



Development and Application of a Tool for Optimizing Composite Matrix Viscoplastic Material Parameters

Pappu L. N. Murthy
Glenn Research Center, Cleveland, Ohio

Paria Naghipour Ghezeljeh
Ohio Aerospace Institute, Brook Park, Ohio

Brett A. Bednarczyk
Glenn Research Center, Cleveland, Ohio

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Pappu L. N. Murthy
Glenn Research Center, Cleveland, Ohio

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Brett A. Bednarczyk
Glenn Research Center, Cleveland, Ohio

National Aeronautics and
Space Administration

Glenn Research Center
Cleveland, Ohio 44135

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Pappu L. N. Murthy
National Aeronautics and Space Administration
Glenn Research Center
Cleveland, Ohio 44135

Paria Naghipour Ghezjeljeh
Ohio Aerospace Institute
Brook Park, Ohio 44142

Brett A. Bednarczyk
National Aeronautics and Space Administration
Glenn Research Center
Cleveland, Ohio 44135

Abstract

This document describes a recently developed analysis tool that enhances the resident capabilities of the Micromechanics Analysis Code with the Generalized Method of Cells (MAC/GMC) (Refs. 1 to 3) and its application. MAC/GMC is a composite material and laminate analysis software package developed at NASA Glenn Research Center. The primary focus of the current effort is to provide a graphical user interface (GUI) capability that helps users optimize highly nonlinear viscoplastic constitutive law parameters by fitting experimentally observed/measured stress-strain responses under various thermo-mechanical conditions for braided composites. The tool has been developed utilizing the MATrix LABoratory (MATLAB) (The Mathworks, Inc., Natick, MA) programming language (Ref. 4). Illustrative examples shown are for a specific braided composite system wherein the matrix viscoplastic behavior is represented by a constitutive law described by seven parameters. The tool is general enough to fit any number of experimentally observed stress-strain responses of the material. The number of parameters to be optimized, as well as the importance given to each stress-strain response, are user choice. Three different optimization algorithms are included: (1) Optimization based on gradient method, (2) Genetic algorithm (GA) based optimization and (3) Particle Swarm Optimization (PSO). The user can mix and match the three algorithms. For example, one can start optimization with either 2 or 3 and then use the optimized solution to further fine tune with approach 1. The secondary focus of this paper is to demonstrate the application of this tool to optimize/calibrate parameters for a nonlinear viscoplastic matrix to predict stress-strain curves (for constituent and composite levels) at different rates, temperatures and/or loading conditions utilizing the Generalized Method of Cells. After preliminary validation of the tool through comparison with experimental results, a detailed virtual parametric study is presented wherein the combined effects of temperature and loading rate on the predicted response of a braided composite is investigated.

Introduction

The Micromechanics Analysis Code with Generalized Method of Cells (MAC/GMC) is NASA developed software (Refs. 1 and 2). It can perform a comprehensive composite material and laminate analysis by utilizing the generalized method of cells (GMC) family of micromechanics theories (Ref. 3). These theories provide access to the local stress and strain fields in the composite material that are crucial for assessing damage initiation and progression in composite structures. The software package is built on a user-friendly framework, along with a library of local inelastic, damage, and failure models. Further,

application of simulated thermo-mechanical loading, generation of output results, and selection of repeating unit cell (RUC) architectures to represent the composite material have been automated in MAC/GMC. Finally, classical lamination theory, wherein GMC is used to model the composite material response of each ply, along with a recursive multiscale GMC for woven and braided composites, have been implemented within MAC/GMC. Thus, the full range of GMC composite material capabilities is available for analysis of arbitrary laminated/woven/braided configurations as well. The many features that are available in the code as well as the procedures to actually setup and run a problem are described in the MAC/GMC User's Manuals (Refs. 1 and 2).

Impact analysis of composites is of interest because it enables the assessment of deformation and damage that might occur during the service life of composite parts. However, high strain rate effects coupled with highly nonlinear viscoplastic deformation of certain matrix materials under thermomechanical loading conditions pose some unique challenges. These need to be captured accurately in order to model the response of composite structures under impact loading. Current MAC/GMC code has inbuilt constitutive laws to represent such behavior. The matrix material constitutive behavior is represented with the aid of a multi parameter viscoplastic law, wherein the parameters need to be determined by fitting to carefully selected experimental stress-strain response curves. The task is not trivial because of the complex nonlinear nature of the material constitutive law, requiring a nonlinear regression fitting to determine the parameters.

In order to determine the optimized constitutive law parameters a graphical user interface (GUI) based tool has been developed utilizing the MATLAB programming language. The tool is general enough to fit any number of experimentally observed stress-strain responses of the material that have been generated for a given material with a design of experiments. Furthermore, the parameters to be optimized, as well as the importance given to each stress-strain response curve, are kept as user choices. Thus the user may opt for only a subset of the parameters as design variables, as well as specify different weights to each of the experimentally observed stress-strain response. The parameters are extracted by minimizing the error between the experimentally observed stress-strain response and the corresponding responses predicted by MAC/GMC. For the minimization, three different optimization algorithms are utilized herein: (1) Optimization based on the gradient method, (2) Genetic algorithm (GA) based optimization, and (3) Particle Swarm Optimization (PSO). The user can use these algorithms sequentially, with the optimized results of one serving as the starting point for another. It is generally recommended to use either Genetic or PSO to zero in on plausible parameters followed by a fine tuning of the parameters by using the Gradient based algorithm.

“Virtual Testing,” which provides material properties via simulation, can be valuable in situations where testing would be impractical. MAC/GMC (Refs. 1 and 2), can predict the multiaxial nonlinear data needed as input for the elastoplastic orthotropic material model (LS-DYNA MAT 213) (Ref. 5). The successful utilization of the Parameter Optimization Tool in the development of a virtual testing platform and all the required preliminary constituent-level and composite-level validations are demonstrated herein.

This report is organized as follows. First the optimization algorithms and objective function implemented in the Multiobjective Viscoplastic Parameter Optimization Tool are described. This is followed by an overview of the modified Bodner-Partom viscoplastic material constitutive model (Refs. 6 and 7) to which the tool has been applied. Next, a detailed description of the Multiobjective Viscoplastic Parameter Optimization Tool GUI and its functionality is given. Results are then presented which demonstrate and validate the application of the tool to a neat resin material as well as a triaxially braided composite whose matrix material is this same resin. For both the neat resin and the composite, stress-strain responses are predicted under various rates, temperatures, and loading conditions and then validated through comparison with available experimental results. The validated Multiobjective Viscoplastic Parameter Optimization Tool, coupled with the MAC/GMC software, constitute a virtual material testing platform, which can be used to generate the required sets of stress-strain curves for use in LS-DYNA MAT213 (Ref. 5).

Optimization Algorithms

Three different approaches to find the optimum parameters that minimize the error between target and predicted stress-strain responses with an optimum set of design parameters are available within the tool. These are (1) Gradient Based, (2) Genetic Algorithm, and (3) Particle swarm optimization.

Gradient Based Optimization

Gradient based optimization is the conventional, basic optimization procedure wherein it is assumed that the objective function is differentiable and a derivative of the function with respect to each of the design variables is available either explicitly or via finite difference scheme. The procedure starts with user given feasible starting design set of parameters. A search direction is constructed by using the first derivatives of an objective function with respect to each of the design parameters. MATLAB's internal function "fmincon" is utilized to perform the gradient based optimization. For further details of the algorithm the user may refer to (Ref. 8).

Genetic Algorithm

Genetic algorithms (GAs) are often considered as part of the Evolutionary Computational (EC) approaches or the evolutionary algorithms (Ref. 9). They are also referred to as global search algorithms. Essentially, evolution acts as type of natural optimization process based on the concepts of competition, reproduction, and mutation. Genetic algorithms are the most popular among ECs and the dominant use has been in optimization. The main difference between the conventional gradient based optimization and GA is that GA works with a starting population of eligible candidates that satisfy our constraints of upper and lower bounds. In contrast, in Gradient based approaches, as discussed above, the process starts with just one eligible candidate solution and attempts to improve it sequentially, while terminating the process when no further improvement is possible. In this context, the improvement means reduction in the error between target and the predicted solutions in the least square sense. The GA typically starts with a population of candidates and then improves this population from generation to generation. This involves four parts. The first part is keeping some of the best candidates as they are. These candidates are known as the elite candidates. Next, among the remaining population, a certain number of candidates (children) are generated by the so called "crossover" between the better candidates (parents). This number is arbitrary. In the present GA implementation, the same number of additional candidates are chosen by introducing Gaussian perturbations to the parents. Thus, for example if the number of children is set to 10, the algorithm creates 10 candidates by cross over and 10 more by introducing the Gaussian perturbations. The remaining population is made by generating fresh candidates, which are mixed with the existing ones and their mutations. Suppose that, for a given generation, the number of elite candidates from the previous generation is six, the number of mutations is 10, and the total population is 100. The 10 Gaussian noise candidates will be generated along with 74 freshly populated candidates. Then the six elite candidates from the total population are identified, and the process repeats. If the GA is successful, the population of solutions will cluster at the global optimum after some number of generations.

Another important difference between the conventional gradient algorithms and GA is that, while in the former, gradients of the objective function are required to perform the search operations, in the latter, the gradients are never required. So, for all cases where the functions are discontinuous or gradients can simply be not obtainable, GAs are perhaps the only possible avenue to perform the search for the optimum. In addition, since the process is not sequential, the algorithm adapts nicely to parallelization of the processes for improved computational performance. Readers interested in more details pertaining to GAs are advised to refer to textbooks such as Reference 9.

Particle Swarm Optimization (PSO)

Particle swarm optimization (PSO) is a population based stochastic optimization technique developed by Eberhart and Kennedy (Ref. 10). It is analogous to the social behavior of bird flocking or fish schooling. PSO shares many similarities with evolutionary computational techniques such as Genetic Algorithms (GA) in the sense that it attempts to solve a problem by having a population of candidate solutions satisfying all the constraints. The candidate solutions are usually termed “particles”. The particles fly through the problem space (design space) by closely following the current best set of particles. At the end of each iteration, based on the individual performance of particles, they are moved according to simple mathematical formulae over the particle’s position and velocity. Each particle’s movement is influenced by its local best known position, but is also guided toward the best known positions in the search space. The best known position is the position of the particle that is closest to the optimum. In the present case, this is the candidate having the least amount of error compared to the target values. Compared to GA, the advantages of PSO are that the actual implementation of the code is quite simple and there are very few parameters to adjust. PSO has been successfully applied in many areas: function optimization, artificial neural network training, fuzzy system control, and other areas where GA can also be applied.

