**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 refined data is then iteratively calibrated to best fit a Lagoudas-Hartl constitutive model. The program is open-source allowing for other features and SMA models to be added. The focus on automated and intuitive generation of figures and model fitting greatly assist experimentalists, modelers, and designers to iterate on novel shape memory alloy materials and applications.

**Introduction**

Shape memory alloy actuators have found uses in the fields of aerospace, biomedical, civil, robotics, and more by virtue of their high actuation energy density and solid-state operation [1]. The inherent complexity of SMAs is an opportunity for more space- and weight-efficient assemblies, but a challenge from a design perspective. A notional process for developing a shape memory alloy engineering system could be divided into six stages (detailed graphically in Fig. 1). Step 1 requires identifying one’s system requirements which entails discerning a suitable range of material requirements (i.e., stiffness, actuation strain, transformation temperatures). These material requirements directly drive step 2, i.e., choosing the precise SMA composition. Finding relations between composition and material properties have recently been streamlined with NASA’s SMA database tool [2], [3].

The arduous journey of turning a material concept into a reality involves the many iterations between Steps 3-5, i.e., processing, characterization, and model fitting. Processing differences during manufacturing can affect the material properties, such as reducing an ingot into a wire or tuning print parameters for additively manufactured SMAs [4]. Characterization enables the simultaneous assessment of the new processing techniques and responses to loading conditions (i.e., tension, compression, or torsion). Rigorous engineers may seek to validate the behavior of a new material within the original system requirements. This can be done by fitting the characterization data to a model that captures the full thermomechanical constitutive response (i.e., the relationship between temperature, stress, and strain). With a calibrated constitutive model (such as the Lagoudas [5] or Brinson [6] models) engineers can design the system to confirm the behavior of the unique nonlinearities inherent of SMAs. Iteration of these steps will likely occur multiple times to reach requirements. Once the constitutive model accurately represents the SMA behavior and the material satisfies requirements, the SMA device can then be integrated into the engineering system.

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Figure : 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.

Such design processes involve many disciplines and can be a daunting endeavor for small teams or new adopters of SMA technology. Characterization hardware is complex; due to the various external state variables that govern shape memory material behavior, extracting a stress-strain-temperature history often requires synchronization of multiple metrologies (i.e., thermocouples, load cells, and strain gauges). Development requires significant time and effort, but the greater SMA community has developed tools to expedite certain stages.

The composition-processing-property space for SMAs is becoming well understood, and many recently developed tools enable quick discovery of new alloys [nasa][7], [8], [9]. 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 [10], [11], [12]. 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 [2], [3]. 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]. [20]-focused

In this work, we detail a streamlined open-source, GUI-based 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 constitutive models (depicted schematically in Figure 2). For iterative calibration, REACT allows the user to choose bounds and lock-in values to further increase speed and accessibility. The tool is written in python but requires no programming experience to use; it is available on GitHub under the GNU General Public License [x]. Two modules accomplish the essential tasks of data processing and constitutive model calibration.

