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A model world

In economics, climate science and public health, computer models help us decide how to act. But can we trust them?

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Here's a simple recipe for doing science. Find a plausible theory for how some bits of the world behave, make predictions, test them experimentally. If the results fit the predictions, then the theory might describe what's really going on. If not, you need to think again. Scientific work is vastly diverse and full of fascinating complexities. Still, the recipe captures crucial features of how most of it has been done for the past few hundred years.

Now, however, there is a new ingredient. Computer simulation, only a few decades old, is transforming scientific projects as mind-bending as plotting the evolution of the cosmos, and as mundane as predicting traffic snarl-ups. What should we make of this scientific nouvelle cuisine? While it is related to experiment, all the action is *in silico* — not in the world, or even the lab. It might involve theory, transformed into equations, then computer code. Or it might just incorporate some rough approximations, which are good enough to get by with. Made digestible, the results affect us all.

As computer modelling has become essential to more and more areas of science, it has also become at least a partial guide to headline-grabbing policy issues, from flood control and the conserving of fish stocks, to climate change and — heaven help us — the economy. But do politicians and officials understand the limits of what these models can do? Are they all as good, or as bad, as each other? If not, how can we tell which is which?

Modelling is an old word in science, and the old uses remain. It can mean a way of thinking grounded in analogy — electricity as a fluid that flows, an atom as a miniature solar system. Or it can be more like the child's toy sense of model: an actual physical model of something that serves as an aid to thought. Recall James Watson in 1953 using first cardboard, then brass templates cut in the shape of the four bases in DNA so that he could shuffle them around and consider how they might fit together in what emerged as the double-helix model of the genetic material.

Computer models are different. They're often more complex, always more abstract and, crucially, they're dynamic. It is the dynamics that call for the computation. Somewhere in the model lies an equation or set of equations that represent how some variables are tied to others: change one quantity, and working through the mathematics will tell you how it affects the rest. In most systems, tracking such changes over time quickly overwhelms human powers of calculation. But with today's super-fast computers, such dynamic problems are becoming soluble. Just turn your model, whatever it is, into a system of equations, let the computer solve them over a given period, and, voila, you have a simulation.

In this new world of computer modelling, an oft-quoted remark made in the 1970s by the statistician George Box remains a useful rule of thumb: 'all models are wrong, but some are useful'. He meant, of course, that while the new simulations should never be mistaken for the real thing, their features might yet inform us about aspects of reality that matter.

To get a feel for the range of models currently in use, and the kinds of trade-offs and approximations model builders have to adopt, consider the certifiably top-notch modelling application that just won its authors the 2013 Nobel Prize for chemistry. Michael Levitt, professor of structural biology at Stanford University, along with professors of chemistry Martin Karplus of Harvard and Arieh Warshel of the University of Southern California, were honoured for modelling chemical reactions involving extremely large molecules, such as proteins. We know how these reactions work in principle, but calculating the full details — governed by quantum mechanics — remains far beyond our computers. What you can do is calculate the accurate, quantum mechanical results for the atoms you think are important. Levitt's model simply treats the rest of the molecule as a collection of balls connected by springs, whose mechanical behaviour is easier to plot. As he explained in Nature in October: 'The art is to find an approximation simple enough to be computable, but not so simple that you lose the useful detail.'

Because it's usually easy to perform experiments in chemistry, molecular simulations have developed in tandem with accumulating lab results and enormous increases in computing speed. It is a powerful combination. But there are other fields where modelling benefits from checking back with a real, physical system. Aircraft and Formula One car designs, though tested aerodynamically on computers, are still tweaked in the wind-tunnel (often using a model of the old-fashioned kind). Marussia F1 (formerly Virgin Racing) likewise uses computational fluid dynamics to cut down on expensive wind-tunnel testing, but not as a complete substitute. Nuclear explosion simulations were one of the earliest uses of computer modelling, and, of course, since the test-ban treaty of 1996, simulated explosions are the only ones that happen. Still, aspects of the models continue to be real-world tested by creating extreme conditions with high-power laser beams.