An Interactive Polymer Building Toolkit for Molecular Dynamics Simulations: PolyMAPS

Xiaoli Yan, Santanu Chaudhuri

Abstract

PolyMAPS is an open-source library that helps researchers to initialize LAMMPS[1] molecular dynamics simulations. It introduces an integrated workflow by combining preparation, launching, visualization, and analysis into a single Jupyter[2] notebook. PolyMAPS enables users to build small or polymeric molecules in a user-friendly interactive 3D plotting system that supports reading and writing systems in LAMMPS data file format. Hence, PolyMAPS demonstrates the potential of reducing the learning difficulties of new users of the LAMMPS software.

1. Introduction

Many open-source preprocessing tools are developed for molecular dynamics (MD) simulations for simulation software such as LAMMPS, GROMACS[3], CP2K[4], etc. Analysis and building tools, such as Moltemplate[5], Packmol[6], VMD[7], EMC[8], OVITO[9], Avogadro[10], etc., are mostly designed by experienced scientists who are very familiar with simulation workflow. These are all excellent software packages that specialize in their own domains, and they are made freely available to the scientific community by diligent scientists and engineers. However, a reasonably complex simulation system is usually built, simulated, and analyzed by multiple different pieces of open-source software that require various styles of user interface and experience. Commercial software packages with pre-designed workflows, such as Scienomics MAPS[11], Materials Studio[12], etc., can sometimes simplify the process. These issues could lead to steep learning curves and tremendous entry barriers for the students and beginner scientists who are relatively new to this knowledge domain. For the entry-level audiences in the field of MD simulations, an intuitive and graphical interface would help significantly to begin with; and a unified programming interface is helpful for the users to develop customized functionalities in the long run.

Input and output file formats of different simulation-related software packages vary considerably due to different software specialties and architectures. In many situations, the same piece of information describing the same molecular system appears in various file formats during the prototyping stage of a
simulation, e.g.: LAMMPS uses its own specialized and customizable file formats for static systems[13] and trajectories[14]; XYZ[15] file can contain static systems and trajectories that contains atoms but not bonds; PDB[16] file can record static systems and trajectories with both atoms and bonds, but it has certain limitations since it was developed in the 1970s, etc. In addition, many old file formats have redundant information due to compatibility issues. Software packages, like OpenBabel[17]–[19] and RDkit[20], become convenient when files are being converted from one format into another. On the other hand, the Simplified Molecular-Input Line-Entry System (SMILES)[21]–[23] has become popular in recording small molecules in the cheminformatics community since it is portable and readable to both humans and machines[24]–[26]. SMILES notation and its variants have also been employed in the field of polymeric science given its capability and flexibility in describing molecular structures with linear and branched topologies. BigSMILES[27] has been the avant-garde in exploring the possibility of abstracting compositional information with specialized SMILES notations and syntax.

There are many open-source visualization packages that excel in their own domain expertise, such as VMD and OVITO, but a similar learning barrier exists here. VMD has both Tcl[28], Python command interfaces, and a well-organized GUI, but not all functionalities are available through GUI. OVITO has a Python command interface and a comprehensive GUI menu with functionalities well-documented on its website, and it even supports querying information via mouse-hovering over atoms. The visualization windows of both programs are clickable to manipulate the view angle and zooming of molecular systems. VMD’s GUI and command line are both free, but Ovito’s GUI requires a license when the Python scripting module is involved. Another noticeable effort has similarities to this work is Polymer Structure Predictor (PSP)[29]. It also has a Jupyter-based interface and in place visualization, and its visualization is based Py3Dmol[30], a Python-interfaced 3Dmol.js. Although being an interactive and portable 3D visualization library, py3Dmol lacks the capability of tooltip on mouse hover for in place information querying. A fancier approach is the Game-Engine-Assisted Research platform for Scientific computing (GEARS)[31], which leverages the existing graphics and physics technology from popular game engines, like Unity[32] and Unreal[33], to analyze and visualize LAMMPS simulations. The user
interface to input commands to the system via virtual reality headsets and controllers offers the users an immersive experience that is beyond the common working atmosphere in a classroom or an office.