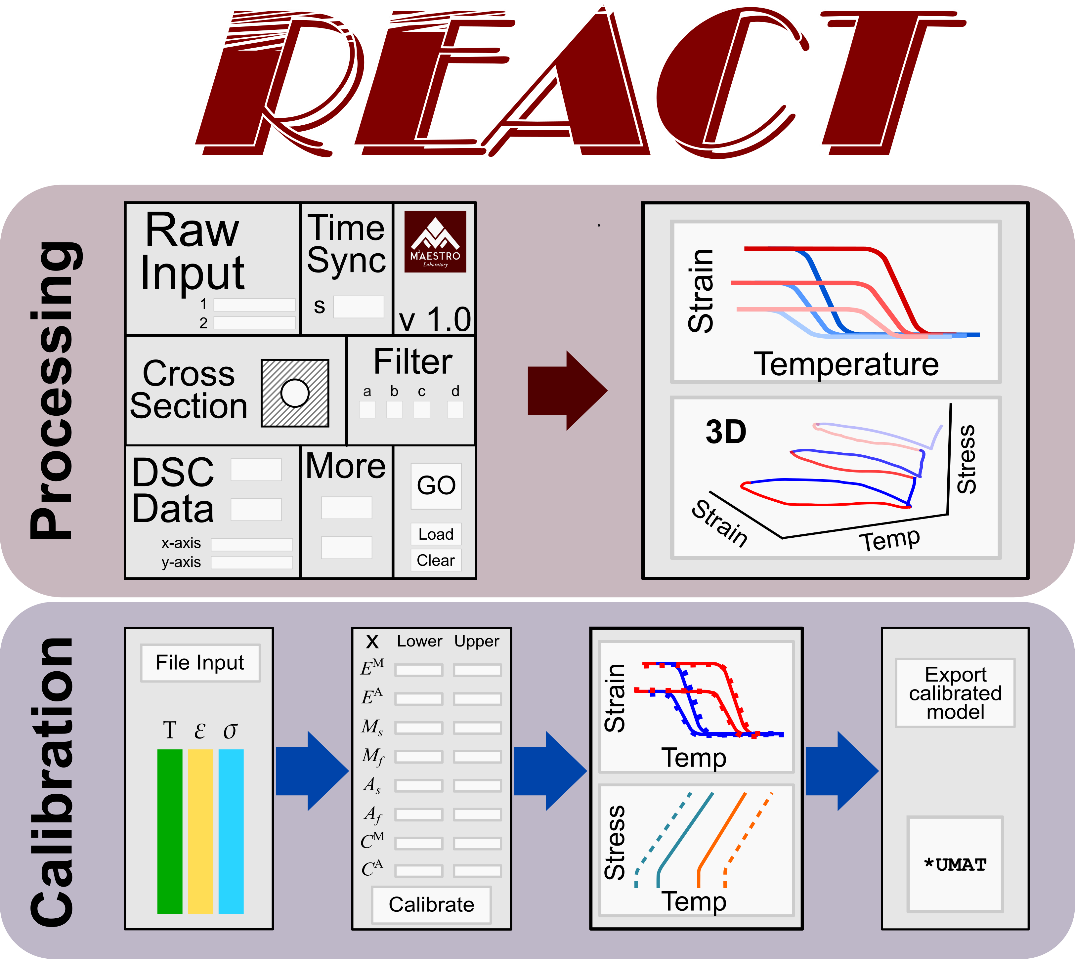


Figure : SMA-REACT allows the user to load their own data, specify known model parameters, and find an optimal calibration that best approximates experimental response.

**Method description**

(Add some meta-text of what this section is, and why it’s different than documentation). Full code documentation of the processing module can be found online [link to your cool wiki].

**Data Processing Module**

Shape memory alloy characterization requires acquisition of at least stress, strain, and temperature histories. Sometimes these histories rely on different telemetries and must be synchronized into a single data file. The SMA REACT processing module extracts data from multiple inputs such as a load frame and external thermocouples and automatically synchronizes them onto the same time series. 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 module of the tool, Model Calibration.

**Model Calibration Module**

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. this intended

A deterministic amount of data can allow for derived closed-form analytical expressions for simple models [17], [18]. However, when the operating stress regime of the SMA spans many stress regions and requires multiple (> 3) experimental tests, these analytical methods become overdetermined. Numerical optimization must be employed to find the combination of model parameters that best fit experimental data, demonstrated within [19], [21], [22], [23]. 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 from the processing module, the model calibration module finds the best fit of constitutive model parameters (martensitic elastic modulus, austenite start temperature, etc.) based on the Lagoudas one-dimensional constitutive model. The developed calibration routine leverages hybrid optimization to minimize error between model prediction and experimental data. Hybrid optimization comprises a global optimization (i.e., a genetic algorithm) to identify a starting point for a local gradient-based optimization (i.e., SLSQP). 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.

Our tool leverages the genetic algorithm NSGA-II [24], [25] for the global search and then SLSQP implemented in SciPy [26] 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 restrict SLSQP to 100 maximum iterations. Though REACT calibrates for only one SMA model at the moment, the developed framework in REACT can be expanded to consider other constitutive models, higher dimensional models (e.g., 3D models with anisotropic effects), and different loading modes (e.g., superelasticity).

**The one-dimensional Lagoudas SMA constitutive model: A brief primer**

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 temperature- and strain-driven implementation of this model for wider applicability in standard finite element suites. In this section, we will omit a full model derivation (see Lagoudas et al. [5] for more information) , but rather highlight the seventeen unique but dependent model parameters that need calibrated and their effects on constitutive behavior.

