A Parametric Sensitivity Study in MHD Modeling for Exploding Wires Using DAKOTA in ALEGRA

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Abstract

We present a parameter study of simulated exploding copper wires using the ALEGRA MHD finite element code integrated with the DAKOTA statistical software package. We examine the effects of varying input parameters to the histories of voltage and current and compare ensemble views of the results to experiment. The integrated DAKOTA statistical capability is used to propogate the uncertainties in the laboratory wire diameter, wire length, and circuit resistance to the numerical results and demonstrate the sensitivity of the solution to variations in each parameter. Our approach is to model previous work done for aluminum wires with an attempt to utilize the integrated ALEGRA-DAKOTA capabilities to provide more automation and take advantage of additional tools and techniques.

I Introduction

While individual forward simulations of nonlinear physical systems can provide insight into the physics and can be of some help in decision making, the incorporation of uncertainties as an integral part of an analysis is essential for increasing the confidence of the simulation results. Performing sensitivity analyses on input parameters and propogating uncertainties from the inputs to the outputs simply provides much more information for use in evaluating the simulation results.

Using a previous validation study performed by Doney *et al.* [4] as a model, we utilize an integrated statistical capability in the ALEGRA MHD finite element code to perform a parameter sensitivity analysis of exploding copper wire simulations. The goal is to exercise and evaluate the ability to perform this type of study using the additional tools and techniques afforded by this integrated simulation and statistical capability.

We start by introducing the integrated DAKOTA capability, then describe the target experiment, followed by the computational setup. We then analyze the simulation results and follow up with some conclusions.

II Integrated Uncertainty Quantification

ALEGRA is a finite element code with the capability to model nonlinear resistive magnetohydrodynamics (MHD) and multimaterial shock hydrodynamics [7]. It performs forward simulations initialized with settings for the geometry, the boundary conditions, the material models and their parameters, and many other configurations that affect the simulation outcome. Ideally these initialization parameters would be known precisely, however, most often there are uncertainties in experimental measurements. Compounding this issue is the fact that many times one must make algorithmic trade-offs to achieve robustness—often in the form of "knobs" whose values are not easily determined.

Here, we utilize the DAKOTA software package [1] to better understand the sensitivities to the uncertain input parameters. DAKOTA is a rich, flexible analysis tool for performing sensitivity analyses, uncertainty quantification, and optimization as well as many other capabilities. In the current context, ALEGRA (the simulation code) produces a value or values in response to input parameters. The common use of DAKOTA is to run a stand-alone executable that samples the input parameter distributions, invokes scripts which launch ALEGRA with the input values, and finally, the response function value is extracted from the output files and handed back to DAKOTA. The analyst must write these scripts and manage the directories and files in this mode of operation.

Recently, the DAKOTA package has been integrated into the ALEGRA simulation code to form a single executable. In this integrated mode, the analyst supplies the DAKOTA specifications within the ALEGRA input deck as well as the response functions to be used, and the rest is automated. The motivation behind this integration is to reduce the level of effort required to add uncertainty quantification and sensitivity analysis as an integral part of performing ALEGRA simulations.

The simulations performed in the exploding wire study were all done with this ALEGRA-DAKOTA integrated feature. Of the limited number of built-in response functions currently available in ALEGRA, the maximum value of a quantity (such as voltage) and the time of that maximum were used. To gain statistical information, DAKOTA samples the input distributions and invokes many forward ALEGRA simulations. The resulting data include the response values as well as current and voltage traces.

III Experimental Setup

By discharging a capacitor through a wire, it is possible to cause an explosion by nonlinear resistive heating. The wire goes through two phase changes as its internal energy increases, first melting and then vaporizing. Histories of the voltage across the wire and the current passing through it provide a signature of these transitions. Simulated voltage and current traces which are typical of a copper wire explosion are shown in Figure 1. The timings of the current and voltage peaks depend sensitively on the timing of the phase changes and, therefore, they effectively test the equation of state and conductivity models.

