

1. What are you trying to do?

I will try to extend the theory of elongated and conical viral capsids to include the additional lattices reported in the recent *Nature Communications* article (Luque and Reguera, 2010; Twarock and Luque, 2019).

2. How is it done today?

Currently the theory of elongated and conical viral capsids only includes hexagonal lattices.

3. What is new in your approach?

The mathematical theory behind elongated and conical viral structures assumes a hexagonal lattice. Exchanging the hexagonal lattice for one of the additional Archimedean lattices will result in new structure to be explored and characterized. This will include deriving the radius of each cap, length, positions of proteins, protein stoichiometry rules, icosahedral class P, *T*-numbers, and the icosahedral lattice.

4. Who cares?

Our lab, structural biologists

5. What difference will it make?

- a. Viral capsids are useful for studying viruses as they tend to be conserved over time and are strongly related to virus replication strategies and evolutionary histories. Unraveling the mathematics behind the elongated and conical structures equipped with these new lattices offers new ways to understand such capsids which previously were difficult to classify. This in turn will aid in characterizing the corresponding virus.

6. What are the risks and payoffs?

The main risk is that the extending of the theory for the elongated and conical structures is not feasible in the given time frame. This is highly unlikely for the elongated structures, but is possible for the conical structures.

The main pay off is that a set of previously unclassified or misclassified viruses is now classifiable. This will enhance our understanding of such viruses as it is our hypothesis that the structural classifications are tied to viral replication strategies and types of capsid protein folds.

7. How much will it cost?

Funding for my entire masters (funding>TA salary).

8. How long will it take?

I will produce code for ChimeraX to model the 5-fold elongated structures by the beginning of the summer of 2022. The 2-fold and 3-fold cases will be done by the end of the summer. The mathematics of the conical structures will be done by no later than December 2022.

9. What are the midterm and final check points for success?

- a. The first milestone is to have working code for the 5-fold elongated structures (followed by the 3-fold and then 2-fold as they are more complicated).
- b. The second milestone is to have a solid mathematical foundation from which conical structures can be modeled. This will involve deriving all of the

expressions described above (3). This is one of the final check points for success and will be done no later than December 2022.

- c. If this is all achieved, coding in ChimeraX to model the conical structures will follow.