Table :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 (at zero-stress) |  | K |
| Stress-influence coefficients |  | Pa/K |
| **Transformation strain properties** |  |  |
| Minimum transformation strain |  | m/m |
| Maximum transformation strain |  | m/m |
| 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 [27]).
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[[1]](#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 coefficients** () define the smoothness of the transition between elastic response and transformation, or vice versa. They are bounded between 0 and 1 and are ordered from one to four, corresponding to a hot-to-cold actuation loop (i.e., ).

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) [11].

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 (see Lagoudas et al. for more information [5]). For these reasons, calibration must leverage numerical optimization to ensure a robust fit of experimental data.

**Calibration via numerical optimization**

Mupdatingthe 17 model parameters to find a best fit to experimental data is a tedious and process.The REACT model calibration module instead uses numerical optimization to find the best fit. Further, the user can specify material property bounds or property values. Prior knowledge of certain properties (e.g., Young’s moduli from tensile tests), will greatly minimize error between model prediction and experiment by varying all other material properties.  Depending on the size of the dataset, each calibration process can execute in less than 10 minutes, and even 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.

**Implementation example**

To show the utility of SMA-REACT, we will calibrate a constitutive model to best fit data from literature. We first identify the critical material property bounds from experimental data, then iteratively update these bounds and others based on the optimization solution. Calibration best practices are discussed, and the ease of using our GUI tool is displayed.

**Experimental data**

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Figure : To demonstrate the utility of SMA-REACT, we will calibrate a constitutive model to fit published experimental data [28].

To calibrate an accurate SMA constitutive model to capture actuator behavior, *n* constant force thermal cycling tests are needed, where *n* is preferably greater than 4. Each test requires stress-strain-temperature histories. We use an experimental dataset for a Ni50.5Ti27.2Hf22.3 alloy from Bigelow et al [28]. The six different constant force cycles, non-zero coefficients of thermal expansion, and nonlinear relationship between applied stress and transformation strain make this data set a great calibration example. Add a tie-in sentence here.

**Identifying material property bounds**



To produce an accurate calibration using SMA-REACT, the optimizer must be provided with bounded material parameters. The better the bounds, the more likely the optimizer will not get stuck in a local minima. To this end, we will calibrate select parameters analytically and discuss rules of thumb for other parameters.

The most important property bounds are the transformation temperatures. If the transformation temperatures are incorrectly bounded, the optimizer may converge to non-physical results (i.e., a phase diagram where martensite temperatures are higher than austenite temperatures) in an attempt to minimize error between model and experimental data. Transformation temperatures for each tested stress level can be estimated via the tangent method or similar (see Figures 5 a) and b)). 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. 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 . Bounds for each transformation temperature are typically 10-20 K around each parameter (i.e., for an estimated of 150 K, the lower and upper bounds would be 130 K and 170 K, respectively).

The average slope of the martensite and austenite 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 [27]), and the Lagoudas model compensates for this via the transformation surfaces (), where the stress-influence coefficients at the calibration stress are a contributing factor. The stress-influence coefficient bounds are then set to vary by 1 MPa/K in each direction.

Austenite elastic modulus can also be estimated from constant-stress force cycling data by extracting the total strains and a temperature well above at each tested stress level. Then, by designating this temperature , Hooke’s law becomes:

Austenite elastic modulus is the best-fit linear coefficient from this equation (see Figure 5 c)).

Estimating the rest of the material properties (Martensite elastic modulus, transformation strain properties, coefficient of thermal expansion, smooth hardening coefficients) requires a nonlinear curve fitting routine. In practice, the estimating the properties detailed above and applying best practices for the remaining properties results in a sufficient calibration.

|  |  |  |
| --- | --- | --- |
| a) Constant-stress force cycling data for five distinct stress levels. | b) Estimates for 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.* |

*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.*

Table 2 shows typical bounds for a preliminary calibration. As mentioned previously, Austenite elastic modulus, transformation temperatures, and stress-influence coefficients can be easily estimated via linear regression. Martensite elastic modulus is commonly lower than the austenite elastic modulus, so common practice entails setting a lower bound equal to one-half the estimated austenite value. Relatively low bounds for the coefficient of thermal expansion are suggested for preliminary calibration to properly restrict the optimizer to find reasonable values for transformation properties. These bounds can be modified based on material response; inspecting the slope of the strain-temperature response in either martensite or austenite can help guide the analyst.

