MOLECULES IN 3D

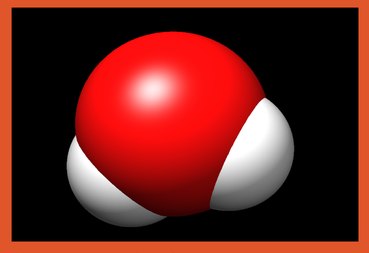
Advancing Academics With Hands-On Bio Data!

THE PURPOSE

- The Department of Biochemistry and Biophysics (DBB) has been using 3D printing to enhance student understanding of various biological structures and their function.
- So far, OSU's DBB has only been able to 3D print monochromatic models, lacking the important information that color can convey, such as atom type and hydrophobic surfaces.
- Recently, the OSU Biochemistry department has purchased two 3D printers (ZMorph and the Rostock MAX Delta) and a multi-material printing interface (Palette+) that allows printing with up to four different filaments.
- The proposed solution: Develop a robust workflow that includes both software and hardware components and results in colored 3D prints.

THE REQUIREMENTS

- All software used must be free or open-source.
- A python pipeline which streamlines the workflow will work together with the multi-filament interface and the 3D printer to produce 3D objects.
- The workflow will be able to take in a single biological file type or non-biological file and create a polychromatic 3D object file that can be printed with the hardware.



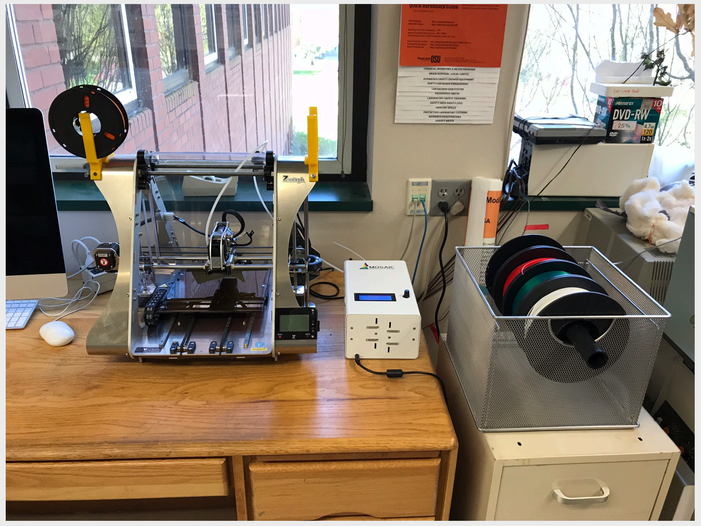
A a water molecule representation in Chimera.

Oregon State University

THE DESIGN

For this project, the technologies best-suited for the project's requirements and goals were determined to be:

- 3D Printer: ZMorph
- Multifilament Interface: Mosaic Manufacturing Palette+
- Computing Platform: MacOS
- Filament Type: Polylactic Acid (PLA)
- Non-biological File Type: Stereo-Lithography (STL)
- Biological File Type: Protein Data Bank (PDB)
- 3D Slicing Software: Ultimaker's Cura
- Programming Language: Python
- Hardware Communication: Direct USB
- Conversion Software: UCSF Chimera



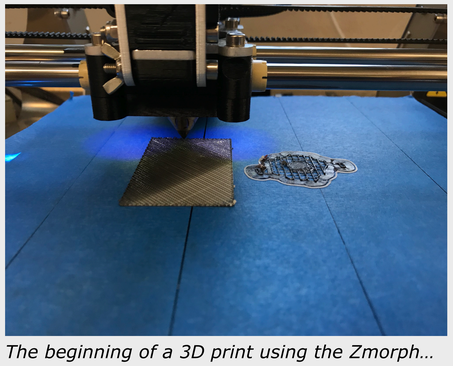
The lab set up in ALS 2157. Pictured are the Mac computer, ZMorph, Palette+, and filament feed.

THE PROCESS

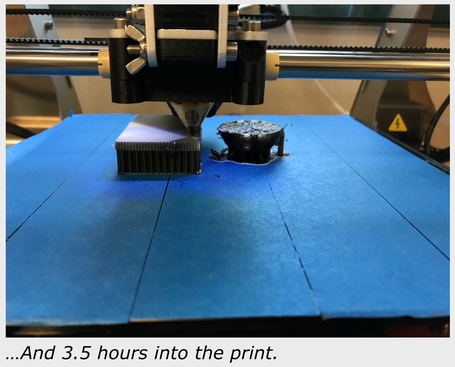
Development began by researching and defining the technologies to be used in the project's workflow. Once these had been determined and the requirements had been discussed, the python pipeline was outlined. Work with the hardware was delayed due to not yet having the Palette+, and once the Palette+ was installed in the lab, it was in need of servicing.

Software development began with an outline of code, to identify an efficient organization. Third party software tools were then tested for their ability to be started from a command-line environment, before adding system calls to said software inside the workflow code. Lastly, file validation was added to the pipeline.

During the initial development of the hardware, interfacing the Palette+ with the other workflow components proved to be a significant challenge, as the Palette+ was designed to be compatible with a wide variety of 3D printers and slicing software. Another major issue that impeded our hardware progress was lack of adhesion between the PLA filament and the Zmorph's print bed during prints. Once methods to minimize this issue were discovered, successful prints could still not be 100% guaranteed due to feed issues. Ultimately, print failures were because of limitations of the hardware, and not the workflow.

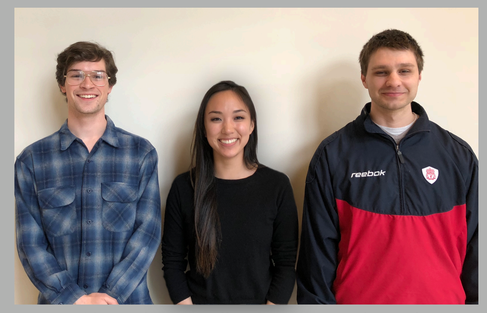


The beginning of a 3D print using the Zmorph…



…And 3.5 hours into the print.

THE TEAM



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THE RESULTS

- A software tool was created per the requirements outlined by the client. The Python script functions as a software pipeline, executing third party open-source software tools sequentially. The script handles invalid input and alters the path through the pipeline according to the format of the file supplied. Most of the user's interaction with the script will consist of usage of the third party software. The script's main purpose is essentially functioning as the guiding hand for the user, alleviating the need for investigation into 3D printing software.
- Configuration and installation of hardware have been mostly successful. The 3D printer can use the files produced by the software deliverable and works with the multifilament interface to produce polychromatic printed objects. General issues are encountered from print to print, but this can be expected owed to the volatile nature of recently invented technology.