As the capacitor is discharged, first the current becomes very large due to the wire's low resistance at ambient conditions. Resistive heating causes the wire to melt and expand, and the voltage across the wire begins to rise rapidly as the material conductivity drops [8]. The current peaks and falls as the wire expands. As the wire vaporizes, the voltage rises abruptly to a maximum and immediately falls off precipitously. The current, meanwhile, passes through a local minimum before rising once again as current redistributes itself throughout the vaporized wire material. Finally, the current falls off as the voltage difference disappears.

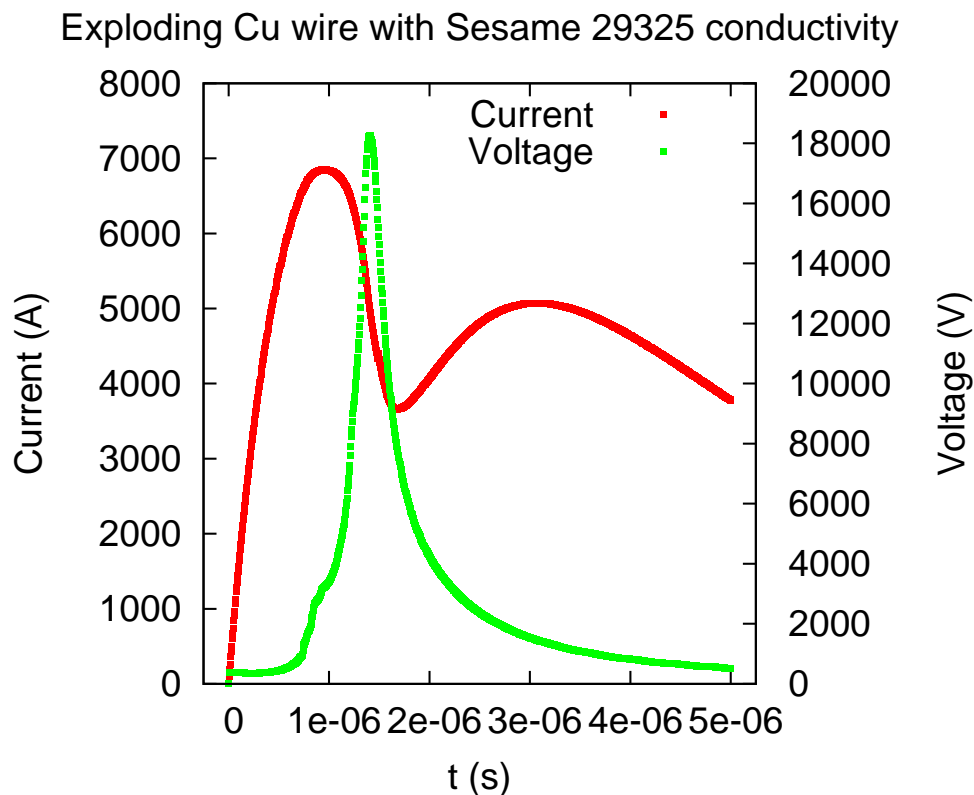## Exploding Cu wire with Sesame 29325 conductivity

Figure 1: Simulated current and voltage histories typical of a copper wire explosion.

In the various contexts in which exploding wires are studied, the moment of wire burst is often of interest. It is typically found to be a distinct and recognizeable point in time. The instant of peak voltage is commonly taken to represent the time of burst [8]. After this time, the voltage quickly collapses as the wire material transitions rapidly to low densities and high temperatures. The rapid change in volume generates shock waves which emanate into the surrounding material.

DeSilva and Vunni [2] recently performed a series of tests on copper wires. The experimental setup was the same as that described in Doney *et al.* [4]. Each wire was placed in series with an RLC circuit with a 1.15-μH inductor and a 1.88-μF capacitor charged to 19.98 kV. Multiple experiments with this setup were performed, and three of the resulting datasets are used here for comparison to simulations.