Transformation strain properties are the most difficult property group to accurately estimate during a preliminary calibration. This is due to the exponential nature of the transformation strain function (see \_\_\_) and the large sensitivity of transformation strain properties on overall calibration error. A calibration that accurately predicts all other properties will drastically underperform a calibration that incorrectly predicts thermoelastic and transformation properties but accurately predicts transformation strain properties. The minimum transformation strain or critical stress at which transformation strain manifests , or both, are commonly set to zero for preliminary calibrations. Setting both of the aforementioned parameters to zero is indicative of a material that exhibits no two-way shape memory effect.

Smooth hardening coefficients are typically the last parameters to be refined. As we do in the next section, these parameters are commonly set to 1 for preliminary calibrations to reduce the number of active design variables. When thermoelastic properties and transformation strain properties have converged, the smooth hardening coefficients and transformation temperatures are refined.

Table 2: Common starting bounds for each parameter of the Lagoudas constitutive model. Note that these are guidelines and should be modified after a preliminary calibration.

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Mathematical Symbol** | **Bounds (SI)** |
| **Thermoelastic properties** |  |  |
| Austenite elastic modulus |  | Eq. 2, Figure 5c) |
| Martenite elastic modulus |  |  |
| Coefficient of thermal expansion |  |  |
| **Transformation properties** |  |  |
| Transformation temperatures (at zero-stress) |  | Figure 5b) |
| Stress-influence coefficients |  | Figure 5b) |
| **Transformation strain properties** |  |  |
| Minimum transformation strain |  | [0, 0.01][[2]](#footnote-4) |
| Maximum transformation strain |  | [0.01, 0.05] |
| Critical stress at which transformation strain manifests |  | [0, 50E6]4 |
| Transformation strain rise time |  | [1E-8, 1E-6] |
| **Smooth hardening properties** |  |  |
| Smooth hardening coefficients |  | [0, 1][[3]](#footnote-5) |

Following the best practices detailed in the previous section, we can perform a preliminary calibration. Then, if any parameter converged to an optimization bound, these bounds were modified for any subsequent calibration until each parameter converged to a value within the set bounds. Afterwards, the smooth hardening coefficients and transformation temperatures were optimized to further decrease calibration error. Table 3 shows the calibration process; the preliminary calibration obtained an error of 1.51% when compared to experiment, and iterative calibration further improved that result.

Table : Estimating bounds via simple rules allows the optimization enables a calibration within 2% error. SMA-REACT enables quick parameter tuning to further improve the calibration.

|  |  |  |
| --- | --- | --- |
| **Calibration Number** | **Mean squared error** | **Notes** |
| 1 | 1.51% | Estimated bounds (see section BLANK.BLANK). . . |
| 2 | 1.34% | Widened bounds on thermoelastic and transformation strain properties. Maintained transformation temperature bounds. . . |
| 3 | 1.31% | Froze all properties besides transformation temperatures and smooth hardening coefficients. |

