

## The two faces of simulation

Simulation is a respectable scientific activity. Even since computers swept the world of science, simulation has been a favoured pastime of engineers, physicists, chemists and even biologists. It is comforting, and often comfortable, to work with mathematical models, which will hopefully, predict the behaviour of real world systems. Increasingly, powerful, number crunching, computers are being used to predict the course of monsoons, the properties of atoms and molecules and to chart the spread of pathogenic organisms that cause infectious disease. The protein folding problem, in structural biology, is a popular windmill; many simulators, like Don Quixote set their own targets and claim success. Computer simulations are at the heart of subjects as diverse as fluid mechanics and computational biology and central to every aspect of engineering design. Simulations, sometimes disguised as projections, enter our daily lives whenever we have elections; forecasts, apparently supported by quantitative analysis, both right and wrong, abound. In modern science, simulations are ubiquitous. It was therefore with some amusement that I greeted the news from the football World Cup, that the FIFA's disciplinary committee had decided that their target was *simulation*. The immediate provocation was the faking of an injury by the Brazilian striker Rivaldo in the match against Turkey. The act, which attracted a red card for a Turkish player and a post-match fine for Rivaldo, when the FIFA committee recognized his simulation of injury, is a commonplace occurrence on soccer fields. When I turned to the dictionary it became clear that the common meaning of *simulate* is *to make a pretense of*. Indeed, the term 'simulation' often appears to be used in a pejorative sense and as in the case of football, it simply appears to be another description of the act of faking. Simulation appears widespread in sport and is at its most obvious in some arenas, like the wrestling circuses on television. Sometimes, simulation is more sophisticated and hard to detect, as in the case of fixed cricket matches. But, as Rivaldo must have realized, the resolution of the close-up video camera shot can distinguish a genuine injury from a clever simulation. Reflecting on Rivaldo's predicament, I came to the inescapable and obvious conclusion that the word *simulation* must have different meanings in sport and science.

But, does simulation, in the sporting sense, occur in science? Faking is not an entirely unknown phenomenon

in science, although the term 'simulation' is almost never used to describe the concoction of fraudulent data. In thinking about fraud in science, several questions spring to mind. Is dishonesty rare in science? Are there many forms of deviant behaviour amongst scientists? Does right always triumph over wrong in the world of science? Many years ago, David Hull drew upon the emerging field of sociobiology, to conclude that unlike many others, 'research workers police themselves coldly, dispassionately, almost cruelly' (*Animal Behaviour*, 1978, **26**, 685). Hull came to his rather naive conclusion, even as science was poised to move explosively forward across a broad front of disciplines. In a critique that appeared a few years later, a more realistic assessment was forthcoming: '... while science does have certain means through its norms, to encourage honesty, it must also reflect the nature of the society in which it is nurtured. A corrupt society will produce a corrupt science' (Manwell, C. and Ann Baker, C. M., *Search*, 1981, **12**, 151). The issue of misconduct in science has been openly debated in the United States and Europe over the past several years; these discussions have been fuelled by many famous cases of publication of doctored data, with the John Darsee and Mark Spector cases from Harvard and Cornell attracting much attention. The Baltimore-Imanishi Kari imbroglio lasted for what appeared to be an eternity, throwing up several questions on the tactics of investigators, who sometimes turn a legitimate inquiry into a witch hunt. Many of these cases were from the field of biomedical research, where competition is intense, the rewards for success immense and the pace of advance frenetic. To scientists in distant disciplines, these cases of data fabrication and manipulation seemed to be determined by the mores of a field, that appeared to be advancing with reckless abandon. Although there have been a fair number of frauds in more sedate fields, these have rarely been characterized by the imagination and effrontery displayed by the 'simulators' in biomedical research. Physics and the burgeoning disciplines of 'nanomaterials' and 'nanotechnology' have therefore been shocked by a new, high profile case of apparent 'simulation'.

In a remarkable period between 2000 and 2001, researchers at Bell Laboratories produced one spectacular result after another, in what appeared to be a major revolution in molecular ('nano') electronics. The successes of

the Bell Labs group ranged from the development of organic photovoltaic diodes, field effect transistors made of films of pentacene, observation of superconductivity at 117 K in a doped fullerene and most dramatically, the announcement of the single molecule transistor. Most of the papers reporting these findings appeared in *Science* and *Nature* attracting widespread acclaim. The path to Stockholm appeared clear until allegations of data faking appeared in editorial offices. The 23 May issue of *Nature* (p. 367) displays two figures from separate articles in *Science* and *Nature*; the experimental curves appear identical down to the last wiggle of noise, although the experiments are different. And, as more people scrutinize the prolific outpouring from the Bell Labs, more worms appear to be surfacing. In the eye of the storm is the young star Jan Hendrik Schön, who at 31, has an extraordinary output of over 100 papers, many of them in high impact journals. In the background are senior and respected colleagues and coauthors. For a while it seemed that Schön had the Midas touch; but now his world appears to be crumbling as questions of reproducibility and authenticity of data are raised by colleagues and competitors (*Nature*, 2002, **417**, 367 and 473; *Science*, 2002, **296**, 1376 and 1584; *Physics World*, June 2002, p. 5). Are the Bell Labs results a case of 'simulation'? The final verdict must come only when a full-fledged inquiry report becomes public. But, one might recall a famous allegation made in 1986 that Stanley Prusiner's claim of an infectious protein particle, the prion, was questionable (Taubes, G., *Discover*, 1986, **7**, 28; Garfield, E., *Current Contents*, 1987, **14**, 88). Prusiner, of course, established his claims to the satisfaction of the Nobel committee, which awarded him the Medicine or Physiology prize in 1997.

Allegations of 'simulation' are often hard to substantiate and in many cases can do irreparable damage to the accused. In an extraordinary episode, the Austrian biolo-

gist Paul Kammerer was suspected of faking the data he produced, demonstrating the inheritance of acquired characteristics (Lamarckian evolution) in the amphibian *Alytes obstetricans*. Kammerer's work attracted attention in the early 1920s, resulting in remarkably vituperative attacks in the columns of *Nature*. He shot himself, 'on an Austrian mountain path', in 1926. Arthur Koestler's narration of the life and times of Paul Kammerer (*The Case of the Midwife Toad*, Random House, 1972) must remain the most compelling investigation of a case of alleged misconduct. But, we might do well to recall one of the obituary references to Kammerer that Koestler quotes:

*'In diesem Lande genial zu sein  
Ist von der Kirche und dem Staat verboten'  
(To be a genius in this country  
Forbidden is by Church and State.)*

In considering misconduct and dishonesty in science, researchers and managers of science in India might also introspect. Are cases of plagiarism, 'simulation', false claims and misappropriation of credit investigated, when allegations are made and evidence produced? Or is there a general tendency to push all disturbing issues under the carpet, pretending that 'simulation' rarely happens? Is there a general reluctance to pursue purposeful enquiry, where *prima facie* cases have been established? Even more disturbingly, do we reward and encourage unethical practices by pretending that they do not occur; on occasion, elevating and celebrating 'simulators'? Do we train students to have sufficient respect for the methods of science and to value integrity above success? In an environment where corruption seems to be endemic, scientific institutions need to be watchful.

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