Computational Fabrication of Macromolecules: Enhancing Understanding of Biological Mechanisms

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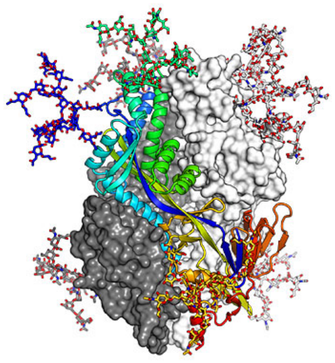
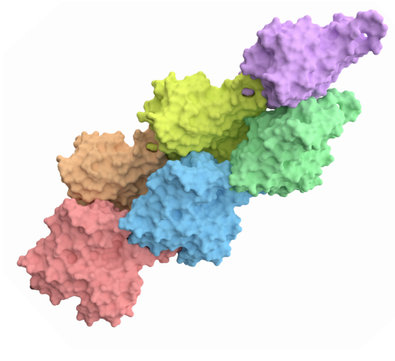
Tangible models are widely used for visualization in education as well as in laboratory settings **but...**



Macromolecular structures are very complex and require adequate representations, **therefore...**

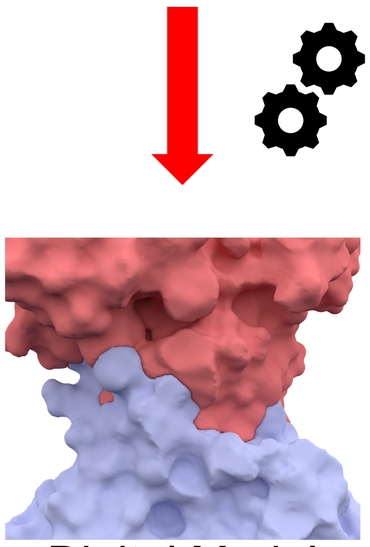


Digital modeling and fabrication techniques are required for the efficient reproduction of complex biological models

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 a educational or laboratory setting.

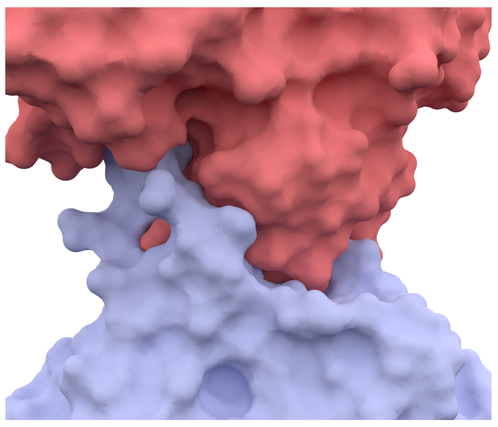
Method

PDB Representation



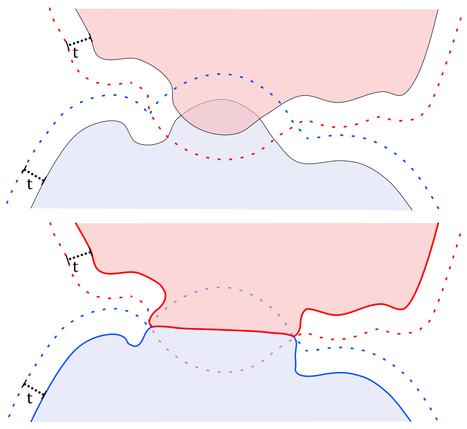
Digital Model

Tangible Model



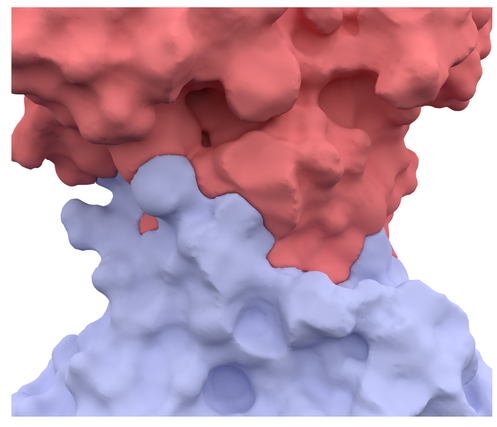
SES Extraction

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

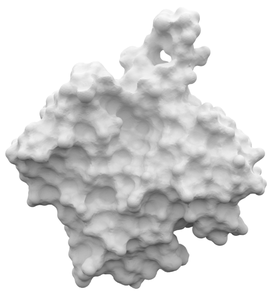


Surface Interpolation

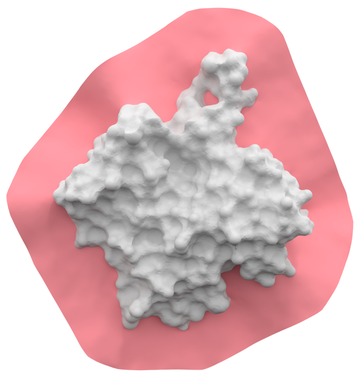
We define an interpolation scheme to automatically generate perfectly matching surfaces, smoothly altering the surface locally to interaction sites. We consider as interaction sites those surface regions whose distance from another monomer is less than a predefined threshold t (t=1.4Å in our examples). 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.



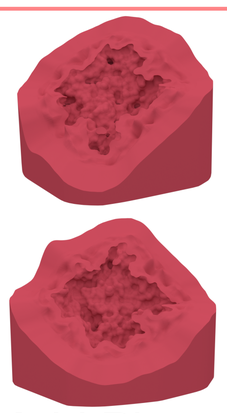
Matching Surfaces



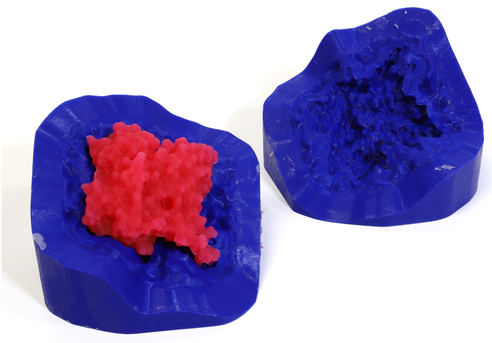
Interpolating SES



Parting Surface



Mold Pieces



Silicone Casting

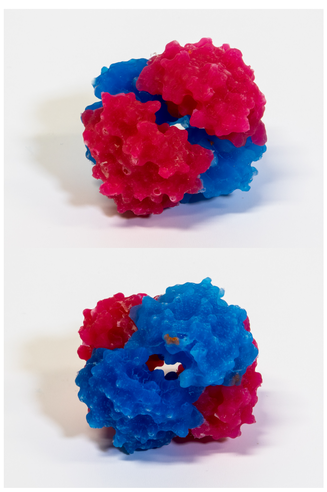
Given the interpolating SES, we define the geometry of the corresponding rigid mold pieces. The key problem in computational mold design is deciding how the mold should open up to allow for the cast extraction. This amounts to the definition of valid parting directions and surfaces of the mold. To do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

The molds 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 proteic 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*)

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