Uncertainty Visualization Prototypes for Materials Modeling

Kristin Potter[*], Thomas Otahal[†], Nathan Fabian[†], V. Gregory Weirs[†], and Laura McNamara[†]

[*]Sandia National Laboratories [†]Scientific Computing and Imaging Institute

1 INTRODUCTION

Material models describe the behavior of a specific material or class of materials and are used as inputs to multiphysics numerical simulations. Because the models are based on theory, they often require empirical information to calibrate or specify free parameters and results from the models may define ranges of possible values or a collection of valid scenarios. Sources of uncertainty within simulations are abundant; this work focuses on the uncertainty arising from variability in the material models and aims at understanding how users comprehend, incorporate, and utilize this qualitative information and how to enhance understanding through visual representations.

Our approach begins with understanding who the users of the material models are and how they are working with uncertainty information. To this end, we have conducted focus groups to engage modelers, analysts and code developers from the Sandia material modeling community in discussions on how visualization can help them understand the impact of material uncertainties in their workflow. The focus groups provided us with detailed insights into the challenge of developing usable and useful representations of material models and associated uncertainties for a user community with a wide range of interests and applications for such visualizations.

To facilitate discussion, we developed four visualization prototypes, each of which present uncertainty within a material model in a unique way. Participants evaluated specific features of each prototype and described scenarios in which different elements could prove helpful. We present each of the prototypes used in the focus group here, using results from a simplified equation of state simulation which produced seven realizations of a material surface.

2 POINT CLOUD

The first prototype implements a technique presented in [3] that renders a cloud of three dimensional points at a variable distance normal to a surface. The emphasis of this prototype is to show uncertainty in the exact location of the surface. The distance each point is away from the surface is random within a range defined by the amount of uncertainty about the surface location at a particular point. The algorithm creates a cloud of points that are further away from the surface in regions of high uncertainty, and closer to the surface in regions of lower uncertainty. Additionally, the transparency of each point can be varied with the uncertainty, thus points of higher uncertainty become more transparent. This creates a visual effect that feeds the expectation of the human visual system, where regions of low uncertainty appear crisp and solid, and regions of higher uncertainty appear hazy and indistinct. In addition, the points can be colored by another scalar value, such as temperature, and thus simultaneously convey data and uncertainty information.

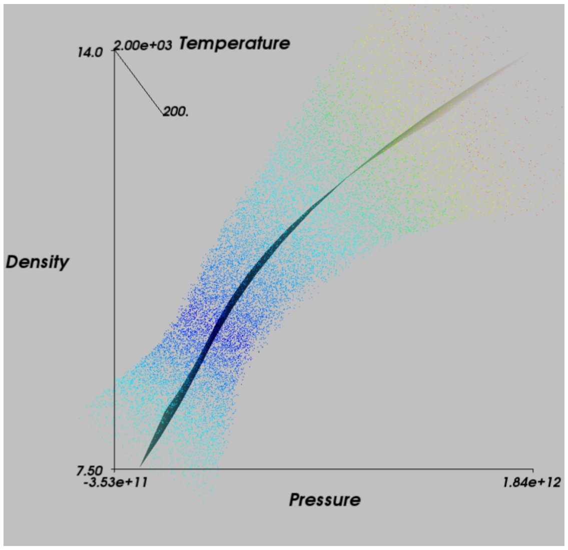

Figure 1: View of the point cloud prototype. The mean surface of the dataset can be seen in the middle of the point cloud. The point cloud is blue and opaque in regions of lower standard deviation and more red and transparent in regions of higher standard deviation, near the top of the figure.

2.1 Surface Animation

The second prototype is based on a technique described by [2] that uses animated visual vibrations of the points defining a surface to show uncertainty in the surface location. The animation draws a fixed semi-transparent surface at the mean and sweeps another solid surface through one standard deviation above and below the mean surface, with the animation transition defined by the sinusoid equation:

$$V = \frac{csin(2\pi pt + \frac{\pi}{2}) + 1}{2} + f \tag{1}$$

where V is the location of the vertex along the surface normal, c is the amplitude of the oscillation, p is the period, f is the floor of the oscillation, and t is time. The sinusoid defines a smooth transition between the floor and amplitude over time for each vertex in the surface mesh. If the floor and amplitude for each vertex corresponds to the uncertainty at that point on the surface, then the viewers eye will naturally be drawn to areas of high uncertainty as the surface animates. Other oscillation functions could be used that cause more rapid transitions between states, such as step and sawtooth functions. Figure 2 shows a snapshot of a single frame of the animation.

