

"Fellows of the Royal Society have for 350 years played a key part in the development of the scientific method." John Gribbin, page 429

Mind the gap: future depends on sciences and humanities

Why do we continue to undermine Earth's life-support system, on which our survival depends, despite a wealth of information documenting its deterioration? Your Editorial on the need for a more productive relationship between natural and social scientists is timely (*Nature* **462**, 825–826; 2009).

As natural scientists, we must not see the social sciences and humanities as an add-on to our own expertise, or as subservient to our supposedly more refined or objective ways of knowing. Integrating insights from different perspectives will help to break down the social and political barriers that obstruct ways of finding a sustainable future (J. Fischer *et al. Trends Ecol. Evol.* **12**, 623–624; 2007). Disciplines such as economics, institutional theory, history, philosophy and sociology can contribute to framing the right questions: smart science alone is unlikely to result in wiser decisions or better outcomes.

Integration between disciplines to tackle sustainability issues is already under way. Most recently, an initiative called the Millennium Assessment of Human Behavior (P. R. Ehrlich *Bull. Ecol. Soc. Am.* **90**, 325–326; 2009) has been launched to give a voice to important insights outside the realm of the natural sciences.

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Mind the gap: social sciences can reveal community needs

The benefits you detail in your Editorial from collaboration between social and natural sciences (*Nature* **462**, 825–826; 2009) can be extended to people

like me. I develop software to support research and therefore need insight into how the research community functions.

The molecular biologists I work for are generous with their time in explaining their speciality. But to be useful, software must be compatible with the habits and attitudes of the community it serves. Most people participate in communities without being consciously aware of the norms they are following. I need to elicit the tacit knowledge from those I work for. Some of this is recorded by sociologists of science, and some is accessible if I can learn to use ethnographic methods.

The pace of change means that scientific communities regularly face new challenges requiring them to restructure themselves. For example, today's molecular biologists are gaining insight into the larger macromolecular machines of the cell. This progress depends on collaborations that combine techniques from different subdisciplines. To lead such restructuring, it is not sufficient to be recognized as a successful, ambitious researcher: an unusual level of insight into the functioning of the research community is needed as well.

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Safeguarding the integrity of protein archive

Your News story 'Fraud rocks protein community' (*Nature* **462**, 970; 2009) discusses allegations that 12 Protein Data Bank (PDB) entries are based on fabricated data. Pending verdicts on these entries from the US Department of Health and Human Services Office for Research Integrity, we wish to clarify PDB policies and actions.

The PDB archive, which is managed by the Worldwide PDB (wwPDB; wwpdb.org), houses

more than 62,000 entries for macromolecular structure models and their experimental data. It is maintained for the public good. Deposited structures are validated using community-developed standards, and any related corrections are made by depositors before release and publication.

Entries can be replaced on written request from the depositor(s) if better data have become available or the interpretation of existing data has changed. Entries can be withdrawn (that is, rendered obsolete) by the senior author, or by journal editors when the published paper describing the entry is retracted.

An author's employer (in this case, the University of Alabama at Birmingham) may request removal of an entry, but this request must be fully documented and the original paper describing the entry must be retracted. This ensures due process for the author(s) and the scientific integrity of the PDB archive. To date, the paper describing one of the 12 PDB entries in question has been retracted (*J. Biol. Chem.* **284**, 34468; 2009), and the corresponding PDB entry (PDB code 1BEF) has been made obsolete by the wwPDB at the request of the publisher.

To ensure that PDB entries are validated using state-of-the-art methods, wwPDB validation task forces have been convened for X-ray crystallography and nuclear magnetic resonance spectroscopy. Their recommendations will be reviewed and incorporated into wwPDB's deposition and annotation procedures.

wwPDB encourages all journals publishing macromolecular structures to stipulate accompanying submission of wwPDB validation reports. These will help editors and referees to assess the reliability of structural data and their interpretation. A few journals have already indicated their interest.

With the support of the structural-biology community,

the mission of the wwPDB is to safeguard the integrity and improve the quality of the PDB archive. It is the public availability of atomic coordinates and experimental data that enables errors and possible fabrications to be detected in the first place. Current validation procedures were designed to identify occasional honest mistakes, not to guard against rare cases of malfeasance.

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Nature would like to make clear that the misconduct investigation by the University of Alabama concluded in December 2009 that H. M. K. Murthy acted alone in generating allegedly falsified protein structures. He denies the allegations.

Science friction as fantasy irritates religious sensibilities

I was amazed to read the story 'Divine diseases' in your Futures science-fiction section (*Nature* **462**, 1088; 2009). I am not a Catholic and I do not believe in transubstantiation, but this gratuitously offensive junk has no place in a serious scientific journal.

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