

# MesoCraft – 3D Modeling Software for Creating Mesoscale Atomistic Models

KAUST Nanovisualization

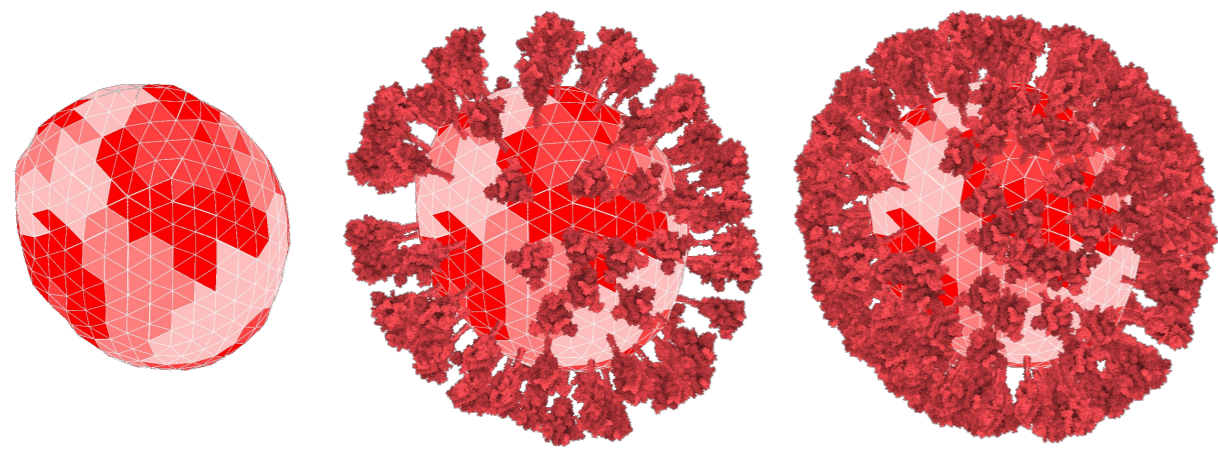
**Abstract:** **MesoCraft** is a new 3D modeling tool implementing visual-programming approach. The software is built on top of **marion** rendering library. It provides the user with the capabilities of loading, rendering and manipulating several modalities (protein data, volumetric data, meshes) and overlaying them inside one rendering view. The modeling algorithm is based on statistical and rule-based modeling approaches that are rapid to author, fast to construct, and easy to revise. Biological information can be incorporated by interactively defining the rules that spatially characterize the biological entity, such as mutual interactions among macromolecules, and their distances and orientations relative to other structures. These rules are defined through an intuitive 3D interactive visualization as a visual-programming feedback loop.

## Building Blocks

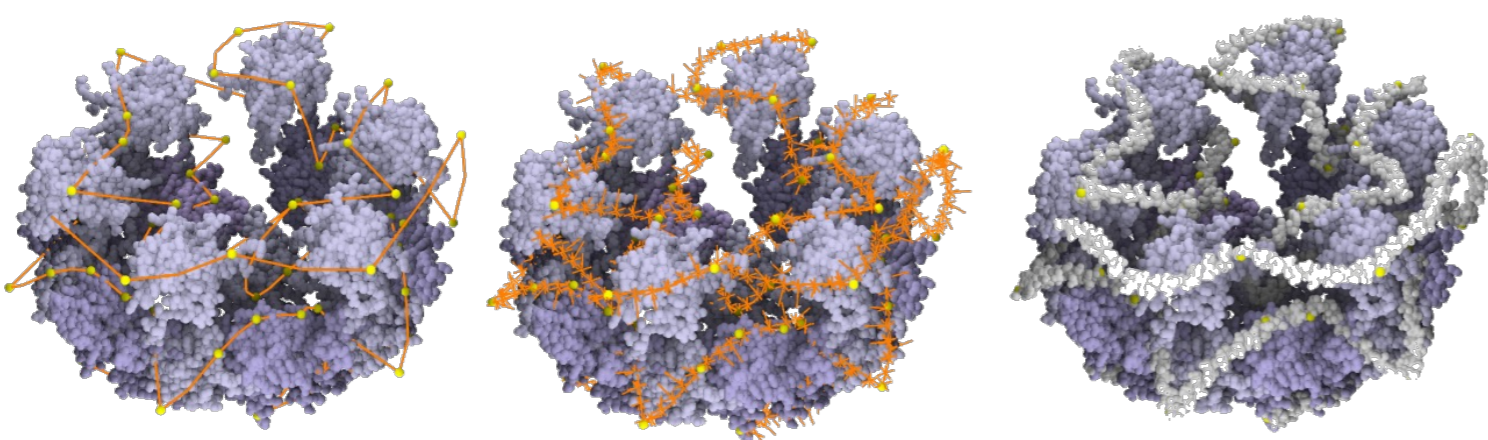


Elementary building blocks are **protein** models (generally available in online databases) and **primitives**. The relations (**rules**) between building blocks are defined directly in 3D environment by the user.

