Uncertainty in the Development and Use of Equations of State Models

V. Gregory Weirs¹, Nathan Fabian², Kristin Potter², Laura McNamara², and Thomas Othalh¹
¹Sandia National Laboratories. ²Scientific Computing and Imaging Institute

Abstract
The research objective of this project is to determine effective visualization techniques for uncertainty of equation of state material models. The ultimate goal is to develop a software tool to be used within the material modeling stakeholder community for understanding material model behavior, including material model uncertainty. Focus groups were used to identify and understand the needs of potential users (the focus group participants) regarding material model visualization and analysis, with the intent of ensuring the usability, utility, and adoptability of the software eventually developed.

Material Modeling
Material models describe the behavior of a specific material or class of materials and are used as inputs to multiphysics numerical simulations. Material models range from the relatively simple to the highly complex, and model formulations vary widely depending on the problem of interest. An equation of state (EOS) describes relationships between thermodynamic variables for a given material. Any given two variables, all other variables can be computed through the EOS under the assumption of thermodynamic equilibrium. EOS models can cover a very wide range of conditions, and different physical phenomena dominate material behavior in different regimes [1]. Uncertainties are abundant throughout the models workflows due to the complexity of a material’s behavior, and the expertise and time required to create an accurate model, the first source of uncertainty comes from inaccurate model forms. Better models can suffer from uncertain parameters values that can come either from experimental measurements or theoretical approximations.

The Distributed Workflow of Material Modeling
Material model development and use exist in a distributed information workflow: a particular model is developed by material modelers, incorporated into a continuum engineering simulation code by developers, used by analysts when they run simulations for specific applications, and, finally, acted upon by a decision maker. Each of these different groups is a stakeholder in the material model, but their knowledge about the material behavior and their use of the material model vary widely. In addition, the meaning of material model uncertainty also varies widely across these stakeholders and the uncertainty at a particular stage is affected by the accumulation of uncertainties throughout the workflow. While the different types of stakeholders were known previously, the most valuable result from the focus groups is the clarification of how these stakeholders interact and how and why they think about material model uncertainty.

Focus Groups
A focus group is a structured group interview, facilitated by a moderator, in which participants explore an issue or set of issues of research importance. All focus groups begin with the same basic principle: exchanges among participants facilitate the expression of ideas, knowledge, behaviors, and opinions that may be invisible to individualized methods (such as a questionnaire or a one-on-one interview). Focus groups enable researchers to access a broader range of skills and experiences than those represented by listening to others express ideas and opinions can spur participants to remember and share information that might not have emerged in a one-on-one setting. However, focus groups should only serve as a starting point for technology design and evaluation, since they only capture information on what users “say they do” - not how they actually do it [2]. The design of the focus groups involves identifying participants, developing a script, organizing and moderating the meetings, and recording and analyzing feedback.

Findings
After reviewing and analyzing the feedback from the focus groups, several themes emerged. These themes can be separated into two categories: direct feedback on the prototypes themselves and more general needs of the material model stakeholders. The most important feedback for us was to discover what the needs of the material model stakeholders are regarding visualization. These types of responses will guide the future development of visualization tools for material modeling. While our prototypes were designed to be sketches of possible visualizations, comments aimed directly at the presented systems identified specific features necessary in a fully developed visualization system. Feedback of this sort will be incorporated in the future visualization systems, ensuring their usability and effectiveness.

Direct Feedback
The feedback directly related to the prototypes can be summarized as the following points:
- Unconnected points convey a sense of uncertainty, but sacrifice the structure of possible realizations
- Users want control over the display of data and statistics
- A large number of surfaces, or surfaces with greater geometric complexity, will be difficult to present simultaneously
- The shape of the EOS surface does not provide enough context; special curves (isentropes, isochersms, Hugoniot, phase boundaries) or explicit labeling are needed as references; analysis need simulation data to provide context
- There is an existing 2D visual language for material models that can be used directly, or leveraged to provide context to 3D representations; 3D views give an overall picture but 2D plots are “more quantitative”

Needs of the Community
More general feedback on the material modeling community are as follows:
- Analysts need access to more information to select an EOSs for particular applications
- Comparative visualizations for EOS properties, including uncertainty, are desired
- Simulation of visualization of EOS and simulation data are useful for “idealized” failed simulations, (b) determining if a simulation relies on EOS data in uncertain regimes, and (c) gaining insight into simulation results
- Material model visualization can alleviate communication bottlenecks across the distributed workflow
- Material model visualization would be useful as a training and learning tool for experienced practitioners as well as those new to the field
- Material model visualization would aid decision makers
- Material model visualization would be useful to identify regions of large uncertainty and gaps in knowledge
- Material model provenance, or lack thereof, is a non-quantitative measure of uncertainty