For an average MD simulation, a typical workflow can be defined with the following steps:

1) building single molecule (or monomer) geometry and topology,
2) force field parameterization and assignment,
3) generating a polymeric or bulk or interfaced system for studying a group of specific properties,
4) launching simulation software suite with computational resource allocation,
5) generating plots and tables from the captured outputs of the simulation.

At each step, the user should have much access to visual inspection and in place information queries as possible to minimize the effort in prototyping. This work is proposing a generalized and lightweight workflow, Polymeric Molecule Assembly Programming System (PolyMAPS), for prototyping and analyzing polymeric systems. The essence of designing a comprehensive workflow for MD simulations is to integrate as many functionalities as possible into one software environment as possible. Thus, by significantly reducing the learning barrier of programming and different types of pre- and post-processing software. The PolyMAPS workflow is designed to initiate a LAMMPS simulation for testing and demonstration purposes, so there are limitations in each part of the software's functionalities due to the computational and graphics capabilities of a Jupyter notebook. The input and output system leverages the portability of SMILES notation and the robustness of native file formats supported by LAMMPS. Simulation systems with a very large number (>100,000) of atoms are out of the scope of this work.

2. Methodology

The center of the PolyMAPS workflow is a Jupyter notebook with Python[34] kernel. As a general-purpose programming language, Python has been widely welcomed in the data science
community. Instructions written in Python using NumPy[35], SciPy[36], and Pandas[37] packages are implemented to manipulate the coordinates and other parameters of atoms and molecules. An interactive visualization tool is developed based on Plotly[38] to demonstrate the atoms and bonds with their corresponding indices and atom information.

Figure 1. Molecular simulation building workflow:

In stage 1, the program starts with either a monomer segment or a complete molecule in the LAMMPS data format[39]. If a complete molecule is already defined, stage 1 can be skipped. A linear polymer chain will require a copy of the left terminal segment, a copy of the right termination segment, and copies of the monomers forming the linear polymer chain. Typically, a termination segment has one linkage anchor, and a monomer segment has two linkage anchors. Branched polymeric systems can also be formed by defining monomers with more than 2 linkage anchors. With a user-defined degree of polymerization, the program can generate a linear
polymer chain with 3D coordinates and the correct bond linkage between monomer segments. The built polymer chain is packaged as a molecule in LAMMPS data format for further processing. The atomic partial charge and atom types are also determined in this stage.

In stage 2, the force field parameters are assigned to the molecule that was built in stage 1. For example, the Charmm general force field[40] (CGenFF) files are parsed, and the related parameters are loaded into Pandas data frames by screening all the atom types. By matching all the possible permutations of the many-body interactions from the loaded parameter data frames: angle, dihedral, and improper, all interactions are detected and assigned to the corresponding selection of atoms automatically. OPLS-AA[41] force field is also supported by directly using an externally generated LAMMPS data file from the LigParGen[42]–[44] website. Then, the workflow can skip stages 1 and 2, and go straight to stage 3.

In stage 3, a larger scale system that is statistically meaningful can be built using the defined molecules. Packmol is commonly used in the community in order to generate randomly initialized systems for MD simulations. However, the supported file formats are limited to XYZ, PDB, and Tinker. For XYZ, no bonding information is present before or after the coordinates’ manipulation; for PDB and Tinker, bonding information can be defined and preserved through the process, but converting the Packmol output file to LAMMPS data format with angle, dihedral, improper and partial charges could be challenging. PolyMAPS offers the user the opportunity to choose how to manipulate atomic coordinates by separating this process from the simulation initialization workflow. Users can choose whether to use Packmol or to generate new atomic coordinates manually in Python or with LAMMPS built-in functions.

A single molecule system with assigned force field parameters and box boundaries will act as a building block to prepare a more complicated system for computational studies. By
duplicating the existing building blocks and stacking them into a larger system using user-defined box sizes, a bulk polymer system can be built. This is achieved by invoking the "replicate" command from LAMMPS. Mixing different types of molecules is also supported for complex systems such as aqueous solutions, multi-phase segregation systems, multi-phase dispersion systems, etc.

In stage 4, users can define the LAMMPS simulation condition with either a text file-based command interface or the PyLAMMPS[45] interface within the Python environment. For small and simple systems, users can launch jobs locally, but for larger and complex systems that require computational cluster access, a job submission script generator is provided. Templates and sample scripts for the Torque[46] system and the Slurm[47] system are provided.

