**Abstract**

Our tool provides an intuitive workflow that imports and processes raw unfiltered shape memory alloy mechanical (tensile/compression), thermal (DSC), or thermomechanical (tensile/compression with environmental chamber) data to produce customizable figures and systematically derived material data. This toolset can extract data from multiple inputs such as tensile test data and external thermocouples and automatically synchronize them onto the same time series. With raw force and displacement data, the SMA REACT can calculate strains and stresses based on various sample geometries. Coupling temperature, stress, and strain data, this tool can apply customizable filters and remove systematic errors within the dataset, periodically prompting the user for filter approval. The program then produces various figures to help visualize the complex shape memory alloy material behavior.

**Introduction**

The fundamental understanding and industrial application of shape memory alloys (SMAs) continues to grow. In particular, SMA actuators have gained the attention of engineers by virtue of their high actuation energy density and have found uses in the fields of aerospace, biomedical, and robotics [1]. A notional process for developing a shape memory alloy engineering system could be divided into six stages (detailed graphically in Fig. 1). Identifying system requirements is critical first stage. These decisions will then guide the material requirements (i.e., stiffness, actuation strain, transformation temperatures), which depend on the precise composition of the SMA itself. Engineers then process the SMA by various means, whether it involves melting processes like vacuum induction melting (VIM), subsequent cold working processes such as wire drawing, and final heat treatments [2].

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Figure 1: The typical SMA development process involves many discrete steps. This work provides an easy constitutive model calibration tool, the Rendering of Experimental Analysis and Calibration Tool, to enable SMA component design.

Stage four involves thermomechanical testing to assess the material response for the particular loading condition in question (i.e., tension, compression, or torsion). At this stage, engineers may need to alter the composition and processing to satisfy system requirements. For a rigorous system design, a material model should capture the full thermomechanical constitutive response (i.e., the relationship between temperature, stress, and strain). The design team then calibrates a constitutive model (examples of which include those published by Brinson [3] and Lagoudas [4], among others) to best fit the thermomechanical characterization data in the operating regime of interest. With a calibrated constitutive model, engineers can design the system to exploit the unique nonlinearities inherent of SMAs. Finally, the SMA device is integrated into the larger system. The design process involves many disciplines, which can be a daunting endeavor for small teams or new adopters of SMA technology.

Each stage of this development process requires significant time and effort, but the greater SMA community has developed tools to speed certain development stages. The composition-processing-property space for SMAs is becoming well understood, and many recently developed tools enable quick discovery of new alloys [5], [6], [7]. ASMADA, the Automatic Shape Memory Alloy Data Analyzer, identifies heating and cooling cycles of SMAs and extracts SMA material properties according to ASTM standard E097 [8], [9], [10]. The Shape Memory Materials Analysis and Research Tool (SM2ART), also known as SMAnalytics, provides an extensive open-source database of tested shape memory alloys and their standard properties [11], [12]. Many research groups have published user material models (i.e., UMATs) to interface with open-source and commercial finite element solvers [13], [14], [15], [16].

However, while many published methods detail SMA actuator calibration [17], [18], [19] and commercial software suites enable superelastic calibration (add Abaqus citation here), no open-source, low-barrier-to-entry SMA actuator calibration tool exists. The various external state variables that govern shape memory material behavior often require synchronization of various datasets from different instruments, slowing the SMA development process. These barriers make SMA design and integration difficult for newcomers in the field or those engaged in multi-disciplinary efforts.

In this work, we detail a streamlined open-source tool to help both material scientists and design engineers analyze their thermomechanical data and calibrate an appropriate SMA constitutive model. We deem this tool REACT, for the Rendering of Experimental Analysis and Calibration Tool. REACT provides an intuitive workflow that imports and processes raw unfiltered shape memory alloy mechanical (tensile/compression), thermal (DSC), or thermomechanical (tensile/compression with environmental chamber) data to produce customizable figures and systematically derived material data (depicted schematically in Figure 2). The tool comprises two graphical user interfaces (GUIs), written in python and available on GitHub under the GNU General Public License. These two GUIs accomplish separate essential tasks in the SMA development process: data processing and constitutive model calibration.

