Advanced Simulation and Computing

Los Alamos NATIONAL LABORATORY

News and Operational Highlights

FEBRUARY 5, 2025

NEW RESOURCE FOR EJECTA MODEL VALIDATION

Mathematical Solutions for Asay Foil Trajectories

The production of ejecta from shocked metal surfaces is a ubiquitous phenomenon with important applications to stockpile stewardship. This drives two mission-relevant needs: One, to develop predictive physics models for ejecta production under a variety of conditions. Two, to quantitatively validate the utility of those models using experimental data. On the first front, Los Alamos researchers have developed an ejecta source model based on the evolution of a Richtmyer-Meshkov fluid instability [1].

Validating this model against high-quality experimental data requires calculating the model's predicted measurements. Piezoelectric pins and Asay foils are complementary diagnostics that retrieve information about the dynamic ejecta cloud with different sensitivities and failure modes. For this reason, they are frequently fielded together. Pin measurements are relatively straightforward to predict because they remain fixed in space, but Asay foils are more challenging because they are accelerated by their interaction with the ejecta cloud and thus exhibit a time-dependent trajectory. Consequently, ejecta model validation based on momentum diagnostic data has, until now, been restricted to pin data, which can become unreliable when heavy dynamic loading can cause the pins' response to become nonlinear or cause the pin to fail completely.

Los Alamos researchers have overcome this difficulty by deriving the solution for calculating the full, time-dependent trajectory of a thin Asay foil moving under the influence of an ejecta cloud generated by a generic ejecta source model [2]. This innovative result required solving an integro-differential equation of motion whose functional form rendered it incompatible with known techniques for handling such problems.

An ability to forward-calculate this trajectory is a major advance: in an experiment, the total ejecta mass—a quantity crucial for ejecta model validation—is inferred from the observed trajectory. Yet, until now, there existed no method for assessing the inference method.

Using this new computational tool, LANL researchers forward calculated a variety of foil trajectories, applied various experimental methods for inferring the dynamic ejecta accumulation, and then compared the results to the true result (known from the forward calculation). Under certain well-understood and frequently satisfied conditions, a commonly used approximation can severely underestimate the total mass. However, a more exact solution published by the authors recreates the true result with near perfection (Figure 1).

For more information, contact **Gowri Srinivasan** (gowri@lanl.gov), V&V Program Manager. We acknowledge the work of Ian Tregillis and Physics Validation Project Leader Aaron Koskelo.

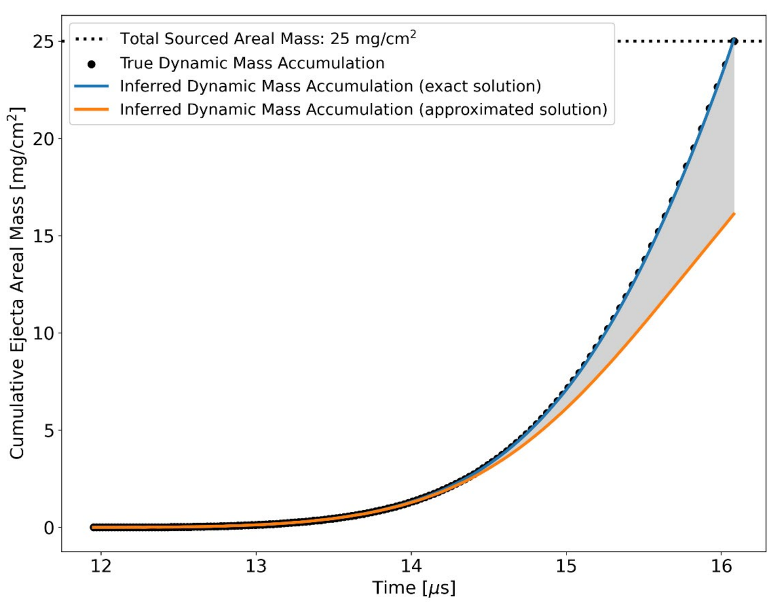

Figure 1 Los Alamos researchers used a newly developed technique to calculate the trajectory of a 100 *μm* titanium Asay foil subjected to 25 mg/cm^2 of tin ejecta generated over the course of 1 *μs* by the Los Alamos ejecta source model. Next, researchers fed that theoretical trajectory into two different data analysis methods for extracting the dynamic ejecta mass accumulation from a foil velocity measurement, comparing the results to the true answer (black circles). In this example, a commonly used approximate solution (orange) underestimates the total ejecta mass by 40%, whereas the authors' exact solution (blue) exactly reproduces the correct answer. The shaded gray region shows the discrepancy.