The algorithm that is implemented here is sometimes referred to as accelerated particle swarm optimization and is described in detail in Reference 11. There are two parameters that control the updated candidates, β and Υ . β affects the fixed part of the correction to the population and varies between 0 and 1. It is the fraction of the location of the best particle (design vector) from the previous generation that is added to $(1 - \beta)$ times the current candidate position to get the fixed part of the current population. This is then augmented with random noise that is equal to α times a random number which is picked from the standard normal distribution (zero mean and a standard deviation 1). α varies from generation to generation and is equal to Υ^i where “ i ” is the iteration number and Υ is a parameter between 0 and 1. As the iterations (generations) progress, the magnitude of the random noise correction diminishes. This is because, as the generations progress, the particles are tending towards the best possible solution and therefore do not need diversity that was needed initially to better scope the entire design space. Many different versions of PSO exist, and some are extremely fast but might end up in local minima. Conversely, some are slow but have better chance of locking on the global minimum. The one that is implemented in the current code is fairly robust in finding global minima quickly. The default values are set as $\beta = 0.5$ and $\Upsilon = 0.75$. As β increases, the convergence is faster, and similarly, as Υ decreases, the convergence is faster. These parameters can be accessed by the user via the “Advanced Options” panel in the optimization tool GUI, as described below.

Objective Function

The objective of the parameter optimization is to minimize the error between the simulated versus target stress-strain responses for all datasets. Let Nds be the number of stress-strain responses. Let W_i be the weight for response dataset number i . Let y_0 be the target and y be the simulated responses. We can construct the following objective function, which is based on a combined weighted root mean square error,

$$RMSErr = \sum_{i=1}^{Nds} \sqrt{Err_i W_i} \quad (1)$$

where,

$$Err_i = \sum_{j=1}^{N_j} (y_j - y_{0j})^2 \quad (2)$$

Here, y_j and y_{0j} are the predicted and the target stress values at strain x_j and N_j is the number of target values (i.e., stress-strain points) in the i^{th} response dataset. Err_i is the total square error for the i^{th} dataset. $RMSErr$ is the weighted root mean square error for all the datasets combined. The same objective function is used for all the three optimization schemes.

Viscoplastic Material Constitutive Model

The Parameter Optimization Tool has been specialized herein for application to the Bodner-Partom viscoplastic model (Ref. 6), as modified by Goldberg et al. (Ref. 7) to include hydrostatic effects. Note, however, that the tool can be easily modified to handle any viscoplastic constitutive model. The flow rule in the model by Goldberg et al. (Ref. 7) is given by,

$$\dot{\epsilon}_{ij}^I = 2D_0 \exp\left[-\frac{1}{2}\left(\frac{Z}{\sigma_e}\right)^{2n}\right] \left(\frac{\hat{\sigma}_{ij}}{2\sqrt{J_2}} + \alpha_t \delta_{ij}\right) \quad (3)$$

where a dot over a symbol denotes a time-derivative, δ_{ij} is the Kronecker delta, J_2 is the second invariant of the deviatoric stress tensor, whose components are $\hat{\sigma}_{ij}$, and,

$$\sigma_e = \sqrt{3J_2} + \sqrt{3}\alpha_t \sigma_{kk} \quad (4)$$

The evolution equations for the internal state variables, Z and α_t , are given by,

$$\dot{Z} = q(Z_1 - Z) \sqrt{\frac{2}{3} \dot{\epsilon}_{ij}^I \dot{\epsilon}_{ij}^I} \quad (5)$$

$$\dot{\alpha}_t = q(\alpha_1 - \alpha_t) \sqrt{\frac{2}{3} \dot{\epsilon}_{ij}^I \dot{\epsilon}_{ij}^I} \quad (6)$$

where

$$\dot{\epsilon}_{ij}^I = \dot{\epsilon}_{ij} - \dot{\epsilon}_m^I \delta_{ij} \quad (7)$$

and $\dot{\epsilon}_m^I$ is the mean inelastic strain rate. In the above equations, D_0 , Z_1 , α_1 , q , and n are material parameters, as are the initial values of the state variables Z and α_t , denoted by Z_0 and α_0 .

This viscoplastic constitutive model has been implemented within the MAC/GMC micromechanics software (Refs. 1 and 2) such that it can simulate the behavior of the matrix material within a unidirectional, laminated, woven, or braided composite (as well as the neat resin matrix itself).

Description of the Multiobjective Viscoplastic Parameter Fitting Tool

The neat PR520 resin stress-strain curves depicted in Figure 1 were used to demonstrate the capabilities of the Parameter Optimization Tool. These room-temperature results, which were generated as part of the experimental program described in Reference 7, were conducted at different strain rates, with three tests representing torsion (pure shear) and two tests representing tension. Because the employed constitutive model does not admit post-yield softening as observed in the torsion results, the three experimental torsion curves were capped at their maximum values and subsequently treated as perfectly plastic. Since these capped experimental curves were provided to the Parameter Optimization Tool, it is the goal of the tool to match these capped curves as closely as possible.

It should also be noted that the Parameter Optimization Tool is designed only to optimize a material's viscoplastic constitutive model parameters, not its elastic constants. Therefore, the elastic constants must be provided. For the PR520 epoxy resin at room-temperature, the isotropic Young's modulus is 3.54 GPa and the Poisson's ratio is 0.38.

To use the Multiobjective Viscoplastic Parameter Fitting Tool, the user must provide (in addition to various settings) the following basic input data:

1. A number of target (usually experimental) stress-strain curves, stored in Microsoft Excel.
2. The same number of MAC/GMC input files that simulate these stress-strain curves utilizing the Reference 7 constitutive model and the associated output X-Y type stress-strain data.
3. The names of the X-Y plot output files, as specified in the above MAC/GMC input files.

Note that the contents of the target stress-strain curve Microsoft Excel files used herein are given in the Appendices, along with MAC/GMC input files. The tool is a standalone Microsoft Windows program and must be placed in the same folder as the folder that contains all the MAC/GMC input files, and the Excel files containing stress-strain response data. Installation of the full MATLAB program is not necessary, however, the run time libraries must be installed. These can be installed from MATLAB website for free.

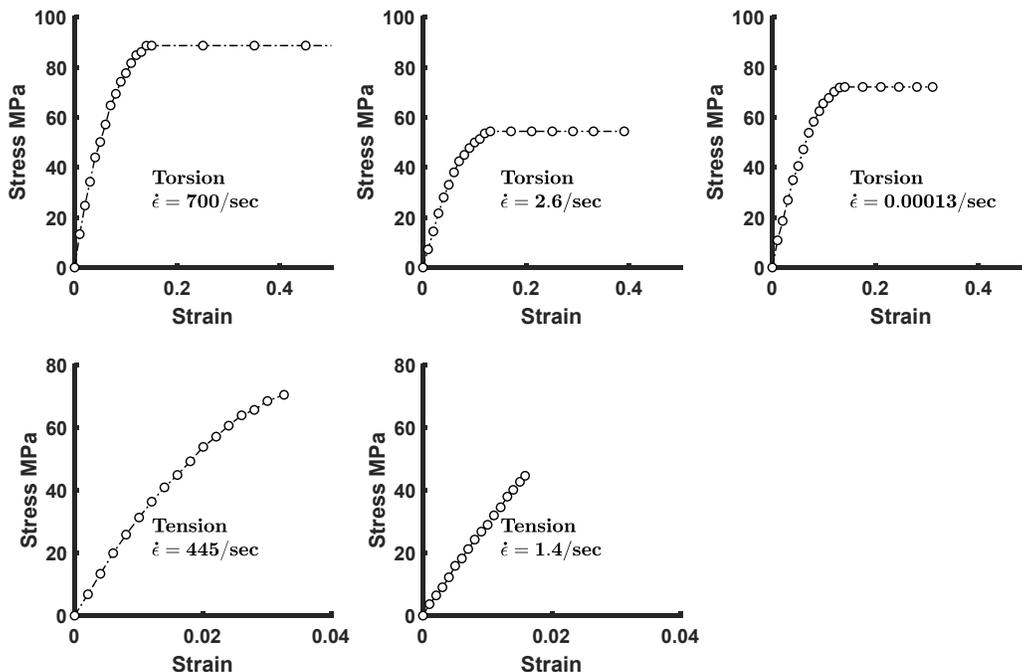


Figure 1.—Room-temperature, rate-dependent stress-strain responses for PR520 material used in a braided composite whose properties are to be used as input for MAT213.

Figure 2, shows the GUI layout of the Multiobjective Viscoplastic Constitutive Law Parameter Fitting Tool. The figure presents all available windows, buttons, graphic panels, and tables and appears somewhat cluttered. The intention of including this figure is to indicate every possible item that the GUI contains. However, when the program is executed, the actual design of the GUI follows context sensitive windows, tables and buttons in the sense that, depending on the user choice, only the appropriate windows and buttons are shown, and all the other details are suppressed. This keeps a clean and uncluttered look to interface when it is in use. Furthermore, context-sensitive helpful tips for all the user choices are provided to give appropriate hints pertaining to the inputs just by hovering the mouse pointer over the button on box. The next few paragraphs provide a step-by-step introduction to the GUI's tables, buttons, and boxes that require user interaction.