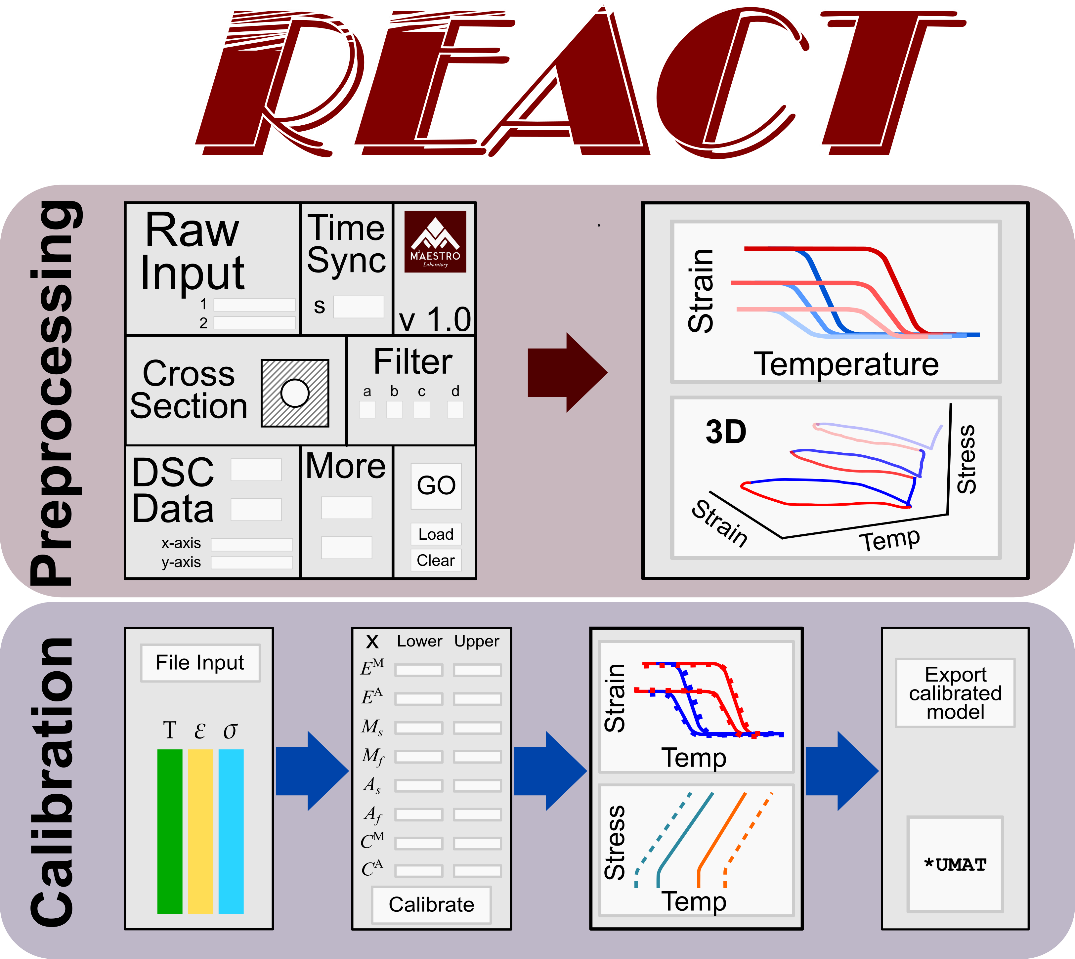


Figure 2: SMA-REACT allows the user to load their own data, specify known model parameters, and find an optimal calibration that best approximates experimental response.

**Method description**

**Data-preprocessing**

Experiments and characterization on shape memory alloy devices require at minimum the data acquisition of stress, strain, temperature histories. Sometimes these data sources rely on different telemetries and must be synchronized into a single data file.

The SMA REACT pre-processing GUI extracts data from multiple inputs such as a load frame and external thermocouples and automatically synchronizes them onto the same time series[[1]](#footnote-1). With unfiltered force and displacement data, REACT can calculate strains and stresses based on various sample geometries. Coupling temperature, stress, and strain data, this tool can apply customizable filters and remove systematic errors within the dataset. The program then produces various figures to help visualize the complex shape memory alloy material behavior. Users can export this processed data to the next phase of the tool, Model Calibration.