[1] Hammerberg, J.E., Buttler, W.T., Cherne, F.J., Andrews, M.J., et al. A Source Model for Ejecta, *J. Dyn. Beh. Mat.*, 2017. **3**:316.

[2] Tregillis, I.L. and Koskelo, Aaron. An implicit solution for Asay foil trajectories generated by separable, sustained-production ejecta source models, *J. Appl. Phys.*, 2024. **136**:114502.

NUCLEAR PHYSICS

Improved Fission Modeling

A significant challenge in nuclear physics is an accurate theoretical understanding of the nuclear fission process. Currently, inaccuracies persist in the predicted fission cross section and no unified description of the whole fission process exists. A project between Los Alamos National Laboratory (LANL) and CEA Bruyeres-le-Chatel under the DOE/NNSA-CEA/DAM agreement on Cooperation on Fundamental Science Supporting Stockpile Stewardship aims to resolve these issues. Recently, scientists at LANL proposed an innovative technique to calculate nuclear fission cross sections by solving a 1D quantum tunneling problem [1]. This new method allows fission cross sections to be predicted with a few model parameters, while traditional fission models require many more tuning knobs. Figure 1 is the calculated fission cross section of Pu-239 compared with its evaluated data based on all available experimental data. A pronounced structure is due to an interference effect in the tunneling.

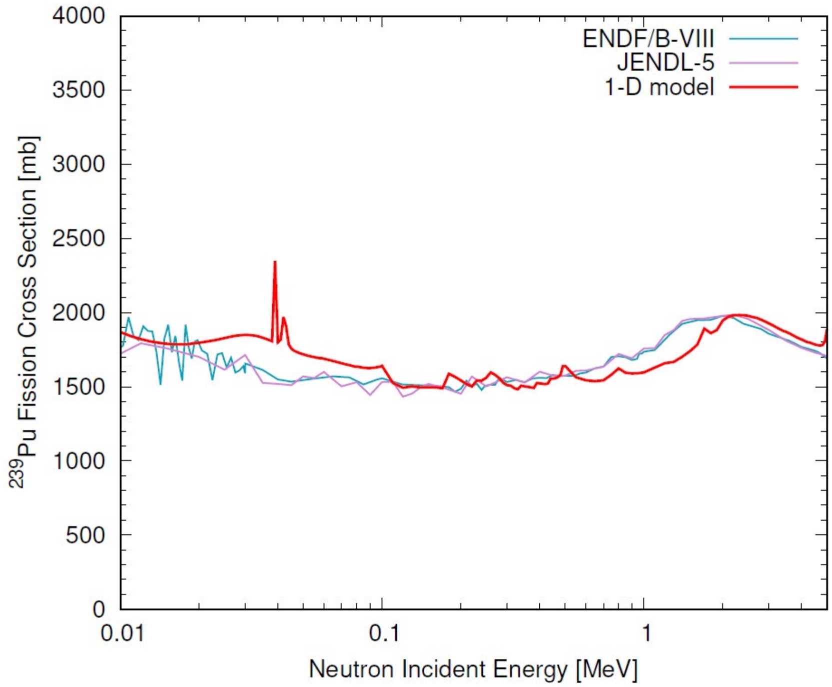

Figure 1 A new calculation of the Pu-239 fission cross section using a 1D quantum tunneling model (red) compared with existing evaluated data.

This technique opens a new path forward—a multi-dimensional tunneling problem—that includes microscopic knowledge of the fission process. For example, solving a 2D problem (nuclear elongation axis and mass asymmetry axis) could provide the fission cross section and the fission fragment distribution simultaneously. Through combination with the LANL fission fragment decay model [2], other fission observables can now be obtained, such as the average number of prompt and delayed neutrons, neutron spectra, and independent and cumulative fission product yields.

