Group Actions Applied to Virus Architecture

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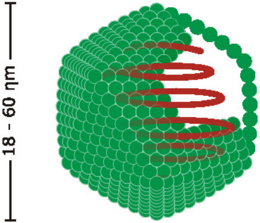
joint work with A. Devillers (UWA) and R. Twarock (Univ. of York, UK)

Workshop on Symmetry in Graphs,
Maps and Polytopes

October 25th, 2011 = 200th anniversary of Galois!!!

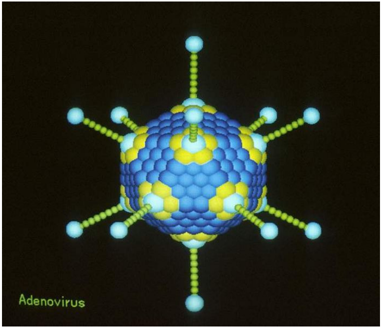
Fields Institute, Toronto, 24–27 October 2011

Viruses

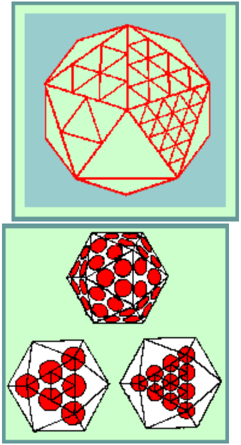


- 1956 Crick and Watson: “The only reasonable way to build a protein shell is to use the same type of molecule over and over again.” “subunits would be packed so as to provide each with an identical environment. This is possible only if they are packed symmetrically.” They predicted *cubic* symmetry.
- Later: icosahedral symmetry is preferred in virus structure.

1962 Caspar and Klug theory



- subunits of few different types in *quasi-equivalent* environments.
- triangulations of icosahedron faces with *capsomers* in corners of triangles.



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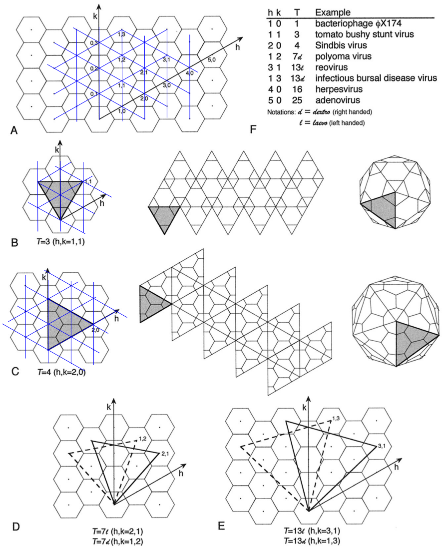
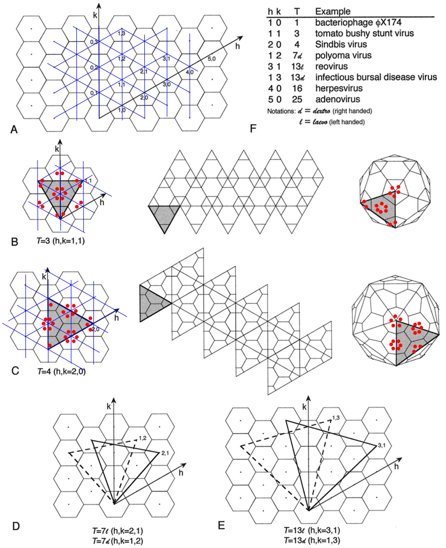
Triangular lattice



- (h, k) are co-ordinates of vertex of icosahedron.
- embedding of icsahedron in triagular lattice.
- A capsomer in corner of each triangle.
- T number is square of distance between two icosahedron vertices. This is exactly $h^2 + hk + k^2$.
- There are $60T$ capsomers, clustered as 12 pentamers and $10(T-1)$ hexamers.

Triangular lattice



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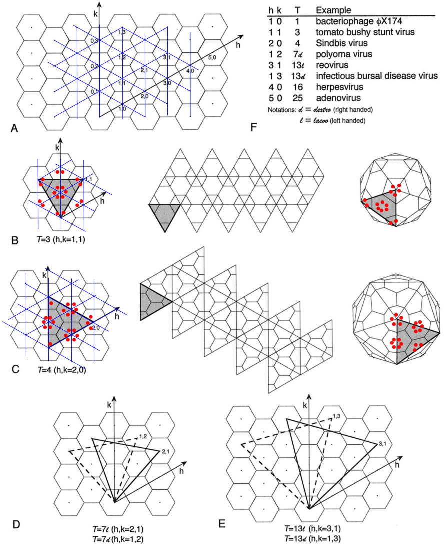

