Canonically, material property calibration is a manual and iterative process requiring a lot of tribal knowledge and intuition and operation by one who is skilled in the art. The interplay between different material properties and their effects on system performance increases the time required to not only formulate a set of material properties that best matches the experimental data, but also to best match the resulting system behavior (the behavior of the component needed analyzed).

For shape memory alloys, the ideal manual calibration routine is as follows. First, elastic properties E^M and E^A are calibrated from two separate elastic tensile tests. In the absence of a low-temperature tensile test, the young’s moduli in martensite is left as a free variable. Then, a series of constant force thermal cycling tests are performed. From this dataset, all remaining free variables need to be calculated iteratively. Zero-stress transformation temperatures and stress-influence coefficients can be estimated by assuming the transformation surfaces are constant slopes. The coefficient of thermal expansion can be calculated by measuring the change in strain with respect to temperature in regions of the experiment where transformation is not occurring. If both elastic moduli have been computed, the current transformation strain as a function of stress can be calculated for each tested stress level by rearranging Hooke’s law:

Then, the associated material properties can be computed (k, sigma\_crit, h\_min, h\_sat). Finally, smooth hardening coefficients can be found by manually varying these and changing the transformation temperatures and stress-influence coefficients to best match experimental data. This final step takes the longest amount of time and requires the most amount of a priori knowledge about shape memory alloy behavior, and could potentially result in a poor fit depending on the experimental data.

For this work, due to the inherent interdependence of so many material properties, and assuming that the driving factor for calibration is *proper fit of experimental data*, we can approach the calibration problem as a numerical optimization problem. For constant force thermal cycle experiments, strain is measured as a function of temperature at certain stress levels. We seek a set a material properties that best matches the experimental data over this set of experiments. Mathematically, this represents: (optimization statement where **x**=design variables and the objective function is an error metric between epsilon(T;sigma)\_model and epsilon(T;sigma)\_experiment).

Because of the aforementioned material property interdependence, we use a hybrid optimization scheme to best balance global searches with local optima; when multiple experiments are conducted, this optimization problem is overdetermined so there may exist many local optima.

Hybrid optimization consists of two main stages: global optimization followed by a local search on the best set of design variables that the global optimization found. The global optimization searches the entire space and hopefully finds the small region where the best solution lies. Then, based on that point, a gradient-based optimization is implemented to find the mathematical optimum point in that smaller subset of the design space. This process is depicted in figure BLANK, where the design space has many local optima but only one true optimal point. The hybrid optimization has a better chance of finding the true optimum because the preliminary global optimization acts as a “Greedy design of experiments” – it selectively samples points based on knowledge gained in the past.

Our tool leverages the genetic algorithm NSGA-II for the global search and then SLSQP implemented in SciPy for the local search, although the tool is modular and other optimization algorithms can be easily inserted in lieu of the ones discussed herein. The population size for NSGA-II is commonly set to 100 and the genetic algorithm is typically run for at least 10 generations, while SLSQP is set to run for approximately 100 maximum iterations. All optimization parameters are modifiable in the GUI.

The current implementation of the tool, in a GUI-based format, allows the SMA designer to specify both optimization parameters and material property bounds and values. If certain properties are known a priori (e.g., the Young’s moduli from tensile tests), these values can be defined and the optimization will minimize error between model prediction and experiment by varying all other material properties. In this way, our GUI allows the designer greater flexibility than previous methods, but the typical iterative method can still be used. The only difference is the speed in which different combinations of material properties and their respective bounds can be tested. Each calibration routine can be executed in less than 10 minutes, depending on the size of the optimization, and the results are easily digestible for those who are not innately familiar with the Lagoudas SMA constitutive model. In this way, our tool provides a high-throughput, low-barrier-to-entry calibration method that we hope to increase use of SMAs in practice.

**Hartl’s calibration procedure**

To calibrate the 17 unknown parameters by hand, two separate types of experiments are needed and then iterative calibration is still required. *Make a note that this can apply to a range of different typles of tests (tensile/compressive/torsion)*. First, based on either DSC or a priori knowledge of the zero-stress transformation temperatures of the material, isothermal tests must be performed at t < M\_f and T > A\_f. From this data, both Young’s moduli can be calibrated.

Next, at least four isobaric tests at different stress levels must be performed to calibrate the rest of the material properties. The coefficient of thermal expansion (assumed to be constant with respect to temperature and material phase) can be calculated from a “tail” or both of the “tails” of the isobaric test. Then, for each isobaric test, the change in strain between austenite and martensite can be calculated via hooke’s law:

The current transformation strain for that particular stress level can then be computed:

If 4 isobaric tests are conducted, the parameters of H\_cur can then be computed numerically. *Maybe I need to add something here or before that describes what stress levels to pick*. Cite the ASTM standard.

The zero-stress transformation temperatures and stress-influence coefficients can also be estimated. Estimates for transformation temperatures at each stress can be found via tangent fit. It also may be called the intersection point. This estimate is equivalent to a Lagoudas model calibration with smooth hardening parameters set to n\_i = 1. With all estimates for zero-stress transformation temperatures computed, best fit a line through each transformation surface, and the intersection with the stress=0 axis is the transformation temperature. Additionally, the slope of the transformation surface is an estimate for the stress influence coefficients.

At this point, all material properties are estimated; to fully capture the true strain-temperature response, iterative calibration of each smooth hardening coefficient is necessary until a satisfactory fit is accomplished. However, due to the interdependencies highlighted earlier, each change of n\_i will need to be accompanied by a change in transformation temperature and perhaps stress-influence coefficient. Herein lies a crucial nuance of calibrating the Lagoudas constitutive model: the model defines the transformation temperatures as the point at which transformation begins (i.e., the state where the transformation criteria is activated), rather than the tangent. In past work, manually updating smooth hardness coefficients, transformation temperatures, and stress-influence temperatures to best fit experimental data has been the most time-intensive part of calibration.