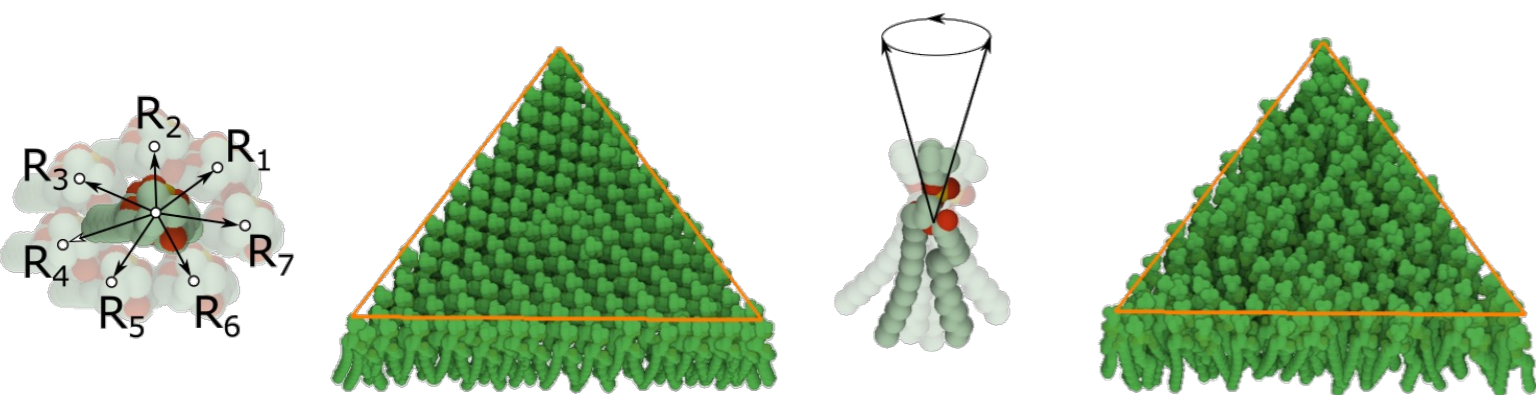
## Rules



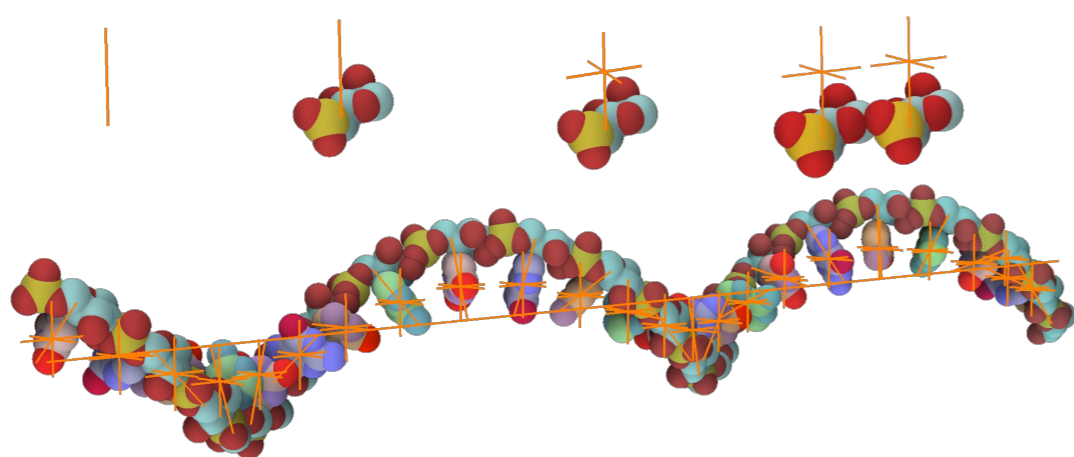
**Distance rule** – generates new elements at a specified distance to the parent. The distance can be either a constant or modeled probability distribution that is sampled each time a new element is created.