The experiments incorporated uncertainties due to variabilities in certain parameters, which were investigated in an uncertainty analysis by Doney *et al.* for experiments on aluminum wires. These same measurement uncertainties are investigated here for copper wires. The uncertain parameters include the wire length and diameter, and the driving circuit resistance external to the wire. Values and uncertainty ranges for these parameters can be seen in Table I. This is not an exhaustive list of the uncertain parameters involved in the experiments and probability distributions are not known, but we think they are appropriate for the purposes of this study.

Table I: Experimental Parameters and Their Uncertainty

Resistance (Ω)	2.00 ± 0.10
Wire Length (mm)	16.5 ± 0.83
Wire Diameter (μm)	126.26 ± 1.89

IV   Computational Setup

The exploding-wire experiments were modeled in a two-dimensional cylindrical (r-z) mesh. The wire extended along the z-axis, and steel electrodes were inserted at both ends of the wire. The remainder of the mesh was filled with water. The simulation was driven by a circuit using a fully coupled lumped element model, with time integration of the circuit model provided by a differential algebraic equation solver [5].

The copper equation of state (EOS) was modeled with the Sesame 3320 EOS table [6]. The electrical conductivity of copper was modeled using two implementations of the Lee-More-Desjarlais model [3]: the standard implementation which runs inline under ALEGRA, and a more recently developed, quantum-molecular-dynamics- (QMD-) tuned version of the LMD model. We will refer to this as the "QLMD" model. It is currently only available in tabular form as Sesame 29325.

As for water, ALEGRA simulations were performed using the Sesame 9150 EOS table. The electrical conductivity of water was modeled using the Sesame 29150 model. The minimum resolved conductivity in ALEGRA (called the "void conductivity") was set to 0.01 S/m for the simulations in this study.

In order to ensure simulation fidelity, it is important to have a sufficiently fine mesh. For exploding wire simulations, it is also important to have the mesh extend to a sufficient radial distance so that the full inductance in the simulated field is captured. However, increasing resolution and mesh size both increase the computing time, so the resolution and extent of the mesh must be chosen in order to find accurate results with reasonable computing times. Following Doney *et al.* [4], we chose a mesh with about 3.8 elements per wire radius and with a radial extent of 400 wire radii.

For the DAKOTA specification, we selected a parameter study using Latin Hypercube sampling (LHS) from a user-specified, normal (Gaussian) distribution of the three input parameters. The mean and standard deviations for each input parameter were chosen to be the values from Table I. For example, the mean resistance was 2.00 with a standard deviation of 0.10. It should be emphasized that we do not know what the probability distribution is for these uncertain input parameters. A uniform distribution could have been chosen as well, but that would mean selecting a lower and upper bound.

The response functions were chosen as the peak values for voltage and current, as well as the times at which those peaks occur. The code returned probability distributions on this user-specified response function (wire burst time) and a matrix of correlation coefficients characterizing the sensitivity of the burst time to the uncertain parameters. The individual simulations (one for each input sample) were selected to remain present after the job finished, so as to allow further analysis of the results.

This computational setup was executed using 32 compute nodes (containing 8 cores each) for the QLMD case. Each ALEGRA simulation ran on 8 compute nodes, which means there were 4 concurrent ALEGRA simulations. For the LMD case, 64 compute nodes were used with 8 simula-

tions running concurrently on 8 nodes each. A separate aluminum wire study was also performed using 72 compute nodes with 6 concurrent simulations on 12 nodes each.

V   Results

The data from multiple forward simulations can be examined and visualised in a number of different ways. One common desire is to compare the data from experiment to the analogous data from the simulation. This means combining the multiple simulation results together in order to provide a single view.

