A Comprehensive Resource for Modeling, Simulation, and Experiments

ACCURATELY predicting how materials will perform under a variety of conditions is essential to countless research programs in national security, lasers, and energy. For the past two decades, Livermore scientists have combined experiments and simulations to predict the performance of materials and help researchers understand how and why materials change over time and ultimately fail. This predictive capability is particularly important for stockpile stewardship, the National Nuclear Security Administration's (NNSA's) program to ensure the safety and reliability of the nation's nuclear stockpile.

Recent experiments at Livermore's High Explosives Applications Facility (HEAF) and National Ignition Facility (NIF) and at Sandia National Laboratories' Z-pinch machine are providing new experimental data about material properties at a record pace. At the same time, other scientists are perfecting new computer models that more faithfully reflect how materials perform under different conditions, especially extreme pressures and temperatures.

Until recently, researchers had to search in different locations for the most relevant data on past experiments to help plan and guide new experiments and simulations. Likewise, Livermore code developers did not have one single resource to support their efforts to build new computer models and refine older ones. In response, a team of physicists, materials scientists, engineers, and computer scientists has developed MIDAS (Material Implementation, Database, and Analysis Source). This Web-based program is strictly access controlled and designed to be a comprehensive central repository for material properties, experimental data, and computer models. MIDAS is used in experiments and simulations involving materials of interest to stockpile stewardship and other national security programs.

The MIDAS development effort is headed by physicist Meijie Tang, together with Peter Norquist, Nathan Barton, Kevin Durrenberger, Jeff Florando, Armand Attia, and Janine Taylor. The effort is sponsored by the Advanced Simulation and Computing

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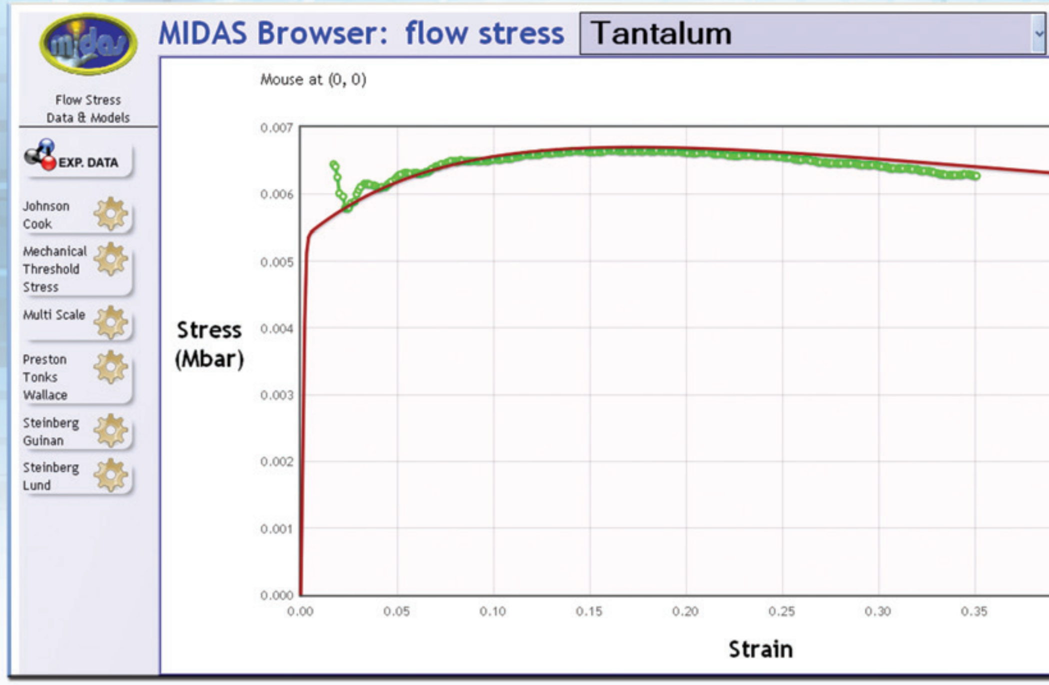


(a) A MIDAS user investigates the strength of tantalum by comparing how closely a standard stress–strain model called Preston–Tonks–Wallace (red line) matches, or fits with, experimental data (green line). (b) Another MIDAS screen shows the relevant parameters used in running the Preston–Tonks–Wallace model. (c) The Experimental Data Panel from the MIDAS browser window lists the selected data from an experiment on tantalum, which was conducted at 293 kelvins and a strain rate of 0.003 per microsecond. Clicking on the Info button would display documentation on the experiment.

Campaign's Physics Engineering Models thrust, led by Brad Wallin. Advanced Simulation and Computing is a key component of NNSA's mission to extend the lifetime of nuclear weapons in the nation's aging stockpile. NNSA's ability to model the extraordinary complexity of nuclear weapons systems is essential to maintaining confidence in the stockpile.

