

Computational Modelling of Irregular Virus Shells as flattened polyhedra

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Abstract

Most viruses have shells made of protein called “capsids”, which adopt polyhedral shapes. Many programs and databases for studying capsids assume that the polyhedra corresponding to them have evenly-spaced vertices, but it is now known that many viruses (including HIV, figure 1a) do not have this property. As part of theoretical work on “irregular” virus capsids, we present a program for creating models of these polyhedra in a manner that makes use of a computational origami method and algorithm, treating them as essentially being made of paper. The software is accessible for the general public, and allows for building of theoretical models of virus capsids, which is useful for setting up molecular dynamics simulations, and for creating illustrations for publications and presentations.

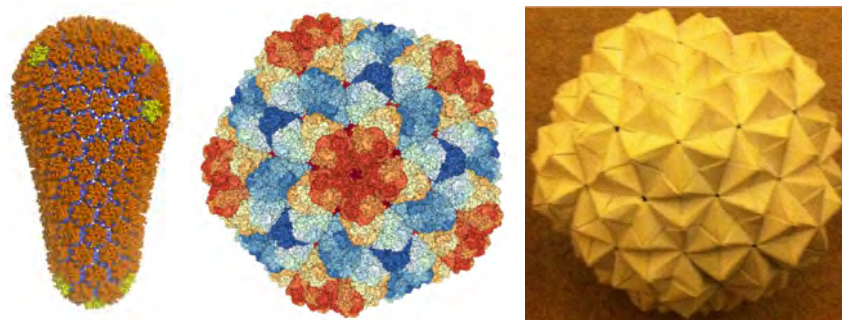


Figure 1: Left to right: capsid of HIV virus[1]; capsid of rice dwarf virus[2]; icosahedrally symmetric modular origami model with the same pattern of triangles as seen on rice dwarf virus.

In general we can make the following set of mathematical assumptions about capsids (figure 1): they are closed surfaces made of at least 60 identical proteins connected to one another. They can be grouped into equilateral triangles, each of which contains three proteins. The equilateral triangles are joined either six around a corner or five around a corner (figure 2). If the equilateral triangles are joined in a six (a “hexamer”), their corners will be flat within the capsid, and if they are joined in a five (a “pentamer”), curvature is introduced. Apart from the smallest viruses, most of the surface of the capsid is made of hexamers and is therefore “paper-like” (zero gaussian curvature), the corners/pentamers being exceptional. Capsids always have precisely 12 pentamers.



Figure 2: Closeup of six-fold and five-fold joins of origami units[3] and HIV capsid proteins[1].

We have created a browser-based program called “Irreg” for creating models of capsids, figure 3. It displays a flat tiling of hexagons (the circular background in 3a), out of which a “net” (the black outline in 3a) can be “cut out and wrapped up” into a capsid model (figure 3c and 3d). The program can display both folded and unfolded models simultaneously, similar to origami-design programs like “freeform origami” and “Treemaker”. The code and user interface for Irreg makes use of the fact that virus capsids must always be polyhedra with 60-degree “angular defect” at their vertices, a result we will derive. Wrapping up the net requires calculation of appropriate dihedral angles, which is non-trivial, and so we have used a folding algorithm developed by Stefan Sechelmann and Erik Demaine[4].

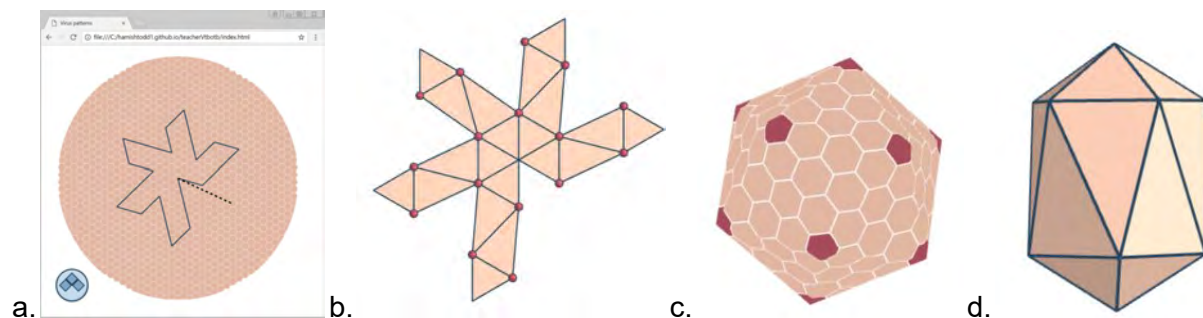


Figure 3: Images from “Irreg”: A. screenshot; B. net for irregular virus; C. “wrapped up” model of HK97 virus, tiled with hexagons and pentagons; D. “wrapped up” model of T4 virus, plain

References

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