The simulation results in this study were aggregated (independently of DAKOTA) into envelope plots as a way to visualize the trace behaviors. See Figures 2 and 3. These figures were created by computing the mean and standard deviation of the current/voltage across all simulations at each time value, then using that to paint a band of width two standard deviations centered around the mean. The minimum and maximum bounds are also shown. Finally, the values from each of the three experiments were overlaid. This allows a direct comparison of simulation to experiment within the context of a full UQ study. In this way, uncertainty inherent to the system is incorporated into whatever judgments are made in the validation analysis, as described by Doney *et al.* [4].
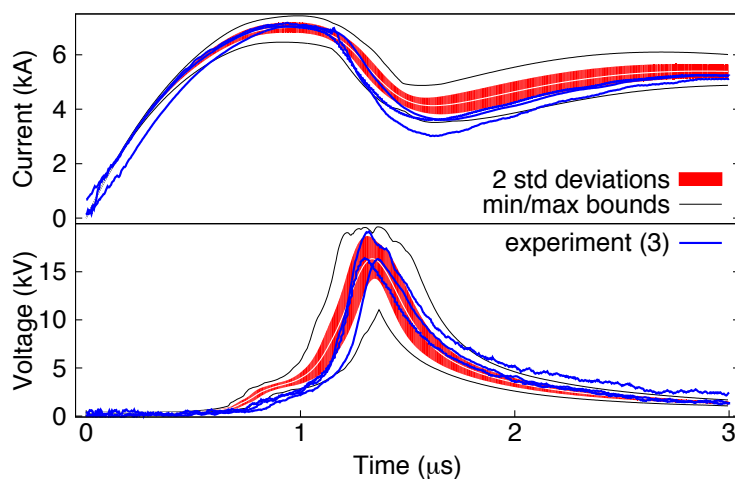

Figure 2: An ensemble of the simulated current and voltage traces as a function of time using the QLMD model overlayed with the experimental values. The red zone has a width of 2 standard deviations and is centered around the mean value.

It can also be very useful to determine the impact of each parameter on various output quantities of interest (i.e., the parameter sensitivities.) As part of the default output from DAKOTA, the partial correlation matrix between the input parameters and the output parameters is provided. The correlation is a measure of dependence between two quantities; zero means no dependence, while plus or minus one represents the strongest dependence possible.

The correlation between our input parameters and the time of peak voltage is shown graphically in Figure 4. The correlation coefficient as reported by DAKOTA is shown the upper left corners.
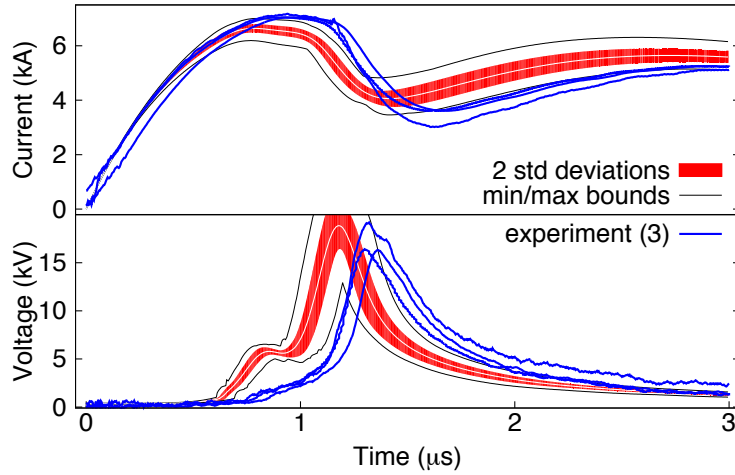
Figure 3: An ensemble of the simulated current and voltage traces as a function of time using the standard LMD model overlayed with the experimental values.

One can see graphically how the slope of the regression line matches the value of the correlation. This representation of the UQ study output shows a relatively strong correlation to the wire diameter and resistance; larger values of either of these cause the time of peak voltage to occur later in time. Increased wire diameter allows for greater cross-sectional area for current flow, leading to lower current densities and lower Joule heating rates. Increased circuit resistance diminishes the total current fed to the wire during the capacitor discharge, leading to delayed onset of wire burst and diminished peaks in current and voltage. It also reduces the prominence of the local minimum for the current (occurring around 1.6 μs). The data also show that a much weaker correlation exists for the wire length, which has no direct influence on the current density in the wire. In all three cases, the scatter in the data shown in Figure 4 results from the interaction of effects from each of the three uncertain paramaeters.