In stage 5, simulation result visualization can be achieved by using the interactive plotting capabilities of Plotly. A LAMMPS log parsing script is provided for the default log style. Selected properties of the system and computational performance metrics can be visualized in the same Jupyter notebook. In case a .xyz trajectory file is generated by LAMMPS, the workflow can help convert it to a regular .xyz trajectory with element symbols instead of atom type numbers. Using Py3Dmol[48], the trajectory animations can be visualized in the Jupyter notebook. An alternative trajectory visualization tool with interactive features is implemented using Plot.ly. Both the regular .xyz trajectory file format and customized LAMMPS trajectory dump format are supported.

3. Results and discussion
   a. Case study: preparing a batch of simulation jobs
For traditional computation clusters, Torque and Slurm are common resource management software. Manually managing parallelly launched jobs with an independent set of simulation parameters could be challenging. A simple job script generating system is implemented in PolyMAPS to organize the simulation files and directory.

![Diagram of simulation jobs with parameters A1 and A2]

Figure 2. A batch of simulation jobs with two independent parameters A1 and A2. A1 has m levels of values, and A2 has n levels of values. Each job is defined by a combination of (A1, A2) values, and each job occupies a folder in the root directory.

PolyMAPS allows users to define the number of independent parameters with individual levels of values and then generates the directories and files with corresponding parameters. For example, a set of simulations with temperatures and pressure within the cartesian product of {283 K, 303 K, 323 K, 343 K, 363 K} × {1 atm, 2 atm}, a total of 10 folders with 10 independent copies of simulation will be prepared.
In addition to the folders holding all the simulation files and resource management scripts, a short bash script is also generated in the root folder. This bash script serves as an automated submission scheduler for the files generated above so that the user need not to access individual directories and submit the jobs manually.

b. Launching MD simulations inside a Jupyter notebook to generate polymers

A polymeric structure with custom terminations, monomer, and polymerization scheme can be defined and generated using the PolyMAPS functionalities. The building process of a system with polyethylene oxide (PEO) molecules is demonstrated.
Figure 3. Building blocks of a polyethylene oxide molecule: (a) head termination block: OH-CH2-X with anchor position X (labeled with pink color); (b) monomer block: CH2-O-CH2-X with anchor position X (labeled with pink color); (c) tail termination block: CH2-OH; (d) assembled PEO molecule. Atom color code: hydrogen as red, carbon as grey, oxygen as white.

As shown in Fig. 3, a polyethylene oxide (PEO) with a degree of polymerization 4 can be decomposed into 2 termination blocks: OH-CH2-X, CH2-OH, and a repetitive monomer block: CH2-O-CH2-X. Letter X is used to denote the anchoring position of the next building block’s first atomic position. For example, when a monomer block is being attached to a head block, the monomer block is first translated so that the left-most carbon atom overlaps with the anchoring position of the head block, site X from the head block is removed, and bonding information is updated.
Once a polymer molecule’s atomic positions and bonding connectivities are all defined, the force field assignment process is ready to take place. PolyMAPS is designed to be force field agnostic so that the same molecule can be simulated with different flavors of force field parameterization schemes under a little amount of effort. Here, the assignment of CGenFF is demonstrated. Since the PEO molecule is documented in the force field files from CGenFF: top_all36_cgenff.rtf[49], the related atom types, bond types, angle types, dihedral types, and improper types are parsed and loaded into the Jupyter notebook as Pandas data frames, as shown below in Table 1~4.

| at   | epsilon | Rmin/2 | eps, 1-4 | Rmin/2, 1-4 | Comment                  |
|------|---------|--------|----------|------------|-------------------------|
| 1 HGA2 | -0.035  | 1.34   | 0        | 0          | # alkane, igor, 6/05    |
| 2 HGP1 | -0.046  | 0.2245 | 0        | 0          | # polar H                |
| 3 CG321 | -0.056  | 2.01   | -0.01    | 1.9        | # alkane (CT2), 4/98, yin, adm jr, also used by viv |
| 4 OG301 | -0.1    | 1.65   | 0        | 0          | # ether; LJ from THP, sng 1/06 |
| 5 OG311 | -0.1921 | 1.765  | 0        | 0          | # og MeOH and EtOH 1/06 (was -0.1521 1.7682) |