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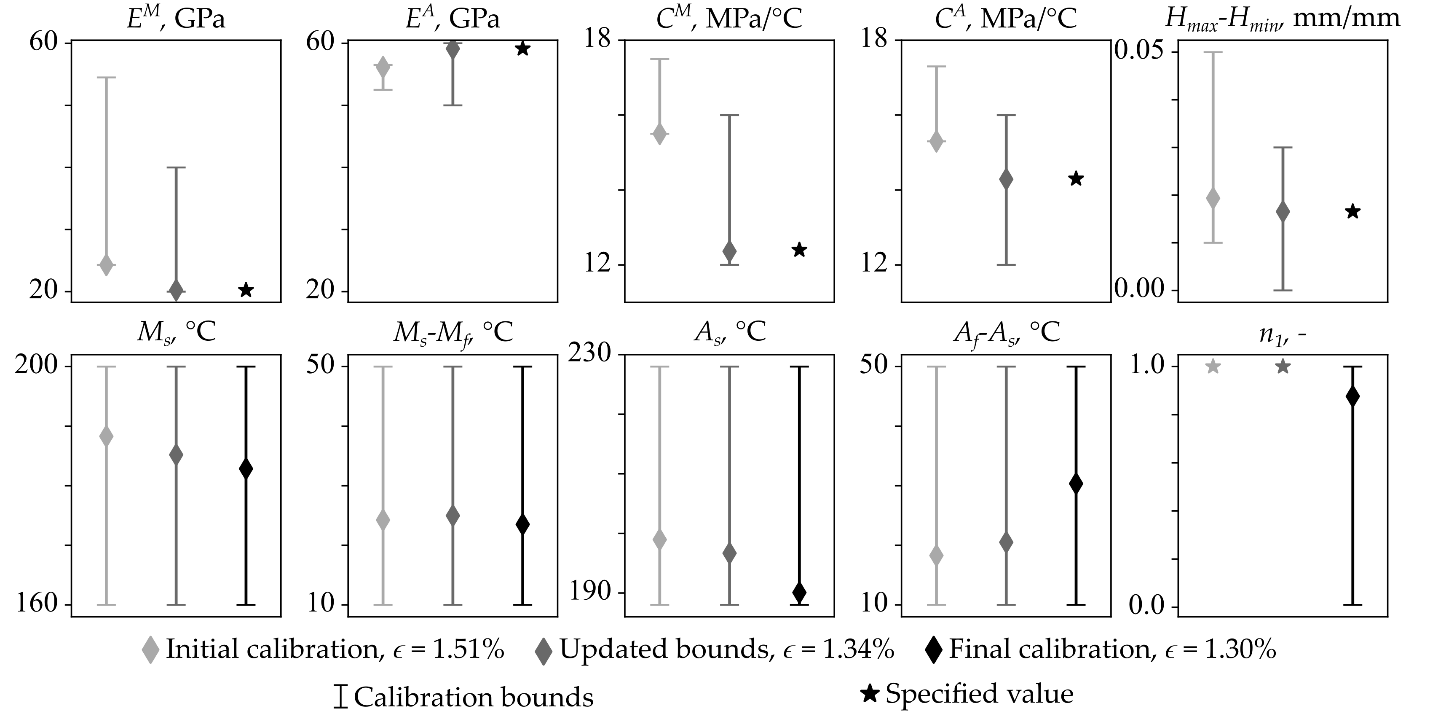


Figure 4: Evolution of selected model parameters for the calibration example. Initial bounds identified from experimental data and best practices (see Table 2) were then refined if the value converged to a bound (e.g., ). All properties besides transformation temperatures and smooth hardening coefficients were set for the final calibration.

