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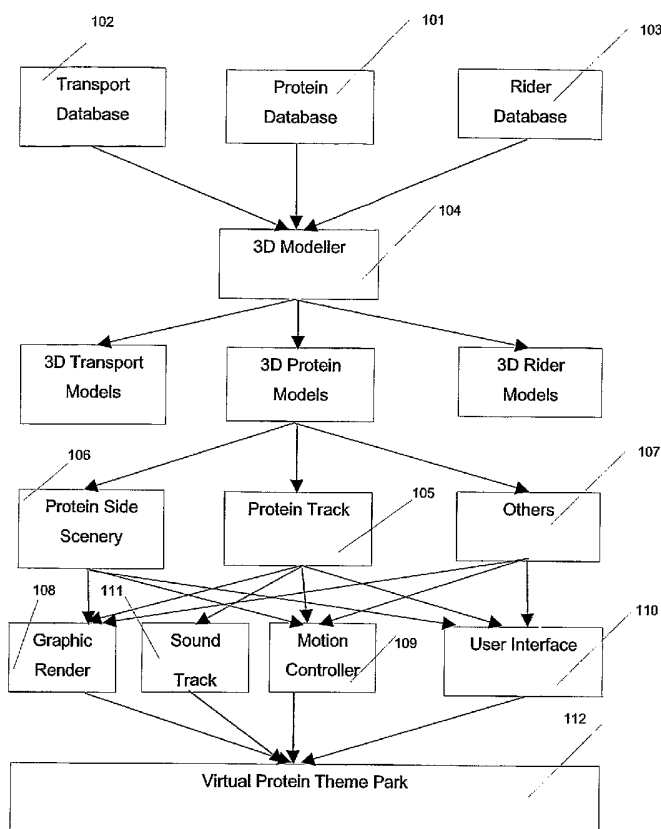
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(54) Title: VIRTUAL PROTEIN THEME PARK



(57) Abstract: A virtual theme park has attractions which are based upon protein chains at large scale, the users being able to use these protein tracks with virtual transports such as roller coasters, water rides, ski rides, skate scooters, skate boards, racing cars, bicycles, motorcycles, etc. The proteins are those proteins including pathogens which representing diseases of animals or humans. The virtual riders may be presented as the disease vector or target, for instance a mosquito to navigate a dengue fever related protein, a cow to navigate a BSE prion. The motion effects and sound effects are modelled based on the protein structure.



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## **Virtual Protein Theme Park**

### **Background of the Invention**

Amusement parks are traditionally areas in which a collection of amusement games are placed for peoples entertainment. Typically many of the games have an element of perceived danger and part of the entertainment involves providing sufficient user involvement in the danger that the users adrenalin level is raised.

Where the amusements have some common theme the amusement parks are typically known as "theme parks" with a theme of perhaps, movie background, or of fantasy. Some amusement parks combine several theme parks within the amusement park.

Over time the games, now known as "rides" have increased in technical complexity to provide more perceived danger in the more extreme rides. A century ago the most extreme roller coaster generated heavy positive gravity force (G) and mild negative G on a straight line run with patrons seated in a carriage whereas recent extreme rides generate a little less positive G and a little more negative G on a spiral descending or ascending course with the standing patrons. The design of such a ride is a highly specialized engineering exercise in maintaining the users within a very limited G envelope while ensuring that the carriages have sufficient kinetic energy to run from the top of the ride to the bottom at a safe speed whether loaded or unloaded. While retarders or linear induction motors may assist this process the design is nevertheless an expert field even with computer aided design.

Advances in the use of virtual reality have now made it possible to provide an environment which can imitate a theme park ride with no danger at all, and such rides have been in use for some time. These rides typically imitate a vehicle in which the user is seated, and provide a virtual environment which is that of a space trip, a dangerous flight, a trip back in

time or some other journey with a perceived danger. Other environments such as the CAVE (Cave Advanced Virtual Environment) allow a user to walk through a virtual environment which may include such things as a walk across Moscow's Red Square or through a giant protein.

While such environments are available they do not generally provide an experience which similar to that which is expected by users used to current theme parks with roller coasters, water chutes, railways etc.

Computer games are available which emulate theme parks and which may include roller coasters, chutes and vehicle rides (eg Roller Coaster Tycoon) but these games use a flat screen display and are not virtual reality enabled. Providing the required functionality for a virtual reality environment exceeds the capabilities of these games.

### **Summary of the Invention**

The present invention relates to providing an architecture to build a virtual theme park with the protein structure in which users (students, visitors and game players) can gain various knowledge of bio-molecules through an edutainment ride.

It is known to create three dimensional protein models and programs for doing this are described in "Ribbon: a stereo cartoon drawing program for proteins. J Appl. Cryst. 21 (1988) 572-576" and known from various software programs such as MOLMOL, VMD, Kinemages and CHIME.

In accordance with one object of the invention a method of presenting an emulation of a protein to a viewer comprises presenting at least one three dimensional emulation of the protein as an attraction in a virtual reality theme park wherein the viewer may interact with the emulated protein in real time.

Preferably the protein structure as displayed is derived from molecular information obtained by analysis of a substance and held in a database.

Preferably when the protein as displayed has a main track, path, or backbone the emulation provides a ribbon, tube or half-pipe as the emulation of the track, path or backbone.

Preferably the emulation includes scenery provided by models representing amino acids and H-bonds of the protein.

Preferably the viewer's viewpoint may be associated with the emulated main track and constrained to the main track along it.

Preferably the viewer's viewpoint may be located in or on a virtual transport such as a vehicle or carrier.

Preferably the protein represented is a pathogen such as viruses, prions and bacteria and the viewer's viewpoint is as a host (human or animal) whose species is a vector of or is affected by the pathogen.

Preferably the view is created from databases of molecular structure, of virtual reality representations of hosts and of virtual reality representations of vehicles or carriers.

In another aspect the invention comprises an assemblage of three-dimensional emulations of proteins presented in a virtual reality environment such that the proteins act as attractions in a virtual reality theme park.

Preferably the viewer may transfer between attractions in a virtual reality transport including vehicles and carriers.

Preferably the transport may be a wheeled vehicle, a sliding vehicle or an airborne or spaceborne carrier.

Preferably the transport may be rid by an emulation of a host.

Preferably the vehicle or carrier may be an emulation of an animal, bird or insect.

Preferably many users may concurrently use the same virtual reality theme park.

Preferably users may interact with the theme park by use of whole body virtual reality components.

In yet another aspect the invention lies in a theme park wherein at least one of the attractions is based on the appearance of at least part of a protein in a virtual reality environment.

These and various other features as well as advantages which characterize the present invention will be apparent upon reading of the following detailed description and review of the associated drawings.

### **Brief Description of the Drawings**

Fig. 1 shows a block diagram of the manner in which the virtual theme park is generated.

Fig. 2 is a diagram showing the modelling of protein track.