**Model calibration**

Constitutive model calibration is a vital link between understanding SMA behavior and designing to exploit SMA performance. The inherent complexity of SMAs is an opportunity for more space- and weight-efficient assemblies, but a challenge from a design perspective. For many applications, selecting a particular SMA component based on transformation temperature and maximum transformation strain is insufficient; the transformation temperatures and actuation strain in the *operating stress regime* must be well characterized and predictable.

In the past, designers have calibrated SMA models analytically, relied on their intuition, or employed numerical optimization. When a deterministic amount of data is available, analysts can derive closed-form analytical expressions for simple models [17], [18]. However, when the operating stress regime of the SMA spans many stress regions and requires many (>3) experimental tests, these analytical methods become overdetermined. More recently, many groups have adopted numerical optimization to find the combination of model parameters that best fit experimental data [19], [20], [21], [22]. These approaches help to speed the process, but exist as purpose-built codes and are have limited applicability outside the authors’ specific application or research group.

Given filtered and synchronized experimental data, the SMA REACT calibration GUI finds the best fit of constitutive model parameters (martensitic elastic modulus, austenite start temperature, etc.). Following the thermodynamically consistent model derived by Lagoudas et al., the developed calibration routine leverages hybrid optimization[[2]](#footnote-2) to minimize error between model prediction and experimental data. Our tool enables the user to customize the optimization routine as well as the model parameters to be optimized (e.g., bounds and free variables). Outputs from the calibration routine include a set of model parameters to be used in future analyses (i.e., material properties for FEA) and a thermodynamically consistent phase diagram based on calibrated model parameters. We focus on the Lagoudas one-dimensional constitutive model, but one could leverage the developed framework and extend the software to consider other constitutive models, higher dimensional models (e.g., 3D models with anisotropic effects), and different loading modes (e.g., superelasticity).

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 hybrid optimization problem. For constant force thermal cycle experiments (ASTM citation), strain is measured as a function of temperature at certain stress levels. We seek a set of material properties such that the calibrated constitutive model best matches the experimental data over this set of experiments. Our tool leverages the genetic algorithm NSGA-II [23], [24] for the global search and then SLSQP implemented in SciPy [25] for the local search, although the tool is modular and can be modified to use other optimization algorithms. For all example calibrations in this text, we specify the population size and number of generations to be 100 and at least 10, respectively for NSGA-II. We constrain SLSQP to 100 maximum iterations. All relevant optimization parameters are modifiable in the GUI.

**One-dimensional Lagoudas SMA Constitutive Model**

The Lagoudas shape memory alloy constitutive model uses the Gibbs' free energy to derive a thermodynamically consistent relationship between stress and strain. In this work, we leverage the commonly used temperature- and strain-driven implementation of this model for wider applicability in standard finite element suites. From the perspective of model calibration, seventeen unique but dependent model parameters must be found to best match experimental data. In this section, we will omit a full model derivation, but rather highlight the seventeen model parameters that need calibrated and their effects on constitutive behavior. See \_\_ for more information.

Table 1:The one-dimensional reduction of the Lagoudas SMA constitutive model requires calibration of 17 unique but dependent parameters.

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Mathematical Symbol** | **Units (SI)** |
| **Thermoelastic properties** |  |  |
| Elastic moduli |  | Pa |
| Coefficient of thermal expansion |  | 1/K |
| **Transformation properties** |  |  |
| Transformation temperatures |  | K |
| Stress-influence coefficients |  | Pa/K |
| **Transformation strain properties** |  |  |
| Minimum transformation strain |  | mm/mm |
| Maximum transformation strain |  | mm/mm |
| Critical stress at which transformation strain manifests |  | Pa |
| Transformation strain rise time |  | 1/Pa |
| **Smooth hardening properties** |  |  |
| Smooth hardening coefficients |  | - |

The Lagoudas one-dimensional constitutive model comprises four interdependent parameter groups.

