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# RaY

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## Recent developments in mathematical virology

Pierre-Philippe Dechant

Pro Vice Chancellor's Office, York St John University  
York Cross-disciplinary Centre for Systems Analysis, University of York

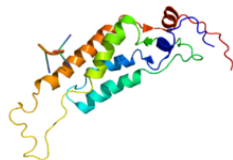
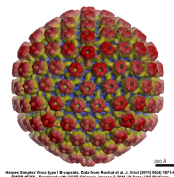
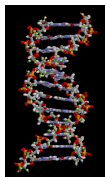
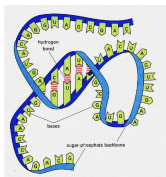
Non-linear Algebra in Applications, ICERM  
November 15, 2018

- 1 Virus structure and dynamics
  - Icosahedral symmetry
  - Tiling theory
  - Extended structures
  - Giant viruses
- 2 Virus assembly
  - MS2 and Packaging Signals
  - Virus-like Particles
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- 3 Disease dynamics
  - Intracellular – Replication
  - Immunological – Infection Dynamics
  - Modelling

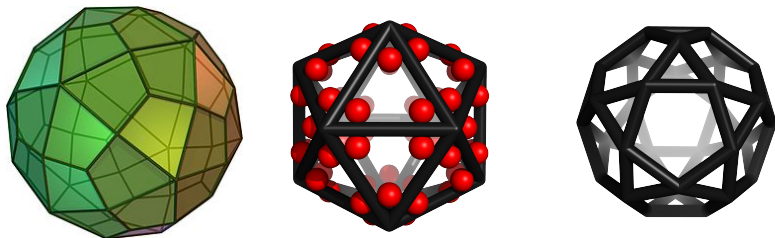
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# What is a Virus?

- Transported piece of **genetic information** that e.g. can run a programme in a host cell
- **Genome**: RNA or DNA
- Fragile – needs to be protected by a **protein** shell: **capsid**
- **Gene** → mRNA → **protein** (transcription and translation)
- Each **protein** = amino acid chain folds into a 3D shape: one **geometric building block**

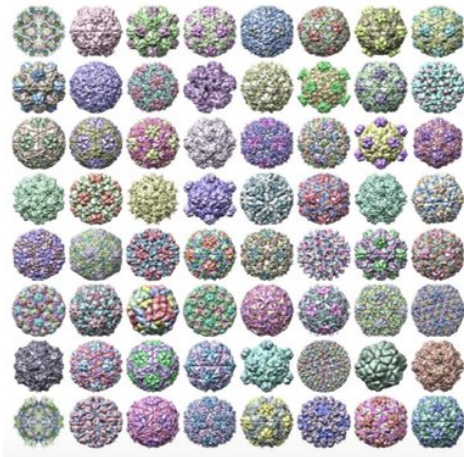


## Watson and Crick: The Icosahedron

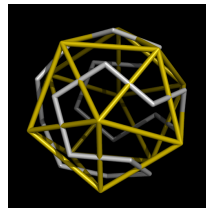
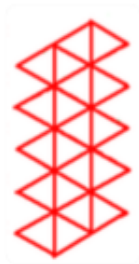
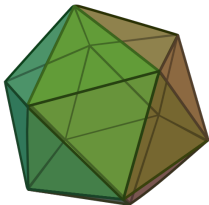


- **Crick&Watson**: Genetic economy  $\rightarrow$  symmetry  $\rightarrow$  icosahedral is largest
- **Rotational** icosahedral group is  $I = A_5$  of order 60
- **Full** icosahedral group is the **Coxeter group**  $H_3$  of order 120 (including reflections/inversion); generated by the **root system icosidodecahedron**

# Many viruses are icosahedral

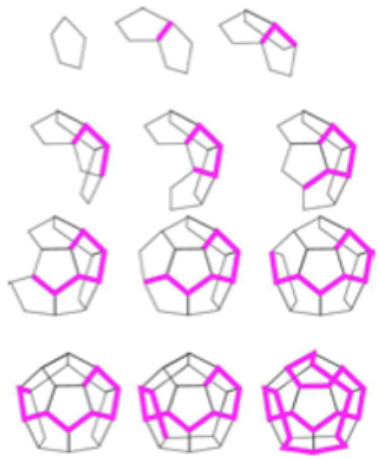
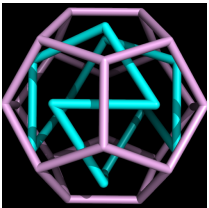


# Assembling an Icosahedron

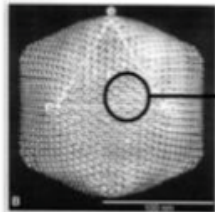


- Assemble from 20 identical triangular building blocks
- The order of addition gives a **Hamiltonian path** on the dual dodecahedron

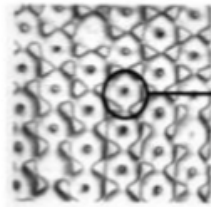
# Assembling a dodecahedron



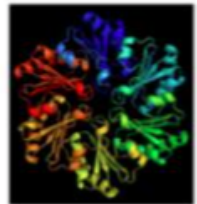
# More than just icosahedral symmetry?



Protein shell  
(viral **capsid**)



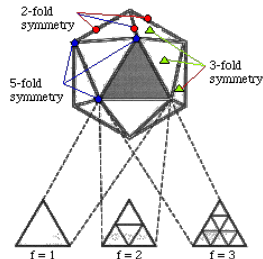
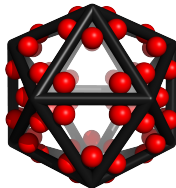
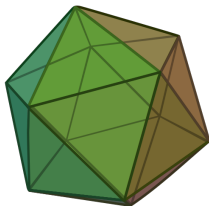
Protein clusters  
(**capsomeres**)



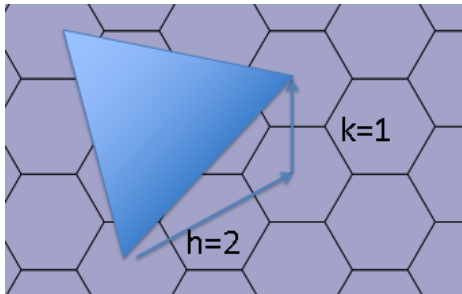
a cluster of 6  
proteins  
(hexamer)

## Caspar and Klug: Triangulations

- Mathematical upper limit of **60** for **equivalent** subunits, but biologically want to do better!
- Gene  $\rightarrow$  can already make a **triangle**  $\rightarrow$  might as well make **many!**
- Caspar-Klug ideas of quasi-equivalence and **triangulations**



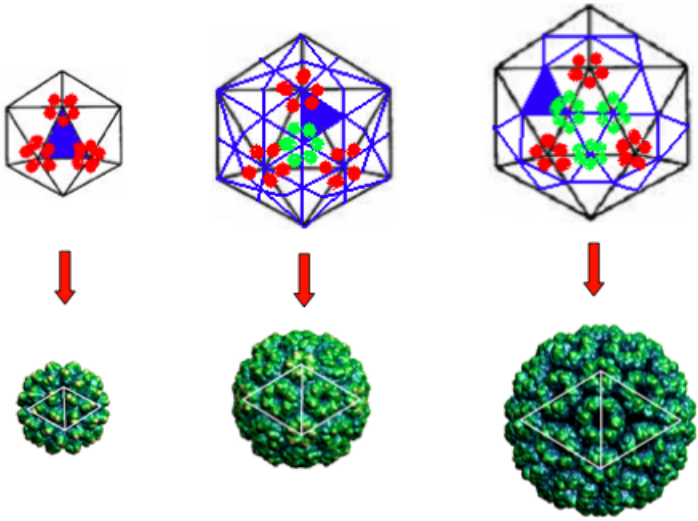
# Viruses: Caspar-Klug triangulations $T = h^2 + hk + k^2$