Fig. 3 shows determination protein orientation using the crossing number

Fig. 4 shows roller coastering on the half pipe of a protein track.

Fig. 5 shows bicycling inside the full pipe of the protein track.

Fig. 6 shows motorcycling on the half pipe of the protein track.

Fig. 7 shows car racing on the half pipe of the protein track.

Fig. 8 shows riding on a scooter on a protein track

Fig. 9 shows riding on a skateboard on a protein track

Fig. 10 shows skiing on a protein track

Fig. 11 shows aerobatic flying inside the protein surface

Fig. 12 shows mosquito manoeuvring inside the protein surface

### **Detailed Description**

Referring now to Fig. 1 a system for producing virtual protein theme park based on various bio-molecules stored in protein database 101 is shown where the system provides a transport database 102 appearing in the virtual theme park, together with a rider database 103. The protein

database holds protein structure data obtained through either X-ray crystallography or Nuclear Magnetic Resonance (NMR) such data may be held in a known manner, as for instance the format used in the Protein Data Bank (PDB <http://www.pdb.org>). Data examples in protein database are viruses, bacteria and prions – all organisms which infect animals or humans. The rider database collects hosts (confirmed or suspected) relevant to a protein including pathogens whose structure information is saved in database 101. For instance, chimpanzees are members of the rider database as they are hosts of the HIV protein which is related to AIDS disease. The transport database collects avatars of different types of transportation tools suitable for theme park riding.

The 3D modeller 104 of the virtual protein theme park creates (1) 3D protein models based on the protein database information; (2) 3D transport models based on the transport database information; and (3) 3D rider models based on the rider database.

The models so created have a road track component 105 which can be modelled based on the protein secondary structures and which represent the track surface; a road side scenery component 106 which can be modelled based on the protein amino acids and which represents the scenery local to the track; and other components 107 which include hydrogen bonds (H-bonds), etc.

Referring to Fig. 2 a method for modelling protein tracks and controlling motion when riding along the protein tracks in virtual protein theme park is shown. The method utilizes the polypeptide chain 200 which provides geometric and biological information for modelling of track or backbone trajectory 201, by moving frame 202 along the backbone trajectory and sweeping the path of pipe 203 (half or full) for the protein secondary structure. There are about 20 different types of amino acids and all of them consist of a common central carbon ( $C\alpha$ ), a hydrogen atom, an amino group, and a carboxyl group and a varied side chain (R) attached to  $C\alpha$ . Amino acids are joined end-to-end via peptide bonds formed in synthesis, which lead the amino group of one amino acid attached to the carboxyl

group and eliminate water. The main chain of protein consists of  $C\alpha$ , C, and N.

With a given set of points, conventional free-form curve modelling techniques such as B-spline or NURB curve interpolation or approximation can easily generate a smooth curve. From the atom coordinates, the backbone trajectory can be constructed to pass through or near all the backbone atoms. In our approach, however, we just choose the  $C\alpha$  atoms as the sampling points. This is due to the following observations. First,  $C\alpha$  atoms seem more important because they are the connecting points between peptide planes. Second, as the backbone atoms ( $C\alpha$ , C, N,  $C\alpha$ ) in a peptide plane can be rather close to each other, the curve interpolating all the atoms may produce zig-zag shapes.  $C\alpha$  atom coordinates are able to produce a reasonable backbone curve while the additional degrees of freedom could be used to control over the normal vectors. Third, reducing sampling points can speed up the curve modelling procedure.

Surface modelling of the backbone is required to present more significant information of the secondary structure. A sweeping technique is used to model the typical helical, strand and loop structures. Thus the moving frames along the trajectory of a protein are expected.

There are many moving frames along a trajectory and many methods have been proposed to compute the frame, for instance those of F. Klok, "Two moving coordinate frames for sweeping along a 3D trajectory." *Computer Aided Geometric Design* 3, 1986, 217–229; H.W. Guggenheimer, "Computing frames along a trajectory." *Computer Aided Geometric Design* 6, 1989, 77–78 and B. Jüttler, "Generating rational frames of space curves via Hermite interpolation with Pythagorean hodograph cubic splines." *Geometric Modeling and Processing '98*, Bookplus Press, 1998, 83–106.

A typical well-known frame is Frenet frame. Traditional differential geometry, as for instance described by G Farin, "*Curves and surfaces for computer aided geometric design: a practical guide*", 3<sup>rd</sup> edition, (Academic press), 1993 or I.D. Faux and MJ Pratt, "*Computational geometry for design*



*and manufacturing*", (Ellis Horwood Limited, Chichester, UK), 1979, gives a simple way to compute its triplet (tangent, normal and binormal). The Frenet frame, however, has an intrinsic problem related to the normal or binormal vectors. Sometimes these vectors suddenly change directions at some points along the path. This is because the Frenet frame is pathological (see M.G. Wagner and B. Ravani, "Curves with rational Frenet-Serret motion." *Computer Aided Geometric Design* 15,1997, 79–101[3]:) when the curve is perfectly straight for some distance or when the curvature vanishes momentarily, the Frenet frame is undefined. To overcome this a modified approach is taken with the biological properties of the protein backbone to provide a more natural solution. Specifically, the  $C\alpha$ -O vectors are used to provide an initial normal. But the  $C\alpha$ -O vectors may flip in the neighbouring peptide planes. This could lead to a sudden twisting of the sweeping surface. Therefore a simply averaging technique is employed to smooth the normal vector distribution, which allows a natural transition.

For each point on the trajectory, we have **tangent**, **normal** and **binormal** that are unit vectors. Thus we can define tangent, normal and binormal curves. First we generate a NURB curve for the path from the coordination of  $C\alpha$  of a given backbone of a protein. The tangent curve is then created from the path with the shift of the tangent vector. The normal and binormal curves can be constructed in a similar way once the normal and binormal vectors are found. We use the amide plane and the  $C\alpha$ -O vectors to determine the normals. The smooth normals along the path are constructed through a weighted interpolation technique. At the end, the bi-normals along the trajectory are formed by the cross product of tangent and normal vectors.

Fig. 3 shows a method for determining an optimal orientation with a given protein polypeptide. The visualization of the protein is subject to the coordinates of the peptide atoms obtained through X-ray crystallography or NMR. However, the original view of a given protein may not be good for building the protein theme park. Any protein can be rotated in the three

dimensional space. To quantify the orientation, it is possible to introduce a "crossing number" concept based on the projection theory.

Geometrically, protein polypeptides can be represented by polygonal lines (polylines) in 3D space. For a given direction in the 3D space, the 3D polylines can be projected along this direction to form 2D polylines in any planes perpendicular to this direction. Thus, the crossing number, or intersection number, of the 2D projected polylines can be used to characterize the visual complexity to an onlooker of the original 3D polylines. The crossing number of a protein is calculated using an algorithm for a given orientation of a protein from a parametric representation of the polylines. Thus, protein orientation determination is therefore a problem of optimising the crossing numbers in the whole 3D space. The orientation corresponding to the maximum crossing number gives the most complicated view while the minimum crossing number gives the least complicated view.