Table 1. LJ interaction parameters

| at1  | at2  | Kb     | b0   | Comment                |
|------|------|--------|------|------------------------|
| 1 CG321 | CG321 | 222.5  | 1.53 | # PROT alkane update, adm jr., 3/2/92 |
| 2 CG321 | OG301 | 360    | 1.145 | # diethylene, alex       |
| 3 CG321 | OG311 | 428    | 1.42 | # PROT methanol vib fit EMB 11/21/89 |
| 4 CG321 | HGA2  | 309    | 1.111 | # PROT alkane update, adm jr., 3/2/92 |
| 5 OG301 | OG311 | 300    | 1.461 | # PBG, yxu, RNA          |
| 6 OG311 | HGP1  | 545    | 0.96  | # PROT EMB 11/21/89 methanol vib fit; og tested on MeOH ElOH,... |

Table 2. Bond interaction parameters
Table 3. Angle interaction parameters

| at1     | at2     | at3     | at4     | Kchi | n   | delta | comment                                      |
|---------|---------|---------|---------|------|-----|-------|----------------------------------------------|
| CG321   | CG321   | CG321   | CG321   | 0.0645 | 2   | 0     | # LIPID alkane, 4/04, jbk (Jeff Klauda)      |
| CG321   | CG321   | CG321   | CG321   | 0.14975 | 3   | 180   | # LIPID alkane, 4/04, jbk                   |
| CG321   | CG321   | CG321   | CG321   | 0.09458 | 4   | 0     | # LIPID alkane, 4/04, jbk                   |
| CG321   | CG321   | CG321   | CG321   | 0.11251 | 5   | 0     | # LIPID alkane, 4/04, jbk                   |
| CG321   | CG321   | CG321   | OG301   | 0.16   | 1   | 180   | # methylpropylether, 2/12/05, ATM            |
| CG321   | CG321   | CG321   | OG301   | 0.39   | 2   | 0     | # methylpropylether                         |
| CG321   | CG321   | CG321   | OG301   | 0.195  | 3   | 0     | # PROT alkane update, admjr, 3/2/92         |
| OG301   | CG321   | CG321   | OG301   | 0.25   | 1   | 180   | # 1,2 dimethoxyethane, 2/12/05, ATM         |
| OG301   | CG321   | CG321   | OG301   | 1.24   | 2   | 0     | # 1,2 dimethoxyethane                       |
| OG301   | CG321   | CG321   | HGA2    | 0.19   | 3   | 0     | # alkane, 4/98, yin and mackerell            |
| OG311   | CG321   | CG321   | HGA2    | 0.195  | 3   | 0     | # PROT alkane update, admjr, 3/2/92         |
| HGA2    | CG321   | CG321   | HGA2    | 0.22   | 3   | 0     | # LIPID alkanes                             |
| CG321   | CG321   | OG301   | CG321   | 0.57   | 1   | 0     | # 1,2 dimethoxyethane, 2/12/05, ATM         |
| CG321   | CG321   | OG301   | CG321   | 0.29   | 2   | 0     | # 1,2 dimethoxyethane                       |
| CG321   | CG321   | OG301   | CG321   | 0.43   | 3   | 0     | # 1,2 dimethoxyethane                       |
| HGA2    | CG321   | OG301   | CG321   | 0.284  | 3   | 0     | # diethyllether, alex                       |
| CG321   | CG321   | OG311   | HGP1    | 1.13   | 1   | 0     | # og ethanol                                |
| CG321   | CG321   | OG311   | HGP1    | 0.14   | 2   | 0     | # og ethanol                                |
| CG321   | CG321   | OG311   | HGP1    | 0.24   | 3   | 0     | # og ethanol                                |
| HGA2    | CG321   | OG311   | HGP1    | 0.18   | 3   | 0     | # og methanol                               |

Table 4. Dihedral interaction parameters

After the force field parameters are assigned to the molecule, the packaged molecule is stored in LAMMPS data format with atomic coordinates, topology definitions, and box boundaries. This LAMMPS data file is already a syntactically correct simulation for LAMMPS, but a system with a large number of the same molecule is needed in reality. A more complex system that is statistically meaningful can be generated by treating the built molecule with fixed boundaries as a new level of building blocks. During this process, replications and linear transformations can be applied to the atomic coordinates while no force field parameter or bonding topology of the molecule is isolated and preserved. For
instance, a 4-by-4-by-1 group of PEO molecules can be realized by utilizing the built-in command “replicate” from LAMMPS.