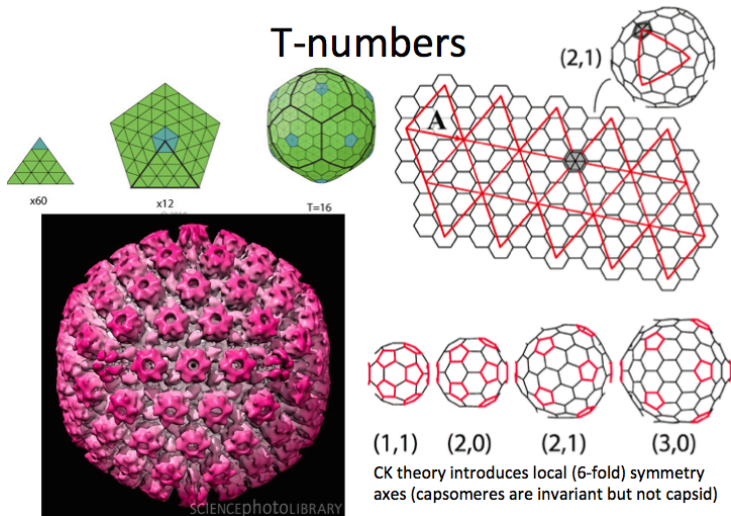
**integer** steps  $h$  and  $k$  in hexagonal directions give allowed triangulation numbers  $T = h^2 + hk + k^2$

$T$  **orbits** so  $60T$  proteins,  $60$  of which form **12** pentamers, and  $60(T - 1)$  form  **$10(T - 1)$**  hexamers

# Viruses: Caspar-Klug triangulations $T = h^2 + hk + h^2$



# Viruses: Caspar-Klug triangulations



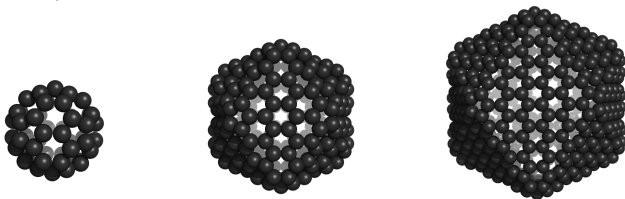
## The status quo for 40 years

- New insights in the 2000s from **Reidun Twarock** who essentially founded the field and other mathematical physicists (e.g. Anne Taormina etc)



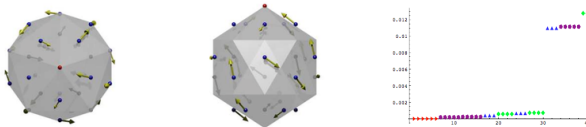
# Fullerenes

- other icosahedral objects in nature: football-shaped **fullerenes**
- Different shells with icosahedral symmetry: e.g.  $C_{60}$ ,  $C_{240}$ ,  $C_{540}$
- Follow Caspar-Klug-like layouts (e.g.  $T = h^2$  and  $T = 3h^2$  families)



# Vibrations of capsids and fullerenes

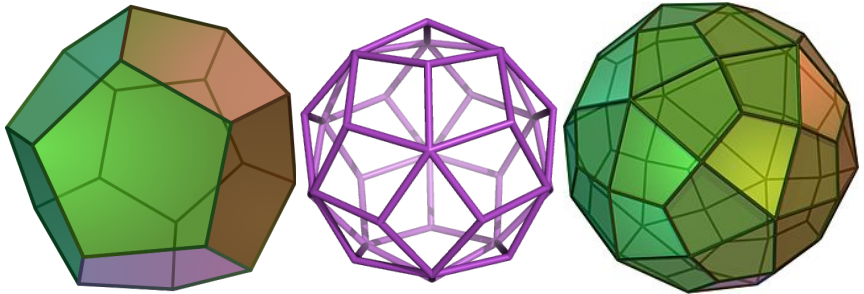
- **Normal modes/vibrations** of icosahedral capsids given by **representation** theory of the icosahedral group
- E.g.  $\Gamma_{\text{Icos}}^{\text{disp}} = \Gamma^1 + 3\Gamma^3 + \Gamma^{3'} + 2\Gamma^4 + 3\Gamma^5$
- Pioneered by Anne **Taormina**, Kasper **Peeters** and Francois **Englert**



$J$	1	$20C_2$	$15C_2$	$12C_2$	$12C_2'$
1	1	1	1	1	1
2	2	0	-1	$\sigma$	$\sigma$
3	3	0	-1	$\sigma$	$\sigma$
4	4	1	0	-1	-1
5	5	-1	1	0	0
Icos perm	12	0	0	2	2
$\chi_{\text{Icos}}$	36	0	0	$2\sigma$	$2\sigma$
Dodec	20	2	0	0	0
perm					
$\chi_{\text{Dodec}}$	60	0	0	0	0
IHD perm	30	0	2	0	0
$\chi_{\text{IHD}}$	90	0	-2	0	0
tr	30	0	0	0	0
perm					
$\chi_{\text{tr}}$	180	0	0	0	0

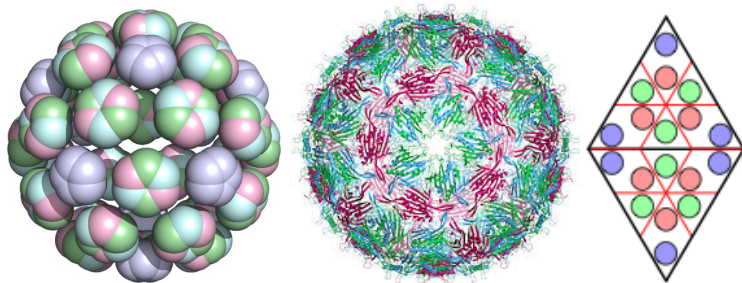
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## More general icosahedral tilings



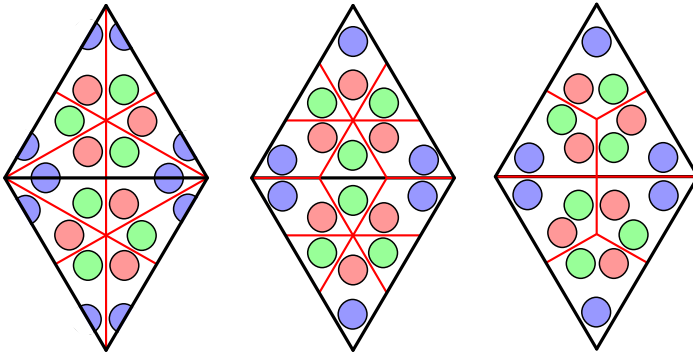
Other **tile shapes** can also give icosahedral tilings: **pentagons** (dodecahedron), **rhombuses** (rhombic triacontahedron), **kites** (deltoidal hexecontahedron)

# triangulations vs other quasi-equivalent tilings



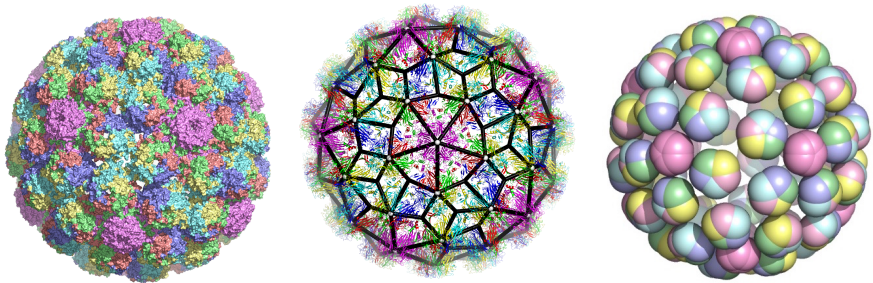
Two **viral surface** layouts: a  $T = 4$  **triangulation** (e.g. HBV) and a **rhombus** tiling (MS2) for a pseudo  $T = 3$  **triangulation**

## Other quasi-equivalent tilings



Three  $T = 3$  capsids: Polio, MS2 and Pariacoto

# A puzzle: non-quasiequivalent tilings – Penrose



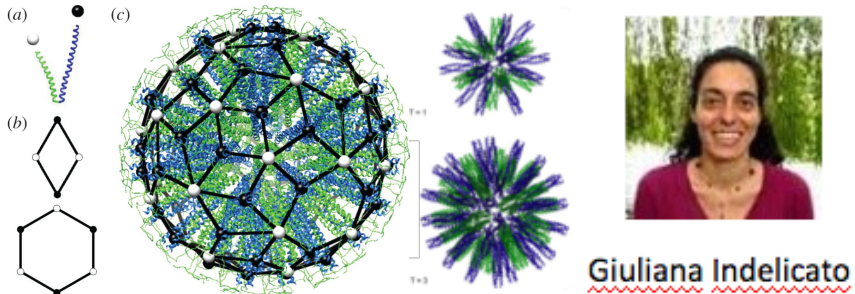
More general icosahedral tilings: Cryo-EM **reconstruction** of HPV, a **kite-rhombus** tiling and a pseudo  $T = 7$  **triangulation**.