Using this technique, we can build a virtual protein theme park by determining the protein crossing numbers. For instance, a front view with a minimum crossing number may give the viewers an overall idea about the virtual protein theme park as there are less overlaps of the protein secondary structure in this direction. Naturally, as a viewer moves around the theme park, the number of crossing lines, or the apparent complexity, of the viewed protein will change.

The road track component can be modelled either as half or full pipes in the form of  $\alpha$ -helix,  $\beta$ -strand, and loops using a protein structure modelling method based on traversing the protein and determining the protein polypeptide information along the protein. The roadside component can be modelled either as trees or balloons based on the amino acid information. All other components such as H-bonds related to protein secondary structure may be added to the main track.

The transport models are created using CAD techniques and saved in the VRML (virtual reality modelling language) format. Typical transport models include aeroplanes, rockets, racing cars, roller coaster cars, trains, motorcars, motorbikes, bikes, skateboards, skiing boards and skateboard scooters.

The rider models used are mostly determined from the protein given. Should the protein be a pathogen, the rider could be the host (confirmed or suspected) of the pathogen or the relevant disease. Examples include kids as riders of the hand-foot-mouth disease protein.

The graphic renderer 108 then renders all the 3D models and updates the graphics display in either stereo or normal fashion during their life cycle. For stereo view, the rendered graphic images can be in various modes of active stereo, passive stereo, auto stereo or anaglyph. The dynamic motion of the rendered models are governed by the motion controller 109 through the user interface 110. Conventional control devices such as a steering wheel could be part of the controller. The transport(s) and rider(s) can be conveniently controlled to provide the motions related to acceleration and deceleration, steering and switching, and free driving. The sound track 111 can be added to the motion of transport(s) and rider(s) along the protein track. The sound track may be created based on the protein amino acids and  $\alpha$ -helical,  $\beta$ -strand, and loops which can be mapped into music notes with possible a combination of music equipments. Everything assembled together forms a virtual protein theme park which can be interactively visualized by users 112 (game players or students).

Fig. 4 shows a portion of a protein backbone with a train of "carriages" acting as a roller coaster train.

Fig 5 shows a series of bicycles with riders inside a protein chain configured in pipe format.

Fig. 6 shows a motorcycle within a half pipe format.

Fig. 7 shows a car driven by a chimpanzee on a protein backbone configured as a cupped ribbon.

Fig. 8 shows a goat kid riding a scooter through a half pipe.

Fig 9 shows a man riding a skateboard on a half pipe track.

Fig 10 shows a man on a skis in a cupped ribbon track.

Fig 11 shows a bird in flight around a protein molecule

Fig 12 shows the path of a mosquito through a protein molecule.

Within a virtual protein theme park, several games are intended to be included and examples of these are, but are not limited to, roller coasters, bicycling, motorcycling, car racing, scooter riding, skating, skiing, etc.

### **Industrial applicability**

The inventive system of protein theme park can be applied to build real and physical theme park. Computer game on protein theme park can also be developed. The invention has a potential for design of educational toys such as bead-coasters and roller-coasters related to protein structure. Educational models of proteins can also be prototyped.

**What is claimed is:**

1. A system for providing users edutainment experience on protein structure in a virtual protein theme park in a VR environment comprising  
means for modeling of ride tracks, ride transports and riders for the virtual protein theme park in three dimensions;  
means for visualizing of the modelled protein theme park in a stereo view; and  
means for riding with the modelled virtual theme park in a VR environment.
2. A system as claimed in claim 1 wherein the VR environment allows six degrees of freedom.
3. A system as claimed in claim 1 wherein the protein is a virus, a bacterium, a prion, a pathogen, or any bio-molecule.
4. A system as claimed in claim 2 wherein the VR environment may associate the viewer's viewpoint with the major ride track of the protein and be constrained to follow this track.
5. A system as claimed in claim 4 wherein the major ride track is a protein backbone of the protein secondary structure.
6. A system as claimed in claim 1 wherein the virtual protein theme park may model virtual moving effects by riding on a virtual transport while following the track of the protein.
7. A system as claimed in claim 6 wherein the virtual protein theme park may model virtual sound effects by mapping the amino acids, and helix, strand and coil into music notes while riding following the track of the protein.

8. A system as claimed in claim 1 wherein the displayed protein track is derived from protein structure data held from protein crystallographic and nuclear magnetic resonance imaging investigations.
9. A system as claimed in claim 5 wherein the protein track is represented in the form of NURBS or tessellation of quadrilateral and triangular meshes for display.
10. A system as claimed in claim 8 wherein the protein track is held in a database and the displayed protein track is derived from algorithms acting against the data.
11. A system as claimed in claim 10 wherein the algorithms to construct the protein track using a sweeping technique is based on the trajectory and its moving frame.
12. A system as claimed in claim 11 wherein the algorithms to construct the trajectory and the moving frame of the protein track uses the coordinates of the polypeptide atoms.
13. A system as claimed in claim 1 wherein the displayed transport is held in a database and the displayed transport is derived from design methods acting against the data.
14. A system as claimed in claim 1 wherein the displayed rider is derived from pathogens or diseases related to proteins.
15. A system as claimed in claim 14 wherein the displayed rider is held in a database and the displayed rider is derived from design methods acting against the data.
16. A system as claimed in claim 1 wherein the riding may be controlled by a user with a steering wheel and foot pedal.

17. A system as claimed in claim 1 wherein the virtual protein theme park is associated with the protein crossing number to determine the optimal view.
18. A method of presenting an emulation of a protein theme park to a viewer comprising presenting at least one three dimensional emulation of the protein track, the ride transport, and the rider as an attraction in a virtual reality environment wherein the viewer may interact with the emulated protein park in real time.
19. A method as claimed in claim 1 wherein the protein track as displayed is derived from protein structure information obtained by analysis of a substance and held in a database.
20. A method as claimed in claim 1 wherein the theme park as displayed has a main track whose emulation provides a tube or half-tube as the emulation of the protein backbone.
21. A method as claimed in claim 4 wherein the emulation includes scenery provided by models representing amino acids and H-bonds of the protein.
22. A method as claimed in claim 4 wherein the viewer's viewpoint may be associated with the emulated main track and constrained to track along it.
23. A method as claimed in claim 4 wherein the viewer's viewpoint may be located in or on a virtual transport and a virtual rider.
24. A method as claimed in claim 1 wherein the protein represented is a disease protein and the viewer's viewpoint is as an animal whose species is a vector of or is affected by the disease.
25. A method as claimed in claim 23 wherein the view is created from databases of protein structure, of virtual reality representations of riders and of virtual reality representations of transports.

