for access to modelling tools drives further modelling. Clear agreements must govern credit attribution and the ethics of data use.

Maximizing the utility of information is a major attraction for investors in the MGI's infrastructure. Expensive data sets obtained, for example, from national synchrotron and neutron-diffraction facilities should be archived and leveraged to the greatest extent possible for searching and citation, as should data from massive supercomputer simulations.

Open-access rules are desirable, following the example of the National Science Foundation-funded nanoHUB for nanometre-scale modelling and simulation tools, as well as the LAMMPS molecular-dynamics code and the DREAM.3D software for meshing three-dimensional microstructures.

AMANDA BARNARD

Embrace uncertainty

Head of the Virtual Nanoscience Laboratory, Commonwealth Scientific and Industrial Research Organisation, Parkville, Australia

The MGI is opening up styles of collaborative working that raise technological and personal challenges. Materials scientists must become more comfortable with uncertainty. They must relinquish control, trust their fellow scientists, and resist the urge to redo everything 'just to be sure'.

Delivering new science from existing data requires the pooling of resources. Some insights and breakthroughs cannot be made any other way. One method may probe scales or achieve resolutions that others cannot. Electron microscopy can resolve subatomic features on surfaces, but optical microscopy shows how light reflects from them.

It is difficult to combine results from different sources. Errors arise from idiosyncrasies in experimental or computational techniques. Many experimentalists know the frustration of reproducing results that vary with laboratory conditions. Even theory-based computational methods can yield different answers.

Mixing data from different origins often introduces more uncertainty than a simple sum of the measurement or statistical errors stemming from the pure data sets. To benefit from data sharing, we must learn to live with that.

The other sort of uncertainty that MGI users must embrace is the human element — our opinions of the people who created the original data and of their competence. Scientists are trained to be sceptical as well as objective. To move materials research forward quickly, we need to assume that each contributor is highly capable, and let the quality of the data speak for itself.

The MGI's value will only come if we can draw from it as easily and confidently as we give to it.

FRANCOIS GYGI

Make simulations reproducible

Professor of computer science, University of California, Davis

The most rapid rewards of the MGI could come from sharing simulations of materials structures.

Numerical simulations are not as reliable and reproducible as their theoretical and computational basis would suggest. They often give differing results owing to the complexity of approximations and the number of parameters used.

Overcoming these difficulties is essential for designing new materials. More robust predictions from simulations of the formation of defects in the lattice of a material, for example, improves our ability to optimize the materials' strength or electronic properties.

> ***"Universal data formats and centralized databases are not always necessary."***

Data are reliable only if they can be independently verified and reproduced by different research groups, ideally using different tools. Sharing data freely will make such cross-validation possible.

When disseminating simulation data, researchers must bear two points in mind. First, simulation software should be openly accessible, not just results. Software vendors must not forbid — as some currently do — publication of raw results or performance data out of fear that comparisons may show their product in an unfavourable light. The scientific community should fight this trend.

Second, universal data formats and centralized databases are not always necessary. The materials community could adopt existing frameworks for data sharing. For example, a vast amount of open-source software already supports the World Wide Web Consortium standards for publishing and exchanging data on the Internet, such as the Extensible Markup Language (XML).

With a modest investment, researchers can publish their own data on their own servers in ways that others can access readily. By encouraging the development of domain-specific web tools, we will lower the barriers to data cross-verification and validation.

PETER B. LITTLEWOOD

Probe the infinite variety

Associate laboratory director for physical sciences and engineering, Argonne National Laboratory, Illinois

From synchrotrons to scanning-electron microscopes, nanotechnology tools have been honed in the information revolution. Now, through the MGI, we need to invent molecular manufacturing by expanding our vision to include the infinite variety of materials.

There are fundamental hurdles. Despite the initiative's ambitious name, atoms are not genes. The biological genome is both a theory and an algorithm for execution. In materials science, quantum mechanics can doom attempts to translate perfectly from code to function.

This theoretical impasse simply reflects the diversity of materials. Tiny variations in composition or structure can produce entirely new functions. The semiconductor industry depends on a delicate salting of silicon with minute concentrations of other atoms.

Yet chemistry can be systematic. Since Dmitri Mendeleev formulated the periodic table, we have exposed patterns of materials' structure and function, now sifted with the aid of powerful computers and high-throughput experiments. We are building, if not a single 'genome', a patchwork of tools matched to material type, property and function. The MGI will expand that.

But the brute-force approach of the modern electronics industry cannot be scaled up to make lightweight structural materials, batteries or solar cells. Here, production must be measured in megatonnes and square kilometres. The MGI has to help us beyond design and into synthesis — our goal being the engineering of programmable matter that builds itself. ■

CORRECTION

The Comment 'Melting glaciers bring energy uncertainty' (*Nature* **502,** 617–618; 2013) wrongly said that Himalayan glaciers lost 174 gigatonnes of water each year for the period 2003–09. This was not the annual rate, but the total amount for that period. And the Indus depends on glacial waters for up to half of its flow, not half of its flow, as stated.