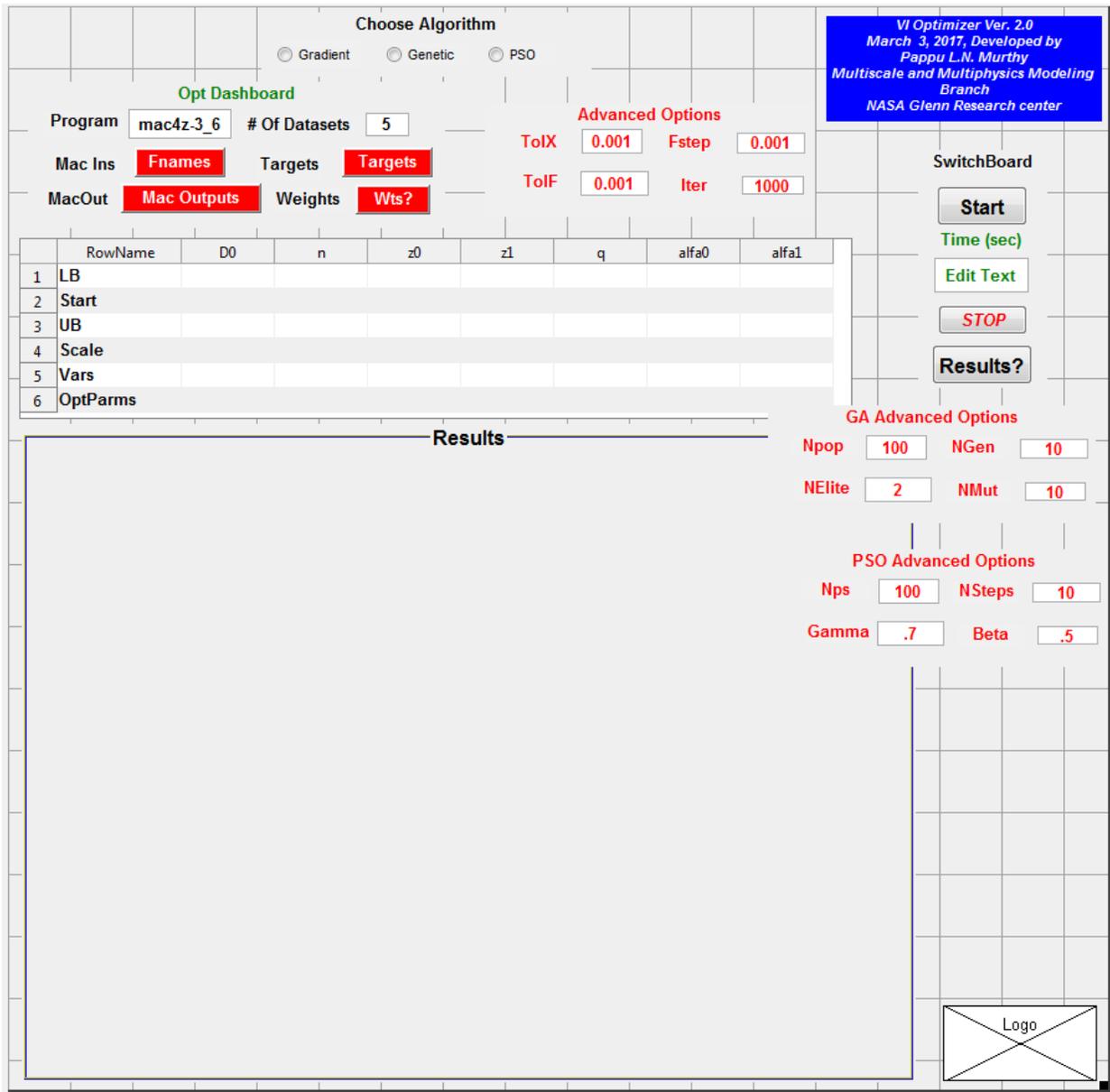


Figure 2.—Multiobjective Viscoplastic Constitutive Law Parameter Fitting Tool graphical user interface layout.

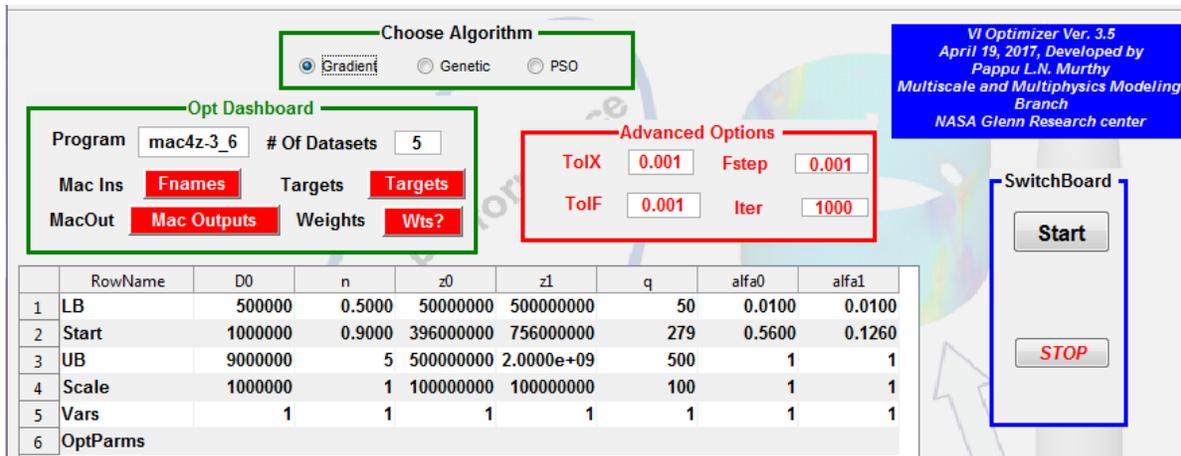


Figure 3.—Shown are the boxes that appear after user selects the option “Gradient” from the button group “Choose Algorithm”.

The program is started by double clicking the *.exe file which, along with the MAC/GMC input and Excel data files, are required to be present in the same folder. The program starts by showing some input dialogue boxes, as seen in Figure 3. As a next step the user chooses one of the optimization algorithms from the button-group titled “Choose Algorithm,” which has three choices: Gradient, Genetic, and PSO. Choosing one leads to the opening of four boxes of input, as shown below the “Choose Algorithm” box in Figure 3. Of these four boxes, the red outlined box is the only one that is different for each of the algorithms. The red box is denoted “Advanced Options,” and as the name indicates, the first time user need not be concerned with these details. These options pertain to some advanced settings with good default values are already provided. The various inputs for each of the boxes are described.

Opt Dashboard

There two editable boxes and four buttons in the “Opt Dashboard” section of the GUI.

Editable Box “Program”: The user should fill this box with the name of the MAC/GMC executable file. It is currently defaulted to “mac4z-3_6”. Note that the “.exe” extension should be omitted.

Editable Box “# of Datasets”: The number of experimental stress-strain curves provided by the user for fitting purposes is filled in here. The default is 5.

Button “Fnames”: Pushing this button opens an input dialogue and spaces where in the user provides MAC/GMC input data filenames, without the extension “.mac” (Fig. 4(a)). The MAC/GMC executable program uses these input files to simulate the stress-strain curves. The number of filenames should be same as the number of datasets, and the simulation defined in each MAC/GMC input file must correspond to each set of target data provided in Microsoft Excel format (see “Targets” below).

Button “Mac Outputs”: Pushing this button opens an input dialogue and spaces where in the user provides the output file names that MAC/GMC used to write the respective stress-strain X-Y data. These must be specified without the extension, so that the optimization algorithm can read and use the predicted response. Note that these names must be identical to those specified in each MAC/GMC input file under the Keyword *XYPLOT (Ref. 1) (see Appendix A).

Button “Targets”: The User specifies the Microsoft Excel full file names with extension (e.g., xls, xlsx) containing the experimentally obtained stress-strain data. Each file should contain two columns, the first of which is strain and the second of which is stress (see Appendix B).

Button “Weights”: Here the user may specify the weighting to be given to each of the target responses to bias the fitting toward or away from each target response. For example, the default weighting of 1 will apply equal weight to each target response.

All the buttons are colored red at start and they turn green once pushed and the appropriate inputs are provided by the user.

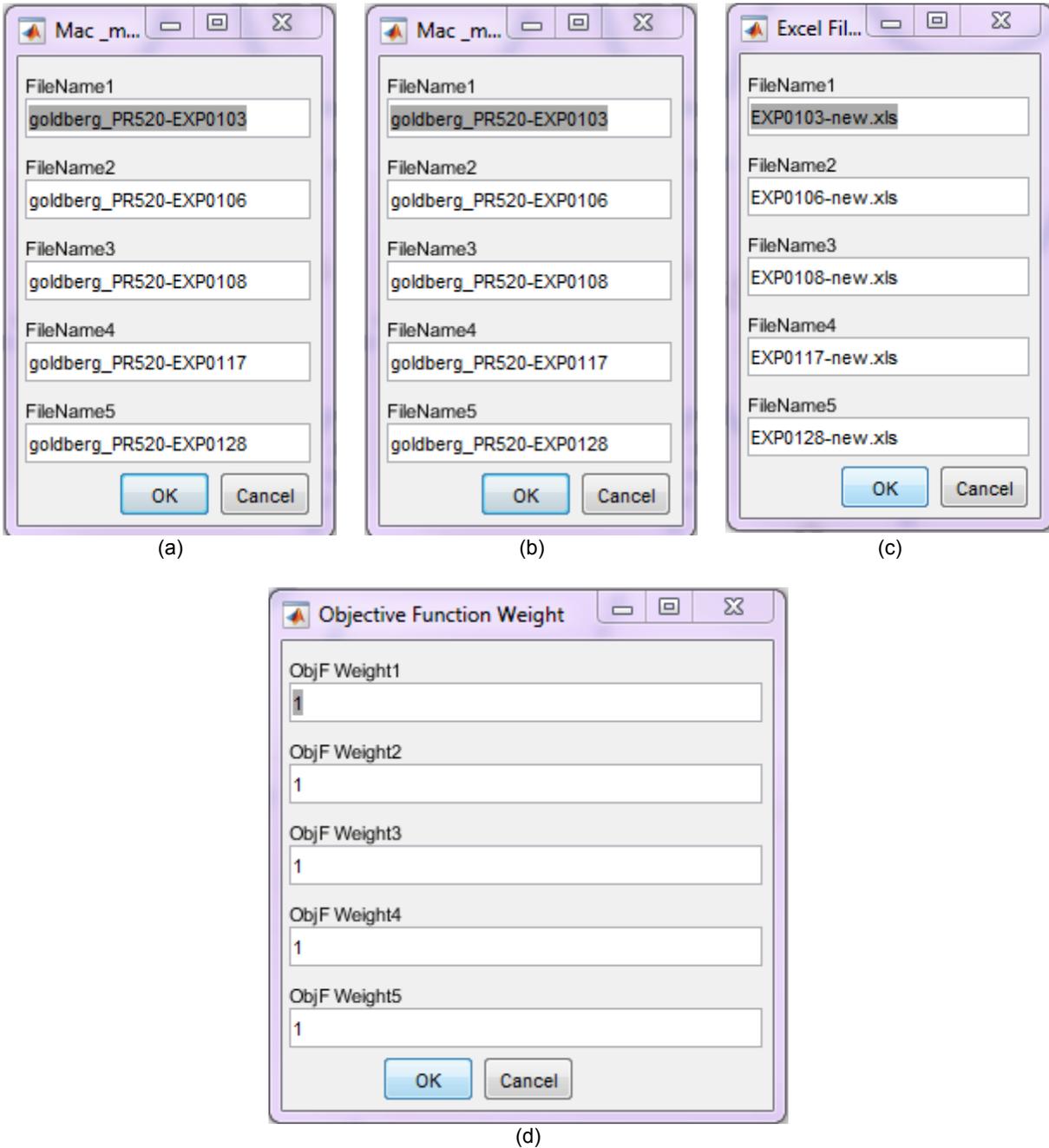


Figure 4.—“Opt Dashboard” push buttons and their respective inputs. (a) Button “Fnames”. (b) Button “Mac Outputs”. (c) Button “Targets”. (d) Button “Wts?”.