26. A method as claimed in claim 17 wherein the orientation of the virtual protein theme park is determined by the optimal view with protein crossing number.
27. An assemblage of three dimensional emulations of proteins presented in a virtual reality environment such that the proteins act as attractions in a virtual reality theme park.
28. An assemblage as claimed in claim 27 wherein the viewer may transfer between attractions in a virtual reality transport.
29. An assemblage as claimed in claim 28 wherein the transport may be a wheeled vehicle, a sliding vehicle or an airborne or spaceborne vehicle.
30. An assemblage as claimed in claim 29 wherein the transport may be an emulation of an animal, bird or insect.
31. An assemblage as claimed in claim 27 wherein many users may concurrently use the same virtual reality theme park.
32. An assemblage as claimed in claim 31 wherein users may interact with the theme park by use of whole body virtual reality components.
33. A theme park wherein at least one of the attractions is based on the appearance of at least part of a protein in a virtual reality environment.



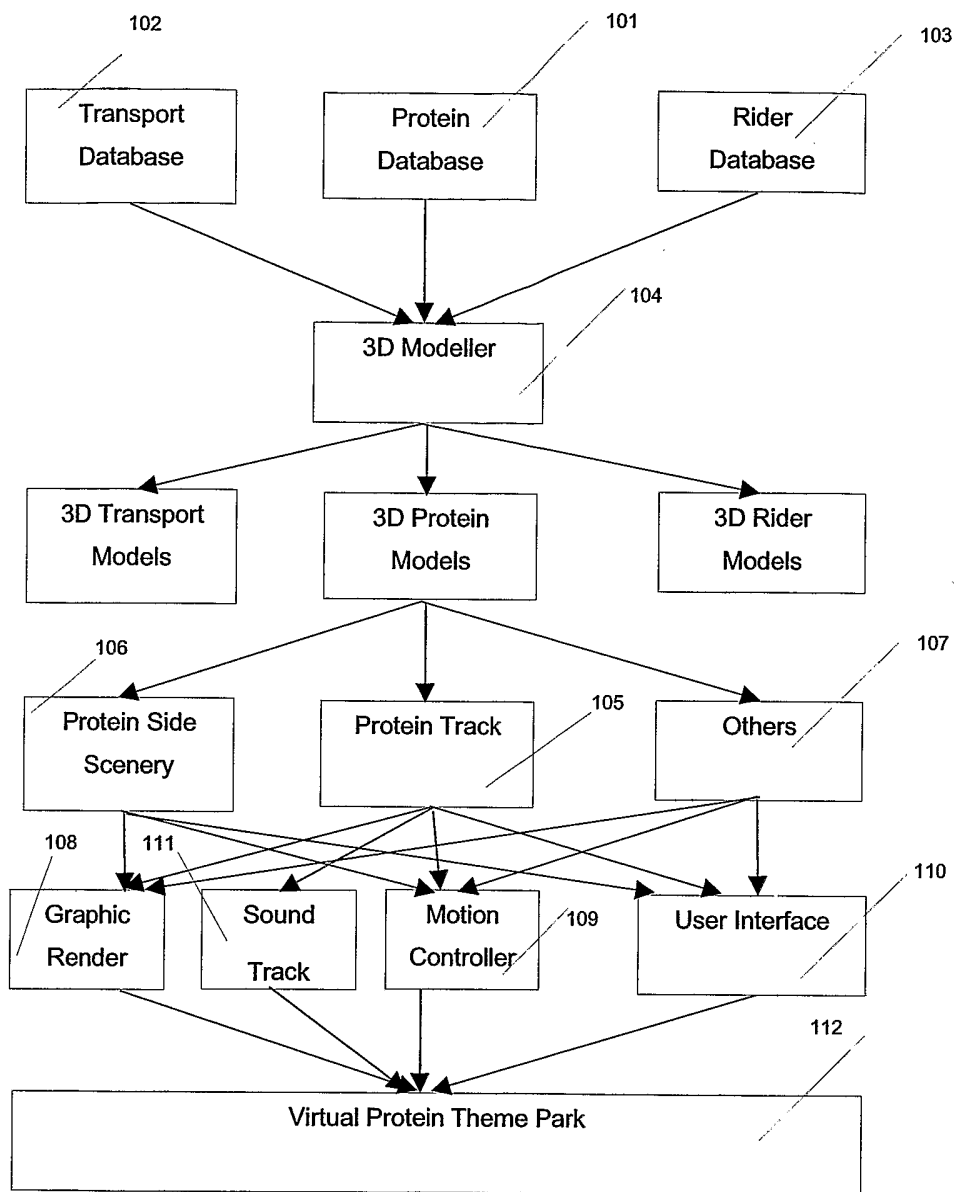
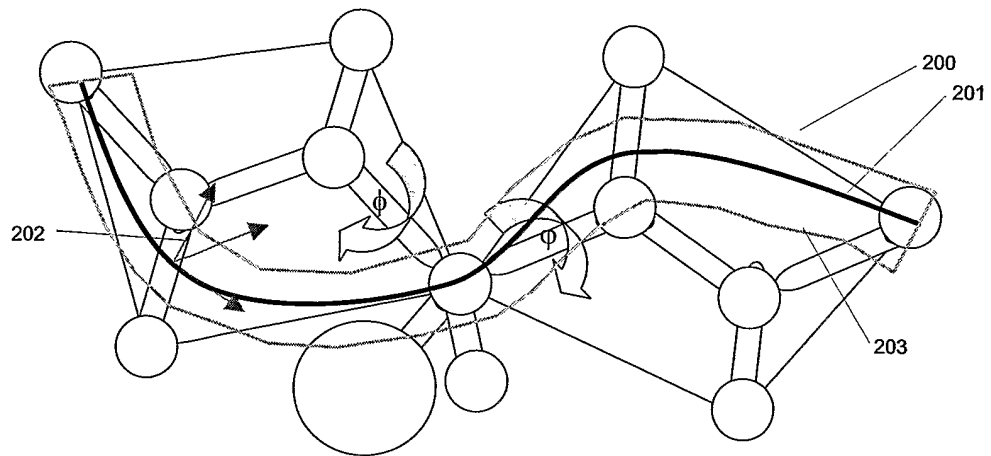


