Imaging technologies need trained practitioners

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letters

Imaging technologies need trained practitioners

I was dismayed by the statement attributed to Angela Gronenborn in David Kramer's piece (PHYSICS TODAY, February 2008, page 27) that nuclear magnetic resonance (NMR) "technology is less mature than x-ray crystallography, which has evolved to the point where it is considered 'black box,' meaning experimenters don't need to be conversant in the technology to use it." I agree that it has become substantially easier to collect x-ray diffraction images, analyze them, use that information to solve the phase problem, view electron density, and build a crystal structure. However, I strongly disagree that the devices, algorithms, or field is so complicated as to be hidden or mysterious—a so-called black box—to the user or that a user doesn't need to be conversant with the technology to use it.

Do we really want scientists in any field to use software, instrumentation, and technologies that they don't understand? Are we training undergraduates, graduate students, and postdoctoral research fellows adequately, or at a minimal level to produce a noncritical set of data? At a time when scientific research and technology are changing so rapidly, and are more accessible, don't we wish to encourage researchers to understand as much as they can? That is the correct paradigm.

I appreciate the fact that it's easier to include crystallography as a central investigative tool in all major fields of scientific research. However, that also means that it's easier to collect data incorrectly due to overlaps, overexposure, poor sample quality, or incompleteness, or to process it rapidly and incorrectly as with poor indexing, wrong unit cell, wrong space group, or twinning, and still arrive at some sort of electron density and resultant structure. Anyone using crystallography needs to be critical at each step. Several recent retractions of protein structures published in high-profile journals attest to the increased lack of critical analysis. We should not confuse ease with transparency and ignorance with rigor for any technology. A major fault with our present educational hegemony is that the fundamentals of crystallography are no longer adequately presented in science courses. Crystallography, like NMR, is an incredibly powerful tool and continues to develop and thrive on the challenge of investigating larger, more dynamic, and more complex biological and chemical systems. It is liberated and expansive because of its maturity.

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Gronenborn replies: My comment comparing nuclear magnetic resonance and x-ray crystallography as structural techniques was intended to highlight the younger nature of NMR versus crystallography. Crystallographers and NMR spectroscopists worth their salt would never advocate blind use of technologies without a thorough understanding of their basic principles, strengths, and limitations. Problems arising from loose interpretation and misuse of technology without critical analysis of the origin, quality, and reproducibility of generated data are, unfortunately, too common. But not every scientist is a methods developer or is, as David Kramer puts it in his report, well "conversant in the technology." Success in the complex structural-biology tasks that lie ahead can be ensured only through rigorous education and training of students to critically and carefully use all methodologies available.

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Cocktail party at the beginning of the universe

I've just finished reading the feature article by Daniel Eisenstein and Charles Bennett about cosmic sound waves (PHYSICS TODAY, April 2008, page 44). As an acoustical engineer, I am especially drawn to the 1 part in 10^5 smoothness of the cosmic microwave background (CMB) fluctuations and the attendant "sound wave" analogy. I'm wondering whether your readers appreciate the elegance of this analogy.

Although 1/100 000 may at first seem tiny, acousticians deal in such ratios daily. Consider that an atmospheric pressure fluctuation of 1 bar, expressed in decibels, is approximately 194 dB, while a typical sound level measured in a crowded room of moderate size full of loudly talking people might easily approach 80 dB, a pressure ratio well below 10^{-5}. Thus lively conversation superimposed on atmospheric pressure looks exactly like the *Wilkinson Microwave Anisotropy Probe*'s CMB anisotropy. So a proper analogy for the CMB fluctuations might be the cocktail party at the beginning of the universe. Acoustically, one part in 10^5 smoothness is not a terribly small variation but rather should be regarded as quite normal. We should expect to be able, in a sense, to extract portions of the intelligible conversation from among the din. CMB analysts are working with what would be analogous to a snapshot of an instant in that cocktail party conversation rather than having to wrestle, as acousticians must, with a fully dynamic situation. In Eisenstein and Bennett's figure 2, the three peaks in the power spectral density function at 0.6°, 0.4°, and 0.2° reveal hints of that conversa-