Tang says that Livermore researchers are always seeking to enhance their understanding of how materials age in the extreme environments found within nuclear warheads. They also need to assess the likely effects of these changes under conditions relevant to weapons performance. For both purposes, researchers need robust models that permit true-to-life simulations.

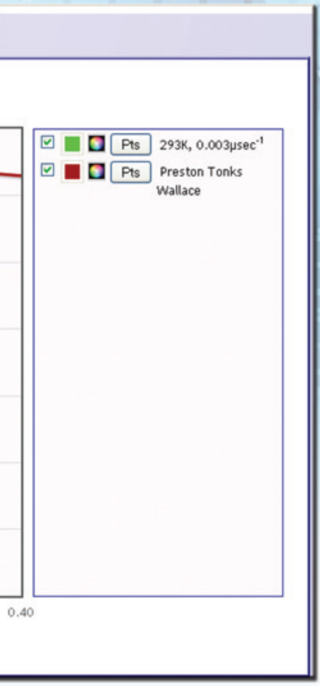
Material Properties Key to Simulations

"Many simulations are performed at the Laboratory, and all depend on using the most accurate material properties generated by experiments or theories," says Tang. She notes, however, that accurate properties can be difficult to obtain. A common repository of experimental results for dozens of materials relevant to stockpile stewardship does not yet exist.

Even when the most relevant data are located, thorough documentation, such as the exact experimental conditions and the purity of materials used in the experiments, may be missing. Researchers also may not have access to the latest models or revisions to the most popular models. In addition, when a newer model is developed, scientists may not have the needed source code to implement the model into their application codes. Plus, few tools help researchers determine the best parameters to use for a given physical regime when they run a simulation or prepare to conduct an experiment.

In the past, Livermore scientists traditionally relied on a "bluebook," developed by the late Livermore scientist Dan Steinberg. The bluebook contains standard strength data and equation-of-state models and parameters for many materials. However, researchers continually need to include new materials, new experimental data, advanced models and the relevant source codes, and new model "fits" showing to what degree a particular model matches experimental results—all of which the bluebook does not easily accommodate.

In place of a printed bluebook, MIDAS provides a simple Web-based program that houses, organizes, and deploys experimental data, models, and their parameters for a growing list of materials. It also provides a flexible interface to the hydrocode applications. When fully developed, MIDAS will provide a comprehensive resource application and framework for many material properties. For now, the team has focused on the all-important material strength data and the related models. Currently, 42 material data sets are available, with up to six models for each



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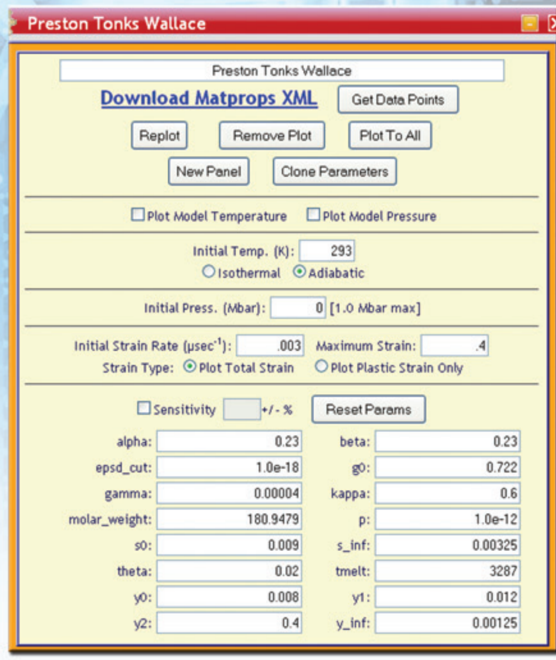

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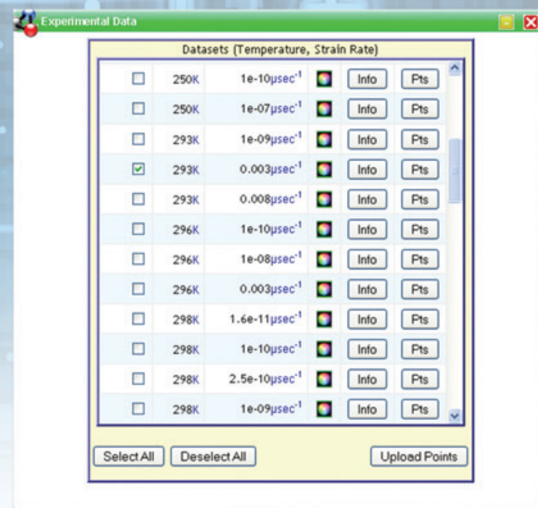


material. Tang's goal is for MIDAS to accommodate a much larger amount of data, more types of material properties, and more models and parameters for materials of interest under different temperature and pressure regimes.