Fig 1

**Fig 2**

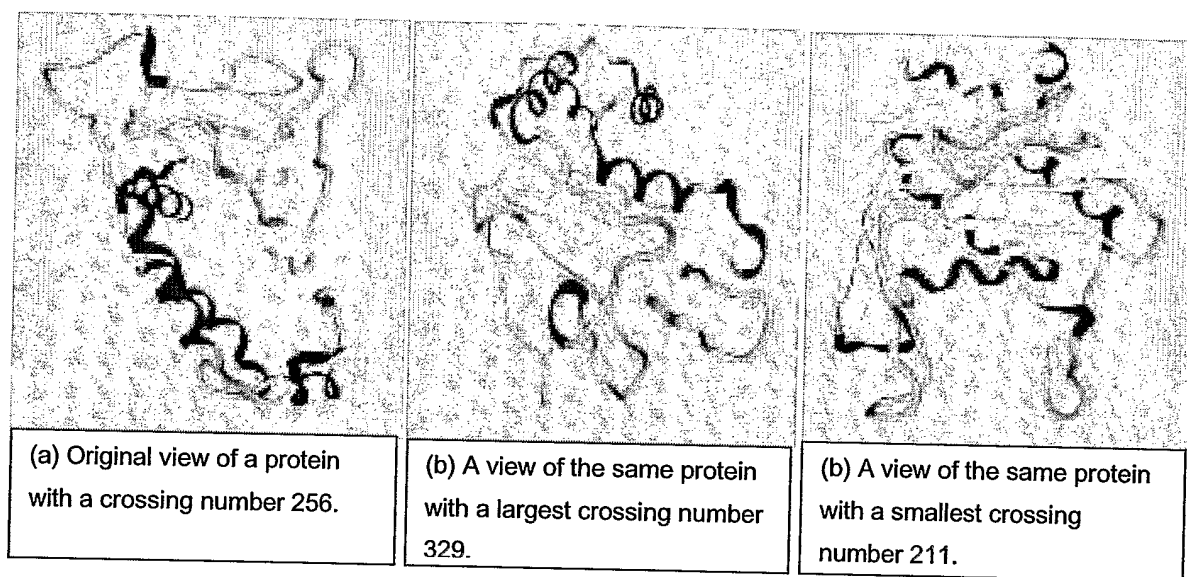
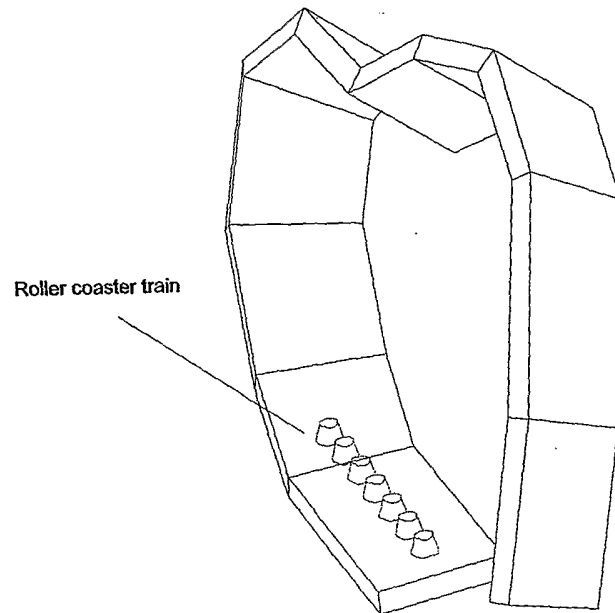


Fig 3



**Fig 4**

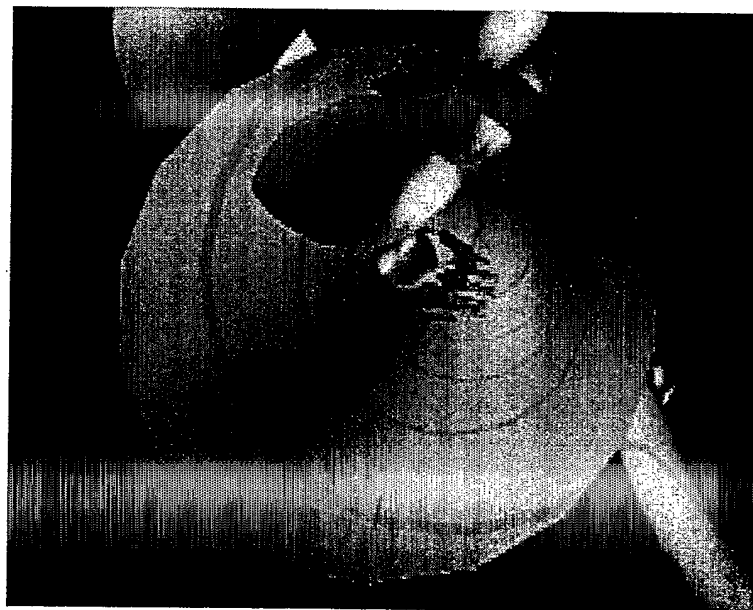
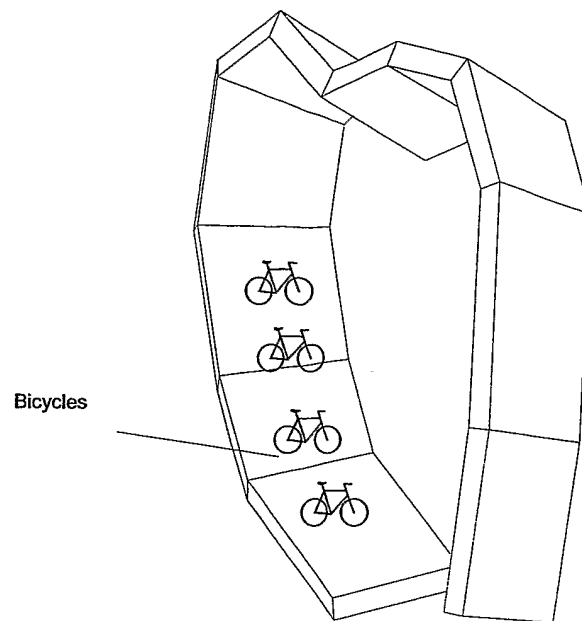