Figure 4. A ready-to-simulate system with 16 PEO molecules with an orthogonal simulation box. A mouse-hovering tip enables immediate information query for any atoms in the 3D system.

A relaxation simulation can be run on the polymer box with an energy minimization followed by an NPT ensemble. The simulation temperature is set at 300 K, pressure at 1 atm, and time step at 1 fs/step. The minimization process ends in 500 steps, followed by 200,000 steps of NPT ensemble.
The measured temperature converges at 299 ± 11.5 K, pressure at -32 ± 2653.0 atm, density at 1.10 ± 0.021 g/cm³, potential energy at 19.6 ± 18.96 kCal/mol. The large fluctuations of temperature, energy, and pressure are expected due to the small size of the simulation[50]. The calculated density can be compared to an experimental result of 1.124~1.126 g/cm³[51] with only -4%~--0.2% error. The simulation is conducted on a personal laptop with i7-8750H with 10 MPI tasks. The LAMMPS version is the v2021.08.31[52] distributed by Conda[53]. The total simulation CPU time is 7 minutes 14 seconds.

The NPT simulation trajectory dumped in both .xyz format and LAMMPS custom format can both be loaded into the Plot.ly-based visualization tool. The visualization interface is similar to the LAMMPS data file visualizer (Fig. 4) but with animation.

Figure 5. Simulation analysis: temperature vs. time (upper left), pressure vs. time (upper right), density vs. time (lower left), potential energy vs. time (lower right). All properties converge in 200 ps.
capabilities. The play and pause buttons can control the animation display, and a sliding bar is available for users to wind and rewind the trajectory animation.

Figure 6. Plot.ly-based visualization tool with slide bar animation play control and hover text information of all atoms

The building blocks of the polymer can be edited by accessing the .lmp files. Users can define any building blocks and modify the polymer building loop in order to generate linear polymers. Mixing different monomers can produce copolymer molecules. With one or more three-anchor monomers involved, a nonlinear polymer molecule with branches can also be generated.
c. Viscosity measurement by simulation

Viscosity calculation by MD simulation is supported by LAMMPS. Here a study of 3 liquid molecules with the Green-Kubo method of viscosity calculation is demonstrated. The Green-Kubo\cite{54}, \cite{55} method calculates the viscosity by sampling the autocorrelation function of all three off-diagonal stress tensor elements over long time periods. The dynamic viscosity of the fluid can be expressed as

\[ \eta = \frac{V}{k_B T} \int_0^\infty \langle P_{xz}(t_0) P_{xz}(t_0 + t) \rangle_{t_0} dt \]

Eq. (1) \cite{56}

where V is the volume of the simulation box, k_B is the Boltzmann constant, T is temperature, P_{xz} is the off-diagonal stress tensor element, and t is the simulation time.

The simulation condition is configured as the following: the temperature at 300 K, time step 0.1 fs/step, autocorrelation length 100,000 steps, total simulation time 2,000,000 steps. The molecule is replicated 8,000 times in LAMMPS and equilibrated under an NPT ensemble for more than 10 ns. The production run is conducted under an NVT ensemble.

The three liquid molecules under examination are water, cyclohexanone, and 2-(2-Methoxyethoxy)ethanol (DEGME). Each type of liquid molecule is generated by the LigParGen server with the OPLS-AA force field. Water molecule is parameterized as tip4p/2005\cite{57}. The initialized simulation box can be visualized with PolyMAPS as in Fig. 7.
Given the data point number limitation of Plot.ly, rendering 3D interactive plots with more than 10,000 atoms can be slow depending on the locally available computation resource.

|                              | water (tip4p/2005) | cyclohexanone | DEGME     |
|------------------------------|--------------------|---------------|-----------|
| **Experimental Viscosity**   | 0.854 [58]         | 2.2 [59]      | 3.48 [60] |
| (mPa*s) at 25°C              |                    |               |           |
| **Green-Kubo Viscosity**     | 0.79919 (-6.4%)    | 2.2461 (+2.1%)| 3.5493 (+2.0%) |
| (mPa*s) at 300 K             |                    |               |           |

Table 5. Viscosity calculation compared against experimental values; percentage error is included in the parenthesis.
The simulated system can predict the viscosity values of water, cyclohexanone, and DEGME within 10% relative error.

