

## Introduction to Volume 3 Issue 2

Steven I. Gordon  
Editor  
Ohio Supercomputer Center  
Columbus, OH  
sgordon@osc.edu

### Forward

This issue of JOCSE provides a diverse set of approaches to computational science education along with several very sophisticated student projects. Kim *et al* describe a comprehensive framework for learning about sustainable design through a series of steps to design a bicycle pedal and to evaluate the impacts of production on several sustainability measures. They have developed a Sustainable Product Development Collaboratory that allows students to make changes in the product design and to then see its impacts on energy use and the carbon footprint of the production process.

Gadepally et al use a combination of an analogous physical system and simulation environment to demonstrate the principles of building autonomous vehicles. Students in a summer workshop use a programmable Roomba and program it to avoid obstacles on a physical course setup to represent city streets. This is augmented by a related simulation environment where various commands can be tested. In that process, they learn the mathematical concepts, programming tools, and modeling processes that are used by engineers creating and testing such systems.

Toth and Franco present a virtual lab focused on the screening of drugs as part of a medicinal chemistry course. Students are introduced to the process of screening drugs using a supercomputer program to identify inhibitors for a number of diseases. Students used a typical workflow that included identifying a protein that has been found to be a good drug target, discovering whether its 3D structure has been solved, using a docking program to screen potential compounds, and generating a visualization of the final docking results.

The student papers in this issue demonstrate the diverse skills that students have acquired through internship experiences. Those include the generation of metadata that allows annotation of scientific datasets, the porting and testing of a parallel version of a computational chemistry code, and test-

ing the speedup of codes using GPUs. Each of those projects has made a significant impact on the academic careers and future career goals of the participating students.

We hope the issue provides insights that you can use in your classrooms. Make sure you also encourage others to start reading and contributing to JOCSE so that we broadly share our experiences in computational science education.