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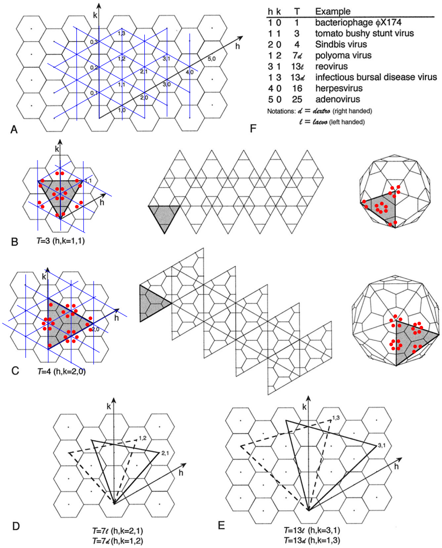

h k	T	Example
1 0	1	bacteriophage ϕX174
1 1	3	tomato bushy stunt virus
2 0	4	Sindbis virus
1 2	7d	polyoma virus
3 1	13ℓ	reovirus
1 3	13d	infectious bursal disease virus
4 0	16	herpesvirus
5 0	25	adenovirus

Notations: d = *dextro* (right handed)
ℓ = *laevo* (left handed)

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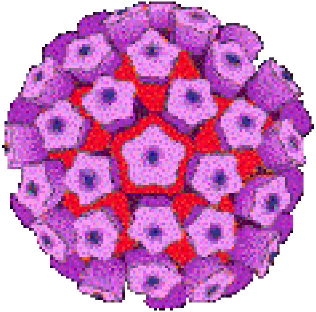

- Has more pentamers!
- $T = 7$
- Twarock 2004: Use other tiles!
- Capsomers only at corners which have same angle
- Rhombs and kites tiling also explains dimer and trimer interactions.

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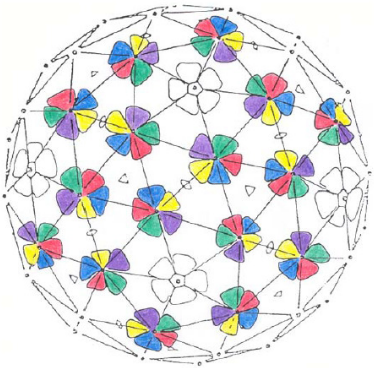

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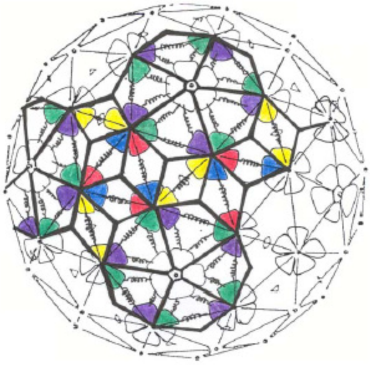

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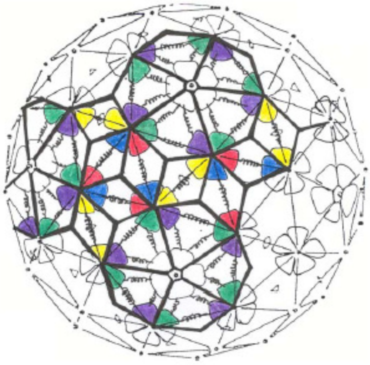

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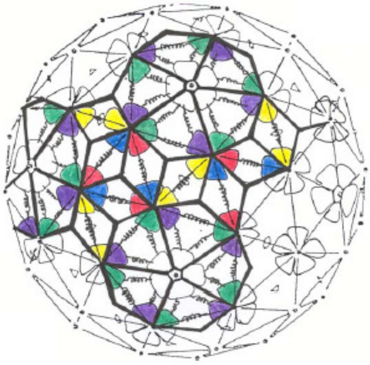

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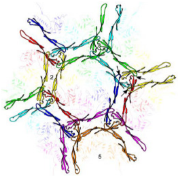
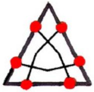
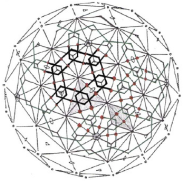
Viral Tiling Theory







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- Also dynamical properties of the capsid. How genetic material is released; resonant frequencies of the capsid

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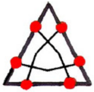

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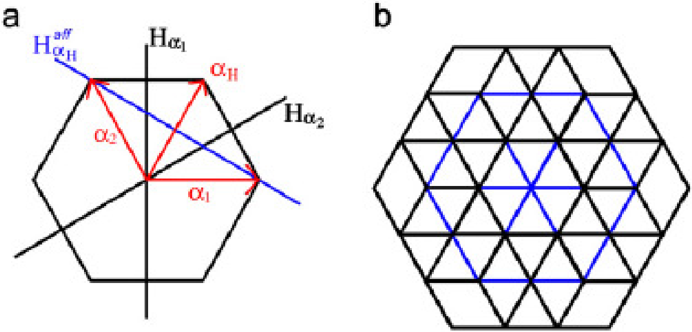
Aperiodic tilings, quasicrystals

