## Modelling and Simulation





Role: Lecturer in Biomedical Sciences Specialises in: The use of Virtual Learning Environments in undergraduate education, in e-Learning, and Bioinformatics. Research area: Biochemistry of ubiquitin and ubiquitin-like proteins.

# What was the teaching and learning issue that the purchase of this technology sought to address?

We teach medical students and science students - biochemistry and neuro-science. Both these groups of students need some kind of understanding of three dimensions as applies to the life sciences. The technology we bought was designed to deepen this understanding through the production of various three-dimensional, and sometimes interactive, images.

## Why is an understanding of threedimensions so valuable to your students?

The medical students have to deal with the shape and structure of organs and skeletons. In text books these are always represented in two dimensions. They do dissections but they can only do these during timetabled class times so we wanted them to be able to look at a 3D representation of a bone in their own time.

We might have particular objectives that we want them to understand about this particular structure. The one we are doing at the moment is the pelvis. They have difficulty understanding the concept of the pelvic floor. So we are trying to facilitate this by using virtual reality to display the pelvis. We put the structure on a turntable. The turntable rotates and a camera takes hundreds of images. These are digitally stitched together and it looks 3D. Then you can zoom in and rotate and really get a feel for how the structure works. This would be available for them to look at and investigate in their own time rather than having to be bound by timetables.

# How do you visualise much smaller things, like molecules for example?

It is a very different process. The biochemists for example, are interested in the molecular level - we are looking at the 3D structure of molecules and proteins like DNA for example. Their function and what they do is tied up with their shape. You can't actually see these structures, so conventions have been developed



of representing them that makes sense to humans. The software we purchased creates these representations based on data that has been collected experimentally.

Most methods involve crystallising the proteins, which are then bombarded with x-rays which are diffracted and scattered. The pattern is analysed by computers and it tells us where all the atoms are in space. The computer then renders that into an image. This works well for small molecules, but proteins are thousands of molecules. The software we have allows us to look at these representations for proteins as well as molecules.

We wanted students to understand the three dimensional nature of molecules better. We purchased software of the kind that is used in a research setting. It allows you to look at the structures and change them. So, say there was a mutation in the molecule, how would this change its 3D structure? These are all the things that a biochemist has to get an understanding of. You don't really get this from looking at a flat representation in the pages of a text book or on a slide displayed on a screen. On the computer, the students can rotate the molecule. They can zoom in on it, they can modify it and see what changes that makes. They can do various calculations. It brings it to life in a highly visual and interactive way.

# How do the students view these images? You mentioned the Wow! Factor....

You can project these images onto a screen with stereoscopic projection. So you project two

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# "I did find the virtual reality pelvis very useful. Being able to rotate it, provided me with a better understanding, as the pelvis could be seen in a 3D fashion when access to the dissecting room was not available." **Second-year medical student comments on the 3D pelvis**

images at slightly offset and watch it through special glasses. You really get a feel for the shape of it. You can't really examine it, or quantify it, but it just makes an impression. You can rotate it and manipulate it whilst it is being projected.

The students are impressed. It is a whizz-bang approach. The parents love it on Open Days! We are going to use it as part of a master class in March in partnership with the Widening Participation team: "The Molecules of Life in 3D". The visiting students will use the molecular graphics software to investigate protein structure for themselves and then we will use the stereo projector to view these molecules in stereoscopic 3D.

## What do students get out of it?

The technology makes these structures real for them. We have a practical lab-based module where the students investigate proteins in various ways. As part of that, they spend a couple of weeks using this software in various ways, to make modifications and calculations, and we assess them on it. Often this is their first exposure to this sort of thing and they do find it hard! But sometimes it is going to be hard. Bioscience is a difficult area!

# What can you envisage this technology facilitating in the future?

In the future, we would like to generate our

own 3D images of this protein - to actually collect the data so that we can get the students to crystallise a protein. We would then send it away for the x-ray analysis to be done - this process is very expensive and there are very few places in the country where it can be done. Once they get the data back they can visualise a protein that they crystallised themselves. And then you could say well, is it possible to generate different kinds of structure? We could crystallise it in slightly different shapes and then look at what difference this makes! We haven't done it before. It would be technically challenging, it might not work, but it would be really great even just to have a go at it. It would bring the bio-informatics (the use of the software) more tightly integrated with the students' actual hands-on labs work. It would be their own structure that they solve, not the one they got from someone else. We'll see!

# Can this technology be used in other disciplines?

At the moment, the molecule modelling software is only really used in Biology, Bioscience and Pharmacy. But with the turntable set-up, you could put anything on there. Archaeologists could bring some of their artefacts down here and have a go! It would be a safe way for students to be allowed to investigate fragile archaeological artefacts that are not appropriate for handling in other ways. We would love that!

We are even thinking of trying to go down to

a much smaller scale. One of the biologists has asked me about chicken embryos. You could do them at different stages. It would be challenging as they are really small, but it is feasible.

# It looks like you have come a long way, but I don't imagine it has all been plain sailing!

There was a long learning curve and there is still a long way to go. We have got a lot of stuff to do with the rig and the photographs for example. We want to make it more interactive. It's possible

to create hotspots on the image, so you could click on the image and it would pop up a message telling you what that is, or even pop-up an image of a cross section through it at that point. The technology is there, now we just need the time to develop it!



Images of made using the molecular modelling software