Technologies of Scientific Visualization

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During the past 15 years or so, a community of scholars in the arts and humanities has examined issues of epistemology in scientific imaging of nanoscale objects and explored the question: How do technology and aesthetics affect the relationship between an atom or a molecule and an image of the atom or molecule? Recently this community reached out to scholars examining other methods of scientific visualization such as images of outer space from the Hubble Telescope and brain imaging.

Annamaria Carusi, Andrew Balmer and Brigitte Nerlich organized the multidisciplinary conference Images and Visualisation: Imaging Technology, Truth and Trust, generously supported by the European Science Foundation, to explore these issues. The conference took place at the Norrköping campus of Linköping University in Sweden, September 2012. While the conference offered many excellent presentations, we present here a selection of papers that illustrate the value and the challenges of the three most salient themes that emerged: color, scale and technology.

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Visualizing the 'Invisible'

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Abstract

The ability of scientists to image and manipulate matter at the (sub)atomic scale is a result of stunning advances in microscopy. Foremost amongst these was the invention of the scanning probe microscope, which, despite its classification as a microscope, does not rely on optics to generate images. Instead, images are produced via the interaction of an atomically sharp probe with a surface. Here the author considers to what extent those images represent an accurate picture of 'reality' at a size regime where quantum physics holds sway, and where the image data can be acquired and manipulated in a variety of ways.

Keywords: scientific visualization; scanning probe microscopy; imaging atoms; molecules; quantum physics

Let me start by quoting from the foreword to this package of *Leonardo Transactions* [1], where Toumey, Nerlich, and Robinson state "After considering a three-part relationship between a nanoscale object, the technology for creating an image of the object, and the image itself, there is reason to conclude that a picture of an atom or a molecule cannot possibly look like the atom or the molecule. The phrase 'look like' does not apply to phenomena at the quantum level… "

From the perspective of a physicist whose research focuses on the imaging, manipulation, and spectroscopic probing of individual atoms and molecules, this is a fascinating statement to tease apart. In my opinion – which, I would argue, is in line with the general consensus in the field of nanoscience – scanning probe microscope images of a molecule can certainly "look like" the molecule in question. The strongest evidence I can produce to support my assertion is given in Fig. 1A. This is an atomic force microscope (AFM) image of pentacene (five fused benzene rings – see ball-and-stick model in Fig. 1B) where the molecular architecture is clearly revealed in the image [2]. What is particularly striking about this AFM image is just how closely it matches the textbook ball-and-stick model of the molecule, vindicating, to a large extent, chemists' and physicists' intuitive – some might say 'naive' – worldview at the nanoscale.

Before tackling the tricky semantic issues underlying what precisely we might mean by an image "looking like" an object, it is instructive to consider just how the image in Fig. 1 was created. Atomic force microscopy is one of a family of techniques which fall under the scanning probe microscopy (SPM) banner [3]. (Note that in the following I will use "SPM" as shorthand for both scanning probe microscopy and scanning probe microscope). At one level, SPMs are conceptually even simpler to understand than conventional optical microscopes (or, indeed, any optical imaging system, such as a digital camera). Instead of using optical elements such as lenses and mirrors to bend light rays so as to form a magnified – and, it must be said, fundamentally distorted (due to aberrations, deficiencies, and fundamental physical limits in even the most technologically advanced optics) – image of an object, an SPM exploits interactions between a sharp tip and a surface. Those interactions can span a wide variety of physicochemical effects (which I won't discuss here), but when the tip is atomically sharp, i.e. terminated in a single atom, it is possible to build up an image on the basis of the formation of a chemical bond between tip and surface atoms. Or, more fundamentally, submolecular resolution of the type shown in Fig. 1 becomes possible by exploiting the interactions between the electrons at the tip apex and those of the molecule on the surface.

The image in Fig. 1 was acquired by taking an exceptionally sharp tip apex, deliberately terminated by a single CO molecule, and moving it back and forth across the pentacene molecule [2]. At each pixel in the image – and a pixel in this case can be a very small fraction of the diameter of an atom in size – a measurement is made of the strength of the interaction between the tip and the molecule. More accurately, the forces between the tip atom and the molecule are measured by electrically measuring the changes in the frequency of a microscopic tuning fork to which the tip is attached [4]. This frequency is just outside the range of human hearing – it's approximately 25 kHz – but if the pitch were slightly lower it would not be too much of an exaggeration to say that the image is formed by 'listening' to how the tuning fork reacts to the interaction of the tip with the molecule. (Indeed, one can very easily transpose the oscillations of the tuning fork to lower frequencies, amplify the (electrical) signal from the fork, and in essence 'listen' to the interactions of atoms).

Instead of generating a 'soundscape', however, a visual image is built up by color coding the changes in frequency of the oscillations of the tuning fork as it moves back and forth across the molecule. This produces what scanning probe microscopists call a frequency shift image (note that the grey scale on the right hand side of Fig. 1(A) has units of Hz). It is possible – although in many cases not mathematically trivial – to convert the frequency shift image into a map of the variation in forces between the tip and the sample, or to generate a potential energy landscape.

