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Tangible visualization of molecular dynamics simulations using 3-D printing

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ABSTRACT

Molecular dynamics (MD) simulations are vital tools in modern research as they can provide molecular and atomic level insights into macroscopic behaviors of organic, inorganic, biological and hybrid materials. The analytical process of translating structural coordinates into a complex 3-D structure can be a challenging and engaging computational exercise for students. Here, we describe a detailed methodology for transforming the outputs of MD simulations into tangible forms through the use of dual-extrusion 3-D printing on a commercially available 3-D printer that we operate in our laboratory. Additionally, the printed 3-D structures can provide unique educational opportunities outside of traditional lecture halls and away from computer workstations environments as they provide a tangible representation of data when a digital copy is unavailable or inconvenient to share. We believe that 3-D printing can become a valuable complementary technique with MD and other forms of simulations in the chemical sciences. 3-D printers truly can be used to make just about anything, and this manuscript provides just one example of how this emerging technology can be applied within chemical engineering. As more chemical engineering educators become familiar with 3-D printing, we foresee a number of educational and applied uses including printing of highly complex patterned/porous surfaces, custom laboratory parts/equipment and even functional unit operations.

1. Introduction

Molecular dynamics (MD) simulations are growing ever more important in many diverse research fields, ranging from pharmaceuticals to electrochemical systems. Over the last 10–20 years, there has been rapid development and adoption of high-quality software packages for performing MD simulations, and this helps lower some of the programming barriers for novice researchers. Also, this software development allows for more thorough benchmarking and code optimization within the community of experts. In tandem with the core simulation software development, there have been equally impressive developments related to user-interfaces, educational and training resources, and visualization. An excellent combination of these aspects is highlighted with the Etomica project at The University of Buffalo (Etomica, 2014). It provides an intuitive, user-interface for performing a range of different molecular-level simulations, coupled with a real-time visualization of the system, and it is accompanied by a variety of problem sets for both undergraduate and graduate-level students. We have regularly used the Etomica modules in our graduate-level thermodynamics course at The University of Alabama.

For the past several years, 3-D printing has been a topic of increasing interest to the general public (Anonymous, 2011), underscored by President Obama's remarks about the

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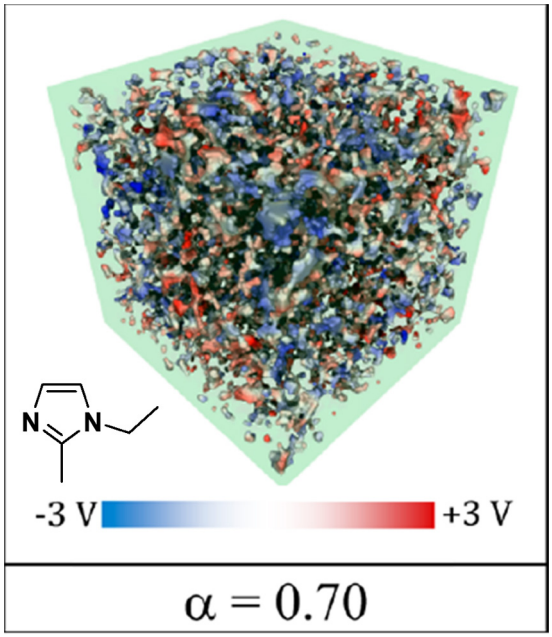

Fig. 1 – MD simulation of the free volume space within 1-ethyl-2-methylimidazole used as a basis for both theoretical evaluations of solvent thermophysical properties and for 3-D printing.

potential of 3-D printing to *"change the way we make almost everything"* during his 2013 State of the Union Address (Obama, 2013). However, this "Third Industrial Revolution" (Anonymous, 2012) has not been without controversy as firearms produced via 3-D printing have already been successfully discharged (Sperry, 2013; Vella, 2013).

While there is very strong online presence of 3-D printing enthusiasts sharing files and experience through repositories such as Thingiverse (Makerbot Industries), there is only a small, but growing, number of publications in the literature discussing the research and education impacts of 3-D printing focused on topics in chemical sciences and engineering. (Anderson et al., 2013; Balowski et al., 2013; Dragone et al., 2013; Gross et al., 2014; Kitson et al., 2012; Kitson et al., 2013; Ladd et al., 2013; Scalfani and Vaid, 2014; Sun et al., 2013; Symes et al., 2012) Chemical & Engineering News recently highlighted the interest among chemical research groups in using 3-D printing as a tool to save money by printing certain lab supplies at a fraction of the catalog cost (Wolf, 2013).