4. Conclusion and future work

PolyMAPS provides researchers with a new approach to initialize simulations in Jupyter notebook with Python language and popular libraries, such as NumPy, SciPy, Pandas, Plotly, and Py3Dmol. The simulation initialization process is separated into 3 parts: atomic coordinates, molecular topology, and force field parameters. Users still reserve the ability to choose whether to use PolyMAPS or other software to process these 3 types of information. PolyMAPS provides an in place analysis and visualization interface to molecular systems defined in LAMMPS data format. A simple batch job preparation and submission system is provided so that high-throughput simulations are possible in computational clusters. Users can now look up atomic and bonding information directly in the 3D interactive plot. PolyMAPS has significantly reduced the learning curve and the number of tools for LAMMPS users by integrating all simulation processes into a single Jupyter notebook.

PolyMAPS is still in the early stages of development, so features and capabilities are limited to LAMMPS simulation initialization and partial result analysis. The computational job management system can be improved with existing tools, such as FireWorks[61]. The visualization is developed using the Plot.ly python library inside the Jupyter notebook, so the 3D image rendering quality and interaction responsiveness are limited by the WebGL[62] library. Aesthetically, the WebGL-based rendering engine of Plot.ly does support lighting, but this will only increase the already-too-heavy
computation load in the rendering process. Most of the existing visualization tools, like VMD and Ovito, support 3D lighting rendering. In the future, the interactive plotting interface can be improved by leveraging more hardware acceleration with more atoms in the system and better 3D lighting effects on the atoms and bonds.

5. Code Availability

A demonstrative notebook is available on Google Colab at:

https://colab.research.google.com/drive/1ka95GbuGGca6J-Vf807kTWf3vLdvmWXc?usp=sharing.

References:

[1] S. Plimpton, “Fast Parallel Algorithms for Short-Range Molecular Dynamics,” *Journal of Computational Physics*, vol. 117, no. 1, Mar. 1995, doi: 10.1006/jcph.1995.1039.

[2] T. Kluyver *et al.*, “Jupyter Notebooks – a publishing format for reproducible computational workflows,” in *Positioning and Power in Academic Publishing: Players, Agents and Agendas*, 2016, pp. 87–90. doi: 10.3233/978-1-61499-649-1-87.

[3] H. J. C. Berendsen, D. van der Spoel, and R. van Drunen, “GROMACS: A message-passing parallel molecular dynamics implementation,” *Computer Physics Communications*, vol. 91, no. 1–3, Sep. 1995, doi: 10.1016/0010-4655(95)00042-E.

[4] T. D. Kühne *et al.*, “CP2K: An electronic structure and molecular dynamics software package - Quickstep: Efficient and accurate electronic structure calculations,” *The Journal of Chemical Physics*, vol. 152, no. 19, May 2020, doi: 10.1063/5.0007045.

[5] A. I. Jewett *et al.*, “Moltemplate: A Tool for Coarse-Grained Modeling of Complex Biological Matter and Soft Condensed Matter Physics,” *Journal of Molecular Biology*, vol. 433, no. 11, May 2021, doi: 10.1016/j.jmb.2021.166841.
[6] L. Martínez, R. Andrade, E. G. Birgin, and J. M. Martínez, “PACKMOL: A package for building initial configurations for molecular dynamics simulations,” *Journal of Computational Chemistry*, vol. 30, no. 13, Oct. 2009, doi: 10.1002/jcc.21224.

[7] W. Humphrey, A. Dalke, and K. Schulten, “VMD: Visual molecular dynamics,” *Journal of Molecular Graphics*, vol. 14, no. 1, Feb. 1996, doi: 10.1016/0263-7855(96)00018-5.