# Architecture

- **Triangulations:** Buckminster Fuller geodesic domes
- **kite-rhombus tiling:** the new Amazon HQ



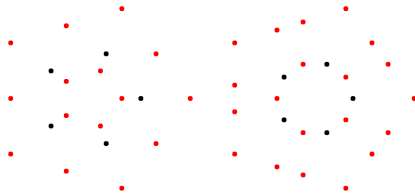
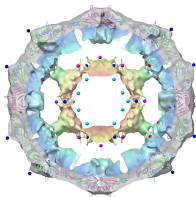
# Self-assembling protein nanoparticles



Quantized e.g. in mass spec - predict units by symmetry. Particles eg. for vaccine design

## More general symmetry still?

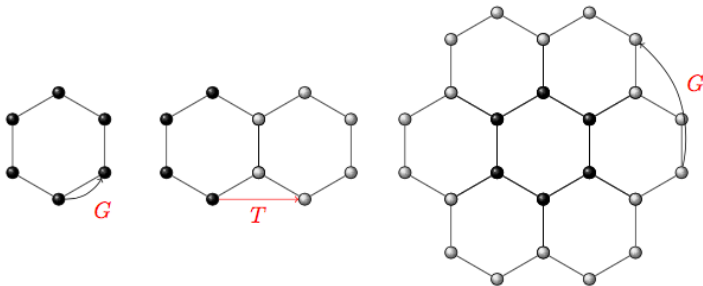
- Improves the limit to  $60T$ , but only in terms of **surface structures** (12 pentagons and rest hexagons).
- Making the symmetry non-compact might allow more general symmetry, **simultaneously constraining** different 'radial levels'
- Non-compact generator is a **translation** – motivates looking into **affine extensions** of icosahedral symmetry
- There is an **inherent length scale** in the problem – given by size of nucleic acid/protein molecules



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## Affine extensions - $A_2$

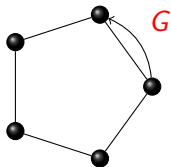
Unit translation along a vertex of a unit hexagon



A **random** translation would give 6 secondary hexagons, i.e. 36 points. Here we have **degeneracies** due to '**coinciding points**', and building up the hexagonal lattice.

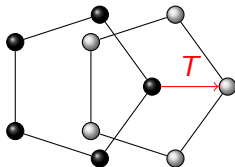
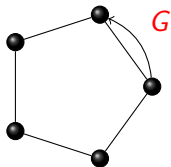
# Affine extensions of non-crystallographic groups?

Unit translation along a vertex of a unit pentagon



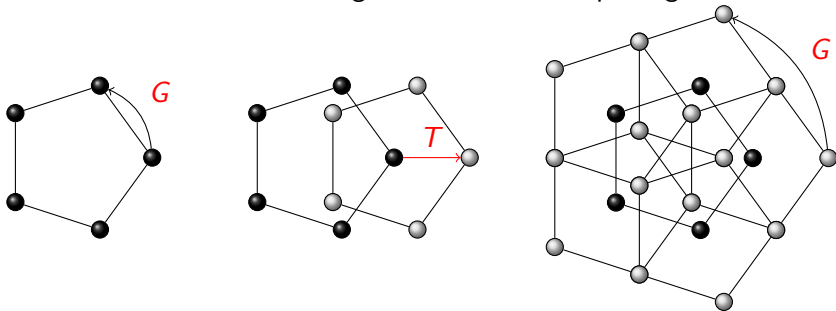
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# Affine extensions of non-crystallographic groups?

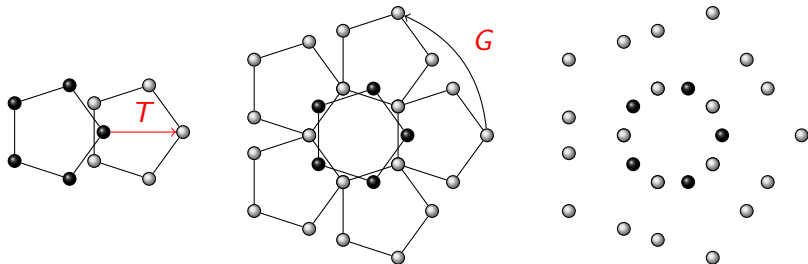
Unit translation along a vertex of a unit pentagon



A **random** translation would give 5 secondary pentagons, i.e. 25 points. Here we have **degeneracies** due to '**coinciding points**'.

# Affine extensions of non-crystallographic root systems?

Translation of length  $\tau = \frac{1}{2}(1 + \sqrt{5}) \approx 1.618$  (golden ratio)

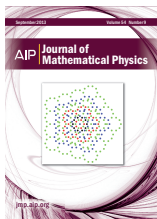


Cartoon version of a **virus** or **carbon onion**. Would there be an **evolutionary benefit** to have more than just compact symmetry?

The problem has an **intrinsic length scale**.

# Affine extensions of non-crystallographic Coxeter groups

- 2D and 3D **point arrays** for applications to viruses, fullerenes, quasicrystals, proteins etc
- Two complementary ways** to construct these



## Know your onions

Acta Cryst. A 70, 162-167 (2014)

Many viruses have icosahedral symmetry. So do certain 'carbon onions' — Russian doll-like arrangements of nested fullerenes. Pierre-Philippe Dechant and colleagues argue that viruses and carbon onions share the same formation principle: affine symmetry. Imagine a set of points lying on the vertices of a regular pentagon. Duplicate the set, and translate it, then repeatedly rotate the combined set over  $72^\circ$  about the midpoint of the original pentagon. This results in a new set of points obeying five-fold symmetry, set with a 2D shell structure that is more complex than that of the pentagon. A similar application of the 3D icosahedral group results in a set of points that are nodes in the highly complex protein network structure of, for example, the Herpesvirus virion.

Dechant *et al.* found that affine symmetry explains the structure of experimentally observed carbon onions — a non-trivial result given that all carbon atoms in each of the nested fullerene molecules must be three-connected, that is, bound to three neighbouring carbons. In particular, they identified the extended group that, starting from buckminsterfullerene (the 'buckyball'), generates the onion  $C_{20} @ C_{40} @ C_{60}$ .

well-known effect for photons, and it turns out to hold for other quantum particles too. James Fokianos and colleagues have performed the Hong–Ou–Mandel quantum interference experiment using plasmons, which are quantized surface plasma waves. Pairs of photons are fed into a specially designed plasmonic waveguide that mixes the paths of the light-excited surface plasmons in the same way as a beam splitter. The outcome is converted back into photons and measured by two detectors. As in the purely photonic case, the characteristic dip in coincidence rate is there, showing that the photons remain indistinguishable when they are converted into plasmons and back. **IG**

Written by Mary Chu, Kiko Giorgani, Abigail Kopper, Bert Verberck and Adam Wilson

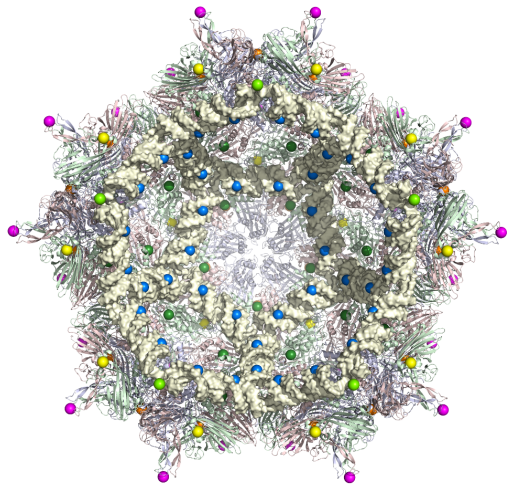
NATURE PHYSICS • VOL 10 | APRIL 2014 | www.nature.com/naturephysics

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## Other ideas

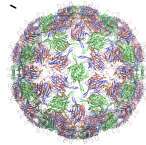
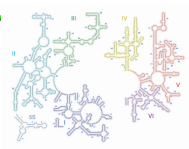
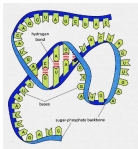
- **Project** symmetry orbits in 6D to get finite extended icosahedral **point arrays** (Emilio Zappa)
- Use projection to find **3D tiles** to model viruses (David Salthouse)
- Use projection to model transitions between capsids via **lattice transitions** in 6D (Giuliana Indelicato)

