Virtual science

...Rustum Roy

A gradual, but enormous, change has come over the practice of science in the last 50 years. I have been intimately immersed in it, both in the US and around the world.

As a chemistry MS student in India, I was exposed to one lecture and at least five hours of lab work every day. Chemistry, at least, was about hands-on experiments. At Penn State in the mid-1940s, under E. F. Osborn, I was taught that no one should dare claim anything as a scientific result that had not been repeated *experimentally* several times. That is what it took – experimental data – to establish a 'fact', those sacred units, the first principles of science.

And even that was only the beginning. No isolated fact was enough. A pattern, a 'gestalt', made the fact much more significant as it fell into place in a jigsaw. I cut my teeth on complex ternary and quaternary phase equilibria. From thousands of points – with apologies to Seurat – emerged our pointillist diagram of reality: a model, a 'picture' based on arrays of facts. Of course, one could misinterpret either individual data points, or the picture that emerged. And the product was not particularly eye-catching – simple black lines on a white background: inelegant but invaluable. That, we believed was real science, or the science of reality: experimental, repeatable, factual.

Today, I open the pages of any major journal and I am confronted with the most beautiful multicolored figures, drawings, and images. I am stunned by their elegance and aesthetics, especially in many biological structures and nano-images. And then I pull myself up short. I look at the axes, I read the legend, and very often what do I find? That this is actually only a 'cartoon' or a computer-generated image: no experiments, no repetition, no facts – virtual science.

As a crystal chemist, I have some idea of what it takes to accurately represent on a sheet of paper the three-dimensional aggregation of four elements (ions) that appear, for example, in the structure of mica. I marvel, then, at all the multicolored ribbons in double and triple helices presented to me as the structure of some biological living unit. Are these the same representations of reality? What Patterson Function or Fourier transform linked the real data to these images?

Why has this happened? Part of my explanation is that we have, more or less, run out of *significant* (to humanity) science, of new ideas, matched to the huge workforce we have created, and the huge amounts of public money we consume. And as always, our enormous *engineering* ingenuity has given us some new instruments (*cf.* historian De Solla Price's attribution of special significance to instruments): the computers and the software. These are the tools that have allowed us to create virtual science. And today, the real and virtual science are intergrown like 'wheat and tares' in the Biblical parable. They are so interconnected that Jesus' injunction may still be a wise one – it will be difficult to uproot the virtual without affecting the real, but wait for the harvest!

In our own materials field, we have no shortage of virtual science. One does not need to be for or against theory and modeling but, as scientists, our challenge is to use these new abilities effectively. And how well have we done so far? Not to put too fine a point on it: not very. Essentially all the exciting new materials, from yttrium barium cuprate to nanotubes, have come by empirical trial and error. The first principle predictions have yet to reach their first victory.

So why are the current plethora of *purely* theoretical papers published at all? Because virtual science has been given a special cachet in today's world. Well what is the harm, you may say? Here is what: thousands of researchers from all over the world may waste enormous amounts of time, effort, and money chasing will-o'-the-wisps.

What should we learn from this? I am not against theory, or modeling, or the use of elegant figures. As a scientist, I would simply implore my colleagues to preserve our traditional values – label axes and explicitly describe the relation of the figure to data. I have also suggested to funding agencies that modelers and theorists should be encouraged to find a collaborator (as many already have done) who is doing parallel experiments to feedback data into the joint work. That, in my view, is the minimum interdisciplinarity in our field that would not only justify theory and modeling, but also make them vastly more effective.

And in the end, I go back to our roots – the earliest 'first principles' of western science. Aristotle, in his *Nicomachean Ethics* (I. Vii. 17-22), wrote, "Nor again must we in all matters alike demand an explanation of the reason why things are what they are; in some cases it is enough if the fact that they are so is satisfactorily established. This is the case with first principles; and the fact is the primary thing – it is a first principle."