Algorithm Input Details Table

The next set of input details are common to all three algorithm choices. It consists of a table of details related to the seven parameters of the material constitutive law. The seven parameters are D_0 , Z_1 , α_1 , q , n , Z_0 , and α_0 as explained above. The user must provide the lower bound (LB), the upper bound (UB), and starting values for these parameters, as well as scaling values for these parameters. The scaling parameter provides the tool with a sense of the relative magnitudes of each of the parameters. This is important because the parameters typically vary widely in magnitude from each other, and it is recommended that these are scaled in such a manner the resulting scaled parameter values are all of same order of magnitude. Appropriate defaults are provided for all of these and thus the user usually needs only to choose the starting values. Row 5 values (Fig. 3) toggle between 0 and 1 to enable users to turn parameters on (1) or off (0) in the fitting optimization process. If a parameter is turned off (0), it will be kept at its start value and not optimized to improve the fit. In Figure 3, all the values are set to the default value of 1, meaning all seven parameters will be treated as active variables. Once the minimization of the error is accomplished, row 6 is populated with the appropriate optimum values for the parameters.

Advanced Options

The advanced options are intended for fine tuning the optimization algorithms and are specific to each of the three algorithms. The default values should provide a sufficient starting point for most users. Figures 5(a) to (c) show these option panels for each algorithm.

Gradient Advanced Options

ToIX	0.001	Fstep	0.001
ToIF	0.001	Iter	1000

(a)

GA Advanced Options

Npop	100	NGen	10
NElite	2	NMut	10

(b)

PSO Advanced Options

Nps	100	NSteps	10
Gamma	.7	Beta	.5

(c)

Figure 5.—Advanced options for the three different optimization algorithms that are supported by the tool. (a) Advanced Options for the Gradient based algorithm. (b) Advanced Options for the Genetic algorithm. (c) Advanced Options for the Particle Swarm Optimization.

Advanced Options for the Gradient Option

For the gradient based algorithm there are four advanced options TolX, Fstep, TolF, and Iter, as shown in Figure 5(a). For further details of these the user is advised to check MATLAB help files under the “fmincon” algorithm (Ref. 8). A brief description of these are given below:

1. TolX: Termination tolerance on x, the design vector.
2. Fstep: Step size used to compute the numerical derivatives and is known by the name “FiniteDifferenceStepSize” by the MATLAB algorithm “fmincon”.
3. TolF: Termination tolerance on the function value.
4. Iter: Number of iterations allowed to terminate the optimization process.

Advanced Options for the Genetic Algorithm

For Genetic Algorithm (GA), the advanced options are shown in Figure 5(b). Each of the four boxes of the inputs are explained below:

1. NPop: The number of candidate solutions that satisfy the upper and lower bounds. Based on this number, the program generates candidates by using a uniform probability distribution between the upper and lower bounds. For example shown a population consisting of 100 has been chosen.
2. NGen: The number of generations the GA is required to perform the search operations, after which the optimization stops. Here we have chosen this number to be 10.
3. NElite: After performing the fitness calculations (that is the square of the error between prediction and target) for each candidate, the top candidates which give rise to the lowest error are considered elite and are preserved for the next generation as they are. The number of elite candidates must be even and is typically 2 or higher. In this example, 2 has been chosen.
4. NMut: This is the number of cross over, or Gaussian noise, candidates to be chosen by the algorithm. In the example shown here, NMut = 10. It should be noted that in the algorithm it is hardcoded to have the Gaussian and cross over candidates to be equal, however, in general they can be different.

Advanced Options for the PSO Algorithm

For the particle swarm optimization algorithm the advanced options are shown in Figure 5(c). Each of these are explained briefly here:

1. Nps: Number of particles constituting the total population.
2. NSteps: Number of steps before the process is terminated.
3. Gamma: Particle swarm algorithm γ parameter (see discussion in “Optimization Algorithm” Section).
4. Beta: Particle swarm algorithm β parameter (see discussion in “Optimization Algorithm” Section).

SwitchBoard

After completing all the necessary input the user pushes the button “Start” to begin the fitting optimization (on right in Fig. 3). Once the algorithm completes it indicates the CPU time taken to complete the procedure. The red “Stop” button, if pushed at any time aborts the program. Figure 6 shows the switchboard and its contents at the end of successful gradient based algorithm run. As the run completes, the “SwitchBoard” shows a box that indicates the total CPU time taken in seconds (here it is 253.8677 s) and a push button labeled “Results?”. In addition, row 6 of the algorithm input details



Figure 6.—Contents of Switchboard at the end of a successful Gradient based algorithm run.

table, “Opt Parm”, is populated with optimum parameters that the tool determined by performing the optimization. During the execution at the end of each iteration, the code outputs two figures. The first one shows the progress of each design variable and the computed least square error (objective function value) as a function of iteration number. The second figure shows a comparison of target and predicted stress-strain curves at the end of each iteration. These figures are output only for the Gradient based algorithm and are meant for monitoring the code progress towards an optimum set of design variables. Once the optimum set of design variables is determined, the code depicts a dialogue box showing “all the operations are completed”. At this point the user may push the “Results” button to see how the code performed in matching the target stress-strain response curves with the predictions based on the optimum set of design variables (row 6).

Results and Discussion

In this section, results are presented that first validate the optimized material parameters (and associated viscoplastic model) for neat PR520 epoxy resin. Next, the Parameter Optimization Tool is applied to determine parameters optimized for the in-situ resin response within a multiscale MAC/GMC model of a triaxially braided T700/PR520 carbon/epoxy composite, with the model results and again validated vs. experimental data. The ability to generate virtual stress-strain curve data for the composite, suitable for use in LS-DYNA MAT 213 (Ref. 5), is also demonstrated, followed by presentation of a parametric study wherein the combined effect of temperature and loading rate on the predicted composite response is investigated.

Application to Monolithic Resin Material

As an illustrative example we chose a cascading approach where we first try to get a feasible optimum design vector by using the Genetic Algorithm based optimization followed by a Gradient based optimization to arrive at the best possible solution. Genetic Algorithm based optimization often becomes computationally intensive, however, for those problems with many local minima in which no good starting point can be easily found. In such cases GA can be used to arrive at a good starting point from which a Gradient search method can be used to quickly zero in on the best possible solution. Here we chose a population of 1000, NElite = 10, NGen = 20, and NMut = 80. The algorithm was run overnight for this problem. The total time taken was 13622 s and the results are shown in Figure 7.

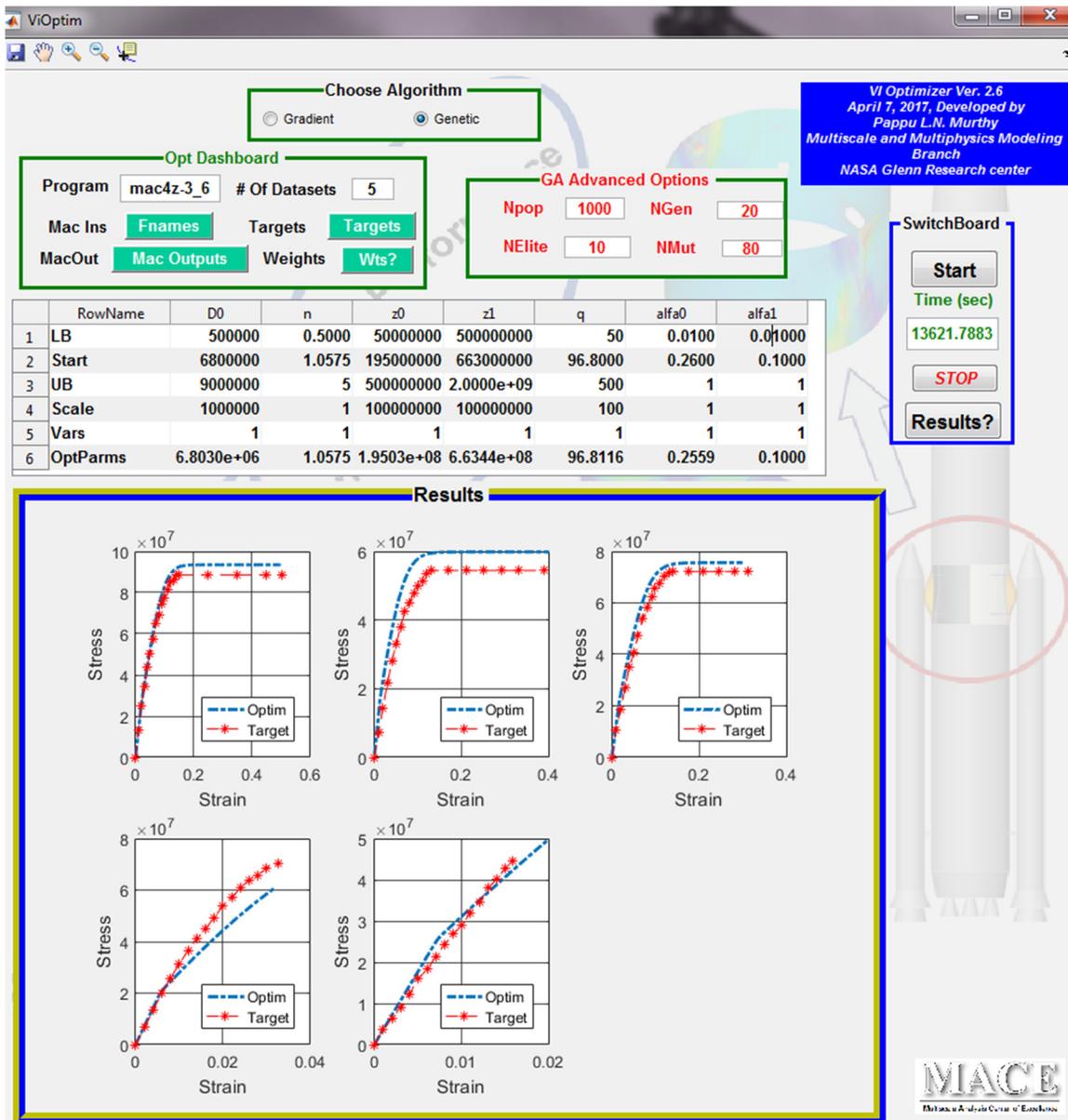


Figure 7.—GA based optimization results.

