization of biological systems that are at the core of molecular simulations.

In order to maximize the impact of the resource and encourage students to learn, we will develop a website that collates necessary background information required to understand molecular simulation and to apply these simulations to study biological systems. Podcasts and interactive content will summarize relevant topics from physics, chemistry, biology, algorithm design, and computer science, while worked examples will allow students to apply simulations to a number of biological systems. The resource will be designed as a step-by-step, self-taught course with interactive content and quizzes that allow both the student and the instructor to assess progress.

I have recently developed a two-day practical class that teaches undergraduate students to use a simulation software to fold small proteins. This class was supervised by Hayden Fennell and was very well received. Expanding this class to a self-contained teaching resource will not only improve knowledge transfer to students, but allow researchers in experimental groups to train in computational techniques.

At present the lack of suitable training tools, which allow experimental researchers to assess the utility of computational techniques for their research, is impeding cross-disciplinary collaboration. The proposed project will address this by developing an electronic teaching resource in a field of growing interest. To my knowledge, no such resource currently exists at Johns Hopkins, and related resources at other Universities are too broad in scope and complexity to be useful.

The technology fellow will develop the online learning tool, the key content of which has already been developed and tested in the classroom. The fellow will adapt this content into a comprehensive online resource, using his knowledge of web-based programming, development of interactive multi-media content, and scientific writing. The benefit of this system is that once developed it allows rapid and inexpensive training of students in simulation techniques.

Together with the fellow, I will design the overall resource layout and sketch out the individual tasks required for completion of the project (i.e., website development, collation and summarizing of the background material, podcasts, interactive content, etc.). The completed resource will be tested in the Fall *Biomaterials Laboratory* (510.430). This will allow us to assess if the project has been successfully implemented and obtain feedback on future improvements of the resource, which will be hosted and maintained as a public resource on my laboratory server. This will benefit all departments interested in adding bio-simulation to their portfolio of techniques (e.g. Medical School, Biomedical Engineering, Chemical Engineering, and Materials Science), by allowing rapid training of their undergraduate or graduate students.