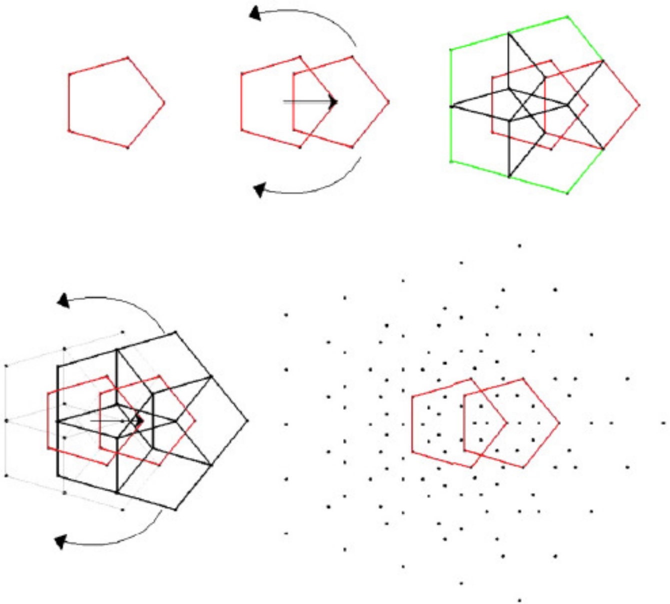
- *crystallographic groups* stabilize a lattice (i.e. a $\mathbb{Z}$-span of a basis).
- Coxeter groups of type H_3 and H_4 are not crystallographic.
- H_3 is the icosahedral group.
- There are “lattice-like” structures...

Affine extensions



We extend the group $sl(3,\mathbb{C})$ with a translation. This yields a triangular lattice.

Affine extension of H_2



Affine extension of H_2

- We extend the group C_5 with a translation T. This yields a dense orbit.
- If we restrict the number of times we are allowed to use the translation, we get part of quasi-lattice.
- For $s \in \mathbb{N}$ we define $M^s = \{$ words made from $C_5 \cup \{T\}$ where T appears at most s times $\}$.

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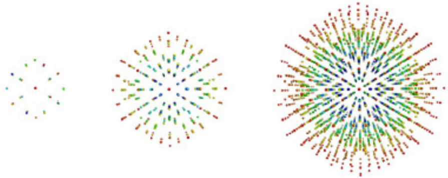
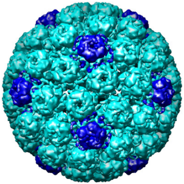
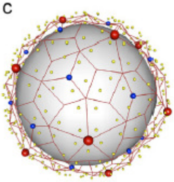


Layers in capsid structure





(Keef, Twarock, Elsawy 2008)

Other translations?

- Consider a finite group $G \leqslant GL(\mathbb{R}^k)$. Example: $\mathcal{I}$.
- For $v \in \mathbb{R}^k$ we can look at the orbit $G(v)$, a *starting configuration*. Example: the 12 vertices of an icosahedron.
- Locate the axes of (rotational) symmetry of $G(v)$.
- A translation T along an axis of symmetry is called admissible if there are at least two elements $u_1, u_2 \in G(v)$ for which Tu_1 and Tu_2 both on (different) axes of symmetry.

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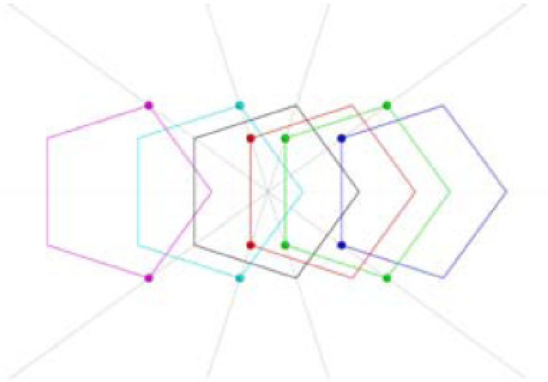
Admissible translations for C_5



Admissible translations for $\mathcal{I}$

	five fold	three fold	two fold
v vertex	3	4	6
v center of face	4	3	5
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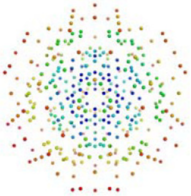

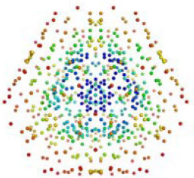

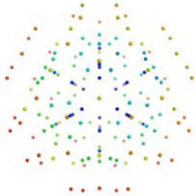

$$M^1 = \mathcal{I} \cup \{g_1 T g_2 \mid g_1, g_2 \in \mathcal{I}\}$$

Application

- VIPER database contains data about capsids of many viruses.
- Choose a virus.
- Compare outer layer to 41 outer layers we have.
- Scale the whole model.
- For Paricoto virus we get a good prediction of the fine structure of the capsid.
- You can combine several clouds.
- Group theoretical X-ray analysis of viruses!

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