**Relative rule** – specifies the location of new elements with respect to a vertex belonging to the proxy geometry.

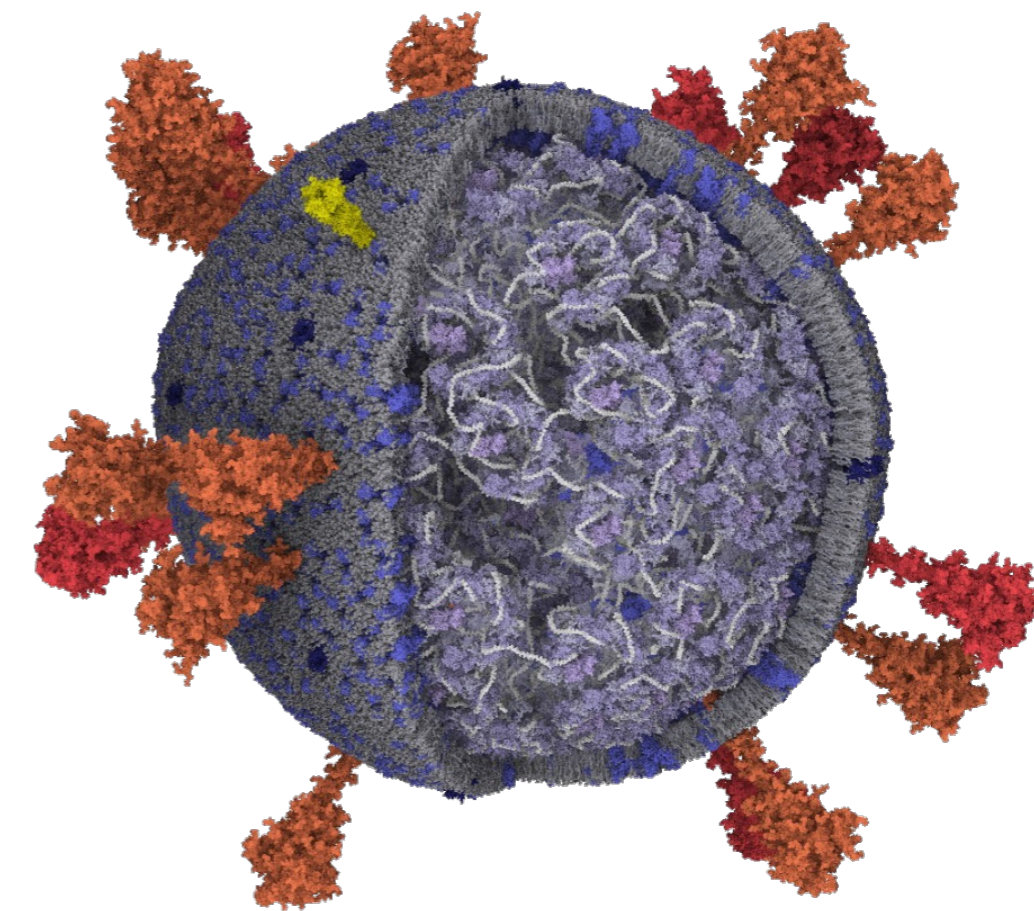


**Siblings rule** – generates new elements and adds them as siblings to the same parent in the hierarchy. A new element is generated by transforming the coordinate system of the input element.