Another way to view the sensitivity on a parameter (at least in this case) is to graph multiple traces but color each trace by the value of the parameter of interest. In Figure 5 we can see the effect of resistance on the voltage and current traces. Increasing the resistance causes lower peaks for both traces and reduces the local minimum for the current (occurring at around 1.6 μs.) The voltage peak shift is also apparent. To reduce the noise of the graph, only those simulations were shown whose wire diameter and wire length was close to the mean (within one standard deviation.)

Given enough samples, the probability distribution functions of the inputs can be propogated to distributions on the outputs. The form of the output distribution may not be known, but a histogram can be created as an approximation. We ran a 729 sample DAKOTA simulation using an aluminum wire and looked at the output distribution of peak kinetic energy of the wire (the burst time.) The large number of samples was made more feasible by reducing the final simulation time to just after the peak occurs. Figure 6 shows the histogram of the sampled external resistance and of the burst time response. Note that while the inputs were sampled from normal distributions, the output does not appear to be a normal distribution. It shows some skew toward later times and there is evidence of a long right hand tail.
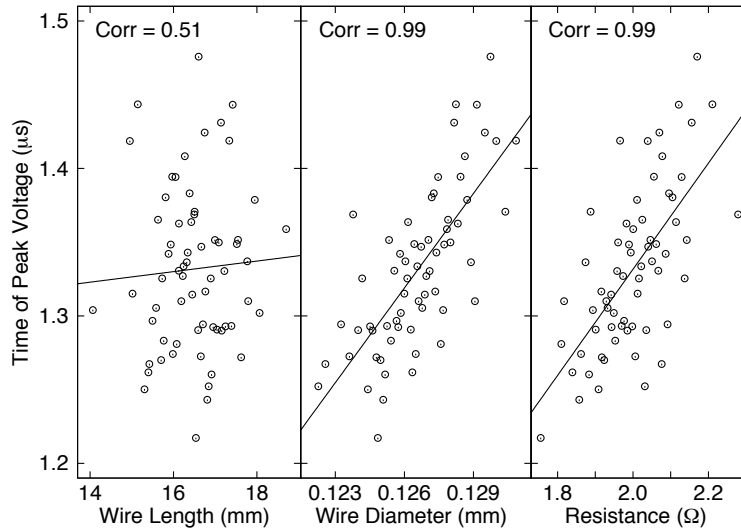
Figure 4: The correlation between the input parameters and the time of peak voltage for each simulation. The partial correlation values are given in the upper left as reported by DAKOTA. The lines are a linear regression fit of the points.

Lastly, the UQ analysis also allows us to investigate the quality of our metric for wire burst time. Previous work on exploding wires has used the time of peak voltage as the burst time, but there has been some debate as to whether the time of peak radial velocity of the wire material might be a better mark. Since the kinetic energy is easily available from the simulations and would peak at the same time as velocity in this situation, we compare the time of peak kinetic energy of the wire with the time of peak voltage. In Figure 7, the trace of each quantity for an arbitrary sample simulation is shown along with a scatter plot (upper right) of the values for each definition of burst time. Points lying on the diagonal have equal values for each definition. Having multiple simulations provides confidence that there is no significant difference between the two possible definitions of the burst time for the conditions considered here.

VI   Conclusions

Based on the analysis presented here, we observe that DAKOTA integrated with ALEGRA provides powerful utility for modeling of systems with inherent uncertainty. Postulated uncertainties in parameters of the setup, represented as probability distributions on inputs, are propagated through the forward simulations in automated fashion, yielding results with their own distributions of probability. The coupling or correlation of each of the uncertain parameters to the simulation response function is quantified, with uncertainties incorporated.

