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Virtual bodies, real treatments

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01 October 2008
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Helen Thomson

NORMALLY, being diagnosed with lung cancer, a defective heart and a nasty skin disease before breakfast would be a spectacularly bad start to the day. Fortunately this is no ordinary person: it is the virtual physiological human (VPH), the ultimate guinea pig whose cells will replicate, blood will flow, and body react like a real human - albeit within a very complex computer model. With no ethical concerns and at vastly reduced costs, the VPH could be the perfect way to test new drugs and novel treatments.

So, in 2008, how near the real world is the VPH? Vital reactions, interactions and the functions of entire body organs are already being replicated using complex algorithms. These studies are all separate, however, so the plan is to combine them to create a virtual human complex enough to stand in for living, breathing humans.

Understandably big pharma is eyeing this development with considerable interest. The industry's productivity is plummeting. While it has successfully developed treatments for many relatively simple diseases such as chicken pox, tuberculosis and diabetes, it is stumbling over the complex interactions of big conditions such as Alzheimer's, heart disease and stroke. Worse, the patents on many drugs launched in the 1990s will expire over the next few years, leaving the industry very exposed financially.

The creation of a VPH would bring huge savings to big pharma. "The biggest gains will be in clinical trials," predicts Simon Young, principal scientist in discovery bioscience at AstraZeneca. "We'll be interested in being able to use fewer people in less time." Efficacy tests of new medicines would also be cheaper. Aventis and Novartis are already interested, and a recent report by PricewaterhouseCoopers goes so far as to predict that virtual research will "transform the pharmaceutical industry by 2020".

While small-scale models are already used to predict the targets and effects of drug treatments, Young says testing these reactions on multiple virtual molecular targets at the same time will enable scientists to get a far better idea of what the drug does and how it works. "If it means we can shave even a year off development time, then it will be taken on board very rapidly," he adds.

Big picture

Human biology is evolving much as physics did, and now needs a big theory or theories to move it forward. Denis Noble, professor of cardiovascular physiology at the University of Oxford, says that in order to continue exploring the human body, our methods have had to change. "We've burrowed down to the bottom of biology - we've found the genes and components of what we're made of," he says. Understanding the interactions of these components is incredibly difficult without using theoretical predictions, though. "You can't understand the solar system without computing it theoretically, and that is the point we have come to in biology," says Noble.

> "Human biology needs a big theory - or theories - to move it forward"

He should know. Noble was the first researcher to develop a computational model of the heart in the 1960s, and after four decades of improvements his cardiac system is now one of the most highly developed examples of applying a computer simulation to biological processes. Today, Noble uses his models to help pharmaceutical companies develop better drugs. For example, CV Therapeutics of Palo Alto, California, used Noble's simulations to understand the actions of ranolazine, a drug used to treat angina. His simulations confirmed the company's belief that a potentially dangerous side effect of ranolazine was counteracted by a different, positive, effect of the drug.

Not surprisingly, the European Commission is very interested in this kind of bioinformatics. Last year, it allocated ¬72 million to VPH projects in the hope that a common framework can be established that will eventually stitch

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together the research into a functional virtual human.

Current models under this umbrella include Genius, or Grid-enabled neurosurgical imaging simulation, developed by Marco Mazzeo and Peter Coveney of University College London. This generates unique 3D models of blood flow in a patient's brain, and will, among other things, help doctors to identify aneurisms - swellings in the brain's blood vessels - and deal with them safely. Other groups are developing everything from virtual kidneys to a virtual immune system. Once completed, these models can be used by researchers to compare observations from an individual suffering from a specific disease, such as HIV, with those of a large group suffering from the same condition in order to predict how well a patient is likely to react to a drug. As well as making treatments safer for patients, big pharma can use the models to test new drugs by predicting the likely outcome from a vast range of molecular targets.

Creating these models is hard: each interaction needs millions of calculations and cannot be done on a single computer or even a cluster of processors. Instead, most researchers use "the Grid", a vast network of millions of linked computers which work together (see "The Grid"). It was developed in 1999 at CERN, the European centre for particle physics near Geneva, Switzerland, to help compute the vast amount of data that will be generated by the Large Hadron Collider.

Only integrate

From IT specialists to biologists, the growing interest in VPH presents opportunities and plenty of career paths for those who want to create their own virtual reality. But getting to grips with the intricacies of grid technology and bioinformatics is no easy ride. "The scale of some of these projects is so broad that it's impossible for someone to have all the skills needed," says Coveney. "You need to stitch together these teams: the sum of the whole is definitely greater than the parts. And there's no one-stop shop where you can get it all."

What we need, Coveney believes, is more doctoral training that bridges the gaps in interdisciplinary areas. This has been recognised by the EU's Network of Excellence initiative, which is developing the right kind of educational programmes. Meanwhile, if you want to impress future employers you could have a go at straddling IT and biology. The minimum requirement is a strong mathematical background, according to top practitioners such as Noble, because it is generally easier to translate physical mathematics to medicine than vice versa.

