Improving human-data interaction to speed nanomaterials innovation

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Data is only as good as humans' ability to analyze and make use of it.

In materials research, the ability to analyze massive amounts of data—often generated at the nanoscale—in order to compare materials' properties is key to discovery and to achieving industrial use. Jeffrey M. Rickman, a professor of materials science and physics at Lehigh

University, likens this process to candy manufacturing:

"If you are looking to create a candy that has, say, the ideal level of sweetness, you have to be able to compare different potential ingredients and their impact on sweetness in order to make the ideal final candy," says Rickman.

For several decades, nanomaterials—matter that is so small it is measured in nanometers (one nanometer = one-billionth of a meter) and can be manipulated at the atomic scale—have outperformed conventional materials in strength, conductivity and other key attributes. One obstacle to scaling up production is the fact that scientists lack the tools to fully make use of data—often in the terabytes, or trillions of bytes—to help them characterize the materials—a necessary step toward achieving "the ideal final candy."

What if such data could be easily accessed and manipulated by scientists in order to find real-time answers to research questions?

The promise of materials like DNA-wrapped single-walled carbon nanotubes could be realized. Carbon nanotubes are a tube-shaped material which can measure as small as one-billionth of a meter, or about 10,000 times smaller than a human hair. This material could revolutionize drug delivery and medical sensing with its unique ability to penetrate living cells.

A new paper takes a step toward realizing the promise of such materials. Authored by Rickman, the article describes a new way to map material properties relationships that are highly multidimensional in nature. Rickman employs methods of data analytics in combination with a visualization strategy called parallel coordinates to better represent multidimensional materials data and to extract useful relationships among properties. The article, "Data analytics and parallel-coordinate materials property charts," has been published in *npj Computational Materials*, a Nature Research journal.

"In the paper," says Rickman, "we illustrate the utility of this approach by providing a quantitative way to compare metallic and ceramic properties—though the approach could be applied to any materials you want to compare."

It is the first paper to come out of Lehigh's Nano/Human Interface Presidential Engineering Research Initiative, a multidisciplinary research initiative that proposes to develop a human-machine interface to improve the ability of scientists to visualize and interpret the vast amounts of data that are generated by scientific research. It was kickstarted by a $3-million institutional investment announced last year.

The leader of the initiative is Martin P. Harmer, professor of materials science and engineering. In addition to Rickman, other senior faculty members include Anand Jagota, department chair of bioengineering; Daniel P. Lopresti, department chair of computer science and engineering and director of Lehigh's Data X Initiative; and Catherine M. Arrington, associate professor of psychology.

"Several research universities are making major investments in big data," says Rickman. "Our initiative brings in a relatively new aspect: the human element."

According to Arrington, the Nano/Human Interface initiative emphasizes the human because the successful development of new tools for data visualization and manipulation must necessarily include a consideration of the cognitive strengths and limitations of the scientist.

"The behavioral and cognitive science aspects of the Nano/Human Interface initiative are twofold," says Arrington. "First, a human-factors research model allows for analysis of the current work environment and clear recommendations to the team for the development of new tools for scientific inquiry. Second, a cognitive psychology approach is needed to conduct basic science research on the mental representations and operations that may be uniquely challenged in the investigation of nanomaterials."

Rickman's proposed method uses parallel coordinates, which is a method of visualizing data that makes it possible to spot outliers or patterns based on related metric factors. Parallel coordinates charts can help tease out those patterns.

The challenge, says Rickman, lies in interpreting what you see.

"If plotting points in two dimensions using X and Y axes, you might see clusters of points and that would tell you something or provide a clue that the materials might share some attributes," he explains. "But, what if the clusters are in 100 dimensions?"

According to Rickman, there are tools that can help cut down on numbers of dimensions and eliminate non-relevant dimensions to help one better identify these patterns. In this work, he applies such tools to materials with success.

"The different dimensions or axes describe different aspects of the materials, such as compressibility and melting point," he says.

The charts described in the paper simplify the description of high-dimensional geometry, enable dimensional reduction and the identification of significant property correlations and underline distinctions among different materials classes.

From the paper: "In this work, we illustrated the utility of combining the methods of data analytics with a parallel coordinates representation to construct and interpret multidimensional materials property charts. This construction, along with associated materials analytics, permits the identification of important property correlations, quantifies the role of property clustering, highlights the efficacy of dimensional reduction strategies, provides a framework for the visualization of materials class envelopes and facilitates materials selection by displaying multidimensional property constraints. Given these capabilities, this approach constitutes a powerful tool for exploring complex property interrelationships that can guide materials selection."

Returning to the candy manufacturing metaphor, Rickman says: "We are looking for the best methods of putting the candies together to make what we want and this method may be one way of doing that."

New frontier, new approaches

Creating a roadmap to finding the best methods is the aim of a 2½-day, international workshop called "Workshop on the Convergence of Materials Research and Multi-Sensory Data Science" that is being hosted by Lehigh University in partnership with The Ohio State University.

The workshop—which will take place at Bear Creek Mountain Resort in Macungie, PA from June 11-13, 2018—will bring together scientists from allied disciplines in the basic and social sciences and engineering to address many issues involved in multi-sensory data science as applied to problems in materials research.

"We hope that one outcome of the workshop will be the forging of ongoing partnerships to help develop a roadmap to establishing a common language and framework for continued dialogue to move this effort of promoting multi-sensory data science forward," says Rickman, who is Principal Investigator on an National Science Foundation (NSF) grant, awarded by the Division of the Materials Research in support of the workshop.

Co-Principal Investigator, Nancy Carlisle, assistant professor in Lehigh's Department of Psychology, says the conference will bring together complementary areas of expertise to allow for new perspectives and ways forward.

"When humans are processing data, it's important to recognize limitations in the humans as well as the data," says Carlisle. "Gathering information from cognitive science can help refine the ways that we present data to humans and help them form better representations of the information contained in the data. Cognitive scientists are trained to understand the limits of human mental processing- it's what we do! Taking into account these limitations when devising new ways to present data is critical to success."

Adds Rickman: "We are at a new frontier in materials research, which calls for new approaches and partners to chart the way forward."

More information: Jeffrey M. Rickman, Data analytics and parallel-coordinate materials property charts, *npj Computational Materials* (2018). DOI: 10.1038/s41524-017-0061-8

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