

Implementation Of Bacilliform Viral Capsid Models

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> Intro -----

The objective is the enhancement of the [democapsid](#) browser app with elongated icosahedral constructions for modeling bacilliform viruses or nanomaterials. Users can export high-quality vector graphics models (thanks to [Paper.js](#)) for use in figures and publication. Code is available under the MIT License.

> Discussion -----

Prior to [democapsid](#), no application existed for the parameterized construction of capsid models, especially for bacilliform viruses. This user-friendly app generates simple, scalable vector graphics (SVG) models for use in publication-quality figures. Planned work includes algorithms to reduce runtime, address z-ordering artifacts due to edge cases, and add other tiling patterns.

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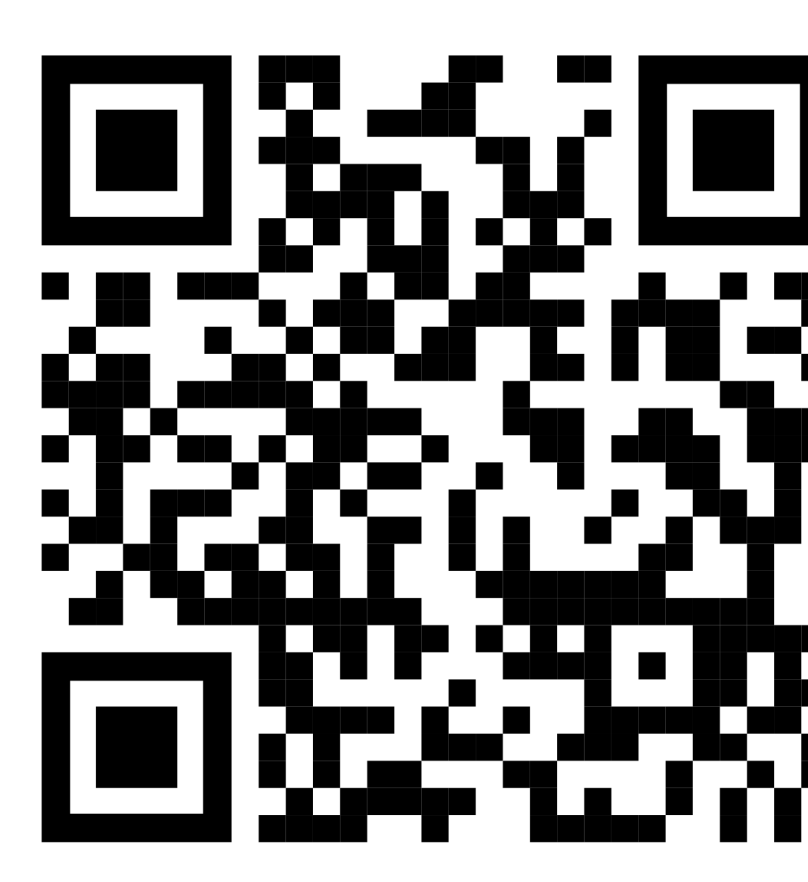
> Methods -----

[GitHub App]



- [1] Select elongated (along the 2-, 3-, or 5-fold axis) or equilateral (all) capsid.
- [2] Calculate required unit faces based on Caspar-Klug parameters and hexagonal tiling.
- [3] Arrange faces into net. [4] Calculate 3D vertex coordinates based on the regular icosahedron axial end cap and then fold the next adjacent face until the end vertex intersects with the constraining cylinder. Solve numerically using a hybrid bracketing-bisection method to obtain the angle and apply Rodrigues' rotation formula. Compute remaining points based on symmetry constraints. [5] Affine transform and order faces.

[GeoGebra]



	<u>Axes</u>	<u>Caspar-Klug</u>	<u>Face</u>	<u>Net</u>	<u>Coordinates</u>	<u>Projection</u>
<u>Equilateral</u>						
<u>5-Fold</u>						
<u>3-Fold</u>						
<u>2-Fold</u>						

<u>Tri</u>	<u>Snub</u>	<u>RhombiTri</u>	<u>DualTri</u>	<u>DualSnub</u>	<u>DualRhombiTri</u>

Alt.Hex-Tiling

> Results -----

Reproduction of capsid models and cryo-EM structures with facet, pattern, and parameters indicated:

[Adenovirus]

$h = 5, k = 0, \text{ laevo} \rightarrow T = 5^2 + (5)(0) + 0^2 = 20$

(Prasad & Schmid, 2011)

[Trihexagonal Capsids]

Left : Basilisk phage, $T = 3^2 + (3)(0) + 0^2 = 9$
 Middle: HSV-1, $T = 4^2 + (4)(0) + 0^2 = 16$
 Right : phage λ, $T = 2^2 + (2)(1) + 1^2 = 7$

(Twarock & Luque, 2019)

[Bacteriophage T4]

$h_1 = 3, k_1 = 1, h_2 = 4, k_2 = 2, \text{ laevo}$
 $T_{\text{end}} = 3^2 + (3)(1) + 1^2 = 13$
 $T_{\text{mid}} = 4^2 + (4)(2) + 2^2 = 20$

(Fokine et al., 2004)

[SVG Models]

Import into design or office software, convert to shape, scale, and customize.