After the experiences in performing the simulations in this paper, we can easily say that having DAKOTA integrated into ALEGRA greatly simplifies the effort required to execute UQ simulations. DAKOTA also provides a number of useful UQ measures by default, such as the partial correlations from input parameters to output responses. However, the more complete analysis required a number
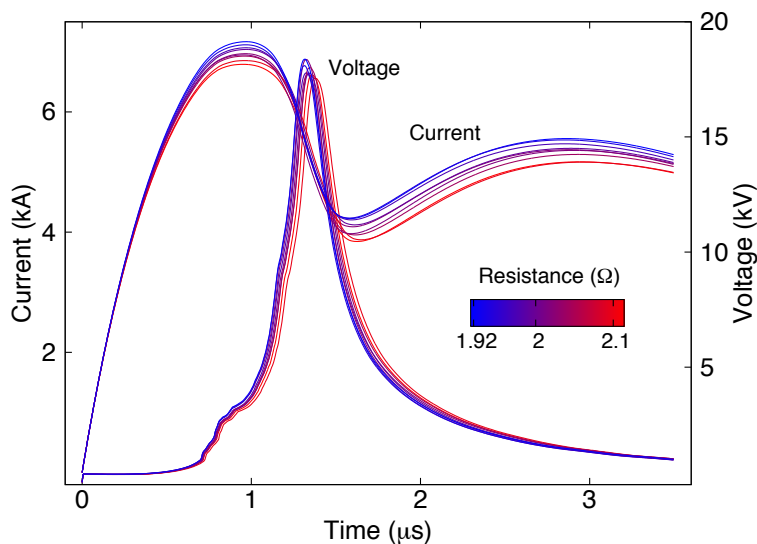
Figure 5: For those simulations whose wire length and diameter are within one standard deviation around the mean, the voltage and current traces are shown colored by the value of the resistance. Blue for a lower resistance up to red for a higher resistance.

of post-processing activities to extract and distill simulation results into a form that enabled a conclusion to be made or a question to be answered. These included the trace envelope technique, the multiple colored trace graph, the correlation scatter plots, as well as the histogram of burst times. We conclude that there is significant room for opportunity in providing analysts with tools and techniques for more easily extracting and visualising UQ results.

In the course of this analysis, it is also shown that the QLMD model for copper electrical conductivity is a significant improvement upon the standard LMD model, bringing the difference between experimental and simulated current and voltage traces to within less than one standard deviation, based on a postulated normal distribution. For the standard LMD model, the peak current and voltage lie well outside the standard-deviation swath plotted in Figure 3. The analysis also shows the time of maximum voltage very nearly corresponds with the time of maximum wire kinetic energy, suggesting that the two are equally adequate diagnostics for the burst time.