The GA algorithm led to the following optimum set of design parameters:

$D_0 = 6.803 \times 10^6$ s, $n = 1.0575$, $Z_0 = 1.9503 \times 10^8$ Pa, $Z_1 = 6.6344 \times 10^8$ Pa, $q = 96.8116$, $\alpha_0 = 0.2559$, $\alpha_1 = 0.10$. The quality of the fit can be seen from the Figure 7 in the “Results” panel. Although, results are close to target response, it is clear a better fit can probably still be pursued. At this point we used the following starting point that is close to the GA design point and chose to optimize with Gradient based approach. The starting point is

$D_0 = 6.8 \times 10^6$ s, $n = 1.0575$, $Z_0 = 1.95 \times 10^8$ Pa, $Z_1 = 6.63 \times 10^8$ Pa, $q = 96.8$, $\alpha_0 = 0.26$, $\alpha_1 = 0.1$.

The Gradient based approach is able to improve the solution significantly. The CPU time taken was 253.8677 s. The optimum design parameters are listed below:

$D_0 = 6.3358 \times 10^6$ s, $n = 0.9546$, $Z_0 = 1.421 \times 10^8$ Pa, $Z_1 = 7.353 \times 10^8$ Pa, $q = 92.0838$, $\alpha_0 = 0.01$, $\alpha_1 = 0.01$.

The results of Gradient based approach are shown in Figure 8.

As discussed in the Introduction, the Multiobjective Viscoplastic Parameter Optimization Tool along with MAC/GMC form the basis for a “Virtual Testing” platform. Given some experimental data, either on the scale of the constituent materials of a composite or that of a composite material itself, optimized constitutive model parameters for the constituent materials can be determined. Then, other data (e.g., stress-strain responses under other types of loading, at other temperatures, or at other loading rates) can be predicted for either constituents or composites. The predicted virtual data, in combination with available experimental data, can then be used as input for characterization of other models. A perfect example of such a model is the LS-DYNA MAT 213 elastoplastic orthotropic material model (Ref. 5). This constitutive model requires as input 12 stress-strain curves in the form of tabular data for each temperature and each applied strain rate. Some of these curves are difficult to obtain experimentally and the ability to obtain virtual data to fill in gaps in the experimental data can be quite valuable.

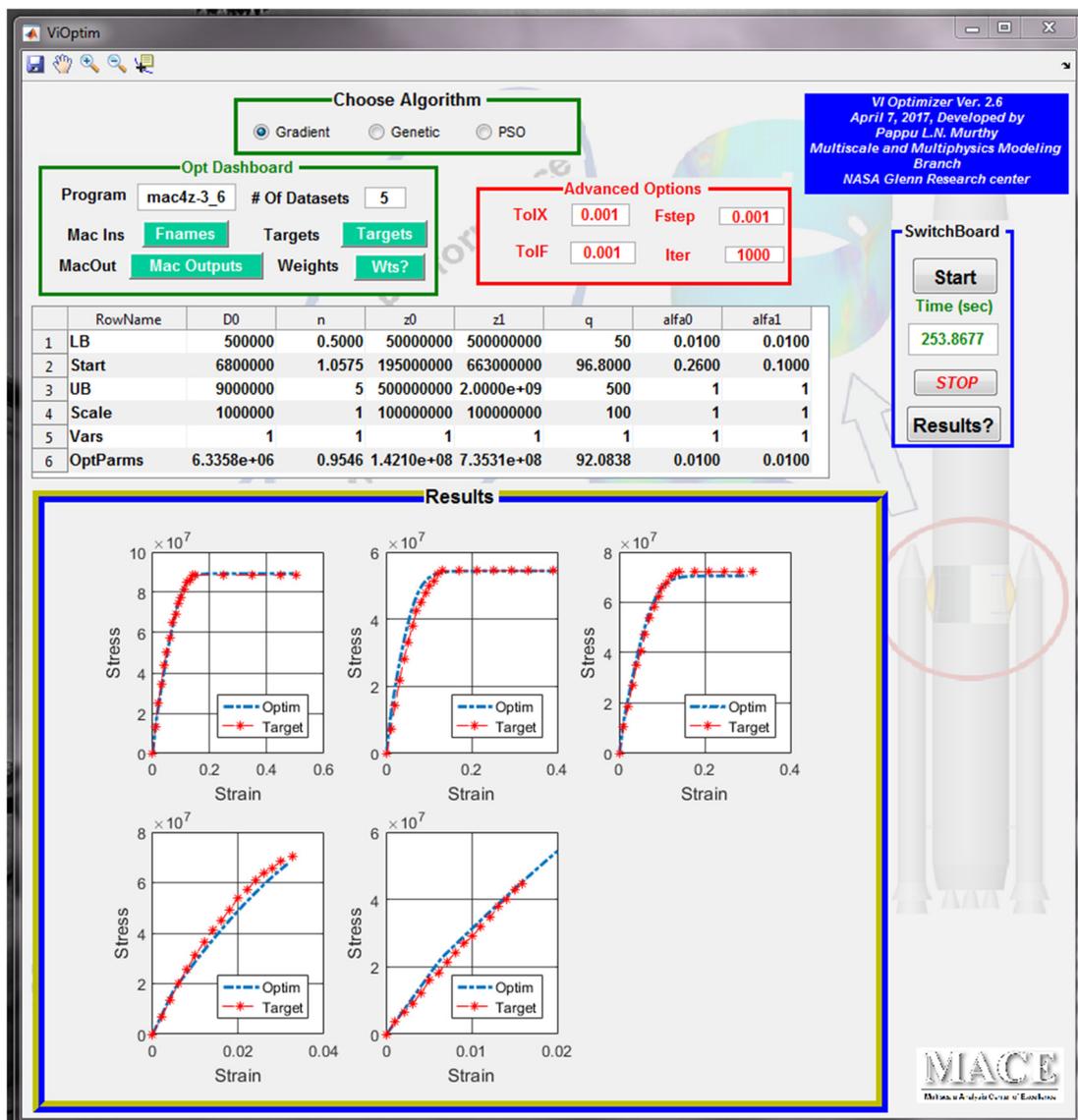


Figure 8.—Illustrative example showing the use of Genetic Algorithm followed by a fine tuning with Gradient approach. The results shown above are by Gradient Based optimization.

Figure 9 compares the predicted nonlinear PR520 resin behavior at varying temperatures, loading rates, and loading scenarios where the previously optimized model parameters have been employed. viscoplastic parameters were determined utilizing the Multiobjective Viscoplastic Parameter Optimization Tool at room temperature to reproduce the reported stress-strain response of PR520 resin (Fig. 8). An example of neat resin elastic and viscoplastic parameters at room temperature, as they appear in the MAC/GMC input file, are provided in Appendix A (Files 1-5). Note that these files provide starting points for the Parameter Optimization Tool, and they are not updated with the output from the parameter optimization. This is why the viscoplastic parameters (specified using “VI=” under the *CONSTITUENTS keyword) in the Appendix A files do not match the output from the optimization tool shown in Figure 8.

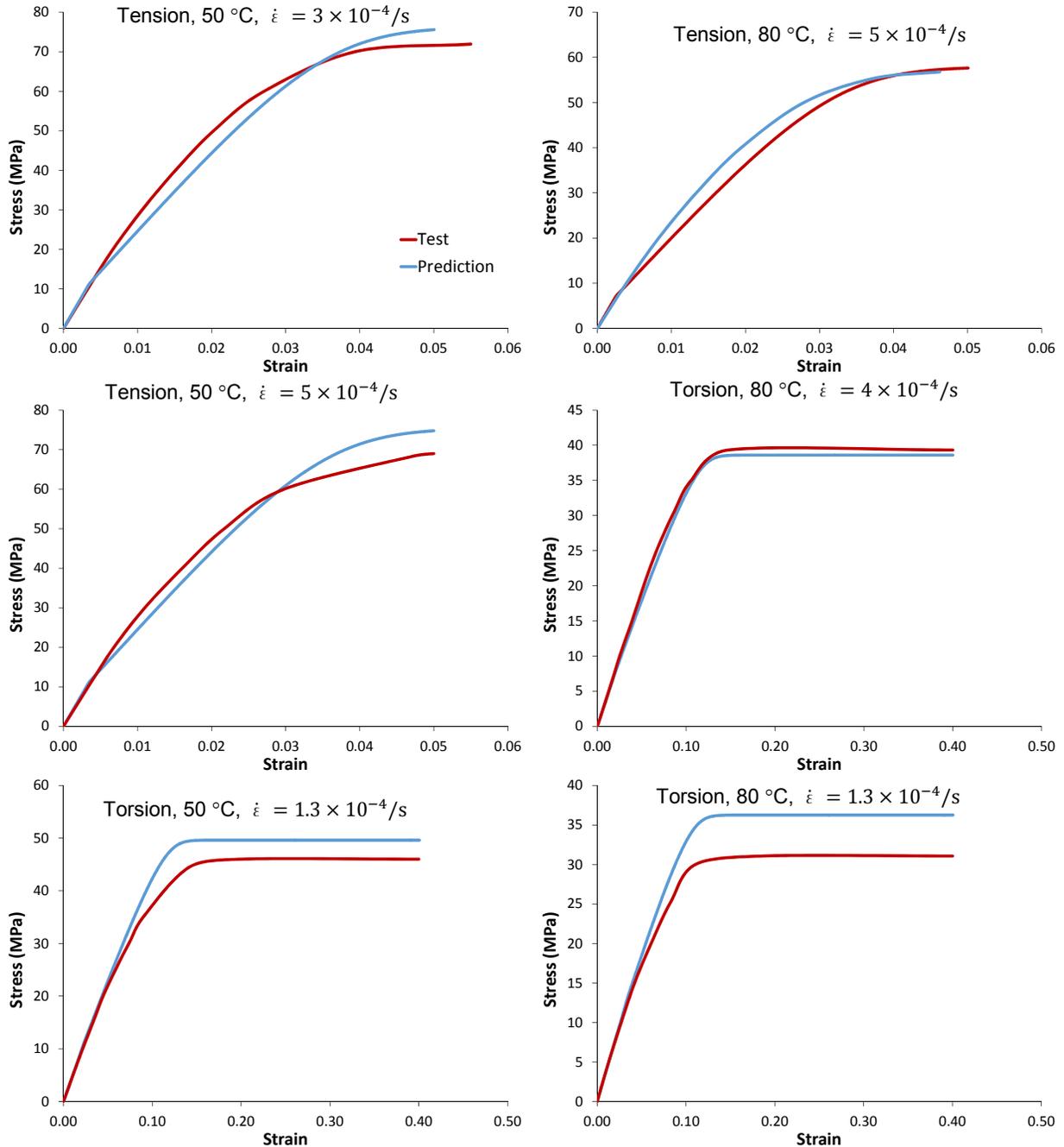


Figure 9.—Tensile and torsional (shear) stress-strain responses of Neat resin (PR520) at various rates and temperatures. Note that the scales are different across the plots.