# Use in Mathematical Virology



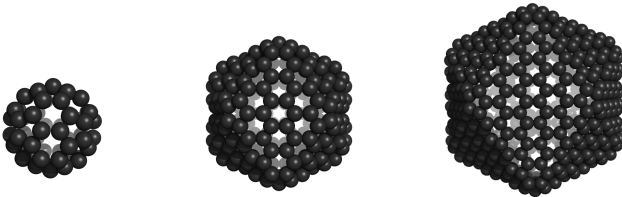
# New insight into RNA virus assembly

- There are **specific interactions** between **RNA** and coat protein (**CP**) given by icosahedral **symmetry** axes
- Essential for **assembly**, as only this RNA-CP interaction turns CP into **right geometric** shape for **capsid formation**
- **Hamiltonian cycle** visiting each RNA-CP contact once – dictated by symmetry
- Even the RNA has an **icosahedrally ordered component**



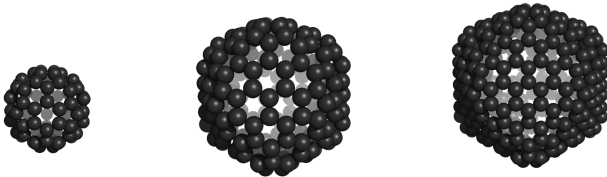
## Extension to fullerenes: carbon onions

- Extend idea of affine symmetry to other icosahedral objects in nature: football-shaped **fullerenes** (with Jess Wardman)
- Recover different shells with icosahedral symmetry from affine approach: **carbon onions** ( $C_{60} - C_{240} - C_{540}$ )



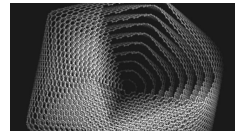
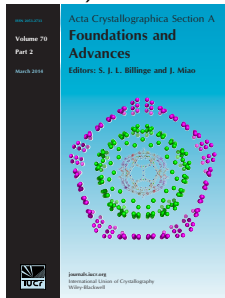
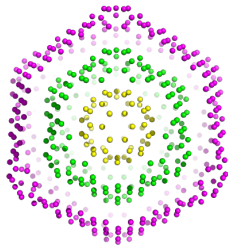
## Extension to fullerenes: carbon onions

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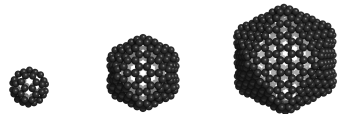
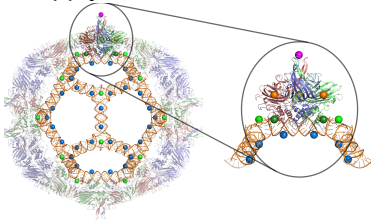
# Viruses and fullerenes – symmetry as a common thread?

- Get nested arrangements like Russian dolls: **carbon onions** (e.g. Nature 510, 250253)



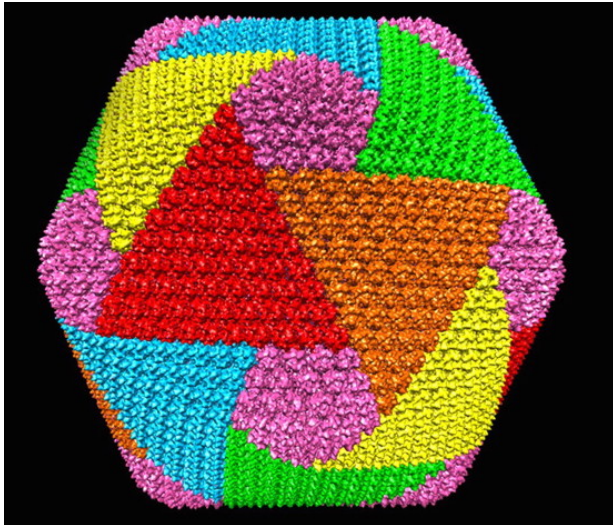
## Two examples

- Non-compact symmetry that relates **different structural features** in the same polyhedral object when there is an additional **length scale**
- **Novel symmetry principle** in Nature, shown that it seems to apply to at least **fullerenes** and **viruses**

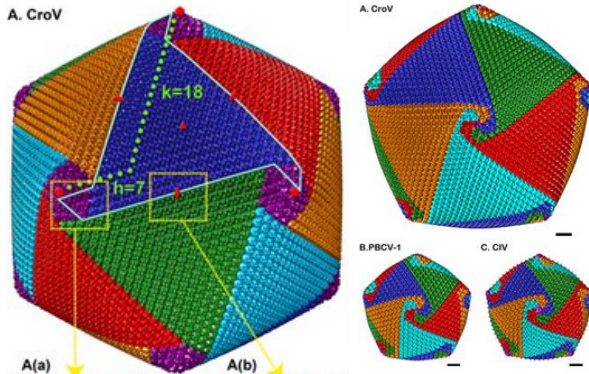


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# Giant viruses

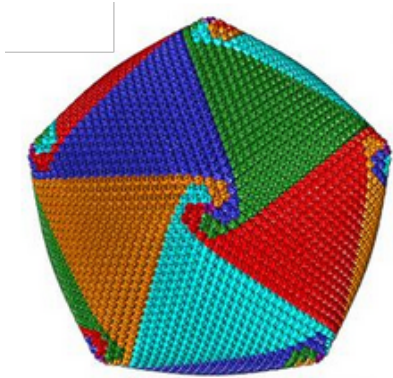


# A common approach – little hooks



Pentasymmetrons and trisymmetrons

# A common approach – little hooks

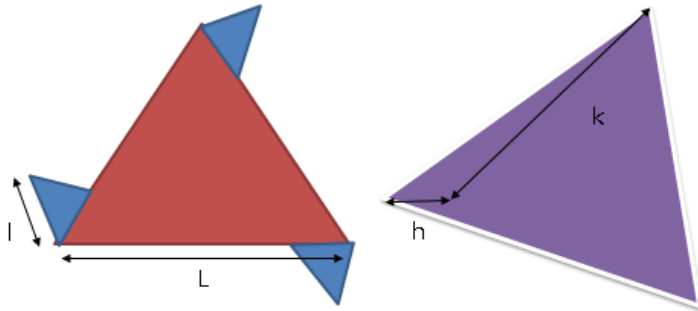


Pentasymmetrons and trisymmetrons

## A family of solutions: $h = 7$ – and some gaps

- Chilo iridescent virus:  $T = 147$ ,  $h = 7$  and  $k = 7$
- Paramecium bursaria Chlorella virus 1:  $T = 169$ ,  $h = 7$  and  $k = 8$
- Phaeocystis pouchetti virus:  $T = 219$ ,  $h = 7$  and  $k = 10$
- Faustovirus:  $T = 277$ ,  $h = 7$  and  $k = 12$
- Pacman virus:  $T = 309$ ,  $h = 7$  and  $k = 13$
- Cafeteria roenbergensis:  $T = 499$ ,  $h = 7$  and  $k = 18$

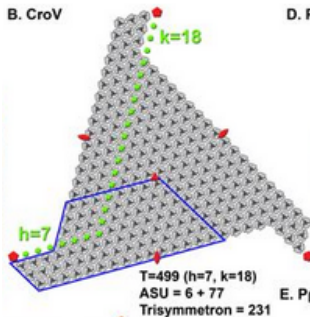
## Count areas?



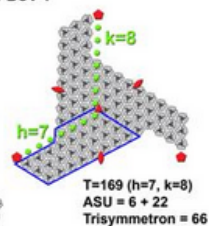
When is there an **equivalent** description in terms of Caspar-Klug  $h$  and  $k$ ?

# Count hexagons

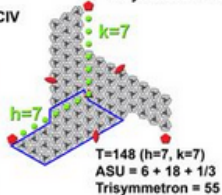
B. CroV



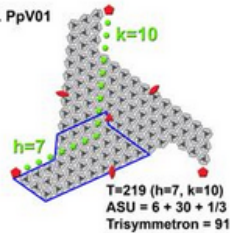
D. PBCV-1



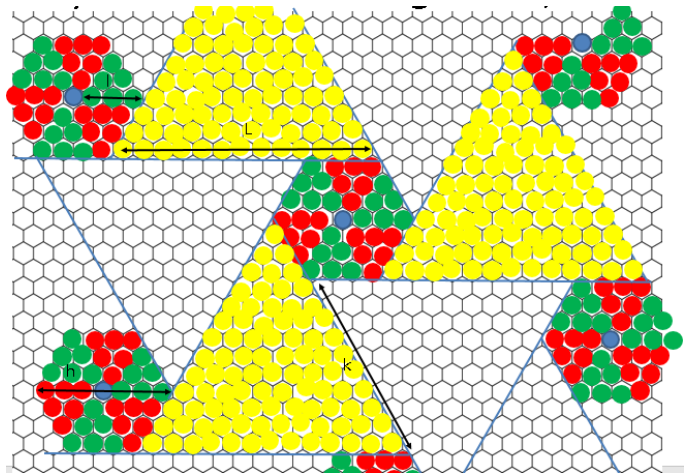
C. CIV



E. PpV01



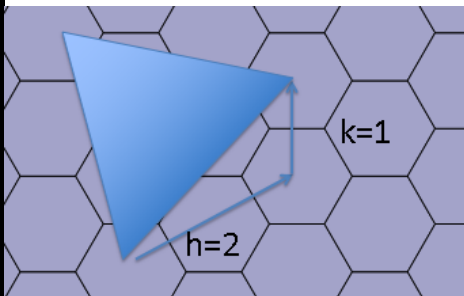
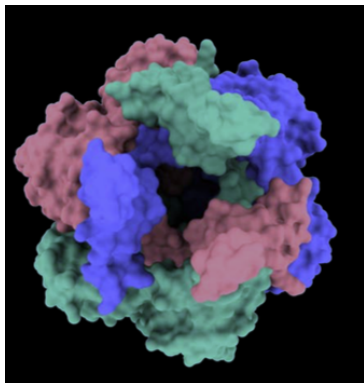
# Trisymmetrons and Pentasymmetrons – how to count