There are several programmes in the UK that aim to help you do just that: the University of Oxford, the University of Manchester, the University of Warwick and University College London all offer good courses, says Noble. And he reckons the growing number of graduates working on VPH projects at PhD and postdoc level is a sure sign that the field is making good progress.

Perhaps the best way to forge a career in VPH, though, is to get involved in a university project that is collaborating with industry. "Novartis, Roche and GlaxoSmithKline are all interested in this research and by working with them, you get a natural showcase to prove what you can do. When the technology becomes good enough for them to use, they are likely to recruit from academics they have collaborated with because they know your track record," Noble says.

"Getting involved in a collaboration is likely to help forge your career"

Young agrees: "Pharmaceutical companies would be worried about laying out millions on technology that is unproven, so collaborations are definitely the way forward." Since the industry is keeping a watchful eye on this technology, clearly the best way to get ahead is to have a foot in both camps. "There are lots of IT specialists and loads of candidates with pharmaceutical knowledge, but hardly any pharmaceutical applicants with a good grounding in IT skills," says Young.

Getting a good grounding in a variety of disciplines, including communication skills, will make your CV stand out from the crowd. As Young says: "When I'm hiring, I want someone who can talk to a computer programmer about software improvements, to a hardware programmer about Linux clusters, someone who can tell me what shape the molecule is, and then talk to clinicians about what dose to use."

So, the bottom line is this: with increased processing power, more integrated projects and a vast potential to change the way we develop treatments for disease, VPH is a technology worth getting stuck into. Going virtual, physiologically or otherwise, is "a piecemeal approach rather than a big bang," says Young. And no black holes...

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From issue 2676 of New Scientist magazine, 01 October 2008, page 52-55

Words of wisdom

Working on the virtual physiological human (VPH)

"I like the aspect of having something that I invented becoming a drug."

Lewis Whitehead, research investigator at Novartis

"It's exciting that physical science and engineering-style modelling is now moving into medicine. That hasn't happened a great at deal until now."

Peter Coveney, director of computational science at University College London

"There's a very robust job market for biological and computational skills in pharma and regulatory industries."

Donald Stanski, global head of modelling and simulation at Novartis

The Grid

THE Grid is the most powerful processing tool in the world. This is not that surprising since it was developed at CERN, the European centre for particle physics at Geneva, Switzerland, to help with the truly epic job of computing the data generated by the Large Hadron Collider. Its processing power makes it 10,000 times quicker than a regular broadband connection, downloading an average movie in mere seconds.

Its awe-inspiring capabilities make it the only network able to run the millions of complex algorithms needed to develop the virtual physiological human (VPH). It is made up of several networks based all over the world, allowing packets of data to be split up and processed simultaneously.

While the LHC experiments could not exist without the Grid, being able to apply Grid technologies to other disciplines has been a bonus, says Roger Jones from Lancaster University's particle physics research group. "It has been very interesting to meet people from many different walks of life who are facing similar challenges and tell them about solutions that may apply to them," he says.

Although the Grid is now being used for biomedicine and drug discovery rather than just physics, James Catmore, a high-energy particle physicist at CERN, thinks we've only just scratched the surface. "I believe that eventually any computer, anywhere in the world, will be able to contribute to distributed processing using the Grid," he says.

Anyone who has written their own programs can use the Grid without too much trouble, says Peter Love, a research associate at Lancaster University. However, most Grid users just use pre-existing applications, and as more non-computer experts get interested in the technology, it will inevitably become simpler to use, says Catmore.

Even non-specialists can get involved, especially if you like getting information out to the world. Press officers, science journalists and communication professionals are currently in demand for projects that use the Grid.

Eventually, the Grid could even change the way companies handle their finances. "Most computers are sitting idle for most of the time, particularly at night in large companies, so it makes perfect sense to use those spare hours to do work for other organisations, scientists included," says Catmore.

"I think a system of accounting will be developed whereby organisations or individuals will be given credits when they allow their computers to do Grid work, and those using the Grid's processors will be charged accordingly."

Spreading computing power around the world, the essence of any grid computing, is the only practical way to let thousands of scientists all over the world access and process data reliably and fairly, Catmore says.

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"the Grid" Is A Concept, Not An Entity

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By Chris Samuel
Mon Oct 06 01:00:24 BST 2008

Sigh, the Grid was not developed at CERN! CERN have their own grid (LCG), but there are many others around the world, often predating LCG.

Foster and Kesselman coined the term "Grid" back in the late '90's, and Globus (a widely used grid toolkit created by them) has been around since 1997.

Worth checking the Globus paper archive for more information here:

http://www-unix.globus.org/alliance/publications/papers.php

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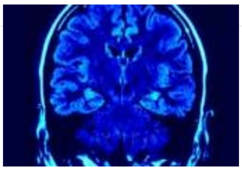

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