While the viscoplastic parameters remained unchanged from the reported values, elastic modulus was adjusted from 3.5 GPa at 23 °C to be 3.2 GPa at 50 °C, and 2.5 GPa at 80 °C. As it can be seen in Figure 9, the model can predict the stress-strain responses with minimal error in majority of the cases. Details of the plotted experimental results are reported in Reference 7. A higher percentage of error (~16 percent) is observed at higher temperatures ($T = 80$ °C), which might stem from the fact that viscoplastic parameters were left unchanged across different temperatures. This was mainly done to assess the predictive capability of the Multiobjective Viscoplastic Parameter Optimization Tool across various temperature profiles, instead of calibrating the model for every given temperature value, which could also be done.

Application to a Triaxially Braided T700/PR520 Composite

Once the predicted nonlinear PR520 behavior was validated at the various temperatures and rates (Fig. 9), the mechanical response of a T700/PR520 braided composite system was predicted and validated. Figure 10 shows the geometry of the multiscale model of the braided composite simulated using the Multiscale Generalized Method of Cells (MSGMC) capability within MAC/GMC. The procedure and geometry employed follows that presented in References 12 and 13, in which MSGMC was applied to model the elastic response and viscoplastic response, respectively, of triaxially braided composites. A typical architecture of the triaxial braided composite is shown in Figure 10(a) with the indicated repeated unit cell. It is composed of three significant volumes: pure matrix, axial tows, and braided tows. Straight axial fiber tows and braided fiber tows are oriented at an angle θ (braid angle). The architecture being analyzed is assumed to be an idealized homogenized RUC with the transversely isotropic elastic fibers and a viscoplastic resin (Fig. 10(c) and (d)). The present homogenization methodology represents the triaxial braided composite with its constituent materials (fiber and matrix), where the constitutive models are applied. Larger scale stress state and moduli are determined through the GMC homogenization methods (Ref. 3). Further details about microstructural parameters in defining a triaxial braided composite architecture can be found in Reference 12. For the triaxial braided composite analyzed here, resin PR520 properties are calibrated through Multiobjective Viscoplastic Parameter Optimization Tool and the transversely isotropic T700 fiber properties are acquired from Reference 7 ($E_A = 230$ GPa, $E_T = 15$ GPa, $\nu_A = 0.2$, $\nu_T = 0.2$, $G_A = 15$ GPa). The subcell dimensions shown in Figure 10(c) are: $h_1 = 0.0022$, $h_2 = 0.00251$, $d = 0.00018$, with the length units being arbitrary. The fiber volume fractions shown in Figure 10(c) are: $Vf_1 = 0.8$, $Vf_2 = 0.7467$, $Vf_3 = 0.3733$. As discussed in Reference 12, the fiber volume fractions account for the regions of pure resin that are homogenized into the subcells. These subcell dimensions and fiber volume fractions result in an overall composite fiber volume fraction of 0.56.

Rather than using the previously optimized neat resin material parameters, the ability of the optimization tool to utilize composite level stress-strain data as input was employed to back out in-situ data for the resin in the composite. This is a key capability that enables the tool to function even in cases where neat resin data is unavailable. Two available composite level stress-strain curves were used for this purpose (transverse tension and in-plane shear), along with the gradient based optimization method.

The multiscale model of the T700/PR520 composite was subjected to simulated tensile and shear loading at room-temperature at a strain rate of 5×10^{-5} /s and compared to available experimental data in Figure 11. For the two stress-strain curves used to determine the in-situ resin viscoplastic parameters, the simulated response is labeled as “correlation,” whereas, the remaining simulations represent predictions. In cases where there was no available experimental data, the simulations represent virtual test data, and the associated plots in Figure 11 are labeled as such. Examining Figure 11, the stress-strain response of the composite is reproduced with relatively acceptable error (< 20 percent) for all loading cases. The error observed for compression seems to be the highest (~20 percent). This may be due to the complex nature of composite nonlinear deformation under compression, which depends on various interacting

mechanisms other than just matrix viscoplasticity. Therefore, it can still be stated that the model's predictive capability is fairly good for various loading scenarios at room-temperature. The virtual data reported in Figure 11 (without one-to-one comparison with experiments) seems to fall in a reasonable range, when compared to similar available data in literature (Ref. 14).

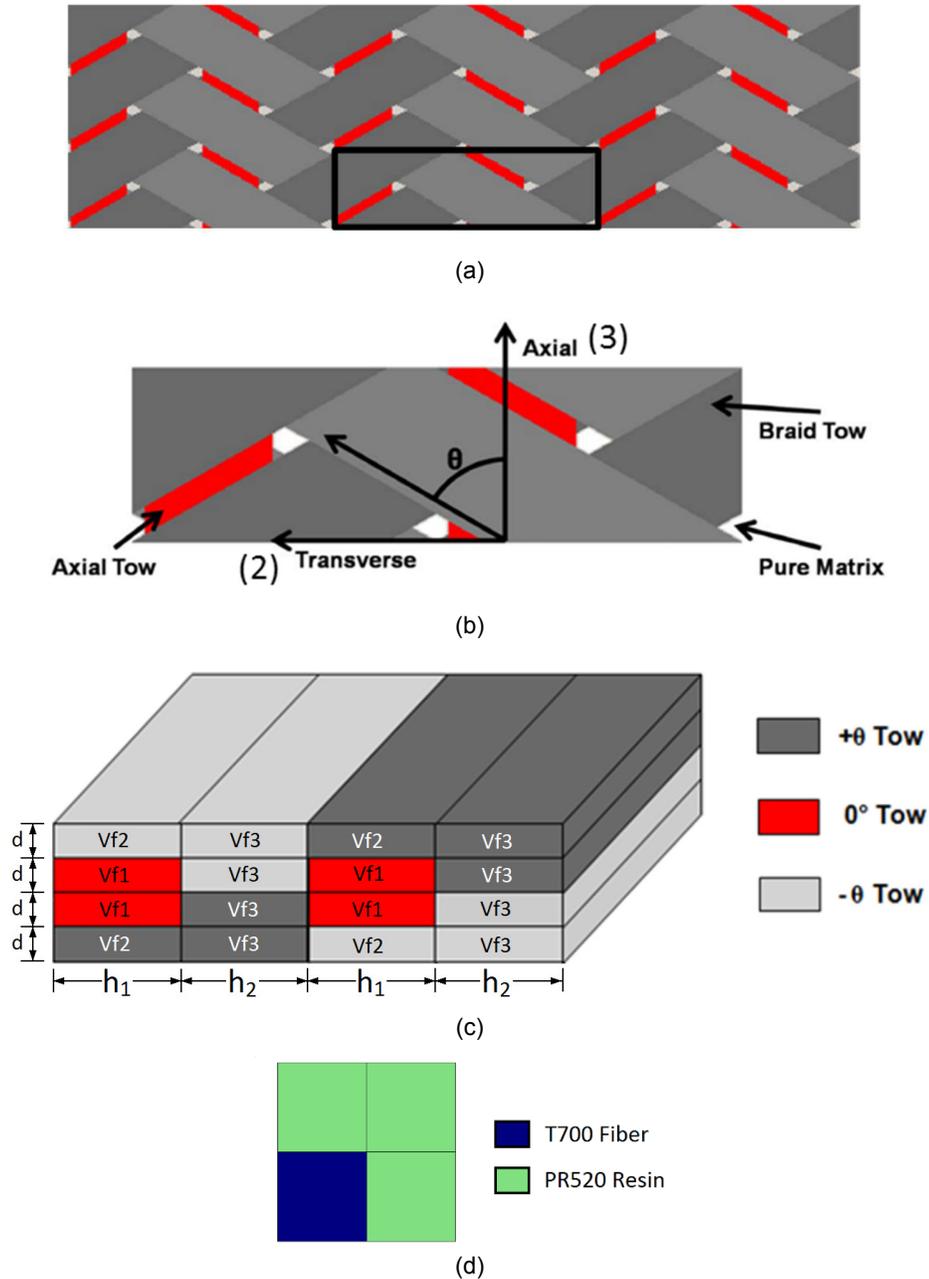


Figure 10.—MAC/GMC multiscale model of a triaxially braided composite (T700/PR520). (a) Triaxial braid pattern with repeating unit cell identified. (b) Top view of the triaxial braid repeating unit cell. (c) MAC/GMC idealization of the triaxial braid repeating unit cell (Ref. 12), with subcell dimensions (h_1 , h_2 , d) and fiber volume fractions (Vf_1 , Vf_2 , Vf_3) denoted. (d) Repeating unit cell used to model the unidirectional composite within each tow.