1. **Thermoelastic properties** include the elastic moduli for each material phase ( and for austenite and martensite, respectively) and the coefficient of thermal expansion . Note this model formulation assumes the coefficient of thermal expansion is constant with respect to material phase; this allows the use of simpler nonlinear solution methods (i.e., Convex Cutting Plane).
2. **Transformation properties** include zero-stress transformation temperatures and stress-influence coefficients . Zero-stress transformation temperatures define the start and end of transformation at zero stress (denoted by the character for the material phase and the subscript for the start and end). Stress-influence coefficients define how transformation temperatures change with respect to stress and are assumed to be constant with respect to material phase; the slope of the stress-temperature phase diagram at the *calibration stress[[3]](#footnote-3)* gives these two values.
3. **Transformation strain properties** define the evolution of transformation strain with respect to stress and are crucial to understand if the material exhibits sufficient transformation strain at the design stress. The transformation strain is approximated as an asymptotic exponential function, where and are the minimum and maximum transformation strain, defines the critical stress at which transformation strain manifests, and is the *rise time*, or how quickly the transformation strain increases from to .
4. **Smooth hardening properties** define the smoothness of the transition between elastic response and transformation, or vice versa. They are numerical values bounded between 0 and 1.

As mentioned earlier, the seventeen material properties that define shape memory alloy constitutive response are unique but interdependent. For example, a change in smooth hardening coefficient will cause a change in the corresponding zero-stress transformation temperature. 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 are activated), rather than the tangent (which is the definition used in ASTM E3097) [9]. 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.

Many other material properties are interdependent; a change in transformation strain properties will be reflected in both the strain-temperature response and the shape of the transformation surfaces. While the stress-influence coefficients are single numbers for each phase, they are only one part of the mathematical expression to define the transformation surface in stress-temperature space. For these reasons, calibration must leverage numerical optimization to ensure a robust fit of experimental data.



**Calibration via numerical optimization**

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 the SMA designer has prior knowledge of certain properties (e.g., Young’s moduli from tensile tests), they can define these properties 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 and helps speed the iterative calibration process.

Depending on the size of the optimization, each calibration routine can execute in less than 10 minutes, and those who are not innately familiar with the Lagoudas SMA constitutive model can easily digest the results. 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.

**Do we need this section?**

**Implementation example**

To show the utility of SMA-REACT, we discuss a sample dataset and calibrate the Lagoudas SMA constitutive model both analytically and numerically using the GUI. We detail an iterative tuning process to refine the calibration, demonstrating the ease of the GUI.

**Experimental data**

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Figure 4: To demonstrate the utility of SMA-REACT, we will calibrate a constitutive model to fit published experimental data [26].

To calibrate an accurate SMA constitutive model to capture actuator behavior, *n* isobaric (constant force thermal cycling) tests, where *n* is preferably greater than 4, are required. Each test requires stress-strain-temperature histories.

We use experimental data of a Ni50.5Ti27.2Hf22.3 alloy from Bigelow et al [26]. NiTiHf is a relevant material system, with many members of the SMA community exploring Hf additions for high-temperature performance [26], [27], [28]. The quality and quantity of data (i.e., six different constant force thermal cycles), non-zero coefficients of thermal expansion, and nonlinear relationship between applied stress and transformation strain make this data set an ideal example of the SMA-REACT tool.

**Conventional calibration procedure**

The 17 unknown parameters that define the Lagoudas SMA constitutive model can be calibrated without a global optimization strategy by estimating parameter groups (e.g., transformation temperatures, thermoelastic properties, etc.) sequentially. However, due to the nonlinearities present in the model with respect to the current transformation strain (H\_cur) and smooth hardening coefficients (n\_i), optimization, or nonlinear curve fitting, is still required. We will discuss one method to find these parameters without using a global optimization strategy, as this method can serve as a good baseline with which to compare the optimized calibration.

|  |  |
| --- | --- |
| a) Constant-stress force cycling data for five distinct stress levels. | b) Zero-stress transformation temperatures and stress-influence coefficients at the calibration stress are extracted directly from CFTC data. |
| c) Austenite elastic modulus are found via Hooke's law at the reference temperature, which is a model parameter defined by the analyst. | d) Nonlinear curve fitting is necessary to find transformation strain properties, martensite elastic modulus, and coefficient of thermal expansion. |

*Figure 5: Given constant-stress thermal cycling (CFTC) data for several stress levels, the Lagoudas SMA constitutive model can be calibrated using local curve-fitting routines. However, this method still relies on many manual iterations to find smooth hardening coefficients (not shown above). In each subfigure above, the parameters found are displayed in the grey box in the lower-right corner.*