Fig. 5

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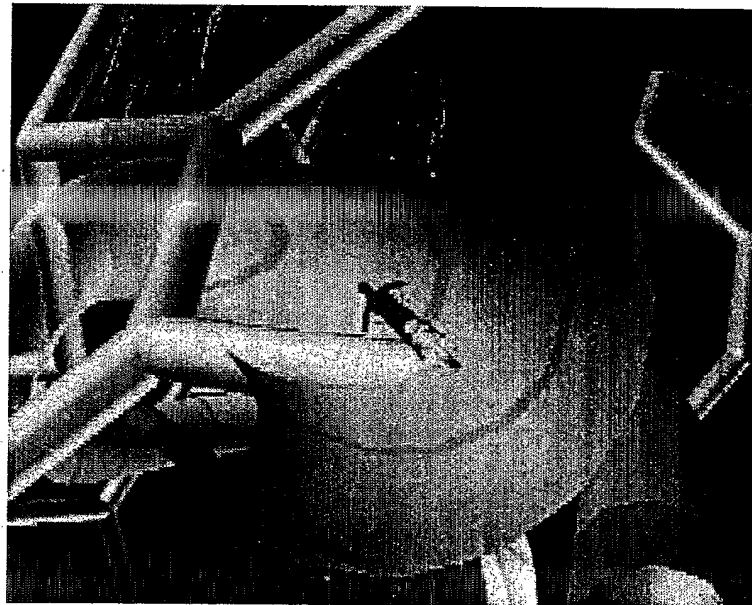
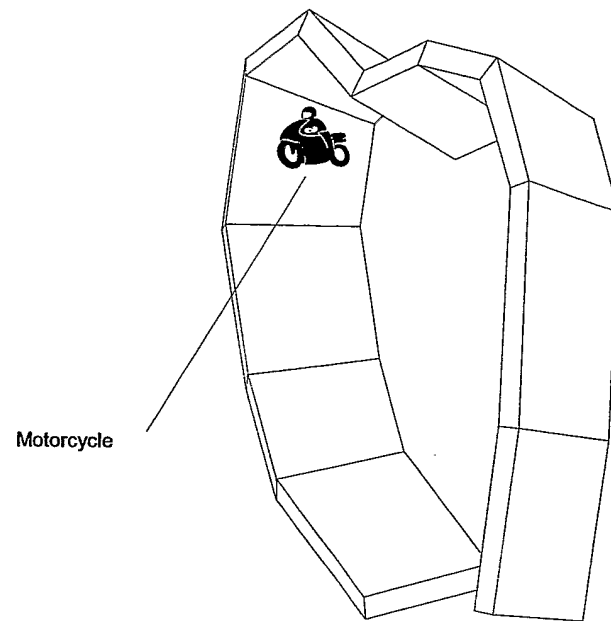


Fig 6

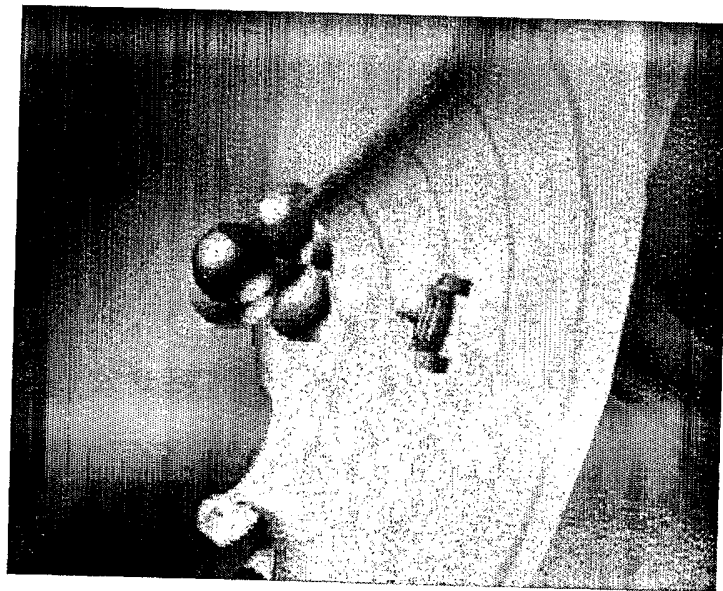
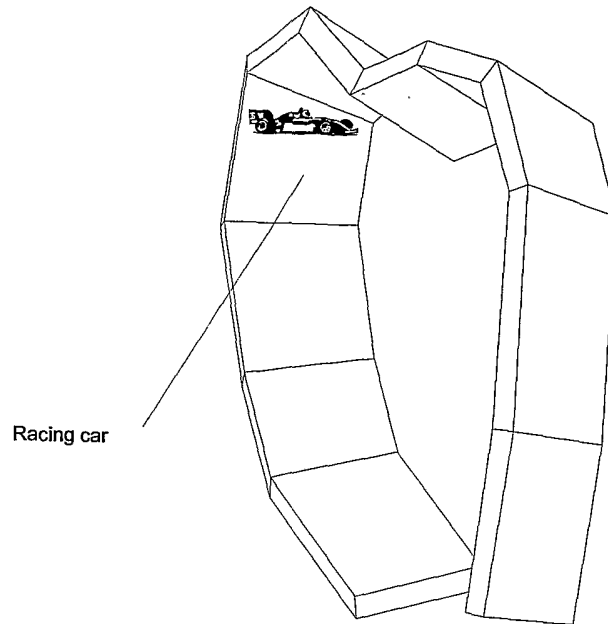


Fig 7.

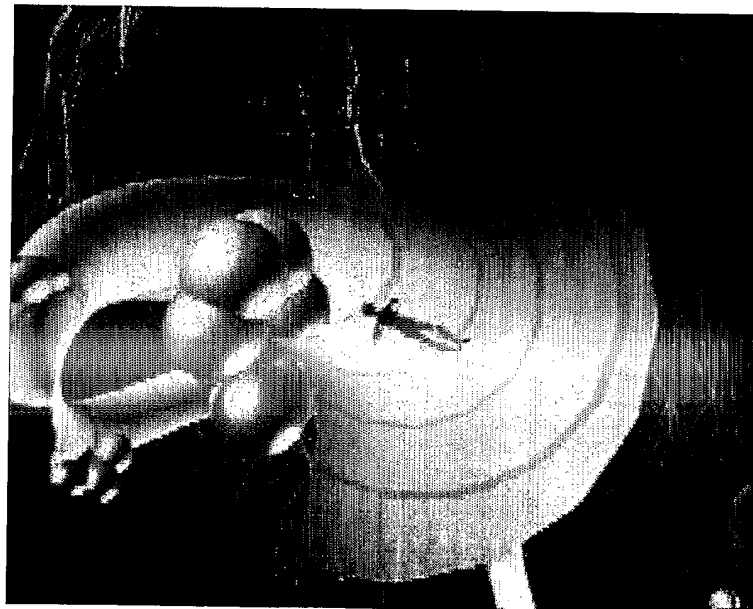
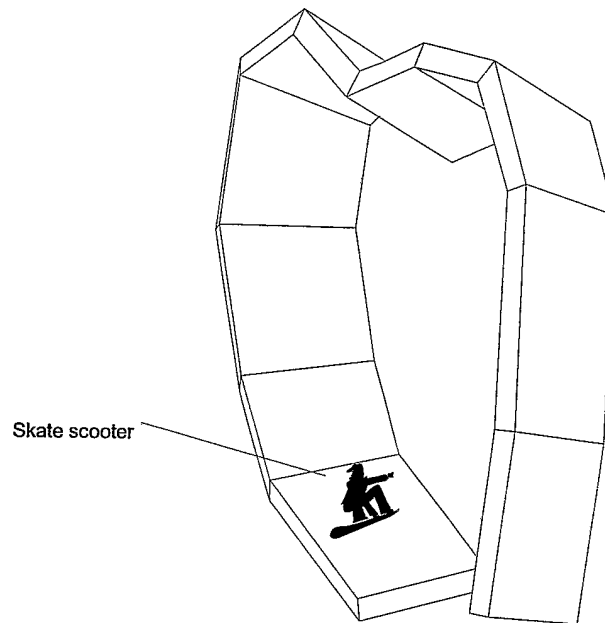


Fig 8.