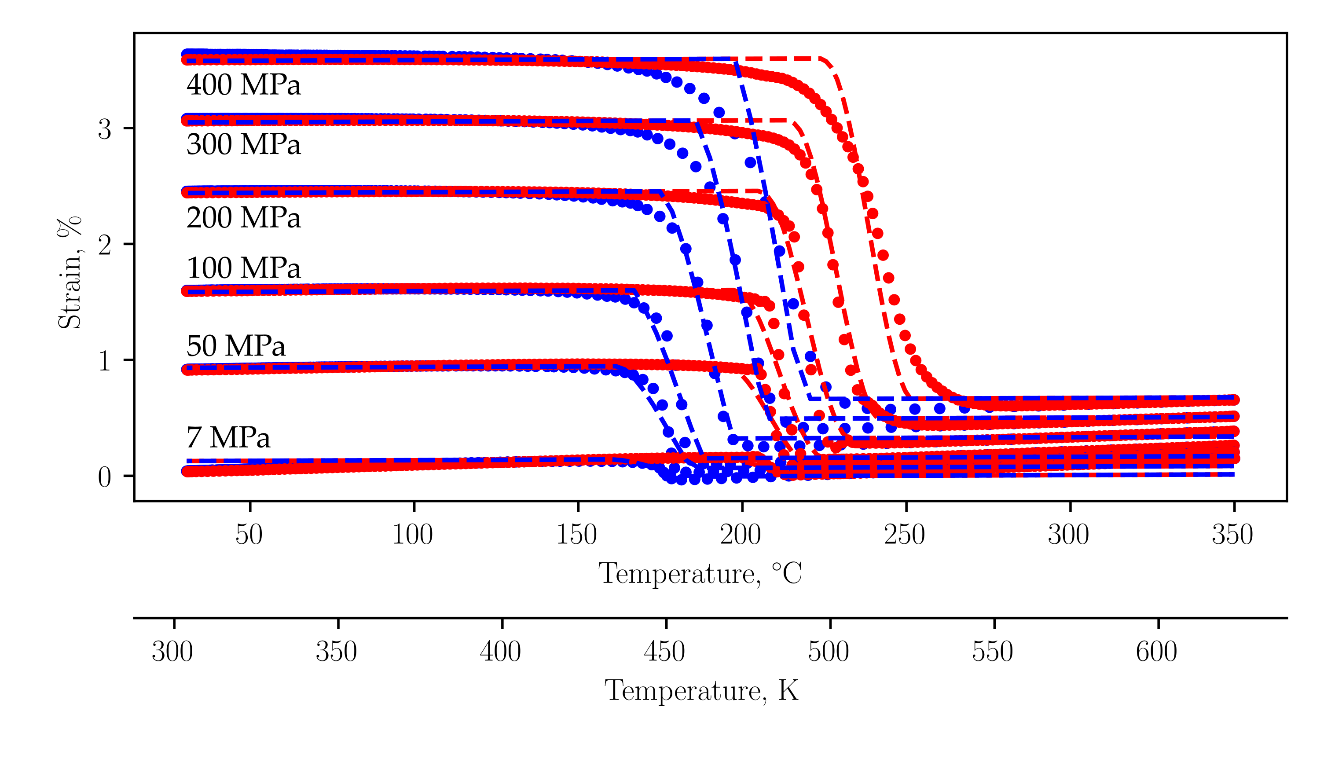


Figure : The final calibration agrees with the experimental data to within 1.31% mean squared error.

The final numerical calibration is depicted in Figure 5. The model predicts the elastic response in martensite accurately, 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 [28]), 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 great 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 [23]) or by simply calibrating the model at the stress levels that matter most.

However, this calibration is not perfect, mainly due to model deficiencies. In reality, the coefficient of thermal expansion varies with material phase. 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 educated guesses , 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, python programming experience, or relatively clean datasets

**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 [6], [30], [31], [32], or any usability enhancements for more robust data import or export. In particular, we believe integration with other open-source tools, such as the Shape Memory Materials Database and SMAnalytics would be very enabling to the greater SMA community [2]. 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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**Appendix: Full calibration property history**

Table 4: Calibration property history for the example discussed in section BLANK.BLANK. Values displayed with a red background converged to a bound, while those with a blue background were specified and not optimized.

|  |  |  |  |
| --- | --- | --- | --- |
|  | **Calibration** | | |
| **Property** | **1** | **2** | **3** |
| **(GPa)** | 24.3 | 20.2 | 20.2 |
| **(GPa)** | 56.1 | 59.1 | 59.1 |
| **(1/)** | 1.00E-6 | 1.07E-6 | 1.07 |
| **()** | 188 | 185 | 183 |
| **()** | 24.2 | 25.0 | 23.5 |
| **()** | 199 | 197 | 190 |
| **()** | 18.3 | 20.5 | 30.4 |
| **(MPa/)** | 15.5 | 12.4 | 12.4 |
| **(MPa/)** | 15.3 | 14.3 | 14.3 |
| **(mm/mm)** | 0 | 0 | 0 |
| **(mm/mm)** | 1.94E-2 | 1.65E-2 | 1.65E-2 |
| **(mm/mm)** | 0 | 0 | 0 |
| **(1/MPa)** | 1.00E-2 | 1.14E-2 | 1.14E-2 |
| **(-)** | 1 | 1 | 0.877 |
| **(-)** | 1 | 1 | 0.412 |
| **(-)** | 1 | 1 | 0.505 |
| **(-)** | 1 | 1 | 0.288 |

1. The calibration stress is *a priori* defined by the designer. Common practice dictates selecting a value close to the design working stress of the material. [↑](#footnote-ref-3)
2. The minimum transformation strain and critical stress at which transformation strain are commonly set to zero for preliminary calibrations and only optimized if modeling two-way shape memory behavior is essential. [↑](#footnote-ref-4)
3. We recommend setting smooth hardening coefficients to 1 for preliminary calibrations. [↑](#footnote-ref-5)