First, transformation temperatures for each tested stress level can be estimated via the tangent method or similar. If a “zero-stress” isobaric test (i.e., 7 MPa or lower) was performed, the transformation temperatures found for this test can be taken as the zero-stress transformation temperatures etc. Otherwise, each zero-stress transformation temperature can be found via the x-intercept of a linear regression of the transformation temperatures as a function of stress. This estimate is equivalent to a Lagoudas model calibration with smooth hardening parameters set to . The average slope of the start and finish transformation surfaces for martensite and austenite for a specified stress range about the user-determined *calibration stress* can be taken as the stress-influence coefficients ( and ). Note that the stress-influence coefficients should not be derived from the average slope from estimated transformation temperatures at all stress levels; most shape memory alloys exhibit a nonlinear change in transformation temperature with respect to stress (see Figure 3(b) in [26]), and the Lagoudas model compensates for this via the transformation surfaces (), where the stress-influence coefficients at the calibration stress are a contributing factor.

With transformation temperatures and stress-influence coefficients estimated, thermoelastic properties and transformation strain properties can be calculated. Austenite elastic modulus can be found by extracting the total strains and a temperature well above at each tested stress level. Then, by designating this temperature such that , Hooke’s law becomes:

Austenite elastic modulus is the best-fit linear coefficient from this equation.

At this point, the analyst has two choices in terms of calculating the rest of the thermoelastic and transformation strain properties. First, the coefficient of thermal expansion can be calculated separately by extracting the total strain at another temperature :

Alternatively, coefficient of thermal expansion can be found concurrently with the other thermoelastic and transformation strain properties via a nonlinear system of equations. At a temperature , Hooke’s Law can be written as:

where

In this equation, there are six unknowns: and . Ideally, to calibrate these six unknowns, one will have performed six or more constant-force thermal cycle tests. However, for shape memory materials that do not exhibit two-way shape memory effect, both and can be set to zero, reducing the number of required tests to four. If the coefficient of thermal expansion was calibrated based on elastic response, the other five parameters are calibrated in the same way as described above.

Both of these approaches to calculate the remaining thermoelastic properties and transformation strain properties may introduce modeling errors. TIf , the strain due to thermal expansion will be incorrectly predicted across the tested temperature range. However, this is a limitation of the one-dimensional reduction of the Lagoudas constitutive model; assuming thermal expansion is invariant of material phase allows for the use of simpler nonlinear solution methods (i.e., Convex Cutting Plane).

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. Due to the interdependencies highlighted earlier, each change of smooth hardening coefficient will need to be accompanied by a change in the associated transformation temperature and perhaps stress-influence coefficient (i.e., a change in will need to be accompanied by a change in and ). Without global numerical optimization, the best model calibration will be found via manual changes and the analyst’s intuition.

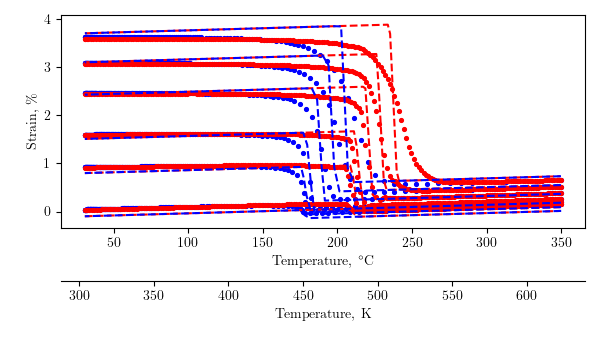


Figure 9: Conventional analytical/numerical calibration techniques produce a passable solution, but rely on user iterations to fine-tune model response.

The resulting conventional calibration, with , is shown in Figure 5. The mean squared error between model and experiment is 3.13% (see equation BLANK), which for many applications could suffice. Transformation temperatures and transformation strain properties are well-captured, as the model bisects the experimental curves as a function of stress (i.e., the martensite elastic response is under-predicted at low levels of applied stress but over-predicted at high levels of applied stress). However, there are several areas that could be improved. The coefficient of thermal expansion is too high, as shown by the large deviance between model and experiment in Martensite, especially immediately before forward transformation. This calibration routine still requires a nonlinear curve fitting procedure to find the transformation strain properties, as well as requiring more intuition about the relationship between model parameters and constitutive response.