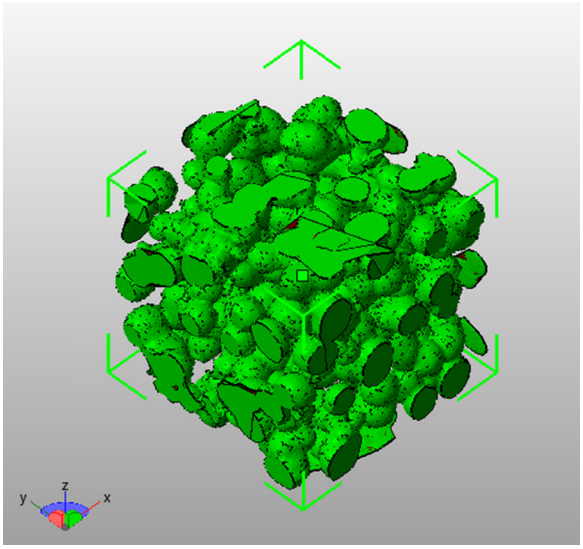

Fig. 2 – Model of free volume within 1-methyl-2-ethylimidazole obtained by MD simulation as shown in Netfabb.

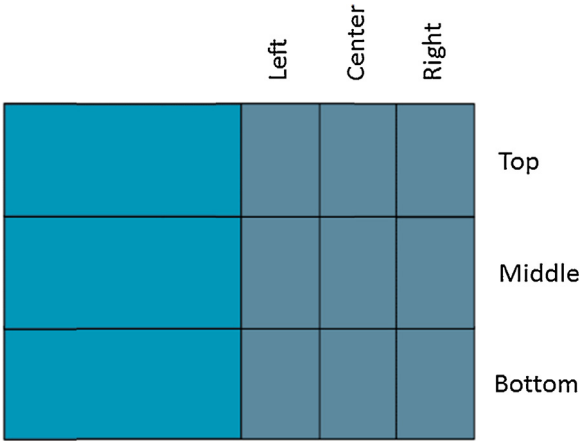

Fig. 3 – Schematic of cutting pattern applied in Netfabb to the MD simulation output .stl file.

Bara's group recently published on the opportunities and challenges of using 3-D printing coupled with computer-aided design (CAD) and computational fluid dynamics (CFD) as a powerful design and manufacturing process by which chemical process unit operations (e.g. mass transfer devices) could be designed, studied, tested and optimized in a rapid, versatile and almost entirely digital feedback loop (Bara et al., 2013). Here, we extend our experience with 3-D printing to discuss an endeavor in which we employ 3-D printing to fabricate tangible visualizations of MD simulations and share our methodologies in detail so that others can adopt this technique. From our experiences, when students see 3-D printed models in our offices or labs, it generates an immediate interest and typically prompts a discussion regarding research or chemical engineering concepts that may not have otherwise occurred. Furthermore, 3-D printed objects serve as excellent visual aids at poster sessions, on a walk across campus, etc.

With the advent of "off the shelf" 3-D printers that are about the same physical size as a household microwave oven (Pepitone, 2013), we now have the ability to transform many of our molecular models into tangible structures, and this opens the door for new forms of communication and education. In many cases, it is challenging to describe or explain the

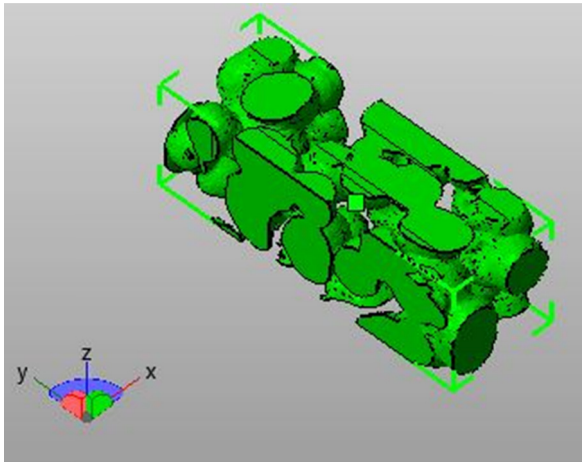

Fig. 4 – Example of one of the nine parts cut from the full model in Fig. 2.