2.2 Bounding Statistics

The third prototype uses statistics similar to the traditional boxplot [4] to bound the valid regions of the simulation. The minimum, maximum, and mean surfaces are calculated point-wise, as well as the standard deviation between all surfaces in the simulation. The user is given control over the display of the statistical sur-

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[*]e-mail:kpotter@sci.utah.edu

[†]e-mail:{vgweirs, ndfabia, tjotaha, lamcnam}@sandia.gov

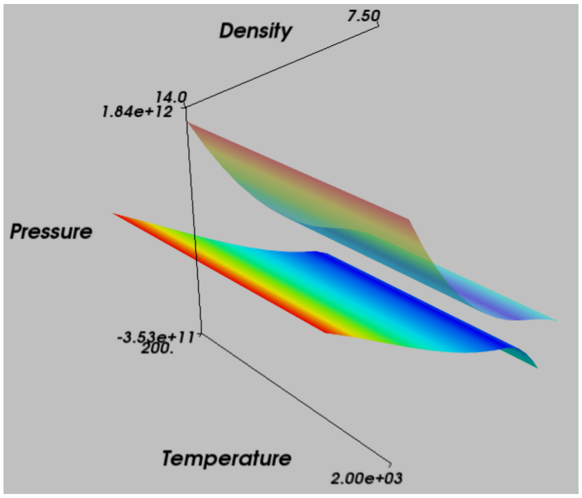

Figure 2: Isometric view of the dataset with the animation stopped at the point of maximum amplitude. The top surface represents the fixed mean surface, and the bottom surface sweeps through a region defined by one standard deviation distance above and below the mean surface. The surfaces are colored by standard deviation, with the largest point of deflection away from the mean surface in the red area of the bottom surface.

faces through a graphical interface which also provides options to show each of the simulation surfaces and contextual surfaces such as the mean +/- standard deviation. Data values can be colormapped onto the mean surface and the user may choose which data values are displayed. Figure 3 shows a screenshot of the prototype. The mean surface is shown centrally and flanked by the minimum and maximum surfaces which have reduced transparency to reduce visual clutter. A single surface from the simulation is shown in blue, below the mean surface. The main goal of this prototype is to show the range of possible outcomes, as well as indicate where the data is most likely to reside.

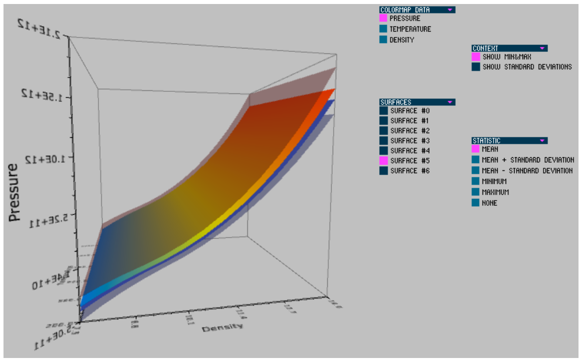

Figure 3: Prototype using bounding statistics and a graphical user interface to explore the dataset. The mean surface is shown centrally along with the minimum and maximum surfaces (with reduced transparency) and a single surface from the simulation (in blue). Through a series of buttons, the user can control which statistical surface to display, contextualize surfaces within statistical bounds, and show the original simulation surfaces.

2.3 View Dependent Opacity

The final prototype uses a model similar to the Blinn lighting model [1], in that the view angle is compared with the normal of the surface at each individual point. Instead of using this to modulate the lighting, it is instead used to modulate the opacity of the surface at each point, as shown in Figure 4. At a high level this technique is used to represent a collection of surfaces, each rendered individually with a transparency associated to confidence in the surface. Thus, when the viewer is directly above the surface, the opacity is determined entirely by the surface's transparency, e.g., $\sigma_{x,y}/N$. When the viewer is at an oblique angle, the surface becomes solid, regardless of the underlying surface's transparency. In the case of this prototype, the transparency is established by the standard deviation of the surfaces as a whole at each position and is divided evenly between all surfaces, that is $\sigma_{x,y}/N$, where N is the number of surfaces rendered.

Figure 4: Two views of an object embedded in a collection of surfaces. On the left, viewed from above, the transparency is set by the surface property. The object can be clearly seen through the surfaces. On the right, viewed from the side, the surfaces are opaque and the object's position along the normal of the surfaces can be seen.

Intuitively, the motivation behind this approach can be understood by considering objects embedded within this collection of surfaces. When viewed from nearly overhead, the surfaces are transparent and objects inside are clearly visible. This allows the viewer to easily determine where the object is positioned on a 2D plane normal to the surfaces. When viewed from the side, because the surfaces become opaque, the embedded object's position along the normal of each of the surfaces becomes more apparent. This approach is not useful when the surfaces are very close together relative to the size of the surfaces.

ACKNOWLEDGEMENTS

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. This publication is based on work supported in part by Award No. KUS-C1-016-04, made by King Abdullah University of Science and Technology (KAUST) and an award from DOE NETL.

REFERENCES

[1] J. F. Blinn. Models of light reflection for computer synthesized pictures. In *SIGGRAPH '77 Proceedings of the 4th annual conference on Computer graphics and interactive techniques*, New York, NY, 1977.

[2] R. Brown. Animated visual vibrations as an uncertainty visualisation technique. *Proceedings of the 2nd international conference on Computer graphics and interactive techniques in Austalasia and Southeast East Asia GRAPHITE 04*, 1(212):84, 2004.

[3] G. Grigoryan and P. Rheingans. Point-based probabilistic surfaces to show surface uncertainty. *IEEE Transactions on Visualization and Computer Graphics*, 10(5):546–573, 2004.

[4] J. W. Tukey. *Exploratory Data Analysis*. Addison-Wesley, 1977.