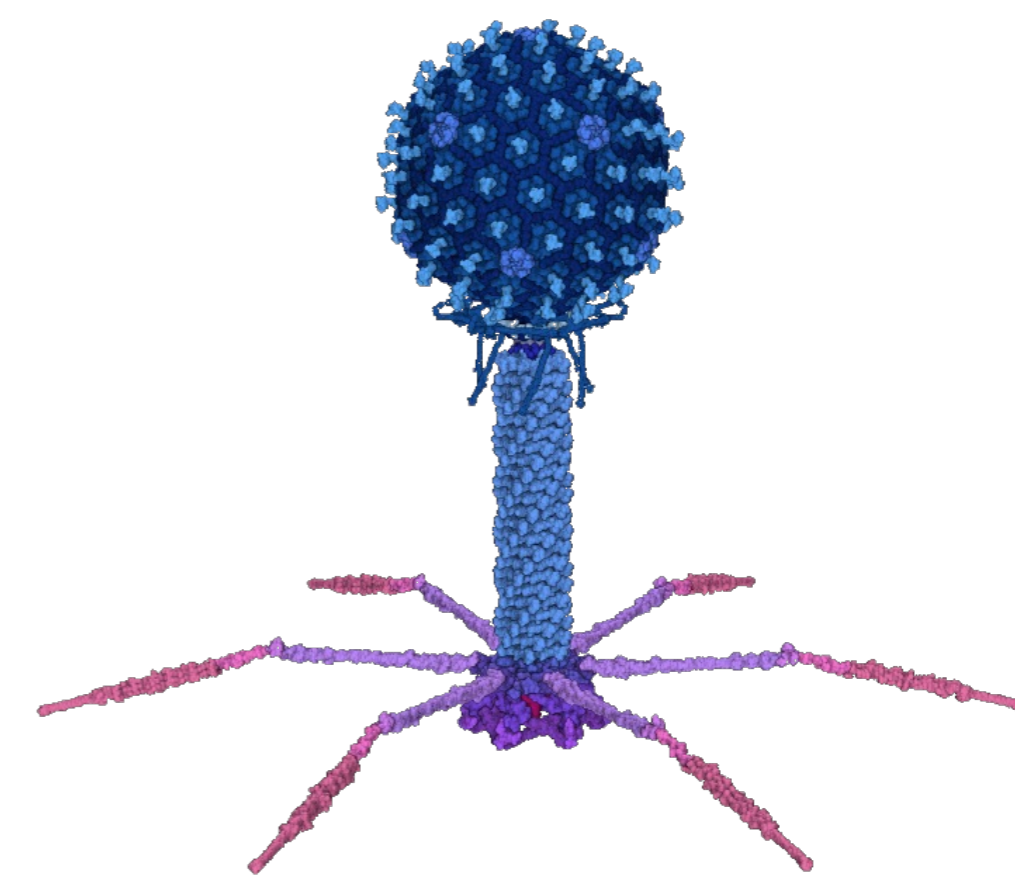


**Siblings-parent rule** - specifies a transformation to the sibling element as in the siblings rule. However, after applying the transformation, the new element is snapped to a given distance from the proxy geometry.

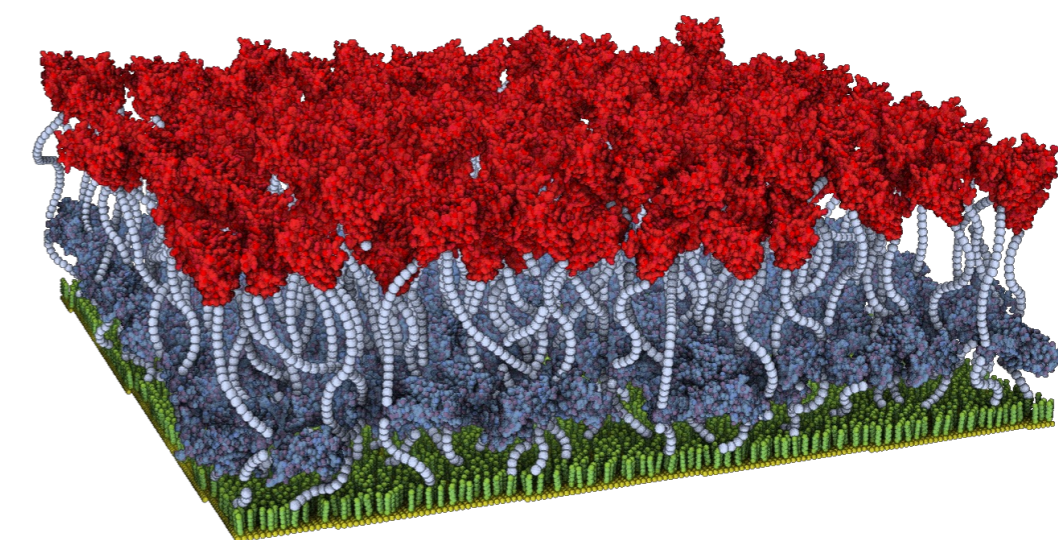
## Generated Models



**SARS-CoV-2**  
~ 200 000 elements (~14M of atoms)  
collaboration with Sai Li (Tsinghua university) & Scripps Institute



**T4 bacteriophage**  
~ 700 elements (~6.2M of atoms)  
collaboration with WISE students



**SARS-Cov-2 tester**  
~ 36 000 elements (~0.5M of atoms)  
collaboration with Stefan Arold's group, work in progress

## Future Work

Collaborative virtual reality environment for modeling of mesoscale models, where scientists can directly share and integrate their knowledge. Furthermore, we would like to re-implement the whole environment into online (web-based) project. In such a system, the exchanging of knowledge could happen online without the necessity of physical presence.

## References

Ngan Nguyen, Ondrej Strnad, Tobias Klein, Deng Luo, Ruwayda Alharbi, Peter Wonka, Martina Maritan, Peter Mindek, Ludovic Autin, David Goodsell, Ivan Viola. **Modeling in the Time of COVID-19: Statistical and Rule-based Mesoscale Models.** *IEEE Transactions on Visualization and Computer Graphics*, 2020.