**Calibration via numerical optimization**

The conventional calibration shown above is used as a starting point for a global numerical calibration using SMA-REACT. Because the current optimization strategy includes a preliminary genetic algorithm followed by a gradient-based algorithm, the previously found model parameters were used to determine bounds for each model parameter (i.e., the conventional calibration estimated austenitic elastic modulus as BLANK, so the bounds were set to BLANK and BLANK). This allows the optimizer to start in the neighborhood of feasible solutions, but gives it freedom to explore for a better performing result.

Then, based on the values to which the optimization converged, the parameters that converged to the bounds were further inspected, bounds were widened, further improving the calibration accuracy. This process of inspecting the converged results and comparing to the optimization bounds was repeated three times until each parameter converged to a value well within the set bounds. Thus, a local optimum is found, and with a large enough initial population in the genetic algorithm, we are confident that this is near the globally optimal calibration for this model formulation.

Table 2: The SMA-REACT tool allows further refinement of the calibrated solution.

|  |  |  |
| --- | --- | --- |
| **Calibration Number** | **Mean squared error** | **Notes** |
| 1 | 3.13% | Analytical calibration, . |
| 2 | 2.09% | Numerical calibration with bounds around analytical values |
| 3 | 1.57% | Widened bounds on and . |
| 4 | 1.46% | Widened bounds on and . Fixed and . |
| 5 | 1.43% | Widened bounds on . Fixed everything but transformation temperatures and . |

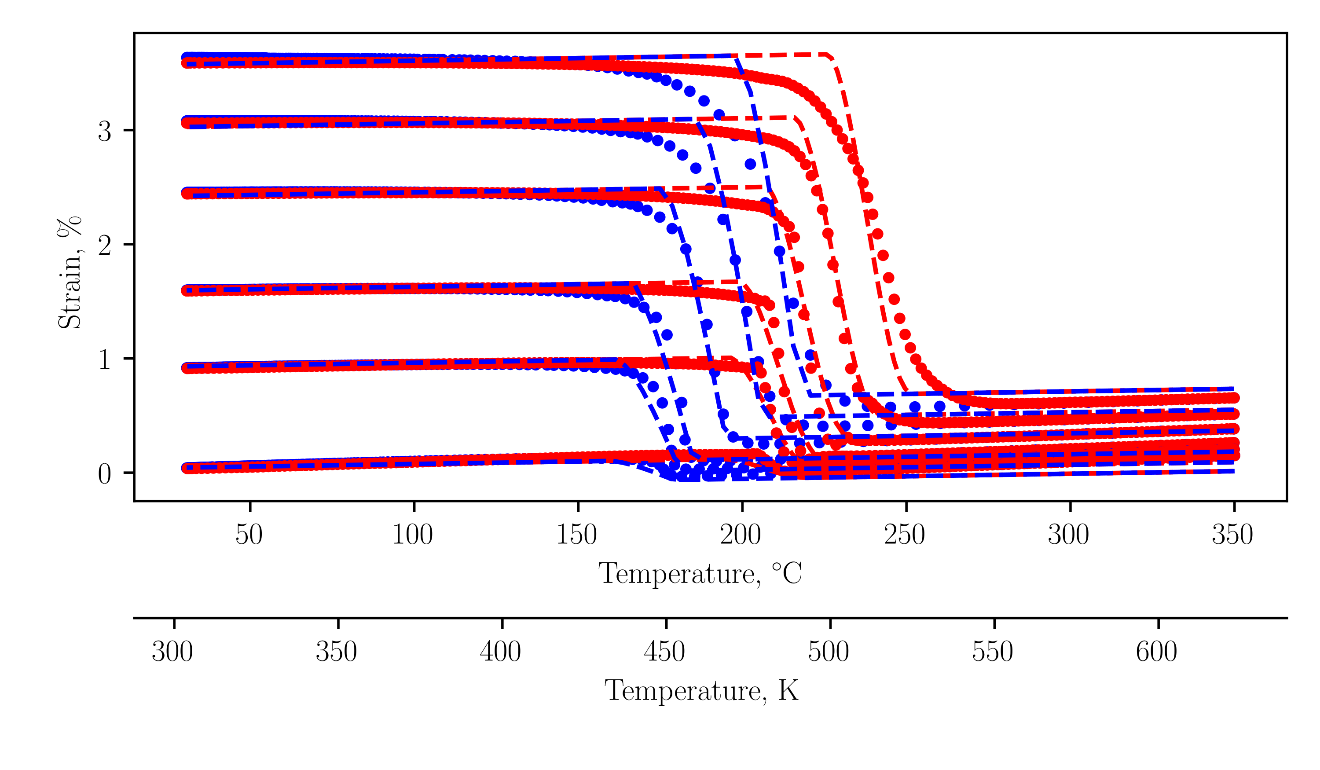


Figure 10: The final calibration agrees with the experimental data to within 1.5% mean squared error.

