EXPANDABLE POLYHEDRAL VIRUSES – KINEMATICS IN BIOLOGY

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Publications and/or Exhibitions:

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Abstract: *The word "mechanism" is commonly associated with technical sciences. Altogether, there are some bright examples of them among living organisms such as in certain polyhedral viruses that are able to change their diameter by means of a symmetric rotational-translational motion. Mechanical modeling of this mechanism can provide deeper insight to natural kinematical processes and can give hints for structural engineering. First stage of modeling is the physical one that was built to simulate the observed motions, and then a numerical modeling follows done by computer analysis. Compound symmetric structures with multiple sets of independent infinitesimal displacements – as occur in this analysis – require efficient tools to interpret the motions in a physically plausible form: in our practice the group theory*

was explored. Finally, some general conclusions are drawn about infinitesimal mobility of the physical model, extended to a family of slightly different polyhedral mechanisms.

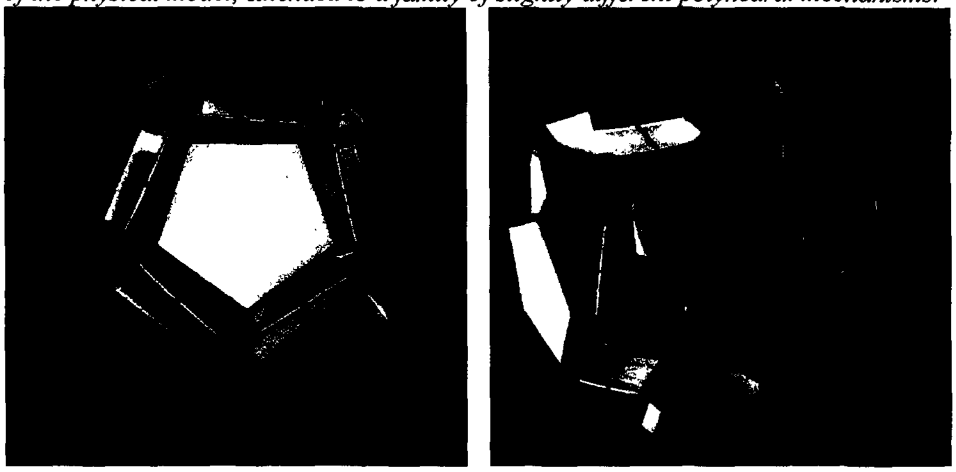

Fig. 1: Cardboard model of an expandable dodecahedral virus, closed and expanded.

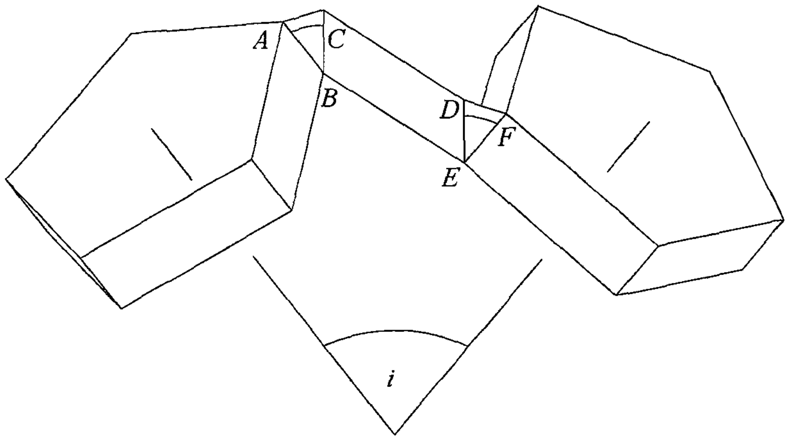

Fig. 2: Two pentagonal prisms and their connection

1 PHYSICAL MODEL

Biologists recently discovered some virus species that represent real mechanisms in nature. These structures are built of pentamers and hexamers (pentagonal and hexagonal faces) that are able to rotate and translate about their own axis if the pH of the environment changes. All this highly symmetric displacement is constrained by double protein links between two adjacent faces (Speir et al., 1995).

In terms of structural mechanics, the question is how to model the protein links in these viruses in order to get the same type of mechanism like the original one? Our cardboard model is one of the possible answers where double links are substituted by single but planar ones, composed of triangular and rectangular elements. For the sake of simplicity, only twelve pentamers are used that produced a dodecahedral arrangement (Fig. 1). All members except for the hinges are supposed to be rigid, so all mechanisms must be inextensional.

It is quite straightforward that linking structure between adjacent faces essentially determines the kinematical behavior of the structure. In this particular case, adjacent faces are connected to each other by means of a linkage composed of four ("fold"-type) hinges and a triangle (*ABC*), a rectangle and again a triangle (*DEF*) among them (Fig.2). Following just this one-parameter finite motion shown in Fig. 1, a direct relationship can be established between the amount of rotation of each face and the diameter of the circumscribed sphere of the structure: to the rotation of $\pi/5$ (from the thoroughly closed configuration to the open state) belongs a 1.77 times larger diameter. Note that a fully expanded configuration means a truncated icosahedral form – like a soccer ball – and means a point of kinematical bifurcation, but the real range of expansion for the viruses does not include this extreme configuration.

It can be verified on the physical model, however, that the structure has other – probably not finite – mechanisms: it is possible, for example, to lift infinitesimally just one face prism while the others remain fixed. The existence of this "face mechanism" can be easily proved through elementary geometrical arguments: it is evident that face mechanism means a pure translation in closed state, but pure rotation at the bifurcation point.

2 NUMERICAL ANALYSIS

Due to the design principles, the structure is able to imitate the expanding motion of viruses. At the same time, however, the structure might have other kind of mechanisms, coupled to the previous one. To discover these additional motions, a detailed cinematic analysis was done in two steps (Kavas & Tania, 2001). First: just by counting cinematic constraints and unknowns it turned out that the structure must have at least six infinitesimal mechanisms (rigid body motions are not considered among them), second: the singular value decomposition of the compatibility matrix has shown nine more mechanisms.

Regarding the possibility of coupling, it is quite complicated to interpret such a big amount of independent systems of displacements. To make this task easier, some considerations on symmetry were introduced by means of group theory (Kangwai, 1997). The result is that twelve of the fifteen mechanisms come from the individual infinitesimal translation-rotation of each face, while the remaining three ones belong to a certain symmetry group (T3) (Fowler et al., 2002) but their physical meaning is not clarified yet – they are very likely to be also infinitesimal that would mean that only one of the mechanisms (the totally symmetric expansion) is finite, as experimented in nature. Note that in this case many of independent self–stress-states must occur in the structure that are not investigated till the moment.

Interestingly enough, the analysis above can also be carried out for other expandable structures based on trivalent polyhedra, i. e. tetrahedron and cube (Fowler et al., 2002): according to the results, the six mechanisms by counting and face mechanisms plus three T3-mechanisms by matrix analysis are unchanged that supposes a more general cinematic property behind this kind of virus models.

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