We propose a fabrication technique for the fast and cheap production of 3D replicas of proteins. We leverage silicone casting with rigid molds, to produce flexible models which can be safely extracted from the mold. Our tangible models are easily manipulated to simulate the biological interaction mechanisms between proteins, easing the understanding of fundamental principles of macromolecular organization in an educational or laboratory setting.

Method

PDB Representation

For complex polymeric structures, extracting the Solvent Extruded Surfaces (SES) individually for the single monomers, often leads to difficult to match or even intersecting surfaces at interaction sites.

SES Extraction

Surface Interpolation

Matching Surfaces

We define an interpolation scheme to automatically generate perfectly matching surfaces, smoothly altering the surface locally to interaction sites. We consider as interaction sites those surface regions whose distance from another monomer is less than a predefined threshold \( t = 1.4 \text{Å} \) in our examples. The resulting surface is a bisector surface between the offset surfaces of monomers in correspondence of the interaction site and smoothly adapts to the original surface elsewhere.

Interpolating SES

Parting Surface

Mold Pieces

Silicone Casting

Given the interpolating SES, we define the geometry of the corresponding rigid mold pieces. The key problem in computational mold design is deciding how the mold should open up to allow for the cast extraction. This amounts to the definition of valid parting directions and surfaces of the mold. To do so, we use an approach based on a volumetric analysis of the melt extraction paths, approximated as shortest walks from the interior of the mold towards the exterior, as in [AMG* 19].

Tangible Model

The mold pieces geometry is defined as prism-like structures. In addition, the mold generation algorithm automatically accounts for the creation of the required air vents and material inlets. The resulting mold pieces are 3D printed and used to cast multiple replicas of the desired monomer, allowing for the efficient production of complex polymers and macromolecules.

Preliminary Results

We have presented an ongoing work on the efficient fabrication of tangible protein models, using silicone casting. To validate our preliminary results we tested the technique on two different proteinic structures: Actin polymers and Hemoglobin tetramers. Thanks to our interpolating SES, monomers can be easily matched together to form complex polymers.

F-Actin

Hemoglobin

Future Works

- Automatize whole pipeline (symmetry detection)
- Magnet docking (automatic or user-defined)
- Surface annotation (using haptic features)
- Conduct user studies (educational/lab settings)