For more information, contact **D. J. Luscher** (djl@lanl.gov), PEM Program Manager. We acknowledge the technical contributions of Toshihiko Kawano, Amy Lovell, Ionel Stetcu, Matthew Mumpower, and Patrick Talou.

[1] T. Kawano, P. Talou, and S. Hilare, "Solving the one-dimensional penetration problem for the fission channel in the statistical Hauser-Feschbach theory," *Physical Review C*, 109, April 2024. DOI: 10.1103/PhysRevC.109.044610

[2] A. Lovell, T. Kawano, S. Okamura, I. Stetcu, M. Mumpower, and P. Talou, "Extension of the Hauser-Feschbach fission fragment decay model to multichance fission," *Physical Review C*, 103, January 2021. DOI: 10.1103/PhysRevC.103.014615

OPACITY EFFORTS

New Approach Produces Mutually Consistent Equation of State and Opacity Values

Opacity is used to predict the generation and transport of x-rays in hot matter. A disagreement between theoretical opacity models and opacity measurements carried out at the Z-pinch facility at SNL and preliminary results from the opacity campaign at the National Ignition Facility at LLNL have prompted efforts to test and improve theoretical atomic models. Recently, a multi-laboratory opacity analysis is identifying approaches for improving the accuracy of ASC simulations.

LANL's previous plasma equation-of-state (EOS) models described plasma effects self-consistently but did not include atomic structure of sufficient fidelity to yield accurate opacity calculations. LANL's PEM-atomic hybrid EOS-opacity effort has developed a new relativistic, variational formalism and computer code (**Starrett et al, Phys. Rev. E 2024**) that produces consistent and high-fidelity EOS and opacities. This represents a breakthrough in consistent EOS and opacity modeling and improves both LANL's EOS and opacity efforts. Accurate EOS was demonstrated through agreement with trusted simulations based on density functional theory.

Predictions of excitation energies were made and compared to experiments in the dense plasma regime and were found to be in **good agreement**. Some differences were observed for highly charged states; however, we understand their origin. The new method developed is a major step forward, and code development for applying the method to materials of interest is underway. Very recently, we began to compare predictions of the opacity of oxygen (an ongoing target of Z-machine and NIF opacity measurements) from the new model to the Opacity LIBrary (OPLIB) database (Figure 1).

For more information, contact **D. J. Luscher** (djl@lanl.gov), PEM Program Manager. We acknowledge the work of Eddy Timmermans, Charles Starrett, Trinity Thelen, Chris Fontes, Joseph Kasper, Brian Tran, and Jackson White.

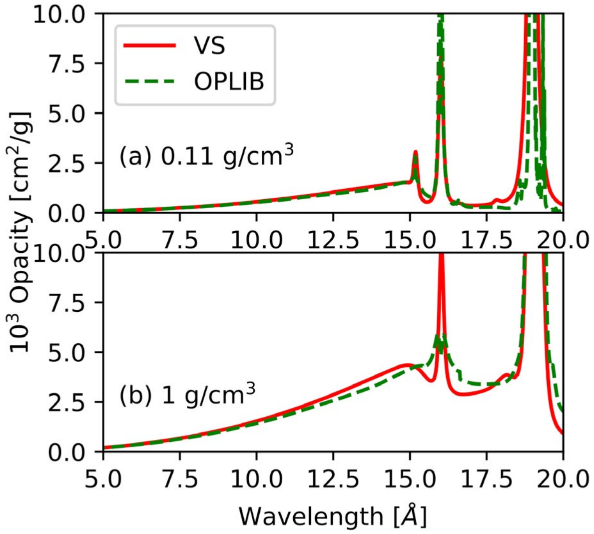

Figure 1 The figure shows predictions of the new model (VS) and OPLIB for oxygen at a temperature of ~2 000 000 K, and two different plasma mass densities (0.11 and 1 g/cm^3). Agreement between the methods is encouraging at the lower density, while some differences at high density point to the importance of including self-consistent plasma effects in the new model.