## Trisymmetrons and Pentasymmetrons – how to count

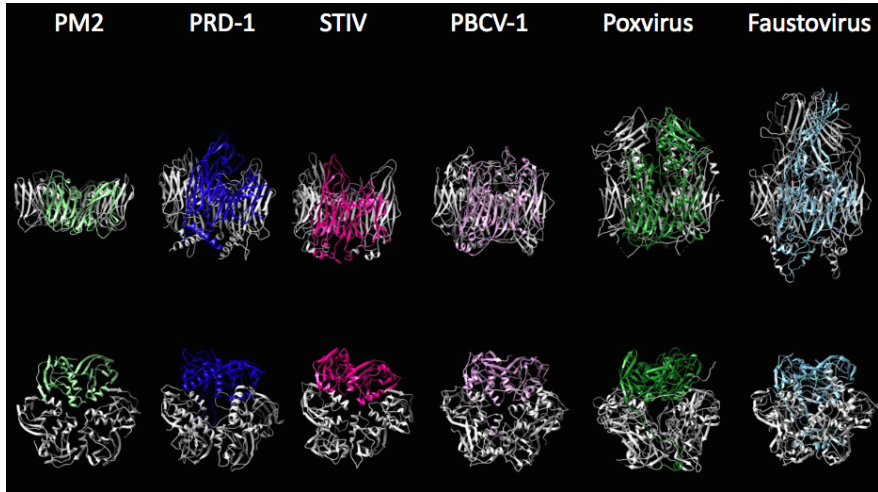
- Each has  $I(I+1)/2$  or  $L(L+1)/2$  hexamers
- So in total  $20(3I(I+1)/2 + L(L+1)/2)$
- Caspar-Klug theory predicts  $10(T-1) = 10(h^2 + hk + k^2 - 1)$
- So for **which**  $h, k, I, L$  can there be equality?
- Turns out for  $h = 2I + 1$  and  $k = L - I$  this **holds identically**
- So can have **odd**  $h$  and **any**  $k$

## Major capsid protein

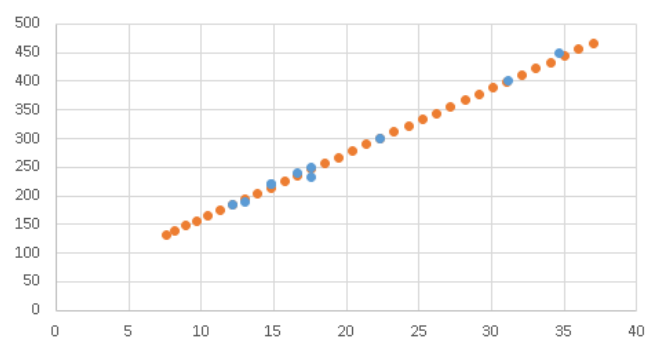


$T$  is an **area**, so  $\sqrt{T}$  gives **size** of triangle and thus also **particle diameter**

# Major capsid protein – evolutionary conservation

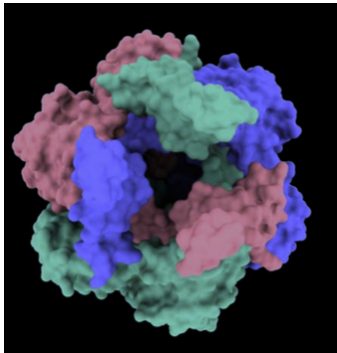


# Scaling

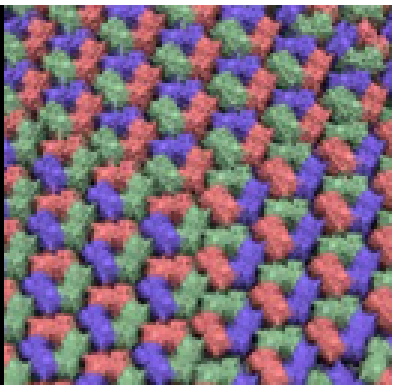
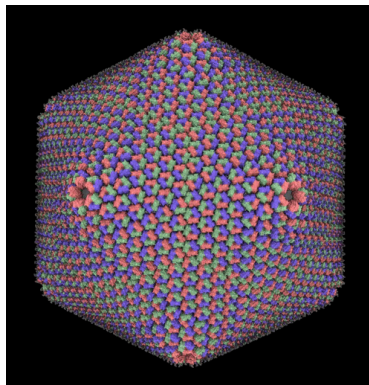


Missing points allowed geometrically but less **stable**? Or just not yet **discovered**? **Predict** Tetraselmis virus 1 TetV-1 of  $257\text{nm} \pm 9\text{nm}$  is exactly  $T = 343$ . **Predict holes in family exist and sizes** given by this scaling

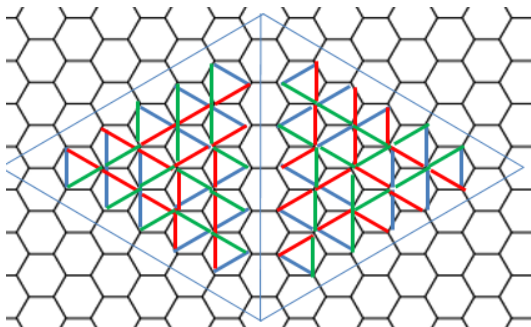
# Major capsid protein – trimer / pseudo-hexamer



# Decorations – threefold and giants



## Decorations – threefold and giants

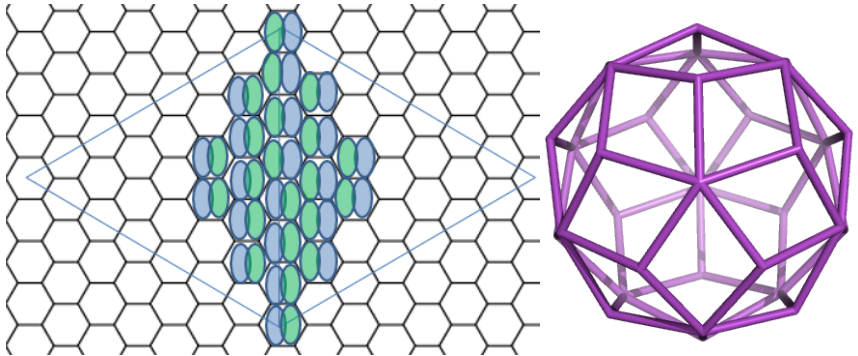


Use hexagonal tiling unit with **decorations** that partially **break** the symmetry: 6, 3, 2, 1

If respect the **3-fold** axis, then still have **partial lattice** symmetry!