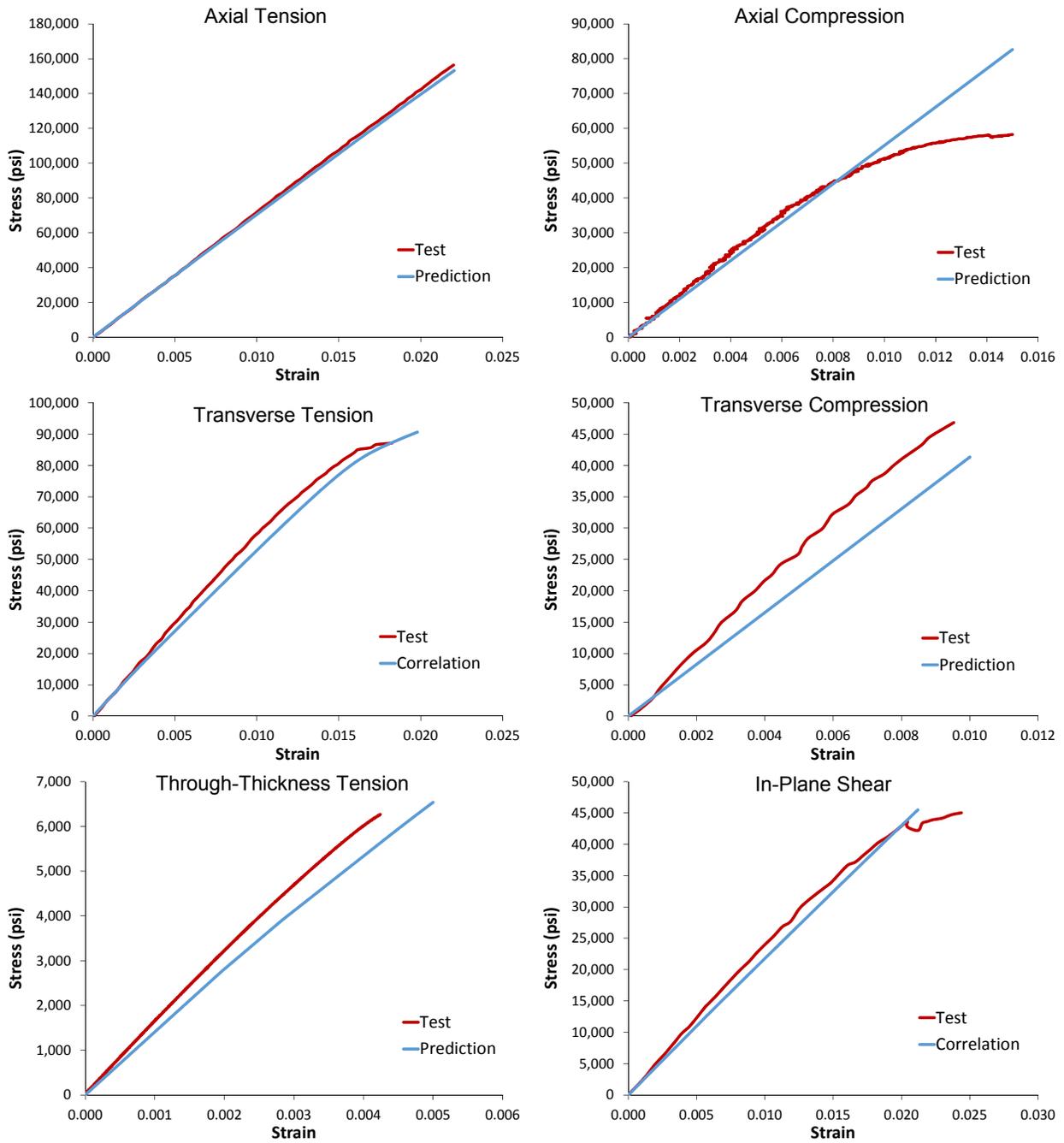


Figure 11.—Stress-strain responses under various loading conditions of the triaxially braided T700/PR520 composite at room temperature and 5×10^{-5} strain rate. Note that the scales are different across the plots.

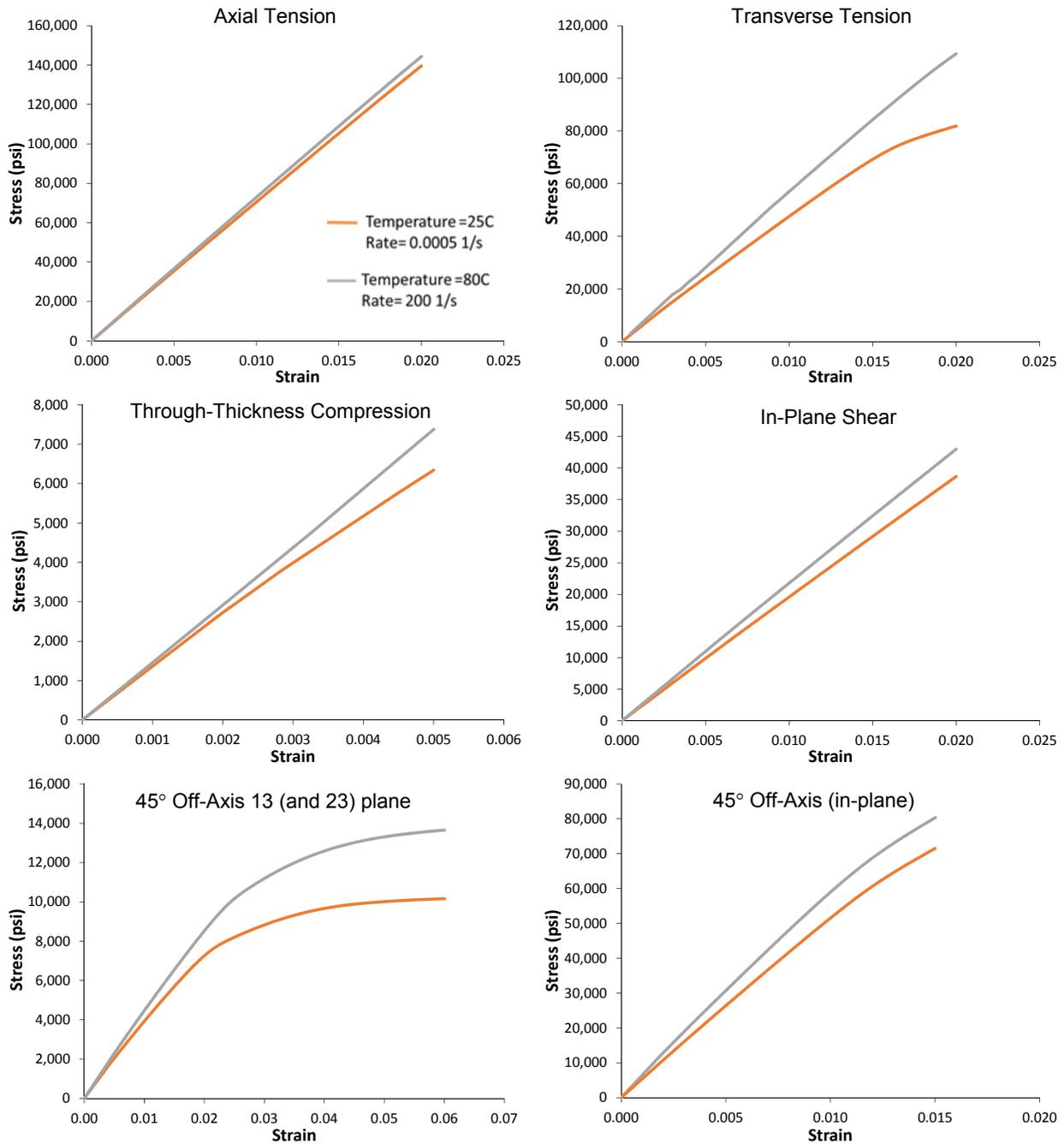


Figure 12.—Parametric study showing combined effect of temperature and loading rate on the stress-strain response of the braided T700/PR520 composite. Note that the scales are different across the plots.

Performing composite parametric studies to evaluate the “virtual testing” predictions over the full range of temperatures and rates for composite systems constitutes the final step for a viable virtual testing platform. After validating the composite response through available tests at room temperature, parametric studies were conducted to examine the influence of rate and temperature variation on the mechanical behavior of the composite system for various loading scenarios. Sample parametric study results are shown in Figure 12, wherein room-temperature/low rate and high-temperature/high rate results are compared. As shown, variation of temperature and rate has a relatively minor effect, except for the 45° off-axis shear loading. Note that the 13 and 23 plane 45° off-axis shear results were nearly identical, so

only the 13 plane results are shown. Also, although not shown, the rate was increased in various increments (from 0.00005 to 200 /s) and the resulted stress-strain curves were obtained for every case. A noticeable difference in stress-strain response (for the presented loading scenarios) was only observed when the rate reached approximately 100 /s. Therefore, it was not deemed necessary to illustrate redundant stress-strain curves with no distinct difference in this section. Further parametric studies on different composite systems are necessary to obtain a better understanding of rate/temperature influence on a given system.

Conclusion

The Multiobjective Viscoplastic Constitutive Law Parameter Fitting Tool helps in fitting experimentally observed stress-strain responses generated at different temperatures and different strain rates to a seven parameter Bodner-Partom constitutive law. The fit can be performed for a neat matrix material (as done herein) or for the composite-scale response. The software supports any number of stress-strain response curves as well as the importance given to these responses in the form of weights. Furthermore, three different algorithms (gradient based, genetic and particle swarm) provide flexibility to be used sequentially or individually in order to zero in on an optimum set of constitutive law parameters with a reasonable amount of computational resources.

The constitutive law parameters for the modified Bodner-Partom model generated by the tool were utilized within a multiscale micromechanics model in MAC/GMC to predict the response of braided composites that were then compared with experimental stress-strain curves. Two available composite level stress-strain curves (transverse tension and in-plane shear) were used to back-out in-situ data for the resin in the composite. Utilizing these in-situ properties, remaining composite stress-strain curves were predicted successfully with an acceptable margin of error for most of the loading cases. Some higher deviation in compression was observed which might be due to complicated nature of a composite behavior under compression. The tools discussed herein form the basis of a virtual test platform, wherein stress-strain curves that are extremely difficult to obtain experimentally can be predicted using the model. This can be very valuable in minimizing experimental costs and filling in experimental gaps.

Appendix A.—Input Data for MAC/GMC Executable, (see Refs. 1 and 2 for details)

File 1: Goldberg PR520-EXPO123.mac: (The input deck is meant to output axial tensile stress for an applied rate (1.4 /s) and temperature (23 °C). The rate is the strain/time ratio).

MAC/GMC - effective properties

```
*CONSTITUENTS
  NMATS=1
# -- PR520 Resin Pa
  M=1 CMOD=12 MATID=U MATDB=1 &
    EL=3.54E9,3.54E9,0.38,0.38,1.28261E9,45.E-6,45.E-6 &
    VI=1E6,1.07,206977131.37,868911452.11,348.72,0.2548,0.126
*RUC
  MOD=1 M=1
*MECH
  LOP=1
  NPT=2 TI=0.,0.014 MAG=0.,0.02 MODE=1
*THERM
  NPT=2 TI=0.,0.014 TEMP=23.,23.
*SOLVER
  METHOD=1 NPT=2 TI=0.,0.014 STP=0.00003
*XYPLOT
  FREQ=1
  MACRO=1
  NAME=goldberg_PR520-EXP0128 X=1 Y=7
  MICRO=0
*PRINT
  NPL=6
*END
```

File 2: Goldberg PR520-EXPO123.mac: (The input deck is meant to output axial tensile stress for an applied rate (5×10^{-5} /s) and temperature (23 °C). The rate is the strain/time ratio).