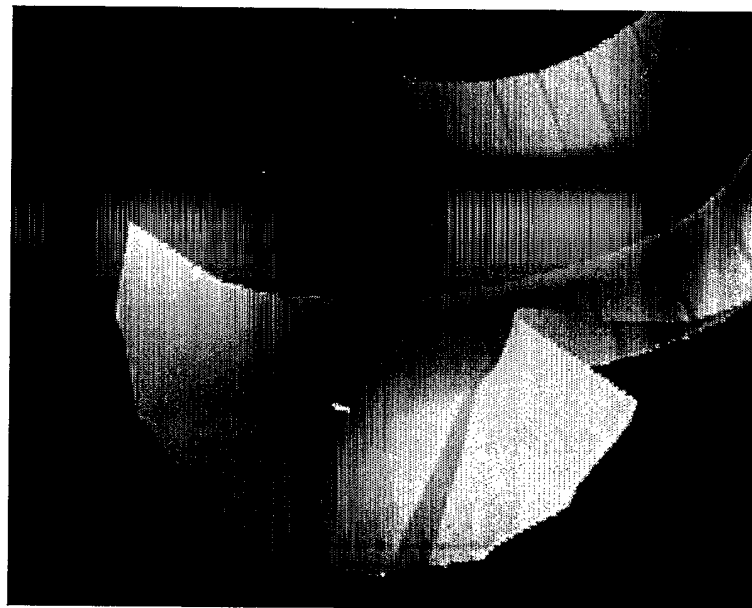
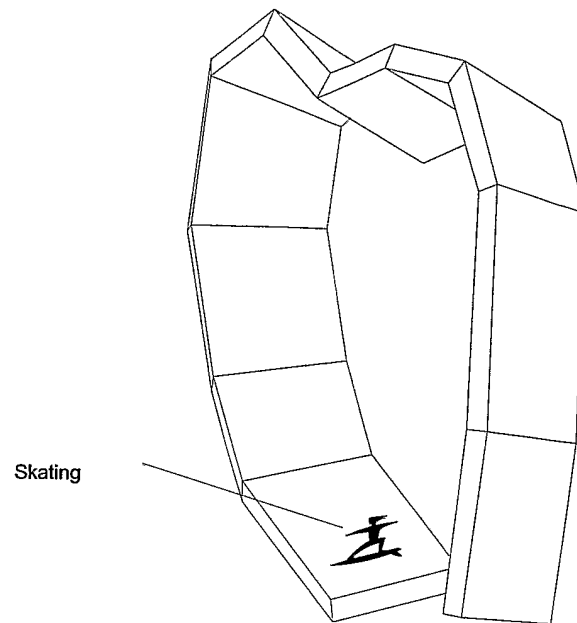


Fig 9.

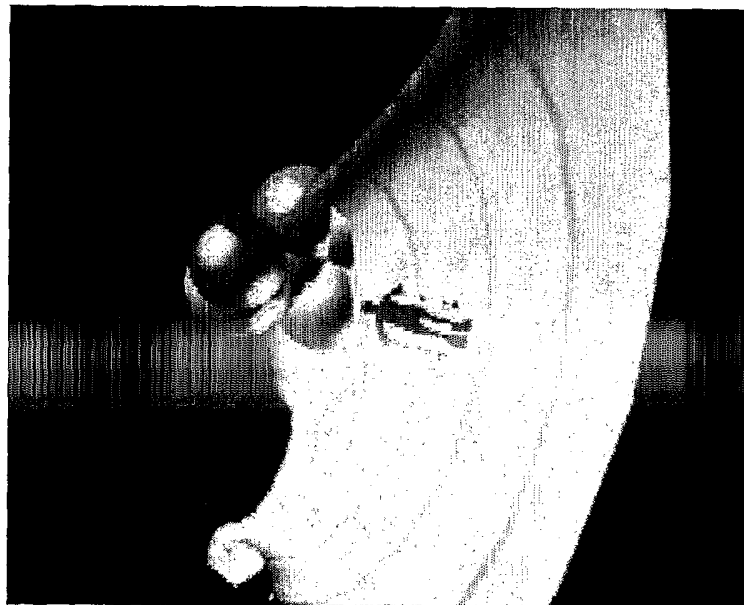
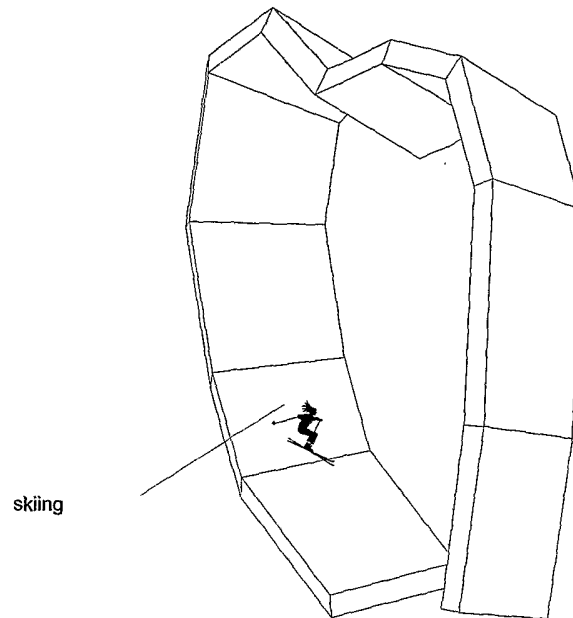


Fig 10.