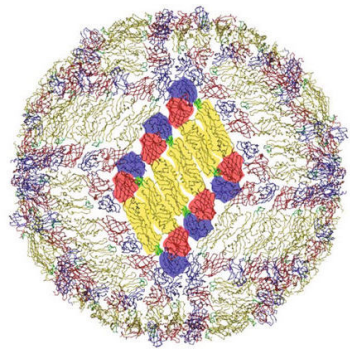
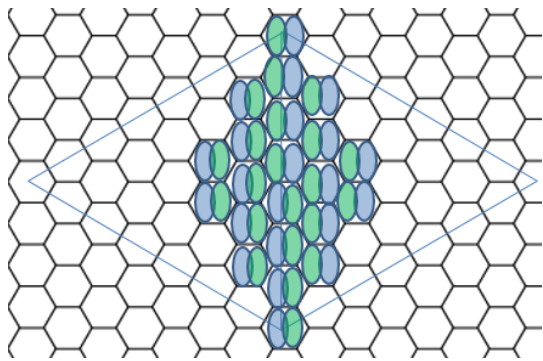
Defects/domain walls at the other symmetry axes

## Decorations – twofold case



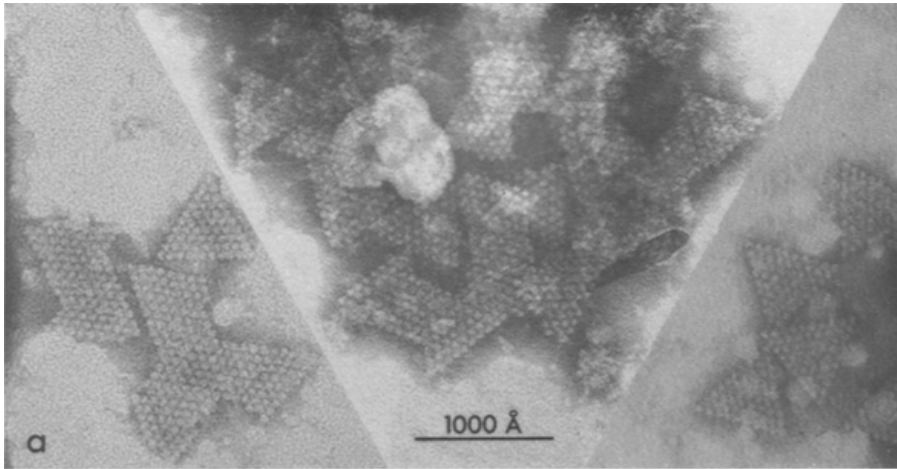
Symmetric with respect to **2-fold** axis – quasi-lattice symmetry  
Looks like a rhombic triacontahedron all over again

# Decorations – twofold and Zika

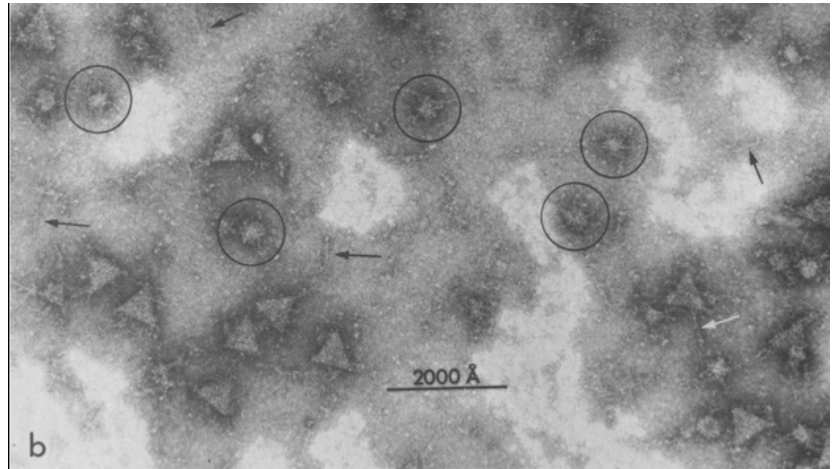


This is exactly what **Zika** looks like

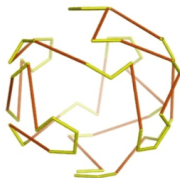
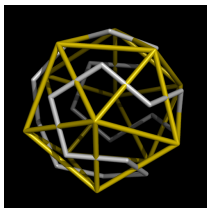
# Trisymmetrons and Pentasymmetrons



# Major capsid protein - trimer, pseudohexamer



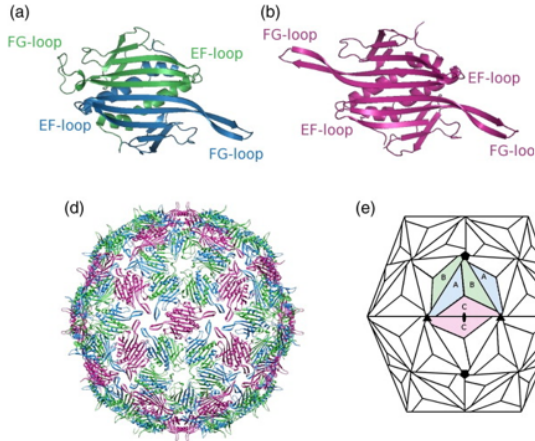
# Build from prearranged blocks? Back to Hamiltonian paths



- Are the trisymmetrons and pentasymmetrons **preformed**? (or is that just what virions **fall apart** into?)
- If **trisymmetrons** are assembled then we're back to a **Hamiltonian path** for the icosahedron
- If **pentasymmetrons** then get a slightly **new polyhedron**

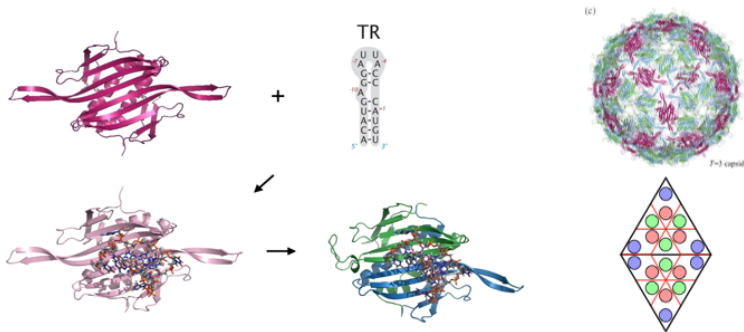
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# MS2 tiling and dimeric building blocks: A/B and C/C



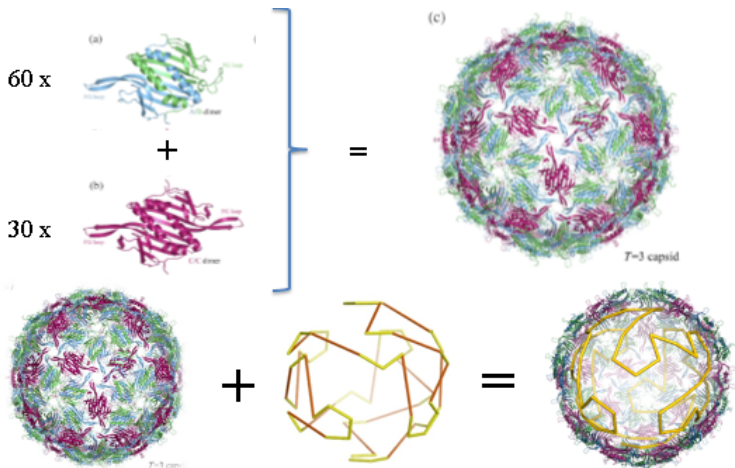
## Need to bind RNA in 60 places

The TR sequence is known to **initiate assembly** by associating with the **maturation protein**. It forms a **stemloop** and it has been shown that the **stemloop changes the conformation** of the **symmetric C/C dimer** to the **asymmetric A/B dimer** (allosteric switch).



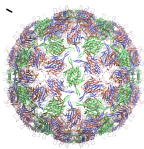
Peter Stockley (Leeds), Neil Ranson (Leeds), Eric Dykeman (York)

# MS2 Hamiltonian path

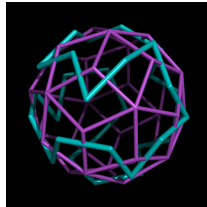
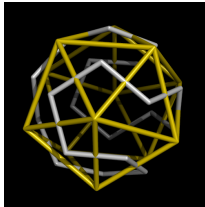
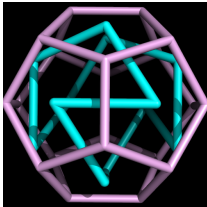


# New insight into RNA virus assembly

- More realistic examples for MS has **60 vertices** with 41,000 paths
- The RNA is actually **circularised** by Maturation Protein: only **66 cycles**
- With thermodynamical **assembly kinetics** and **5-fold averaging** experiments **uniquely** identified an **evolutionarily conserved** cycle
- **Patents** for new **antiviral strategies** and **virus-like nanoparticles** e.g. for **drug delivery** (Twarock group)



