**Introduction**

- Quasiequivalence [1] allows using the same interaction to specify inequivalent bond geometries.
- An approximate symmetry.
- Polymorphism a direct consequence: spheres, tubes, and cones all allowed by same bond in slightly different conformations.
- Quasiequivalent models have found minimal-energy equilibrium structures.
- Icosahedral symmetry favorable [2]
- Facetedness controlled by ratio of elastic stiffnesses [3]
- Tubes/cones under very specific constraints [4]
- Equilibrium models cannot determine assembly pathways.
- Growth models can investigate
- What is mechanism for assembly?
- How do icosahedral viruses assemble symmetrically? (i.e. for triangulation number \( T > 1 \), how do the pentamers end up in the right places?)
- For cones, which end (big or small) assemblies first?
- How does the ensemble of grown capsids compare with experimental measurements of real capsids?

**Methods**

Given a set of model parameters, we produce an ensemble of capsids, one at a time:

1. Begin with a pentameric template of five triangles around a point.
2. Determine the lowest energy structure for the incomplete capsid.
3. Use the local geometry to determine where to bind triangles.
4. Repeat steps 2–4 until capsid is complete, or until completion becomes impossible.
5. Measure capsid size, shape, etc.

**Results: Success**

Fraction of successfully completed capsids versus average size

**Results: Size**

Average size of capsids versus spontaneous curvature

**Future Directions**

- We plan to use more realistic interactions based on protein modelling.
- Our newest model: individual proteins and add hexamers and pentamers instead of trimers.
- Simpler growth rules; better describes more viruses
- Concentration effects, membrane and genome interactions
- Likely important for conical capsids like HIV
- We are most interested in experimental measurements (size, shape, frequency of occurrence) of the appugal and defective capsids — these will shed the most light on the details of assembly mechanisms.

**References**


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