[8] I. Cabeza de Vaca, Y. Qian, J. Z. Vilseck, J. Tirado-Rives, and W. L. Jorgensen, “Enhanced Monte Carlo Methods for Modeling Proteins Including Computation of Absolute Free Energies of Binding,” *Journal of Chemical Theory and Computation*, vol. 14, no. 6, Jun. 2018, doi: 10.1021/acs.jctc.8b00031.

[9] A. Stukowski, “Visualization and analysis of atomistic simulation data with OVITO—the Open Visualization Tool,” *Modelling and Simulation in Materials Science and Engineering*, vol. 18, no. 1, p. 015012, Jan. 2010, doi: 10.1088/0965-0393/18/1/015012.

[10] M. D. Hanwell, D. E. Curtis, D. C. Lonie, T. Vandermeersch, E. Zurek, and G. R. Hutchison, “Avogadro: an advanced semantic chemical editor, visualization, and analysis platform,” *Journal of Cheminformatics*, vol. 4, no. 1, p. 17, Dec. 2012, doi: 10.1186/1758-2946-4-17.

[11] SCIENOMICS, “Materials And Processes Simulations (MAPS).” SCIENOMICS LLC, Paris, 2021.

[12] D. S. BIOVIA, “MATERIALS STUDIO.” Dassault Systèmes, San Diego, 2021.

[13] “LAMMPS Data File.” https://docs.lammps.org/read_data.html#format-of-a-data-file (accessed Apr. 26, 2022).

[14] “LAMMPS Dump Trajectories.” https://docs.lammps.org/dump.html (accessed Apr. 26, 2022).

[15] “XYZ File Format.” https://people.math.sc.edu/Burkardt/data/xyz/xyz.html (accessed Apr. 26, 2022).

[16] “Protein Data Bank File Format.” https://www.umass.edu/microbio/rasmol/pdb.htm (accessed Apr. 26, 2022).

[17] N. M. O’Boyle, M. Banck, C. A. James, C. Morley, T. Vandermeersch, and G. R. Hutchison, “Open Babel: An open chemical toolbox,” *Journal of Cheminformatics*, vol. 3, no. 1, p. 33, Dec. 2011, doi: 10.1186/1758-2946-3-33.

[18] N. M. O’Boyle, M. Banck, C. A. James, C. Morley, T. Vandermeersch, and G. R. Hutchison, “Open Babel: An open chemical toolbox,” *Journal of Cheminformatics*, vol. 3, no. 1, Dec. 2011, doi: 10.1186/1758-2946-3-33.

[19] “The Open Babel Package.” http://openbabel.org.

[20] “RDKit, Open-Source Cheminformatics.” github.com/rdkit/rdkit.

[21] D. Weininger, “SMILES, a chemical language and information system. 1. Introduction to methodology and encoding rules,” *Journal of Chemical Information and Modeling*, vol. 28, no. 1, pp. 31–36, Feb. 1988, doi: 10.1021/ci00057a005.
[40] K. Vanommeslaeghe et al., “CHARMM general force field: A force field for drug-like molecules compatible with the CHARMM all-atom additive biological force fields,” *Journal of Computational Chemistry*, 2009, doi: 10.1002/jcc.21367.

[41] M. J. Robertson, J. Tirado-Rives, and W. L. Jorgensen, “Improved Peptide and Protein Torsional Energetics with the OPLS-AA Force Field,” *Journal of Chemical Theory and Computation*, vol. 11, no. 7, Jul. 2015, doi: 10.1021/acs.jctc.5b00356.

[42] W. L. Jorgensen and J. Tirado-Rives, “Potential energy functions for atomic-level simulations of water and organic and biomolecular systems,” *Proceedings of the National Academy of Sciences*, vol. 102, no. 19, May 2005, doi: 10.1073/pnas.0408037102.

[43] L. S. Dodda, I. Cabeza de Vaca, J. Tirado-Rives, and W. L. Jorgensen, “LigParGen web server: an automatic OPLS-AA parameter generator for organic ligands,” *Nucleic Acids Research*, vol. 45, no. W1, Jul. 2017, doi: 10.1093/nar/gkx312.