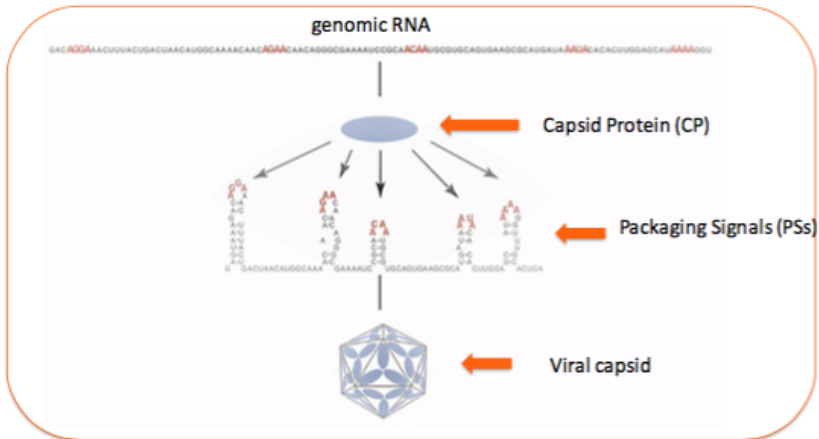
## Hamiltonian cycles on icosahedral solids



- So **interaction contacts** are given by the **symmetry**
- Orbits of the interaction points have to be visited by the **RNA exactly once**
- Even the RNA has an **icosahedrally ordered component**
- **Hamiltonian cycles** for dodecahedron, icosahedron and rhombic triacontahedron

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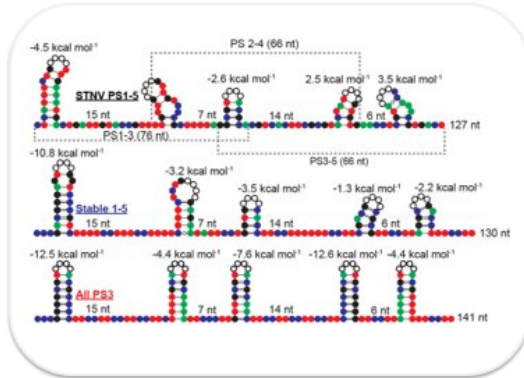
# Multiple dispersed Packaging Signals paradigm





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  - **Virus-like Particles**
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# Engineering Packaging Signals to make VLPs



Improved sequences assemble twice as efficiently (Nikesh Patel).  
Potential applications to vaccines or drug delivery.

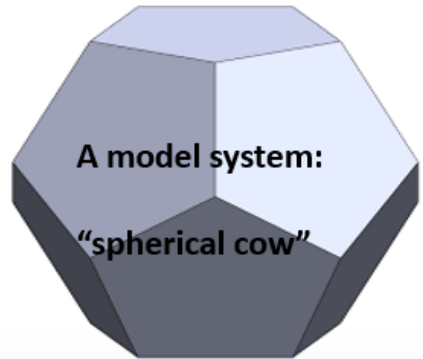
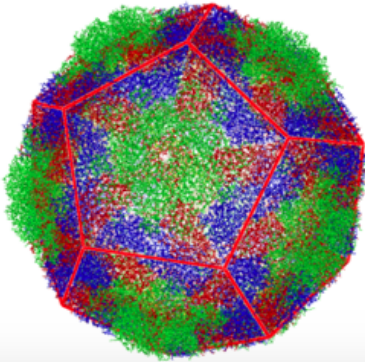
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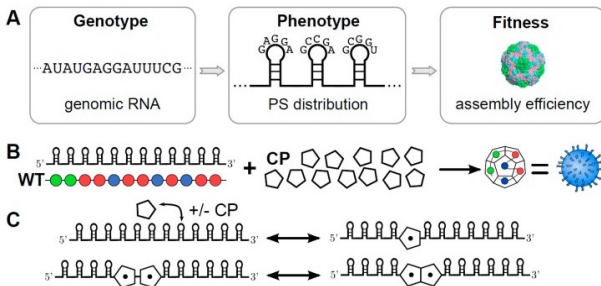
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# Dodecahedral cow (Rich Bingham)



# Viral evolution and quasispecies

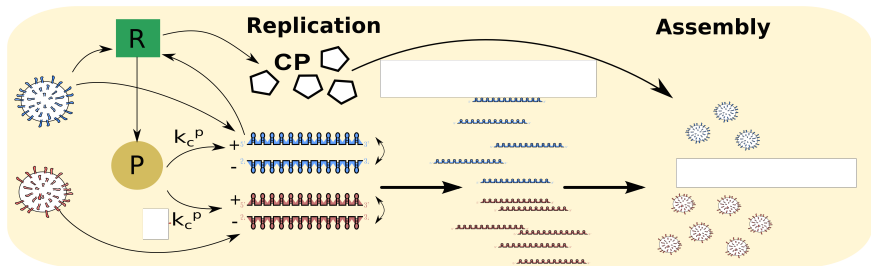


A **phenomenological** genome space of 12 packaging signals with 3 binding **affinity** bands (weak, medium, strong). Can compute the **whole** space explicitly in terms of **assembly efficiency**.

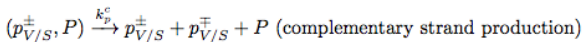
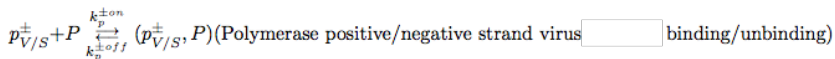
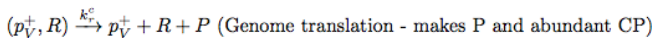
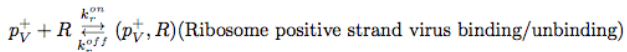
# Simulations

- **Stochastic** simulations rather than ODE models because of discrete nature and low numbers
- **Gillespie** algorithm that selects a random reaction to occur (Eric Dykeman)
- Couple an **intracellular** model (replication) with an **infection model** (immune system)

# Intracellular model: replication

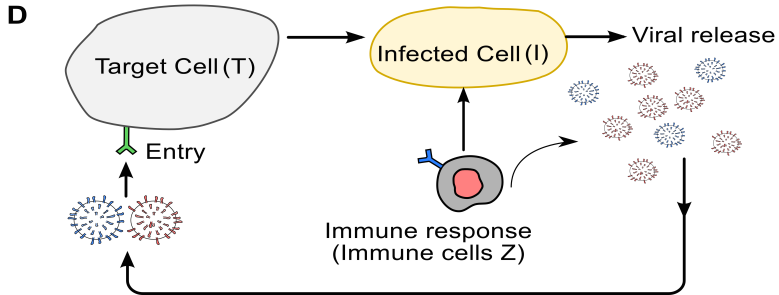


# Intracellular reactions

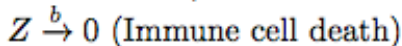
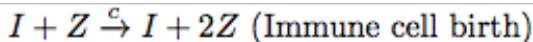
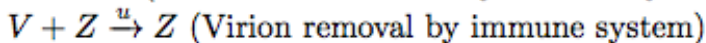
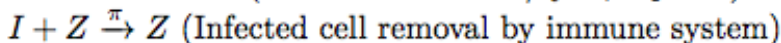
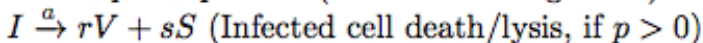
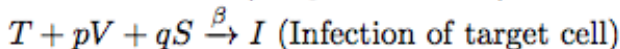
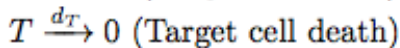
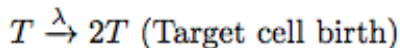


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# Infection model: immune system