MIDAS allows registered users to view and interact with experimental data, references, and corresponding material strength models. The program accesses components already in existence at Livermore, including databases of materials properties, experimental results, and material model source codes. In the current phase of development, much of the MIDAS effort has focused on the computer framework required to provide easy interfaces between these components.

A registered user signing onto MIDAS could, for example, choose to view all experimental data that reference the hard metal tantalum and select a strength model for the material. The browser then plots the experimental data and the modeled results on a graph known as a stress–strain plot. (See the box on p. 22.) The user can easily determine to what degree data from past experiments fit various strength models. The user can then modify the model parameters to see how those changes affect the corresponding stress–strain behavior. Another feature downloads the model parameters examined at the browser so a user can add the data to their application codes. If a user is unsure what parameters are needed, MIDAS provides "blessed" or default parameters.

Only Pedigreed Data Permitted

Most experimental data on the Web site is "pedigreed"; that is, scientists can attest to the veracity of the data and the purity of materials used for the experiment. Says materials scientist Florando, "A researcher reviewing a previous experiment on tantalum needs to know the amount of impurities as well as microstructural features, such as the size of the tantalum grains." Such detailed knowledge is critical because these features dictate the overall mechanical behavior. In addition, examining the compiled experimental data can reveal where the MIDAS team needs to add experimental data. The team is currently engaging the broad scientific community to obtain additional experimental data.

MIDAS also serves as a central location for documentation of the various models and their source codes. Users can easily compare differences between model versions. MIDAS links the model version with its developer because a user may need to know the model development history and background. Users can also test the sensitivity of model fits to various parameters in the models. Additional plot types, such as strength versus temperature, provide more insight into rate- and temperature-dependent material behavior.

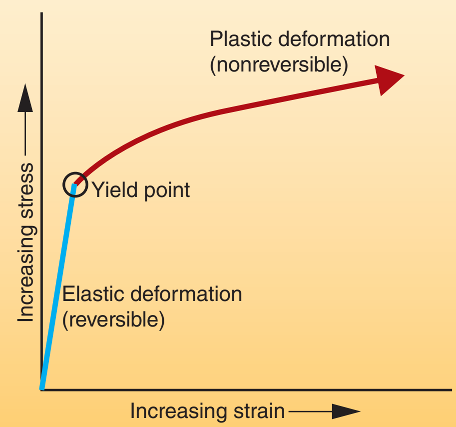
MIDAS users will be encouraged to upload new experimental data and model fits. However, all uploaded data will be checked and reviewed to ensure completeness and quality before these resources become part of the central database.

The Stress and Strain on Materials

A typical model represents a small piece of "physics" for a given material under a set of physical forces. For example, one of the simplest models that Livermore scientists use is for obtaining a stress–strain curve, a graph that shows the relationship between the stress (intensity of the applied force) and the strain (relative deformation) of a particular material.

The nature of the stress–strain curve varies from material to material. Livermore materials scientist Jeff Florando explains, "If one takes a small metal spring and starts to pull it a little bit and lets go, the spring goes back to its original shape, which is called elastic deformation and represents the initial linear portion of the stress–strain curve." If one continues to pull, the spring begins to permanently or plastically deform and does not return exactly to its original shape. The point at which the material transitions from elastic to plastic deformation is called the yield point. On the example stress–strain plot (at right), it is the point where the line starts to curve. If a person continued to pull on the spring, it would eventually break.

Bending samples of gold and aluminum produces different results because the metals have different properties. Models account for these material differences. The more accurate the model, the better the modeled results will match, or fit to, experimental data. And the closer this fit, the more confidence scientists will have in using the information in simulation codes.



A stress–strain plot shows the relationship between the intensity of the applied force (stress) and the resulting relative deformation (strain) of a particular material. The point at which the line starts to curve is called the yield point. It indicates a material's transition from elastic (reversible) to plastic (nonreversible) deformation.

The model source library will soon be able to interface with Livermore application codes written in programming languages such as C, C++, and FORTRAN. Application codes simulate an entire system such as a weapon system or a NIF experiment. The codes involve multiscale modeling, which solves physical problems that have important features at multiple spatial or temporal scales (or both). Florando explains, "We want our source codes to seamlessly feed the pertinent parameters from the material properties database into an application code."

The number of Livermore researchers now using MIDAS continues to grow. The development team plans to make the Web-based program available to other DOE national laboratories as well as the Department of Defense Joint Munitions Program and the U.S. Army Research Program.

Although the current focus is on materials strength, the MIDAS team wants to integrate other properties such as fracture, failure, and high-explosives properties. The team is also developing the capability to examine temperature change and material strength during deformation. The plan is to add to the list of materials and eventually include important compounds. "The overall goal," says Tang, "is to make people's jobs easier, and in so doing, advance stockpile stewardship as well as scientific understanding of what makes materials age and ultimately fail."

—Arnie Heller

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