[44] L. S. Dodda, J. Z. Vilseck, J. Tirado-Rives, and W. L. Jorgensen, “1.14*CM1A-LBCC: Localized Bond-Charge Corrected CM1A Charges for Condensed-Phase Simulations,” *The Journal of Physical Chemistry B*, vol. 121, no. 15, Apr. 2017, doi: 10.1021/acs.jpcb.7b00272.

[45] “PyLammps Tutorial,” 2021.

[46] G. Staples, “TORQUE---TORQUE resource manager,” 2006. doi: 10.1145/1188455.1188464.

[47] A. B. Yoo, M. A. Jette, and M. Grondona, “LNCS 2862 - SLURM: Simple Linux Utility for Resource Management.”

[48] N. Rego and D. Koes, “3Dmol.js: molecular visualization with WebGL,” *Bioinformatics*, vol. 31, no. 8, Apr. 2015, doi: 10.1093/bioinformatics/btu829.

[49] “CGenFF: Topology for the Charmm General Force Field v. 4.4 for Small Molecule Drug Design.”

[50] H. C. Andersen, “Molecular dynamics simulations at constant pressure and/or temperature,” *The Journal of Chemical Physics*, vol. 72, no. 4, Feb. 1980, doi: 10.1063/1.439486.

[51] Sigma-Aldrich, “Polyethylene glycol 200,” 2021.

[52] “conda-forge / packages / lammps 2021.08.31.” 2021.

[53] “Anaconda Software Distribution, Anaconda Documentation.” Anaconda Inc., 2020.

[54] M. S. Green, “Markoff Random Processes and the Statistical Mechanics of Time-Dependent Phenomena. II. Irreversible Processes in Fluids,” *The Journal of Chemical Physics*, vol. 22, no. 3, Mar. 1954, doi: 10.1063/1.1740082.

[55] R. Kubo, “Statistical-Mechanical Theory of Irreversible Processes. I. General Theory and Simple Applications to Magnetic and Conduction Problems,” *Journal of the Physical Society of Japan*, vol. 12, no. 6, Jun. 1957, doi: 10.1143/JPSJ.12.570.

[56] D. J. Evans and G. P. Morriss, “Transient-time-correlation functions and the rheology of fluids,” *Physical Review A*, vol. 38, no. 8, Oct. 1988, doi: 10.1103/PhysRevA.38.4142.
[57] J. L. F. Abascal and C. Vega, “A general purpose model for the condensed phases of water: TIP4P/2005,” The Journal of Chemical Physics, vol. 123, no. 23, Dec. 2005, doi: 10.1063/1.2121687.

[58] J. C. Crittenden, R. R. Trussell, D. W. Hand, K. J. Howe, and G. Tchobanoglous, MWH’s Water Treatment. Hoboken, NJ, USA: John Wiley & Sons, Inc., 2012. doi: 10.1002/9781118131473.

[59] E. M. Pearce, “Kirk-Othmer encyclopedia of chemical technology, 3rd ed., Vol. I, Wiley-Interscience, New York, 1978.,” Journal of Polymer Science: Polymer Letters Edition, vol. 16, no. 5, May 1978, doi: 10.1002/pol.1978.130160508.

[60] F. Nees, “Kirk/Othmer Encyclopedia of Chemical Technology. Vol. 1: A to Alkaloids. Vol. 2: Alkanolamines to Antibiotics (Glycopeptides). 4. Auflage. (Reihenherausgeber: J. I. Kroschwitz). Herausgegeben von M. Howe-Grant. Wiley, Chichester. Vol. 1: 1991. XXII, 1087 S., geb. 135.00 £ – ISBN 0-471-52669-X; Vol. 2: 1992. XXVIII, 1018 S., geb. 135.00 £ – ISBN 0-471-52670-3,” Angewandte Chemie, vol. 105, no. 2, Feb. 1993, doi: 10.1002/ange.19931050249.

[61] A. Jain et al., “FireWorks: a dynamic workflow system designed for high-throughput applications,” Concurrency and Computation: Practice and Experience, vol. 27, no. 17, pp. 5037–5059, Dec. 2015, doi: 10.1002/cpe.3505.

[62] Tony Parisi, WebGL: Up and Running, 1st ed. O’Reilly Media, Inc., 2012.