It would be useful in future work to check that the assumptions with regard to mesh extent and resolution that were used for aluminum also hold for these simulations with copper. Currently, however, there is a limitation of the integrated DAKOTA capability that makes such an analysis difficult. The reason is due to the fact that higher resolution or greater mesh extents require more computational resources for a given forward simulation. But the number of compute nodes for each simulation is not variable within DAKOTA and cannot adapt to the size of the problem. We think this is another area of opportunity which could have a significant impact on the ease of performing UQ studies.
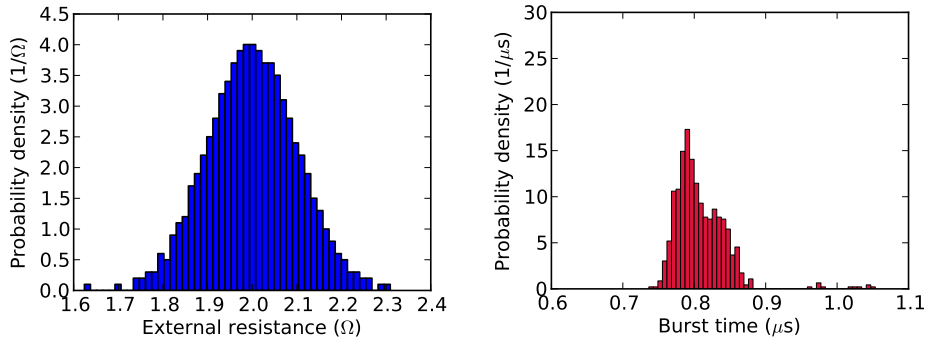
Figure 6: Histograms of the sampled resistance and the kinetic energy burst time responses for a 729 sample aluminum wire simulation.
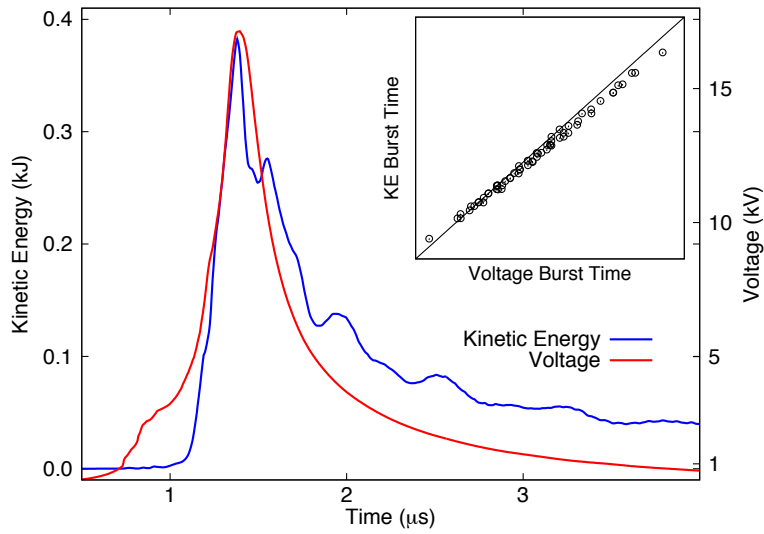

Figure 7: The traces of kinetic energy of the wire and voltage across the wire for a sample simulation with QLMD. The inset compares the time of peak voltage and time of peak kinetic energy for each simulation (points lying on the diagonal have equal values.)

References

[1] B.M. Adams et al. DAKOTA, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 5.0 User's Manual. Technical report SAND2010-2183, Sandia National Laboratories, Albuquerque, NM, December 2009. http://dakota.sandia.gov.

[2] A. W. DeSilva and G. B. Vunni. Electrical conductivity of dense Al, Ti, Fe, Ni, Cu, Mo, Ta, and W plasmas. *Phys. Rev. E*, 83(037402), 2011.

[3] M. P. Desjarlais. Practicle improvements to the Lee-More conductivity near the metal-insulator transition. *Contrib. Plasma Phys.*, 41(2-3):267–270, 2008.

[4] R. L. Doney, G. B. Vunni, and J. H. Niederhaus. Experiments and simulations of exploding aluminum wires: validation of ALEGRA-MHD. Technical report ARL-TR-5299, U.S. Army Research Laboratory, 2010.

[5] A. C. Hindmarsh, P. N. Brown, K. E. Grant, S. L. Lee, R. Serban, D. E. Shumaker, and C. S. Woodward. SUNDIALS: suite of nonlinear and differential/algebraic equation solvers. *ACM T. Math. Software*, 31(3):363–396, 2005.

[6] G. I. Kerley. Equations of state for copper and lead. report KTS02-1, Kerley Technical Services, 2002.

[7] A. C. Robinson, W. J. Rider, et al. ALEGRA: an arbitrary Lagrangian-Eulerian multimaterial, multiphysics code. In *Proceedings of the 46th AIAA Aerospace Sciences Meeting, Reno, NV*, January 2008. AIAA-2008-1235.

[8] T. J. Tucker and R. P. Toth. EBW1: A computer code for the prediction of the behavior of electrical circuits containing exploding wire elements. Technical report SAND-75-0041, Sandia Laboratories, 1975.