The central question of course is, Just how accurate a picture of reality is the frequency shift map and the molecular image derived from it? For many scientists, particularly chemists, there is almost a visceral quality to the image of Fig. 1(A) – it just "feels" right! The results of many other experiments have previously been 'decoded' in order to indirectly determine the structure of pentacene (and countless other mole-

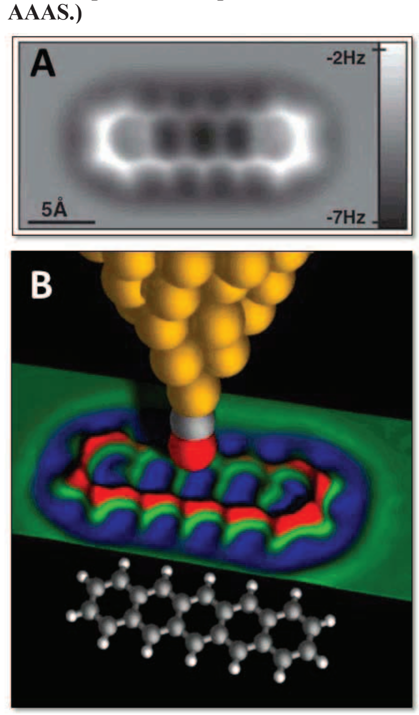

Fig. 1(A). An atomic force microscope image of a pentacene molecule. (B) schematic diagram (and false-colour experimental data) showing the experimental geometry. An atomically sharp tip terminated in a carbon monoxide molecule was used to acquire the image. A ball-and-stick model of the pentacene molecule is also shown. (From Leo Gross, Fabian Mohn, Nikolaj Moll, Peter Liljeroth, and Gerhard Meyer, "The Chemical Structure of a Molecule Resolved by Atomic Force Microscopy," *Science* 325 (2009) pp. 1110-1114. Reprinted with permission from AAAS.)

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cules); what makes Fig. 1(A) so different is that it is as direct a measurement as one can get (with current technology) of the molecular framework.

From many perspectives the image shown in Fig. 1(A) is just as a valid a picture of reality as, for example, a photograph of the AFM (and its associated bulky vacuum equipment) used to acquire the snapshot of the molecule. The photograph is formed by the interaction of photons of light with the AFM system, with the optics and light collection unit in the camera (a charge-coupled device (CCD)), and, ultimately, with the eyes of the observer. But in many ways our eyes give us a remarkably narrow and constrained view of the world around us – they are sensitive to just a thin sliver of the electromagnetic spectrum. In addition, *every* image – regardless of its origin – is a convolution of the signal from the object (be it optical, electrical, magnetic, auditory etc…) with the properties of the imaging system. In SPM, as in any other microscopy, we aim to minimize the contribution of the imaging system to get as true a picture of the object as possible.

The argument that light – i.e. a stream of photons – should hold a privileged position in our perception of the world around us doesn't hold up to scrutiny. (Einstein's relativity notwithstanding!) Just because we don't use light to form an image, why should that mean it's any less valid a representation of reality? Ultrasound scans don't use traditional optical techniques as the basis of their image generation technology, nor do magnetic resonance scanners. Yet few would claim that ultrasound and MRI scans don't provide an accurate representation of what's going on in our bodies. Some might argue that a key difference between the image shown in Fig. 1(A) and those produced by ultrasound and MRI scans is the ultrahigh resolution: for the AFM 'micrograph' not only are the atoms of the molecule seen but so too are the bonds. Isn't our picture of reality at the atomic/molecular level governed by quantum mechanics? How then can we speak of definite atomic positions – isn't the essence of quantum physics the intrinsic uncertainty in the positions of atomic and sub-atomic entities?

This is a common fallacy. The Heisenberg uncertainty principle involves *two* complementary quantities (position and momentum, or energy and time) – there is a fundamental limit to the *product* of uncertainties in these quantities. There is nothing in quantum physics that rules out the observation of atoms and the electronic charge arising from chemical bonds, and Fig. 1(A) of course bears this out. Moreover, we can manipulate molecules just like that shown in Fig. 1(A) using the AFM tip – we can translate, rotate, and, if we're lucky, pick them up and put 'em down. Far from the ethereal, 'other-worldly' character usually associated with the quantum domain, scanning probe microscopists can interact in a very tangible and direct sense with the nanoscopic realm: molecules and atoms can be plucked, poked, positioned, pulled, prodded, and pushed [5 - 7]. Via haptic interfaces, the forces associated with these events can be fed back to the microscopists to enhance the 'immersion' in the quantum realm.

This is not to say that there aren't very many weird and entirely non-intuitive aspects of quantum physics. There certainly are. But probe microscopists visualize the quantum world in a variety of ways – visual, auditory, tactile – and find that in the majority of cases, far from being phantoms of no substance, atoms and molecules have a compelling 'solidity'. The stunning images of single molecules provided by scanning probe microscopes indeed 'look like' the molecules themselves. Or, at the very least, the pictures of reality derived from SPMs are no less valid than those obtained from the light-based techniques – photography, microscopy, telescopy – with which, through virtue of their perceived direct connection to our visual cortex, we are rather more comfortable and familiar. We need, however, to revise our understanding of what is meant by something being invisible. Photons are not always required to see the light.

References

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