MAC/GMC - effective properties

```
*CONSTITUENTS
  NMATS=1
# -- PR520 Resin Pa
  M=1 CMOD=12 MATID=U MATDB=1 &
    EL=3.54E9,3.54E9,0.38,0.38,1.28261E9,45.E-6,45.E-6 &
    VI=1E6,1.07,206977131.37,868911452.11,348.72,0.2548,0.126
*RUC
  MOD=1 M=1
*MECH
  LOP=1
  NPT=2 TI=0.,600. MAG=0.,0.032 MODE=1
*THERM
  NPT=2 TI=0.,600. TEMP=25.,25.
*SOLVER
  METHOD=1 NPT=2 TI=0.,600. STP=1
*XYPLOT
  FREQ=1
  MACRO=1
  NAME=goldberg_PR520-EXP0117 X=1 Y=7
  MICRO=0
*PRINT
  NPL=6
*END
```

File 3: Goldberg PR520-EXPO123.mac: (The input deck is meant to output out-of-plane shear stress (Torsion) for an applied rate (2.6 /s) and temperature (23 °C). The rate is the strain/time ratio).

```
MAC/GMC - effective properties
*CONSTITUENTS
  NMATS=1
# -- PR520 Resin Pa
  M=1 CMOD=12 MATID=U MATDB=1 &
  EL=3.54E9,3.54E9,0.38,0.38,1.28261E9,45.E-6,45.E-6 &
  VI=1E6,1.07,206977131.37,868911452.11,348.72,0.2548,0.126
*RUC
  MOD=1 M=1
*MECH
  LOP=6
  NPT=2 TI=0.,0.115 MAG=0.,0.3 MODE=1
*THERM
  NPT=2 TI=0.,0.115 TEMP=25.,25.
*SOLVER
  METHOD=1 NPT=2 TI=0.,0.115 STP=0.0002
*XYPLOT
  FREQ=1
  MACRO=1
  NAME=goldberg_PR520-EXP0108 X=6 Y=12
  MICRO=0
*PRINT
  NPL=6
*END
```

File 4: Goldberg PR520-EXPO123.mac: (The input deck is meant to output out-of-plane shear stress (Torsion) for an applied rate (1.3×10^{-4} /s) and temperature (23 °C). The rate is the strain/time ratio).

```
MAC/GMC - effective properties *CONSTITUENTS
  NMATS=1
# -- PR520 Resin Pa
  M=1 CMOD=12 MATID=U MATDB=1 &
  EL=3.54E9,3.54E9,0.38,0.38,1.28261E9,45.E-6,45.E-6 &
  VI=1E6,1.07,206977131.37,868911452.11,348.72,0.2548,0.126
*RUC
  MOD=1 M=1
*MECH
  LOP=6
  NPT=2 TI=0.,3076. MAG=0.,0.4 MODE=1
*THERM
  NPT=2 TI=0.,3076. TEMP=25.,25.
*SOLVER
  METHOD=1 NPT=2 TI=0.,3076. STP=5
*XYPLOT
  FREQ=1
  MACRO=1
  NAME=goldberg_PR520-EXP0106 X=6 Y=12
  MICRO=0
*PRINT
  NPL=6
*END
```

File 5: Goldberg PR520-EXPO123.mac: (The input deck is meant to output out-of-plane shear stress (Torsion) for an applied rate (700 /s) and temperature (25 °C). The rate is the strain/time ratio).

```
MAC/GMC - effective properties *CONSTITUENTS
  NMATS=1
# -- PR520 Resin Pa
  M=1 CMOD=12 MATID=U MATDB=1 &
    EL=3.54E9,3.54E9,0.38,0.38,1.28261E9,45.E-6,45.E-6 &
    VI=1E6,1.07,206977131.37,868911452.11,348.72,0.2548,0.126
*RUC
  MOD=1 M=1
*MECH
  LOP=6
  NPT=2 TI=0.,0.000714 MAG=0.,0.5 MODE=1
*THERM
  NPT=2 TI=0.,0.000714 TEMP=25.,25.
*SOLVER
  METHOD=1 NPT=2 TI=0.,0.000714 STP=0.000001
*XYPLOT
  FREQ=1
  MACRO=1
  NAME=goldberg_PR520-EXP0103 X=6 Y=12
  MICRO=0
*PRINT
  NPL=6
*END
```

File 6: goldberg triax test: (The input deck is meant to output transverse axial stress for an applied rate (5×10^{-5} /s) and temperature (25 °C). The rate is the strain/time ratio).

```
MAC/GMC - effective properties
*CONSTITUENTS
  NMATS=2
# -- T700 fiber - Pa
  M=1 CMOD=6 MATID=U MATDB=1 &
    EL=230.E9,15.E9,0.2,0.2,15.E9,-99.E-6,-99.E-6
# -- PR520 Resin Pa
  M=2 CMOD=12 MATID=U MATDB=1 &
    EL=3.54E9,3.54E9,0.38,0.38,1.28261E9,45.E-6,45.E-6 &
    VI=1775518,1.969662,1.51E8,6.33E8,249.05,0.477916,0.1
# Axial tension 3, transverse tension 2, and in-plane shear 4.
*MSGMC
  NA=1 NB=4 NG=1
  D=0.00070
  H=0.00220,0.00251,0.00220,0.00251
  L=0.00272
# -- gamma = 1
  SM=-17,-18,-19,-20
*MSMATS
  NMATS=11
  MSM=-17 DIM=3 ARCHID=99
  NA=4 NB=1 NG=1
  D=0.00018,0.00018,0.00018,0.00018
  H=1.00000
  L=1.00000
# -- gamma = 1
  SM=-23
  SM=-21
```

```

SM=-21
SM=-22
MSM=-18 DIM=3 ARCHID=99
NA=4 NB=1 NG=1
D=0.00018,0.00018,0.00018,0.00018
H=1.00000
L=1.00000
# -- gamma = 1
SM=-27
SM=-27
SM=-24
SM=-24
MSM=-19 DIM=3 ARCHID=99
NA=4 NB=1 NG=1
D=0.00018,0.00018,0.00018,0.00018
H=1.00000
L=1.00000
# -- gamma = 1
SM=-22
SM=-21
SM=-21
SM=-23
MSM=-20 DIM=3 ARCHID=99
NA=4 NB=1 NG=1
D=0.00018,0.00018,0.00018,0.00018
H=1.00000
L=1.00000
# -- gamma = 1
SM=-25
SM=-25
SM=-26
SM=-26
MSM=-21 DIM=2 ARCHID=1 VF=8.000000e-01 F=1 M=2
D1=0.00000,0.00000,1.00000
D2=0.00000,1.00000,0.00000
D3=-1.00000,0.00000,0.00000
MSM=-22 DIM=2 ARCHID=1 VF=7.466667e-01 F=1 M=2
D1=0.00000,0.86603,0.50000
D2=1.00000,0.00000,0.00000
D3=0.00000,0.50000,-0.86603
MSM=-23 DIM=2 ARCHID=1 VF=7.466667e-01 F=1 M=2
D1=0.00000,-0.86603,0.50000
D2=1.00000,0.00000,0.00000
D3=-0.00000,0.50000,0.86603
MSM=-24 DIM=2 ARCHID=1 VF=0.3733 F=1 M=2
D1=-0.17795,0.85220,0.49202
D2=0.00000,0.50000,-0.86603
D3=0.98404,0.15411,0.08897
MSM=-25 DIM=2 ARCHID=1 VF=0.3733 F=1 M=2
D1=0.17795,0.85220,0.49202
D2=0.00000,0.50000,-0.86603
D3=0.98404,-0.15411,-0.08897
MSM=-26 DIM=2 ARCHID=1 VF=0.3733 F=1 M=2
D1=-0.17795,-0.85220,0.49202
D2=0.00000,0.50000,0.86603
D3=0.98404,-0.15411,0.08897
MSM=-27 DIM=2 ARCHID=1 VF=0.3733 F=1 M=2

```

```
D1=0.17795,-0.85220,0.49202
D2=0.00000,0.50000,0.86603
D3=0.98404,0.15411,-0.08897
*MECH
  LOP=2
  NPT=2 TI=0.,600. MAG=0.,0.03 MODE=1
*THERM
  NPT=2 TI=0.,600. TEMP=25.,25.
*SOLVER
  METHOD=1 NPT=2 TI=0.,600. STP=0.9
*XYPLOT
  FREQ=1
  MACRO=1
  NAME=goldberg_triax_test X=2 Y=8
  MICRO=0
*PRINT
  NPL=6
*END
```


Appendix B.—Target Stress-Strain Response Files

EXP0103.xls: Experimental data (first column: strain- second column: stress (Pa)) for torsion test (rate = 700 /s, temperature = 23 °C)

0	0
0.01008	13320000
0.02016	24734000
0.03006	34250000
0.03996	43984000
0.04998	50133000
0.06018	57125000
0.07014	64719000
0.08034	69359000
0.09006	74234000
0.10002	77633000
0.11022	81641000
0.12012	84820000
0.13008	86078000
0.14004	88609000
0.15006	88617000
0.25006	88617000
0.35006	88617000
0.45006	88617000
0.5037	88617000

EXP0106.xls: Experimental data (first column: strain- second column: stress (Pa)) for torsion test (rate = 1.3e-4 /s, temperature = 23 °C)

0	0
0.010031	7212500
0.020062	14428000
0.030094	21641000
0.040125	28022000
0.050125	33016000
0.060156	38009000
0.070187	42450000
0.080219	44947000
0.09025	47719000
0.10028	49941000
0.11031	51328000
0.11991	53547000
0.13081	54378000
0.17081	54378000
0.21081	54378000
0.25081	54378000
0.29081	54378000
0.33081	54378000
0.39025	54378000

EXP0108.xls: Experimental data (first column: strain- second column: stress (Pa)) for torsion test (rate = 2.6 /s, temperature = 23 °C)

0	0
0.010032	10822000
0.020063	18591000
0.030063	26916000
0.040094	34959000
0.050125	40509000
0.060157	47169000
0.070625	53828000
0.080219	58269000
0.091125	62431000
0.098533	65481000
0.109433	67703000
0.119903	70200000
0.130343	71859000
0.140373	72137000
0.175373	72137000
0.210373	72137000
0.245373	72137000
0.280373	72137000
0.310873	72137000

EXP0117.xls: Experimental data (first column: strain- second column: stress (Pa)) for tension test (rate = 5e-5 /s, temperature = 23 °C)

0	0
0.002081	6793700
0.004031	13369000
0.006006	19944000
0.008025	25856000
0.010044	31337000
0.012019	36381000
0.014006	40981000
0.016019	44925000
0.018031	49306000
0.020044	53912000
0.022062	57200000
0.024006	60706000
0.026019	63994000
0.028	65744000
0.03005	68594000
0.032631	70562000

EXP0128.xls: Experimental data (first column: strain- second column: stress (Pa)) for tension test (rate = 1.4 /s, temperature = 23 °C)

0	0
0.001013	3650000
0.00205	6443700
0.003019	9025000
0.004031	12250000
0.005006	15900000
0.006044	18262000
0.007019	21269000
0.008025	24281000
0.009069	26856000
0.010044	29006000
0.011013	32012000
0.01205	34594000
0.013094	38031000
0.014006	40181000
0.015044	42756000
0.01585	44694000

References

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