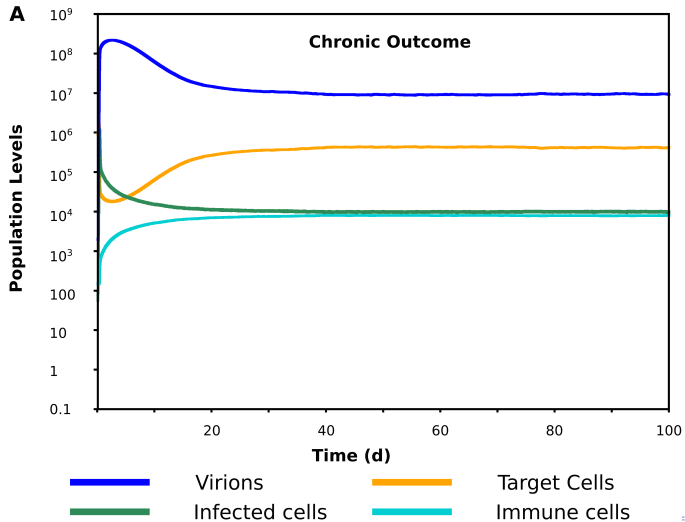


## Immune cell reactions

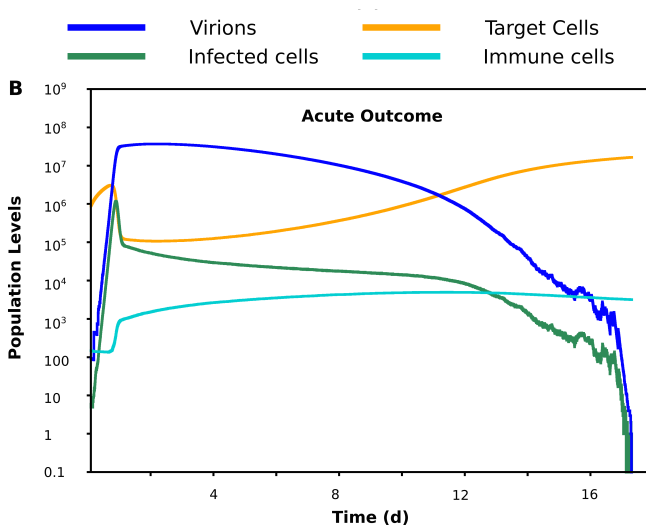


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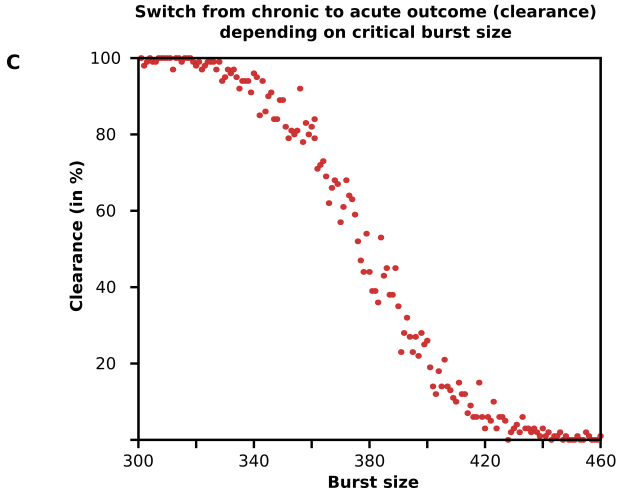
# Chronic infections



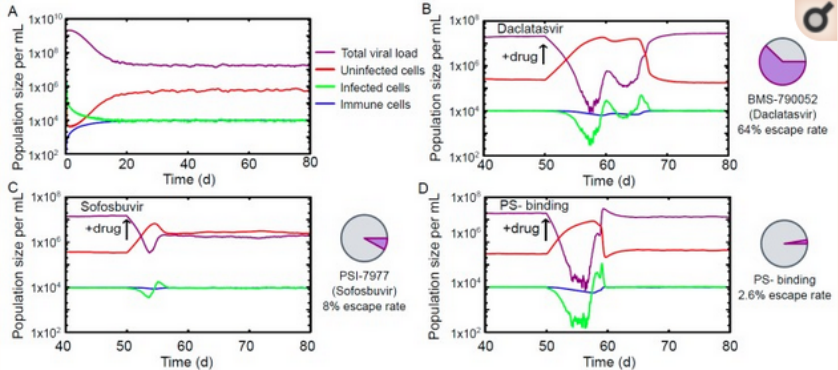
# Acute infections



# Transition between chronic and acute



# Evolutionarily stable drugs



# Summary of mathematical virology

- a truly diverse **interdisciplinary** endeavour: group theory, tiling theory, dynamical systems, graph theory, computational modelling, biophysics, bioinformatics, biochemistry, cell biology, structural biology, immunology
- **curiosity**-driven and **impactful**: from understanding a structural puzzle to a new generation of **anti-virals** – by accident

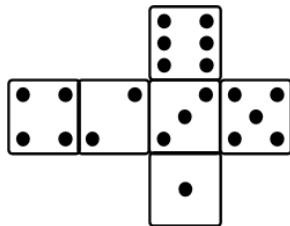
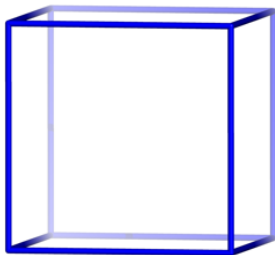
## Other algebraic interests

- **exceptional** root systems/geometries
- (reflexive) **polytopes**
- **Clifford** algebras
- **ADE** correspondences

Thank you!  
LGBTQ+ lunch at 1pm.

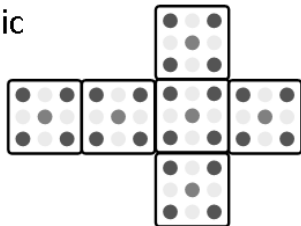
## Symmetry averaging

- As an example use the symmetry of a **cube**
- (axes of 4-fold, 3-fold and 2-fold symmetry)
- **Dice have approximately** cubic symmetry, but have slightly **asymmetric** features (the faces)



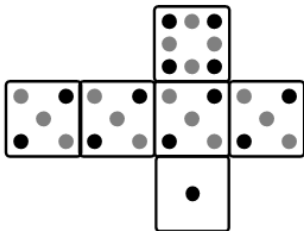
## Symmetry averaging

- As an example use the symmetry of a **cube**
- **Approximately** cubic symmetry, but have slightly **asymmetric** features (the faces)
- Experiment averages over all **orientations**
- **Washes out** all asymmetric features

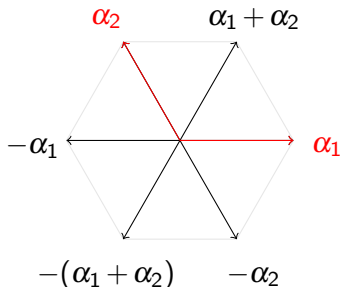


## Symmetry averaging

- Assume we have a **distinguished face**, e.g. 1 is always at the bottom
- The 6 can be in **two** configurations
- Average over **the other 4 faces**



# Root systems



reflection/Coxeter groups

**Root system**  $\Phi$ : set of vectors  $\alpha$  in a **vector space** with an **inner product** such that

- $\Phi \cap \mathbb{R}\alpha = \{-\alpha, \alpha\} \forall \alpha \in \Phi$
- $s_\alpha \Phi = \Phi \forall \alpha \in \Phi$

**Simple roots**: express every element of  $\Phi$  via a  **$\mathbb{Z}$ -linear combination**.

$$s_\alpha : v \rightarrow s_\alpha(v) = v - 2 \frac{(v|\alpha)}{(\alpha|\alpha)} \alpha$$

# Affine extensions

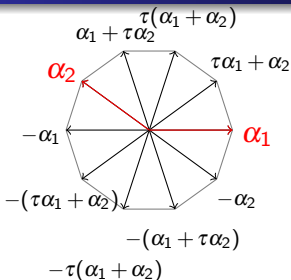
An **affine Coxeter group** is the extension of a Coxeter group by an **affine reflection in a hyperplane not containing the origin**  $s_{\alpha_0}^{aff}$  whose geometric action is given by

$$s_{\alpha_0}^{aff} v = \alpha_0 + v - \frac{2(\alpha_0 | v)}{(\alpha_0 | \alpha_0)} \alpha_0$$

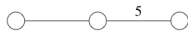
**Non-distance preserving:** includes the **translation generator**

$$Tv = v + \alpha_0 = s_{\alpha_0}^{aff} s_{\alpha_0} v$$

# Non-crystallographic Coxeter groups $H_2 \subset H_3 \subset H_4$



$$A = \begin{pmatrix} 2 & -\tau \\ -\tau & 2 \end{pmatrix}$$



$$A = \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -\tau \\ 0 & -\tau & 2 \end{pmatrix}$$



$$A = \begin{pmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -\tau \\ 0 & 0 & -\tau & 2 \end{pmatrix}$$

$H_2 \subset H_3 \subset H_4$ : 10, 120, 14,400 elements, the only Coxeter groups that generate **rotational symmetries of order 5** linear combinations now in the **extended integer ring**

$$\mathbb{Z}[\tau] = \{a + \tau b \mid a, b \in \mathbb{Z}\}$$

**golden ratio**

$$\tau = \frac{1}{2}(1 + \sqrt{5}) = 2 \cos \frac{\pi}{5}$$

$$x^2 = x + 1$$

$$\tau' = \sigma = \frac{1}{2}(1 - \sqrt{5}) = 2 \cos \frac{2\pi}{5}$$

$$\tau + \sigma = 1, \tau\sigma = -1$$