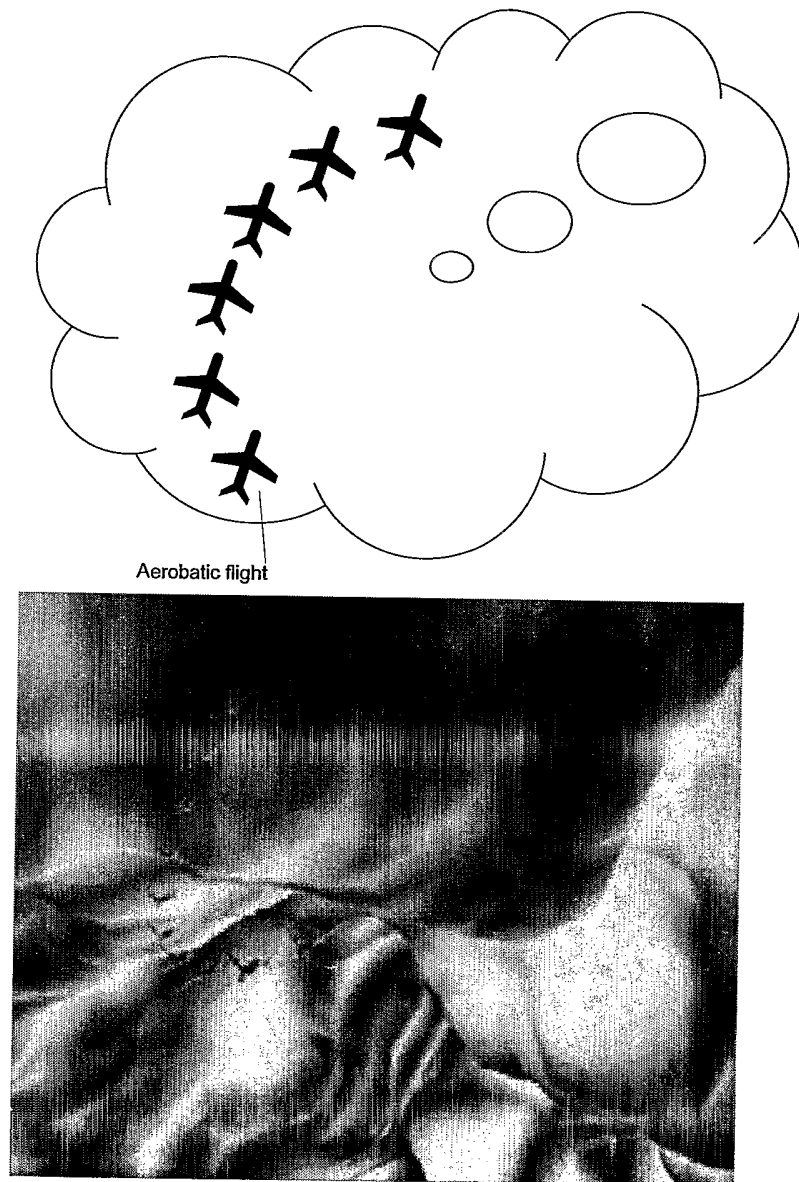


Fig 11

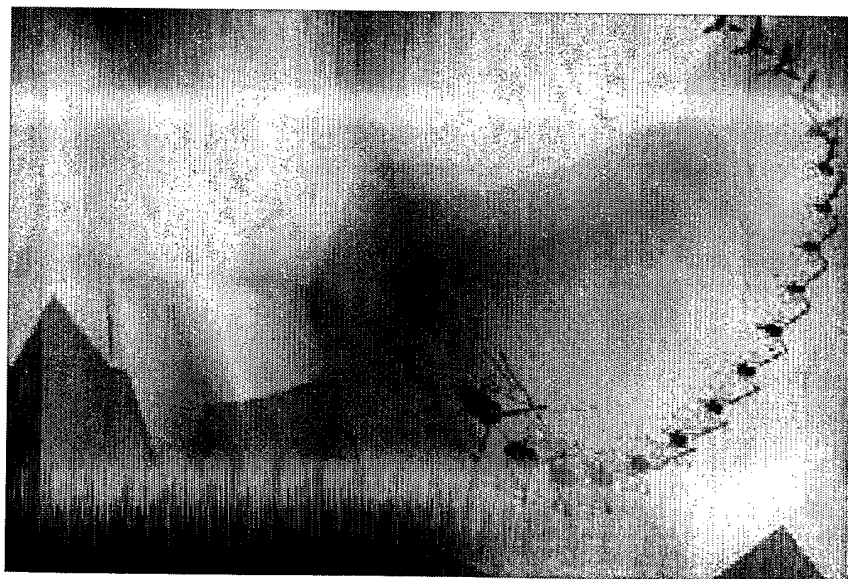
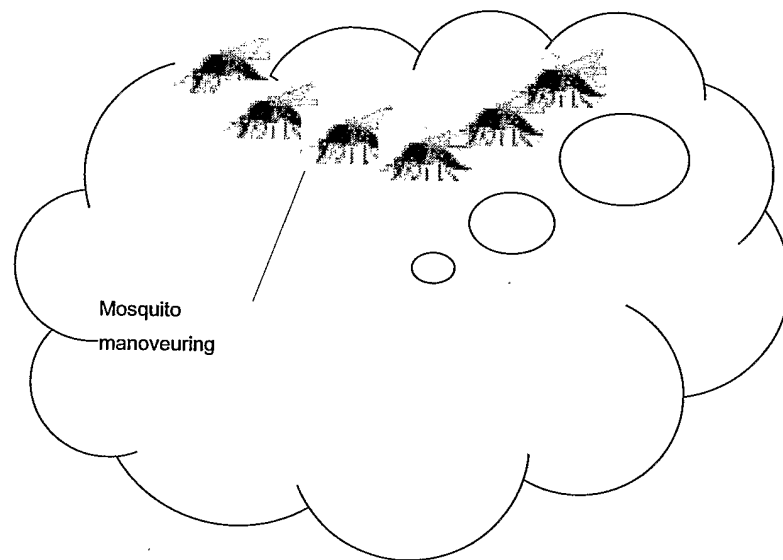


Fig. 12

# INTERNATIONAL SEARCH REPORT

International application No.

**PCT/SG2004/000286**

**A. CLASSIFICATION OF SUBJECT MATTER**

Int. Cl. <sup>7</sup>: A63F 13/10 G09B 9/00 G09B 5/00 G06F 17/00

According to International Patent Classification (IPC) or to both national classification and IPC

**B. FIELDS SEARCHED**

Minimum documentation searched (classification system followed by classification symbols)

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

WPAT. Keywords: molecule, protein, virtual, reality, 3D, stereo, model, theme park and similar terms

USPTO. Keywords: molecule, protein, virtual reality and similar terms

**C. DOCUMENTS CONSIDERED TO BE RELEVANT**

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	US 5185561 A (GOOD et al.) 9 February 1993 Whole document	
A	US 2003107178 A (WESTON) 12 June 2003 Whole document	
A	US 5884230 A (SRINIVASAN et al.) 16 March 1999 Whole document	



Further documents are listed in the continuation of Box C



See patent family annex

* "A" document defining the general state of the art which is not considered to be of particular relevance	"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
"E" earlier application or patent but published on or after the international filing date	"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
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"O" document referring to an oral disclosure, use, exhibition or other means	"&" document member of the same patent family
"P" document published prior to the international filing date but later than the priority date claimed	

Date of the actual completion of the international search  
**8 November 2004**

Date of mailing of the international search report

**12 NOV 2004**

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# INTERNATIONAL SEARCH REPORT

Information on patent family members

International application No.

**PCT/SG2004/000286**

This Annex lists the known "A" publication level patent family members relating to the patent documents cited in the above-mentioned international search report. The Australian Patent Office is in no way liable for these particulars which are merely given for the purpose of information.

Patent Document Cited in Search Report		Patent Family Member			
US	5185561				
US	2003107178				
US	5884230	AU	33037/97	AU	67799/94
		US	5557535	WO	9425860
				US	5453937
				WO	9748060
Due to data integration issues this family listing may not include 10 digit Australian applications filed since May 2001.					
END OF ANNEX					