The final numerical calibration is depicted in Figure 6. The model predicts the elastic response in martensite almost perfectly, which signifies that both the martensitic elastic modulus and transformation strain properties are well calibrated. Transformation temperatures show good agreement at low levels of applied stress. At higher levels of applied stress, the model-predicted transformation overshoots the experimental data and predicts a smaller hysteresis. This is because the transformation temperatures are not a linear function of stress (i.e., the stress-influence coefficients are not constant, see figure 3b in Bigelow [26]), and because the smoothness of transformation initiation is not constant with stress (compare the 100 MPa transformation into austenite with the analogous location at 300 MPa). This calibration is a perfect example of the utility of numerical optimization; the optimizer finds the best global fit of data, especially regarding the austenite transformation temperatures. For lower stresses, is too low, and is too high. At intermediate stresses, like 100 and 200 MPa, the transformation temperatures are almost perfect. Then, at 300 MPa, is too high and is too low. This could be better fit at the relevant stresses by biasing the solution to prioritize fitting certain stress levels (see [22]) or by simply calibrating the model at the stress levels that matter most.

However, this calibration is not perfect, mainly due to model deficiencies. The coefficient of thermal expansion is not constant for austenite and martensite. Clearly, the coefficient of thermal expansion in austenite is larger than that in martensite. This is a model deficiency because the current model uses a convex cutting plane assumption for numerical integration and could be improved in future work.

Regardless, these five optimizations improved calibration accuracy by over 50% compared to the conventional calibration, and were accomplished in less than an hour on a lightweight laptop with a low-performance processor (Intel Core m3-6Y30 CPU @ 0.90 GHz with 4 Gb RAM). This calibration routine can be performed by general analysts, designers, or material scientists, without the need for exotic hardware or python programming experience.

**Conclusions and further refinements**

SMA-REACT is an open-source, easy-to-use tool for characterization data post-processing and shape memory alloy constitutive model calibration. While we have focused on the Lagoudas constitutive model and actuator (i.e., constant force thermal cycling) behavior, the tool is easily extensible to other constitutive models or loading modes. By framing the calibration routine as a numerical optimization problem, SMA-REACT can find robust calibrations that outperform conventional (i.e., by hand) calibrations by 50% or more, without requiring detailed knowledge of programming, optimization, or the Lagoudas constitutive model. This allows the tool to be approachable for a wide range of students and professionals working on shape memory alloys. The speed at which model calibrations can be fine-tuned allows for rapid iterations to converge to a satisfactory model calibration, which can then be used in commercial finite element suites like ABAQUS.

We distribute the SMA-REACT toolset and source code under the GNU General Public License, which allows anyone to run, study, share, and modify the code. We invite any modifications that users may find useful, including, but not limited to, alternative loading modes (i.e., superelasticity or combined superelasticity/shape memory [29]), alternative constitutive models [3], [30], [31], [32], or any usability enhancements for more robust data import or export. In particular, we believe seamless integration with NASA tools such as the Shape Memory Materials Database would be very enabling to the greater SMA community [11]. SMA-REACT aims to reduce the barrier between materials scientists and engineers, and will hopefully enable more widespread adoption of shape memory alloys in engineering applications.

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1. Full documentation of the pre-processor can be found in the code documentation (link). [↑](#footnote-ref-1)
2. Hybrid optimization comprises two stages: global optimization followed by a local search on the best set of design variables that the global optimization found. The global optimization (i.e., a genetic algorithm) searches the entire space and provides a starting point for a local gradient-based optimization (i.e., SLSQP) to find the mathematically optimum solution. [↑](#footnote-ref-2)
3. The calibration stress is *a priori* defined by the designer, and common practice dictates selecting a value close to the design working stress of the material. Get a citation on this. Talk to Hartl? [↑](#footnote-ref-3)